

Unimolecular Decay strongly limits the Atmospheric Impact of Criegee Intermediates

– Supporting Information –

L. Vereecken, A. Novelli, D. Taraborrelli

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A. Summary of the key findings

Nomenclature (section B) : To designate the absolute configuration of complex carbonyl oxides, we propose the IUPAC Z and E stereodescriptors also in use for other systems with a π -system. Relying solely on the *syn*- and *anti*-designators is potentially ambiguous.

Stereoisomers (section H) : Stereoisomerisation is found to be negligible for all substituents examined in this work, such that both carbonyl oxide stereoisomers effectively act as separate species. The relative energy of the stereoisomers depends strongly on the substituents, with CH_3 in *syn*-position yielding the most stable isomers, and β -oxo-substituents in *syn*-position the most reactive CI.

Main unimolecular reactions (section J, L, N, O, P) : The main channels are alkyl-1,4-H-migration, allyl-1,4- and allyl-1,6-H-migration, and 1,3- and 1,5-ring closure. For large, hetero-substituted Criegee intermediates, secondary ozonide formation or other complex intramolecular pathways could become dominant. H-migration typically forms vinyl hydroperoxides (VHP), a processes that is stereo-specific, with *E*-VHP being the near-exclusive product.

Ester/acid channel (section N) : The longest-lived SCI have no migratable H-atom nor *syn*- β -unsaturation, and decay by 1,3-ring closure with lifetimes of seconds to an hour. Even though this channel, forming dioxiranes that re-arrange to acids or esters, is traditionally considered a slow reaction, it can still attain high rate coefficients, e.g. for *syn*-oxo-SCI we predict $k(298\text{K}) \geq 10^4 \text{ s}^{-1}$.

SAR for unimolecular decay (section R) : The loss rate for Criegee intermediates can be predicted readily based on the substitution patterns, where the rate coefficient and reaction class is mostly determined by the substituent in *syn*-position of the carbonyl oxide, and only to a lesser extent by the substituent in *anti*-position.

SAR for the reaction with H_2O (Section S.5) : Several estimation methods for the rate coefficient of the carbonyl oxide + H_2O reaction are examined. Our preferred structure-activity relationship is tuned to the available experimental and high-quality theoretical data, but also incorporates the reaction trends obtained from a systematic series of quantum chemical and theoretical kinetic calculations.

SAR for the reaction with $(\text{H}_2\text{O})_2$ (Section T.4) : Several estimation methods for the rate coefficient of the carbonyl oxide + $(\text{H}_2\text{O})_2$ reaction are examined. Our preferred structure-activity relationship is based on the theoretical data for the SCI + H_2O reaction, but tuned to the available literature experimental and high-quality theoretical data for SCI + $(\text{H}_2\text{O})_2$.

Group additivity trends (section H.3, N.3, S.7) : The relative energy of stereoisomers, the rate coefficient for 1,3-ring closure, and the reaction of SCI + H_2O can be modeled using a group additivity paradigm. This could simplify the development and application of SARs for specific reaction classes.

Concentration of CI in pristine environments (Section U.3, V.2) : The concentration of SCI in rural environments is predicted to be of the order of $1 \times 10^4 \text{ molecule cm}^{-3}$, both for isoprene- and monoterpene-dominated sites (Amazonia, Sierra Nevada). Global modeling shows maximum peak values less than $1 \times 10^5 \text{ molecule cm}^{-3}$, and very low average concentrations, $\leq 3 \times 10^3 \text{ molecule cm}^{-3}$, across the globe. The equatorial belt shows the highest concentrations. Sources of SCI are the biogenic VOC, with many complex SCI species contributing to the population.

Concentration of CI in urban environments (Section U.3, V.2) : The ozonolysis of small, anthropogenic unsaturated hydrocarbons is the main source of SCI in urban environments (Mexico City), with predicted peak concentrations remain below $1 \times 10^5 \text{ molecule cm}^{-3}$ even for polluted areas. The SCI population is dominated by smaller SCI such as CH_2OO , CH_3CHOO , and $(\text{CH}_3)\text{COO}$.

Loss process contributions (Section U.3, V.2) : Unimolecular decay constitutes an important loss process of the carbonyl oxides, predicted to account for more than half of the SCI loss for biogenic SCI. The reaction with water is the second most important loss path, with H_2O and $(\text{H}_2\text{O})_2$ both contributing equally. SCI loss to SO_2 , NO_2 or acids has minor to negligible contribution, with a combined contribution $\leq 10\%$.

Impact of CI on atmospheric chemistry (section W): Due to the low predicted SCI concentrations, the impact on the atmosphere is minimal. Only around the equatorial belt, and regionally in polluted environments, are non-negligible contributions to SO_2 oxidation found, of about the same order of magnitude as the OH-driven oxidation path. In these regions, SCI might also constitute a gas phase loss path to carboxylic acids.

B. An updated standard nomenclature for carbonyl oxides

The π -system in the carbonyl oxide moiety in Criegee intermediates has a strong double-bond character (see Figure 1),¹⁻³ making inversion of the outer oxygen orientation relative to the carbon atom substituents difficult, as discussed in more detail below. For most practical purposes, the two stereoisomers of an asymmetric CI therefore act as two separate chemical species, similar to the stereoisomers of olefins or oximes.

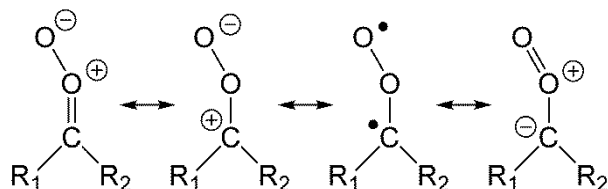
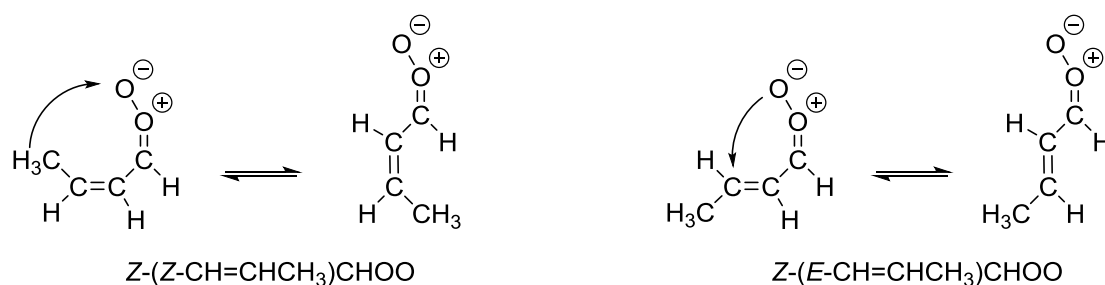


Figure 1: Lewis structures representing contributions to the carbonyl oxide wave function. The Lewis structure on the left is the representation of the wave function that best reflects^{1,3,4} the carbonyl oxide reactive properties, and is the recommended representation if a single Lewis structure is used.

Traditionally, the two stereoisomers are labelled as *syn*- and *anti*-CI. However, as most studies on substituted CI examined CH_3CHOO , with generalizations to larger CI where the carbonyl oxides could not necessarily be speciated, the term '*syn*' and '*anti*' have become overloaded in this context with the meaning 'follows the H-migration VHP channel leading to OH' versus 'follows the 1,3-ring closure channel leading to esters/acid', respectively (see Figure 4). For a carbonyl oxide with two alkyl substituents, *i.e.* where both stereoisomers have similar accessible pathways, *syn/anti* designations are therefore potentially ambiguous.

The strong double bond character of the $>\text{C}=\text{OO}$ bond in carbonyl oxides, and the concomitantly high barrier for stereoisomerisation (see section H), makes carbonyl oxides similar to olefins or oximes, and we propose to use the *E/Z* stereodescriptors for unambiguous naming of the absolute carbonyl oxide orientation based on the Cahn-Ingold-Prelog (CIP) precedence of the substituents.⁵⁻⁷ E.g. *syn*- CH_3CHOO will be named *Z*- CH_3CHOO and has the outer oxygen atom pointing towards the CH_3 group, while *E*-(CH_3)(C_2H_5) COO has the ethyl substituent opposite of the oxide side. This naming scheme will be especially useful for disambiguation in complex CI such as obtained from terpenoid ozonolysis. As an additional mnemonic aid in the current manuscript, we will label doubly substituted CI as $(\text{R}_1)(\text{R}_2)\text{COO}$, where the R_1 substituent is always on the *syn*-side of the oxide outer oxygen, e.g. *Z*-(C_2H_5)(CH_3) COO compared to its stereoisomer *E*-(CH_3)(C_2H_5) COO . Figure 2 and Figure 3 show an extensive list of substituted CI, and their notation.

For olefinic moieties such as in unsaturated carbonyl oxides or in vinyl hydroperoxide, we use the IUPAC *E/Z* stereodescriptors also used for alkenes. It should be noted that the stereo-orientation of the olefinic moiety can be critical in determining the fate of the CI, even after accounting for all internal rotations, as in the example below:



Here, *Z*-(*Z*- $\text{CH}=\text{CHCH}_3$) CHOO will undergo a 1,6-allyl-H-migration (curved arrow, see section L for more information) whereas *Z*-(*E*- $\text{CH}=\text{CHCH}_3$) CHOO will undergo a 1,5-ring closure (curved arrow, see section R).

Molecules bearing a conjugated π -system, e.g. butadiene or isoprene, have conformers showing different stereo-orientation of the double bonds; for the CI studied in this work we find conjugated systems in β -vinyl ($\text{C}=\text{C}-\text{C}=\text{OO}$) and β -oxo ($\text{O}=\text{C}-\text{C}=\text{OO}$) carbonyl oxides. We use the IUPAC *s-cis* and *s-trans* nomenclature to designate the conformers accessible through rotation of the internal single bond. Most of the conjugated oxides considered have periplanar double bonds, though for a few CI the *s-cis* structure is not an energetic minimum. For these, an *s-gauche* structure is formed where the double bonds are non-periplanar (e.g. $\text{Z}-(\text{Z}-\text{CH}=\text{CHCH}_3)\text{CHOO}$). As discussed in more detail in section G, the rotamers are expected to be in a (near-)equilibrium distribution, such that the *s-trans* and *s-cis/gauche* conformers act as a single reactant pool.

C. Carbonyl oxides substituents

1. Substituted CI characterized explicitly using theoretical calculations

Figure 2 shows the list of substituents considered in this work, spanning H, alkyl, β - and γ -vinyl, and β -oxo substituents, where the latter three are considered with a range of methyl substitution. Not all permutations of these substituents are considered, nor are all substitution permutations on unsaturated moieties considered, for reasons of computational cost. The range of CI substituents considered was selected to enable kinetic analysis of all relevant reaction channels across the terpenoids emitted to the atmosphere, and many of their first-generation reaction products. Figure 3 shows all carbonyl oxides considered in this work, where for most structures all applicable unimolecular reaction channels were considered (see section D). Note that for each reactant and transition state, all rotational conformers are characterized, and included in the kinetic analysis (see section F).

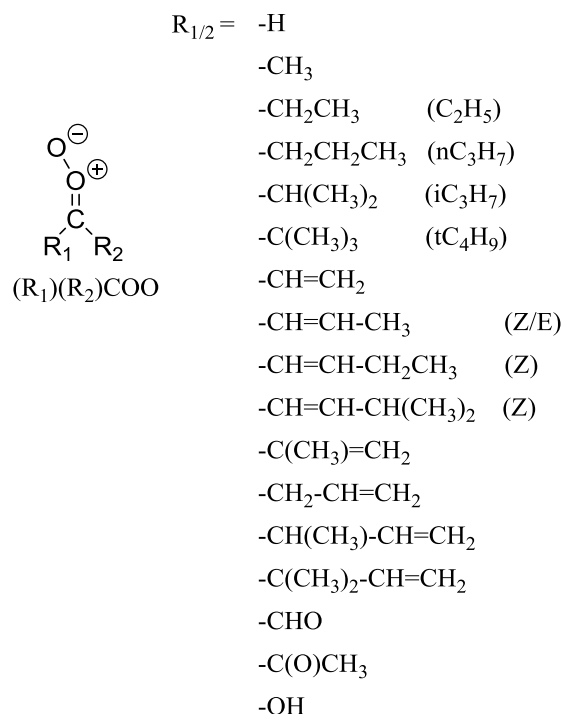


Figure 2: List of substituents considered in the quantum chemical and theoretical kinetic studies in this work. For alkyl substituents, we use the common abbreviations iso-propyl (iC₃H₇) and tert-butyl (tC₄H₉). For asymmetrically substituted vinyl groups, we do not in all cases consider both the *Z*- and *E*- conformer.

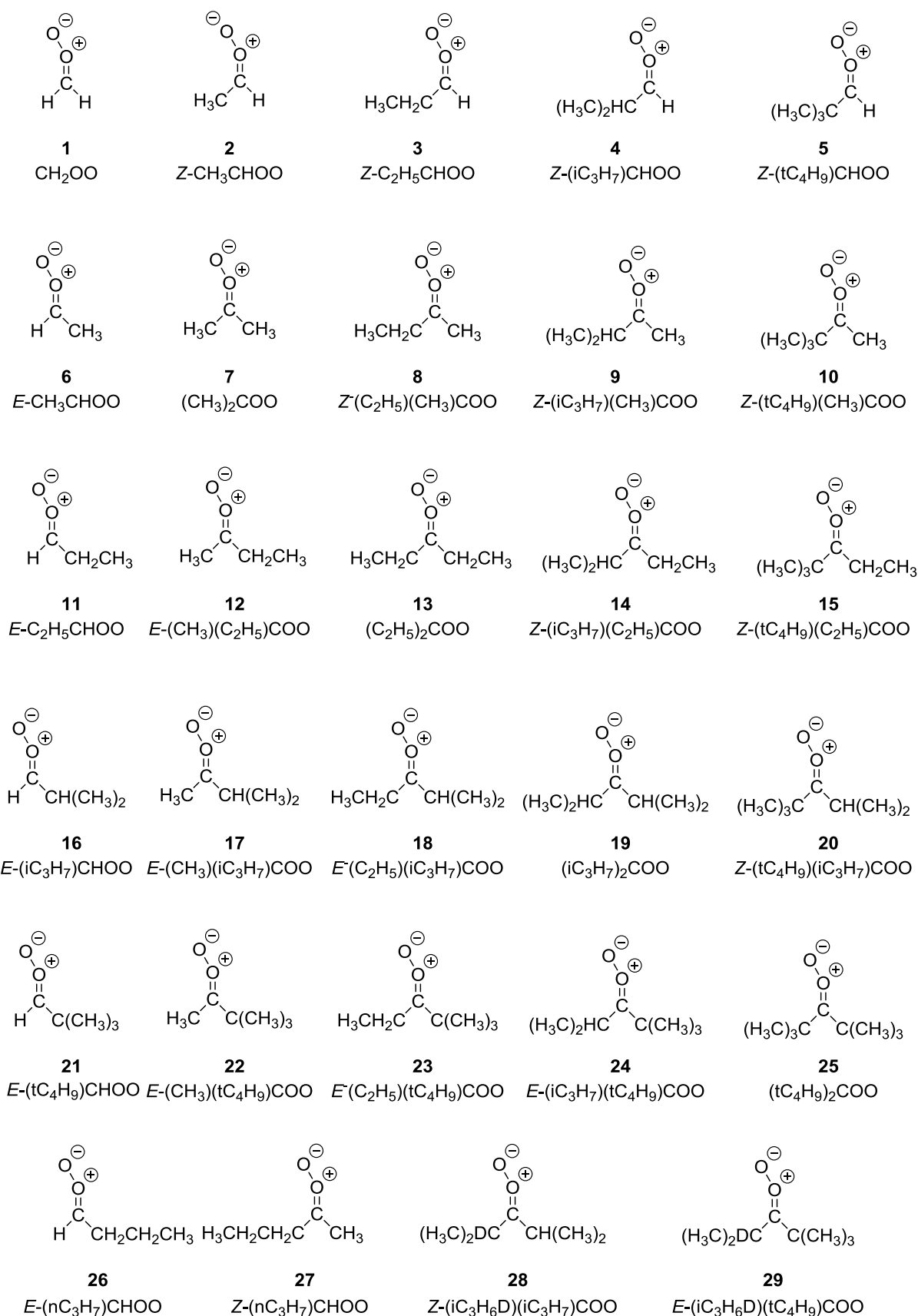


Figure 3: Carbonyl oxides considered in the theoretical calculations this work. For each reactant and TS, a full analysis of the conformational space is performed.

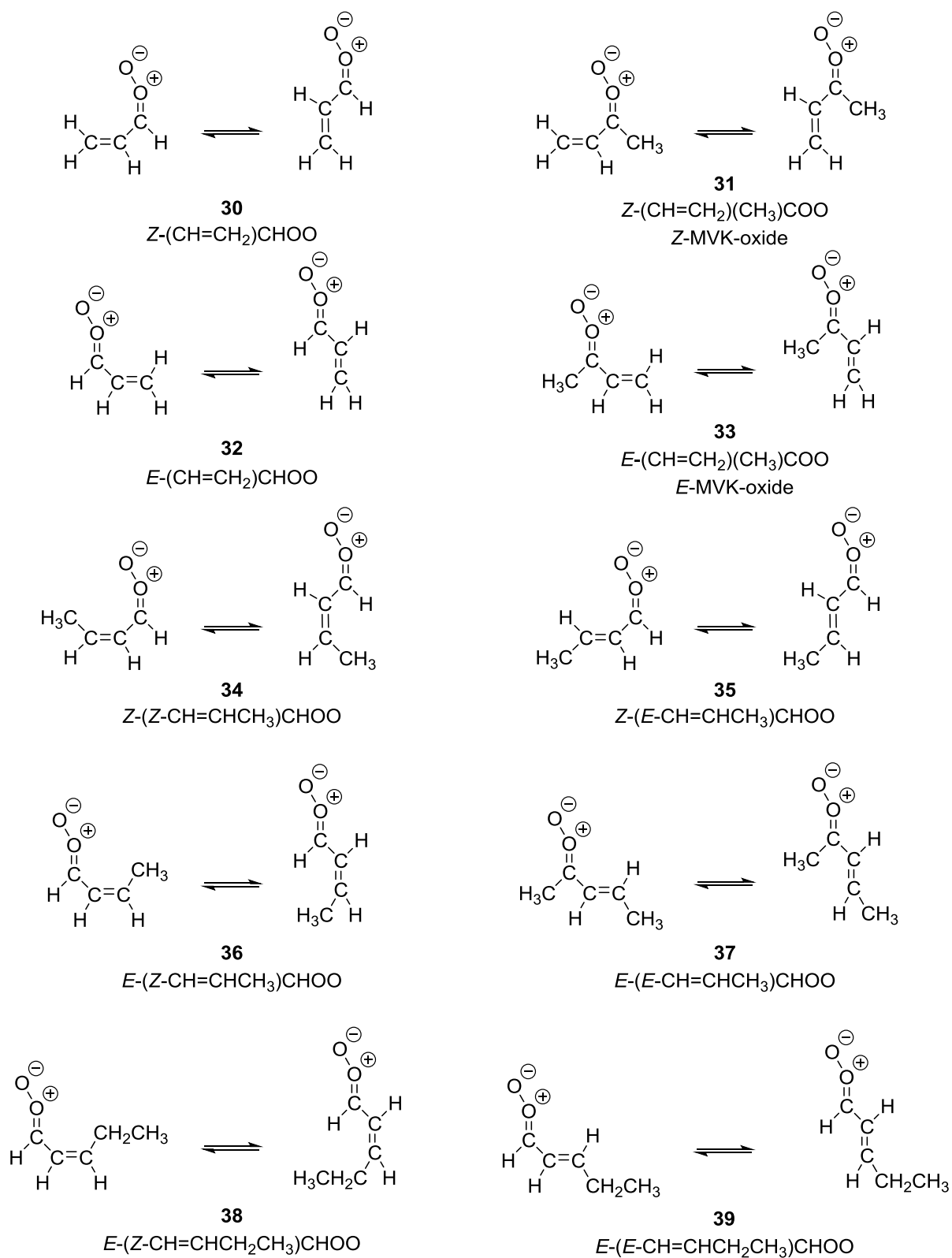


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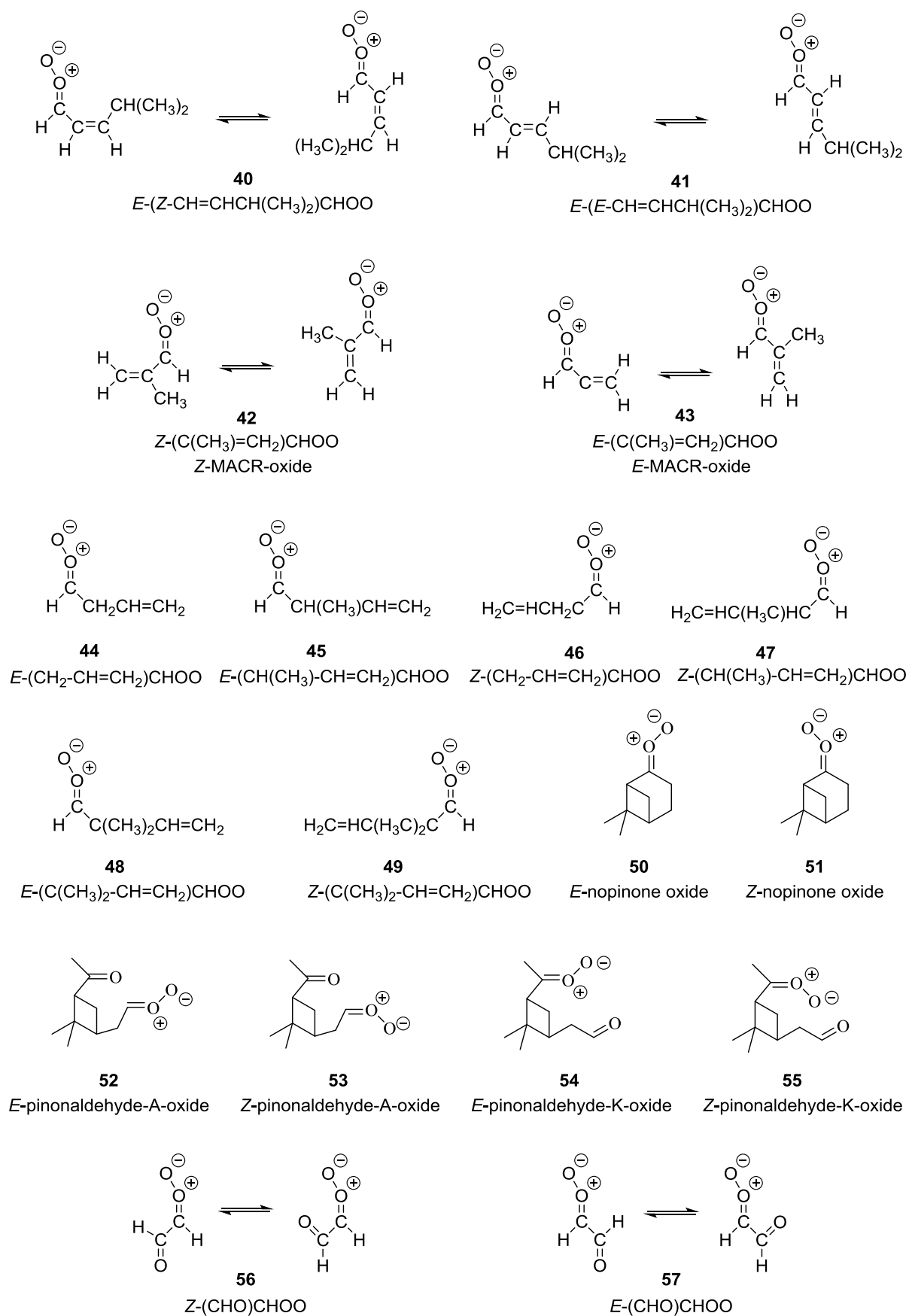


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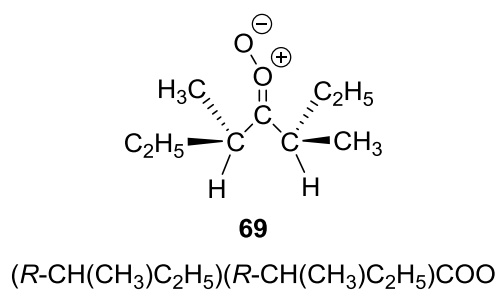
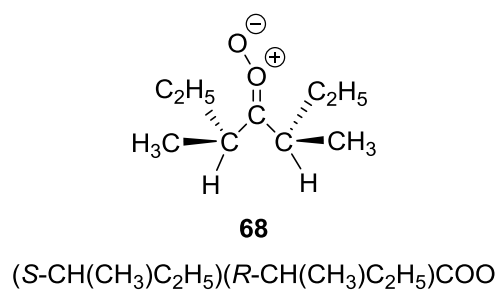
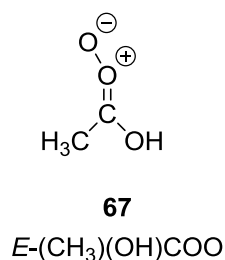
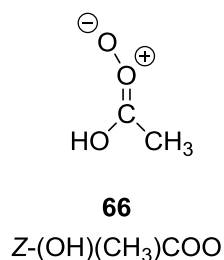
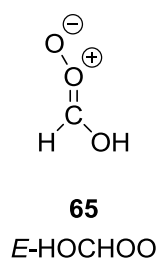
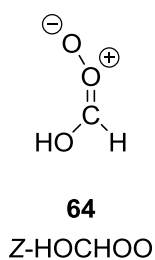
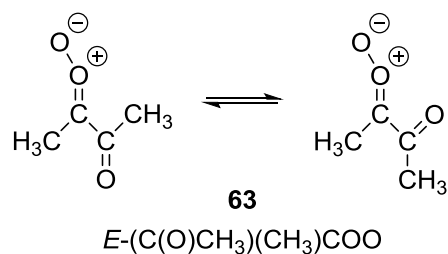
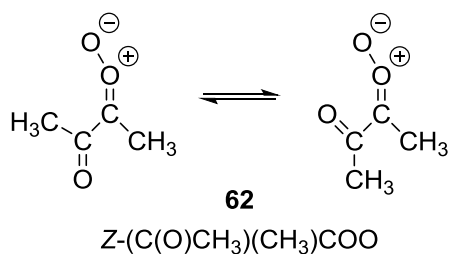
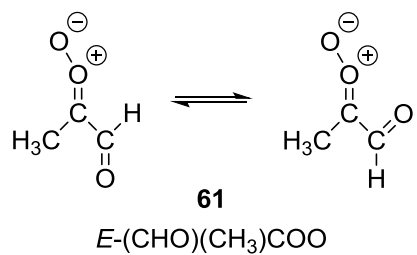
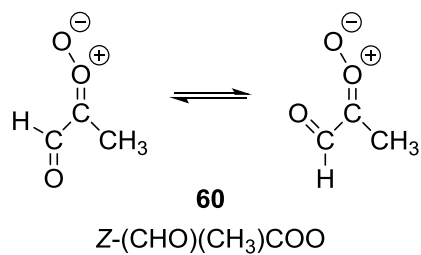
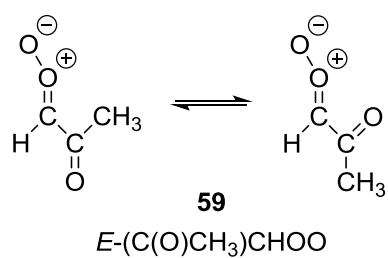
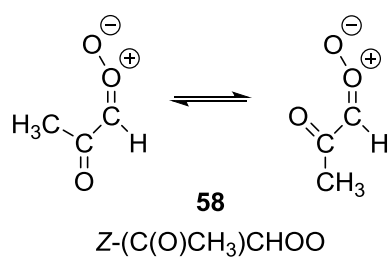
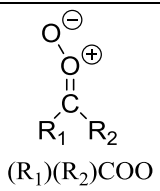
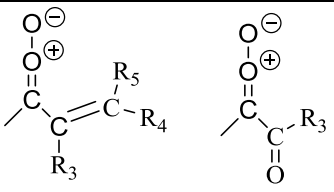


Figure 3 continued.

2. Structure-Activity relationships: substituent naming conventions

The combinations of substituents used allow the construction of Structure-Activity Relationships (SAR) that is applicable to most of the unsaturated compounds present in the troposphere. Table 1 lists the notational conventions used in the SARs in this work.

Table 1: SAR naming convention for carbonyl oxide substituents

Substituent label	Definition
R ₁ , R ₂	These are the substituents implanted on the carbon in the carbonyl oxide moiety, where R₁ is always on the <i>syn</i>-side of the oxide O-atom, and R₂ on the <i>anti</i>-side, as indicated in the scheme on the right. These substituents can represent the following moieties: H-atoms, alkyl groups (any branching, any chain length), β-, γ- and other vinyl substituents, β-, γ- and other oxo-substituted chains, and generally substituted alkyl chains where the functional group is at least in γ-position, where it is currently assumed to assert only a minor influence. Some additional substitution patterns are discussed explicitly elsewhere in this supporting information. 
R ₃ , R ₄ , R ₅	Substituents implanted on unsaturated substituents, specifically vinyl- and oxo-groups (see scheme on the right). We always use the same naming for the site-specific and stereo-specific positions, i.e. R₃, R₄ and R₅ are always as indicated in the schemes on the right. These substituents can represent all of the moieties as for R₁ and R₂, though one should consider that no explicit data is available for multi-unsaturated CI (i.e. conjugated alkadiene or cumulene/ketene functionalities adjacent to the carbonyl oxide moiety). 
R ₆ , R ₇	These substituents can represent all of the moieties as for R₁, but are implanted in a position of the molecule that is not defined explicitly by R₁ through R₅.
R _a , R _b , R _c , R _d ,...	These substituents allow for the same moieties as R₁, except for H-atoms. This is used to define the branching order of the bearing C-atom, i.e. -CH₃, -CH₂R_a, -CHR_aR_b, -CR_aR_bR_c are primary, secondary, tertiary and quaternary carbon atoms with exactly 3, 2, 1, and 0 H-atoms, respectively.
R', R'', R'''	These substituents represent either an H-atom, or a substituent without (easily) mobile H-atoms on the connecting carbon, e.g. -tC₄H₉, -C(R_a)=CR₄R₅, a cyclic moiety where ring strain or geometric constraints prevents H-migration (e.g. nopinone oxide), etc. These labels are used to signify compounds for which no H-migration path is accessible.

D. Reaction mechanisms available to CI

The unimolecular chemistry of CI has been reviewed extensively,^{4,8-11} we refer to these texts for more details. The reaction processes are depicted in Figure 4 and Figure 5.

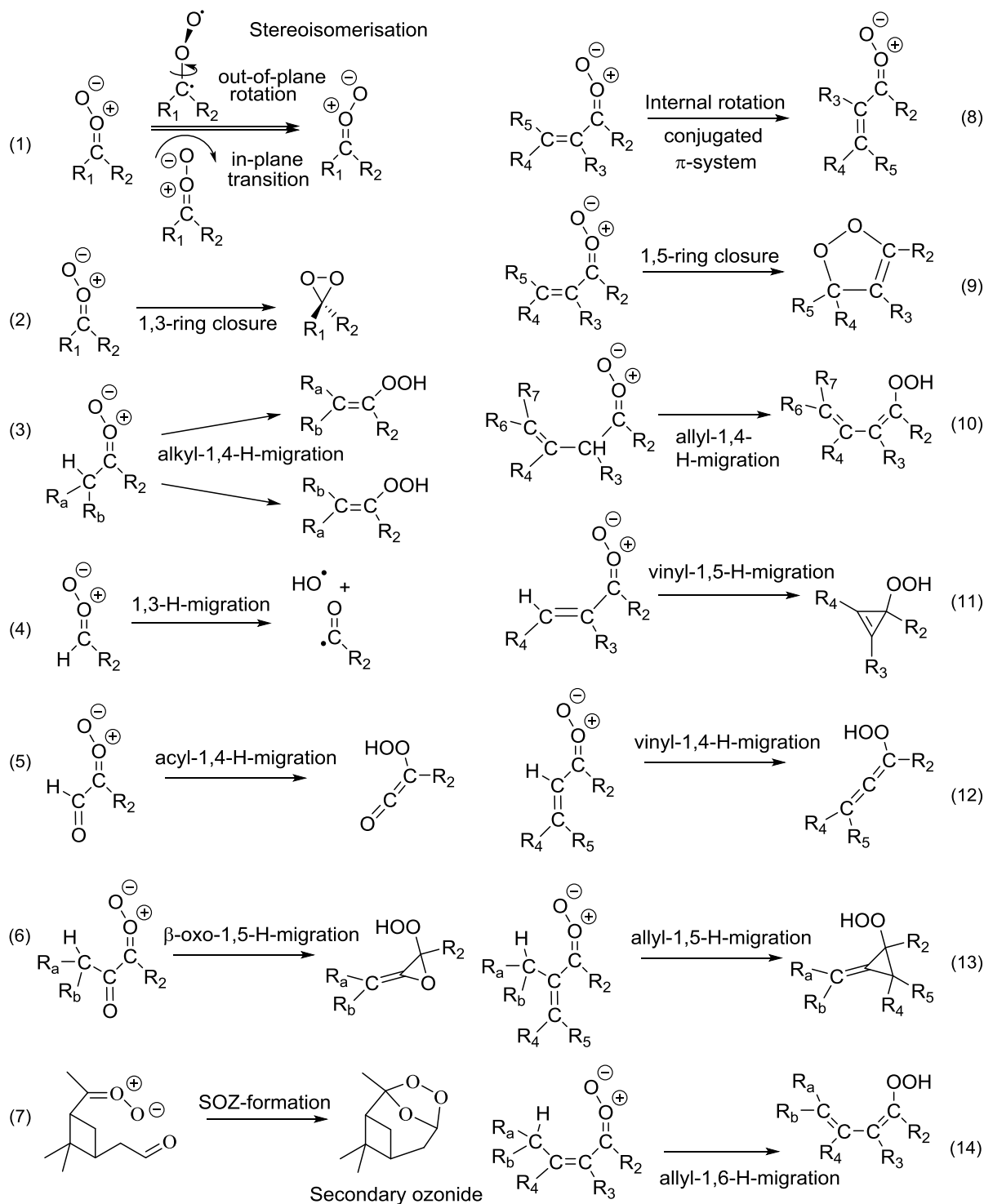
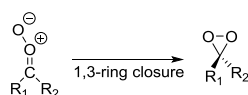
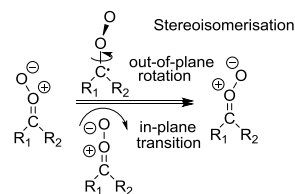


Figure 4: The reaction classes for alkyl-substituted, unsaturated, and oxo-substituted carbonyl oxides considered in this work. See text below for a short description and cross-references to the relevant sections.

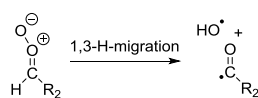
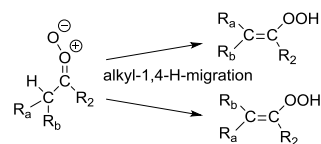
The *Z/E* stereo-isomerisation of CI (**reaction 1**) can occur through two channels: an out-of-plane rotation of the outer oxygen around the C–O axle, and an in-plane transition of the outer oxygen involving a linearization of the COO moiety. For unsaturated CI, one could also consider the analogous stereo-isomerisation of the olefinic moiety (not shown). The olefinic stereo-isomerisation barrier is less high in β -unsaturated CI than in the corresponding reaction for isolated double bonds, as the reaction proceeds via a bi-radical system that is stabilized by delocalization over the carbonyl oxide double bond. This reaction is discussed in detail in section H.



discussed in detail in section N.

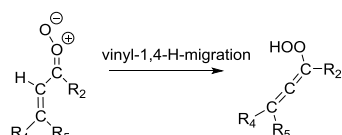
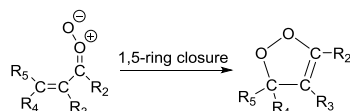
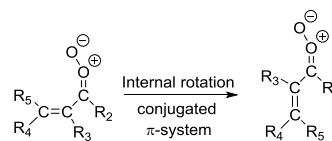
The ester channel (**reaction 2**) is in principle accessible to all carbonyl oxides, and involves a 1,3-ring closure forming a dioxirane, which in turn can re-arrange to an acid or ester. We only consider the initial ring closure in this work. This reaction is

The vinyl hydroperoxide (VHP) channel is accessible to substituted CI where an alkyl-hydrogen atom undergoes a 1,4-H-migration (**reaction 3**), forming a vinyl hydroperoxide, which is typically thought to dissociate readily forming an OH radical and a vinoxy radical, or to re-arrange forming a hydroxy-alkene. Dynamics studies have shown that the OH formation can also occur directly without isomerisation to VHP at high excitation energies,¹² but this process is not important at thermal dissociation energies^{12,13} where the bulk of the reaction occurs by tunneling through the barrier. The 1,4-H-migration can yield *Z*- or *E*-stereoisomers of the VHP products; these could show different chemical behavior though no information is available to our knowledge. As shown below, formation of the *Z*-isomer contributes only for a negligible fraction, < 4% at 298 K; we therefore report the rate coefficient for total VHP formation, and mention the $k(T)$ for *Z*-VHP formation separately. This reaction is discussed in detail in section J.

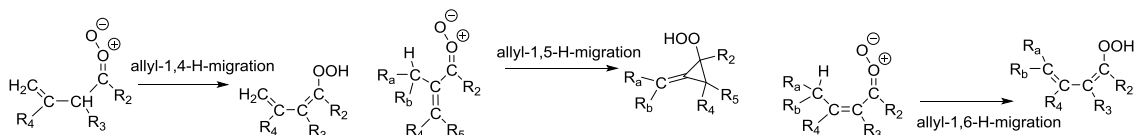


E-RCHOO carbonyl oxides (*anti*-RCHOO) can undergo a 1,3-H-migration (**reaction 4**), forming a hydroperoxide-alkyl radical that spontaneously falls apart to an acyl radical and OH; it is the main source of OH formation in ethene ozonolysis. The fragment could conceivably recombine to form a carboxylic acid, though the large energy release only makes this feasible for very large CI that can redistribute the excess energy sufficiently long to undergo collisional stabilization.

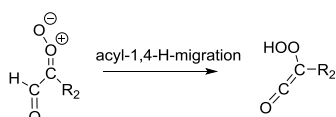
Complex CI have multiple conformers with different spatial orientations of the substituents. For alkyl substituents, this internal rotation is well known, but internal rotation along the single bond in the conjugated π -systems of β -unsaturated CI (**reaction 8**, both for vinyl- and oxo-substitution) is also feasible, similar to internal rotation^{14,15} in butadiene and isoprene. This reaction has been described for many β -unsaturated CI, but the impact of this isomerisation on CI kinetics has not been fully appreciated. This reaction is discussed in detail in section G.



Z- β -unsaturated CI can undergo a 1,5-ring closure (**reaction 9**, section O) forming a cyclic peroxide. This reaction has already been proposed by Kuwata et al.³ for methyl vinyl ketone oxide formed in the isoprene ozonolysis. These CI can also undergo vinyl-H-migrations, from either the inner or outer olefinic carbon: vinyl-1,4-H-migration (**reaction 12**, section K) forms a cumulene hydroperoxide, but has higher barriers than 1,5-cyclization, as already shown by Kuwata et al.³ Vinyl-1,5-H-migration (**reaction 11**, section M) formally leads to a singlet diradical structure that readily cyclises to a hydroperoxy-substituted cyclopropene.

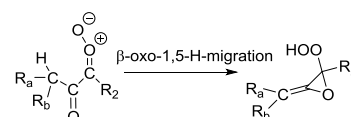


The double bond in β -unsaturated CI can assist the migration of alkylic H-atoms through allyl resonance stabilisation (**reaction 10**, allyl-1,4-H-migration in section L), by stabilization effects of a conjugated π -system (**reaction 13**, allyl-1,5-H-migration in section M), and by alleviating ring strain and allowing H-migration across a larger span (**reaction 14**, allyl-1,6-H-migration in section L). These reactions can have lower barriers than the traditional alkyl-1,4-H-migration; an exception is the allyl-1,5-H-migration (reaction 13) which formally forms a singlet biradical intermediate that readily cyclizes to a three-membered ring.



Acyl-1,4-H-migration in β -oxo-substituted CI, forming a ketene (**reaction 5**, section K), typically has a higher barrier than the analogous alkyl-1,4-H-shift owing to the

increased ring strain in the TS, which overwhelms any advantage that might be granted by the weaker acyl C–H-bond. Similar to β -vinyl-substituted CI, a β -ketone CI can undergo a β -oxo-1,5-H-migration (**reaction 6**, section M), formally forming a singlet biradical intermediate that cyclizes to an unsaturated epoxide.



For carbonyl-substituted CI, an internal ring closure can lead to secondary ozonides (SOZ, 1,2,4-trioxalane). This is particularly important for the ozonolysis of endocyclic double bonds, due the tethering of the two fragments after breaking of the primary ozonide. While the barrier for the reaction of CI with carbonyl compounds are typically low, leading to significant yields of SOZ,^{16–22} Vereecken and Francisco⁴ suggested that at least 6 connecting carbon atoms between the oxide and carbonyl moieties are needed to prevent excessive ring strain. In this respect, the intramolecular bicyclic SOZ formation in pinonaldehyde oxide (**reaction 7**) represents an edge case, where the 4-membered ring causes a higher reaction barrier than the corresponding non-cyclic CI would have. SOZ formation is discussed in detail in section P.



Other unimolecular reactions of CI have been described in the literature (see Table 5),^{4,8} but will not be studied here. A recent publication by Nguyen et al.²³ proposed a roaming $O(^1D)$ -migration with insertion in a C–H bond (**reaction 15**), leading directly to a carboxylic acid. However, we found that their calculations are severely impacted by spin-contamination, with an $S^2 > 1.00$ prior to annihilation of the first contaminant at both the UDFT and UHF level of theory, and still 0.03 (DFT) or 0.08 (HF) after annihilation. The root problem is that the UCCSD(T)/B3LYP level of theory is fundamentally unable to describe the $O(^1D)$ moiety, with a predicted $O(^3P)$ to $O(^1D)$ energy splitting of 11.4 kcal mol^{−1} as opposed to the best available value²⁴ of 45.369 kcal mol^{−1}. The proposed reaction process is thus more akin to a spin-forbidden transition over the $O(^3P)$ + carbonyl triplet surface. Harding and Klippenstein,²⁵ have made similar observations, and Chen et al.²⁶ have characterized the roaming channel with a barrier of 52.3 kcal mol^{−1}; we therefore consider this roaming channel negligible. One could also consider the O-atom elimination from the CI, leading either to $O(^1D)$ + carbonyl (**reaction 16**) or to $O(^3P)$ + a triplet carbonyl (**reaction 17**); these channels have been characterized as highly endothermic.^{23,27–32} The 1,5-ring closure reaction (**reaction 18**) in β -oxo carbonyl oxides forms a primary ozonide (POZ), and was already described in the acetylene + O_3 study by Cremer et al.²⁸ These authors, and our own exploratory calculations, show that this reaction has a large exit barrier and is never competitive. Note that this process is not limited to alkyne ozonolysis, but can occur in the CI formed in β -oxo-olefine ozonolysis (e.g. methyl-vinyl-ketone or methacrolein).

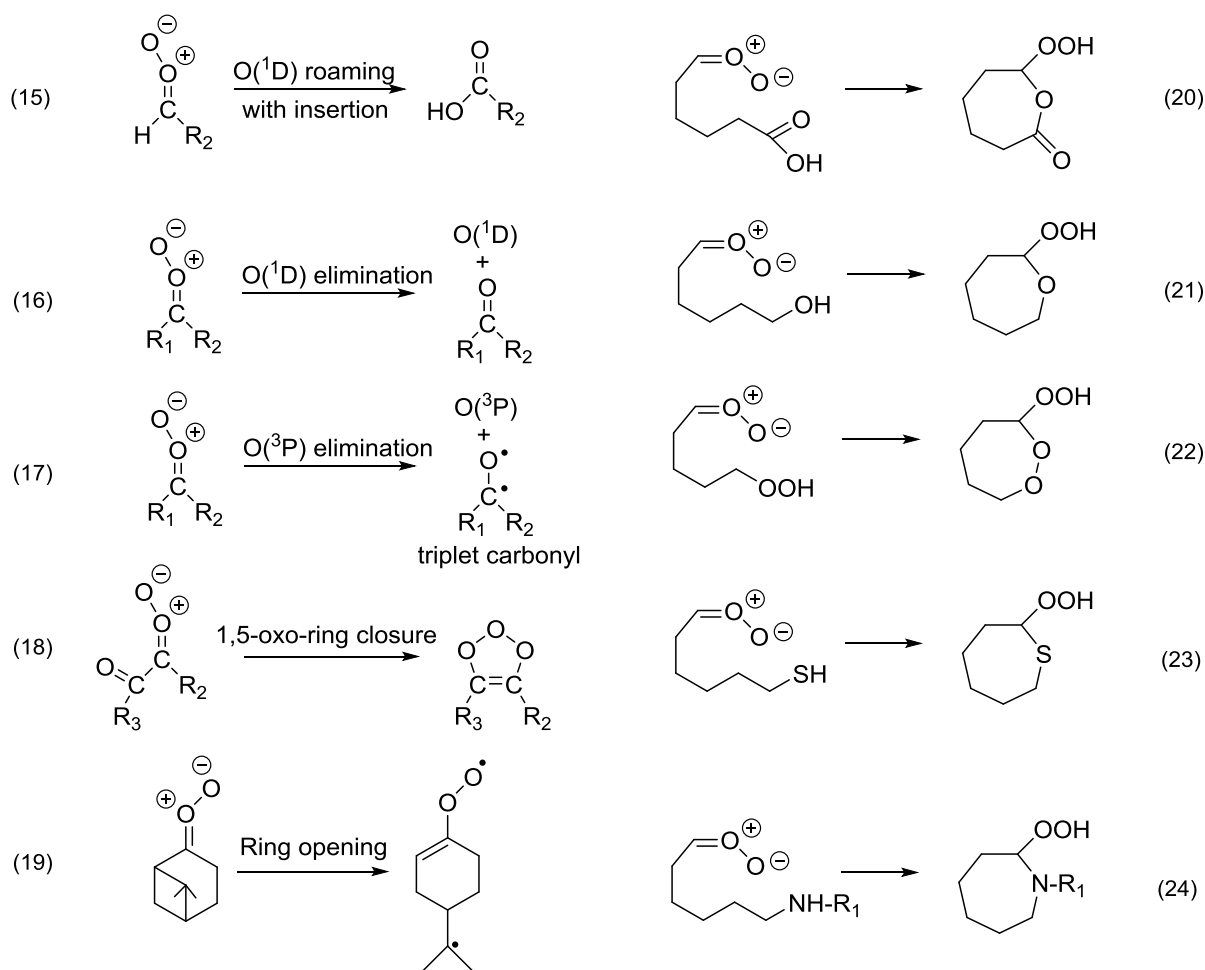


Figure 5: Carbonyl oxide unimolecular reaction classes that are not characterized in detail in this work.

Finally, there are many possible intramolecular interactions of the CI moiety with other functionalities in the molecules. This includes ring opening reactions (**reaction 19**) for CI with a strained ring in β -position, which was found to have high barriers in nopinone oxide.³³ In addition to SOZ formation (**reaction 7**), CI can also undergo ring closure with an acid functionality (**reaction 20**), as well as a hydroxy- (**reaction 21**), hydroperoxide- (**reaction 22**), sulfide (**reaction 23**) and amine group (**reaction 24**), etc. The feasibility of these reactions, and their kinetics, depends strongly on the molecular structure, i.e. moiety separation, ring strain, entropy of the cyclisation, etc., and this chemistry is thus hard to generalize. Similar to SOZ formation described higher, we propose that at least 6 connecting carbon atoms between the oxide and co-reacting moieties are needed to prevent excessive ring strain. Given that these reactions are highly specific to particular molecules, we do not include these reactions in our structure-activity relationships at this time. However, some of these reactions could represent a fast additional CI loss processes in the ozonolysis of specific compounds. In addition to reactions 20, 21 and 22, one should consider furthermore that carboxylic acids and -OH moieties can catalyze H-migration reactions,^{34–41} and could thus significantly speed up many of the other elementary reactions characterized in this work.

E. Literature SCI rate coefficients

1. Selected data for unimolecular reactions

Table 2: Selected literature data based on recent experimental work and post-CCSD(T) theoretical work for unimolecular reactions. Barrier height E_b in kcal mol⁻¹, rate coefficient $k(T)$ in s⁻¹. Only the energetically most favorable reaction path is considered here (1,3-ring closure for CH₂OO and *anti*-CH₃CHOO, 1,4-H-migration for all other). See Vereecken and Francisco,⁴ Vereecken et al.,⁸ or section E.8 for a more extensive list of data.

CI	E_b	$k(T)$	T / K	Methodology ^a	Reference
CH ₂ OO		0.19±0.07	297	E: C ₂ H ₄ ozonolysis; titration CI with SO ₂	Berndt et al. 2015 ⁴²
	18.9	0.25	297	T: CHEAT1 modified ; RRKM	Berndt et al. 2015 ⁴²
	19.0	0.3	298	T: W3X-L//CCSD(T)-F12 ; CVTST	Long et al. 2016 ³⁹
	19.1	0.3	298	T: HEAT-345(Q) ; SCTST	Nguyen et al. 2015 ⁴³
		< 11.6	293	E: RI ₂ photolysis ; cavity ring down	Chhantyal-Pun et al. 2016 ⁴⁴
		8.8±13	298	E: C ₂ H ₄ ozonolysis; Relative to CI + SO ₂	Newland et al. 2015 ⁴⁵
	18.6	0.6	298	T: CCSD(T)/aVTZ//M06-2X ; CTST	This work
	19.0	0.3	298	T: adjusted to literature data	This work ^b
	17.1	166	298	T: HEAT modified ; RRKM	Fang et al. 2016 ⁴⁶
	17.0	328	298	T: W3X-L//CCSD(T)-F12 ; CVTST	Long et al. 2016 ³⁹
<i>syn</i> -CH ₃ CHOO		122	298	T+E: mHEAT + RRKM + exp. k(E)	Fang et al. 2016 ⁴⁷
		288±275	298	E: C ₄ H ₈ ozonolysis; Relative to CI + SO ₂	Newland et al. 2015 ⁴⁵
		76±25	298	E: C ₄ H ₈ ozonolysis	Fenske et al. 2000 ⁴⁸
		20±10	≤293 ^c	E: C ₄ H ₈ ozonolysis ; OH LIF	Novelli et al. 2014 ⁴⁹
		> 3	297	E: C ₄ H ₈ ozonolysis; titration CI with SO ₂	Berndt et al. 2015 ⁴²
	16.4	257	298	T: CCSD(T)/aVTZ//M06-2X ; CTST	This work
	16.8	136	298	T: adjusted to literature data	This work ^b
	15.6	55.4	298	T: W3X-L//CCSD(T)-F12 ; CVTST	Long et al. 2016 ³⁹
		> 3	297	E: C ₄ H ₈ ozonolysis; titration CI with SO ₂	Berndt et al. 2015 ⁴²
	15.3	104	298	T: CCSD(T)/aVTZ//M06-2X ; CTST	This work
<i>anti</i> -CH ₃ CHOO	15.7	53	298	T: adjusted to literature data	This work ^b
	16.5	279	298	T: CCSD(T)-F12/CBS//B2PLYPD3 ; RRKM	Fang et al. 2016 ⁵⁰
	16.1	387	298	T: CCSD(T)/aVTZ//M06-2X ; CTST	This work
	16.5	205	298	T: adjusted to literature data	This work ^b
(CH ₃) ₂ COO	16.2	369	298	T: HEAT modified ; RRKM	Fang et al. 2016 ⁴⁶
		276	298	T+E: mHEAT + RRKM + exp. k(E)	Fang et al. 2017 ⁵¹
		305±70	293	E: RI ₂ photolysis ; cavity ring down	Chhantyal-Pun et al. 2017 ⁴⁴
		1000±200 ^d	298	E: TME ozonolysis; Relative to CI + SO ₂	Newland et al. 2015 ⁴⁵
		361±49	298	E: TME ozonolysis; UV absorption	Smith et al. 2016 ⁵²
	15.9	400	298	T: QCISD(T)/CBS//B3LYP; SCTST	Smith et al. 2016 ⁵²
	15.7	906	298	T: CCSD(T)/aVTZ//M06-2X ; CTST	This work
	16.1	478	298	T: adjusted to literature data	This work ^b

^a Concise description of experimental (E:) and theoretical (T:) methodologies. See references for more details.

^b CCSD(T)/aug-cc-pvTZ//M06-2X data with CTST/Eckart rate coefficients after adjusting the barrier height by +0.4 kcal mol⁻¹ (see methodology description in section F)

^c These measurements may have been affected by expansion cooling in the probe nozzle.

^d Relative rate converted using $k((\text{CH}_3)_2\text{COO} + \text{SO}_2) = 1.6 \times 10^{-10} \text{ cm}^3 \text{ molecules}^{-1} \text{ s}^{-1}$ (see below)

Table 3: Intramolecular secondary ozonide (SOZ) formation in substituted carbonyl oxides, listing barrier heights E_b (kcal mol⁻¹), rate coefficient k (s⁻¹) at 298 K, and parameters for a Kooij equation fit $k(T)=A \times T^n \times \exp(-E_a/T)$ for the temperature range 200-450 K.

Carbonyl oxide	E_b	$k(298K)$	A / s^{-1}	n	E_a / K	Reference
<i>n</i> -OCHC ₄ H ₈ CHOO	5.1					Chuong et al. 2004 ¹⁷
<i>n</i> -OCHCH ₂ CHOO	15.7					Kuwata et al. 2011 ¹⁶
β-caryophyllene CI-1a	12.3	5.3				Nguyen et al. 2009 ⁵³
β-caryophyllene CI-1b	10.6	486				Nguyen et al. 2009 ⁵³
β-caryophyllene CI-2a	8.1	1100				Nguyen et al. 2009 ⁵³
β-caryophyllene CI-2b	13.3	7.4				Nguyen et al. 2009 ⁵³
α-phellandrene CI1a	13.6 ^a					Mackenzie-Rae et al. 2016 ⁵⁴
α-phellandrene CI1b	6.5 ^a					Mackenzie-Rae et al. 2016 ⁵⁴
α-phellandrene CI2a	4.2 ^a					Mackenzie-Rae et al. 2016 ⁵⁴
α-phellandrene CI2b	5.8 ^a					Mackenzie-Rae et al. 2016 ⁵⁴
α-phellandrene CI3a	14.4 ^a					Mackenzie-Rae et al. 2016 ⁵⁴
α-phellandrene CI3b	9.3 ^a					Mackenzie-Rae et al. 2016 ⁵⁴
α-phellandrene CI4a	6.7 ^a					Mackenzie-Rae et al. 2016 ⁵⁴
α-phellandrene CI4b	7.5 ^a					Mackenzie-Rae et al. 2016 ⁵⁴
Z-pinonaldehyde-K-oxide	13.5	8.7	8.72×10^{13}	-1.31	6702	This work
Z-pinonaldehyde-A-oxide	16.0	2.8×10^{-2}	6.21×10^{13}	-1.54	7914	This work

^a $\Delta G^\ddagger(298K)$ from a single-conformer analysis

2. Rate coefficient estimates for the reaction of SCI with H₂O

Table 4: Barrier heights (kcal mol⁻¹) and rate coefficients (cm³ molecule⁻¹ s⁻¹) available in the literature on the CI + H₂O reaction. Relative position of R₁ and R₂ as in Figure 1.

R ₁	R ₂	E_b ^a	$k(298K)$	Ref.
H	H		$< 4 \times 10^{-15}$ (Exp)	Welz et al. 2012 ⁵⁵
			$10^{-12} - 10^{-15}$ (Exp)	Leather et al. 2012 ⁵⁶
			$(2.5 \pm 1) \times 10^{-17}$ (Exp)	Ouyang et al. 2013 ⁵⁷
			$< 9 \times 10^{-17}$ (Exp)	Stone et al. 2014 ⁵⁸
			$(3.2 \pm 1.2) \times 10^{-16}$ (Exp)	Berndt et al. 2015 ⁴²
			$(1.3 \pm 0.4) \times 10^{-15}$ (Exp)	Newland et al. 2015 ⁴⁵
		2.0	$1.66-5.60 \times 10^{-15}$	Anglada et al. 2011 ¹
		1.9	5.9×10^{-17}	Anglada et al. 2002 ³⁸
		4.3	5.8×10^{-18}	Ryzhkov and Ariya 2004 ⁵⁹
		2.8	3.69×10^{-16}	Lin et al. 2016 ⁶⁰
		2.2	3.05×10^{-15}	Anglada and Solé 2016 ⁶¹
CH ₃	H	2.8	2.32×10^{-18}	Chen et al. 2016 ²⁶
		3.5	2.4×10^{-16}	Long et al. 2016 ³⁹
			$< 4 \times 10^{-15}$ (Exp)	Taatjes et al. 2013 ⁶²
			$< 2 \times 10^{-16}$ (Exp)	Sheps et al. 2014 ⁶³
		5.3	$2.39-3.23 \times 10^{-18}$	Anglada et al. 2011 ¹
		7.0	7.23×10^{-21}	Kuwata et al. 2010 ⁴⁰
		5.8	4.2×10^{-20}	Anglada et al. 2002 ³⁸
		1.2	7.33×10^{-21}	Ryzhkov and Ariya 2004 ⁵⁹
		7.0	1.98×10^{-19}	Lin et al. 2016 ⁶⁰
		6.0	2.89×10^{-18}	Anglada and Solé 2016 ⁶¹
		7.5	1.9×10^{-19}	Long et al. 2016 ³⁹
CH ₂ -C ₈ H ₁₃ O	H	10.5 ^c		Jiang et al. 2013 ^{64 c}
			$(1.0 \pm 0.4) \times 10^{-14}$ (Exp)	Taatjes et al. 2013 ⁶²
			$(2.4 \pm 0.4) \times 10^{-14}$ (Exp)	Sheps et al. 2014 ⁶³
			$(2.3 \pm 2.1) \times 10^{-14}$ (Exp)	Newland et al. 2015 ⁴⁵
		-1.2	$1.68-2.03 \times 10^{-13}$	Anglada et al. 2011 ¹
		0.6	2.87×10^{-16}	Kuwata et al. 2010 ⁴⁰
H	CH ₃	-0.7	2.5×10^{-15}	Anglada et al. 2002 ³⁸

		-5.3	4.0×10^{-16}	Ryzhkov and Ariya 2004 ⁵⁹
		0.3	3.4×10^{-14}	Lin et al. 2016 ⁶⁰
		-1.2	1.35×10^{-13}	Anglada and Solé 2016 ⁶¹
CH ₃	CH ₃	1.2	5.2×10^{-15}	Long et al. 2016 ³⁹
			$< 1.5 \times 10^{-16}$ (Exp)	Huang et al. 2015 ⁶⁵
			$(2.1 \pm 0.6) \times 10^{-15}$ (Exp)	Newland et al. 2015 ⁴⁵
		3.6	3.87×10^{-17}	Anglada et al. 2011 ¹
		4.0	7.5×10^{-19}	Anglada et al. 2002 ³⁸
		4.0	1.4×10^{-19}	Ryzhkov and Ariya 2004 ⁵⁹
		3.6	2.41×10^{-17}	Anglada and Solé 2016 ⁶¹
CH ₃	CH ₂ -CH ₂ -C ₆ H ₉ O	9.2		Jiang et al. 2013 ^{64 c}
CH ₃	-cyc-C ₆ H ₈ -CH ₃	8.5		Jiang et al. 2013 ^{64 c}
<i>E</i> -nopinone oxide (bicyclic)		2.07		Lin et al. 2014 ⁶⁶
CH ₃	<i>s-trans</i> -CH=CH ₂	8.2	$(1.4 \text{ s}^{-1})^b$	Aplincourt and Anglada 2003 ³⁷
		6.8	2.93×10^{-19}	Anglada et al. 2011 ¹
		9.8	1.62×10^{-21}	Kuwata et al. 2010 ⁴⁰
		6.8	3.35×10^{-19}	Anglada and Solé 2016 ⁶¹
CH ₃	<i>s-cis</i> -CH=CH ₂	6.8	$(8.8 \text{ s}^{-1})^b$	Aplincourt and Anglada 2003 ³⁷
		5.2	1.97×10^{-18}	Anglada et al. 2011 ¹
		7.6	3.43×10^{-20}	Kuwata et al. 2010 ⁴⁰
		5.2	2.91×10^{-18}	Anglada and Solé 2016 ⁶¹
<i>s-trans</i> -CH=CH ₂	CH ₃	6.1	$(49 \text{ s}^{-1})^b$	Aplincourt and Anglada 2003 ³⁷
		4.7	1.39×10^{-18}	Anglada et al. 2011 ¹
		4.3	1.87×10^{-17}	Anglada and Solé 2016 ⁶¹
<i>s-cis</i> -CH=CH ₂	CH ₃	7.5	$(15 \text{ s}^{-1})^b$	Aplincourt and Anglada 2003 ³⁷
		5.8	8.31×10^{-18}	Anglada et al. 2011 ¹
		5.8	3.65×10^{-18}	Anglada and Solé 2016 ⁶¹
H	<i>s-trans</i> -C(CH ₃)=CH ₂	3.9	$(3.8 \times 10^3 \text{ s}^{-1})^b$	Aplincourt and Anglada 2003 ³⁷
		1.9	1.89×10^{-15}	Anglada et al. 2011 ¹
		1.9	2.91×10^{-15}	Anglada and Solé 2016 ⁶¹
H	<i>s-cis</i> -C(CH ₃)=CH ₂	2.1	$(4.6 \times 10^4 \text{ s}^{-1})^b$	Aplincourt and Anglada 2003 ³⁷
		0.2	1.36×10^{-14}	Anglada et al. 2011 ¹
		0.2	1.67×10^{-14}	Anglada and Solé 2016 ⁶¹
H	C(CH ₃)=CH ₂		$1.2 \times 10^{-15 d}$	Newland et al. 2016 ⁴⁵
<i>s-trans</i> -C(CH ₃)=CH ₂	H	2.4	$(5.8 \times 10^4 \text{ s}^{-1})^b$	Aplincourt and Anglada 2003 ³⁷
		4.7	4.86×10^{-18}	Anglada et al. 2011 ¹
		4.7	6.87×10^{-18}	Anglada and Solé 2016 ⁶¹
<i>s-cis</i> -C(CH ₃)=CH ₂	H	3.9	$(1.6 \times 10^4 \text{ s}^{-1})^b$	Aplincourt and Anglada 2003 ³⁷
		6.8	5.58×10^{-19}	Anglada et al. 2011 ¹
		6.8	2.25×10^{-19}	Anglada and Solé 2016 ⁶¹
F	F	-8.0	4.65×10^{-9}	Anglada et al. 2011 ¹
H	n-C ₁₂ H ₂₃		$10^{-3} \times k_{\text{acid}}$ (Exp)	Tobias and Ziemann 2001 ⁶⁷
cyc-OCH ₂ CH ₂ O-COO		-7.1	7.06×10^{-11}	Anglada et al. 2011 ¹
cyc-CH=CH-COO		-4.0	1.23×10^{-11}	Anglada et al. 2011 ¹

^a Energy barrier relative to the separated reactants CI + H₂O. The reaction proceeds through a strong pre-reactive complex CI--H₂O which is not considered here.

^b Value in brackets is the unimolecular reaction of the CI--H₂O complex to the hydroxy-hydroperoxide.

^c Limonene, single-conformer analysis only

^d Bulk rate coefficient assigned to *E*-(C(CH₃)=CH₂)CHOO as it is the only (non-CH₂OO) isoprene-derived CI that is predicted to have a high rate coefficient with H₂O.

3. Rate coefficient estimates for the reaction of SCI with (H₂O)₂

Table 5: Barrier heights (kcal mol⁻¹) and rate coefficients (cm³ molecule⁻¹ s⁻¹) available in the literature on the CI + (H₂O)₂ reaction. Relative position of R₁ and R₂ as in Figure 1.

R ₁	R ₂	E _b (H ₂ O) ₂ ^a	k(298K) (H ₂ O) ₂	Ref
H	H		(6.5 ± 0.5) × 10 ⁻¹² (Exp)	Chao et al. 2015 ⁶⁸
			(4.0 ± 1.2) × 10 ⁻¹² (Exp)	Lewis et al. 2015 ⁶⁹
			(7.4 ± 0.6) × 10 ⁻¹² (Exp)	Smith et al. 2015 ⁷⁰
			131 × k(H ₂ O)	Ryzhkov and Ariya 2006 ⁷¹
		-8.9	2.07 × 10 ⁻¹²	Ryzhkov and Ariya 2004 ⁵⁹
		-6.6	5.44 × 10 ⁻¹²	Lin et al. 2016 ⁶⁰
		-8.5	1.67 × 10 ⁻¹⁰	Anglada and Solé 2016 ⁶¹
		-10.0	2.66 × 10 ⁻¹¹	Chen et al. 2016 ²⁶
CH ₃	H	-5.9	1.2 × 10 ⁻¹⁶	Ryzhkov and Ariya 2004 ⁵⁹
		-3.2	2.56 × 10 ⁻¹⁴	Lin et al. 2016 ⁶⁰
		-5.9	4.83 × 10 ⁻¹³	Anglada and Solé 2016 ⁶¹
H	CH ₃	-10.1	2.0 × 10 ⁻¹²	Ryzhkov and Ariya 2004 ⁵⁹
		-7.5	1.6 × 10 ⁻¹¹	Lin et al. 2016 ⁶⁰
		-9.9	5.93 × 10 ⁻¹⁰	Anglada and Solé 2016 ⁶¹
CH ₃	CH ₃	-4.3	5.78 × 10 ⁻¹⁷	Ryzhkov and Ariya 2004 ⁵⁹
		-6.1	3.72 × 10 ⁻¹³	Anglada and Solé 2016 ⁶¹
CH ₃	<i>s-trans</i> -CH=CH ₂	-1.5	9.23 × 10 ⁻¹⁶	Anglada and Solé 2016 ⁶¹
CH ₃	<i>s-cis</i> -CH=CH ₂	-4.0	1.27 × 10 ⁻¹⁴	Anglada and Solé 2016 ⁶¹
<i>s-trans</i> -CH=CH ₂	CH ₃	-4.3	4.71 × 10 ⁻¹⁴	Anglada and Solé 2016 ⁶¹
<i>s-cis</i> -CH=CH ₂	CH ₃	-2.4	5.42 × 10 ⁻¹⁵	Anglada and Solé 2016 ⁶¹
H	<i>s-trans</i> -C(CH ₃)=CH ₂	-6.2	3.31 × 10 ⁻¹²	Anglada and Solé 2016 ⁶¹
H	<i>s-cis</i> -C(CH ₃)=CH ₂	-8.0	2.21 × 10 ⁻¹¹	Anglada and Solé 2016 ⁶¹
<i>s-trans</i> -C(CH ₃)=CH ₂	H	-4.9	1.08 × 10 ⁻¹⁵	Anglada and Solé 2016 ⁶¹
<i>s-cis</i> -C(CH ₃)=CH ₂	H	-2.0	2.39 × 10 ⁻¹⁵	Anglada and Solé 2016 ⁶¹

^a Energy barrier relative to the separated reactants CI + (H₂O)₂. The reaction proceeds through a strong pre-reactive complex CI--(H₂O)₂ which is not included here.

4. Rate coefficient estimates for the reaction of SCI with SO₂

For the rate coefficient k_{SO_2} for the reactions of SCI with SO₂ we rely mostly on the available literature data for SCI species CH₂OO (**1**), Z-CH₃CHOO (**2**), *E*-CH₃CHOO (**6**) and (CH₃)₂COO (**7**), as listed in Table 6. Direct experimental data are available for CH₂OO (**1**) by five different groups, with a very good agreement across the different measurements; we adopt the average value of 3.7 × 10⁻¹¹ cm³ molecules⁻¹ s⁻¹. For *E*-CH₃CHOO (**6**) and Z-CH₃CHOO (**2**) several groups measured the rate coefficient directly by following the decay of the SCI. For this study, the average value of 1.4 × 10⁻¹⁰ and 2.7 × 10⁻¹¹ cm³ molecule⁻¹ s⁻¹ for *E*-CH₃CHOO (**6**) and Z-CH₃CHOO (**2**), respectively, was used. The indirect values by Berndt et al.⁷², obtained by measuring H₂SO₄ formation, were omitted from the averaging as these values differ by more than two orders of magnitude from the other literature data; the reason for this large discrepancy has not been reliably established yet.^{4,9,10} For (CH₃)₂COO (**7**) we rely on the average rate coefficient of 1.6 × 10⁻¹⁰ cm³ molecules⁻¹ s⁻¹ across the most recent direct studies; as before we exclude the Berndt et al.⁷² rate coefficient.

These values are all within one order of magnitude, and theoretical studies do not predict an energy barrier for the reaction of SCI with SO₂,^{4,8,73,74} suggesting that the rate coefficients for other SCI are likely to remain with this range. With this in mind, we adopt the value for *E*-CH₃CHOO (**6**) for all *E*-RCHOO, the value for Z-CH₃CHOO (**2**) for all Z-RCHOO, and the value for (CH₃)₂COO (**7**) for all di-substituted CI. An exception is Z-nopinone oxide (**51**), where the rate coefficient of 4 × 10⁻¹¹ cm³ molecule⁻¹ s⁻¹ from the study of Ahrens et al.⁷⁵ is used. Note that this value depended on the assumption that the lifetime of *E*-nopinone oxide (**50**) was ≤ 0.02 s, an assumption shown in section Q.1 to hold.

Table 6: Experimental rate coefficients k_{SO_2} at 298K ($\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$) for the reaction of stabilized CI with SO_2 .

SCI	k_{SO_2}	Source
CH_2OO	3.8×10^{-11}	Sadezky et al., 2008 ⁷⁶
	3.9×10^{-11}	Welz et al., 2012 ⁷⁷
	3.4×10^{-11}	Stone et al., 2014 ⁵⁸
	3.5×10^{-11}	Liu et al., 2014 ⁷⁸
$E\text{-CH}_3\text{CHOO}$	3.9×10^{-11}	Chhantyal-Pun et al., 2015 ⁷⁹
	1.4×10^{-13}	Berndt et al., 2012 ⁷²
	6.7×10^{-11}	Taatjes et al., 2013 ⁶²
$Z\text{-CH}_3\text{CHOO}$	2.2×10^{-10}	Sheps et al., 2014 ⁶³
	1.4×10^{-13}	Berndt et al., 2012 ⁷²
	2.4×10^{-11}	Taatjes et al., 2013 ⁶²
$(\text{CH}_3)_2\text{COO}$	2.9×10^{-11}	Sheps et al., 2014 ⁶³
	2.0×10^{-11}	Smith et al., 2014 ⁸⁰
	7.7×10^{-13}	Berndt et al., 2012 ⁷²
	1.3×10^{-10}	Huang et al., 2015 ⁶⁵
1-Me-cyclohexene-CI	1.3×10^{-10}	Chhantyal-Pun et al., 2017 ⁴⁴
	2.2×10^{-10}	Chhantyal-Pun et al., 2017 ⁴⁴
	9.3×10^{-14}	Berndt et al., 2012 ⁷²
Z-nopinone oxide	4.0×10^{-11}	Ahrens et al., 2014 ⁷⁵

It should be noted that the rate coefficients of $\text{CI} + \text{SO}_2$ do not follow the CI stability trends, e.g. the rate coefficient for $(\text{CH}_3)_2\text{COO}$ is significantly higher than for $Z\text{-CH}_3\text{CHOO}$ and more like that of $E\text{-CH}_3\text{CHOO}$, despite the stability of $(\text{CH}_3)_2\text{COO}$ being similar to that of $Z\text{-CH}_3\text{CHOO}$. As many CI formed in the atmosphere are di-substituted, generalizing this trend leads to a high average SO_2 conversion rate. In this respect, it is interesting that Z-nopinone oxide was measured by Ahrens et al. at a comparatively lower rate coefficient;⁷⁵ note that the exoergicity of the $\text{SO}_2 + \text{Z-nopinone oxide}$ reaction is similar to that for $(\text{CH}_3)_2\text{COO}$, i.e. the reaction is not significantly affected by ring strain or steric hindrance. Berndt et al.⁷² likewise observed a lower relative rate for 1-Me-cyclohexene-derived CI, which implies that neither the *Z*- and *E*-di-substituted CI, nor the *E*-RCHOO CI formed from this compound, react fast with SO_2 . This interpretation, however, assumes that the relative rate measurements are reliable; the absolute rate coefficients values in Berndt et al.⁷² are systematically underestimated compared to the remaining literature.

5. Rate coefficient estimates for the reaction of SCI with NO_2

Data on the $\text{SCI} + \text{NO}_2$ reaction (see Table 7) is very scarce. For the modeling study, we employ a rate coefficient of $4 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for all SCI, biased to the high side to investigate if this reaction can contribute to SCI loss or affect the NOx cycle.

Table 7: Rate coefficients ($\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$) for reactions of SCI with NO_2

SCI	$k_{NO_2}(298\text{K})$	Reference
CH_2OO	7×10^{-12}	Welz et al., 2012 ⁵⁵
	1.5×10^{-12}	Stone et al., 2014 ⁵⁸
	4.4×10^{-12}	Vereecken and Nguyen, 2017 ⁸¹
$Z\text{-CH}_3\text{CHOO}$	2×10^{-12}	Taatjes et al., 2013 ⁶²
$E\text{-CH}_3\text{CHOO}$	2×10^{-12}	Taatjes et al., 2013 ⁶²
$(\text{CD}_3)_2\text{COO}$	2.1×10^{-12}	Chhantyal-Pun et al., 2017 ⁴⁴

The product formation from these reactions has been the subject of considerable debate, with environmental chamber studies by Ouyang et al.⁵⁷ finding mostly formation of $\text{NO}_3 + \text{carbonyl}$, in agreement with early low-level theoretical work by Presto and Donahue.⁸² If NO_3 is formed, this reaction could have an impact on the NOx cycle.⁸³ However, more recent experimental work by Taatjes et al.⁶² and Caravan et al.⁸⁴ did not detect NO_3 in low-pressure photo-ionization experiments, placing an upper limit of 30% on the NO_3 yield. Their observation of a product mass equivalent to the $\text{CI} + \text{NO}_2$ adduct suggests that addition is the main product pathway. A recent multi-reference theoretical study by Vereecken and Nguyen⁸¹ predicted formation of the α -nitro-peroxy radical adduct, in agreement with these latter experimental studies.

6. Rate coefficient estimates for the reaction of SCI with acids

The reaction of SCI with acids has been well studied, though direct measurements remain scarce. Early experimental data^{85–92} showed fast reactions of CI with carboxylic acids, and relative reaction rates suggested a rate coefficients $k(298\text{K})$ of the order of $\sim 1 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ or above. Table 8 lists recent measurements of the rate coefficients, which suggests that all reactions of SCI with oxoacids have rate coefficients near or above the collision limit, while hydricids (i.e. acids without an oxygen atom) appear to react slower. These rate coefficients are in agreement with theoretical mechanistic studies,^{35,93–100} showing that oxoacids react by a fast 1,4-insertion while hydricids react through a less favorable 1,2-insertion mechanism. In the analysis of the field data, the reactions of SCI with acids are not permuted across all acids; rather, we use an average rate of reaction with the sum of acids, for which we use $2.4 \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for most SCI. CH_2OO appears to have slightly lower rate coefficients, where we use $1.2 \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$. As for the reactions of SCI with SO_2 , we also take advantage of the direct information on RCHOO reactions; we employ 2.1×10^{-10} and $3.8 \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the reactions of Z-RCHOO and E-RCHOO , respectively, as averaged from the corresponding rates in Table 8. In the modeling study, we have separated out the reaction with HCOOH ; the corresponding data from Table 8 was used. The reaction of SCI with acids has been reported to catalyze H-migration in SCI;^{35,41} for these reactions, the acid is not removed and thus these reactions would not represent an acid loss process. However, it is generally accepted^{88,90,93–96,101} that the reaction proceeds by a barrierless adduct formation yielding hydroperoxymethylesters, which should be the dominant channel⁹³ in all cases.

Table 8: Experimental rate coefficients ($\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$) for reactions of SCI with acids

Reaction	$k_{\text{acid}}(298\text{K})$	Reference
$\text{CH}_2\text{OO} + \text{HCOOH}$	1.1×10^{-10}	Welz et al., 2014 ⁷⁷
$\text{CH}_2\text{OO} + \text{CH}_3\text{COOH}$	1.3×10^{-10}	Welz et al., 2014 ⁷⁷
$\text{CH}_2\text{OO} + \text{HNO}_3$	5.4×10^{-10}	Foreman et al., 2016 ¹⁰²
$\text{CH}_2\text{OO} + \text{HCl}$	4.6×10^{-11}	Foreman et al., 2016 ¹⁰²
$\text{E-CH}_3\text{CHOO} + \text{HCOOH}$	5×10^{-10}	Welz et al., 2014 ⁷⁷
$\text{E-CH}_3\text{CHOO} + \text{CH}_3\text{COOH}$	2.5×10^{-10}	Welz et al., 2014 ⁷⁷
$\text{Z-CH}_3\text{CHOO} + \text{HCOOH}$	2.5×10^{-10}	Welz et al., 2014 ⁷⁷
$\text{Z-CH}_3\text{CHOO} + \text{CH}_3\text{COOH}$	1.7×10^{-10}	Welz et al., 2014 ⁷⁷
$(\text{CH}_3)_2\text{COO} + \text{HCOOH}$	$4.5 \times 10^{-10 \text{ a}}$	Sipilä et al., 2014 ¹⁰³
$(\text{CH}_3)_2\text{COO} + \text{HCOOH}$	$5.4 \times 10^{-10 \text{ a}}$	Sipilä et al., 2014 ¹⁰³

^a Relative rate converted using $k((\text{CH}_3)_2\text{COO} + \text{SO}_2) = 1.6 \times 10^{-10} \text{ cm}^3 \text{ molecules}^{-1} \text{ s}^{-1}$ (see above)

7. Rate coefficient for the reaction of SO_2 with OH

An important reaction for assessing the impact of CI on SO_2 oxidation is the competing reaction of $\text{SO}_2 + \text{OH}$, the only known reaction that is a contributing gas phase source of H_2SO_4 . Rate coefficients at 298K are listed in Table 9. A recent re-analysis of this reaction by Blitz et al.^{104,105} finds a lower rate coefficient than earlier recommendations by IUPAC or JPL, which reduces the yield of H_2SO_4 through the OH channel compared to earlier modeling and field studies, and concomitantly allows for a higher impact on H_2SO_4 formation by the $\text{CI} + \text{SO}_2$ reactions. We are only aware of one study¹⁰⁶ that indicates the H_2SO_4 budget could not be closed without invoking an additional gas phase oxidant for SO_2 .

In this work, we opt to use the most recent value of Blitz et al.^{104,105} in our analysis of the field data, but use an averaged rate coefficient¹⁰⁷ of $1 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ in the modeling study as for these latter calculations we prefer to run with the unmodified MOM model.

Study	Rate coefficient
Paraskevopoulos et al., 1983 ¹⁰⁸	$k(298\text{K}, 1\text{atm}) = 9.3 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$
Wine et al., 1984 ¹⁰⁹	$k_{\infty}(298\text{K}) = 1.3 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$
Cobos and Troe, 1985 ¹¹⁰	$k_{\infty}(298\text{K}) = 2.1 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$
Fulle et al., 1999 ¹¹¹	$k_{\infty}(298\text{K}) = 3.6 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$
Blitz et al., 2003 ¹¹²	$k_{\infty}(298\text{K}) = 2.0 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$
JPL recommendation, 2011 ¹¹³	$k_{\infty}(300\text{K}) = 1.6 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$
IUPAC recommendation, 2012 ¹¹⁴	$k_{\infty}(298\text{K}) = 2.0 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$
Blitz et al., 2017 ¹⁰⁴	$k_{\infty}(295\text{K}) = 7.2 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$
Blitz et al., 2017 ¹⁰⁵	$k_{\infty}(295\text{K}) = 7.8 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$

There is significantly more experimental and theoretical data available on unimolecular reactions of CI than listed under section E.1. There is, however, significant variation across the literature data, owing to experimental uncertainties and difficulties, or the applications of lower levels of theory, which is why we have selected a subset of the data that we feel is among the best available. Still, it is useful to give an overview of all the available literature for reference purposes; the collected data is given in Table 10, in a format similar to an earlier review by Vereecken and Francisco.⁴ The study on α -phellandrene ozonolysis by MacKenzie-Rae et al.⁵⁴ is not included in this overview. These authors reported $\Delta H(298K)$ and $\Delta G(298K)$ barrier heights, which include thermal correction based on a single conformer, i.e. not accounting for internal rotation, making the values less reliable. In all cases, it is recommended to consult (and reference) the original publication when using values from this table.

R ₁	R ₂	Process	Barrier (kcal mol ⁻¹)	k(298K) (s ⁻¹)	Reference
H	H	O-loss	47.0		Cremer et al., 1993 ³¹
			32.4		Anglada et al., 1996 ²⁹
			51.2		Nguyen et al., 2007 ³⁰
			49.2		Lehman et al., 2013 ³²
			≤ 54 ^a		Lehman et al., 2013 ³²
			≤ 47 ^a		Lehman et al., 2013 ³²
			16.5 (anion)		Karton et al. 2013 ¹¹⁵
			54.2		Nguyen et al., 2015 ²³
			47.0		Dawes et al., 2015 ¹¹⁶
			49.0 ± 0.3		Li et al., 2015 ¹¹⁷
		ester channel	17.7		Gutbrod et al., 1996 ¹¹⁸
			24.0		Anglada et al., 1996 ²⁹
			19.9		Aplincourt and Ruiz-López, 2000 ⁹⁵
			20.7		Kroll et al., 2001 ¹¹⁹
			20.6		Selçuki and Aviyente, 2001 ¹²⁰
			19.8	0.024	Zhang and Zhang, 2002 ^{121,122}
			23.8		Bach et al., 1992 ¹²³
				0.19±0.07 ^a	Berndt et al., 2015 ⁴²
			18.9	0.03-0.58 ^f	Berndt et al., 2015 ⁴²
			18.2	0.3	Olzmann et al., 1997 ¹²⁴
			<19.7 ^g		Kalinowski et al., 2014 ¹²⁵
			19.2		Cremer et al., 1993 ³¹
			18.9		Chen et al., 2002 ¹²⁶
			19.0		Li et al., 2014 ¹²⁷
			22.8		Cremer et al., 1988 ¹²⁸
				≤ 11.6±8.0 ^a	Chhantyal-Pun et al., 2015 ⁷⁹
			19.6		Fang and Fu, 2002 ¹²⁹
			19.0		Nguyen et al. 2014 ¹³⁰
			19.1		Nguyen et al. 2015 ⁴³
			18.7		Nguyen et al., 2015 ²³

			19.4		Nguyen et al., 2015 ²³
				-8.58±13 ^a	Newland et al., 2015 ⁴⁵
			19.40	0.34 ⁱ	Chen et al. 2016 ²⁶
			19.03	0.31 ⁱ	Long et al. 2016 ³⁹
		1,3-H-shift	30.8		Gutbrod et al., 1996 ¹¹⁸
			32.0	1.2×10 ⁻¹²	Zhang and Zhang, 2002 ^{121,122}
			30.8		Olzmann et al., 1997 ¹²⁴
			32.5		Chen et al., 2002 ¹²⁶
			31.8		Nguyen et al., 2015 ⁴³
			30.67	8.2×10 ^{-9 i}	Chen et al. 2016 ²⁶
			31.64		Long et al. 2016 ³⁹
		syn-anti isom	25.7		Anglada et al., 1996 ²⁹
			25.3		Hull, 1978 ¹³¹
			32.1		Cremer, 1979 ¹³²
		direct-HCOOH	52.33		Chen et al. 2016 ²⁶
			(16.1) ^j		Nguyen et al. 2015 ²³
Alkyl	H	O-loss	34.1		Anglada et al., 1996 ²⁹
			23.8		Gutbrod et al. 1997 ¹³³
			28.4		Anglada et al., 1996 ²⁹
			24.0		Selçuki and Aviyente, 2001 ¹²⁰
		ester channel	24.1		Kuwata et al., 2010 ⁴⁰
			23.6		Kuwata et al., 2011 ¹⁶
			21.3 (C2) ^c		Kuwata et al., 2011 ¹⁶
			24.0 (C14)		Nguyen et al., 2009 ¹⁸
			23.3		Nguyen et al., 2009 ¹⁸
			23.70		Long et al. 2016 ³⁹
		hydroperoxide	14.8		Gutbrod et al. 1997 ¹³³
			21.2		Anglada et al., 1996 ²⁹
			19.1 (C5)		Chuong et al., 2004 ¹⁷
			16.7		Kroll et al., 2001 ¹¹⁹
			17.9	24	Kuwata et al., 2010 ⁴⁰
			12.7 (C2) ^c		Kuwata et al., 2011 ¹⁶
			16.9		Kuwata et al., 2003 ¹³⁴
				76 ^a	Fenske et al., 2000 ⁴⁸
			18.7 (C14)	1.6	Nguyen et al., 2009 ¹⁸
			15.7		Nguyen et al., 2009 ¹⁸
			19.6		Zhang and Zhang, 2005 ¹³⁵
			17.1	166	Fang et al., 2016 ⁴⁶
			≤16.0 eff. ^a		Liu et al., 2014 ¹³⁶
			17.9		Liu et al., 2014 ¹³⁷
			17.4 (C2)		Liu et al., 2014 ¹³⁷
			16.3		Liu et al., 2015 ⁴¹
		syn-anti isom		20±10.0 ^a	Novelli et al. 2014 ⁴⁹
				288±275 ^a	Newland et al., 2015 ⁴⁵
			16.4 (C6O)		Leonardo et al., 2011 ¹³⁸
			15.5 (C4O)		Leonardo et al., 2011 ¹³⁸
				3 ^a	Berndt et al., 2012 ⁷²
				2.5 ^a	Horie et al., 1997 ⁸⁷
				2.9 ^a	Horie et al., 1999 ¹³⁹
				<250 ^a	Taatjes et al., 2013 ⁶²
			16.5		Kidwell et al. 2016 ¹³
			17.01	328 ⁱ	Long et al. 2016 ³⁹
			17.2	124	Nguyen et al., 2016 ¹⁴⁰
				122 ¹	Fang et al., 2016 ⁴⁷
			30.5		Anglada et al., 1996 ²⁹
			33.7		Kuwata et al. 2005 ³
			38.0		Kuwata et al., 2010 ⁴⁰
			33.7		Kuwata et al., 2011 ¹⁶
			32.6		Nguyen et al., 2009 ¹⁸
			38.1		Nguyen et al., 2015 ²³
			25.1		Hull, 1978 ¹³¹
			35.6		Cremer, 1979 ¹³²
		CH ₃ rotation	2.1		Bowman et al., 2015 ¹⁴¹
H	Alkyl	O-loss	31.6		Anglada et al., 1996 ²⁹
			20.6		Anglada et al., 1996 ²⁹
			13.3 (C5)		Chuong et al., 2004 ¹⁷
			16.9		Kroll et al., 2001 ¹¹⁹
			17.1		Selçuki and Aviyente, 2001 ¹²⁰
			15.4	67.3	Kuwata et al., 2010 ⁴⁰

			16.6		Kuwata et al., 2011 ¹⁶
			15.0 (C2O) ^c		Kuwata et al., 2011 ¹⁶
			16.0 (C14)	5.3	Nguyen et al., 2009 ¹⁸
			15.5		Nguyen et al., 2009 ¹⁸
			27.6 (C9)		Zhang and Zhang, 2005 ¹³⁵
			15.63	55.4 ⁱ	Long et al., 2016 ³⁹
		acyl + OH (1,3-H-shift)	30.1		Kuwata et al., 2010 ⁴⁰
			29.2		Kuwata et al., 2011 ¹⁶
			29.8		Kuwata et al., 2011 ¹⁶
			27.6 (C14)		Nguyen et al., 2009 ¹⁸
			32.5		Zhang and Zhang, 2005 ¹³⁵
			29.01		Long et al., 2016 ³⁹
		syn-anti isom	28.3		Anglada et al., 1996 ²⁹
			30.1		Kuwata et al., 2005 ³
			34.5		Kuwata et al., 2010 ⁴⁰
			30.1		Kuwata et al., 2011 ¹⁶
			28.9		Nguyen et al., 2009 ¹⁸
		CH ₃ rotation	1.2		Bowman et al., 2015 ¹⁴¹
Alkyl	Alkyl	ester channel	18.7		Gutbrod et al., 1996 ¹¹⁸
			21.7		Kroll et al., 2001 ¹¹⁹
			21.6		Selçuki and Aviyente, 2001 ¹²⁰
			21.7		Olzmann et al., 1997 ¹²⁴
			22.6 (C13,C1)		Nguyen et al., 2009 ¹⁸
			21.1 (C1,C13)		Nguyen et al., 2009 ¹⁸
			28.2 (cC8,C1)		Zhang and Zhang, 2005 ¹³⁵
			21.0		Leonardo et al., 2011 ¹³⁸
			20.8	3.3×10 ⁻³	Smith et al., 2016 ⁵²
			20.8 (CD3)	3.0×10 ⁻³	Smith et al., 2016 ⁵²
		hydroperoxide	13.6		Gutbrod et al., 1996 ¹¹⁸
			16.0 ^a	6.4±9 ^{a,b}	Kroll et al., 2001 ¹¹⁹
			14.8		Olzmann et al., 1997 ¹²⁴
			16.2	362	Fang et al., 2016 ⁴⁶
			18.6 (C14,C1)	0.57	Nguyen et al., 2009 ¹⁸
			16.6 (C1,C14)	42	Nguyen et al., 2009 ¹⁸
			10.3 (C1,C8)	25.9	Sun et al., 2011 ¹⁴²
			18.6 (cC8,C1)		Zhang and Zhang, 2005 ¹³⁵
			17.1		Liu et al., 2014 ¹³⁷
			≤16.0		Liu et al., 2014 ¹⁴³
			E _A =5.9±1.2 ^a	361±49 ^a	Smith et al., 2016 ⁵²
			15.9 (E _A =8-9)	400	Smith et al., 2016 ⁵²
				3.0±0.4 ^a	Newland et al., 2015 ⁴⁵
				<65±65 ^a	Berndt et al., 2012 ⁷²
			(CD ₃)	<100	Smith et al., 2016 ⁵²
			16.6 (CD ₃)	10.6	Smith et al., 2016 ⁵²
			15.7 (C1,C3O)		Leonardo et al., 2011 ¹³⁸
			19.6 (C1,C6)		Leonardo et al., 2011 ¹³⁸
			16.0		Leonardo et al., 2011 ¹³⁸
			15.77		Li et al., 2016 ¹⁴⁴
				305±70 ^a	Chhantyal-Pun et al., 2017 ⁴⁴
				276 ¹	Fang et al., 2017 ⁵¹
		alkyl rotation	1.2 (C1, C2)		Kuwata et al., 2005 ³
			2.4 (C2, C1)		Kuwata et al., 2005 ³
3-membered ring		ester channel	9.4 (cC3)		Anglada and Bofill, 1997 ¹⁴⁵
		syn-anti isom	20.7		Anglada and Bofill, 1997 ¹⁴⁵
6-membered ring		ester channel	17.1 (bicyclic)	1	Nguyen et al., 2009 ³³
			20.9 (bicyclic)		Nguyen et al., 2009 ³³
			19.7 (bicyclic)		Zhang and Zhang, 2005 ¹³⁵
		hydroperoxide	15.4 (bicyclic)	50	Nguyen et al., 2009 ³³
			16.4 (bicyclic)		Zhang and Zhang, 2005 ¹³⁵
		syn-anti isom	30.0 (bicyclic)		Nguyen et al., 2009 ³³
		ring opening	23.6 (bicyclic)		Nguyen et al., 2009 ³³
9-membered ring		ester channel	23.3 (bicyclic)		Nguyen et al., 2009 ¹⁸
			24.7 (bicyclic)		Nguyen et al., 2009 ¹⁸
		hydroperoxide	20.3 (bicyclic)		Nguyen et al., 2009 ¹⁸
CH ₃	s-cis-CH=CH ₂	ester channel	24.0		Gutbrod et al., 1997 ¹³³
			19.2		Kuwata et al., 2005 ³
			19.5	0.018	Zhang and Zhang, 2002 ^{121,122}
		hydroperoxide	15.5		Gutbrod et al., 1997 ¹³³
			16.9	146	Kuwata et al., 2010 ⁴⁰

CH ₃	s-trans-CH=CH ₂	syn-anti isom vinyl rotation ester channel	17.4	0.11	Kuwata et al., 2005 ³
			18.4		Zhang and Zhang, 2002 ^{121,122}
			21.8		Kuwata et al., 2005 ³
			5.9 (C1, C2H3)		Kuwata et al., 2005 ³
			23.0		Gutbrod et al. 1997 ¹³³
		hydroperoxide	22.2	3.2×10 ⁻⁴	Kuwata et al., 2005 ³
			22.1		Zhang and Zhang, 2002 ^{121,122}
			16.0		Gutbrod et al. 1997 ¹³³
			18.3		Kuwata et al., 2010 ⁴⁰
			18.0		Kuwata et al., 2005 ³
s-cis-CH=CH ₂	CH ₃	syn-anti isom vinyl rotation ester channel	18.8	0.066	Zhang and Zhang, 2002 ^{121,122}
			26.0		Kuwata et al., 2005 ³
			7.6 (C1, C2H3)		Kuwata et al., 2005 ³
			22.0		Kuwata et al., 2005 ³
			22.2		Zhang and Zhang, 2002 ¹²¹
		syn-anti isom vinyl rotation ring closure ester channel	20.6	0.62	Kuwata et al., 2005 ³
			8.0		Kuwata et al., 2005 ³
			11.0		Kuwata et al., 2005 ³
			16.8		Kuwata et al., 2005 ³
			17.5		Zhang and Zhang, 2002 ^{121,122}
H	s-cis-C(CH ₃)=CH ₂	hydroperoxide vinyl (1,4-Hshift) syn-anti isom vinyl rotation ester channel	18.8	6.9×10 ⁻⁴	Kuwata et al., 2005 ³
			21.9		Zhang and Zhang, 200 ^{122,135}
			23.1		Kuwata et al., 2005 ³
			8.0		Kuwata et al., 2005 ³
			24.1		Gutbrod et al. 1997 ¹³³
		1,3-H-shift	14.5	3.6	Zhang and Zhang, 2002 ¹²¹
			13.9		Kuwata and Valin, 2008 ²⁷
			31.6		Gutbrod et al. 1997 ¹³³
			31.6		Zhang and Zhang, 2002 ¹²¹
			32.6		Kuwata and Valin, 2008 ²⁷
H	s-trans-C(CH ₃)=CH ₂	syn-anti isom ester channel	18.2	1.4×10 ⁻¹⁰	Kuwata and Valin, 2008 ²⁷
			20.3		Gutbrod et al. 1997 ¹³³
			16.7		Zhang and Zhang, 2002 ^{121,122}
			16.4		Kuwata and Valin, 2008 ²⁷
			31.1		Gutbrod et al. 1997 ¹³³
		1,3-H-shift	31.2		Zhang and Zhang, 2002 ^{121,122}
			31.2		Kuwata and Valin, 2008 ²⁷
			21.3		Kuwata and Valin, 2008 ²⁷
			25.5		Zhang and Zhang, 2002 ¹²¹
			25.3		Kuwata and Valin, 2008 ²⁷
s-cis-C(CH ₃)=CH ₂	H	1,5-ring closure syn-anti isom ester channel	11.9	2.2	Kuwata and Valin, 2008 ²⁷
			20.4		Kuwata and Valin, 2008 ²⁷
			16.9		Zhang and Zhang, 2002 ^{121,122}
			16.3		Kuwata and Valin, 2008 ²⁷
			36.2		Zhang and Zhang, 2002 ^{121,122}
		1,5-H-shift	35.9	2.2×10 ⁻¹¹	Kuwata and Valin, 2008 ²⁷
			18.6		Kuwata and Valin, 2008 ²⁷
			19.2 ^k		Cremer et al., 2001 ²⁸
			23.6 ^k		Cremer et al., 2001 ²⁸
			36.6 ^k		Cremer et al., 2001 ²⁸
H	CHO	1,4-H-shift ester channel O(¹ D) loss O(3P) loss syn-anti isom	20.6 ^k		Cremer et al., 2001 ²⁸
			16.9 ^k		Cremer et al., 2001 ²⁸
			53.0 ^k		Cremer et al., 2001 ²⁸
			52.0 ^k		Cremer et al., 2001 ²⁸
			17.3 ^k		Cremer et al., 2001 ²⁸
		ester channel O(¹ D) loss O(³ P) loss syn-anti isom 1,4-H-migration	21.8 ^k		Cremer et al., 2001 ²⁸
			55.5 ^k		Cremer et al., 2001 ²⁸
			54.5 ^k		Cremer et al., 2001 ²⁸
			20.0 ^k		Cremer et al., 2001 ²⁸
			barrierless ^d		Selçuki and Aviyente, 2000 ¹⁴⁶
s-syn-OH	H	ester channel	18.8		Selçuki and Aviyente, 2000 ¹⁴⁶
s-anti-OH	H	ester channel	18.1		Selçuki and Aviyente, 2001 ¹²⁰
s-anti-OCH ₃	H	ester channel	12.5		Selçuki and Aviyente, 2001 ¹²⁰
s-syn-OCH ₃	H	ester channel	8.0		Selçuki and Aviyente, 2000 ¹⁴⁶
H	s-syn-OH	ester channel	7.9		Selçuki and Aviyente, 2000 ¹⁴⁶
H	s-anti-OH	ester channel	7.50		Selçuki and Aviyente, 2001 ¹²⁰
H	s-anti-OCH ₃	ester channel	7.93		Selçuki and Aviyente, 2001 ¹²⁰
H	s-syn-OCH ₃	ester channel			
H	Cl	syn-anti isom	1.1		Ljubić and Sabljic, 2002 ¹⁴⁷
H	F	O-loss	27.2		Ljubić and Sabljic, 2005 ¹⁴⁸

		ester channel	11.3	Ljubić and Sabljčić, 2005 ¹⁴⁸
			7.9	Cremer et al., 1988 ¹²⁸
		1,3-H-shift	22.6	Ljubić and Sabljčić, 2005 ¹⁴⁸
Cl	H	syn-anti isom	1.7	Ljubić and Sabljčić, 2002 ¹⁴⁷
F	H	syn-anti isom	2.8	Ljubić and Sabljčić, 2002 ¹⁴⁷
		ester channel	20.0	Ljubić and Sabljčić, 2005 ¹⁴⁸
			17.1	Cremer et al., 1988 ¹²⁸
		syn-anti isom	3.4	Ljubić and Sabljčić, 2002 ¹⁴⁷
H	CN	ester channel	20.9	Selçuki and Aviyente, 2001 ¹²⁰
CN	H	ester channel	22.6	Selçuki and Aviyente, 2001 ¹²⁰
CN	CN	ester channel	22.8	Selçuki and Aviyente, 2001 ¹²⁰
[not applicable]	=O	ester channel	barrierless	Keßel et al., 2017 ¹⁴⁹
=C=O	[not applicable]	cycl. + frag. ^h	< 1 kcal mol ⁻¹	Keßel et al., 2017 ¹⁴⁹

^a experimental data

^b at 100 Torr

^c alkyl substituent is -CH₂-CHO

^d rearranges to performic acid, HC(O)OOH

^e 1,5-H-shift of methyl hydrogen.

^f Range includes fall-off and variation of barrier height.

^g Reported value is without ZPE corrections, which decrease the barrier height

^h cyclizes to a transient 4-membered ring, which decomposes spontaneously to CO₂ + CO

ⁱ T-dependent data available

^j Methodologically flawed result; see Harding and Klippenstein, 2015⁸² Chen et al. 2016,⁸³ and this work for further information.

^k ΔH(298K)

^l Value obtained by combining experimentally observed energy-specific k(E), with RRKM rate coefficient calculations.

F. Theoretical methodology

1. Quantum chemical calculations

The equilibrium structures and transition states for reaction for the unimolecular reactions were studied using the M06-2X level of theory combined with the aug-cc-pVTZ (abbr. aVTZ) basis set,^{150,151} where geometries, vibrational analysis, and IRC calculations were performed using an integral integration grid of 99 radial shells and 590 angular points (superfine grid). Harmonic wavenumbers were scaled by 0.971.^{152,153} For CI and TS with internal degrees of freedom of rotation, all (non-degenerate) conformers were explicitly optimized. The relative energy of the barrier heights was then improved by performing the single point calculations using the CCSD(T)/aug-cc-pVTZ methodology.^{151,154} Most of the critical points have a wave function that is well described using a closed shell formalism. For the isomerisation reactions by internal rotation of the oxide (reaction 1), the lowest SCF wavefunction converges to a singlet biradical; both the UM06-2X and UCCSD(T) calculations performed on these TS used the broken-symmetry method by Noodleman et al.¹⁵⁵ at the SCF level to allow the wave function to break α - β electron symmetry. Note that, unless otherwise indicated, CCSD(T)/aVTZ//M06-2X data will be used through this text, with barriers increased by +0.4 kcal mol⁻¹ for unimolecular reactions (see section F.3 below for a discussion of the reason for this empirical correction).

For a subset of compounds, i.e. CH₂OO and *syn*-CH₃CHOO, we performed an additional set of benchmark calculations. This involved re-optimizing the geometries of the reactants and the TS for 1,4-H-migration and 1,3-ring closure at the CCSD(T)/aVTZ level of theory, and obtaining vibrational frequencies at this level of theory. In addition, single-point CCSD(T)/aug-cc-pVxZ (x=D,T,Q,5,6) energy calculations were performed where feasible to allow extrapolation to the complete basis set (CBS), using the aug-Schwartz4 and aug-Schwartz6 schemes proposed by Martin et al.¹⁵⁶ Finally, for the 1,4-H-shift in *syn*-CH₃CHOO, CCSD(T)/aug-cc-pVxZ (x=D,T,Q) calculations were performed for geometries along the minimum energy pathway; this allows for the derivation of IRCMax¹⁵⁷ energies, as well as to assess tunneling.

For pinonaldehyde oxides, i.e. CI derived from α -pinene ozonolysis, the CCSD(T) calculations proved too computationally expensive to perform for all reactions. We limited ourselves to a number of key reactions, while for the remainder we can estimate the CCSD(T)//M06-2X barrier heights reasonably well from the M06-2X barrier heights. Table 11 lists the average difference in barrier height, per reaction class, between the M06-2X and CCSD(T)//M06-2X levels of theory, allowing us to estimate CCSD(T) data for those channels for which we lack direct CCSD(T) data, albeit with an increased uncertainty. This table lists information on multiple reaction classes; these energy differences are a metric on the systematic differences between the CCSD(T) and M06-2X levels of theory, and can serve as a guide for future work on larger molecules where CCSD(T) calculations are prohibitively expensive.

All calculations were performed using the Gaussian-09¹⁵⁸ and Molpro-2010¹⁵⁹ program suites.

Table 11: Barrier height difference (kcal mol⁻¹) between the M06-2X/aug-cc-pVTZ and CCSD(T)/aug-cc-pVTZ//M06-2X/aug-cc-pVTZ levels of theory, per reaction class. $\Delta E_{\text{DFT} \rightarrow \text{CC}}$ is the average of the differences $E_b(\text{CC}) - E_b(\text{M06-2X})$ of the CCSD(T)/M06-2X barrier height $E_b(\text{CC})$ and the M06-2X barrier height $E_b(\text{M06-2X})$, averaged over a set of n_{obs} carbonyl oxides. The indicated uncertainty is the statistical 1 σ error. Not all reactions studied in this work were included in the averaging. For secondary ozonide formation, we are limited to the pinonaldehyde oxides formed from α -pinene as a reference reactions; the ring strain might make these numbers less suitable as a reference for other compounds.

Reaction class	$\Delta E_{\text{DFT} \rightarrow \text{CC}}$	n_{obs}
1,3-H-shift	-0.153 ± 0.426	12
Alkyl-1,4-H-shift	$+0.591 \pm 0.568$	27
Vinyl-1,4-H-shift	$+0.605 \pm 0.190$	4
Allyl-1,4-H-shift	$+0.861 \pm 0.444$	2
Allyl-1,6-H-shift	$+1.237 \pm 0.266$	3
1,5-ring closure	-1.765 ± 0.328	6
Internal rotation conjugated system	-0.206 ± 0.616	22 (includes both vinyl and oxo)
Stereoisomerisation	$+4.137 \pm 1.663$	41 (includes rotation and inversion)
1,3-ring closure	-2.196 ± 0.456	56
SOZ formation	-1.672 ± 0.274	2 (pinonaldehyde oxide)
CI + H ₂ O	$+1.867 \pm 0.574$	29

2. Theoretical kinetic calculations

The rate coefficients of the unimolecular reactions are calculated in the high-pressure limit using multi-conformer canonical transition state theory (MC-CTST) in a rigid-rotor harmonic-oscillator approximation,^{160,161} augmented in all cases by tunneling corrections based on asymmetric Eckart barriers.^{162,163}

The impact of internal rotation is approximated by explicitly accounting for all conformers in reactant and TS; this also permits stereo-selective rate coefficients where applicable. As we have not characterized all products in detail, we base the Eckart tunneling corrections on standardized reaction exoergicities of 10 kcal mol⁻¹ for acyl+OH formation, 19 kcal mol⁻¹ for VHP formation, 30 kcal mol⁻¹ for dioxirane formation, and 40 kcal mol⁻¹ for hydroxy-hydroperoxide formation; for stereoisomerisation reaction ΔH_r are available in our dataset. The shape of the asymmetric Eckart barrier for exothermic reactions is most sensitive to the forward barrier height and the TS imaginary wavenumber such that improving the reverse barrier height by explicit calculations would have only a minor impact on the uncertainties of the rate predictions. The temperature dependent $k(T)$ is fitted to a Kooij¹⁶⁴ equation $k(T) = A \times T^n \times \exp(-E_a/T)$. As discussed in more detail in sections S and T, the reaction of CI with water has a fairly stable pre-reactive complex, which we assume to be in equilibrium with the free reactants, and to be located -7 kcal mol⁻¹ below the reactants for the purpose of asymmetric Eckart tunneling corrections. For CI + (H₂O)₂, a stability of 11 kcal mol⁻¹ is assumed.

3. Theoretical methodology limitations and benchmarks

The goal of this paper, which requires the examination of a broad selection of substituents, puts severe limitations on the methodologies we can bring to bear, as the CI can have over 11 non-H atoms; some of the barrier height calculations presented here, performed on our Xeon-based JuKinet cluster, required years of cpu time. While many theoretical calculations are available for CI chemistry using a wide variety of methodologies,^{4,8} we feel it is important to strictly apply the same methodology for all CI considered so as not to obscure reactivity trends by methodological variations. The limitations of the methodologies applied here, compared to the state-of-the-art theoretical work available, need to be accounted for explicitly to improve the predictions.

The wave function of carbonyl oxides is complex, consisting predominantly of contributions from zwitterionic configurations with some contribution of biradical configurations.¹⁻³ The multi-reference character of the wave function is borne out by diagnostics in the quantum chemical calculations, such as T1 which reaches values as high as 0.04 to 0.05 while recommended values for single-reference methodologies lie below 0.02 to 0.044.^{165,166} Because of this, the CCSD(T) methodology used here is insufficient to be quantitatively rigorously accurate, with post-CCSD(T) methodologies such as variants of HEAT,^{167,168} W3¹⁶⁹⁻¹⁷³ and others, correct the CCSD(T) barrier heights for CI unimolecular reaction by as much as ~0.5 kcal mol⁻¹, implying systematic rate

coefficient bias of over a factor of 2 for CCSD(T)-based predictions. In the literature, post-CCSD(T) calculations have recently become available for CH_2OO ,^{42–44,39} CH_3CHOO ,^{39,46} $\text{C}_2\text{H}_5\text{CHOO}$,⁵⁰ and $(\text{CH}_3)_2\text{COO}$,⁴⁶ which combined with the scarce experimental data^{42,44,45,48,49} allows us to benchmark our results.

Our kinetic methodology likewise does not use the highest levels of kinetic theory, where the most advanced calculations currently applied to simple CI^{39,44,46,50} use separable internal rotor descriptions based on explicit rotational potential energy surfaces, anharmonic oscillator analysis (VPT2),¹⁷⁴ and multidimensional tunneling (SCTST, SCT).^{175–178} We do account for the different energies and rovibrational characteristics of all conformers of the reactant and TS explicitly, but do not fully introduce the impact of internal rotation on the state density. In this work, the CI examined have up to 8 internal rotors, yet typically ≤ 2 rotors change to a vibrational mode in the TS; cancellation of error will eliminate most of the impact of the remaining rotors. Also, the barriers to internal rotation are higher than ~ 1 kcal mol⁻¹, often even significantly higher; at the low internal energies at room temperature the hindered internal rotors therefore retain a significant vibrational character in the bottom of the rotational energy wells, such that the multiconformer rigid rotor harmonic oscillator model remains applicable to a very good approximation. We limit ourselves to temperatures below 450K, as above those temperatures rotational properties increasingly become important.

Even for the highest barriers for internal rotation, up to 10 kcal mol⁻¹ for rotation around the central $\text{OO}=\text{C}-\text{C}=\text{C}$ single bond in β -unsaturated CI, the rate of internal rotation is generally much faster than the unimolecular isomerisation reaction, by one or more orders of magnitude. Hence, it is valid to assume that the CI conformers are in Boltzmann equilibrium and react as a single reactant pool. Only the 1,6-migration of an allylic H-atom (reaction (14) in Figure 4) or some reactions in heterosubstituted CI have a barrier height for chemical reactions that are comparable to the heights for internal rotation of the conjugated system; this could distort the relative population of the conformers away from a pure Boltzmann equilibrium. The chemical reactions that might induce a non-Boltzmann population are in all cases overwhelmingly dominant, however, and the next fastest competing reaction is several orders of magnitude slower in all cases, making any impact on the rate coefficient irrelevant for typical applications. The rapid internal rotation in β -unsaturated CI appears to have been omitted in the kinetic analysis of some recent work,^{61,107} which affects the predictions in these studies; this will be corrected for when analysing these results. It is important to stress that the assumption of rapid conformer equilibration does not extend to stereo-isomerisation of the oxide or olefinic moieties, where the stereoisomers effectively act as separate species due to the high isomerisation barriers.

Tunneling correction is based on the Eckart potential, which was shown to often perform well compared to multi-dimensional tunneling methodologies.^{e.g. 179} In practice, tunneling corrections are important only for H-migration reactions, whose reaction rates typically exceed those of the competing unimolecular reactions by several orders of magnitude. The uncertainty on the tunneling correction has a direct impact on the predicted CI lifetimes, but the results are robust with respect to the predicted type of the dominant reaction. Improving the level of theory for tunneling beyond Eckart tunneling (e.g. zero-curvature, small-curvature, or multi-dimensional tunneling) requires an excessive additional computational effort, and is outside the scope of the current work.

The impact of pressure under atmospheric conditions is limited, where even the faster reactions are within 10% of the high-pressure limit at 0.01 atm.⁴⁶ We therefore neglect the impact of pressure fall-off in this work relative to the remaining uncertainties.

To partially correct for the limitations of our adopted methodology, we apply a correction to our predictions for unimolecular reactions, where we adjust the barrier heights E_b to match the best available experimental and theoretical rate coefficients $k(T)$. We use a single correction factor for all E_b , irrespective of substitution or reaction type, as currently insufficient information is available to develop a more finely-tuned empirical correction. Given that the multi-reference character of the CI is the main source of error in the barrier height, and given that the CI reactants typically have higher multi-reference character than the TS, it is reasonable to assume that most of the correction reflects a refinement of the reactant energies rather than TS energies, and the correction should therefore be applicable to all reactions equally. Table 2 in section E.1 shows the literature data

we selected as benchmark values for CI unimolecular reactions. Reducing our uncorrected rate coefficients predictions by a factor of 2 brings them in agreement (i.e. within a factor 1.4) with the averaged literature rate data, though clearly this reference average has itself a sizable uncertainty due to the spread in the data. This rate adjustment requires a barrier height increase of ~ 0.4 kcal mol⁻¹, bringing the CCSD(T)//M06-2X barrier height E_b obtained by us to within 0.1 kcal mol⁻¹ of the best available post-CCSD(T) predictions, suggesting that such rate coefficient correction is compatible with benchmark theoretical results, even if it does rely somewhat on cancellation of error. Note that the available reference data is typically for H-migration pathways, such that the comparison includes any bias on the tunneling correction.

For the bimolecular reaction of CI with water molecules (section S and T), larger corrections will need to be made, as we have additional sources of error, e.g. due to the bimolecular nature of the reaction, the pre-reactive complexes, the various possibilities for H-bonding, and a stronger change in steric interactions. Even the best theoretical methodologies currently applied in the literature struggle to reproduce within an order of magnitude either the experimental data or other high-level theoretical data for CI + water reactions; our lower level of theory is thus not expected to yield highly accurate results *a priori*. Pragmatically, we will therefore rely on correlations between our rate predictions and the available literature data; the procedure is expanded on in the relevant sections S and T. The main correction involves an increase of the CCSD(T)//M06-2X reaction barrier by 1.46 kcal mol⁻¹, for CI + H₂O reactions. This exceeds the barrier shift for the unimolecular reactions by about 1 kcal mol⁻¹, and corresponds to a correction factor of ~ 12 on the $k(298\text{K})$ rate coefficient. Still, this remains comparable to the uncertainty of an order of magnitude on much of the available (theory-based) literature data. Additional discussion of the literature data on unimolecular and bimolecular reactions is available in sections E, S, and T.

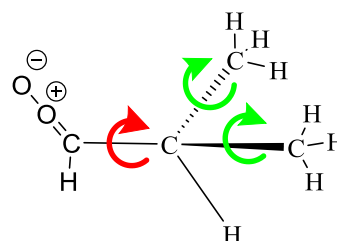
G.Internal rotation of substituents

Complex CI have multiple conformers with different spatial orientations of the substituents, which are in constant flux by internal rotations along single bonds. For internal rotation in the alkyl chains in CI the energy barriers are typically low, of the order of ~ 1 kcal mol⁻¹. E.g. the CH₃ rotation in Z-CH₃CHOO has a barrier of 1.82 kcal mol⁻¹ at our level of theory, and the tC₄H₉ rotation in tC₄H₉CHOO was predicted at 4.53 kcal mol⁻¹. Rotational barriers of similar magnitude have been reported elsewhere^{3,46,50,180} For our current purposes, we can assume that these rotamers are in quasi-equilibrium.

The energy profile for internal rotation depends rather strongly on the substituents, where the energy of the different conformers is affected by interaction of the substituents with the carbonyl oxide moiety, as well as with the substituent on the opposite site of the oxide moiety. This interaction also affects the entropy, even for those CI where the energy of the most stable conformer does not appear to be strongly affected by variations in substitutions. We illustrate that in Table 12, where we list the energy of the different conformers of a series of Z-R₁CHOO, progressively more substituted by methyl groups, where we should note that the interaction of the substituent with the oxide O-atom is most pronounced at the *syn*-side (Z-conformers of R₁CHOO) of the carbonyl oxide. One sees that for most of these CI, the ground state energy remains mostly unchanged (~ 3 kcal mol⁻¹ below the most stable *E*-stereoisomer), but the other conformers increase in energy as the methyl groups interact with the carbonyl oxide O-atom. This unfavorable interaction of the methyl substituent with the carbonyl oxide and the resulting increase of the conformer energies is shown later to cause some non-intuitive reaction trends, e.g. a slowdown of H-migration reactions with increasing substitution (e.g. section J). Substituents on the *anti*-side are less affected, as shown also in Table 12 for the analogous series of *E*-R₁CHOO, where rotamer relative energies remain within 1 kcal mol⁻¹. Finally, the conformer energy can also be affected by substituent-substituent interaction across the carbonyl oxide moiety, especially for bulky groups like iC₃H₇ or tC₄H₉ (not shown).

Table 12: Energy (kcal mol⁻¹) of carbonyl oxide conformers, relative to the most stable *E*-R₁CHOO structure. Only the three main orientations of the alkyl substituent are listed; the degeneracies of the rotation of the additional outer methyl groups is indicated in the last column. The inset figure shows an example of the the rotations.

Carbonyl oxide	Conformer energy Rotation of entire substituent	Outer CH ₃ rotations degeneracy
Z-CH ₃ CHOO	-3.30	1
	-3.30	1
	-3.30	1
Z-CH ₃ CH ₂ CHOO	-2.84	3
	-1.93	3
	-1.93	3
Z-(CH ₃) ₂ CHCHOO	-2.48	9
	-0.37	9
	-0.37	9
Z-(CH ₃) ₃ CCHOO	-0.33	27
	-0.33	27
	-0.33	27
<i>E</i> -CH ₃ CHOO	0.00	1
	0.00	1
	0.00	1
<i>E</i> -CH ₃ CH ₂ CHOO	0.00	3
	0.75	3
	0.75	3
<i>E</i> -(CH ₃) ₂ CHCHOO	0.00	9
	0.36	9
	0.36	9
<i>E</i> -(CH ₃) ₃ CCHOO	0.00	27
	0.00	27
	0.00	27



Example: Rotations in CH(CH₃)₂CHOO

Rotation of 2-propyl (red arrow):

Position H/CH₃ relative to C=O⁺-O⁻
= different energies

Methyl rotation (green arrows):

Each rotation 3-fold degenerate

= 9-fold degeneracy combined

For internal rotation around the single bond in the conjugated π -systems of β -unsaturated CI, barriers of the order of 8 to 11 kcal mol⁻¹ have been reported,^{3,27,37} of a similar value to those found in butadiene and isoprene.^{14,15} Table 13 lists the barrier heights and rate coefficients calculated in this work for the *s-cis* $\leftrightarrow$ *s-trans* isomerisation in β -unsaturated CI, i.e. with a vinyl or carbonyl substituent. The barrier heights are in agreement with the literature data. The isomerisation rates are typically significantly faster by several orders of magnitude than the chemical isomerisations considered in this work, indicating that the *s-cis* and *s-trans* isomers will be in near-equilibrium and should be considered as a single pool of reactants rather than separable species. This has not been accounted for in some earlier studies on unsaturated CI,^{1,37,40,61,121} but is incorporated in this work and will be corrected for in our analysis of the literature data on reactions for CI with H₂O and (H₂O)₂.

Only two reaction types discussed in this work can have energy barriers and rate coefficients comparable to the *s-cis* $\leftrightarrow$ *s-trans* isomerisation in β -unsaturated CI, i.e. the allyl-1,6-H-migration, and the 1,5-ring closure (see sections L and O). While this could lead to a non-equilibrium energy distribution across the conformers, there are no competing reactions, and the same products will be formed for both the *s-cis* and *s-trans* isomers, such that it rarely affects practical applications even if the effective over-all rate coefficient may be slightly lower than reported in this work.

Table 13: Barrier heights (kcal mol⁻¹) and rate coefficients (s⁻¹) for *s-cis* $\leftrightarrow$ *s-trans* internal rotation in β -unsaturated and β -oxo CI, i.e. rotation along the central single bond in conjugated systems. The isomerisation reaction is listed for rotation from the more stable conformer towards the less stable orientation; the reverse rotation has a lower barrier and higher reaction rates.

carbonyl oxide	E _b	k(298K)
<i>E</i> -(CH=CH ₂)CHOO	8.91	5.2×10 ⁶
<i>Z</i> -(CH=CH ₂)CHOO	9.68	7.6×10 ⁵
<i>E</i> -(CH ₃)(CH=CH ₂)COO	7.79	2.4×10 ⁷
<i>Z</i> -(CH=CH ₂)(CH ₃)COO	8.41	6.4×10 ⁶
<i>E</i> -(<i>Z</i> -CH=CHCH ₃)CHOO	8.95	3.4×10 ⁶
<i>Z</i> -(<i>Z</i> -CH=CHCH ₃)CHOO	8.47	4.5×10 ⁶
<i>E</i> -(<i>E</i> -CH=CHCH ₃)CHOO	9.20	3.0×10 ⁶
<i>Z</i> -(<i>E</i> -CH=CHCH ₃)CHOO	10.7	1.4×10 ⁵
<i>E</i> -(C(CH ₃)=CH ₂)CHOO	9.09	3.7×10 ⁶
<i>Z</i> -(C(CH ₃)=CH ₂)CHOO	7.94	1.4×10 ⁷
<i>E</i> -(CHO)CHOO	9.84	1.3×10 ⁶
<i>Z</i> -(CHO)CHOO	8.02	1.6×10 ⁷
<i>E</i> -(CH ₃)(CHO)COO	10.0	8.1×10 ⁵
<i>Z</i> -(CHO)(CH ₃)COO	8.57	3.8×10 ⁶
<i>E</i> -(C(O)CH ₃)CHOO	8.63	6.3×10 ⁶
<i>Z</i> -(C(O)CH ₃)CHOO	6.86	6.4×10 ⁷
<i>E</i> -(CH ₃)(CHO)COO	8.34	7.9×10 ⁶
<i>Z</i> -(CHO)(CH ₃)COO	8.20	9.3×10 ⁵

H. Stereoisomerisation

1. Stereoisomerisation rate coefficients

There have been relatively few studies on the Z/E-stereoisomerisation of carbonyl oxides, mostly focused on CH_2OO ^{29,131,132} and CH_3CHOO ,^{18,23,29,40,131,132} though a few authors present data on larger^{3,33,145} or hetero-substituted¹⁴⁷ CI. The highest level of calculations available yield very high barriers for stereo-isomerisation of alkyl-substituted CI, and despite the lack of information on the impact of substituents, it is generally assumed that all CI have high barriers to stereoisomerisation. Still, Ljubić and Sabljic report low barriers for stereoisomerisation¹⁴⁷, $< 4 \text{ kcal mol}^{-1}$, at the CASSCF(10,9)/cc-pVTZ level of theory for halogen-substituted CI, while Kuwata et al.³ find significantly lowered isomerisation barriers for unsaturated CI, warranting an in-depth study.

For the stereoisomerisation of CI with substituents ranging from H-atoms to $t\text{-C}_4\text{H}_9$, and with γ -unsaturated substituents, we find barriers exceeding 30 kcal mol^{-1} for the rotational pathways (see Table 14), while the in-plane pseudo-rotation pathway has even higher barriers. The resulting very low rate coefficients confirm the current view that thermalized CI stereoisomers should be considered as separable species under atmospheric conditions. For β -unsaturated CI, i.e. oxides with a β -vinyl or β -carbonyl functionality, we find barriers to isomerisation lower by $\sim 9 \text{ kcal mol}^{-1}$, owing to the stabilization of the TS carbon-based unpaired electron orbital by conjugation with the double bond. Even for these unsaturated CI the reaction rates remain below those of the dominant unimolecular reactions by many orders of magnitude, making stereo-isomerisation negligible. These higher-level calculations improve on earlier results by Kuwata et al.³ who found DFT barrier heights comparable to those of some of the other unimolecular reactions, which suggested a potential role for stereo-isomerisation.

Table 14: Stereo-isomerisation in carbonyl oxides by in-plane transition or by internal rotation (out-of-plane) of the outer oxygen. Barrier heights E_b (kcal mol⁻¹) are reported relative to the lowest isomer. Rate coefficients (s⁻¹) are given in both reaction directions.

carbonyl oxide	E_b	$k(298\text{K}) \text{ Z} \rightarrow \text{E}$	$k(298\text{K}) \text{ E} \rightarrow \text{Z}$
H_2COO in-plane	39.0		1.8×10^{-16}
H_2COO out-of-plane	29.8		2.9×10^{-9}
CH_3CHOO in-plane	41.7	4.2×10^{-18}	1.8×10^{-15}
CH_3CHOO out-of-plane	34.6	8.1×10^{-13}	2.3×10^{-10}
$\text{C}_2\text{H}_5\text{CHOO}$ out-of-plane	34.7	8.4×10^{-13}	1.5×10^{-10}
$t\text{C}_4\text{H}_9\text{CHOO}$ out-of-plane	32.9	2.3×10^{-11}	4.5×10^{-11}
$(\text{CH}_3)_2\text{COO}$ out-of-plane	36.2		4.7×10^{-14}
$(\text{C}_2\text{H}_5)(\text{CH}_3)\text{COO}$ out-of-plane	36.7	2.9×10^{-14}	1.4×10^{-14}
$(t\text{C}_4\text{H}_9)(\text{C}_2\text{H}_5)\text{COO}$ out-of-plane	37.7	1.1×10^{-12}	5.1×10^{-15}
$(t\text{C}_4\text{H}_9)(i\text{C}_3\text{H}_7)\text{COO}$ out-of-plane	35.7	5.9×10^{-12}	1.9×10^{-13}
$(\text{CH}_2=\text{CH}=\text{CH}_2)\text{CHOO}$ out-of-plane	34.9	5.1×10^{-13}	8.4×10^{-11}
$(\text{OH})\text{CHOO}$ out-of-plane	34.1	N/A ^a	1.5×10^{-12}
$(\text{CH}=\text{CH}_2)\text{CHOO}$ out-of-plane	24.4	6.7×10^{-6}	6.1×10^{-5}
$(\text{CH}=\text{CH}_2)(\text{CH}_3)\text{COO}$ out-of-plane	27.3	3.7×10^{-6}	8.5×10^{-8}
$(\text{Z-CH}=\text{CH}-\text{CH}_3)\text{CHOO}$ out-of-plane	25.4	4.9×10^{-7}	5.1×10^{-6}
$(\text{E-CH}=\text{CH}-\text{CH}_3)\text{CHOO}$ out-of-plane	26.1	4.9×10^{-7}	1.3×10^{-5}
$(\text{C}(\text{CH}_3)=\text{CH}_2)\text{CHOO}$ out-of-plane	24.9	2.4×10^{-5}	7.3×10^{-6}
$(\text{CHO})\text{CHOO}$ out-of-plane	25.0	6.4×10^{-5}	6.1×10^{-6}
$(\text{C}(\text{O})\text{CH}_3)\text{CHOO}$ out-of-plane	25.7	4.1×10^{-5}	1.5×10^{-6}
$(\text{CHO})(\text{CH}_3)\text{COO}$ out-of-plane	28.0	8.1×10^{-4}	3.6×10^{-8}
$(\text{C}(\text{O})\text{CH}_3)(\text{CH}_3)\text{COO}$ out-of-plane	28.9	9.5×10^{-5}	6.7×10^{-9}

^a Z-HOCHOO is unstable and isomerises without barrier to formic acid (see section R.3)

2. Relative energy of stereoisomers

As already reported extensively,^{4,8–11} the two stereoisomers of a given carbonyl oxide can have strongly different reactivity, where the energetically highest-lying isomer often reacts faster by releasing some of its higher potential energy in the transition state, leading to lower effective barrier heights. Relative energies of the stereoisomers are shown in Table 15 and visualized in Figure 6. The most stable isomers are those where the carbonyl oxide outer O-atom interacts with H-atoms on the β -carbons in the *syn*-substituent R_1 ; an α -H-atom as in *E*-RCHOO, or alkyl chains on the β -carbon are less favorable. For larger alkyl substituents, the preferred conformers within each isomer are therefore those with the largest possible number of β -carbon H-atoms rotated towards the oxide moiety in a staggered formation, while the other conformers have higher energy. If no β -carbon H-atom exists (i.e. R_1 =H or tC_4H_9) or can't reach an optimal orientation (β -unsaturated CI), the carbonyl oxide stabilization is limited, leading to a much smaller energy difference between the *E* and *Z* conformers. For the *anti*-substituent R_2 the β -carbon has an eclipsed conformation with the oxide moiety, with any alkyl group preferentially rotated away from the substituent on the *syn*-side. If the R_2 group is highly branched, it can interact with the R_1 group, affecting the relative energies. 2-oxo-substitution likewise has a strong impact, and oxo-substitution on the *syn*-side can lead to high-energy isomers.

Table 15: Energy (kcal mol⁻¹) of carbonyl oxide stereoisomers relative to lowest-energy isomer.

Carbonyl oxide	<i>Z</i> isomer	<i>E</i> isomer
CH ₃ CHOO	0.00	3.48
C ₂ H ₅ CHOO	0.00	3.27
nC ₃ H ₇ CHOO	0.00	3.11
iC ₃ H ₇ CHOO	0.00	2.87
tC ₄ H ₉ CHOO	0.00	0.78
(CH ₂ –CH=CH ₂)CHOO	0.00	3.62
CH(CH ₃)–CH=CH ₂ CHOO	0.00	2.68
C(CH ₃) ₂ –CH=CH ₂ CHOO	0.00	0.84
(C ₂ H ₅)(CH ₃)COO	0.54	0.00
(iC ₃ H ₇)(CH ₃)COO	0.72	0.00
(iC ₃ H ₇)(C ₂ H ₅)COO	0.17	0.00
(tC ₄ H ₉)(CH ₃)COO	3.75	0.00
(tC ₄ H ₉)(C ₂ H ₅)COO	3.09	0.00
(tC ₄ H ₉)(iC ₃ H ₇)COO	2.26	0.00
(CH=CH ₂)CHOO	0.00	0.98
(CH=CH ₂)(CH ₃)COO	2.59	0.00
(<i>Z</i> -CH=CH–CH ₃)CHOO	0.00	0.76
(<i>E</i> -CH=CH–CH ₃)CHOO	0.00	1.68
C(CH ₃)=CH ₂ CHOO	0.83	0.00
(CHO)CHOO	1.62	0.00
C(O)CH ₃ CHOO	2.09	0.00
(CHO)(CH ₃)COO	5.62	0.00
(C(O)CH ₃)(CH ₃)COO	6.41	0.00

3. Group additivity prediction of the relative energy of stereoisomers

It is clear from Figure 6 that the relative energies follow a clear pattern that could be leveraged to estimate the relative energy of the stereoisomers using a group additivity paradigm. The underlying property of the group factors is the formation enthalpy $\Delta H_f(0\text{ K})$, though we have only relative data ($\Delta\Delta H_f(0\text{ K})$) and the enthalpies ΔH_f themselves can't be predicted purely from our data set. We arbitrarily set the R_1 and R_2 group factors for an H-atom to $F_{R1}(H) = F_{R2}(H) = 0$ (labeling as in Figure 1), i.e. the $\Delta\Delta H_f$ values use CH₂OO as zero. We are mostly sensitive to the group factors of the R_1 group, as the R_2 group has only a minor impact on the relative energies. Furthermore, we don't have many data on the cross-combinations of the substituents, such that group factors remain tentative as the additivity property is not rigorously validated. Finally, the group factors combine many effects that in reality vary independently across the substituents, e.g. inductive effects, (hyper)conjugation, steric

hindrance, electrostatic attraction/repulsion, etc.; this lumping will limit the predictive performance of the group factors when applied to different molecular properties or reaction classes.

To derive the group additivity factors, we divided the substituents into categories; these were selected to be consistent with the substituent groups used in the SARs for SCI unimolecular decay, and SCI reactions with H₂O and (H₂O)₂, and could in principle be reduced to a smaller set with little loss of accuracy. The relative formation enthalpy $\Delta\Delta H_f$ of the individual CI, and the energy difference ΔE_{stereo} between two stereoisomers can then be calculated using the following formulas:

$$\Delta\Delta H_f = F_{R1}(\text{subst. } R_1) + F_{R2}(\text{subst. } R_2)$$

$$\Delta E_{\text{stereo}} = \Delta\Delta H_f(\text{isomer1}) - \Delta\Delta H_f(\text{isomer2})$$

Table 16 shows the derived group additivity factors for a substituent in the R₁ or R₂ position, and Figure 7 shows the predictive performance. Summing the factors for the R₁ and R₂ substituent in a CI gives the relative formation enthalpy of a CI. Doing the same for its stereoisomer and taking the difference in relative formation enthalpy yields the relative energy of the stereoisomers. E.g. *Z*-(C₂H₅)(CH₃)COO has $\Delta\Delta H_f = F_{R1}(\text{C}_2\text{H}_5) + F_{R2}(\text{CH}_3) = -3.30 - 0.04 = -3.34 \text{ kcal mol}^{-1}$, while *E*-(C₂H₅)(CH₃)COO has $\Delta\Delta H_f = F_{R1}(\text{CH}_3) + F_{R2}(\text{C}_2\text{H}_5) = -3.89 - 0.03 = -3.92 \text{ kcal mol}^{-1}$. The energy difference of 0.58 kcal mol⁻¹ corresponds well with the value of 0.54 kcal mol⁻¹ in Table 15, and we correctly predict the *E*-isomer as the most stable form.

Table 16: Group additivity factors F_{R1} and F_{R2} for the determination of the relative energy of stereoisomers of Criegee intermediates with the indicated R₁ and R₂ substituents. For reference to later sections, we also indicate the SAR substituent classes as defined in section C.

Substituent	SAR Substituent class	$F_{R1} / \text{kcal mol}^{-1}$	$F_{R2} / \text{kcal mol}^{-1}$
CH ₃	-CH ₃	-3.89	-0.04
C ₂ H ₅ / n-C ₃ H ₇	-CH ₂ R _a	-3.30	-0.03
CH ₂ -CH=CH ₂	-CH ₂ -CR ₃ =CR ₄ R ₅	-3.62	N/A ^a
iC ₃ H ₇	-CHR _a R _b	-2.94	0.00
CH(CH ₃)-CH=CH ₂	-CHR _a -CR ₃ =CR ₄ R ₅	-2.68	N/A ^a
CH=CH ₂ / CH=CH-CH ₃	-CH=CR ₄ R ₅	-1.17	0.00
tC ₄ H ₉	-CR _a R _b R _c	-0.43	0.00
C(CH ₃) ₂ -CH=CH ₂	-CR _a R _b -CR ₃ =CR ₄ R ₅	-0.84	N/A ^a
C(CH ₃)=CH ₂	-CR _a =CR ₄ R ₅	-0.83	N/A ^a
H	-H	0.00	0.00
CHO	-CHO	+1.70	0.00
C(O)CH ₃	-C(O)R _a	+2.26	-0.07

^a Insufficient cross-substituent data available to determine this F_{R2} . Use 0.00 kcal mol⁻¹ for calculations.

It must be stressed that the factors F_{R1} and F_{R2} do not predict formation enthalpies, and are such as not directly suitable to predict chemical reactivity. Compare for example *Z*-(C(O)CH₃)CHOO and CH₂OO: while it is often the case that the higher F_{R1} factor for the acetyl substituent will lead to faster reaction, this is not covered by the data in Table 16. However, as the group additivity factors reflect relative enthalpy of stereoisomers, they are indicative of the relative reactivity of the stereoisomers within a given reaction class, assuming an Evans-Polanyi relationship. For example, the stereoisomers *Z*-(CHO)(CH₃)COO and *E*-(CH₃)(CHO)COO have a very different "stability", with the *Z*-isomer significantly higher in energy. As we will see in sections N and S, this translates in faster rates for this isomer in the 1,3-ring closure reaction, or in the reaction with H₂O and (H₂O)₂. It is not recommended to use Table 16 to make a statement about the relative reactivity of CI that are not stereoisomers.

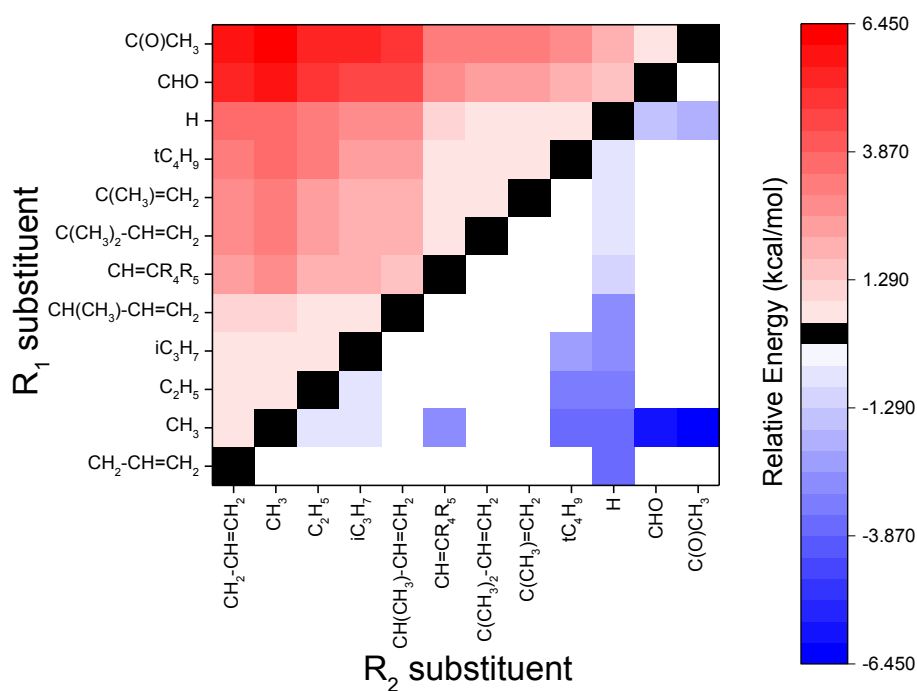
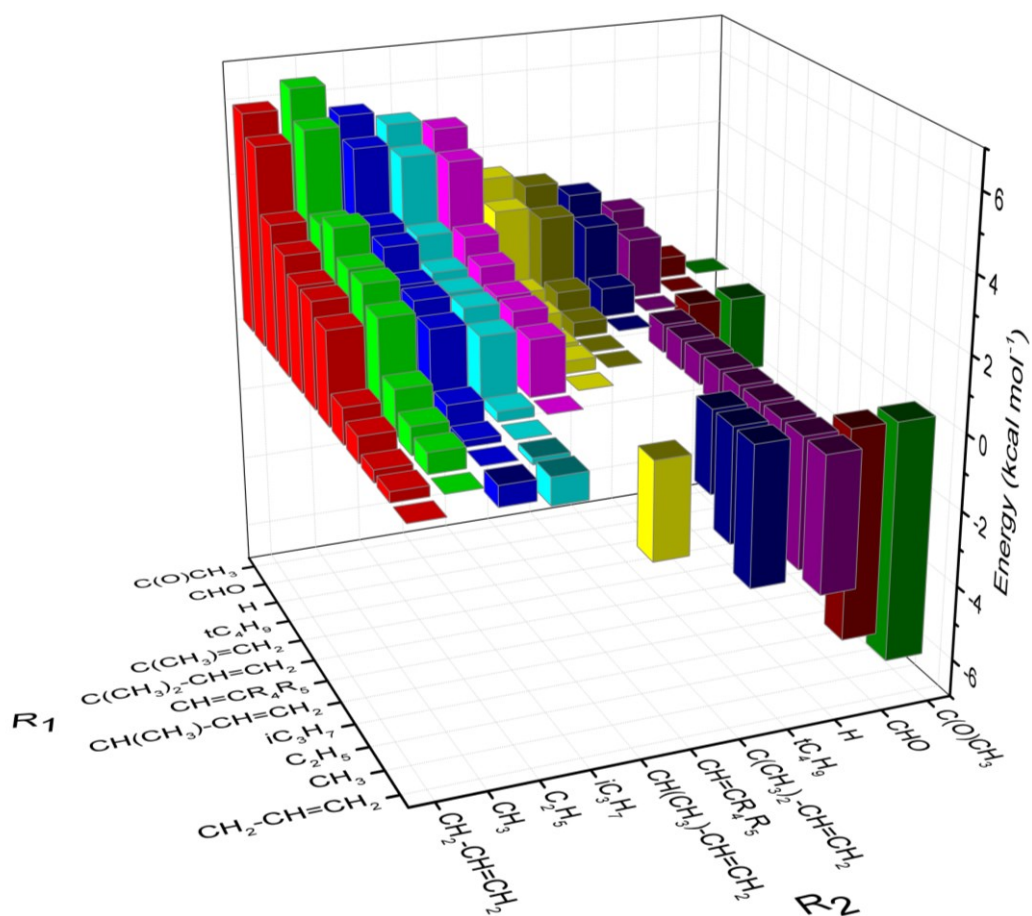


Figure 6: 3D and 2D representation of the energy of a $(R_1)(R_2)COO$ carbonyl oxide relative to its stereoisomer, as a function of substitution (R_1 always in *syn*-position). As both axes show all substituents, the upper-left and lower-right halves are an inversion of each other. The lower right half of each figure (negative energies) shows the data available in Table 15 (some data omitted), while the upper left half (positive energies) shows the same data, amended with the predictions obtained from group additivity.

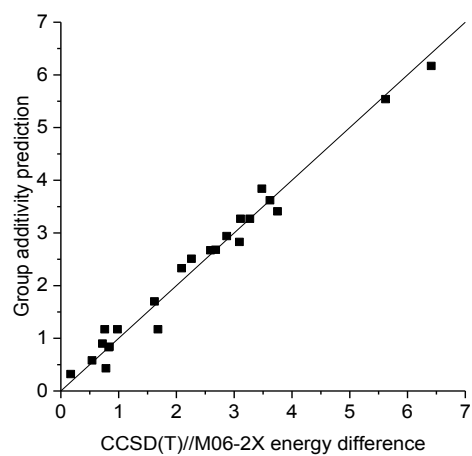
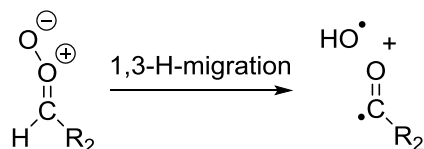


Figure 7: Comparison of the group additivity-predicted relative energy (kcal mol^{-1}) of non-symmetric stereoisomers against the original quantum chemical data. The line represents a 1:1 agreement.

I. 1,3-H-migration in *E*-R₂CHOO (*anti*-RCHOO)



1. Benchmark calculations

To assess the impact of basis set and geometry on the predicted barrier height, we have re-evaluated the 1,3-H-migration in CH₂OO using CCSD(T)/aug-cc-pVQZ single point calculations on the M06-2X geometries, as well as re-optimizing the reactant and TS using CCSD(T)/aVTZ (both geometry and vibrational analysis); the results are summarized in Table 17. Increasing the level of theory leads to slightly higher barriers, where the barrier height obtained from CCSD(T) geometries agrees with the M06-2X-based geometries. Compared to the post-CCSD(T) calculations by Long et al.³⁹ the barrier remains underestimated by ~1 kcal mol⁻¹. The use of CCSD(T) rovibrational data leads to higher rate coefficients, though the difference against M06-2X rovibrational data remains below a factor of 2 at room temperature.

Table 17: 1,3-H-migration in *E*-RCHOO carbonyl oxides, listing barrier heights E_b (kcal mol⁻¹), rate coefficient k (s⁻¹) at 298 K, and parameters for a Kooij equation fit $k(T)=A \times T^n \times \exp(-E_a/T)$ for the temperature range 200–450 K.

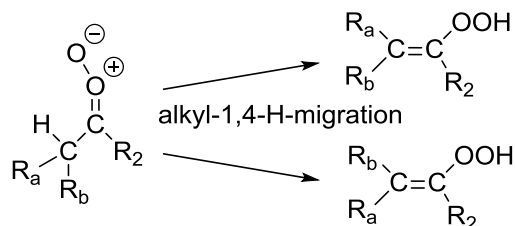
Carbonyl oxide	E_b	$k(298\text{K})$	A / s^{-1}	n	E_a / K	Reference and methodology
CH ₂ OO	30.4 ^a	2.7×10^{-7}				This work (CCSD(T)/aVTZ//M06-2X)
	30.5 ^a	2.0×10^{-7}				This work (CCSD(T)/aVQZ//M06-2X)
	30.8 ^a	2.3×10^{-7}				This work (CCSD(T)/aVTZ//CCSD(T)/aVTZ)
	31.7 ^a					Long et al. (W3X-L//CCSD(T)-F12/DZ-F12) ³⁹
	30.7	1.4×10^{-7}	6.27×10^{-145}	51.3	-7178	This work
<i>E</i> -CH ₃ CHOO	28.3	3.8×10^{-6}	7.59×10^{-132}	47.2	-6178	This work
<i>E</i> -C ₂ H ₅ CHOO	28.2	4.0×10^{-6}	8.56×10^{-132}	47.2	-6093	This work
<i>E</i> -(CH ₂ -C ₈ H ₁₃ O)CHOO ^b	29.0 ^b	1.6×10^{-6}	1.64×10^{-134}	47.1	-6237	This work
<i>E</i> -iC ₃ H ₇ CHOO	28.4	2.4×10^{-6}	2.06×10^{-132}	47.4	-6127	This work
<i>E</i> -tC ₄ H ₉ CHOO	28.3	4.3×10^{-6}	9.18×10^{-132}	47.2	-6076	This work
<i>E</i> -(CH ₂ -CH=CH ₂)CHOO	28.4	1.7×10^{-6}	4.11×10^{-134}	47.9	-6178	This work
<i>E</i> -(CH=CH ₂)CHOO	30.0	3.0×10^{-7}	7.63×10^{-141}	50.1	-6656	This work
<i>E</i> -(Z-CH=CH-CH ₃)CHOO	28.9	1.2×10^{-6}	2.76×10^{-134}	47.9	-6324	This work
<i>E</i> -(E-CH=CH-CH ₃)CHOO	29.0	1.3×10^{-6}	1.91×10^{-134}	48.3	-6352	This work
<i>E</i> -(C(CH ₃)=CH ₂)CHOO	29.9	3.0×10^{-7}	7.87×10^{-141}	50.1	-6567	This work
<i>E</i> -(CHO)CHOO	35.5	1.7×10^{-10}	1.29×10^{-171}	60.2	-8363	This work
<i>E</i> -(C(O)CH ₃)CHOO	34.7	1.3×10^{-9}	3.49×10^{-167}	58.9	-8115	This work
<i>E</i> -(OH)CHOO	21.4	0.25	3.13×10^{-91}	33.9	-4116	This work

^a Barrier height not shifted by 0.4 kcal mol⁻¹ ^b *E*-pinonaldehyde-A-oxide, based on M06-2X/aug-cc-pVTZ data.

2. Reaction trends

Table 17 lists the predicted barrier heights and rate coefficients for 1,3-H-migration in a set of *E*-RCHOO. The barrier height is independent of alkyl-substitution within the uncertainty of the level of theory. For CH₂OO and β-unsaturated CI a slightly higher barrier height is found, while a β-oxo substituent increases the barrier by 5 to 7 kcal mol⁻¹. The rate coefficients are low, and this reaction is never competitive against the 1,3-ring closure reaction also accessible to *E*-RCHOO carbonyl oxides (see section N). $k(T)$ shows a strong temperature dependence and a strong non-linear Arrhenius behavior, with a tunneling factor enhancing the reaction rate by ~10³ at room temperature.

J. Alkyl-1,4-H-migration forming vinyl hydroperoxides (VHP)



1. Benchmark calculations

CCSD(T)/aVTZ IRCMax calculations on the M06-2X/aVTZ minimum energy path for 1,4-H-migration in Z-CH₃CHOO shows that the CC level of theory has its highest energy only 0.063 Å AMU^{0.5} past the M06-2X saddle point, corresponding with the breaking C–H bond elongated by an additional 0.003 Å from its saddle point length of 1.31 Å, and an energy increase of 0.12 kcal mol⁻¹. This level of agreement suggests that the use of M06-2X TS geometries is sufficiently accurate. Complete basis set estimates on this IRCMax geometry shows a slight decrease in barrier height with respect to basis set size, with CCSD(T)/aug-Schwartz(DTQ)/M06-2X/aVTZ energies about 0.13 kcal mol⁻¹ below the CCSD(T)/aVTZ single point barrier (see Table 18). Re-optimizing the geometries at the CCSD(T)/aVTZ level of theory leads to a slightly higher barrier, which at the aug-Schwartz(TQ5) complete basis set limit leads to a 16.5 kcal mol⁻¹ barrier. IRCMax calculations and complete basis set estimates for (CH₃)₂COO yield similar trends, with an IRCMax barrier increase of only 0.1 kcal mol⁻¹ relative to single-point calculations, and a slight decrease of 0.2 kcal mol⁻¹ when increasing the basis set to the CBS limit. Replacing the Eckart tunneling correction for Z-CH₃CHOO H-migration with a zero-curvature WKB approximation based on an CCSD(T)//M06-2X energy profile increases the predicted rate coefficient by a factor 1.9, though the WKB correction using a CCSD(T)//CCSD(T) energy profile matches the Eckart correction within 5%.

Post-CCSD(T) calculations are available in the literature for both $\text{Z-CH}_3\text{CHO}$ and $(\text{CH}_3)_2\text{CO}$; these are listed in Table 2, showing that our adjusted barrier heights and rate coefficients are in fair agreement with the best available theoretical estimates. Still, it remains hard to judge the quality of our predictions, as the post-CCSD(T) rate predictions differ by over a factor of two, and all available experimental thermal rate coefficients (see Table 2) significantly below these predictions. We propose an uncertainty of at least a factor of 3.

2. Reaction trends

The rate coefficient predictions across the relevant range of substituents are listed in Table 18. For CI where the vinyl hydroperoxide product after 1,4-H-migration has two stereoisomers, we list both the total VHP formation, and the rate coefficient for the formation of Z-VHP, which is always a minor channel contributing $< 5\%$ at 298K. The results indicate that, as for stereoisomerism, the rate coefficients are influenced by both the R_1 and R_2 substituents. For most CI, we find rate coefficients in the range of 10^2 to 10^3 s^{-1} , in line with post-CCSD(T) predictions and compatible with energy-specific experimental data.^{39,42,46,50} The rate coefficients show strong non-Arrhenius behavior due to extensive tunneling, which increases the rate coefficient by one to two orders of magnitude at room temperature, and is the main driver for reaction at lower temperatures.

The uncertainty on the predictions makes it unreliable to assign much significance to the relative rates. Still, it is worthwhile to examine the reaction trend in more detail. Increasing the branching on the R₂ substituent can increase the rate of H-migration from the R₁ substituent, but the interaction between these two substituents can lead to a dramatic increase in barrier height when the substituent branching prevents favorable orientations. The R₂ = tC₄H₉ substituent in particular leads to increases in barrier height. The relative energy of the various conformers of the CI (see section G) also affects the reaction entropies, with internal conformer contribution to the CI population diminishing as substituent orientation becomes less favorable. The barrier height by itself therefore does not suffice as the sole indicator to the reactivity of a given CI. For R₁ = iC₃H₇, with only one H-atom available for migration, the aforementioned effects leads to an increase in barrier height and a

concomitantly low rate coefficient in all cases, but also for smaller R₁ substituents it appears that the interaction with the R₂ substituent can be unfavorable. The reaction trend for 1,4-H-migration tends to go against the accepted structure-activity relationship for alkene H-abstractions,^{114,181,182} where H-atoms on more substituted carbon atoms, i.e. those H-atoms with lower bond strengths, are more easily abstracted.

Table 18: Alkyl-1,4-H-migration in carbonyl oxides, listing barrier heights E_b (kcal mol⁻¹), rate coefficient k (s⁻¹) at 298 K, and parameters for a Kooij equation fit $k(T)=A \times T^n \times \exp(-E_a/T)$ for the temperature range 200-450 K.

Carbonyl oxide	E_b	$k(298\text{K})$	A / s^{-1}	n	E_a / K	Methodology, comment
Z-CH ₃ CHOO	16.4 ^a					CCSD(T)/aVTZ//M06-2X
	16.5 ^a					IRCMax CCSD(T)/aVTZ//M06-2X
	16.3 ^a					IRCMax CCSD(T)/CBS(DTQ)//M06-2X
	16.5 ^a	139				CCSD(T)/CBS(TQ5)//CCSD(T)/aVTZ
	16.8	136	3.11×10^{-64}	25.0	-2685	
Z-C ₂ H ₅ CHOO	16.5	205	2.41×10^{-62}	24.3	-2571	Total VHP formation
	20.0	0.6	5.88×10^{-83}	31.0	-3601	Z-VHP formation
Z-nC ₃ H ₇ CHOO	16.5	127	8.54×10^{-63}	24.5	-2490	Total VHP formation
	19.3	0.8	1.43×10^{-79}	29.9	-3343	Z-VHP formation
Z-(CH ₂ -C ₈ H ₁₃ O)CHOO ^b	15.8	634	6.77×10^{-58}	23.0	-2099	Total VHP formation
Z-iC ₃ H ₇ CHOO	18.9	6.7	1.52×10^{-75}	28.7	-3150	
(R-2-butyl) ₂ COO	18.1 ^d	10	5.51×10^{-70}	26.8	-2692	
(S-2-butyl)(R-2-butyl)COO	17.4 ^d	21	6.83×10^{-69}	26.4	-2854	
(CH ₃) ₂ COO	15.7 ^a					CCSD(T)/aVTZ//M06-2X
	15.8 ^a					IRCMax CCSD(T)/aVTZ//M06-2X
	15.6 ^a					IRCMax CCSD(T)/CBS(DTQ)//M06-2X
	16.1	478	7.64×10^{-60}	23.6	-2367	
E-(CH ₃)(C ₂ H ₅)COO	16.5	433	8.63×10^{-61}	23.9	-2390	
E-(CH ₃)(iC ₃ H ₇)COO	16.0	611	4.18×10^{-59}	23.4	-2276	
E-(CH ₃)(C ₈ H ₁₃ O)COO ^c	16.3	250	8.33×10^{-58}	22.8	-2054	
E-(CH ₃)(tC ₄ H ₉)COO	16.3	373	9.26×10^{-61}	23.9	-2362	
E-(CH ₃)(CH=CH ₂)COO	17.5	50	4.36×10^{-67}	25.9	-2737	
E-(CH ₃)(OH)COO	16.0	277	6.08×10^{-59}	23.3	-2074	
Z-(C ₂ H ₅)(CH ₃)COO	15.6	689	5.91×10^{-58}	22.9	-2331	Total VHP formation
	19.2	1.9	1.10×10^{-78}	29.7	-3251	Z-VHP formation
(C ₂ H ₅) ₂ COO	15.9	534	4.72×10^{-59}	23.3	-2358	Total VHP formation
	19.4	2.6	7.46×10^{-79}	29.8	-3246	Z-VHP formation
E-(C ₂ H ₅)(iC ₃ H ₇)COO	15.8	257	4.83×10^{-61}	23.9	-2420	Total VHP formation
	19.0	3.8	2.28×10^{-77}	29.4	-3102	Z-VHP formation
E-(C ₂ H ₅)(tC ₄ H ₉)COO	18.2	121	2.13×10^{-74}	28.5	-2964	Total VHP formation
	19.1	4.2	1.56×10^{-77}	29.5	-3069	Z-VHP formation
Z-(iC ₃ H ₇)(CH ₃)COO	18.3	15	4.45×10^{-73}	28.0	-2967	
Z-(C ₈ H ₁₃ O)(CH ₃)COO ^c	17.0	60	6.95×10^{-66}	25.7	-2391	Total VHP formation
	18.7	1.7	4.19×10^{-77}	29.3	-2917	E-VHP formation
Z-(iC ₃ H ₇)(C ₂ H ₅)COO	18.7	13	8.54×10^{-73}	27.9	-2858	
(iC ₃ H ₇) ₂ COO	17.8	19	1.62×10^{-70}	27.0	-2912	
E-(iC ₃ H ₇)(tC ₄ H ₉)COO	19.7	1.1	8.80×10^{-81}	30.5	-3249	

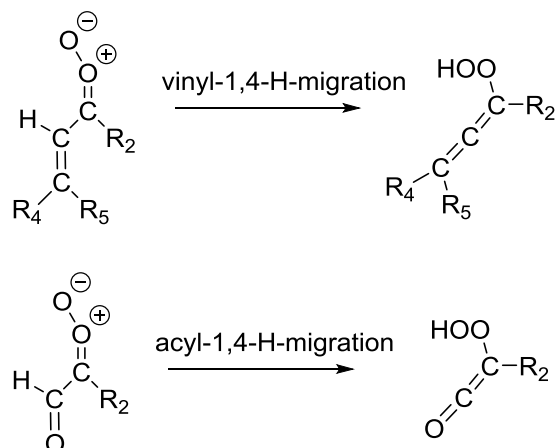
^a Barrier height not shifted by 0.4 kcal mol⁻¹

^b Z-pinonaldehyde-A-oxide.

^c Pinonaldehyde-K-oxide.

^d Based on M06-2X/aug-cc-pVTZ data

K. Vinyl-1,4- and acyl-1,4-H-migration forming cumulene hydroperoxides

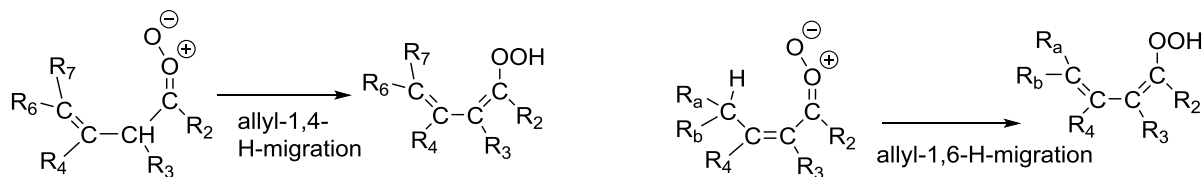


The rate coefficient predictions across the relevant range of substituents are listed in Table 19. In all cases we find high barriers, in agreement with earlier work by Kuwata et al.³ on MVK-oxide, and low rate coefficients despite strong rate enhancement by tunneling, rendering this reaction non-competitive. For both reaction classes this is caused by the higher ring strain compared to the alkyl-1,4-H-migration, and the loss of conjugation stabilization in the TS as the external π -bond rotates to a $\sim 90^\circ$ orientation relative to the carbonyl oxide/VHP moiety π -bond. For acyl-1,4-H-migration, this negates any advantage that might be afforded by the weaker acyl H-C(O) bond.

Table 19: Vinyl- and acyl-1,4-H-migration in β -unsaturated and β -oxo carbonyl oxides forming cumulene and ketene hydroperoxides, respectively, listing barrier heights E_b (kcal mol⁻¹), rate coefficient k (s⁻¹) at 298 K, and parameters for a Kooij equation fit $k(T)=A \times T^n \times \exp(-E_a/T)$ for the temperature range 200–450 K.

Carbonyl oxide	E_b	$k(298\text{K})$	A / s^{-1}	n	E_a / K
Z-(CH=CH ₂)CHOO	23.2	4.7×10^{-3}	5.08×10^{-104}	38.1	-4687
Z-(CH=CH ₂)(CH ₃)COO	21.3	0.09	9.47×10^{-91}	33.9	-3553
Z-(Z-CH=CH-CH ₃)CHOO	21.2	0.11	2.54×10^{-91}	33.9	-3860
Z-(E-CH=CH-CH ₃)CHOO	23.3	3.7×10^{-3}	1.53×10^{-103}	38.0	-4372
Z-(C(O)CH ₃)CHOO	24.4	2.8×10^{-5}	3.05×10^{-52}	21.2	3703
Z-(C(O)CH ₃)(CH ₃)COO	20.6	6.8×10^{-3}	1.07×10^{-33}	14.9	4213

L. Allyl-1,4- and allyl-1,6-H-migration forming β -unsaturated VHP



The 1,4-H-migration in γ -unsaturated CI benefits strongly from the presence of the double bond (see Table 20), stabilizing both the TS and the product. The γ -C=C moiety reduces the barrier height by ~ 2.5 kcal mol $^{-1}$ relative to a saturated γ -substituent, and thus enhances the reaction rate by a factor of 20 at room temperature. Analogous to the alkyl-1,4-H-shift, we find that increasing substitution on the H-bearing carbon atom can lead to higher barriers and slower rate coefficients.

Table 20: Allyl-1,4-H-migration in γ -unsaturated carbonyl oxides forming conjugated vinyl hydroperoxides, listing barrier heights E_b (kcal mol $^{-1}$), rate coefficient k (s $^{-1}$) at 298 K, and parameters for a Kooij equation fit $k(T)=A \times T^n \times \exp(-E_a/T)$ for the temperature range 200–450 K.

Carbonyl oxide	E_b	$k(298\text{K})$	A / s^{-1}	n	E_a / K	Remarks
Z-(CH $_2$ -CH=CH $_2$)CHOO	13.8	4.2×10^3	3.66×10^{-46}	18.9	-1630	
Z-(CH(CH $_3$)-CH=CH $_2$)CHOO	15.8	229	8.89×10^{-58}	22.7	-2269	Total VHP formation
	16.4	31	2.11×10^{-63}	24.4	-2639	Z-VHP formation

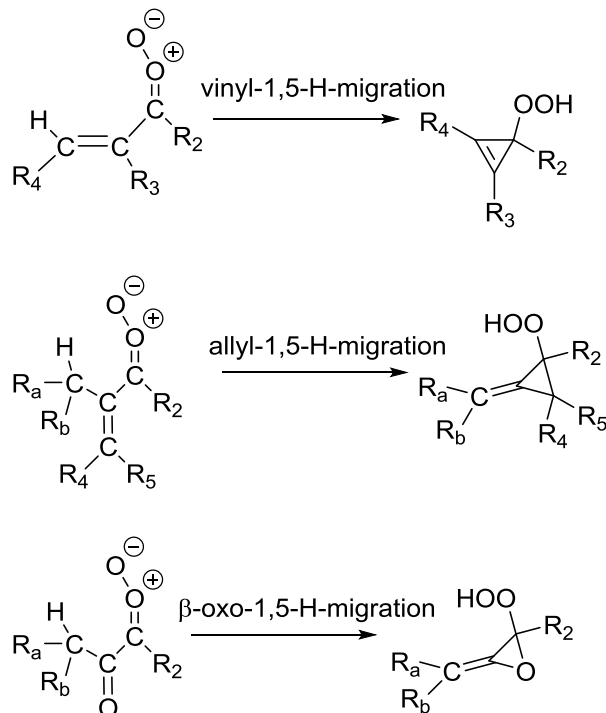
For β -unsaturated CI with a suitably placed H-atom, an allyl-1,6-H-migration leads to a similar conjugated VHP and furthermore benefits from a significantly reduced ring strain in the TS, leading to the lowest reaction barriers found in this work (see Table 21). Tunneling is less important in this reaction relative to other H-migrations in this work, with a rate increase factor of 5 at room temperature only, owing to the low and broad barrier of the reaction. The low barriers lead to a very fast loss process that can be comparable in rate to internal rotation along the single bond in the conjugated C=C-C=COO system. H-abstraction from more substituted C-atoms leads to lower barrier heights, matching the lower C-H bond strength. However, an alkyl substituent that is forced geometrically close to the carbonyl oxide moiety increases the barrier (as also found for e.g. the alkyl-1,4-H-shift, see section J), so the decrease in barrier height by increasing substitution is only active as long as TS conformers exist that allows this additional substituent to avoid the outer O-atom of the oxide. For -CH(CH $_3$) $_2$ and similar moieties, this is no longer possible and concomitantly the barrier increases somewhat, as found e.g. for Z-(Z-CH=CH-CH(CH $_3$) $_2$)CHOO (see Table 21).

Note that the stereo-orientation of the olefinic moiety is important as this channel is not accessible for an R $_4$ alkyl chain which is oriented away from the oxide moiety (see Figure 4). For the moieties considered here, this applies to the E-substituents, i.e. Z-(E-CH=CH-CH $_3$)CHOO and analogues. For these CI, 1,5-ring-closure is the dominant reaction (see section O).

Table 21: Allyl-1,6-H-migration in β -unsaturated carbonyl oxides forming conjugated vinyl hydroperoxides, listing barrier heights E_b (kcal mol $^{-1}$), rate coefficient k (s $^{-1}$) at 298 K, and parameters for a Kooij equation fit $k(T)=A \times T^n \times \exp(-E_a/T)$ for the temperature range 200–450 K.

Carbonyl oxide	E_b	$k(298\text{K})$	A / s^{-1}	n	E_a / K	Remarks
Z-(Z-CH=CH-CH $_3$)CHOO	8.3	4.7×10^6	1.40×10^{-9}	6.77	838	
Z-(Z-CH=CH-CH $_2$ CH $_3$)CHOO	7.6	5.7×10^6	1.57×10^{-8}	6.42	917	Total VHP formation
	9.2	5.1×10^5	1.45×10^{-13}	8.03	909	Z,Z-VHP formation
Z-(Z-CH=CH-CH(CH $_3$) $_2$)CHOO	8.6	2.0×10^6	1.51×10^{-9}	6.83	1210	

M. Vinyl-, allyl-, and β -oxo-1,5-H-migration



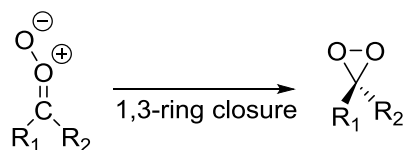
The reaction mechanism for these reactions passes formally over a high-energy singlet biradical intermediate, leading to high barriers for H-migration. For β -oxo-1,5-H-migration and allyl-1,5-H-migration, the reaction proceeds by ring closure to a 3-membered ring without an intermediary energy minimum, as verified by IRC calculations. At our level of theory, the vinyl-1,5-H-migration does lead to a semi-stable biradical intermediate with an energy over 45 kcal mol⁻¹ above the CI, but this cyclises with a very low barrier to a substituted cyclopropene.

These three reaction classes can thus be neglected, as they are never competitive against other unimolecular channels.

Table 22: Vinyl-1,5-H-migration and allyl-1,5-H-migration in β -unsaturated carbonyl oxides, and β -oxo-1,5--migration in β -oxo carbonyl oxides, listing barrier heights E_b (kcal mol⁻¹), rate coefficient k (s⁻¹) at 298 K, and parameters for a Kooij equation fit $k(T)=A \times T^n \times \exp(-E_a/T)$ for the temperature range 200–450 K.

Carbonyl oxide	E_b	$k(298\text{K})$	A / s^{-1}	n	E_a / K	Reaction type
Z-(CH=CH ₂)CHOO	>45					Vinyl-1,5-H-shift
Z-(C(CH ₃)=CH ₂)CHOO	>40					Vinyl-1,5-H-shift
	33.3	1.8×10^{-12}	5.15×10^8	1.23	16125	Allyl-1,5-H-shift
Z-(C(O)CH ₃)CHOO	24.4	2.8×10^{-5}	3.05×10^{-52}	21.2	3703	β -oxo-1,5-H-shift
Z-(C(O)CH ₃)(CH ₃)COO	20.6	6.8×10^{-3}	1.07×10^{-33}	14.9	4213	β -oxo-1,5-H-shift

N. 1,3-Ring closure forming dioxirane



1. Benchmark calculations

1,3-Ring closure to a dioxirane is a reaction path that is available to all CI. To improve our estimates of the barrier height for CH_2OO , we re-optimized the geometries and vibrational frequencies at the CCSD(T)/aVTZ and CCSD(T)/aVQZ levels of theory, and performed single point calculations on the M06-2X and CCSD(T) geometries with basis sets up to aug-cc-pV6Z to estimate the CBS limit (see Table 23). We also performed IRCMax calculations on the M06-2X minimum energy pathway, with basis sets up to aug-cc-pVQZ. We find that these improvements of the level of theory lead to only a slight increase in barrier height. The base level of theory in this work, CCSD(T)/aVTZ//M06-2X with a $+0.4 \text{ kcal mol}^{-1}$ increase of the barrier height, seems to underestimate the CH_2OO ring closure barrier somewhat compared to higher-level calculations. For *Z*- and *E*- CH_3CHOO and $(\text{CH}_3)_2\text{COO}$, we performed complete basis set estimates on the M06-2X geometry (see Table 23). Re-optimizing the geometries for $(\text{CH}_3)_2\text{COO}$ ring closure at the CCSD(T)/aVTZ level of theory yielded essentially the same barrier height as the CCSD(T)/aVTZ//M06-2X, within $0.06 \text{ kcal mol}^{-1}$, again confirming that the M06-2X geometries close mimic the CCSD(T) potential energy surface.

Post-CCSD(T) calculations are available in the literature for both *Z*- CH_3CHOO and $(\text{CH}_3)_2\text{COO}$; these are listed in Table 2, showing that our adjusted barrier heights and rate coefficients are in fair agreement with the best available theoretical estimates and experimental data.

2. Reaction trends

The barrier height and rate coefficient predictions for all CI considered in this work are listed in Table 23. The reactivity trends are strongly linked to the relative energy of the stereoisomers discussed higher. For alkyl- and vinyl-substituted CI, the fastest 1,3-ring closure reactions are accessible to *E*-RCHOO carbonyl oxides, with rate coefficients as high as 10^2 s^{-1} , making it the dominant loss process for these carbonyl oxides. Their barrier height is essentially independent of the substituent ($15.8 \pm 0.5 \text{ kcal mol}^{-1}$), except H_2COO which falls outside the trend. In contrast, the highest barriers to 1,3-ring closure are found for their stereoisomers, *Z*-RCHOO. The barrier is strongly dependent on the R_1 substituent, decreasing when the substituent becomes more substituted on the β -carbon, with β -unsaturated R_1 yielding the lowest barriers. The R_2 substituent has little impact, even if it is unsaturated. The ring closure for these carbonyl oxides remains orders of magnitude slower than 1,4-H-migration, where available. The barrier heights for CI with two alkyl- or vinyl substituents lie between the corresponding *Z*- and *E*-RCHOO extremes. The barrier decreases as the R_1 substituent become more branched on the β -carbon, while elongating the alkyl chain substituents has only a minor impact. For small R_1 , ring closure remains significantly slower than 1,4-H-migration, but for $\text{R}_1 = \text{iC}_3\text{H}_7$ the barrier heights for ring closure become more comparable to those for the VHP channel, and the channel start to compete against H-migration at higher temperatures. At room temperature, though, we never predict more than 10% contribution of ring closure for CI that have a H-atom available for 1,4-H-migration. The impact of the R_2 substituent on the reaction rate depends on the branching of the R_1 substituent, as its influence derives from steric $\text{R}_1\text{-R}_2$ interaction. Indeed, as both substituents become more branched, the barrier height and rate coefficient shows larger variations compared to the values obtained for the smallest, less-interacting R_1 substituents.

Table 23: 1,3-ring closure in carbonyl oxides, listing barrier heights E_b (kcal mol⁻¹), rate coefficient k (s⁻¹) at 298 K, and parameters for a Kooij equation fit $k(T)=A \times T^n \times \exp(-E_a/T)$ for the temperature range 200–450 K.

Carbonyl oxide	E_b	$k(298K)$	A / s^{-1}	n	E_a / K	Methodology
CH ₂ OO	18.6 ^a					CCSD(T)/aVTZ//M06-2X
	19.1 ^a					IRCMaX CCSD(T)/aVQZ//M06-2X
	19.3 ^a	0.2				CCSD(T)/CBS(Q56)//CCSD(T)/aVTZ
	19.3 ^a	0.1				CCSD(T)/CBS(Q56)//CCSD(T)/aVQZ
	19.0	0.3	16.6	4.0	8024	
Z-CH ₃ CHOO	23.2 ^a					CCSD(T)/aVTZ//M06-2X
	24.0 ^a					CCSD(T)/CBS(DTQ)//M06-2X
	23.2 ^a	6.9×10 ⁻⁵				CCSD(T)/aVTZ//CCSD(T)/aVTZ
	23.6	9.2×10 ⁻⁵	1.81×10 ⁴	2.98	10755	
Z-C ₂ H ₅ CHOO	22.9	4.3×10 ⁻⁴	1.26×10 ⁶	2.41	10584	
Z-nC ₃ H ₇ CHOO	22.8	2.8×10 ⁻⁴	2.55×10 ⁵	2.60	10562	
Z-(CH ₂ -C ₈ H ₁₃ O)CHOO ^b	21.6 ^d	9.8×10 ⁻⁴	7.97×10 ²	3.45	9906	
Z-(CH ₂ -CH=CH ₂)CHOO	22.6	3.3×10 ⁻⁴	1.02×10 ⁵	2.73	10460	
Z-iC ₃ H ₇ CHOO	21.9	2.9×10 ⁻³	3.22×10 ⁶	2.36	10219	
Z-tC ₄ H ₉ CHOO	20.9	1.0×10 ⁻²	2.58×10 ⁶	2.32	9710	
Z-(C(CH ₃) ₂ -CH=CH ₂)CHOO	20.5	1.3×10 ⁻²	9.84×10 ⁶	2.09	9625	
Z-(CH=CH ₂)CHOO	19.9	2.5×10 ⁻²	8.03×10 ⁵	2.34	9126	
Z-(Z-CH=CH-CH ₃)CHOO	20.3	7.3×10 ⁻³	7.34×10 ⁴	2.63	9279	
Z-(E-CH=CH-CH ₃)CHOO	20.4	5.3×10 ⁻³	9.11×10 ⁵	2.23	9444	
Z-(C(CH ₃)=CH ₂)CHOO	18.3	3.5×10 ⁻¹	5.52×10 ⁷	1.68	8476	
Z-(CHO)CHOO	14.9	1.4×10 ²	2.49×10 ⁶	2.21	6656	
Z-(C(O)CH ₃)CHOO	15.9	19	5.55×10 ⁵	2.41	7141	
E-CH ₃ CHOO	15.3 ^a					CCSD(T)/aVTZ//M06-2X
	15.9 ^a					CCSD(T)/CBS(DTQ)//M06-2X
	15.7	53	1.69×10 ⁹	1.35	7445	
E-C ₂ H ₅ CHOO	15.6	74	1.57×10 ¹⁰	1.03	7464	
E-(CH ₂ -C ₈ H ₁₃ O)CHOO ^b	14.8	62	3.86×10 ⁵	2.43	6732	
E-(CH ₂ -CH=CH ₂)CHOO	15.6	41	1.64×10 ⁹	1.35	7504	
E-nC ₃ H ₇ CHOO	15.3	92	5.63×10 ⁹	1.20	7380	
E-iC ₃ H ₇ CHOO	15.3	102	9.22×10 ⁹	1.13	7387	
E-tC ₄ H ₉ CHOO	15.2	111	8.51×10 ⁹	1.15	7357	
E-(CH=CH ₂)CHOO	16.7	14	1.08×10 ¹¹	0.80	8139	
E-(Z-CH=CH-CH ₃)CHOO	16.3	26	7.98×10 ¹¹	0.48	8007	
E-(E-CH=CH-CH ₃)CHOO	15.7	71	4.28×10 ¹¹	0.60	7722	
E-(C(CH ₃)=CH ₂)CHOO	16.3	10	5.93×10 ⁸	1.46	7832	
E-(CHO)CHOO	20.7	1.7×10 ⁻²	1.85×10 ⁵	2.72	9444	
E-(C(O)CH ₃)CHOO	19.8	5.7×10 ⁻²	2.36×10 ⁶	2.30	9127	
E-(OH)CHOO	7.13	6.1×10 ⁷	2.06×10 ¹²	0.25	3530	
(CH ₃) ₂ COO	20.4 ^a					CCSD(T)/aVTZ//M06-2X
	21.1 ^a					CCSD(T)/CBS(DTQ)//M06-2X
	20.8	6.4×10 ⁻³	3.84×10 ⁹	1.21	10140	
E-(CH ₃)(C ₂ H ₅)COO	20.9	8.8×10 ⁻³	3.06×10 ¹⁰	0.92	10159	
E-(CH ₃)(iC ₃ H ₇)COO	20.4	9.3×10 ⁻³	2.36×10 ⁹	1.28	9995	
E-(CH ₃)(C ₈ H ₁₃ O)COO ^c	20.8	6.5×10 ⁻³	1.16×10 ¹²	0.33	10337	
E-(CH ₃)(tC ₄ H ₉)COO	21.0	4.2×10 ⁻³	2.06×10 ¹⁰	0.94	10306	
E-(CH ₃)(CH=CH ₂)COO	21.0	4.0×10 ⁻³	3.57×10 ¹¹	0.48	10385	
E-(CH ₃)(CHO)COO	26.0	1.5×10 ⁻⁶	2.30×10 ⁶	2.34	12328	
E-(CH ₃)(C(O)CH ₃)COO	24.9	8.1×10 ⁻⁶	2.93×10 ⁷	1.92	11883	
Z-(C ₂ H ₅)(CH ₃)COO	19.8	2.4×10 ⁻²	4.27×10 ⁷	1.86	9509	
(C ₂ H ₅) ₂ COO	19.8	4.0×10 ⁻²	1.05×10 ⁹	1.46	9627	
E-(C ₂ H ₅)(iC ₃ H ₇)COO	19.4	3.1×10 ⁻²	1.55×10 ⁷	2.02	9396	
E-(C ₂ H ₅)(tC ₄ H ₉)COO	20.3	1.3×10 ⁻²	2.23×10 ⁹	1.33	9961	
Z-(iC ₃ H ₇)(CH ₃)COO	19.8	4.1×10 ⁻²	4.76×10 ¹⁰	0.90	9809	
Z-(C ₈ H ₁₃ O)(CH ₃)COO ^c	19.9	3.1×10 ⁻²	1.75×10 ⁷	2.06	9493	
Z-(iC ₃ H ₇)(C ₂ H ₅)COO	19.8	6.6×10 ⁻²	2.66×10 ¹³	0.05	10108	
(iC ₃ H ₇) ₂ COO	18.8	1.7×10 ⁻¹	3.97×10 ¹¹	0.45	9253	
E-(iC ₃ H ₇)(tC ₄ H ₉)COO	19.1	8.7×10 ⁻²	6.97×10 ¹⁰	0.72	9383	
Z-(tC ₄ H ₉)(CH ₃)COO	19.1	1.7×10 ⁻¹	2.55×10 ¹⁰	1.02	9399	
Z-(tC ₄ H ₉)(C ₂ H ₅)COO	19.1	1.5×10 ⁻¹	5.45×10 ¹¹	0.55	9555	
Z-(tC ₄ H ₉)(iC ₃ H ₇)COO	17.6	1.1	6.83×10 ¹⁰	0.80	8759	
(tC ₄ H ₉) ₂ COO	19.8	7.5×10 ⁻²	1.12×10 ¹¹	0.85	9795	
Z-(CH=CH ₂)(CH ₃)COO	17.2	1.6	3.49×10 ⁹	1.12	8291	
Z-(CHO)(CH ₃)COO	10.8	7.1×10 ⁴	2.76×10 ¹⁰	0.78	5162	
Z-(C(O)CH ₃)(CH ₃)COO	11.3	1.6×10 ⁴	3.95×10 ⁹	1.02	5448	
E-(CH ₃)(OH)CHOO	11.3	4.6×10 ⁴	8.54×10 ¹¹	0.37	5618	

^a Barrier height not shifted by 0.4 kcal mol⁻¹ ^b Pinonaldehyde-A-oxide ^c Pinonaldehyde-K-oxide. ^d based on M06-2X/aug-cc-pVTZ data

The reaction trends seen for alkyl- and vinyl-substituted CI are found to an even larger extent in oxo-substituted CI. The fastest and slowest 1,3-ring closure reactions correspond to the stereoisomers with the largest energy difference, i.e. CI with a β -oxo- and an alkyl substituent such as *Z*- and *E*-(CH₃)(C(O)CH₃)COO. If the alkyl substituent is replaced with a H-atom, the stereoisomer energy difference is less (see section H), and the difference in rate coefficient decreases in accordance, with the absolute $k(T)$ approaching those of the non-hetero-substituted CI.

3. Group additivity SAR for the rate coefficient of 1,3-ring closure

While 1,3-ring closure in CI is not the fastest reaction, it is a reaction class that is available to all CI, providing us with a large amount of data that allows us to further expand on our earlier observations (section H) on the group additivity properties of CI reactivity.

The rate of ring closure in (R₁)(R₂)COO at 298 K can be well predicted by the following group additivity relationship, where Table 24 lists the group additivity factors F_{R1} and F_{R2} obtained by a least-square analysis of $\log(k)$.

$$k_{1,3\text{-ring closure}}(298K) = 10^{(-0.517 + F_{R1} + F_{R2})} S^{-1}$$

Table 24: Group additivity factors F_{R1} and F_{R2} for prediction of the rate coefficient of 1,3-ring closure in Criegee intermediates with the indicated R₁ and R₂ substituents. We also indicate the SAR substituent classes with designators as defined in section C.

Substituent	SAR Substituent class	F_{R1} / kcal mol ⁻¹	F_{R2} / kcal mol ⁻¹
CH ₃	-CH ₃	-3.80	+2.15
C ₂ H ₅ / n-C ₃ H ₇	-CH ₂ R _a	-3.16	+2.20
CH ₂ -CH=CH ₂	-CH ₂ -CR ₃ =CR ₄ R ₅	-2.97	+2.13
iC ₃ H ₇	-CHR _a R _b	-2.62	+2.41
CH(CH ₃)-CH=CH ₂	-CHR _a -CR ₃ =CR ₄ R ₅	N/A ^a	N/A ^a
CH=CH ₂ / CH=CH-CH ₃	-CH=CR ₄ R ₅	-1.49	+1.99
tC ₄ H ₉	-CR _a R _b R _c	-2.17	+2.00
C(CH ₃) ₂ -CH=CH ₂	-CR _a R _b -CR ₃ =CR ₄ R ₅	-1.36	N/A ^a
C(CH ₃)=CH ₂	-CR _a =CR ₄ R ₅	+0.06	+1.50
H	-H	+0.00	0.00
CHO	-CHO	+2.95	-1.37
C(O)CH ₃	-C(O)R _a	+2.18	-0.75

^a Insufficient data available to determine this factor.

As can be seen in Figure 8, the group additivity SAR reproduces the theory-based rate coefficients well, with an average deviation of only a factor of 2 with rate coefficients extending across almost 11 decades. The largest deviations on non-cyclic CI are found for tC₄H₉ substituents, where the SAR prediction deviates as much as a factor of 5 from the original data; the rate coefficients for CI with a tC₄H₉ substituent range across 4.4 decades. The explanation lies most likely in the higher variation of steric interaction of this bulky substituent with the substituent on the opposite side of the carbonyl oxide; at this point, we refrain from trying to introduce cross-terms F_{R1R2} as our data set is not large enough to support this many variables. The largest deviations are found for β -pinene derived nopinone oxides (see section Q.1), where we modelled the two substituents as -iC₃H₇ and -C₂H₅. Deviations between SAR and source data are as high as a factor of 30, showing clearly in Figure 8, and are obviously caused by the ring strain in these CI, where 1,3-ring closure leads to a tricyclic structure.

Finally, we compare the group additivity factors derived for 1,3-ring closure against those obtained in section H for CI stereoisomer relative stability. Figure 9 shows the correlation between the F_{R1} factors, showing a clear correlation, even if large deviations remain. Not surprisingly, and for similar reasons as above, the largest deviation is found for the $F_{R1}(\text{tC}_4\text{H}_9)$ factor. The emergence that a stability group factor of 1 kcal mol⁻¹

corresponds nearly exactly to a reactivity factor of 1 (factor 10 increase in the rate coefficient) is numerical coincidence and specific for the chosen reaction; at room temperature a factor 10 change on a rate coefficient corresponds to a change in reaction energy barrier of $\sim 1.35 \text{ kcal mol}^{-1}$. We have thus shown that CI reactivity is clearly linked to the CI relative stability. As the study on stereoisomerisation group additivity was not sensitive to the F_{R2} parameters, no meaningful correlation can be found (see Figure 9); the key finding is mostly that F_{R2} parameters span a significantly smaller domain than F_{R1} , i.e. the CI reactivity is determined predominantly by the R_1 substituent in *syn*-position to the carbonyl oxide outer O-atom.

Efforts to derive a SAR for CI unimolecular reactions based on group additivities are not overly valuable, as the dominant reaction depends on the CI substitution (see section R below), and the additivity factors do not transfer exactly across different reaction types. The SAR developed here thus serves mostly as an example of how the CI reactivity can be expressed as a function of the substituents near the oxide moiety.

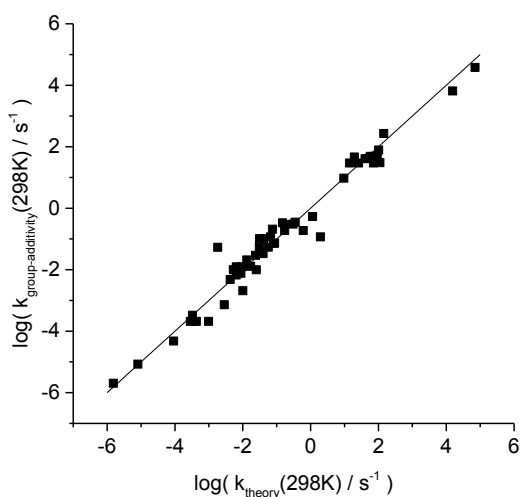


Figure 8: Theory-based rate coefficients for 1,3-ring closure in CI, compared to the group additivity predictions. The line represents a 1:1 ratio.

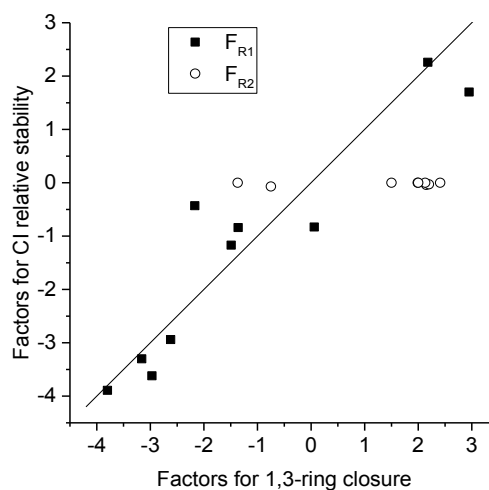
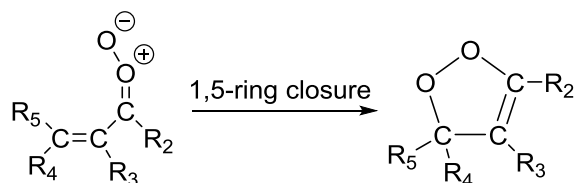


Figure 9: Comparison of the group additivity factors F_{R1} and F_{R2} for 1,3-ring closure versus those for CI relative stability (see section H). The line represents a linear correlation.

O. 1,5-Ring closure forming cyclic peroxides



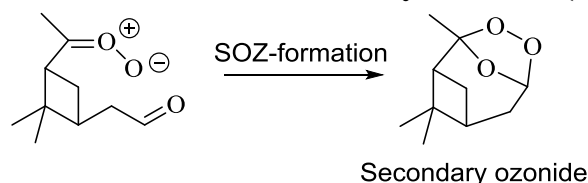
β -unsaturated CI have a double bond in *syn*-position to the oxide moiety and can undergo a 1,5-ring closure reaction. For these processes we find low reaction barriers (see Table 25), in agreement with earlier calculations by Kuwata et al.,^{3,27} leading to rate coefficients exceeding 10^3 s^{-1} . For nearly all β -unsaturated CI, this reaction is the dominant loss process, barring CI that have access to an allyl-1,6-H-migration. This reaction is therefore particularly important in the ozonolysis of conjugated π -systems, such as isoprene, myrcene, α -terpinene and other terpenoids.

The product of this reaction, a cyclic peroxide with a 5-membered ring, is expected to break the O–O bond; Kuwata and coworkers^{3,27} predicted a barrier height of 18 to 21 kcal mol^{-1} for this process. The resulting singlet diradical will re-arrange to either a carbonyl-epoxide or a dicarbonyl.

Table 25: 1,5-Ring closure in β -unsaturated carbonyl oxides, listing barrier heights E_b (kcal mol^{-1}), rate coefficient k (s^{-1}) at 298 K, and parameters for a Kooij equation fit $k(T)=A \times T^n \times \exp(-E_a/T)$ for the temperature range 200–450 K.

Carbonyl oxide	E_b	$k(298\text{K})$	A / s^{-1}	n	E_a / K
Z-(CH=CH ₂)CHOO	12.2	4.0×10^3	2.02×10^{10}	0.66	5727
Z-(Z-CH=CH-CH ₃)CHOO	11.9	2.1×10^3	7.22×10^{10}	0.32	5711
Z-(E-CH=CH-CH ₃)CHOO	11.2	8.4×10^3	2.59×10^{11}	0.21	5496
Z-(Z-CH=CH-CH ₂ CH ₃)CHOO	10.8	9.1×10^3	2.05×10^9	0.86	5129
Z-(E-CH=CH-CH ₂ CH ₃)CHOO	10.7	6.1×10^4	1.69×10^{12}	0.04	5182
Z-(Z-CH=CH-CH(CH ₃) ₂)CHOO	10.9	1.2×10^4	1.18×10^{10}	0.65	5207
Z-(E-CH=CH-CH(CH ₃) ₂)CHOO	10.8	2.7×10^4	2.37×10^{11}	0.33	5322
Z-(C(CH ₃)=CH ₂)CHOO	12.8	2.5×10^3	1.59×10^{11}	0.44	6102
Z-(CH=CH ₂)(CH ₃)COO	11.9	7.7×10^3	2.94×10^{10}	0.65	5617

P. Intramolecular secondary ozonide (SOZ) formation



The only intramolecular formation of secondary ozonides studied explicitly in this work is for pinonaldehyde oxides formed in α -pinene ozonolysis. As already noted, intramolecular SOZ formation involves the formation of a bicyclic structure; ring strain can thus strongly affect the reaction barrier height, while the conversion of modes for internal rotation to skeletal vibrational modes induces a significant entropic disadvantage for these reactions. Due to this entropic hindrance of SOZ ring closure relative to other modes of reaction, chemically excited CI typically do not yield SOZ.¹⁸ On the other hand, if the formed ring is sufficiently large to avoid excessive ring strain, it can be a dominant pathway for stabilized CI, with a low energy barrier to reaction;^{16–22} SOZ have been observed in sizable yields in e.g. sesquiterpene ozonolysis.^{21,53,183} Intramolecular SOZ formation is not only important in the ozonolysis of endocyclic double bonds, but can also occur in secondary ozonolysis of multi-unsaturated VOC, where a carbonyl functionality was formed in the first O_3 - or OH-initiated reaction.

Table 3 in section E.1 lists barrier heights and rate coefficients available in the literature on intramolecular SOZ formation, as well as our current calculations on pinonaldehyde oxide (see Figure 10). For strained systems such as α -pinene and cyclopropene, the barriers to SOZ formation are rather high and the reaction is not competitive, while for systems with less ring strain such as cyclohexene, β -caryophyllene, or α -phellandrene, lower barriers and higher reaction rates are found. In this work, we consider SOZ formation negligible when less than 6 carbon atoms are present between the two reacting moieties,^{4,184} as well as for larger spans if cyclic structures are interfering with the ring closure.

Q. Impact of specific substitutions

1. Impact of cyclic substituents on unimolecular reaction rates

Many of the monoterpenes and sesquiterpenes emitted into the atmosphere are cyclic or bicyclic compounds, with α - and β -pinene the most ubiquitous representatives with an endocyclic and exocyclic double bond, respectively (see Figure 10). The carbonyl oxides formed from their ozonolysis have either a cyclic substituent (pinonaldehyde oxide), or are implanted directly onto a cyclic structure (nopinone oxide), which can affect their reactivity through changes in ring strain or geometric constraints.

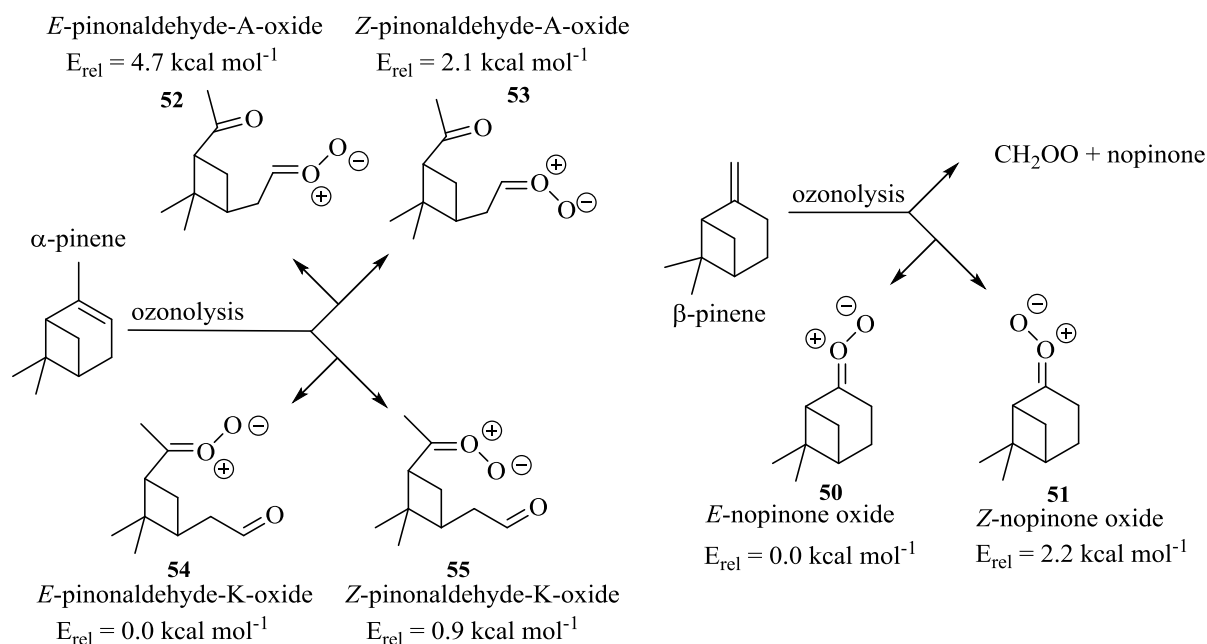


Figure 10: Carbonyl oxides formed from α -pinene and β -pinene ozonolysis. The naming for pinonaldehyde oxide is based on the position of the oxide O-atom, i.e. on the aldehyde (A) or ketone (K) carbonyl moiety.

The chemistry of E - and Z -pinonaldehyde-A-oxide is not expected to be influenced significantly by the cyclic substituent, as it is separated by one $-\text{CH}_2-$ group from the oxide moiety. We find that for all reactions the barrier heights are within $0.8 \text{ kcal mol}^{-1}$ of the values for aliphatic substituents; this is within the expected uncertainty. For pinonaldehyde-K-oxide, the cyclic substituent is implanted directly on the carbonyl oxide C-atom. The most similar non-cyclic CI for which we have data are Z - and E -(iC_3H_7)(CH_3)COO, used here as reference compounds. The relative energy of the stereoisomers matches the reference compound within $0.15 \text{ kcal mol}^{-1}$ (Table 15). For the dominant 1,4-H-migration, the estimated barrier height remains within $1.3 \text{ kcal mol}^{-1}$ of the barrier height for the non-cyclic reference compound both for the E - and Z -isomers, and the rate coefficients within a factor of 4 (see Table 26), i.e. differences that remain within the expected reliability of the predictions. We thus conclude that the presence of an adjacent cyclic substituent, even one as highly strained as a four-membered ring, does not overly disturb the reaction trends as laid out in this work.

Nopinone oxide is an extreme example where the carbonyl oxide is implanted on a strained bicyclic substrate, where (iC_3H_7)(C_2H_5)COO is the closest non-cyclic reference CI available to us. As already discussed by Nguyen et al.,³³ the Z -isomer can not undergo a 1,4-H-migration of the bridgehead hydrogen atom due to the ring strain, indicating a marked difference in reactivity against the reference compound. The barrier to 1,3-ring closure has a barrier significantly lower by over $2.5 \text{ kcal mol}^{-1}$, owing to the changing ring strain. This shortens the lifetime of this stereo isomer significantly, despite the lack of an H-migration channel. 1,4-H-migration in the E -isomer has a barrier slightly higher than the reference compound, though the reaction is only slightly

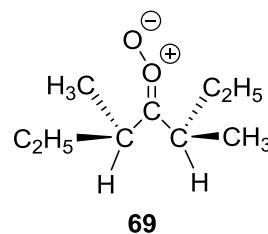
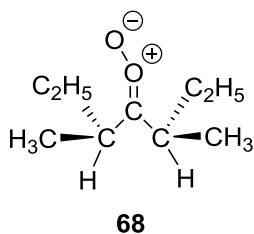
slower due to the differing reaction entropy as a double bond is created in the 6-membered ring (see Table 26). In contrast, the 1,3-ring closure has a higher barrier compared to the reference structure. It is hard to *a priori* predict the reactivity for cyclic carbonyl oxides such as nopinone oxide based on simple trends, and it is recommended that such compounds are explicitly studied individually. The impact of the ring structure is likely to decrease for ring structures with less strain.

Table 26: Reactions of selected monoterpene-derived carbonyl oxides (see Figure 10), listing barrier heights E_b (kcal mol⁻¹), rate coefficient k (s⁻¹) at 298 K, and parameters for a Kooij equation fit $k(T)=A \times T^n \times \exp(-E_a/T)$ for the temperature range 200-450 K. (iC₃H₇)(C₂H₅)COO and (iC₃H₇)(CH₃)COO are listed as reference compounds; their data from Table 18 and Table 23 are repeated here for convenience.

Carbonyl oxide	Reaction	E_b	$k(298\text{K})$	A / s^{-1}	n	E_a / K
Z-(iC ₃ H ₇)(C ₂ H ₅)COO	1,3-ring closure	19.8	6.6×10^{-2}			
	1,4-H-migration	18.7	13			
Z-nopinone oxide	1,3-ring closure	17.2	2.0	1.90×10^9	1.33	8425
E-(C ₂ H ₅)(iC ₃ H ₇)COO	1,3-ring closure	19.4	3.1×10^{-2}			
	1,4-H-migration	18.2	121			
E-nopinone oxide	1,3-ring closure	21.1	1.8×10^{-3}	2.06×10^9	1.23	10358
	1,4-H-migration	15.7	375	5.37×10^{-59}	23.27	-2251
Z-(iC ₃ H ₇)(CH ₃)COO	1,3-ring closure	19.8	4.1×10^{-2}			
	1,4-H-migration	18.3	15			
Z-pinonaldehyde-K-oxide	1,3-ring closure	19.9	3.1×10^{-2}	1.75×10^7	2.06	9493
	1,4-H-migration	17.0	60	6.95×10^{-66}	25.7	-2391
	1,4-H-migration (E-VHP)	18.7	1.7	4.19×10^{-77}	29.3	-2917
E-(CH ₃)(iC ₃ H ₇)COO	1,3-ring closure	20.4	9.3×10^{-3}			
	1,4-H-migration	16.0	611			
E-pinonaldehyde-K-oxide	1,3-ring closure	20.8	6.5×10^{-3}	1.16×10^{12}	0.33	10337
	1,4-H-migration	16.3	250	8.33×10^{-58}	22.8	-2054

2. Impact of substituent chirality on unimolecular reaction rates

To investigate the impact of chirality of the R₁ and R₂ substituents, we examined the alkyl-1,4-H-migration in R,R- and S,R-(2-butyl)₂COO :



At the M06-2X/aug-cc-pVTZ level of theory, these isomers have nearly the same energy, with CI **69** slightly more stable by 0.07 kcal mol⁻¹. The energy difference for the 1,4-H-migration shows a slightly larger difference, with CI **68** having a lower barrier of by 0.7 kcal mol⁻¹. The rate coefficients (see Table 18) remain within a factor of 2, indistinguishable within the uncertainty of the calculations. We conclude that for most monoterpenes, the chirality of the substituents will likely not play a role in determining the CI reactivity.

3. Impact of deuteration on relative unimolecular reaction rates

As H-migration is a main loss channel in unimolecular CI loss, the kinetic isotope effect (KIE) upon deuteration of the migrating H-atom can have a significant impact on the CI lifetime, and the contribution of H-migration channels relative to other channels. The natural incidence of per-H deuteration, 0.016 %, is not high enough to have an impact on atmospheric CI chemistry, so we only cursory examine two examples, (iC₃H₇)₂COO and *E*-(iC₃H₇)(tC₄H₉)COO, selected here as the difference in rate coefficient between 1,3-ring closure and H-migration rate coefficient ratio is smallest. Table 31 lists the rate coefficients upon single deuteration, replacing the tertiary H-atom on the iC₃H₇ group in *syn*-position to the oxide O-atom.

Table 27: Reactions of mono-deuterated CI, with the tertiary H-atom in an iC₃H₇ group replaced with a D-atom.; the non-deuterated cases are also shown for comparison. Listed are barrier heights E_b (kcal mol⁻¹), rate coefficient k (s⁻¹) at 298 K, and parameters for a Kooij equation fit $k(T)=A \times T^n \times \exp(-E_d/T)$ for the temperature range 200–450 K.

Carbonyl oxide	Reaction	E_b	$k(298\text{K})$	A / s^{-1}	n	E_d / K
(iC ₃ H ₇) ₂ COO	1,3-ring closure	18.8	0.17	3.97×10^{11}	0.45	9253
	1,4-H-migration	17.8	19	1.62×10^{-70}	27.0	-2912
Z-(iC ₃ H ₆ D)(iC ₃ H ₇)COO	1,3-ring closure	18.8	0.17	3.02×10^{11}	0.49	9237
	1,4-D-migration	18.6	0.55	4.63×10^{-38}	16.56	2691
<i>E</i> -(iC ₃ H ₇)(tC ₄ H ₉)COO	1,3-ring closure	19.1	8.7×10^{-2}	6.97×10^{10}	0.72	9383
	1,4-H-migration	19.7	1.1	8.80×10^{-81}	30.5	-3249
<i>E</i> -(iC ₃ H ₆ D)(tC ₄ H ₉)COO	1,3-ring closure	19.1	8.1×10^{-2}	6.40×10^{10}	0.73	9402
	1,4-D-migration	20.5	2.9×10^{-2}	4.48×10^{-41}	17.63	3311

As expected, the 1,3-ring closure reaction is hardly affected by deuteration, while the KIE increases the barrier height and decreases tunneling in the 1,4-H-migration, reducing the reaction rate by over a factor 30. For these compounds, the ring closure reaction then becomes a competitive, or even the dominant unimolecular loss channel.

Experimental information on deuterated CI is scarce; direct studies include those of Huang et al.¹⁸⁵ on the CD₂OO UV spectrum, and Chhantyal-Pun et al.⁴⁴ on the reactions of (CD₃)₂COO with SO₂ and NO₂. These latter authors also see a significant reduction in hydroxyacetone yield from (CD₃)₂COO, which suggests an important slow-down of the VHP channel upon deuteration, in agreement with our results. Earlier observation on OH:OD product yield ratios by Kroll et al.¹⁸⁶ led to the conclusion that the acid channel was not affected significantly by deuteration, though later theoretical work by Kuwata et al.¹³⁴ suggested that at least part of the OD radicals observed by Kroll et al. originate in secondary chemistry of the vinoxy radical product.

R. Structure-Activity Relationship (SAR) for unimolecular SCI reactions

1. Temperature-dependent rate predictions for 98 classes of Criegee intermediates

From the theoretical sections above, we conclude that carbonyl oxide stereoisomers should be considered separate species, and that the main loss process is 1,4-H- or 1,6-H-migration forming trans-VHP. If no suitable H-atom is available for migration, 1,3-ring closure and 1,5-ring closure (for β -unsaturated compounds) become the dominant channels; examples include H-, tC_4H_9 -, and $CH=CH_2$ substituents in CI *syn*-position, as well as some cyclic structures such as nopinone oxide. In all cases studied here only one unimolecular reaction is competitive (>90% of the reaction flux), and the total rate coefficient can be equated to that of this dominant pathway. Table 31 summarizes the proposed unimolecular loss rate coefficients as a function of the two CI substituents, selecting the fastest loss channel in each case. For reaction classes for which no direct theoretical information is available, average reactivity trends are extrapolated across R_2 substituents; substituents in this stereo-position have the least impact on the reaction rates and as such don't require extrapolation across too large a rate coefficient range.

2. Examples of converting a CI structure to a SAR CI class

Determining which Criegee intermediates are formed from the ozonolysis, and what CI class this belongs to in the structure activity relationships is done by the following procedure:

- For each double bond, write out the four possible stereo-specific CI structures
- Find the most appropriate R_1 (*syn*-side) and R_2 (*anti*-side) class in the left-hand column and top row of the SAR tables, respectively. Especially for the unsaturated CI, one must pay particular care to the presence or absence of migratable H-atoms, the order (prim. sec. or tert.) of these H-atoms, if present, and the stereo-specific substitution on the unsaturated bonds.
- The intersection of the corresponding row and column lists the rate coefficient at 298K, and the parameters of the Kooij expression for $k(T)$.

Figure 11 and Figure 12 show two examples, one for a substituted alkene, and one for a larger polyunsaturated compound with three double bonds.

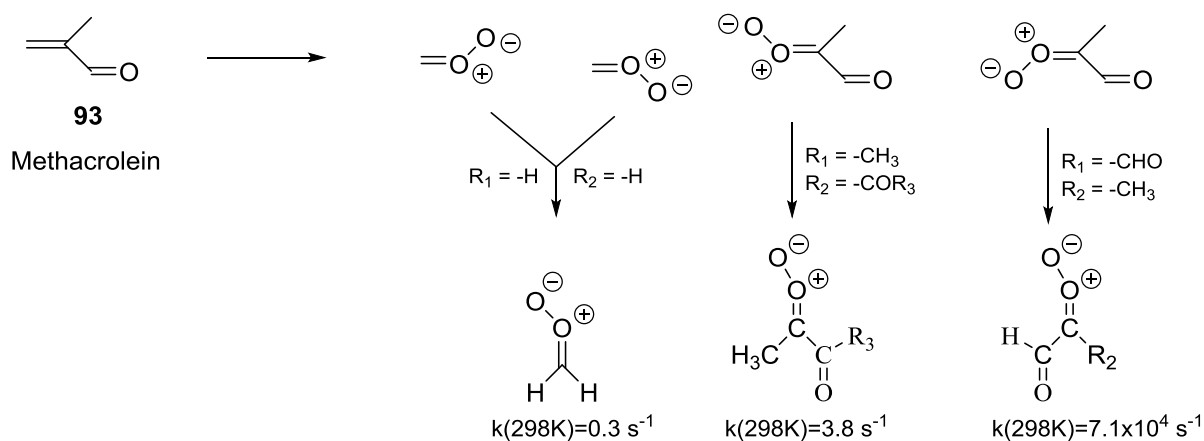


Figure 11: Ozonolysis of methacrolein, CI formed in this reaction, determination of the SAR CI class, and the corresponding rate coefficient for SCI unimolecular decay.

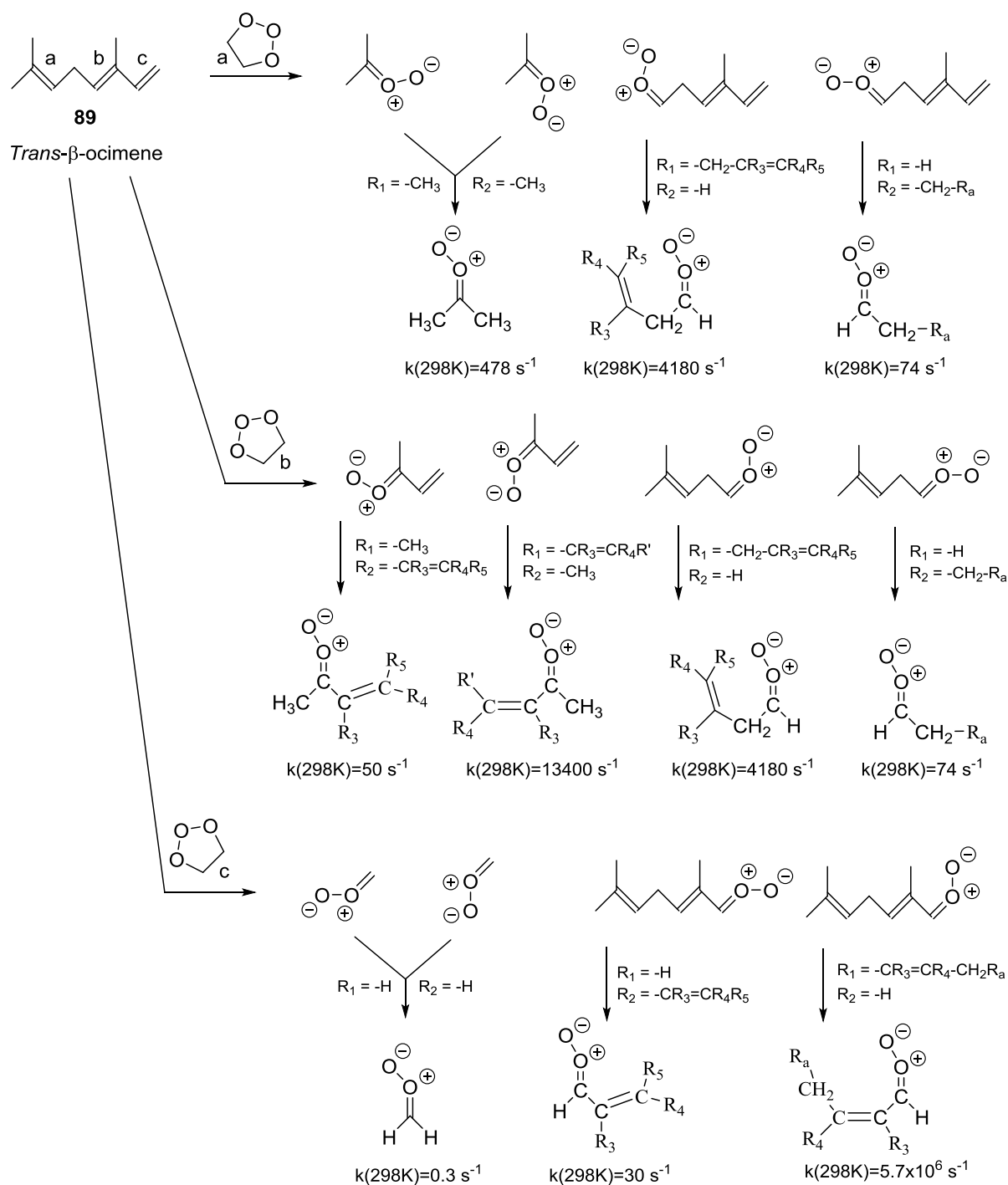


Figure 12: Ozonolysis of β -ocimene, CI formed in reaction on each of its double bonds, determination of the SAR CI class, and the corresponding rate coefficient for SCI unimolecular decay.

3. Handling substituents that are not included in the SAR table

The terpenoids which comprise the bulk of the organic matter emitted to the troposphere are often polyunsaturated; their ozonolysis forms oxygenated products that still retain one or more double bonds which in turn could be attacked by O_3 , forming CI again. Typical examples of such oxygenated products are methyl vinyl ketone (MVK) and methacrolein (MACR) formed in the isoprene oxidation initiated by O_3 , OH and other oxidants. Furthermore, the typical degradation processes in the atmosphere through RO_2 and RO radicals leads to alcohols, nitrate, peroxide, and other heterosubstituted functionalities. A wide variety of heterosubstituted unsaturated compounds are also emitted to the atmosphere, though in lesser concentration than pure hydrocarbons. Such compounds need to be addressed in chemical models, but are outside the scope of our SAR development at this time. In this section, we summarize relevant data from literature, supplemented with some targeted calculations on their unimolecular and bimolecular reactions.

a. -OH and -OR substitution

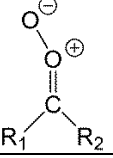
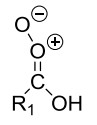
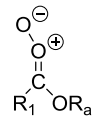
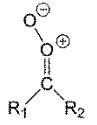
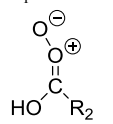
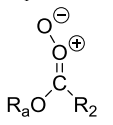
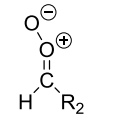
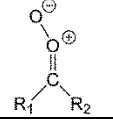
OH-substitution on the carbonyl oxide carbon atom of CH_2OO leads to very fast degradation reactions, where Selçuki and Aviyente^{120,146} predicted that CI with $R_2 = -OH$ (in *anti* position to the oxide O-atom) have barriers for 1,3-cyclisation forming dioxiranes of less than 10 kcal mol⁻¹. Note that these authors make separate predictions for different internal orientations of the OH moiety, but have not examined the -OH internal rotation. At the CCSD(T)//M06-2X level of theory, we find even lower energy barriers for cyclisation (see Table 28), while 1,3-H-migration, 1,4-H-migration, and stereoisomerisation are not competitive. Internal rotation of the OH moiety is fast, allowing access to the lowest TS from all rotamers. Both Selçuki and Aviyente, and this work, finds that *Z*-(OH)CHOO is unstable, with a barrierless 1,4-H-shift to formic peracid, $HC(=O)OOH$. Our calculations also find a similar barrierless isomerisation for *Z*-(OH)(CH₃)COO to peracetic acid; we generalize this and propose that all *syn*-OH-CI are unstable to peracid formation. Calculations on the stereoisomerisation TS for OH-substituted CI show very high multi-reference character (T1 diagnostic = 0.109) and are not reliable at our chosen level of theory.

α -OCH₃-substitution on the carbonyl oxide is reported by Selçuki and Aviyente¹²⁰ to significantly lower the 1,3-ring closure barrier compared to alkyl substituents, with a barrier of ~12.5 kcal mol⁻¹ if $R_1 = -OCH_3$, and 8.0 kcal mol⁻¹ if $R_2 = -OCH_3$, where again we allow for fast internal rotation along the single bonds. We propose at this time that *anti*-OH-, and both *anti*- and *syn*-OR-substituted CI undergo fast 1,3-ring closure reactions. For OR-substituted CI, we estimate the rate coefficients relative to alkyl-substituted CI, using the relative barrier heights reported by Selçuki and Aviyente.¹²⁰ Given the rapid unimolecular isomerisation, competition of bimolecular reactions are of lesser importance. The resulting simplified SAR is summarized in Table 29.

Table 28: Unimolecular reactions of hydroxyl-substituted CI, listing barrier heights E_b (kcal mol⁻¹), rate coefficient k (s⁻¹) at 298 K, and parameters for a Kooij equation fit $k(T)=A \times T^n \times \exp(-E_a/T)$ for the temperature range 200-450 K.

Carbonyl oxide	Reaction	E_b	$k(298K)$	A / s^{-1}	n	E_a / K
<i>E</i> -(OH)CHOO	1,3-ring closure	7.1	6.1×10^7	2.06×10^{12}	0.25	3530
	1,3-H-migration	21.4	0.25	3.13×10^{-91}	33.91	-4116
	Stereoisomerisation	34.1	1.5×10^{-12}	3.08×10^{10}	1.04	17077
	OH Internal rotation	8.2	2.5×10^7	4.29×10^{10}	0.98	3883
<i>Z</i> -(OH)CHOO	1,4-H-migration	0.00	Barrierless isomerisation to $HC(O)OOH$			
<i>E</i> -(CH ₃)(OH)COO	1,3-ring closure	11.3	4.5×10^4	8.54×10^{11}	0.37	5618
	1,4-H-migration	16.0	2.8×10^2	6.08×10^{-59}	23.30	-2074
	Stereoisomerisation	≥ 40	$< 10^{-10}$			
	OH Internal rotation	8.9	8.2×10^6	3.72×10^{10}	1.02	4247
<i>Z</i> -(OH)(CH ₃)COO	1,4-H-migration	0.00	Barrierless isomerisation to $CH_3C(O)OOH$			

Table 29: Predicted total rate coefficients for unimolecular carbonyl oxide decay as a function of the two substituents R_1 and R_2 . Indicated is the mode of reaction, the rate coefficient k (s^{-1}) at 298K, and the parameters of a Kooij equation fit $k(T) = A \times T^n \times \exp(-E_a/T)$ between 200 and 450 K (A in s^{-1} , E_a in K). The SAR substituent notation is defined in section C. Values in green are based directly on theoretical kinetic calculations, whereas values in orange are estimated from the reactivity trends for other substituents.

	$R_2 = -OH$ 	$R_2 = -OR$ 	$R_2 \neq OH/OR$ 
$R_1 = -OH$ 	Barrierless rearrangement to peracid	Barrierless rearrangement to peracid	Barrierless rearrangement to peracid
$R_1 = -OR$ 	No data available	No data available	1,3-Cyclisation $k(298K) = 2.5 \times 10^4$ $A = 1.81 \times 10^4$ $n = 2.98$ $E_a = 4968$
$R_1 = -H$ 	1,3-Cyclisation $k(298K) = 6.1 \times 10^7$ $A = 2.06 \times 10^{12}$ $n = 0.25$ $E_a = 3530$	1,3-Cyclisation $k(298K) = 8.2 \times 10^8$ $A = 1.57 \times 10^{10}$ $n = 1.03$ $E_a = 2633$	See Table 31
$R_1 \neq OH/OR/H$ 	1,3-Cyclisation $k(298K) = 4.6 \times 10^4$ $A = 8.54 \times 10^{11}$ $n = 0.37$ $E_a = 5618$	1,3-Cyclisation $k(298K) = 7.0 \times 10^4$ $A = 3.84 \times 10^9$ $n = 1.21$ $E_a = 5309$	See Table 31

b. Cyclic structures

For α - and β -pinene derived CI, rate coefficients for unimolecular decay and reaction with water are available in this work. We concluded that the impact of cyclic structures often was not very large, unless the carbonyl oxide moiety was implanted directly on the cycle. For most cyclic compounds, then, we propose to treat these as their non-cyclic equivalents, taking care to maintain the same number and type of substituents and migratable H-atoms. This may require duplicating parts of the molecule, i.e. simply "opening" the ring could change the nature of the reaction compared to reaction type found by for the molecular graph of the closed structure. Instead, one must ensure that the double bond studied has the same number and orientation of alkyl substituents up to a distance of 2 bonds (3 if unsaturated) in the molecular graph. For each double bond in the molecule, the following procedure is followed:

Step 1: draw a C=C double bond

Step 2: Attach the same number of C-atoms to each carbon of the double bond as in the cyclic molecule, with the same bond order (single/double bond). Do not close any cycles, but rather duplicate atoms as needed.

Step 3: To each of the carbon atoms added in step 2, add the same number of C-atoms as in the cyclic molecule, with the same bond order (single/double bond). Do not close any cycles, but rather duplicate atoms as needed.

Step 4: If any of the carbons in the cyclic molecule added in step 3 is unsaturated, add the needed carbons to this carbon to achieve the same bond orders. Do not close any cycles, but rather duplicate atoms as needed.

Step 5: Terminate any dangling bonds with H-atoms.

For heteroatoms, the same procedure is followed. Figure 13 depicts several examples of this procedure, showing for each double bond the simplest non-cyclic structure that retains all properties of the cyclic structure, as far as the SAR CI classes are concerned of the SCI generated after ozonolysis.

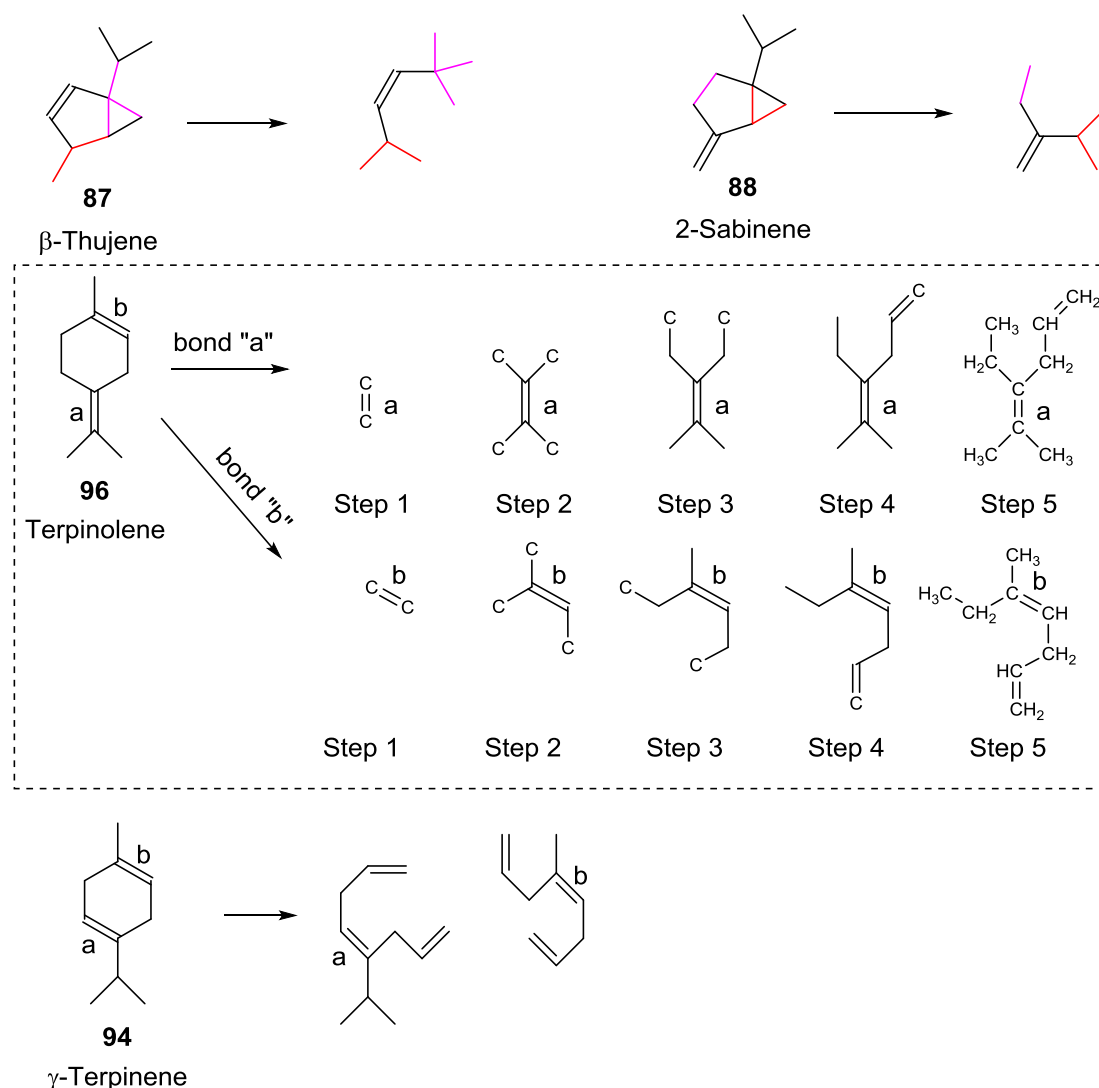


Figure 13: Examples of decyclisation of cyclic terpenes, showing the smallest structure that yields the same SAR SCI reaction class as the parent molecule. For poly-unsaturated structures, each double bond must be treated separately. The topmost examples use color in a simple case to help with the comparison between source molecule and decyclized molecule. For a more elaborate example in the dashed box, each step in the procedure, for each double bond, is given. The bottom example gives the end-result for a complex case with two double bonds in a doubly-unsaturated ring.

c. Other functionalities

The global model contains a few additional functionalities not considered in this work (see Figure 28). These compounds are not critical to the CI concentration in the atmosphere, and we apply the SAR rate coefficients for the corresponding hydrocarbon-substituted CI obtained by replacing hetero-atoms by alkyl groups, as indicated in Table 30.

Table 30: Substituent equivalences used in the global model. Substituent notation is defined in section C.

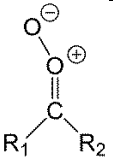
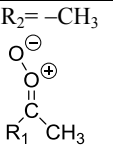
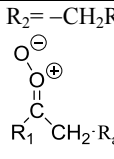
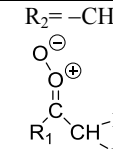
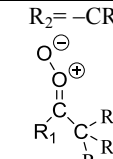
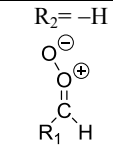
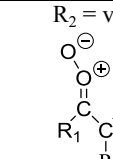
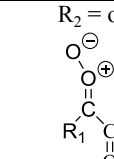
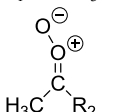
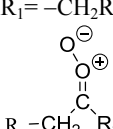
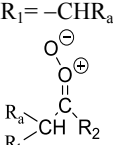
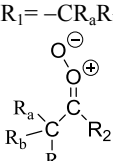
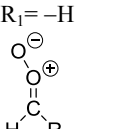
Substituent moiety R_1 / R_2	Treated as SAR substituent
$-\text{CH}_2\text{OH}$	$-\text{CH}_2(\text{R}_a)$
$-\text{C}(\text{CH}_3)_2\text{OH}$	$-\text{C}(\text{R}_a)(\text{R}_b)(\text{R}_c)$
$-\text{CH}_2\text{OR}_3$	$-\text{CH}_2(\text{R}_a)$
$-\text{CH}(\text{CH}_3)\text{OR}_3$	$-\text{CH}(\text{R}_a)(\text{R}_b)$
$-\text{CH}_2\text{OOH}$	$-\text{CH}_2(\text{R}_a)$
$-\text{CH}(\text{OOH})(\text{CH}_2\text{OH})$	$-\text{CH}(\text{R}_a)(\text{R}_b)$
$-\text{C}(\text{R}_a)(\text{OOH})(\text{CH}_2\text{OH})$	$-\text{C}(\text{R}_a)(\text{R}_b)(\text{R}_c)$
$-\text{CH}_2(\text{ONO}_2)$	$-\text{CH}_2(\text{R}_a)$
$-\text{C}(\text{R}_a)(\text{ONO}_2)(\text{OOR}_b)$	$-\text{C}(\text{R}_a)(\text{R}_b)(\text{R}_c)$
$-\text{C}(=\text{O})\text{CH}_2\text{OH}$	$-\text{C}(=\text{O})\text{R}_3$
$-\text{C}(=\text{O})\text{OR}_a$	$-\text{C}(=\text{O})\text{R}_3$
$\begin{array}{c} \text{O} \\ \\ -\text{C}-\text{C}-\text{R}_a \text{ (epoxide)} \\ \quad \\ \text{H} \quad \text{H} \end{array}$	$-\text{CH}(\text{R}_a)(\text{R}_b)$
$-\text{C}_6\text{H}_5$ (phenyl)	$-\text{C}(\text{R}_a)(\text{R}_b)(\text{R}_c)$ Here, it is assumed that 1,5-ring closure onto a double bond in the aromatic ring is geometrically and energetically unfavorable, leaving 1,3-ring closure as the main channel

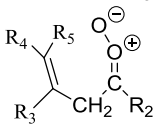
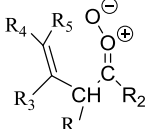
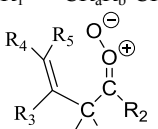
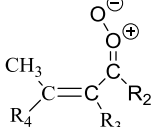
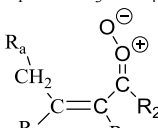
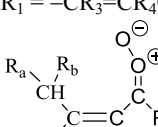
4. Uncertainty analysis

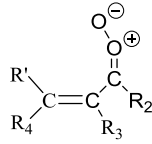
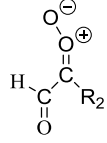
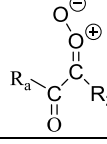
The largest uncertainty on the rate predictions included in the SAR originates in the estimation of the barrier height. The reference rate coefficients from literature upon which we based our correction scheme vary by a factor of 2, and only a handful of rate coefficients are characterized with reasonable accuracy. The level of quantum chemical theory employed in this work, i.e. CCSD(T)/M06-2X + empirical corrections, should predict the reaction barrier heights reasonably well, within chemical accuracy. Even then, the barrier heights carry an uncertainty of at least a few tenths of a kcal mol⁻¹, which at room temperature corresponds to a factor of 2 to 3 on the rate coefficient. For the H-migration reactions, tunneling corrections also have a large impact on the predicted rate coefficient, and the underlying methodology is a 1-dimensional correction building on arbitrarily fixed reaction exoergicities for each type of reaction. Hence, an uncertainty of a factor of 2 on the tunneling correction (which itself is typically on the order of $\times 10^2$) should be assumed, which covers the uncertainties of reaction exoergicity, corner cutting, etc. The combined uncertainty on the predicted rate coefficients is thus estimated at a factor of 5 at room temperature, or ± 1 kcal mol⁻¹ ($\pm 500\text{K}$) on the effective activation energy E_a in temperature-dependent expressions. Exploratory calculations on the length of the substituent alkyl chain, from C₂H₅ to *n*-C₃H₇, show an impact of a factor of ~ 2 , such that as a first estimate we can generalize the reactivity trends to most substituents relevant in the atmosphere within the aforementioned uncertainties. Even for cyclic substituents, the prediction will typically remain applicable (see section Q.1) though for strained cycles larger variations of up to an order of magnitude are to be expected.

The resulting combined uncertainty interval is about an order of magnitude, which is large compared to that of high-quality experimental measurements. For many assessments, however, it is sufficient to determine whether the reaction is significantly faster or slower than competing reactions. In many cases, and especially in atmospheric conditions, the SAR in Table 31 will thus allow for a sufficiently accurate kinetic model. More absolute and relative rate measurements or high-level theoretical predictions are needed to improve on the accuracy of the predictions, though when such reference data become available it is comparatively easy to re-evaluate the corrections used in the SAR development to improve the values. Unfortunately, we have not identified any compounds that have a balanced competition between unimolecular channels; an experimental study of such a system would have enabled a more targeted analysis of the relative uncertainty of the predictions through product analysis.

Table 31: Predicted total rate coefficients for unimolecular carbonyl oxide decay as a function of the two substituents R_1 and R_2 . Indicated is the mode of reaction, the rate coefficient k (s^{-1}) at 298K, and the parameters of a Kooij equation fit $k(T) = A \times T^n \times \exp(-E_a/T)$ between 200 and 450 K (A in s^{-1} , E_a in K). The meaning of the SAR substituents is explained in section C. Note that the theoretical work here does not consider systematic variations for $R_a/R_b/R_c/R_3/R_4/R_5/R'$, and the values listed are for substituents $-H$ (when appropriate), $-CH_3$, $-C_2H_5$, or an average of the prediction for these substituents. Values in green are based directly on theoretical kinetic calculations, whereas values in orange are estimated values based on the reactivity trends for other substituents. The values are standardized in number of digits, see section R.4 for an uncertainty analysis.

	$R_2 = -CH_3$ 	$R_2 = -CH_2R_a$ 	$R_2 = -CHRaR_b$ 	$R_2 = -CRaRbRc$ 	$R_2 = -H$ 	$R_2 = \text{vinyl}$ 	$R_2 = \text{oxo}$ 
$R_1 = -CH_3$ 	1,4-H-migration $k(298K)=478$ $A = 7.64 \times 10^{-60}$ $n = 23.59$ $E_a = -2367$	1,4-H-migration $k(298K)=433$ $A = 8.63 \times 10^{-61}$ $n = 23.94$ $E_a = -2390$	1,4-H-migration $k(298K)=611$ $A = 4.18 \times 10^{-59}$ $n = 23.38$ $E_a = -2276$	1,4-H-migration $k(298K)=373$ $A = 9.26 \times 10^{-61}$ $n = 23.92$ $E_a = -2362$	1,4-H-migration $k(298K)=136$ $A = 3.11 \times 10^{-64}$ $n = 24.95$ $E_a = -2685$	1,4-H-migration $k(298K)=50$ $A = 4.36 \times 10^{-67}$ $n = 25.90$ $E_a = -2737$	1,4-H-migration $k(298K)=3.8$ $A = 7.31 \times 10^{-80}$ $n = 30.08$ $E_a = -3644$
$R_1 = -CH_2R_a$ 	1,4-H-migration $k(298K)=689$ $A = 5.91 \times 10^{-58}$ $n = 22.91$ $E_a = -2331$	1,4-H-migration $k(298K)=534$ $A = 4.72 \times 10^{-59}$ $n = 23.29$ $E_a = -2358$	1,4-H-migration $k(298K)=257$ $A = 4.83 \times 10^{-61}$ $n = 23.93$ $E_a = -2420$	1,4-H-migration $k(298K)=12$ $A = 2.13 \times 10^{-74}$ $n = 28.47$ $E_a = -2964$	1,4-H-migration $k(298K)=205$ $A = 2.41 \times 10^{-62}$ $n = 24.33$ $E_a = -2571$	1,4-H-migration $k(298K)=39$ $A = 1.42 \times 10^{-66}$ $n = 25.62$ $E_a = -2780$	1,4-H-migration $k(298K)=3.0$ $A = 2.38 \times 10^{-79}$ $n = 29.80$ $E_a = -3686$
$R_1 = -CHRaR_b$ 	1,4-H-migration $k(298K)=14$ $A = 4.45 \times 10^{-76}$ $n = 27.97$ $E_a = -2967$	1,4-H-migration $k(298K)=13$ $A = 8.54 \times 10^{-73}$ $n = 27.89$ $E_a = -2858$	1,4-H-migration $k(298K)=19$ $A = 1.62 \times 10^{-70}$ $n = 27.01$ $E_a = -2912$	1,4-H-migration $k(298K)=1$ $A = 8.80 \times 10^{-81}$ $n = 30.47$ $E_a = -3249$	1,4-H-migration $k(298K)=6.7$ $A = 8.54 \times 10^{-63}$ $n = 24.47$ $E_a = -2490$	1,4-H-migration $k(298K)=1.2$ $A = 2.55 \times 10^{-80}$ $n = 30.21$ $E_a = -3387$	1,4-H-migration $k(298K)=0.09$ $A = 4.28 \times 10^{-93}$ $n = 34.39$ $E_a = -4294$
$R_1 = -CRaRbRc$ 	1,3-Cyclisation $k(298K)=0.17$ $A = 2.55 \times 10^{10}$ $n = 1.02$ $E_a = 9399$	1,3-Cyclisation $k(298K)=0.15$ $A = 5.45 \times 10^{11}$ $n = 0.55$ $E_a = 9555$	1,3-Cyclisation $k(298K)=1.1$ $A = 6.83 \times 10^{10}$ $n = 0.80$ $E_a = 8759$	1,3-Cyclisation $k(298K)=0.075$ $A = 1.12 \times 10^{11}$ $n = 0.85$ $E_a = 9795$	1,3-Cyclisation $k(298K)=1 \times 10^{-2}$ $A = 2.58 \times 10^6$ $n = 2.32$ $E_a = 9710$	1,3-Cyclisation $k(298K)=0.13$ $A = 3.76 \times 10^7$ $n = 1.87$ $E_a = 8977$	1,3-Cyclisation $k(298K)=1.6 \times 10^{-4}$ $A = 1.92 \times 10^2$ $n = 3.63$ $E_a = 10331$
$R_1 = -H$ 	1,3-Cyclisation $k(298K)=53$ $A = 1.69 \times 10^9$ $n = 1.35$ $E_a = 7445$	1,3-Cyclisation $k(298K)=74$ $A = 1.57 \times 10^{10}$ $n = 1.03$ $E_a = 7464$	1,3-Cyclisation $k(298K)=102$ $A = 9.22 \times 10^9$ $n = 1.13$ $E_a = 7387$	1,3-Cyclisation $k(298K)=111$ $A = 8.51 \times 10^9$ $n = 1.15$ $E_a = 7357$	1,3-Cyclisation $k(298K)=0.3$ $A = 1.66 \times 10^1$ $n = 4.02$ $E_a = 8024$	1,3-Cyclisation $k(298K)=30$ $A = 1.68 \times 10^{10}$ $n = 1.02$ $E_a = 7732$	1,3-Cyclisation $k(298K)=0.037$ $A = 8.58 \times 10^4$ $n = 2.78$ $E_a = 9085$

$R_1 = -CH_2-CR_3=CR_4R_5$ 	Allyl-1,4-Hmig. k(298K)=14100 $A = 9.00 \times 10^{-42}$ $n = 17.45$ $E_a = -1390$	Allyl-1,4-Hmig. k(298K)=10900 $A = 7.18 \times 10^{-43}$ $n = 17.83$ $E_a = -1417$	Allyl-1,4-Hmig. k(298K)=5250 $A = 7.35 \times 10^{-45}$ $n = 18.47$ $E_a = -1479$	Allyl-1,4-Hmig. k(298K)=247 $A = 3.24 \times 10^{-58}$ $n = 23.01$ $E_a = -2023$	Allyl-1,4-Hmig. k(298K)=4180 $A = 3.66 \times 10^{-46}$ $n = 18.87$ $E_a = -1630$	Allyl-1,4-Hmig. k(298K)=795 $A = 2.16 \times 10^{-50}$ $n = 20.16$ $E_a = -1839$	Allyl-1,4-Hmig. k(298K)=61 $A = 3.63 \times 10^{-63}$ $n = 24.35$ $E_a = -2746$
$R_1 = -CHR_a-CR_3=CR_4R_5$ 	Allyl-1,4-Hmig. k(298K)=493 $A = 2.60 \times 10^{-55}$ $n = 21.92$ $E_a = -2087$	Allyl-1,4-Hmig. k(298K)=433 $A = 4.99 \times 10^{-55}$ $n = 21.85$ $E_a = -1978$	Allyl-1,4-Hmig. k(298K)=649 $A = 9.47 \times 10^{-53}$ $n = 20.97$ $E_a = -2032$	Allyl-1,4-Hmig. k(298K)=38 $A = 5.14 \times 10^{-63}$ $n = 24.42$ $E_a = -2369$	Allyl-1,4-Hmig. k(298K)=23 $A = 8.89 \times 10^{-58}$ $n = 22.68$ $E_a = -2269$	Allyl-1,4-Hmig. k(298K)=40 $A = 1.49 \times 10^{-62}$ $n = 24.16$ $E_a = -2507$	Allyl-1,4-Hmig. k(298K)=3.1 $A = 2.50 \times 10^{-75}$ $n = 28.34$ $E_a = -3413$
$R_1 = -CR_aR_b-CR_3=CR_4R_5$ 	1,3-Cyclisation k(298K)=0.23 $A = 9.73 \times 10^{10}$ $n = 0.79$ $E_a = 9314$	1,3-Cyclisation k(298K)=0.20 $A = 2.08 \times 10^{12}$ $n = 0.32$ $E_a = 9471$	1,3-Cyclisation k(298K)=1.5 $A = 2.61 \times 10^{11}$ $n = 0.57$ $E_a = 8674$	1,3-Cyclisation k(298K)=0.10 $A = 4.27 \times 10^{11}$ $n = 0.62$ $E_a = 9711$	1,3-Cyclisation k(298K)=0.013 $A = 9.87 \times 10^6$ $n = 2.09$ $E_a = 9625$	1,3-Cyclisation k(298K)=0.17 $A = 1.44 \times 10^8$ $n = 1.63$ $E_a = 8893$	1,3-Cyclisation k(298K)=2.1 × 10⁻⁴ $A = 7.32 \times 10^2$ $n = 3.39$ $E_a = 10246$
$R_1 = -(CR_3=CR_4CH_3)$ 	Allyl-1,6-Hmig. k(298K)=1.4 × 10⁷ $A = 1.30 \times 10^{-5}$ $n = 5.52$ $E_a = 1106$	Allyl-1,6-Hmig. k(298K)=1.2 × 10⁷ $A = 2.63 \times 10^{-6}$ $n = 5.77$ $E_a = 1117$	Allyl-1,6-Hmig. k(298K)=1.4 × 10⁷ $A = 2.31 \times 10^{-5}$ $n = 5.42$ $E_a = 1131$	Allyl-1,6-Hmig. k(298K)=4.7 × 10⁶ $A = 5.83 \times 10^{-8}$ $n = 6.24$ $E_a = 1063$	Allyl-1,6-Hmig. k(298K)=4.8 × 10⁶ $A = 1.40 \times 10^{-9}$ $n = 6.77$ $E_a = 838$	Allyl-1,6-Hmig. k(298K)=1.7 × 10⁶ $A = 2.79 \times 10^{-12}$ $n = 7.67$ $E_a = 807$	Allyl-1,6-Hmig. k(298K)=1.3 × 10⁵ $A = 3.29 \times 10^{-25}$ $n = 11.90$ $E_a = -121$
$R_1 = -CR_3=CR_4CH_2R_a$ 	Allyl-1,6-Hmig. k(298K)=1.7 × 10⁷ $A = 1.03 \times 10^{-4}$ $n = 5.22$ $E_a = 1163$	Allyl-1,6-Hmig. k(298K)=1.5 × 10⁷ $A = 2.07 \times 10^{-5}$ $n = 5.48$ $E_a = 1174$	Allyl-1,6-Hmig. k(298K)=1.6 × 10⁷ $A = 1.82 \times 10^{-4}$ $n = 5.12$ $E_a = 1188$	Allyl-1,6-Hmig. k(298K)=5.6 × 10⁶ $A = 4.60 \times 10^{-7}$ $n = 5.95$ $E_a = 1120$	Allyl-1,6-Hmig. k(298K)=5.7 × 10⁶ $A = 1.57 \times 10^{-8}$ $n = 6.42$ $E_a = 917$	Allyl-1,6-Hmig. k(298K)=2.1 × 10⁶ $A = 2.20 \times 10^{-11}$ $n = 7.37$ $E_a = 864$	Allyl-1,6-Hmig. k(298K)=1.6 × 10⁵ $A = 3.69 \times 10^{-24}$ $n = 11.55$ $E_a = -42$
$R_1 = -CR_3=CR_4CHRaR_b$ 	Allyl-1,6-Hmig. k(298K)=6.1 × 10⁶ $A = 9.92 \times 10^{-6}$ $n = 5.62$ $E_a = 1456$	Allyl-1,6-Hmig. k(298K)=5.2 × 10⁶ $A = 2.00 \times 10^{-6}$ $n = 5.88$ $E_a = 1467$	Allyl-1,6-Hmig. k(298K)=5.8 × 10⁶ $A = 1.76 \times 10^{-5}$ $n = 5.53$ $E_a = 1481$	Allyl-1,6-Hmig. k(298K)=2.0 × 10⁶ $A = 4.44 \times 10^{-8}$ $n = 6.35$ $E_a = 1413$	Allyl-1,6-Hmig. k(298K)=2.0 × 10⁶ $A = 1.51 \times 10^{-9}$ $n = 6.83$ $E_a = 1210$	Allyl-1,6-Hmig. k(298K)=7.4 × 10⁵ $A = 2.13 \times 10^{-12}$ $n = 7.77$ $E_a = 1157$	Allyl-1,6-Hmig. k(298K)=5.7 × 10⁴ $A = 3.56 \times 10^{-25}$ $n = 11.95$ $E_a = 251$

$R_1 = -CR_3=CR_4R'$ 	1,5-Cyclisation k(298K)=13400 $A=9.75 \times 10^9$ $n=1.03$ $E_a=5081$	1,5-Cyclisation k(298K)=13400 $A=9.75 \times 10^9$ $n=1.03$ $E_a=5081$	1,5-Cyclisation k(298K)=13400 $A=9.75 \times 10^9$ $n=1.03$ $E_a=5081$	1,5-Cyclisation k(298K)=13400 $A=9.75 \times 10^9$ $n=1.03$ $E_a=5081$	1,5-Cyclisation k(298K)=14300 $A=2.58 \times 10^9$ $n=0.87$ $E_a=5090$	1,5-Cyclisation k(298K)=13400 $A=9.75 \times 10^9$ $n=1.03$ $E_a=5081$	1,5-Cyclisation k(298K)=13400 $A=9.75 \times 10^9$ $n=1.03$ $E_a=5081$
$R_1 = -CHO$ 	1,3-Cyclisation k(298K)= 7.1×10⁴ $A=2.76 \times 10^{10}$ $n=0.78$ $E_a=5162$	1,3-Cyclisation k(298K)= 5.3×10⁴ $A=2.01 \times 10^{10}$ $n=0.82$ $E_a=5212$	1,3-Cyclisation k(298K)= 1.3×10⁵ $A=7.28 \times 10^6$ $n=1.84$ $E_a=4329$	1,3-Cyclisation k(298K)= 8.0×10³ $A=2.95 \times 10^6$ $n=1.96$ $E_a=5099$	1,3-Cyclisation k(298K)= 144 $A=2.49 \times 10^6$ $n=2.21$ $E_a=6656$	1,3-Cyclisation k(298K)= 2.5×10⁴ $A=2.33 \times 10^{10}$ $n=0.71$ $E_a=5303$	1,3-Cyclisation k(298K)= 30 $A=4.06 \times 10^4$ $n=2.70$ $E_a=6730$
$R_1 = -C(O)R_a$ 	1,3-Cyclisation k(298K)= 1.6×10⁴ $A=3.95 \times 10^9$ $n=1.02$ $E_a=5448$	1,3-Cyclisation k(298K)= 1.1×10⁴ $A=2.86 \times 10^9$ $n=1.05$ $E_a=5489$	1,3-Cyclisation k(298K)= 2.7×10⁴ $A=1.50 \times 10^6$ $n=2.02$ $E_a=4620$	1,3-Cyclisation k(298K)= 1.6×10³ $A=1.29 \times 10^5$ $n=2.36$ $E_a=5315$	1,3-Cyclisation k(298K)= 20 $A=5.55 \times 10^5$ $n=2.41$ $E_a=7141$	1,3-Cyclisation k(298K)= 5.2×10³ $A=2.25 \times 10^9$ $n=1.00$ $E_a=5560$	1,3-Cyclisation k(298K)= 6.3 $A=3.92 \times 10^3$ $n=2.99$ $E_a=6987$

S. The reaction of CI with H₂O

1. Literature data

In the atmosphere, the reaction of stabilized CI with water is a major loss process, and was until recently even considered the sole fate of atmospheric thermalized CI. Extensive experimental and theoretical data as a function of the CI substitution is tabulated in Table 4. The predicted rate coefficients are strongly dependent on the SCI substitution, spanning almost 5 orders of magnitude, though the reaction with the water dimer often is faster than the monomer (see section T). The reaction of CI with larger water clusters, (H₂O)_n with $n \geq 3$, has also been studied theoretically.^{26,71,187} The rate of all these reactions is slower or comparable to that of the H₂O or (H₂O)₂ reaction; considering the significantly lower atmospheric concentration of these clusters, the consensus is that these reactions are not relevant for the atmosphere. The reaction of H₂COO with the water analogue H₂S was also studied,^{188,189} compared to the H₂O reaction its reaction barrier is lower by several kcal mol⁻¹, and a rate coefficient was measured as $k(298\text{K}) = (1.7 \pm 0.2) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, independent of pressure. As the concentration of H₂S in the atmosphere is less than 1 ppm even near point sources, this implies pseudo-first order rate coefficients less than 5 s⁻¹. We neglect this reaction in our current analysis.

The products of the CI + (H₂O)_n ($n \geq 1$) reaction are α -hydroxy-alkylhydroperoxides (HOOC(OH)R₁R₂; HAHP), formed by insertion of carbonyl oxide moiety in the water O–H bond, though theoretical work has shown^{37–40,64} that water also catalyzes unimolecular H-migration reactions, potentially increasing the yield of VHP and OH radicals. The reaction rates of these latter channels, however, remain below those for HAHP formation, such that these channels are likely not the source of the OH yield observed^{190–192} for some ozonolysis systems upon increasing the relative humidity. The fate of the HAHP products, observed in the troposphere with concentrations as high as 5 ppb, has been studied^{26,38,89,193,194} but is not discussed in more detail here.

2. Structure-Activity Relationship (SAR) for the CI + H₂O, based on literature data

The scarce experimental data on H₂COO, *Z/E*-CH₃CHOO, (CH₃)₂COO, and a handful of other compounds is not sufficient to cover the range of CI formed in the atmosphere. Combined with the available theoretical data, however, one can obtain a fairly accurate view of the temperature-dependent reactivity of CI towards water as a function of their substitution, even if no direct data is available for many of the CI classes considered in this work.

In this section, we will develop a Structure-Activity Relationship estimating the temperature-dependent rate coefficients for the reactions of CI with H₂O, drawing solely on the literature experimental and theoretical rate data. Due to the dearth of data, these estimations carry a high uncertainty, up to several orders of magnitude for many of the entries. A specific source of uncertainty is that these estimates do not incorporate the relative stability of the Criegee intermediates, and the impact it has on the rate coefficient. Unfortunately, the literature does not carry enough information to apply such reaction trends to the CI + H₂O reaction, and care is recommended when applying the SAR. The SAR is developed mainly to serve as a reference for further developments (see below), and represents a rather conservative view on the CI + H₂O reaction.

The available literature data listed in Table 4 (see section E.2) needs to be harmonized across the different studies. The only rate coefficient on which there is currently consensus is the reaction of *E*-CH₃CHOO + H₂O. We will treat this as our golden standard. It is clear from the available data that even very-high level theoretical methodologies struggle to reproduce this reference reaction, owing to the complexities in treating these reactions *a priori*. This includes difficulties in obtaining an accurate potential energy surface by quantum chemical calculations (where post-CCSD(T) methods are a necessity), the treatment of the flexible H-bonded pre-reactive complexes, the impact of tunneling, etc. For our current purposes, we will therefore select the highest-quality theoretical data only, and adjust the theoretical predictions to match the available experimental data as well as possible.

An additional difficulty is that β -unsaturated CI (i.e. with a $-\text{CR}_3=\text{CR}_4\text{R}_5$ substituent) have been treated in theoretical work^{1,38,61} for specific orientations of the conjugated system separately, i.e. the rapid interconversion of *s-trans* and *s-cis* structures by internal rotation of the central single bond of the conjugated system (see section G, and literature data^{3,15}) has not been taken into account. The resulting rate coefficients are thus not representative of the equilibrium population of these CI. Rather than simply equating the rate coefficient to one of the listed rate coefficients, we can estimate the overall rate coefficient of the equilibrated population using (conformer-specific) partition functions $Q(T)$ for the CI reactants derived from our own rovibrational data. This approximation retains as much of the detailed analysis for the TS as possible, such as variational effects and tunneling κ . Following multi-conformer TST formalism,^{160,195} assuming for notational simplicity that the *s-trans*-conformer has the lowest relative energy $E_{\text{trans}} = 0 \text{ kcal mol}^{-1}$ used as the reference for all other relative energies, and calculating conformer-specific partition functions relative to their individual ground state, we can write:

$$k_{\text{total}}(T) = \frac{k_B T}{h} \kappa_{\text{total}}(T) \frac{Q_{\text{total}}^{\ddagger}(T)}{Q_{\text{total}}(T)} \exp\left(\frac{-E^{\ddagger}}{k_B T}\right)$$

$$k_{\text{total}}(T) = \frac{k_B T}{h} \frac{\kappa_{\text{trans}}(T) \cdot Q_{\text{trans}}^{\ddagger}(T) \exp\left(\frac{-E_{\text{trans}}^{\ddagger}}{k_B T}\right) + \kappa_{\text{cis}}(T) \cdot Q_{\text{cis}}^{\ddagger}(T) \exp\left(\frac{-E_{\text{cis}}^{\ddagger}}{k_B T}\right)}{Q_{\text{trans}}(T) + Q_{\text{cis}}(T) \exp\left(\frac{-E_{\text{cis}}}{k_B T}\right)}$$

$$k_{\text{trans}}(T) = \frac{k_B T}{h} \kappa_{\text{trans}}(T) \frac{Q_{\text{trans}}^{\ddagger}(T)}{Q_{\text{trans}}(T)} \exp\left(\frac{-E_{\text{trans}}^{\ddagger}}{k_B T}\right)$$

$$k_{\text{cis}}(T) = \frac{k_B T}{h} \kappa_{\text{cis}}(T) \frac{Q_{\text{cis}}^{\ddagger}(T)}{Q_{\text{cis}}(T)} \exp\left(\frac{-(E_{\text{cis}}^{\ddagger} - E_{\text{cis}})}{k_B T}\right)$$

$$k_{\text{total}}(T) = \frac{Q_{\text{trans}}(T) \cdot k_{\text{trans}}(T) + Q_{\text{cis}}(T) \cdot k_{\text{cis}}(T) \exp\left(\frac{-E_{\text{cis}}}{k_B T}\right)}{Q_{\text{trans}}(T) + Q_{\text{cis}}(T) \exp\left(\frac{-E_{\text{cis}}}{k_B T}\right)}$$

where $k_{\text{trans}}(T)$ and $k_{\text{cis}}(T)$ are the literature conformer-specific rate coefficients, and $Q_{\text{trans}}(T)$, $Q_{\text{cis}}(T)$ and E_{cis} are available from our work. These latter three parameters likely differ slightly from the original work, but this should introduce only a minor bias, negligible compared to the remaining sources of uncertainty in this SAR. The resulting $k_{\text{total}}(T)$ are then newly fitted to a Kooij equation.

To obtain the temperature-dependence of the rate coefficients, we rely on the best available theoretical kinetic data. Theory-based rate coefficients at 298K are scaled to selected reference values $k(298\text{K})$ by a scaling factor $\exp(\Delta E/T)$, where ΔE represents a shift in effective activation energy. The temperature dependence is modeled using the theoretical data, where rate coefficients at all temperatures are corrected using the same activation energy shift ΔE , i.e. the rate coefficients are not scaled linearly across the temperature range.

We then harmonize the available literature data on CI + H₂O as follows:

a) For CH₂OO + H₂O, we use the geometric average of the available experimental data^{42,45} and highest-level theoretical work,^{1,39,60,61} leading to $k(298\text{K}) = 8.3 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$. The temperature dependence of Long et al.³⁹ is used.

b) For *E*-CH₃CHOO + H₂O, we use the geometric average of the experimental^{45,62,63} and highest-level theoretical work,^{39,60,61} yielding $k(298\text{K}) = 2.2 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$; again, we rely on the work by Long et al.³⁹ for the *T*-dependence. The high rate of reaction of *E*-CH₃CHOO, relative to *Z*-CH₃CHOO, is caused mostly by the higher energy of the *E*-stereoisomer, which helps to reduce the relative energy of the TS. The same high

relative energies for the *E*-stereoisomer were found for other R₂ substituents in *E*-RCHOO CI (see section H); for these higher-energy stereoisomers we also adopt these high rate coefficients.

c) For Z-CH₃CHOO + H₂O, we use the geometric average of the highest-level theoretical work,^{39,60,61} finding $k(298\text{K}) = 4.8 \times 10^{-19} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, and adopt the temperature dependence of Long et al.³⁹. We propose for the current SAR that this rate coefficient applies to all Z-R₁CHOO + H₂O; these stereoisomers are energetically the most stable form.

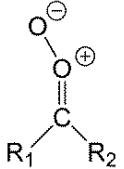
d) For (CH₃)₂COO + H₂O, the highest-level theoretical work is provided by Anglada and coworkers.^{1,61} However, when considering the predictions of these authors for our golden standard *E*-CH₃CHOO, it appears their rate coefficients are overestimated by a factor of ~7.1. This is caused by the level of theory applied, where we already discussed in section F that levels of theory below post-CCSD(T) are prone to underestimation of the barrier heights due to an overestimation of the energy of the CI. Hence, we feel that it is more accurate for our SAR to adjust the barrier height in the Anglada et al. predictions such that their predictions for Z-CH₃CHOO matches the experimental data; this requires an adjustment of only 1.16 kcal mol⁻¹, within the *a priori* error margin for the theoretical calculations. Applying this correction to the Anglada et al. (CH₃)₂COO predictions, we obtain a rate coefficient of $k(298\text{K}) = 4.4 \times 10^{-18} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, with a T-dependence as described by Anglada et al.⁶¹ The rate coefficient obtained experimentally by Newland et al.⁴⁵ is significantly higher than the upper limit obtained Huang et al.,⁶⁵ and higher than all theoretical work on this reaction. As the Newland et al. rate coefficient was obtained from complex experiments interpreted by an extensive kinetic model, we should consider that this rate coefficient carries a larger uncertainty and its value might be overestimated. We chose not to incorporate this higher rate coefficient in our analysis, mostly to avoid underestimating the concentration of CI in the atmosphere.

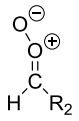
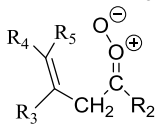
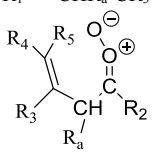
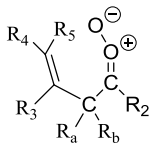
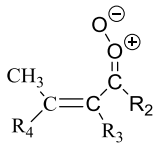
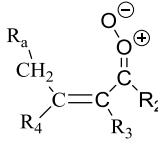
e) For other H₂O reaction of saturated (R₁)(R₂)COO, we have no direct information available. The most straightforward assumption is that these CI react at the same rate as (CH₃)₂COO.

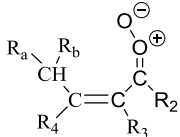
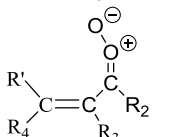
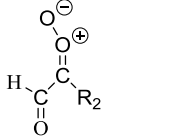
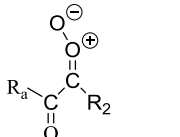
f) For the reaction of H₂O with unsaturated CI, we rely on the theoretical work by Anglada and Solé,⁶¹ where we merge the data on *s-cis*- and *s-trans*-conformers as outlined above. We also adjust the rate coefficient downwards by shifting the barrier by +1.16 kcal mol⁻¹ (a factor of ~7 for $k(298\text{K})$) as discussed in item d.

Table 32 lists the rate coefficient SAR, and gives some indication how a specific entry was obtained.

Table 32: Predicted total rate coefficients for the reaction of carbonyl oxide with H₂O monomers as a function of the two substituents R₁ and R₂. The first line of each entry indicates how the values were obtained, i.e. averaged from experimental and theoretical data (Ex&Th), theoretical data adjusted as described in the text, or data assumed to be similar to other compounds. The rate coefficient *k* (cm³ molecule⁻¹ s⁻¹) is given at 298K, and the parameters of a Kooij equation fit $k(T) = A \times T^n \times \exp(-E_a/T)$ between 200 and 450 K (*A* in cm³ molecule⁻¹ s⁻¹, *E_a* in K). The definition of R_a/R_b/R_c/R₃/R₄/R₅/R' is given in Table 1. Values in green are based directly on experimental and/or theoretical literature data, values in orange are values estimated by similarity to other compounds. **SEE TABLE 35 FOR A SAR THAT ADDITIONALLY INCORPORATES THEORY-BASED REACTION TRENDS (RECOMMENDED).**

	R ₂ = -CH ₃	R ₂ = -CH ₂ R _a	R ₂ = -CHR _a R _b	R ₂ = -CR _a R _b R _c	R ₂ = -H	R ₂ = vinyl	R ₂ = oxo
R ₁ = -CH ₃	Adjusted Th k=4.4×10⁻¹⁸ A= 1.14×10 ⁻¹⁷ n= 0.00 E _a = -2095	As (CH ₃) ₂ COO k=4.4×10⁻¹⁸ A= 1.14×10 ⁻¹⁷ n= 0.00 E _a = -2095	As (CH ₃) ₂ COO k=4.4×10⁻¹⁸ A= 1.14×10 ⁻¹⁷ n= 0.00 E _a = -2095	As (CH ₃) ₂ COO k=4.4×10⁻¹⁸ A= 1.14×10 ⁻¹⁷ n= 0.00 E _a = -2095	Average Ex&Th k=4.8×10⁻¹⁹ A= 8.37×10 ⁻⁴⁹ n= 11.08 E _a = -1606	Adjusted Th k=9.5×10⁻²⁰ A= 1.18×10 ⁻¹⁶ n= 0.24 E _a = 2527	As (CH ₃) ₂ COO k=4.4×10⁻¹⁸ A= 1.14×10 ⁻¹⁷ n= 0.00 E _a = -2095
R ₁ = -CH ₂ R _a	As (CH ₃) ₂ COO k=4.4×10⁻¹⁸ A= 1.14×10 ⁻¹⁷ n= 0.00 E _a = -2095	As (CH ₃) ₂ COO k=4.4×10⁻¹⁸ A= 1.14×10 ⁻¹⁷ n= 0.00 E _a = -2095	As (CH ₃) ₂ COO k=4.4×10⁻¹⁸ A= 1.14×10 ⁻¹⁷ n= 0.00 E _a = -2095	As (CH ₃) ₂ COO k=4.4×10⁻¹⁸ A= 1.14×10 ⁻¹⁷ n= 0.00 E _a = -2095	As R ₁ =-CH ₃ k=4.8×10⁻¹⁹ A= 8.37×10 ⁻⁴⁹ n= 11.08 E _a = -1606	As R ₁ =-CH ₃ k=9.5×10⁻²⁰ A= 1.18×10 ⁻¹⁶ n= 0.24 E _a = 2527	As R ₁ =-CH ₃ k=9.5×10⁻²⁰ A= 1.18×10 ⁻¹⁶ n= 0.24 E _a = 2527
R ₁ = -CHR _a R _b	As (CH ₃) ₂ COO k=4.4×10⁻¹⁸ A= 1.14×10 ⁻¹⁷ n= 0.00 E _a = -2095	As (CH ₃) ₂ COO k=4.4×10⁻¹⁸ A= 1.14×10 ⁻¹⁷ n= 0.00 E _a = -2095	As (CH ₃) ₂ COO k=4.4×10⁻¹⁸ A= 1.14×10 ⁻¹⁷ n= 0.00 E _a = -2095	As (CH ₃) ₂ COO k=4.4×10⁻¹⁸ A= 1.14×10 ⁻¹⁷ n= 0.00 E _a = -2095	As R ₁ =-CH ₃ k=4.8×10⁻¹⁹ A= 8.37×10 ⁻⁴⁹ n= 11.08 E _a = -1606	As R ₁ =-CH ₃ k=9.5×10⁻²⁰ A= 1.18×10 ⁻¹⁶ n= 0.24 E _a = 2527	As R ₁ =-CH ₃ k=9.5×10⁻²⁰ A= 1.18×10 ⁻¹⁶ n= 0.24 E _a = 2527
R ₁ = -CR _a R _b R _c	As (CH ₃) ₂ COO k=4.4×10⁻¹⁸ A= 1.14×10 ⁻¹⁷ n= 0.00 E _a = -2095	As (CH ₃) ₂ COO k=4.4×10⁻¹⁸ A= 1.14×10 ⁻¹⁷ n= 0.00 E _a = -2095	As (CH ₃) ₂ COO k=4.4×10⁻¹⁸ A= 1.14×10 ⁻¹⁷ n= 0.00 E _a = -2095	As (CH ₃) ₂ COO k=4.4×10⁻¹⁸ A= 1.14×10 ⁻¹⁷ n= 0.00 E _a = -2095	As (CH ₃) ₂ COO k=4.4×10⁻¹⁸ A= 1.14×10 ⁻¹⁷ n= 0.00 E _a = -2095	As R ₁ =-H k=3.0×10⁻¹⁵ A= 5.83×10 ⁻¹⁶ n= 0.43 E _a = 836	As R ₁ =-H k=3.0×10⁻¹⁵ A= 5.83×10 ⁻¹⁶ n= 0.43 E _a = 836

$R_1 = -H$ 	Average Ex&Th $k=2.3 \times 10^{-14}$ $A=9.07 \times 10^{-19}$ $n=1.40$ $E_a = -649$	As $R_2 = -CH_3$ $k=2.2 \times 10^{-14}$ $A=9.07 \times 10^{-19}$ $n=1.40$ $E_a = -649$	As $R_2 = -CH_3$ $k=2.2 \times 10^{-14}$ $A=9.07 \times 10^{-19}$ $n=1.40$ $E_a = -649$	As $R_2 = -CH_3$ $k=2.2 \times 10^{-14}$ $A=9.07 \times 10^{-19}$ $n=1.40$ $E_a = -649$	Average Ex&Th $k=8.3 \times 10^{-16}$ $A=6.40 \times 10^{-19}$ $n=1.52$ $E_a = 435$	Adjusted Th $k=3.0 \times 10^{-15}$ $A=5.83 \times 10^{-16}$ $n=0.43$ $E_a = 836$	As $R_2 = -CH_3$ $k=2.2 \times 10^{-14}$ $A=9.07 \times 10^{-19}$ $n=1.40$ $E_a = -649$
$R_1 = -CH_2-CR_3=CR_4R_5$ 	As $(CH_3)_2COO$ $k=4.4 \times 10^{-18}$ $A=1.14 \times 10^{-17}$ $n=0.00$ $E_a = -2095$	As $(CH_3)_2COO$ $k=4.4 \times 10^{-18}$ $A=1.14 \times 10^{-17}$ $n=0.00$ $E_a = -2095$	As $(CH_3)_2COO$ $k=4.4 \times 10^{-18}$ $A=1.14 \times 10^{-17}$ $n=0.00$ $E_a = -2095$	As $(CH_3)_2COO$ $k=4.4 \times 10^{-18}$ $A=1.14 \times 10^{-17}$ $n=0.00$ $E_a = -2095$	As $R_1 = -CH_2R_a$ $k=4.8 \times 10^{-19}$ $A=8.37 \times 10^{-49}$ $n=11.08$ $E_a = -1606$	As $R_1 = -CH_2R_a$ $k=9.5 \times 10^{-20}$ $A=1.18 \times 10^{-16}$ $n=0.24$ $E_a = 2527$	As $R_1 = -CH_2R_a$ $k=9.5 \times 10^{-20}$ $A=1.18 \times 10^{-16}$ $n=0.24$ $E_a = 2527$
$R_1 = -CHR_a-CR_3=CR_4R_5$ 	As $(CH_3)_2COO$ $k=4.4 \times 10^{-18}$ $A=1.14 \times 10^{-17}$ $n=0.00$ $E_a = -2095$	As $(CH_3)_2COO$ $k=4.4 \times 10^{-18}$ $A=1.14 \times 10^{-17}$ $n=0.00$ $E_a = -2095$	As $(CH_3)_2COO$ $k=4.4 \times 10^{-18}$ $A=1.14 \times 10^{-17}$ $n=0.00$ $E_a = -2095$	As $(CH_3)_2COO$ $k=4.4 \times 10^{-18}$ $A=1.14 \times 10^{-17}$ $n=0.00$ $E_a = -2095$	As $R_1 = -CHR_aR_b$ $k=4.8 \times 10^{-19}$ $A=8.37 \times 10^{-49}$ $n=11.08$ $E_a = -1606$	As $R_1 = -CHR_aR_b$ $k=9.5 \times 10^{-20}$ $A=1.18 \times 10^{-16}$ $n=0.24$ $E_a = 2527$	As $R_1 = -CHR_aR_b$ $k=9.5 \times 10^{-20}$ $A=1.18 \times 10^{-16}$ $n=0.24$ $E_a = 2527$
$R_1 = -CR_aR_b-CR_3=CR_4R_5$ 	As $(CH_3)_2COO$ $k=4.4 \times 10^{-18}$ $A=1.14 \times 10^{-17}$ $n=0.00$ $E_a = -2095$	As $(CH_3)_2COO$ $k=4.4 \times 10^{-18}$ $A=1.14 \times 10^{-17}$ $n=0.00$ $E_a = -2095$	As $(CH_3)_2COO$ $k=4.4 \times 10^{-18}$ $A=1.14 \times 10^{-17}$ $n=0.00$ $E_a = -2095$	As $(CH_3)_2COO$ $k=4.4 \times 10^{-18}$ $A=1.14 \times 10^{-17}$ $n=0.00$ $E_a = -2095$	As $(CH_3)_2COO$ $k=4.4 \times 10^{-18}$ $A=1.14 \times 10^{-17}$ $n=0.00$ $E_a = -2095$	As $R_1 = -CR_aR_bR_c$ $k=3.0 \times 10^{-15}$ $A=5.83 \times 10^{-16}$ $n=0.43$ $E_a = 836$	As $R_1 = -CR_aR_bR_c$ $k=3.0 \times 10^{-15}$ $A=5.83 \times 10^{-16}$ $n=0.43$ $E_a = 836$
$R_1 = -CR_3=CR_4CH_3$ 	As $R_1 = -CR_3=CR_4R'$ $k=2.0 \times 10^{-17}$ $A=1.50 \times 10^{-17}$ $n=0.82$ $E_a = 1990$	As $R_2 = -CH_3$ $k=2.0 \times 10^{-17}$ $A=1.50 \times 10^{-17}$ $n=0.82$ $E_a = 1990$	As $R_2 = -CH_3$ $k=2.0 \times 10^{-17}$ $A=1.50 \times 10^{-17}$ $n=0.82$ $E_a = 1990$	As $R_2 = -CH_3$ $k=2.0 \times 10^{-17}$ $A=1.50 \times 10^{-17}$ $n=0.82$ $E_a = 1990$	As $R_1 = -CR_3=CR_4R'$ $k=2.2 \times 10^{-19}$ $A=7.12 \times 10^{-15}$ $n=0.04$ $E_a = 3164$	As $R_2 = -CH_3$ $k=2.0 \times 10^{-17}$ $A=1.50 \times 10^{-17}$ $n=0.82$ $E_a = 1990$	As $R_2 = -CH_3$ $k=2.0 \times 10^{-17}$ $A=1.50 \times 10^{-17}$ $n=0.82$ $E_a = 1990$
$R_1 = -CR_3=CR_4CH_2R_a$ 	As $R_1 = -CR_3=CR_4R'$ $k=2.0 \times 10^{-17}$ $A=1.50 \times 10^{-17}$ $n=0.82$ $E_a = 1990$	As $R_2 = -CH_3$ $k=2.0 \times 10^{-17}$ $A=1.50 \times 10^{-17}$ $n=0.82$ $E_a = 1990$	As $R_2 = -CH_3$ $k=2.0 \times 10^{-17}$ $A=1.50 \times 10^{-17}$ $n=0.82$ $E_a = 1990$	As $R_2 = -CH_3$ $k=2.0 \times 10^{-17}$ $A=1.50 \times 10^{-17}$ $n=0.82$ $E_a = 1990$	As $R_1 = -CR_3=CR_4R'$ $k=2.2 \times 10^{-19}$ $A=7.12 \times 10^{-15}$ $n=0.04$ $E_a = 3164$	As $R_2 = -CH_3$ $k=2.0 \times 10^{-17}$ $A=1.50 \times 10^{-17}$ $n=0.82$ $E_a = 1990$	As $R_2 = -CH_3$ $k=2.0 \times 10^{-17}$ $A=1.50 \times 10^{-17}$ $n=0.82$ $E_a = 1990$

$R_1 = -CR_3=CR_4CHR_aR_b$ 	$As\ R_1=-CR_3=CR_4R'$ $k=2.0\times 10^{-17}$ $A=1.50\times 10^{-17}$ $n=0.82$ $E_a=1990$	$As\ R_2=-CH_3$ $k=2.0\times 10^{-17}$ $A=1.50\times 10^{-17}$ $n=0.82$ $E_a=1990$	$As\ R_2=-CH_3$ $k=2.0\times 10^{-17}$ $A=1.50\times 10^{-17}$ $n=0.82$ $E_a=1990$	$As\ R_2=-CH_3$ $k=2.0\times 10^{-17}$ $A=1.50\times 10^{-17}$ $n=0.82$ $E_a=1990$	$As\ R_1=-CR_3=CR_4R'$ $k=2.2\times 10^{-19}$ $A=7.12\times 10^{-15}$ $n=0.04$ $E_a=3164$	$As\ R_2=-CH_3$ $k=2.0\times 10^{-17}$ $A=1.50\times 10^{-17}$ $n=0.82$ $E_a=1990$	$As\ R_2=-CH_3$ $k=2.0\times 10^{-17}$ $A=1.50\times 10^{-17}$ $n=0.82$ $E_a=1990$
$R_1 = -CR_3=CR_4R'$ 	$Adjusted\ Th$ $k=2.0\times 10^{-17}$ $A=1.50\times 10^{-17}$ $n=0.82$ $E_a=1990$	$As\ R_2=-CH_3$ $k=2.0\times 10^{-17}$ $A=1.50\times 10^{-17}$ $n=0.82$ $E_a=1990$	$As\ R_2=-CH_3$ $k=2.0\times 10^{-17}$ $A=1.50\times 10^{-17}$ $n=0.82$ $E_a=1990$	$As\ R_2=-CH_3$ $k=2.0\times 10^{-17}$ $A=1.50\times 10^{-17}$ $n=0.82$ $E_a=1990$	$Adjusted\ Th$ $k=2.2\times 10^{-19}$ $A=7.12\times 10^{-15}$ $n=0.04$ $E_a=3164$	$As\ R_2=-CH_3$ $k=2.0\times 10^{-17}$ $A=1.50\times 10^{-17}$ $n=0.82$ $E_a=1990$	$As\ R_2=-CH_3$ $k=2.0\times 10^{-17}$ $A=1.50\times 10^{-17}$ $n=0.82$ $E_a=1990$
$R_1 = -CHO$ 	$As\ (CH_3)_2COO$ $k=4.4\times 10^{-18}$ $A=1.14\times 10^{-17}$ $n=0.00$ $E_a=-2095$	$As\ (CH_3)_2COO$ $k=4.4\times 10^{-18}$ $A=1.14\times 10^{-17}$ $n=0.00$ $E_a=-2095$	$As\ (CH_3)_2COO$ $k=4.4\times 10^{-18}$ $A=1.14\times 10^{-17}$ $n=0.00$ $E_a=-2095$	$As\ (CH_3)_2COO$ $k=4.4\times 10^{-18}$ $A=1.14\times 10^{-17}$ $n=0.00$ $E_a=-2095$	$As\ R_1=-CHR_aR_b$ $k=4.8\times 10^{-19}$ $A=8.37\times 10^{-49}$ $n=11.08$ $E_a=-1606$	$As\ R_1=-CHR_aR_b$ $k=9.5\times 10^{-20}$ $A=1.18\times 10^{-16}$ $n=0.24$ $E_a=2527$	$As\ R_1=-CHR_aR_b$ $k=9.5\times 10^{-20}$ $A=1.18\times 10^{-16}$ $n=0.24$ $E_a=2527$
$R_1 = -C(O)R_a$ 	$As\ (CH_3)_2COO$ $k=4.4\times 10^{-18}$ $A=1.14\times 10^{-17}$ $n=0.00$ $E_a=-2095$	$As\ (CH_3)_2COO$ $k=4.4\times 10^{-18}$ $A=1.14\times 10^{-17}$ $n=0.00$ $E_a=-2095$	$As\ (CH_3)_2COO$ $k=4.4\times 10^{-18}$ $A=1.14\times 10^{-17}$ $n=0.00$ $E_a=-2095$	$As\ (CH_3)_2COO$ $k=4.4\times 10^{-18}$ $A=1.14\times 10^{-17}$ $n=0.00$ $E_a=-2095$	$As\ R_1=-CR_aR_bR_c$ $k=4.4\times 10^{-18}$ $A=1.14\times 10^{-17}$ $n=0.00$ $E_a=-2095$	$As\ R_1=-CR_aR_bR_c$ $k=3.0\times 10^{-15}$ $A=5.83\times 10^{-16}$ $n=0.43$ $E_a=836$	$As\ R_1=-CR_aR_bR_c$ $k=3.0\times 10^{-15}$ $A=5.83\times 10^{-16}$ $n=0.43$ $E_a=836$

3. Theoretical calculations on the CI + H₂O reaction

The SAR derived solely on literature data does not fully capture the relative reactivity of the CI as a function of its substituents. To incorporate these reaction trends more faithfully, we have examined the reaction of CI with H₂O by the quantum chemical and theoretical methods described in section F, as a function of a wide range of substituents. Though our data set is not as extensive as for the unimolecular reactions, it will help to confirm reactivity trends, improve on the predicted rate coefficients, and identify compounds that are not well-described by the current literature. The theoretical results clearly shows that accurately predicting the rate coefficients for CI + H₂O reactions *a priori* is difficult, even at high levels of theory, and the computational cost prohibits us from attempting calculations at these levels of theory across a sufficiently wide variety of CI. Instead, we will rely on the best available literature data to obtain an empirical correction on lower-level computational data, and use this to predict reliable temperature-dependent rate coefficients $k(T)$.

The chemical mechanism for CI + H₂O reactions proceeds by the formation of H-bonded pre-reactive complexes, followed by a saddle point transition state to form a hydroxyalkylhydroperoxide product. The reactions of CI + H₂O are relatively slow, and the pre-reactive complexes are likely in equilibrium with the free reactants. In such a case, the properties of the pre-reactive complex cancel out of the kinetic equations, except for the impact the complex has on tunneling through the energy barrier during the H-shift. The approximation we apply is then to assume the pre-reactive complex is not affecting the reaction kinetics, but correct the Eckart barrier in the tunneling corrections to a standardized complex stability of 7 kcal mol⁻¹, a value obtained from explicit quantum chemical calculations in various publications.^{1,26,37-40,59-61,64,66,196} A second approximation is that we assume a fixed reaction exoergicity of -40 kcal mol⁻¹, to avoid the costly explicit characterization of the reaction products by quantum chemical calculations. This will have only a minor effect on the shape of the Eckart barrier used in the tunneling predictions. The transition states for the CI + H₂O reaction are characterized explicitly, i.e. a full conformational analysis is done at the M06-2X level of theory, and the energies are refined at the CCSD(T) level of theory, as explained in the methodology section F. A third approximation is the assumption that all differences between theory-predicted rate coefficient and the literature data can be accommodated by adjusting the barrier height to reaction. As already discussed, the barrier heights of CI reactions are systematically underestimated by our level of theory; other effects that we are not fully incorporating are multi-dimensional tunneling, the effect of the pre-reactive complex, the product stability, variational effects of the TS location along the reaction coordinate, or anharmonicities in the vibrational modes. All these effects we then aim to compensate by altering the barrier height, as described below.

The reference data we use is the room temperature rate coefficients obtained from the literature, harmonized as described above and listed in Table 33. We selected only compounds in our reference set for which data is available for the H₂O as well as the (H₂O)₂ reaction, as both are necessary to describe the impact of moisture on the CI lifetime in the atmosphere. The data selected span several orders of magnitude, and as detailed below our substituent-specific barrier heights will be adjusted uniformly such that our theory-derived rate coefficients match these values as well as possible. Given that the *E*-CH₃CHOO + H₂O reaction is the only reaction for which the experimental data has reached consensus, we will force our prediction to match this value exactly.

Table 33: Reference rate coefficients (cm³ molecule⁻¹ s⁻¹) for deriving the structure activity relationships for the CI + H₂O and CI + (H₂O)₂ reactions, re-evaluated from literature data as explained in sections S and T.

CI	$k_{\text{H}_2\text{O}}(298\text{K})$	$k_{(\text{H}_2\text{O})_2}(298\text{K})$
CH ₂ OO	8.34×10^{-16}	5.78×10^{-12}
Z-CH ₃ CHOO	4.77×10^{-19}	2.56×10^{-14}
<i>E</i> -CH ₃ CHOO	2.27×10^{-14}	1.60×10^{-11}
(CH ₃) ₂ COO	4.40×10^{-18}	1.29×10^{-14}
Z-(CH=CH ₂)(CH ₃)COO	1.98×10^{-18}	7.02×10^{-16}
<i>E</i> -(CH=CH ₂)(CH ₃)COO	9.49×10^{-20}	8.96×10^{-17}
Z-(C(CH ₃)=CH ₂)CHOO	2.24×10^{-19}	8.52×10^{-16}
<i>E</i> -(C(CH ₃)=CH ₂)CHOO	4.17×10^{-16}	1.20×10^{-13}

4. Correlation between literature and theory-based rate coefficients

The theory-predicted rate coefficients and the reference values can be brought into agreement by altering the barrier as follows:

$$E_b = E_{b,\text{CCSD(T)}} + 1.46 \text{ kcal mol}^{-1} - 0.06 \times (E_{b,\text{CCSD(T)}} - E_{b,\text{CCSD(T)}}(E\text{-CH}_3\text{CHOO}))$$

The barrier height is increased by $1.46 \text{ kcal mol}^{-1}$, a correction of similar magnitude as that for some of the theoretical data described earlier in this section, and amounts to a rate coefficient correction at 298K of a factor 11.8. The resulting correlation has a very slight deviation from a 1:1 agreement, which is corrected for by the third term in the equation above, which preserves the barrier $E_b(E\text{-CH}_3\text{CHOO})$ for the $E\text{-CH}_3\text{CHOO} + \text{H}_2\text{O}$ reaction, $-0.925 \text{ kcal mol}^{-1}$ prior to correction, but makes a minor adjustment as the reaction barrier differs more from this reference value. This latter term amounts to a correction of a factor of 2 at most across the full rate coefficient range of 7 decades. This minor correction is significantly smaller than the uncertainty on the reference data and carries no statistical significance; it should be seen only as an effort to numerically adhere as close as possible to the reference data. Figure 14 shows the correlation between the reference values, and the theory-predicted rate coefficients after barrier height corrections. The rate coefficients are reproduced on average within a factor of 1.4, with a largest deviation of a factor 2.2 for $E\text{-(C(CH}_3\text{)=CH}_2\text{)CHOO}$, across a rate coefficient range of 5.5 decades. This excellent reproducibility indicates that our procedure captures all important aspects of the $\text{CI} + \text{H}_2\text{O}$ chemistry, and should yield reliable predictions across a very wide range of rate coefficients. Predictions for the temperature-dependent rate coefficients for a wide range of $\text{CI} + \text{H}_2\text{O}$ reactions are listed in Table 34.

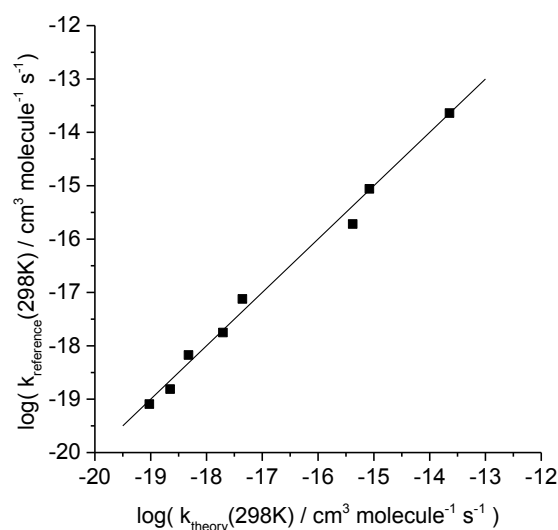


Figure 14: Correlation between the reference rate coefficients for the $\text{CI} + \text{H}_2\text{O}$ reaction, and the theory-based predictions after barrier height corrections. The line represents a 1:1 correlation.

5. Structure-activity Relationship (SAR) for $\text{CI} + \text{H}_2\text{O}$ reaction, incorporating theoretical data

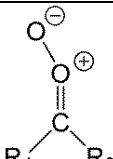
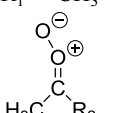
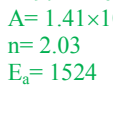
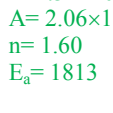
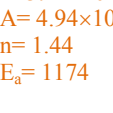
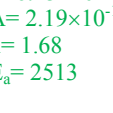
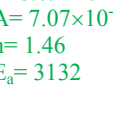
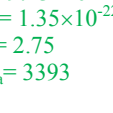
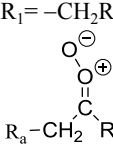
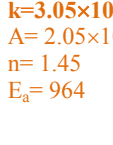
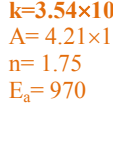
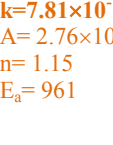
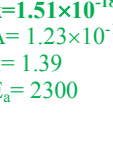
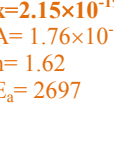
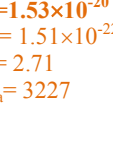
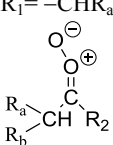
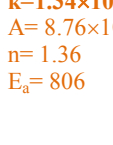
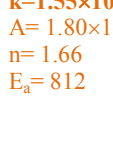
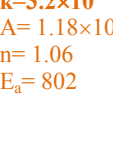
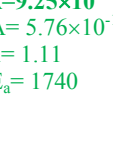
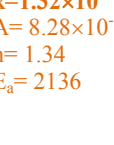
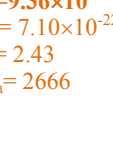
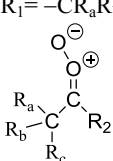
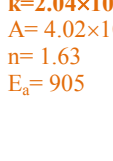
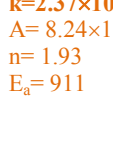
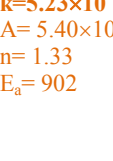
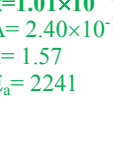
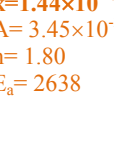
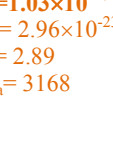
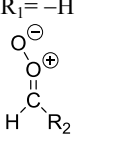
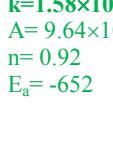
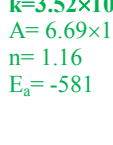
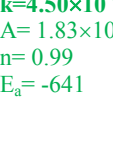
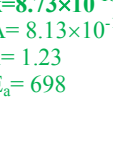
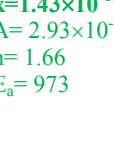
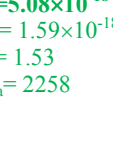
The rate coefficient trends obtained from the adjusted theoretical data are then converted in a Structure-Activity relationship, listed in Table 35. This SAR extrapolates the reactivity trends across a wider range of substituents than available in the theoretical data set; the same SAR substituent classes as used for unimolecular decomposition were used to simplify implementation.

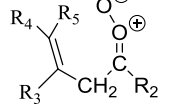
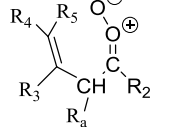
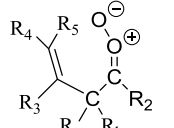
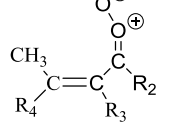
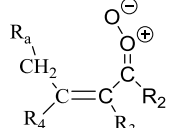
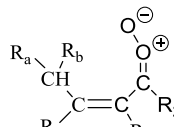
Table 34: Rate constant predictions for the reaction of CI with H₂O monomers obtained after barrier height corrections in the theoretical data, listing barrier heights E_b (kcal mol⁻¹), rate coefficient k (cm³ molecule⁻¹ s⁻¹) at 298 K, and parameters for a Kooij equation fit $k(T)=A \times T^n \times \exp(-E_a/T)$ cm³ molecule⁻¹ s⁻¹ for the temperature range 200-450 K. The first 8 entries correspond to the reference compounds in Table 33.

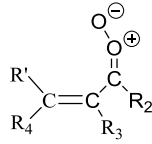
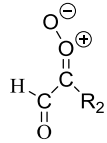
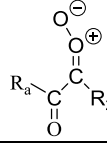
Carbonyl oxide	E_b	$k(298K)$	A	n	E_a / K
CH ₂ OO	2.68	8.7×10^{-16}	8.13×10^{-18}	1.23	698
Z-CH ₃ CHOO	6.56	6.7×10^{-19}	2.19×10^{-19}	1.68	2513
E-CH ₃ CHOO	0.53	2.3×10^{-14}	4.32×10^{-18}	1.27	-405
(CH ₃) ₂ COO	5.05	7.5×10^{-18}	3.87×10^{-20}	1.91	1677
Z-(CH=CH ₂)(CH ₃)COO	5.70	1.8×10^{-18}	2.21×10^{-21}	2.27	1858
E-(CH ₃)(CH=CH ₂)COO	7.95	8.1×10^{-20}	7.07×10^{-19}	1.46	3132
Z-(C(CH ₃)=CH ₂)CHOO	7.53	1.5×10^{-19}	5.88×10^{-19}	1.52	2977
E-(C(CH ₃)=CH ₂)CHOO	3.46	1.9×10^{-16}	2.13×10^{-19}	1.74	929
Z-C ₂ H ₅ CHOO	6.07	1.5×10^{-18}	1.23×10^{-18}	1.39	2300
E-C ₂ H ₅ CHOO	0.22	1.6×10^{-14}	9.64×10^{-18}	0.92	-652
Z-iC ₃ H ₇ CHOO	4.80	9.3×10^{-18}	5.76×10^{-18}	1.11	1740
E-iC ₃ H ₇ CHOO	0.01	3.5×10^{-14}	6.69×10^{-18}	1.16	-581
Z-tC ₄ H ₉ CHOO	5.98	1.0×10^{-18}	2.40×10^{-19}	1.57	2241
E-tC ₄ H ₉ CHOO	-0.08	4.5×10^{-14}	1.83×10^{-17}	0.99	-641
Z-(C ₂ H ₅)(CH ₃)COO	4.36	1.5×10^{-17}	4.19×10^{-20}	1.78	1265
E-(CH ₃)(C ₂ H ₅)COO	4.82	9.1×10^{-18}	1.41×10^{-20}	2.03	1524
Z-(iC ₃ H ₇)(CH ₃)COO	3.76	9.8×10^{-18}	1.66×10^{-20}	1.71	1005
E-(CH ₃)(iC ₃ H ₇)COO	5.14	4.3×10^{-18}	2.06×10^{-19}	1.60	1813
Z-(CHO)CHOO	2.00	7.7×10^{-16}	3.04×10^{-19}	1.59	370
E-(CHO)CHOO	5.80	5.0×10^{-18}	1.59×10^{-18}	1.53	2258
Z-(CHO)(CH ₃)COO	-0.12	1.4×10^{-14}	7.81×10^{-20}	1.68	-757
E-(CH ₃)(CHO)COO	9.97	3.9×10^{-21}	1.09×10^{-19}	1.87	4177
Z-(C(O)CH ₃)(CH ₃)COO	-1.35	5.5×10^{-14}	2.18×10^{-19}	1.43	-1268
E-(CH ₃)(C(O)CH ₃)COO	8.60	1.6×10^{-20}	1.40×10^{-20}	2.07	3472
Z-(CH=CH ₂)CHOO	7.81	8.2×10^{-20}	1.22×10^{-19}	1.73	3059
E-(CH=CH ₂)CHOO	3.75	9.5×10^{-17}	8.39×10^{-19}	1.46	1073
Z-(CH ₂ -CH=CH ₂)CHOO	5.76	1.4×10^{-18}	5.03×10^{-20}	1.84	2120
E-(CH ₂ -CH=CH ₂)CHOO	-0.20	1.8×10^{-14}	5.18×10^{-19}	1.48	-593
Z-(CH(CH ₃)-CH=CH ₂)CHOO	4.67	4.8×10^{-18}	1.55×10^{-20}	1.88	1484
E-(CH(CH ₃)-CH=CH ₂)CHOO	-0.19	3.4×10^{-14}	3.81×10^{-18}	1.21	-656
Z-(C(CH ₃) ₂ -CH=CH ₂)CHOO	5.66	1.4×10^{-18}	7.07×10^{-19}	1.39	2150
E-(C(CH ₃) ₂ -CH=CH ₂)CHOO	-0.51	3.9×10^{-14}	3.40×10^{-18}	1.20	-745
Z-nopinone oxide	2.14	4.2×10^{-16}	8.46×10^{-23}	2.64	-121
E-nopinone oxide	5.16	1.7×10^{-18}	4.08×10^{-22}	2.37	1525
Z-pinonaldehyde-A-oxide ^a	4.55	1.3×10^{-18}	1.72×10^{-26}	3.83	1023
E-pinonaldehyde-A-oxide	0.30	1.6×10^{-14}	4.91×10^{-15}	0.17	-71
Z-pinonaldehyde-K-oxide ^a	6.07	2.4×10^{-19}	1.25×10^{-21}	2.27	2276
E-pinonaldehyde-K-oxide ^a	5.38	9.8×10^{-18}	3.00×10^{-18}	1.06	2132

^a No CCSD(T) data available; barrier height based on M06-2X/aug-cc-pVTZ data only.

Table 35: Predicted total rate coefficients for the reaction of carbonyl oxide with H₂O monomers as a function of the two substituents R₁ and R₂, based on fitting theory-derived reaction trends to a set of literature data. The rate coefficient k (cm³ molecule⁻¹ s⁻¹) is given at 298 K, and the parameters of a Kooij equation fit $k(T) = A \times T^n \times \exp(-E_a/T)$ between 200 and 450 K (A in cm³ molecule⁻¹ s⁻¹, E_a in K). The definition of R_a/R_b/R_c/R₃/R₄/R₅/R' is given in Table 1. Values in green are based directly on experimental and/or theoretical kinetic calculations, values in orange are values estimated by applying (averaged) reaction trends for other substituents.

	R ₂ = -CH ₃	R ₂ = -CH ₂ R _a	R ₂ = -CHR _a R _b	R ₂ = -CR _a R _b R _c	R ₂ = -H	R ₂ = vinyl	R ₂ = oxo
R ₁ = -CH ₃	 $k=7.54 \times 10^{-18}$ $A = 3.87 \times 10^{-20}$ $n = 1.91$ $E_a = 1677$	 $k=9.11 \times 10^{-18}$ $A = 1.41 \times 10^{-20}$ $n = 2.03$ $E_a = 1524$	 $k=4.32 \times 10^{-18}$ $A = 2.06 \times 10^{-19}$ $n = 1.60$ $E_a = 1813$	 $k=3.47 \times 10^{-17}$ $A = 4.94 \times 10^{-19}$ $n = 1.44$ $E_a = 1174$	 $k=6.73 \times 10^{-19}$ $A = 2.19 \times 10^{-19}$ $n = 1.68$ $E_a = 2513$	 $k=8.09 \times 10^{-20}$ $A = 7.07 \times 10^{-19}$ $n = 1.46$ $E_a = 3132$	 $k=9.75 \times 10^{-21}$ $A = 1.35 \times 10^{-22}$ $n = 2.75$ $E_a = 3393$
R ₁ = -CH ₂ R _a	 $k=1.49 \times 10^{-17}$ $A = 4.19 \times 10^{-20}$ $n = 1.78$ $E_a = 1265$	 $k=3.05 \times 10^{-17}$ $A = 2.05 \times 10^{-19}$ $n = 1.45$ $E_a = 964$	 $k=3.54 \times 10^{-17}$ $A = 4.21 \times 10^{-20}$ $n = 1.75$ $E_a = 970$	 $k=7.81 \times 10^{-17}$ $A = 2.76 \times 10^{-18}$ $n = 1.15$ $E_a = 961$	 $k=1.51 \times 10^{-18}$ $A = 1.23 \times 10^{-18}$ $n = 1.39$ $E_a = 2300$	 $k=2.15 \times 10^{-19}$ $A = 1.76 \times 10^{-19}$ $n = 1.62$ $E_a = 2697$	 $k=1.53 \times 10^{-20}$ $A = 1.51 \times 10^{-22}$ $n = 2.71$ $E_a = 3227$
R ₁ = -CHR _a R _b	 $k=9.77 \times 10^{-18}$ $A = 1.66 \times 10^{-20}$ $n = 1.71$ $E_a = 1005$	 $k=1.34 \times 10^{-17}$ $A = 8.76 \times 10^{-20}$ $n = 1.36$ $E_a = 806$	 $k=1.55 \times 10^{-17}$ $A = 1.80 \times 10^{-20}$ $n = 1.66$ $E_a = 812$	 $k=3.2 \times 10^{-17}$ $A = 1.18 \times 10^{-18}$ $n = 1.06$ $E_a = 802$	 $k=9.25 \times 10^{-18}$ $A = 5.76 \times 10^{-18}$ $n = 1.11$ $E_a = 1740$	 $k=1.32 \times 10^{-18}$ $A = 8.28 \times 10^{-19}$ $n = 1.34$ $E_a = 2136$	 $k=9.36 \times 10^{-20}$ $A = 7.10 \times 10^{-22}$ $n = 2.43$ $E_a = 2666$
R ₁ = -CR _a R _b R _c	 $k=1.49 \times 10^{-17}$ $A = 7.64 \times 10^{-21}$ $n = 1.98$ $E_a = 1104$	 $k=2.04 \times 10^{-17}$ $A = 4.02 \times 10^{-20}$ $n = 1.63$ $E_a = 905$	 $k=2.37 \times 10^{-17}$ $A = 8.24 \times 10^{-21}$ $n = 1.93$ $E_a = 911$	 $k=5.23 \times 10^{-17}$ $A = 5.40 \times 10^{-19}$ $n = 1.33$ $E_a = 902$	 $k=1.01 \times 10^{-18}$ $A = 2.40 \times 10^{-19}$ $n = 1.57$ $E_a = 2241$	 $k=1.44 \times 10^{-19}$ $A = 3.45 \times 10^{-20}$ $n = 1.80$ $E_a = 2638$	 $k=1.03 \times 10^{-20}$ $A = 2.96 \times 10^{-23}$ $n = 2.89$ $E_a = 3168$
R ₁ = -H	 $k=2.29 \times 10^{-14}$ $A = 4.32 \times 10^{-18}$ $n = 1.27$ $E_a = -405$	 $k=1.58 \times 10^{-14}$ $A = 9.64 \times 10^{-18}$ $n = 0.92$ $E_a = -652$	 $k=3.52 \times 10^{-14}$ $A = 6.69 \times 10^{-18}$ $n = 1.16$ $E_a = -581$	 $k=4.50 \times 10^{-14}$ $A = 1.83 \times 10^{-17}$ $n = 0.99$ $E_a = -641$	 $k=8.73 \times 10^{-16}$ $A = 8.13 \times 10^{-18}$ $n = 1.23$ $E_a = 698$	 $k=1.43 \times 10^{-16}$ $A = 2.93 \times 10^{-19}$ $n = 1.66$ $E_a = 973$	 $k=5.08 \times 10^{-18}$ $A = 1.59 \times 10^{-18}$ $n = 1.53$ $E_a = 2258$

$R_1 = -CH_2-CR_3=CR_4R_5$ 	$k=4.09 \times 10^{-18}$ $A = 8.45 \times 10^{-21}$ $n = 2.05$ $E_a = 1633$	$k=2.88 \times 10^{-17}$ $A = 8.43 \times 10^{-21}$ $n = 1.89$ $E_a = 784$	$k=3.35 \times 10^{-17}$ $A = 1.73 \times 10^{-21}$ $n = 2.20$ $E_a = 790$	$k=7.38 \times 10^{-17}$ $A = 1.13 \times 10^{-19}$ $n = 1.60$ $E_a = 781$	$k=1.43 \times 10^{-18}$ $A = 5.03 \times 10^{-20}$ $n = 1.84$ $E_a = 2120$	$k=2.04 \times 10^{-19}$ $A = 7.23 \times 10^{-21}$ $n = 2.07$ $E_a = 2516$	$k=1.45 \times 10^{-20}$ $A = 6.20 \times 10^{-24}$ $n = 3.16$ $E_a = 3047$
$R_1 = -CHR_a-CR_3=CR_4R_5$ 	$k=5.04 \times 10^{-18}$ $A = 4.48 \times 10^{-23}$ $n = 2.48$ $E_a = 749$	$k=6.88 \times 10^{-18}$ $A = 2.36 \times 10^{-22}$ $n = 2.13$ $E_a = 550$	$k=8.00 \times 10^{-18}$ $A = 4.84 \times 10^{-23}$ $n = 2.44$ $E_a = 556$	$k=1.76 \times 10^{-17}$ $A = 3.17 \times 10^{-21}$ $n = 1.84$ $E_a = 547$	$k=4.77 \times 10^{-18}$ $A = 1.55 \times 10^{-20}$ $n = 1.88$ $E_a = 1484$	$k=6.78 \times 10^{-19}$ $A = 2.23 \times 10^{-21}$ $n = 2.11$ $E_a = 1881$	$k=4.82 \times 10^{-20}$ $A = 1.91 \times 10^{-24}$ $n = 3.20$ $E_a = 2411$
$R_1 = -CR_aR_b-CR_3=CR_4R_5$ 	$k=2.06 \times 10^{-17}$ $A = 2.25 \times 10^{-20}$ $n = 1.79$ $E_a = 1013$	$k=2.82 \times 10^{-17}$ $A = 1.18 \times 10^{-19}$ $n = 1.44$ $E_a = 813$	$k=3.28 \times 10^{-17}$ $A = 2.43 \times 10^{-20}$ $n = 1.75$ $E_a = 819$	$k=7.22 \times 10^{-17}$ $A = 1.59 \times 10^{-18}$ $n = 1.15$ $E_a = 810$	$k=1.40 \times 10^{-18}$ $A = 7.07 \times 10^{-19}$ $n = 1.39$ $E_a = 2150$	$k=1.99 \times 10^{-19}$ $A = 1.02 \times 10^{-19}$ $n = 1.62$ $E_a = 2546$	$k=1.42 \times 10^{-20}$ $A = 8.71 \times 10^{-23}$ $n = 2.71$ $E_a = 3076$
$R_1 = -CR_3=CR_4CH_3$ 	$k=1.78 \times 10^{-18}$ $A = 2.21 \times 10^{-21}$ $n = 2.27$ $E_a = 1858$	$k=3.48 \times 10^{-18}$ $A = 2.13 \times 10^{-20}$ $n = 1.83$ $E_a = 1589$	$k=4.05 \times 10^{-18}$ $A = 4.37 \times 10^{-21}$ $n = 2.14$ $E_a = 1595$	$k=8.93 \times 10^{-18}$ $A = 2.87 \times 10^{-19}$ $n = 1.4$ $E_a = 1586$	$k=1.18 \times 10^{-19}$ $A = 2.24 \times 10^{-19}$ $n = 1.65$ $E_a = 2989$	$k=1.68 \times 10^{-20}$ $A = 3.22 \times 10^{-20}$ $n = 1.88$ $E_a = 3385$	$k=1.20 \times 10^{-21}$ $A = 2.76 \times 10^{-23}$ $n = 2.97$ $E_a = 3915$
$R_1 = -CR_3=CR_4CH_2R_a$ 	$k=1.78 \times 10^{-18}$ $A = 2.21 \times 10^{-21}$ $n = 2.27$ $E_a = 1858$	$k=3.48 \times 10^{-18}$ $A = 2.13 \times 10^{-20}$ $n = 1.83$ $E_a = 1589$	$k=4.05 \times 10^{-18}$ $A = 4.37 \times 10^{-21}$ $n = 2.14$ $E_a = 1595$	$k=8.93 \times 10^{-18}$ $A = 2.87 \times 10^{-19}$ $n = 1.4$ $E_a = 1586$	$k=1.18 \times 10^{-19}$ $A = 2.24 \times 10^{-19}$ $n = 1.65$ $E_a = 2989$	$k=1.68 \times 10^{-20}$ $A = 3.22 \times 10^{-20}$ $n = 1.88$ $E_a = 3385$	$k=1.20 \times 10^{-21}$ $A = 2.76 \times 10^{-23}$ $n = 2.97$ $E_a = 3915$
$R_1 = -CR_3=CR_4CHRaR_b$ 	$k=1.78 \times 10^{-18}$ $A = 2.21 \times 10^{-21}$ $n = 2.27$ $E_a = 1858$	$k=3.48 \times 10^{-18}$ $A = 2.13 \times 10^{-20}$ $n = 1.83$ $E_a = 1589$	$k=4.05 \times 10^{-18}$ $A = 4.37 \times 10^{-21}$ $n = 2.14$ $E_a = 1595$	$k=8.93 \times 10^{-18}$ $A = 2.87 \times 10^{-19}$ $n = 1.4$ $E_a = 1586$	$k=1.18 \times 10^{-19}$ $A = 2.24 \times 10^{-19}$ $n = 1.65$ $E_a = 2989$	$k=1.68 \times 10^{-20}$ $A = 3.22 \times 10^{-20}$ $n = 1.88$ $E_a = 3385$	$k=1.20 \times 10^{-21}$ $A = 2.76 \times 10^{-23}$ $n = 2.97$ $E_a = 3915$

$R_1 = -CR_3=CR_4R'$ 	$k=1.78 \times 10^{-18}$ $A=2.21 \times 10^{-21}$ $n=2.27$ $E_a=1858$	$k=3.48 \times 10^{-18}$ $A=2.13 \times 10^{-20}$ $n=1.83$ $E_a=1589$	$k=4.05 \times 10^{-18}$ $A=4.37 \times 10^{-21}$ $n=2.14$ $E_a=1595$	$k=8.93 \times 10^{-18}$ $A=2.87 \times 10^{-19}$ $n=1.4$ $E_a=1586$	$k=1.18 \times 10^{-19}$ $A=2.24 \times 10^{-19}$ $n=1.65$ $E_a=2989$	$k=1.68 \times 10^{-20}$ $A=3.22 \times 10^{-20}$ $n=1.88$ $E_a=3385$	$k=1.20 \times 10^{-21}$ $A=2.76 \times 10^{-23}$ $n=2.97$ $E_a=3915$
$R_1 = -CHO$ 	$k=1.41 \times 10^{-14}$ $A=7.81 \times 10^{-20}$ $n=1.68$ $E_a=-757$	$k=1.54 \times 10^{-14}$ $A=5.10 \times 10^{-20}$ $n=1.65$ $E_a=-966$	$k=1.79 \times 10^{-14}$ $A=1.05 \times 10^{-20}$ $n=1.95$ $E_a=-960$	$k=3.95 \times 10^{-14}$ $A=6.86 \times 10^{-19}$ $n=1.35$ $E_a=-969$	$k=7.66 \times 10^{-16}$ $A=3.04 \times 10^{-19}$ $n=1.59$ $E_a=370$	$k=1.09 \times 10^{-16}$ $A=4.37 \times 10^{-20}$ $n=1.82$ $E_a=767$	$k=7.74 \times 10^{-18}$ $A=3.75 \times 10^{-23}$ $n=2.91$ $E_a=1297$
$R_1 = -C(O)R_a$ 	$k=5.46 \times 10^{-14}$ $A=2.18 \times 10^{-19}$ $n=1.43$ $E_a=-1268$	$k=7.46 \times 10^{-14}$ $A=1.15 \times 10^{-18}$ $n=1.08$ $E_a=-1468$	$k=8.66 \times 10^{-14}$ $A=2.35 \times 10^{-19}$ $n=1.39$ $E_a=-1462$	$k=1.91 \times 10^{-13}$ $A=1.54 \times 10^{-17}$ $n=0.79$ $E_a=-1471$	$k=3.70 \times 10^{-15}$ $A=6.84 \times 10^{-18}$ $n=1.03$ $E_a=-131$	$k=5.27 \times 10^{-16}$ $A=9.83 \times 10^{-19}$ $n=1.26$ $E_a=265$	$k=3.75 \times 10^{-17}$ $A=8.43 \times 10^{-22}$ $n=2.35$ $E_a=795$

6. Uncertainty analysis

The experimental determination of the rate coefficient for the E -CH₃CHOO + H₂O reaction carries a large weight in the SAR development, as it is the only data point for which the literature is in consensus, within a factor of 2, and all SAR rate coefficients are directly or indirectly relative to this value. The remaining 7 reference rate coefficients (Table 33) have been averaged from more scattered data, have been systematically scaled to match the E -CH₃CHOO + H₂O reaction, and/or have been derived by combining theory-based conformer-specific rate coefficients into a population-averaged rate coefficient. The *a priori* uncertainty on these reference values is thus rather large, especially for those compounds where the rate coefficients differs significantly from the E -CH₃CHOO + H₂O anchor point. In Figure 14, this corresponds to an uncertainty on the slope of the correlation line, where the E -CH₃CHOO + H₂O anchor point remains relatively well-defined. The largest uncertainties are thus found for the lowest of rate coefficients. In nearly all atmospheric situations, however, these low rate coefficients have a negligible contribution to the chemical fate of the CI, even in high relative humidities. We summarize and simplify by proposing a constant uncertainty of 1 order of magnitude at room temperature for all rate predictions, even if this is possibly an underestimate for $k(T) < 10^{-17}$ cm³ molecule⁻¹ s⁻¹. It should be noted that some of the values for pinonaldehyde oxide are subject to an additional uncertainty of a factor of 3 (see section F), owing to the fact that these are based on M06-2X barrier heights, not CCSD(T) energies.

Comparing the literature-based SAR (Table 32) against the theory-derived SAR (Table 35), we find that the rate coefficients remain in good agreement. Our theoretical predictions thus remain compatible with the available literature data, and represent mostly an expression of the trends obscured by the sparseness of the literature data set. The largest differences are found for the oxo-substituted CI, for which no literature data was available, but where the theory-based data clearly shows that large energy differences exist between the stereoisomers, and that the reactivity of these compounds both for unimolecular reactions and for water-reactions, is impacted strongly by the presence of these type of substituents.

We prefer the use of the theory-derived SAR, as this SAR corresponds well with the literature data, where available, but additionally captures the more subtle impact of different alkyl and vinyl substituents, and the larger impact of heterosubstituents. For the validation of this SAR, an accurately measured rate coefficient in the low end of the rate coefficient range would be invaluable to reduce the uncertainty, but this may be hard to achieve in practice.

7. Other correlations potentially useful for future SAR development

Expanding the current SAR to build upon a larger set of compounds, and cover a wider range of substituents is clearly desirable. From a practical view, however, these efforts will encounter significant computational hurdles, as larger substituents, more internal rotations with a concomitantly higher number of conformers, and other effects lead to more expensive quantum chemical calculations. In this section, we explore a few other correlations that are expected to hold for the CI + H₂O reaction, though not necessarily with the same high correlation coefficient as in the analysis above.

A first correlation proposed is the Evans-Polanyi relation between the barrier height for reaction, and the logarithm of the rate coefficient. Figure 15 shows that this correlation holds rather well for the CCSD(T)/M06-2X barrier heights of the reference compounds. It is also encouraging that a similarly good correlation can be seen for M06-2X data (Figure 16), which might allow one to skip the very expensive CCSD(T) calculations, and still derive fairly good predictions for rate coefficients based solely on the more accessible DFT calculations. In both cases, the average deviation is a factor of ~1.7, with maximum deviations of a factor 2.5. It should be noted that this type of correlation does not incorporate any entropic information, and is thus not expected to perform equally well across all types of conformers.

In sections H and N, we found that the reactivity of CI was fairly well described by group additivity, without the need for extensive cross-group factors, though this latter aspect could be the result of our limited data set. If group additivity holds, it strongly reduces the demands on SAR development, as not all combinations

of substituents need to be explicitly characterized. To investigate such an approach, we apply a group additivity scheme to the barrier height of the $\text{CI} + \text{H}_2\text{O}$ reaction, both for M06-2X and CCSD(T)//M06-2X derived barriers (see Figure 17 and Figure 18). In both cases, we find a very tight correlation using the group additivity terms listed in Table 36, and the following expressions :

$$E_b(\text{CCSD(T)}) = 1.36 \text{ kcal mol}^{-1} + F_{R1} + F_{R2}$$

$$E_b(\text{M06-2X}) = -1.22 \text{ kcal mol}^{-1} + F_{R1} + F_{R2}$$

The comparable quality in correlation for both DFT-based and CCSD(T)-based calculation could again allow a significantly reduced computation burden. One should bear in mind, however, that for many substituents no information on cross terms is available. It is thus not proven that cross-terms can be neglected in all cases.

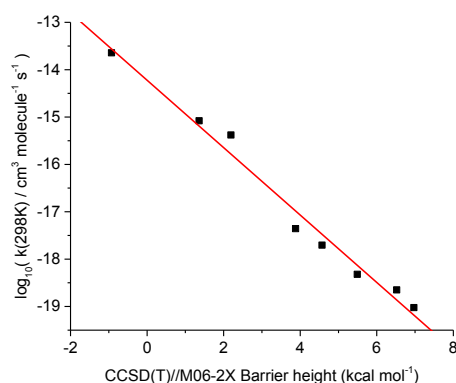


Figure 15: Correlation of the CCSD(T)/aug-cc-pVTZ//M06-2X/aug-cc-pVTZ barrier heights E_b against the reference rate coefficients $k(298\text{K})$. The trend (red line) can be written as $\log_{10}(k(298\text{K}) / \text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}) = -14.22 - 0.711 \times (E_b / \text{kcal mol}^{-1})$

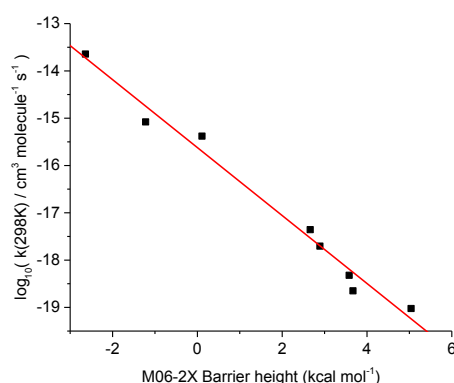


Figure 16: Correlation of the M06-2X/aug-cc-pVTZ barrier heights E_b against the reference rate coefficients $k(298\text{K})$. The trend (red line) can be written as $\log_{10}(k(298\text{K}) / \text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}) = -15.63 - 0.718 \times (E_b / \text{kcal mol}^{-1})$

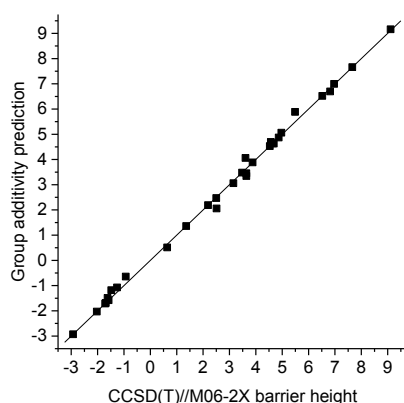


Figure 17: Group additivity predictions for CCSD(T)/M06-2X derived barrier heights (kcal mol^{-1}). The line represents a 1:1 correlation.

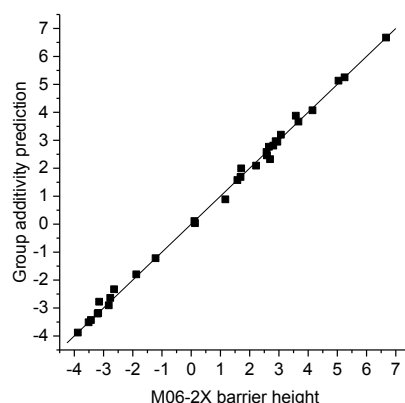


Figure 18: Group additivity predictions for M06-2X derived barrier heights (kcal mol^{-1}). The line represents a 1:1 correlation.

Table 36: Group additivity factors (kcal mol⁻¹) for the prediction of the barrier heights for the CI + H₂O reaction.

Substituent	SAR Substituent class	CCSD(T)//M06-2X barriers		M06-2X barriers	
		F_{R1}	F_{R2}	F_{R1}	F_{R2}
CH ₃	-CH ₃	4.53	-2.00	5.10	-1.11
C ₂ H ₅ / n-C ₃ H ₇	-CH ₂ R _a	3.70	-2.43	4.42	-1.42
CH ₂ -CH=CH ₂	-CH ₂ -CR ₃ =CR ₄ R ₅	3.28	3.07	4.17	-2.29
iC ₃ H ₇	-CHR _a R _b	2.70	-2.54	3.21	-1.55
CH(CH ₃)-CH=CH ₂	-CHR _a -CR ₃ =CR ₄ R ₅	2.12	-3.05	2.91	-1.98
CH=CH ₂ / CH=CH-CH ₃	-CH=CR ₄ R ₅	5.34	1.11	5.29	1.26
tC ₄ H ₉	-CR _a R _b R _c	3.51	-2.94	4.03	-1.96
C(CH ₃) ₂ -CH=CH ₂	-CR _a R _b -CR ₃ =CR ₄ R ₅	3.17	-3.39	3.80	-2.21
C(CH ₃)=CH ₂	-CR _a =CR ₄ R ₅	5.16	0.83	4.89	1.33
H	-H	0.00	0.00	0.00	0.00
CHO	-CHO	-0.85	3.27	-0.58	2.80
C(O)CH ₃	-C(O)R _a	-2.29	1.77	-1.55	1.37

As the barrier height is correlated to the rate coefficient, one can suspect that group additivity remains applicable to the rate coefficients. Expressing the $k(298K)$ data in Table 35 in terms of group additivity (see Table 37 for terms F_{R1} and F_{R2}) yields a fair, but not exceptionally good correlation, as shown in Figure 19, using the following formula:

$$k_{CI+H_2O}(298K) = 10^{(-15.06+F_{R1}+F_{R2})} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$$

When examining Figure 19, one should consider that many of the values in the SAR are obtained by applying reactivity trends across substituents, and are thus intrinsically assumed to adhere to group additivity, which explains much of the correlation. The largest deviations are found when the *syn*-substituent (R_1) is a tertiary carbon, i.e. iC₃H₇, -CH(CH₃)-CH=CH₂, etc., which are only reproduced within a factor of 4, and can be visually distinguished in Figure 19 as points on a line parallel to the 1:1 line (below the 1:1 line for log(k) between -19 and -17, above the 1:1 line for log(k) between -17.5 and -16). The poorer recovery here is related to the rate prediction for Z-(iC₃H₇)(CH₃)COO, which shows a different reactivity trend relative to Z-(iC₃H₇)CHOO, compared to e.g. $R_1 = H, CH_3, C_2H_5$, etc.; this influenced the reactivity trends used in the SAR. We were unable to find a reason for this difference, and it appears to be a property of the CI + H₂O reaction chemistry or an artefact of the level of theory used. If more data becomes available, it will be feasible to assess if group additivity can hold rigorously, or that cross-terms would need to be introduced to maintain a good predictability; our current data set suggests that the latter may be the case. At the same time, the current maximum deviation of a factor of 4 of the group additivity SAR relative to the explicit SAR remains a good result, considering the rate coefficients cover 8 decades, and that for many CI the reaction with H₂O will either be too slow or be dominating, such that a reduced accuracy has little impact on modeling predictions.

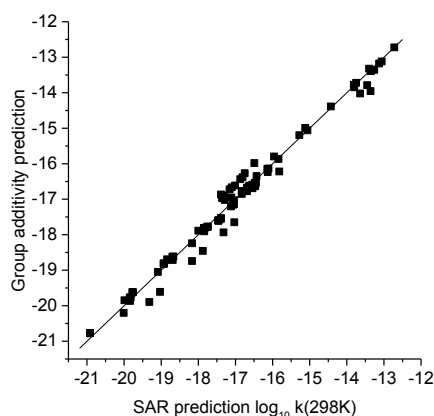


Figure 19: Group additivity predictions for the rate coefficients (cm³ molecule⁻¹ s⁻¹) of the theory-based SAR for CI + H₂O. The line represents a 1:1 correlation. See Figure 14 for a visualisation of the agreement between the theory-based SAR and the reference literature data.

Table 37: Group additivity factors for the prediction of the rate coefficient $k(298\text{K})$ for the $\text{Cl} + \text{H}_2\text{O}$ reaction:

Substituent	SAR Substituent class	F_{R1}	F_{R2}
CH_3	$-\text{CH}_3$	-3.18	1.04
C_2H_5 / $n\text{-C}_3\text{H}_7$	$-\text{CH}_2\text{R}_a$	-2.74	1.21
$\text{CH}_2=\text{CH}=\text{CH}_2$	$-\text{CH}_2-\text{CR}_3=\text{CR}_4\text{R}_5$	-2.84	1.21
$i\text{C}_3\text{H}_7$	$-\text{CHR}_a\text{R}_b$	-2.59	1.27
$\text{CH}(\text{CH}_3)-\text{CH}=\text{CH}_2$	$-\text{CHR}_a-\text{CR}_3=\text{CR}_4\text{R}_5$	-2.87	1.27
$\text{CH}=\text{CH}_2$ / $\text{CH}=\text{CH}-\text{CH}_3$	$-\text{CH}=\text{CR}_4\text{R}_5$	-3.75	-0.81
$t\text{C}_4\text{H}_9$	$-\text{CR}_a\text{R}_b\text{R}_c$	-2.83	1.67
$\text{C}(\text{CH}_3)_2-\text{CH}=\text{CH}_2$	$-\text{CR}_a\text{R}_b-\text{CR}_3=\text{CR}_4\text{R}_5$	-2.75	1.67
$\text{C}(\text{CH}_3)=\text{CH}_2$	$-\text{CR}_a=\text{CR}_4\text{R}_5$	-0.58	-0.81
H	-H	0.00	0.00
CHO	-CHO	0.07	-1.96
$\text{C}(\text{O})\text{CH}_3$	$-\text{C}(\text{O})\text{R}_a$	0.67	-1.96

T. The reaction of CI with (H₂O)₂

1. Literature data

Compared to the reaction of CI with the water monomer, significantly less literature data is available on the CI + (H₂O)₂ reaction. We refer to section S for some general comments on the CI + water reactions; an overview of the available data for the reaction with water dimer is tabulated Table 5 in section E.3. The only rate coefficient where consensus is reached, within a factor of 2, appears to be the CH₂OO + (H₂O)₂ reaction, with three independent rate coefficient measurements; in this work, we will use this value as our golden standard.

2. Structure-Activity Relationship (SAR) for the CI + (H₂O)₂, based on literature data

As for the reaction of CI with water monomers, we will use the available literature data to derive a conservative SAR. The data is first harmonized as follows:

a) For the CH₂OO + (H₂O)₂ reaction, $k(T)$ is obtained from the geometric average of the experimental data, $k(298\text{K}) = 5.8 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, where we use the experimental temperature dependence by Smith et al.⁷⁰, though at low (<250K) and high (>400K) this expression is likely to be inaccurate due to the lack of curvature. The theoretical work by Lin et al.⁶⁰ is in excellent agreement with this value.

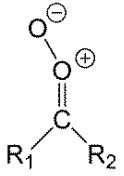
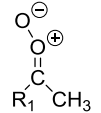
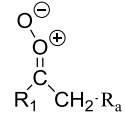
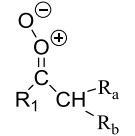
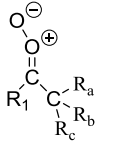
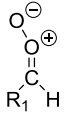
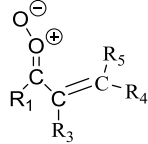
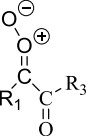
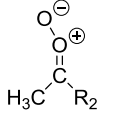
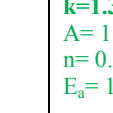
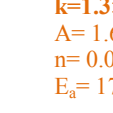
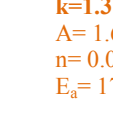
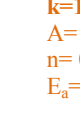
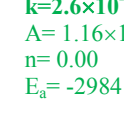
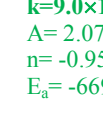
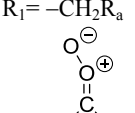
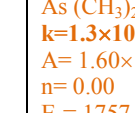
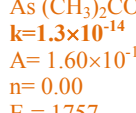
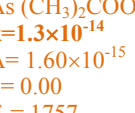
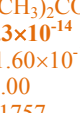
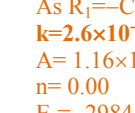
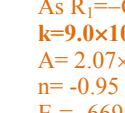
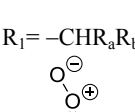
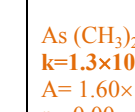
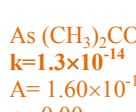
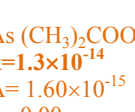
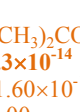
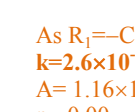
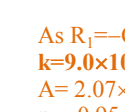
b) For the reaction of *E*-CH₃CHOO with water dimers, we use the rate coefficient expression by Lin et al.,⁶⁰ selected for its good agreement with experiment for the CH₂OO case. As for H₂O, we apply this rate coefficient to the reaction of other *E*-RCHOO with (H₂O)₂, as these can be expected to show similar enhanced reactivity compared to their *Z*-stereoisomer.

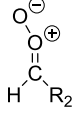
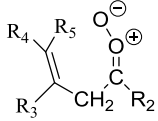
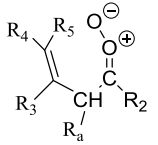
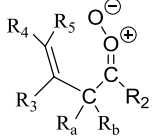
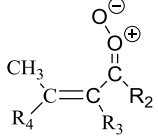
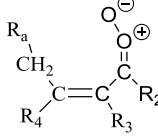
c) For *Z*-CH₃CHOO, we again select the data by Lin et al.⁶⁰ for the reaction with water dimers, owing to its good agreement with experiment for the CH₂OO reaction; we apply this rate coefficient to other *Z*-R₁CHOO + (H₂O)₂ reactions.

d) For the reaction of (H₂O)₂ with (CH₃)₂COO and with unsaturated CI, the best or only systematic data available is the theoretical work by Anglada and Solé (2016).⁶¹ Comparison of their predictions for CH₂OO, *E*- and *Z*-CH₃CHOO against the values adopted in items (a), (b) and (c), suggests that the Anglada and Solé $k(T)$ values might be overestimates. This was also found for the H₂O monomer reactions, and appears to be an artifact of the level of theory applied, leading to an underestimation of the barrier height. The Anglada and Solé predictions⁶¹ can be brought into agreement with the aforementioned values by barrier height corrections of +2.0 kcal mol⁻¹, +2.1 kcal mol⁻¹, and +1.7 kcal mol⁻¹, respectively, i.e. a fairly systematic correction. We choose here to scale the Anglada and Solé rate predictions down by increasing the effective activation energy by $\Delta E = 2.0$ kcal mol⁻¹, which corresponds roughly to the average barrier corrections needed in items (a), (b), and (c). For β -unsaturated CI, we furthermore merge the Anglada and Solé data for *s-trans* and *s-cis* conformers to account for their rapid isomerisation, using the same methodology as used in section S. Finally, we propose similar reactivity trends as for the CI + H₂O reaction, where for those CI for which we have no direct data, we use the (averaged) rate coefficients of simpler substituents (typically CH₃) for which we have data.

Table 38 lists the predicted rate coefficients at 298 K, and gives an Arrhenius/Kooij expression for the temperature-dependence. This table also give some indication how a specific entry was obtained.

Table 38: Predicted total rate coefficients for the reaction of carbonyl oxide with water dimers (H₂O)₂ as a function of the two substituents R₁ and R₂. The first line of each entry indicates how the values were obtained, i.e. averaged from experimental and theoretical data, or assumed to be identical to a similar substitution pattern. The rate coefficient *k* (cm³ molecule⁻¹ s⁻¹) is given at 298K, and the parameters of a Kooij equation fit $k(T) = A \times T^n \times \exp(-E_a/T)$ between 200 and 450 K (*A* in cm³ molecule⁻¹ s⁻¹, *E_a* in K). The definition of R_a/R_b/R_c/R₃/R₄/R₅/R' is given in Table 1. Values in green are based directly on experimental and theoretical literature data, values in orange are values estimated by similarity to other compounds. **SEE Table 40 FOR A SAR THAT ADDITIONALLY INCORPORATES THEORY-BASED REACTION TRENDS (RECOMMENDED).**

	R ₂ = -CH ₃	R ₂ = -CH ₂ R _a	R ₂ = -CHR _a R _b	R ₂ = -CR _a R _b R _c	R ₂ = -H	R ₂ = vinyl	R ₂ = oxo
R ₁ = -CH ₃							
R ₁ = -CH ₂ R _a							
R ₁ = -CHR _a R _b							
R ₁ = -CR _a R _b R _c							
	Theory <i>k</i> = 1.3 × 10⁻¹⁴ <i>A</i> = 1.60 × 10 ⁻¹⁵ <i>n</i> = 0.00 <i>E_a</i> = 1757	As (CH ₃) ₂ COO <i>k</i> = 1.3 × 10⁻¹⁴ <i>A</i> = 1.60 × 10 ⁻¹⁵ <i>n</i> = 0.00 <i>E_a</i> = 1757	As (CH ₃) ₂ COO <i>k</i> = 1.3 × 10⁻¹⁴ <i>A</i> = 1.60 × 10 ⁻¹⁵ <i>n</i> = 0.00 <i>E_a</i> = 1757	As (CH ₃) ₂ COO <i>k</i> = 1.3 × 10⁻¹⁴ <i>A</i> = 1.60 × 10 ⁻¹⁵ <i>n</i> = 0.00 <i>E_a</i> = 1757	Theory <i>k</i> = 2.6 × 10⁻¹⁴ <i>A</i> = 1.16 × 10 ⁻¹⁸ <i>n</i> = 0.00 <i>E_a</i> = -2984	Theory <i>k</i> = 9.0 × 10⁻¹⁷ <i>A</i> = 2.07 × 10 ⁻¹⁵ <i>n</i> = -0.95 <i>E_a</i> = -669	As (CH ₃) ₂ COO <i>k</i> = 1.3 × 10⁻¹⁴ <i>A</i> = 1.60 × 10 ⁻¹⁵ <i>n</i> = 0.00 <i>E_a</i> = 1757
	As (CH ₃) ₂ COO <i>k</i> = 1.3 × 10⁻¹⁴ <i>A</i> = 1.60 × 10 ⁻¹⁵ <i>n</i> = 0.00 <i>E_a</i> = 1757	As (CH ₃) ₂ COO <i>k</i> = 1.3 × 10⁻¹⁴ <i>A</i> = 1.60 × 10 ⁻¹⁵ <i>n</i> = 0.00 <i>E_a</i> = 1757	As (CH ₃) ₂ COO <i>k</i> = 1.3 × 10⁻¹⁴ <i>A</i> = 1.60 × 10 ⁻¹⁵ <i>n</i> = 0.00 <i>E_a</i> = 1757	As (CH ₃) ₂ COO <i>k</i> = 1.3 × 10⁻¹⁴ <i>A</i> = 1.60 × 10 ⁻¹⁵ <i>n</i> = 0.00 <i>E_a</i> = 1757	As R ₁ = -CH ₃ <i>k</i> = 2.6 × 10⁻¹⁴ <i>A</i> = 1.16 × 10 ⁻¹⁸ <i>n</i> = 0.00 <i>E_a</i> = -2984	As R ₁ = -CH ₃ <i>k</i> = 9.0 × 10⁻¹⁷ <i>A</i> = 2.07 × 10 ⁻¹⁵ <i>n</i> = -0.95 <i>E_a</i> = -669	As R ₁ = -CH ₃ <i>k</i> = 9.0 × 10⁻¹⁷ <i>A</i> = 2.07 × 10 ⁻¹⁵ <i>n</i> = -0.95 <i>E_a</i> = -669
	As (CH ₃) ₂ COO <i>k</i> = 1.3 × 10⁻¹⁴ <i>A</i> = 1.60 × 10 ⁻¹⁵ <i>n</i> = 0.00 <i>E_a</i> = 1757	As (CH ₃) ₂ COO <i>k</i> = 1.3 × 10⁻¹⁴ <i>A</i> = 1.60 × 10 ⁻¹⁵ <i>n</i> = 0.00 <i>E_a</i> = 1757	As (CH ₃) ₂ COO <i>k</i> = 1.3 × 10⁻¹⁴ <i>A</i> = 1.60 × 10 ⁻¹⁵ <i>n</i> = 0.00 <i>E_a</i> = 1757	As (CH ₃) ₂ COO <i>k</i> = 1.3 × 10⁻¹⁴ <i>A</i> = 1.60 × 10 ⁻¹⁵ <i>n</i> = 0.00 <i>E_a</i> = 1757	As R ₁ = -CH ₃ <i>k</i> = 2.6 × 10⁻¹⁴ <i>A</i> = 1.16 × 10 ⁻¹⁸ <i>n</i> = 0.00 <i>E_a</i> = -2984	As R ₁ = -CH ₃ <i>k</i> = 9.0 × 10⁻¹⁷ <i>A</i> = 2.07 × 10 ⁻¹⁵ <i>n</i> = -0.95 <i>E_a</i> = -669	As R ₁ = -CH ₃ <i>k</i> = 9.0 × 10⁻¹⁷ <i>A</i> = 2.07 × 10 ⁻¹⁵ <i>n</i> = -0.95 <i>E_a</i> = -669
	As (CH ₃) ₂ COO <i>k</i> = 1.3 × 10⁻¹⁴ <i>A</i> = 1.60 × 10 ⁻¹⁵ <i>n</i> = 0.00 <i>E_a</i> = 1757	As (CH ₃) ₂ COO <i>k</i> = 1.3 × 10⁻¹⁴ <i>A</i> = 1.60 × 10 ⁻¹⁵ <i>n</i> = 0.00 <i>E_a</i> = 1757	As (CH ₃) ₂ COO <i>k</i> = 1.3 × 10⁻¹⁴ <i>A</i> = 1.60 × 10 ⁻¹⁵ <i>n</i> = 0.00 <i>E_a</i> = 1757	As (CH ₃) ₂ COO <i>k</i> = 1.3 × 10⁻¹⁴ <i>A</i> = 1.60 × 10 ⁻¹⁵ <i>n</i> = 0.00 <i>E_a</i> = 1757	As R ₁ = -CH ₃ <i>k</i> = 2.6 × 10⁻¹⁴ <i>A</i> = 1.16 × 10 ⁻¹⁸ <i>n</i> = 0.00 <i>E_a</i> = -2984	As R ₁ = -H <i>k</i> = 1.2 × 10⁻¹³ <i>A</i> = 6.19 × 10 ⁻²⁰ <i>n</i> = 0.77 <i>E_a</i> = -3006	As R ₁ = -H <i>k</i> = 1.2 × 10⁻¹³ <i>A</i> = 6.19 × 10 ⁻²⁰ <i>n</i> = 0.77 <i>E_a</i> = -3006

$R_1 = -H$ 	Theory $k=1.6 \times 10^{-11}$ $A=1.63 \times 10^{-18}$ $n=0.00$ $E_a=-4801$	$As R_2=-CH_3$ $k=1.6 \times 10^{-11}$ $A=1.63 \times 10^{-18}$ $n=0.00$ $E_a=-4801$	$As R_2=-CH_3$ $k=1.6 \times 10^{-11}$ $A=1.63 \times 10^{-18}$ $n=0.00$ $E_a=-4801$	$As R_2=-CH_3$ $k=1.6 \times 10^{-11}$ $A=1.63 \times 10^{-18}$ $n=0.00$ $E_a=-4801$	Average Exp. $k=5.8 \times 10^{-12}$ $A=8.48 \times 10^{-18}$ $n=0.00$ $E_a=-4003$	Theory $k=1.2 \times 10^{-13}$ $A=6.19 \times 10^{-20}$ $n=0.77$ $E_a=-3006$	$As R_2=-CH_3$ $k=1.6 \times 10^{-11}$ $A=1.63 \times 10^{-18}$ $n=0.00$ $E_a=-4801$
$R_1 = -CH_2-CR_3=CR_4R_5$ 	$As (CH_3)_2COO$ $k=1.3 \times 10^{-14}$ $A=1.60 \times 10^{-15}$ $n=0.00$ $E_a=1757$	$As (CH_3)_2COO$ $k=1.3 \times 10^{-14}$ $A=1.60 \times 10^{-15}$ $n=0.00$ $E_a=1757$	$As (CH_3)_2COO$ $k=1.3 \times 10^{-14}$ $A=1.60 \times 10^{-15}$ $n=0.00$ $E_a=1757$	$As (CH_3)_2COO$ $k=1.3 \times 10^{-14}$ $A=1.60 \times 10^{-15}$ $n=0.00$ $E_a=1757$	$As R_1=-CH_2R_a$ $k=2.6 \times 10^{-14}$ $A=1.16 \times 10^{-18}$ $n=0.00$ $E_a=-2984$	$As R_1=-CH_2R_a$ $k=9.0 \times 10^{-17}$ $A=2.07 \times 10^{-15}$ $n=-0.95$ $E_a=-669$	$As R_1=-CH_2R_a$ $k=9.0 \times 10^{-17}$ $A=2.07 \times 10^{-15}$ $n=-0.95$ $E_a=-669$
$R_1 = -CHR_a-CR_3=CR_4R_5$ 	$As (CH_3)_2COO$ $k=1.3 \times 10^{-14}$ $A=1.60 \times 10^{-15}$ $n=0.00$ $E_a=1757$	$As (CH_3)_2COO$ $k=1.3 \times 10^{-14}$ $A=1.60 \times 10^{-15}$ $n=0.00$ $E_a=1757$	$As (CH_3)_2COO$ $k=1.3 \times 10^{-14}$ $A=1.60 \times 10^{-15}$ $n=0.00$ $E_a=1757$	$As (CH_3)_2COO$ $k=1.3 \times 10^{-14}$ $A=1.60 \times 10^{-15}$ $n=0.00$ $E_a=1757$	$As R_1=-CHR_aR_b$ $k=2.6 \times 10^{-14}$ $A=1.16 \times 10^{-18}$ $n=0.00$ $E_a=-2984$	$As R_1=-CHR_aR_b$ $k=9.0 \times 10^{-17}$ $A=2.07 \times 10^{-15}$ $n=-0.95$ $E_a=-669$	$As R_1=-CHR_aR_b$ $k=9.0 \times 10^{-17}$ $A=2.07 \times 10^{-15}$ $n=-0.95$ $E_a=-669$
$R_1 = -CR_aR_b-CR_3=CR_4R_5$ 	$As (CH_3)_2COO$ $k=1.3 \times 10^{-14}$ $A=1.60 \times 10^{-15}$ $n=0.00$ $E_a=1757$	$As (CH_3)_2COO$ $k=1.3 \times 10^{-14}$ $A=1.60 \times 10^{-15}$ $n=0.00$ $E_a=1757$	$As (CH_3)_2COO$ $k=1.3 \times 10^{-14}$ $A=1.60 \times 10^{-15}$ $n=0.00$ $E_a=1757$	$As (CH_3)_2COO$ $k=1.3 \times 10^{-14}$ $A=1.60 \times 10^{-15}$ $n=0.00$ $E_a=1757$	$As (CH_3)_2COO$ $k=1.3 \times 10^{-14}$ $A=1.60 \times 10^{-15}$ $n=0.00$ $E_a=1757$	$As R_1=-CR_aR_bR_c$ $k=1.2 \times 10^{-13}$ $A=6.19 \times 10^{-20}$ $n=0.77$ $E_a=-3006$	$As R_1=-CR_aR_bR_c$ $k=1.2 \times 10^{-13}$ $A=6.19 \times 10^{-20}$ $n=0.77$ $E_a=-3006$
$R_1 = -CR_3=CR_4CH_3$ 	$As R_1=-CR_3=CR_4R'$ $k=6.1 \times 10^{-16}$ $A=5.43 \times 10^{-21}$ $n=0.90$ $E_a=-1939$	$As R_2=-CH_3$ $k=6.1 \times 10^{-16}$ $A=5.43 \times 10^{-21}$ $n=0.90$ $E_a=-1939$	$As R_2=-CH_3$ $k=6.1 \times 10^{-16}$ $A=5.43 \times 10^{-21}$ $n=0.90$ $E_a=-1939$	$As R_2=-CH_3$ $k=6.1 \times 10^{-16}$ $A=5.43 \times 10^{-21}$ $n=0.90$ $E_a=-1939$	$As R_1=-CR_3=CR_4R'$ $k=8.5 \times 10^{-16}$ $A=4.74 \times 10^{-18}$ $n=0.10$ $E_a=-1380$	$As R_2=-CH_3$ $k=6.1 \times 10^{-16}$ $A=5.43 \times 10^{-21}$ $n=0.90$ $E_a=-1939$	$As R_2=-CH_3$ $k=6.1 \times 10^{-16}$ $A=5.43 \times 10^{-21}$ $n=0.90$ $E_a=-1939$
$R_1 = -CR_3=CR_4CH_2R_a$ 	$As R_1=-CR_3=CR_4R'$ $k=6.1 \times 10^{-16}$ $A=5.43 \times 10^{-21}$ $n=0.90$ $E_a=-1939$	$As R_2=-CH_3$ $k=6.1 \times 10^{-16}$ $A=5.43 \times 10^{-21}$ $n=0.90$ $E_a=-1939$	$As R_2=-CH_3$ $k=6.1 \times 10^{-16}$ $A=5.43 \times 10^{-21}$ $n=0.90$ $E_a=-1939$	$As R_2=-CH_3$ $k=6.1 \times 10^{-16}$ $A=5.43 \times 10^{-21}$ $n=0.90$ $E_a=-1939$	$As R_1=-CR_3=CR_4R'$ $k=8.5 \times 10^{-16}$ $A=4.74 \times 10^{-18}$ $n=0.10$ $E_a=-1380$	$As R_2=-CH_3$ $k=6.1 \times 10^{-16}$ $A=5.43 \times 10^{-21}$ $n=0.90$ $E_a=-1939$	$As R_2=-CH_3$ $k=6.1 \times 10^{-16}$ $A=5.43 \times 10^{-21}$ $n=0.90$ $E_a=-1939$

$R_1 = -CR_3=CR_4CHR_aR_b$ 	$As\ R_1=-CR_3=CR_4R'$ $k=6.1\times 10^{-16}$ $A=5.43\times 10^{-21}$ $n=0.90$ $E_a=-1939$	$As\ R_2=-CH_3$ $k=6.1\times 10^{-16}$ $A=5.43\times 10^{-21}$ $n=0.90$ $E_a=-1939$	$As\ R_2=-CH_3$ $k=6.1\times 10^{-16}$ $A=5.43\times 10^{-21}$ $n=0.90$ $E_a=-1939$	$As\ R_2=-CH_3$ $k=6.1\times 10^{-16}$ $A=5.43\times 10^{-21}$ $n=0.90$ $E_a=-1939$	$As\ R_1=-CR_3=CR_4R'$ $k=8.5\times 10^{-16}$ $A=4.74\times 10^{-18}$ $n=0.10$ $E_a=-1380$	$As\ R_2=-CH_3$ $k=6.1\times 10^{-16}$ $A=5.43\times 10^{-21}$ $n=0.90$ $E_a=-1939$	$As\ R_2=-CH_3$ $k=6.1\times 10^{-16}$ $A=5.43\times 10^{-21}$ $n=0.90$ $E_a=-1939$
$R_1 = -CR_3=CR_4R'$ 	Theory $k=6.1\times 10^{-16}$ $A=5.43\times 10^{-21}$ $n=0.90$ $E_a=-1939$	$As\ R_2=-CH_3$ $k=6.1\times 10^{-16}$ $A=5.43\times 10^{-21}$ $n=0.90$ $E_a=-1939$	$As\ R_2=-CH_3$ $k=6.1\times 10^{-16}$ $A=5.43\times 10^{-21}$ $n=0.90$ $E_a=-1939$	$As\ R_2=-CH_3$ $k=6.1\times 10^{-16}$ $A=5.43\times 10^{-21}$ $n=0.90$ $E_a=-1939$	Theory $k=8.5\times 10^{-16}$ $A=4.74\times 10^{-18}$ $n=0.10$ $E_a=-1380$	$As\ R_2=-CH_3$ $k=6.1\times 10^{-16}$ $A=5.43\times 10^{-21}$ $n=0.90$ $E_a=-1939$	$As\ R_2=-CH_3$ $k=6.1\times 10^{-16}$ $A=5.43\times 10^{-21}$ $n=0.90$ $E_a=-1939$
$R_1 = -CHO$ 	$As\ (CH_3)_2COO$ $k=1.3\times 10^{-14}$ $A=1.60\times 10^{-15}$ $n=0.00$ $E_a=1757$	$As\ (CH_3)_2COO$ $k=1.3\times 10^{-14}$ $A=1.60\times 10^{-15}$ $n=0.00$ $E_a=1757$	$As\ (CH_3)_2COO$ $k=1.3\times 10^{-14}$ $A=1.60\times 10^{-15}$ $n=0.00$ $E_a=1757$	$As\ (CH_3)_2COO$ $k=1.3\times 10^{-14}$ $A=1.60\times 10^{-15}$ $n=0.00$ $E_a=1757$	$As\ R_1=-CH_3$ $k=2.6\times 10^{-14}$ $A=1.16\times 10^{-18}$ $n=0.00$ $E_a=-2984$	$As\ R_1=-CH_3$ $k=9.0\times 10^{-17}$ $A=2.07\times 10^{-15}$ $n=-0.95$ $E_a=-669$	$As\ R_1=-CH_3$ $k=9.0\times 10^{-17}$ $A=2.07\times 10^{-15}$ $n=-0.95$ $E_a=-669$
$R_1 = -C(O)R_a$ 	$As\ (CH_3)_2COO$ $k=1.3\times 10^{-14}$ $A=1.60\times 10^{-15}$ $n=0.00$ $E_a=1757$	$As\ (CH_3)_2COO$ $k=1.3\times 10^{-14}$ $A=1.60\times 10^{-15}$ $n=0.00$ $E_a=1757$	$As\ (CH_3)_2COO$ $k=1.3\times 10^{-14}$ $A=1.60\times 10^{-15}$ $n=0.00$ $E_a=1757$	$As\ (CH_3)_2COO$ $k=1.3\times 10^{-14}$ $A=1.60\times 10^{-15}$ $n=0.00$ $E_a=1757$	$As\ R_1=-CH_3$ $k=2.6\times 10^{-14}$ $A=1.16\times 10^{-18}$ $n=0.00$ $E_a=-2984$	$As\ R_1=-H$ $k=1.2\times 10^{-13}$ $A=6.19\times 10^{-20}$ $n=0.77$ $E_a=-3006$	$As\ R_1=-H$ $k=1.2\times 10^{-13}$ $A=6.19\times 10^{-20}$ $n=0.77$ $E_a=-3006$

3. Correlations between literature rate coefficients, and theory-based or graph-based indicators

Similar to the reaction with H_2O , the rate coefficient of the $\text{CI} + (\text{H}_2\text{O})_2$ reaction is determined by the substituents on either side of the carbonyl oxide, and the relative stability of the CI stereoisomer thus formed. It would be worthwhile if we could also incorporate this molecular information into a SAR to fine-tune the rate coefficient predictions, especially for those substituents for which no direct experimental data or high-level theoretical data is currently available.

Due to the increased computational demands of characterizing the $\text{CI} + (\text{H}_2\text{O})_2$ reactions compared to H_2O or unimolecular reactions, we chose not to perform an extensive series of calculations on these reactions. To estimate the rate coefficient, we will attempt to link the available data on the $\text{CI} + \text{H}_2\text{O}$ reaction to the water dimer reaction literature data. Both reactions involve a H-migration to the carbonyl oxide outer oxygen with a concerted OH addition on the carbonyl C-atom, proceed through a pre-reactive complex, have a clearly defined transition state, have similar exothermicity, and as such share many similarities that might allow us to use data on the $\text{CI} + \text{H}_2\text{O}$ reaction to derive reaction trends on the $(\text{H}_2\text{O})_2$ counterpart. Obviously, there are non-negligible differences between these reactions as well, and a lower accuracy of the predictive correlations is expected.

Figure 20 shows that the selected reference literature data on the $\text{CI} + \text{H}_2\text{O}$ and $(\text{H}_2\text{O})_2$ reactions as listed in Table 33 are correlated by a clear trend, with deviation from this trend of a factor of ~ 5 on average; $Z\text{-CH}_3\text{CHOO}$ shows the largest deviation of a factor of 18 and accounts for much of the summed squared residuals in the linear correlation. Figure 21 shows the correlation between the theory-derived $k(\text{CI} + \text{H}_2\text{O})$ against the literature data for $k(\text{CI} + (\text{H}_2\text{O})_2)$, a correlation that is found to be even more pronounced with an average deviation of only a factor of 4, and a maximum deviation of less than a factor of 14 (again for $Z\text{-CH}_3\text{CHOO}$), across 6 orders of magnitude. Combined, these two plots confirm our hypothesis that the rate of reaction for H_2O and $(\text{H}_2\text{O})_2$ are influenced by similar molecular properties. A first-order SAR could thus predict the $\text{CI} + (\text{H}_2\text{O})_2$ rate coefficient within an order of magnitude from the $k(\text{CI} + \text{H}_2\text{O})$ proposed in section S and the trend line obtained from Figure 21.

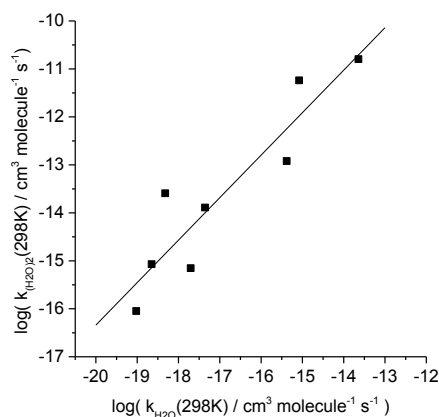


Figure 20: Correlation between the reference rate coefficients at 298K (see Table 33) for the $\text{CI} + \text{H}_2\text{O}$ and the $\text{CI} + (\text{H}_2\text{O})_2$ reactions. The trend line matches $\log_{10}(k(\text{CI} + (\text{H}_2\text{O})_2)) = 1.36 + 0.885 \times \log_{10}(k(\text{CI} + \text{H}_2\text{O}))$ (units $k(298\text{K})$ of $\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$).

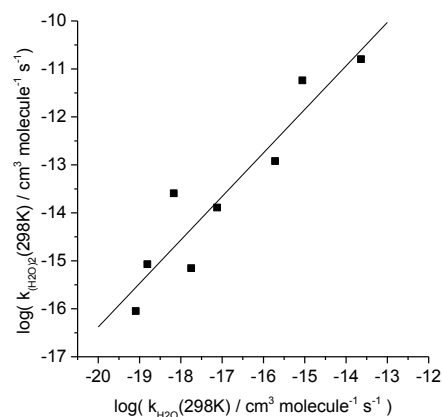


Figure 21: Correlation between the theory-predicted rate coefficients at 298K for the $\text{CI} + \text{H}_2\text{O}$ reaction (see Table 34) and the reference rate coefficients for the $\text{CI} + (\text{H}_2\text{O})_2$ reactions (see Table 33). The trend line matches $\log_{10}(k(\text{CI} + (\text{H}_2\text{O})_2)) = 1.77 + 0.908 \times \log_{10}(k(\text{CI} + \text{H}_2\text{O}))$ (units $k(298\text{K})$ of $\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$).

A more refined approach would be adjust the potential energy surface of the $\text{CI} + \text{H}_2\text{O}$ reaction to more closely mimic the $\text{CI} + (\text{H}_2\text{O})_2$ reaction, but retaining the same molecular properties. The key energetic differences for the PES are the barrier height, which is significantly lower for $(\text{H}_2\text{O})_2$ compared to H_2O , and the

pre-reactive complex, which is several kcal mol⁻¹ more stable with (H₂O)₂ than with H₂O and thus affects the tunneling correction. The reaction exoergicity remains similar, ~ 40 kcal mol⁻¹, at least to the hydroxy-alkylhydroperoxide + H₂O complex, which is the parameter that affects tunneling. Performing theoretical kinetic calculations on a thus modified PES, but using the CI + H₂O rovibrational characteristics, should be somewhat more robust for extrapolations outside the training set, as it estimates the non-linear/non-logarithmic effect of tunneling as a function of the barrier height. Furthermore, such a kinetic model is more straightforward to extend as more data becomes available in future. As before, the key parameter on the PES remains the barrier height to reaction; Figure 22 shows the correlation of the CI + H₂O barrier height against the literature rate coefficients of CI + (H₂O)₂. Most of the reactivity trend can thus be recovered by a suitable estimate of the barrier height. Our kinetic model then consists of calculating the rate coefficients using CTST based on the rovibrational characteristics of the CI + H₂O reactants and TS, but with a pre-reactive complex -11 kcal mol⁻¹ below the reactants, as found in quantum chemical calculations,^{1,26,37-40,59-61,64,66,196} a post-reactive complex -40 kcal mol⁻¹ below the reactants, and relying on a barrier height obtained from the CI + H₂O CCSD(T)//M06-2X barrier height as follows:

$$E_b(\text{CI} + (\text{H}_2\text{O})_2) = 0.85 \times E_b(\text{CI} + \text{H}_2\text{O}) - 2.86 \text{ kcal mol}^{-1}$$

It should be noted that many of the reaction barriers thus obtained are submerged, i.e. the reaction proceeds over a TS that lies below the energy of the separated reactants. The energy lowering of the TS due to H-bonding with the water dimer complexes, and due to a less strained TS ring geometry, are the principal reason why the CI + (H₂O)₂ reaction is significantly faster than the CI + H₂O reaction, allowing it in many cases to become the dominant loss process of CI in the atmosphere.

The rate coefficients thus obtained correlate well with the reference data set from Table 33, as illustrated in Figure 23. The recovery remains similar to the earlier correlations, with an average deviation of a factor of 4, and a largest deviation of a factor of 13.6 for k(Z-CH₃CHOO + (H₂O)₂). Table 39 lists the rate coefficients for all CI for which we have explicit theoretical data on the CI + H₂O reaction.

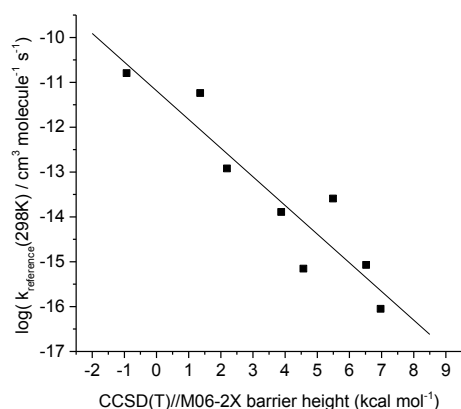


Figure 22: Correlation between the CCSD(T)//M06-2X barrier height for the CI + H₂O reaction, against the reference rate coefficients for the CI + (H₂O)₂ reactions (Table 33).

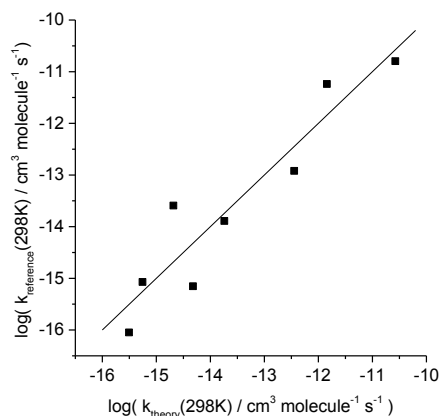


Figure 23: Correlation between the theory-based rate coefficients for the CI + (H₂O)₂ reactions against the reference rate coefficients from Table 33. The line represents a 1:1 correlation.

4. Structure-activity Relationship (SAR) for CI + (H₂O)₂ reaction, incorporating theoretical data

Using the data in Table 39, we again extrapolate the reactivity trends across all combinations of the two carbonyl oxide substituents R₁ and R₂, where we match the substituent classes used earlier in the SAR for unimolecular reaction (see section R) and defined in Table 1. The results SAR is available in Table 40.

5. Uncertainty analysis

The uncertainty on the barrier heights estimated through the above approach carries a rather large uncertainty, which could easily reach ± 1 kcal mol⁻¹ or more. The agreement between the reference rate coefficients for the CI + (H₂O)₂ reactions, and the correlation line that determines the barrier height modifications is on average again a factor of 4, with deviations as high as a factor of 15; this covers uncertainties in tunneling, vibrational anharmonicity, internal rotation, etc. At the same time, the reference rate coefficients are not highly accurate either. For only one rate coefficient (CH₂OO + (H₂O)₂) has consensus been reached across multiple measurements, and this anchor point has a very large influence on our predictions. Many of the other values were derived by large corrections on literature data to bring theoretically predicted values in agreement with this one anchor point, and especially for rate coefficients that are strongly different from the reference point this could introduce large uncertainties on the reference values themselves.

As many of the CI + (H₂O)₂ reaction have submerged barriers, there is the possibility that the assumption in our kinetic model of equilibrium between separated reactants and pre-reactive complex no longer holds rigorously. Indeed, reactions with submerged barriers can show pressure-dependence owing to the contribution of non-thermal nascent complexes to the reaction flux. This introduces another source of errors, which we estimate at about a factor of 3 at room temperature and 1 atm.

Overall, we estimate that the absolute rate coefficients carry an uncertainty of the order of a factor ~ 40 across the entire range of values. There is likely a better overall performance than this value due to cancellation of error, but in view of the very limited set of reference rate coefficients, and the uncertainty on these reference values themselves, we can't test this hypothesis. It should be noted that some of the values for pinonaldehyde oxide are subject to an additional uncertainty of a factor of 3, owing to the fact that their $k(\text{CI} + \text{H}_2\text{O})$ values are based on adjusted M06-2X barrier heights, not CCSD(T) energies.

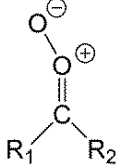
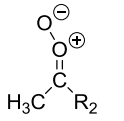
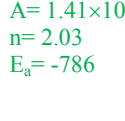
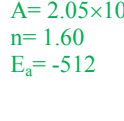
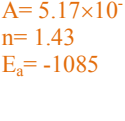
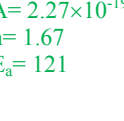
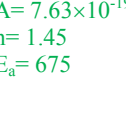
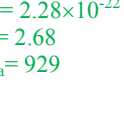
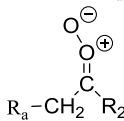
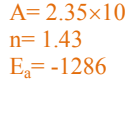
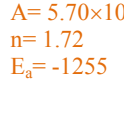
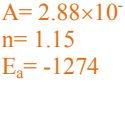
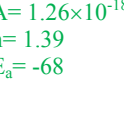
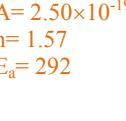
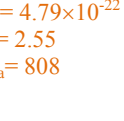
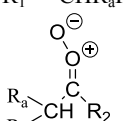
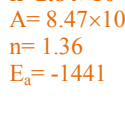
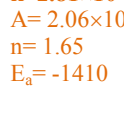
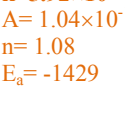
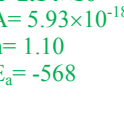
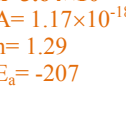
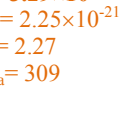
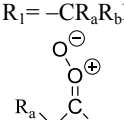
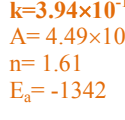
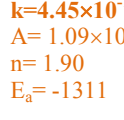
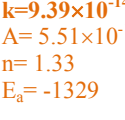
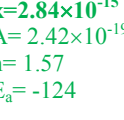
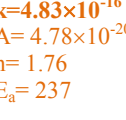
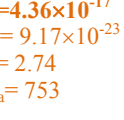
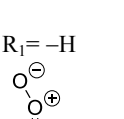
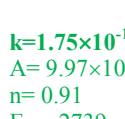
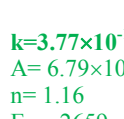
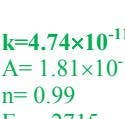
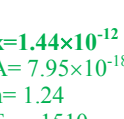
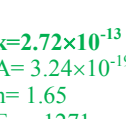
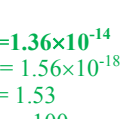
Similar to the CI + H₂O rate coefficient predictions, we should bear in mind that the predicted $k(T)$ is important mostly relative to other loss processes, and in many cases it is sufficient to determine that the reaction of CI with water dimers is negligibly slow, or overwhelmingly fast. More experimental data and high quality theoretical work is needed to calibrate the predictions for those cases where a competition between different reactions is at play, or where absolute steady-state concentrations are required.

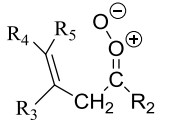
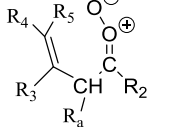
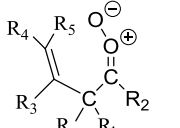
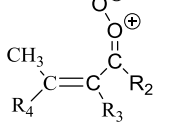
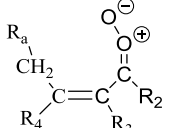
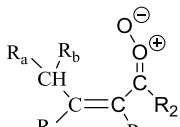
Table 39: Rate constant predictions for the reaction of CI with (H₂O)₂ obtained after barrier height corrections in the theoretical data, listing barrier heights E_b (kcal mol⁻¹), rate coefficient k (cm³ molecule⁻¹ s⁻¹) at 298 K, and parameters for a Kooij equation fit $k(T)=A \times T^n \times \exp(-E_a/T)$ cm³ molecule⁻¹ s⁻¹ for the temperature range 200-450 K. The first 8 entries correspond to the reference compounds in Table 33.

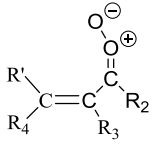
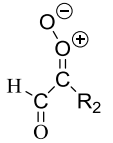
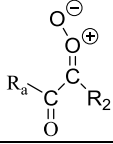
Carbonyl oxide	E_b	$k(298K)$	A	n	E_a / K
CH ₂ OO	-1.70	1.4×10^{-12}	7.98×10^{-18}	1.24	-1510
Z-CH ₃ CHOO	1.81	2.1×10^{-15}	2.27×10^{-19}	1.67	121
E-CH ₃ CHOO	-3.65	2.7×10^{-11}	4.17×10^{-18}	1.27	-2510
(CH ₃) ₂ COO	0.44	1.8×10^{-14}	3.90×10^{-20}	1.91	-643
Z-(CH=CH ₂)(CH ₃)COO	1.02	4.8×10^{-15}	2.25×10^{-21}	2.27	-493
E-(CH ₃)(CH=CH ₂)COO	3.06	3.1×10^{-16}	7.83×10^{-19}	1.45	675
Z-(C(CH ₃)=CH ₂)CHOO	2.68	5.6×10^{-16}	5.95×10^{-19}	1.52	537
E-(C(CH ₃)=CH ₂)CHOO	-1.00	3.6×10^{-13}	2.24×10^{-19}	1.73	-1313
Z-C ₂ H ₅ CHOO	1.36	4.3×10^{-15}	1.26×10^{-18}	1.39	-68
E-C ₂ H ₅ CHOO	-3.93	1.8×10^{-11}	9.97×10^{-18}	0.91	-2739
Z-iC ₃ H ₇ CHOO	0.21	2.1×10^{-14}	5.93×10^{-18}	1.10	-568
E-iC ₃ H ₇ CHOO	-4.12	3.8×10^{-11}	6.79×10^{-18}	1.16	-2659
Z-tC ₄ H ₉ CHOO	1.28	2.8×10^{-15}	2.42×10^{-19}	1.57	-124
E-tC ₄ H ₉ CHOO	-4.20	4.7×10^{-11}	1.81×10^{-17}	0.99	-2715
Z-(C ₂ H ₅)(CH ₃)COO	-0.18	3.2×10^{-14}	4.27×10^{-20}	1.77	-1022
E-(CH ₃)(C ₂ H ₅)COO	0.23	2.1×10^{-14}	1.41×10^{-20}	2.03	-786
Z-(iC ₃ H ₇)(CH ₃)COO	-0.73	1.9×10^{-14}	1.66×10^{-20}	1.71	-1254
E-(CH ₃)(iC ₃ H ₇)COO	0.52	1.1×10^{-14}	2.05×10^{-19}	1.60	-512
Z-(CHO)CHOO	-2.32	1.1×10^{-12}	3.04×10^{-19}	1.59	-1804
E-(CHO)CHOO	1.12	1.4×10^{-14}	1.56×10^{-18}	1.53	-100
Z-(CHO)(CH ₃)COO	-4.24	1.5×10^{-11}	8.07×10^{-20}	1.67	-2828
E-(CH ₃)(CHO)COO	4.88	2.1×10^{-17}	1.09×10^{-19}	1.87	1619
Z-(C(O)CH ₃)(CH ₃)COO	-5.35	4.7×10^{-11}	2.26×10^{-19}	1.43	-3279
E-(CH ₃)(C(O)CH ₃)COO	3.65	6.7×10^{-17}	1.45×10^{-20}	2.06	982
Z-(CH=CH ₂)CHOO	2.94	3.1×10^{-16}	1.28×10^{-19}	1.72	607
E-(CH=CH ₂)CHOO	-0.74	1.9×10^{-13}	8.80×10^{-19}	1.46	-1183
Z-(CH ₂ -CH=CH ₂)CHOO	1.08	3.9×10^{-15}	5.17×10^{-20}	1.83	-234
E-(CH ₂ -CH=CH ₂)CHOO	-4.31	1.8×10^{-11}	5.27×10^{-19}	1.48	-2660
Z-(CH(CH ₃)-CH=CH ₂)CHOO	0.10	1.1×10^{-14}	1.55×10^{-20}	1.88	-819
E-(CH(CH ₃)-CH=CH ₂)CHOO	-4.30	3.6×10^{-11}	3.86×10^{-18}	1.21	-2724
Z-(C(CH ₃) ₂ -CH=CH ₂)CHOO	0.99	3.7×10^{-15}	7.24×10^{-19}	1.38	-200
E-(C(CH ₃) ₂ -CH=CH ₂)CHOO	-4.59	3.9×10^{-11}	3.21×10^{-18}	1.21	-2801
Z-nopinone oxide ^a	-2.15	6.0×10^{-13}	8.83×10^{-23}	2.63	-2278
E-nopinone oxide ^a	0.62	3.7×10^{-15}	4.17×10^{-22}	2.36	-757
Z-pinonaldehyde-A-oxide ^a	-0.16	3.6×10^{-15}	1.74×10^{-26}	3.83	-1266
E-pinonaldehyde-A-oxide ^a	-3.82	1.7×10^{-11}	4.94×10^{-15}	0.17	-2146
Z-pinonaldehyde-K-oxide ^a	1.22	8.9×10^{-16}	1.25×10^{-21}	2.27	-167
E-pinonaldehyde-K-oxide ^a	0.59	3.2×10^{-15}	3.18×10^{-18}	1.05	-275

^a No CCSD(T) data available; barrier height based on M06-2X/aug-cc-pVTZ data only.

Table 40: Predicted total rate coefficients for the reaction of carbonyl oxide with (H₂O)₂ as a function of the two substituents R₁ and R₂, based on fitting theory-derived reaction trends to a set of literature data. The rate coefficient k (cm³ molecule⁻¹ s⁻¹) is given at 298K, and the parameters of a Kooij equation fit $k(T) = A \times T^n \times \exp(-E_a/T)$ between 200 and 450 K (A in cm³ molecule⁻¹ s⁻¹, E_a in K). The definition of R_a/R_b/R_c/R₃/R₄/R₅/R' is given in Table 1. Values in green are based directly on experimental and/or theoretical kinetic calculations, values in orange are values estimated by applying (averaged) reaction trends for other substituents.

	R ₂ = -CH ₃	R ₂ = -CH ₂ R _a	R ₂ = -CHR _a R _b	R ₂ = -CR _a R _b R _c	R ₂ = -H	R ₂ = vinyl	R ₂ = oxo
R ₁ = -CH ₃	 $k=1.82 \times 10^{-14}$ $A=3.90 \times 10^{-20}$ $n=1.91$ $E_a=-643$	 $k=2.12 \times 10^{-14}$ $A=1.41 \times 10^{-20}$ $n=2.03$ $E_a=-786$	 $k=1.06 \times 10^{-14}$ $A=2.05 \times 10^{-19}$ $n=1.60$ $E_a=-512$	 $k=6.84 \times 10^{-14}$ $A=5.17 \times 10^{-19}$ $n=1.43$ $E_a=-1085$	 $k=2.07 \times 10^{-15}$ $A=2.27 \times 10^{-19}$ $n=1.67$ $E_a=121$	 $k=3.12 \times 10^{-16}$ $A=7.63 \times 10^{-19}$ $n=1.45$ $E_a=675$	 $k=4.39 \times 10^{-17}$ $A=2.28 \times 10^{-22}$ $n=2.68$ $E_a=929$
R ₁ = -CH ₂ R _a	 $k=3.22 \times 10^{-14}$ $A=4.27 \times 10^{-20}$ $n=1.77$ $E_a=-1022$	 $k=5.97 \times 10^{-14}$ $A=2.35 \times 10^{-19}$ $n=1.43$ $E_a=-1286$	 $k=6.75 \times 10^{-14}$ $A=5.70 \times 10^{-20}$ $n=1.72$ $E_a=-1255$	 $k=1.42 \times 10^{-13}$ $A=2.88 \times 10^{-18}$ $n=1.15$ $E_a=-1274$	 $k=4.31 \times 10^{-15}$ $A=1.26 \times 10^{-18}$ $n=1.39$ $E_a=-68$	 $k=7.33 \times 10^{-16}$ $A=2.50 \times 10^{-19}$ $n=1.57$ $E_a=292$	 $k=6.61 \times 10^{-17}$ $A=4.79 \times 10^{-22}$ $n=2.55$ $E_a=808$
R ₁ = -CHR _a R _b	 $k=1.92 \times 10^{-14}$ $A=1.66 \times 10^{-20}$ $n=1.71$ $E_a=-1254$	 $k=2.84 \times 10^{-14}$ $A=8.47 \times 10^{-20}$ $n=1.36$ $E_a=-1441$	 $k=2.81 \times 10^{-14}$ $A=2.06 \times 10^{-20}$ $n=1.65$ $E_a=-1410$	 $k=5.92 \times 10^{-14}$ $A=1.04 \times 10^{-18}$ $n=1.08$ $E_a=-1429$	 $k=2.14 \times 10^{-14}$ $A=5.93 \times 10^{-18}$ $n=1.10$ $E_a=-568$	 $k=3.64 \times 10^{-15}$ $A=1.17 \times 10^{-18}$ $n=1.29$ $E_a=-207$	 $k=3.29 \times 10^{-16}$ $A=2.25 \times 10^{-21}$ $n=2.27$ $E_a=309$
R ₁ = -CR _a R _b R _c	 $k=3.04 \times 10^{-14}$ $A=8.81 \times 10^{-21}$ $n=1.96$ $E_a=-1155$	 $k=3.94 \times 10^{-14}$ $A=4.49 \times 10^{-20}$ $n=1.61$ $E_a=-1342$	 $k=4.45 \times 10^{-14}$ $A=1.09 \times 10^{-20}$ $n=1.90$ $E_a=-1311$	 $k=9.39 \times 10^{-14}$ $A=5.51 \times 10^{-19}$ $n=1.33$ $E_a=-1329$	 $k=2.84 \times 10^{-15}$ $A=2.42 \times 10^{-19}$ $n=1.57$ $E_a=-124$	 $k=4.83 \times 10^{-16}$ $A=4.78 \times 10^{-20}$ $n=1.76$ $E_a=237$	 $k=4.36 \times 10^{-17}$ $A=9.17 \times 10^{-23}$ $n=2.74$ $E_a=753$
R ₁ = -H	 $k=2.66 \times 10^{-11}$ $A=4.17 \times 10^{-18}$ $n=1.27$ $E_a=-2510$	 $k=1.75 \times 10^{-11}$ $A=9.97 \times 10^{-18}$ $n=0.91$ $E_a=-2739$	 $k=3.77 \times 10^{-11}$ $A=6.79 \times 10^{-18}$ $n=1.16$ $E_a=-2659$	 $k=4.74 \times 10^{-11}$ $A=1.81 \times 10^{-17}$ $n=0.99$ $E_a=-2715$	 $k=1.44 \times 10^{-12}$ $A=7.95 \times 10^{-18}$ $n=1.24$ $E_a=-1510$	 $k=2.72 \times 10^{-13}$ $A=3.24 \times 10^{-19}$ $n=1.65$ $E_a=-1271$	 $k=1.36 \times 10^{-14}$ $A=1.56 \times 10^{-18}$ $n=1.53$ $E_a=-100$

$R_1 = -CH_2-CR_3=CR_4R_5$ 	$k=2.89 \times 10^{-14}$ $A=4.36 \times 10^{-23}$ $n=2.49$ $E_a=-1505$	$k=5.37 \times 10^{-14}$ $A=2.22 \times 10^{-22}$ $n=2.14$ $E_a=-1692$	$k=6.07 \times 10^{-14}$ $A=5.39 \times 10^{-23}$ $n=2.42$ $E_a=-1661$	$k=1.28 \times 10^{-13}$ $A=2.73 \times 10^{-21}$ $n=1.86$ $E_a=-1679$	$k=3.88 \times 10^{-15}$ $A=5.17 \times 10^{-20}$ $n=1.83$ $E_a=-234$	$k=6.59 \times 10^{-16}$ $A=3.07 \times 10^{-21}$ $n=2.07$ $E_a=-458$	$k=5.94 \times 10^{-17}$ $A=5.89 \times 10^{-24}$ $n=3.05$ $E_a=58$
$R_1 = -CHR_a-CR_3=CR_4R_5$ 	$k=9.68 \times 10^{-15}$ $A=4.36 \times 10^{-23}$ $n=2.46$ $E_a=-1505$	$k=1.25 \times 10^{-14}$ $A=2.22 \times 10^{-22}$ $n=2.14$ $E_a=-1692$	$k=1.42 \times 10^{-14}$ $A=5.39 \times 10^{-23}$ $n=2.42$ $E_a=-1661$	$k=2.99 \times 10^{-14}$ $A=2.73 \times 10^{-21}$ $n=1.86$ $E_a=-1679$	$k=1.08 \times 10^{-14}$ $A=1.55 \times 10^{-20}$ $n=1.88$ $E_a=-819$	$k=1.84 \times 10^{-15}$ $A=3.07 \times 10^{-21}$ $n=2.07$ $E_a=-458$	$k=1.66 \times 10^{-16}$ $A=5.89 \times 10^{-24}$ $n=3.05$ $E_a=58$
$R_1 = -CR_aR_b-CR_3=CR_4R_5$ 	$k=3.99 \times 10^{-14}$ $A=2.64 \times 10^{-20}$ $n=1.77$ $E_a=-1231$	$k=5.17 \times 10^{-14}$ $A=1.34 \times 10^{-19}$ $n=1.42$ $E_a=-1418$	$k=5.85 \times 10^{-14}$ $A=3.26 \times 10^{-20}$ $n=1.71$ $E_a=-1387$	$k=1.23 \times 10^{-13}$ $A=1.65 \times 10^{-18}$ $n=1.14$ $E_a=-1405$	$k=3.73 \times 10^{-15}$ $A=7.24 \times 10^{-19}$ $n=1.38$ $E_a=-200$	$k=6.35 \times 10^{-16}$ $A=1.43 \times 10^{-19}$ $n=1.7$ $E_a=161$	$k=5.72 \times 10^{-17}$ $A=2.74 \times 10^{-22}$ $n=2.55$ $E_a=677$
$R_1 = -CR_3=CR_4CH_3$ 	$k=4.76 \times 10^{-15}$ $A=2.25 \times 10^{-21}$ $n=2.27$ $E_a=-493$	$k=8.60 \times 10^{-15}$ $A=2.16 \times 10^{-20}$ $n=1.83$ $E_a=-738$	$k=9.73 \times 10^{-15}$ $A=5.24 \times 10^{-21}$ $n=2.12$ $E_a=-707$	$k=2.05 \times 10^{-14}$ $A=2.65 \times 10^{-19}$ $n=1.55$ $E_a=-726$	$k=4.33 \times 10^{-16}$ $A=2.42 \times 10^{-19}$ $n=1.64$ $E_a=548$	$k=7.36 \times 10^{-17}$ $A=4.78 \times 10^{-20}$ $n=1.82$ $E_a=909$	$k=6.64 \times 10^{-18}$ $A=9.16 \times 10^{-23}$ $n=2.80$ $E_a=1424$
$R_1 = -CR_3=CR_4CH_2R_a$ 	$k=4.76 \times 10^{-15}$ $A=2.25 \times 10^{-21}$ $n=2.27$ $E_a=-493$	$k=8.60 \times 10^{-15}$ $A=2.16 \times 10^{-20}$ $n=1.83$ $E_a=-738$	$k=9.73 \times 10^{-15}$ $A=5.24 \times 10^{-21}$ $n=2.12$ $E_a=-707$	$k=2.05 \times 10^{-14}$ $A=2.65 \times 10^{-19}$ $n=1.55$ $E_a=-726$	$k=4.33 \times 10^{-16}$ $A=2.42 \times 10^{-19}$ $n=1.64$ $E_a=548$	$k=7.36 \times 10^{-17}$ $A=4.78 \times 10^{-20}$ $n=1.82$ $E_a=909$	$k=6.64 \times 10^{-18}$ $A=9.16 \times 10^{-23}$ $n=2.80$ $E_a=1424$
$R_1 = -CR_3=CR_4CHRaR_b$ 	$k=4.76 \times 10^{-15}$ $A=2.25 \times 10^{-21}$ $n=2.27$ $E_a=-493$	$k=8.60 \times 10^{-15}$ $A=2.16 \times 10^{-20}$ $n=1.83$ $E_a=-738$	$k=9.73 \times 10^{-15}$ $A=5.24 \times 10^{-21}$ $n=2.12$ $E_a=-707$	$k=2.05 \times 10^{-14}$ $A=2.65 \times 10^{-19}$ $n=1.55$ $E_a=-726$	$k=4.33 \times 10^{-16}$ $A=2.42 \times 10^{-19}$ $n=1.64$ $E_a=548$	$k=7.36 \times 10^{-17}$ $A=4.78 \times 10^{-20}$ $n=1.82$ $E_a=909$	$k=6.64 \times 10^{-18}$ $A=9.16 \times 10^{-23}$ $n=2.80$ $E_a=1424$

$R_1 = -CR_3=CR_4R'$ 	$k=4.76 \times 10^{-15}$ $A=2.25 \times 10^{-21}$ $n=2.27$ $E_a=-493$	$k=8.60 \times 10^{-15}$ $A=2.16 \times 10^{-20}$ $n=1.83$ $E_a=-738$	$k=9.73 \times 10^{-15}$ $A=5.24 \times 10^{-21}$ $n=2.12$ $E_a=-707$	$k=2.05 \times 10^{-14}$ $A=2.65 \times 10^{-19}$ $n=1.55$ $E_a=-726$	$k=4.33 \times 10^{-16}$ $A=2.42 \times 10^{-19}$ $n=1.64$ $E_a=548$	$k=7.36 \times 10^{-17}$ $A=4.78 \times 10^{-20}$ $n=1.82$ $E_a=909$	$k=6.64 \times 10^{-18}$ $A=9.16 \times 10^{-23}$ $n=2.80$ $E_a=1424$
$R_1 = -CHO$ 	$k=1.48 \times 10^{-11}$ $A=8.07 \times 10^{-20}$ $n=1.67$ $E_a=-2828$	$k=1.56 \times 10^{-11}$ $A=5.65 \times 10^{-20}$ $n=1.63$ $E_a=-3022$	$k=1.77 \times 10^{-11}$ $A=1.37 \times 10^{-20}$ $n=1.92$ $E_a=-2991$	$k=3.73 \times 10^{-11}$ $A=6.94 \times 10^{-19}$ $n=1.35$ $E_a=-3009$	$k=1.1310^{-12}$ $A=3.04 \times 10^{-18}$ $n=1.59$ $E_a=-1804$	$k=1.92 \times 10^{-13}$ $A=6.02 \times 10^{-20}$ $n=1.78$ $E_a=-1443$	$k=1.73 \times 10^{-14}$ $A=1.15 \times 10^{-22}$ $n=2.76$ $E_a=-927$
$R_1 = -C(O)R_a$ 	$k=4.68 \times 10^{-11}$ $A=2.26 \times 10^{-19}$ $n=1.43$ $E_a=-3279$	$k=6.06 \times 10^{-11}$ $A=1.15 \times 10^{-18}$ $n=1.08$ $E_a=-3466$	$k=6.86 \times 10^{-11}$ $A=2.80 \times 10^{-19}$ $n=1.37$ $E_a=-3435$	$k=1.45 \times 10^{-10}$ $A=1.41 \times 10^{-17}$ $n=0.80$ $E_a=-3454$	$k=4.38 \times 10^{-12}$ $A=6.20 \times 10^{-18}$ $n=1.04$ $E_a=-2248$	$k=7.44 \times 10^{-13}$ $A=1.23 \times 10^{-18}$ $n=1.23$ $E_a=-1887$	$k=6.71 \times 10^{-14}$ $A=2.35 \times 10^{-21}$ $n=2.21$ $E_a=-1372$

U. Field data analysis

1. Literature data

a. Trace gas concentrations

To derive the concentration of a tropospherically relevant mixture of stabilized CI (SCI) we selected four environments characterized by contrasting volatile organic compounds (VOC) composition and trace gases, i.e. a rainforest (Amazonia, Brazil), a polluted mega-city (Mexico city, Mexico) a temperate forest (Sierra Nevada, USA) and a mid-latitude rural area (Hohenpeissenberg, Germany).

The VOC and coreactant concentrations measured in each environment were taken from literature. A short summary of the campaign times is given in Table 41. Chemical structures of the VOCs considered in our analysis are given in Figure 24; it should be noted that not all compounds are present in each environment. Time-dependent data was averaged to obtain an estimate of the average CI concentration for each site. The average concentrations for the Amazonian rainforest were taken mostly from Jardine et al.,¹⁹⁷ enhanced with data on MVK and MACR,¹⁹⁸ H₂O, SO₂ and OH,¹⁹⁹ O₃,²⁰⁰ and organic acids.²⁰¹ For Mexico City we adopted the Velasco et al. data set,²⁰² extended with information on H₂O,¹⁹⁹ SO₂,²⁰³ OH,²⁰⁴ and organic acids.²⁰⁵ The temperate forest in Sierra Nevada, USA is well documented by Bouvier-Brown et al.,²⁰⁶ where we add information on isoprene,¹⁹⁸ and SO₂.²⁰⁷ The concentration of organic acids in this environment is not well-known, we use a lower limit estimate by Wolfe et al.²⁰⁸ Finally, the HOPE 2012 field campaign has a very extensive data set for the rural Hohenpeissenberg (Germany) area, as described by Handisides et al.²⁰⁹ where viable concentrations for organic acids were taken from Grossmann et al.²¹⁰ All concentrations are summarized in Table 42. For all sites, we calculated the concentration of (H₂O)₂ from the relative humidity using K_{eq}(298 K) = 0.04 atm⁻¹ as published by Shilling et al.²¹¹.

Table 41: Summary of field campaign measurement periods

	Amazonia	Mexico City	Temperate forest	Rural area
Campaign name		MCMA 2002 & 2003	BEARPEX 2007	HOPE 2000
Site location	Amazonian forest Brazil	Mexico City Urban site Mexico	Sierra Nevada USA	Hohenpeissenberg Germany
Time period	8 Nov 2013 - 7 Jul 2014	7 Feb - 24 Feb 2002 1 Apr - 5 May 2003	20 Aug - 12 Sep 2007	18 Jun - 21 Jun 2000
Sampling times	rain free periods (13:00 – 16:30)	rush hour period (06:00 – 09:00)	daytime (10:00 – 17:00)	daytime (07:00 – 17:00)
Data accumulation	Time period average	Time period average	Time period average	Time period average

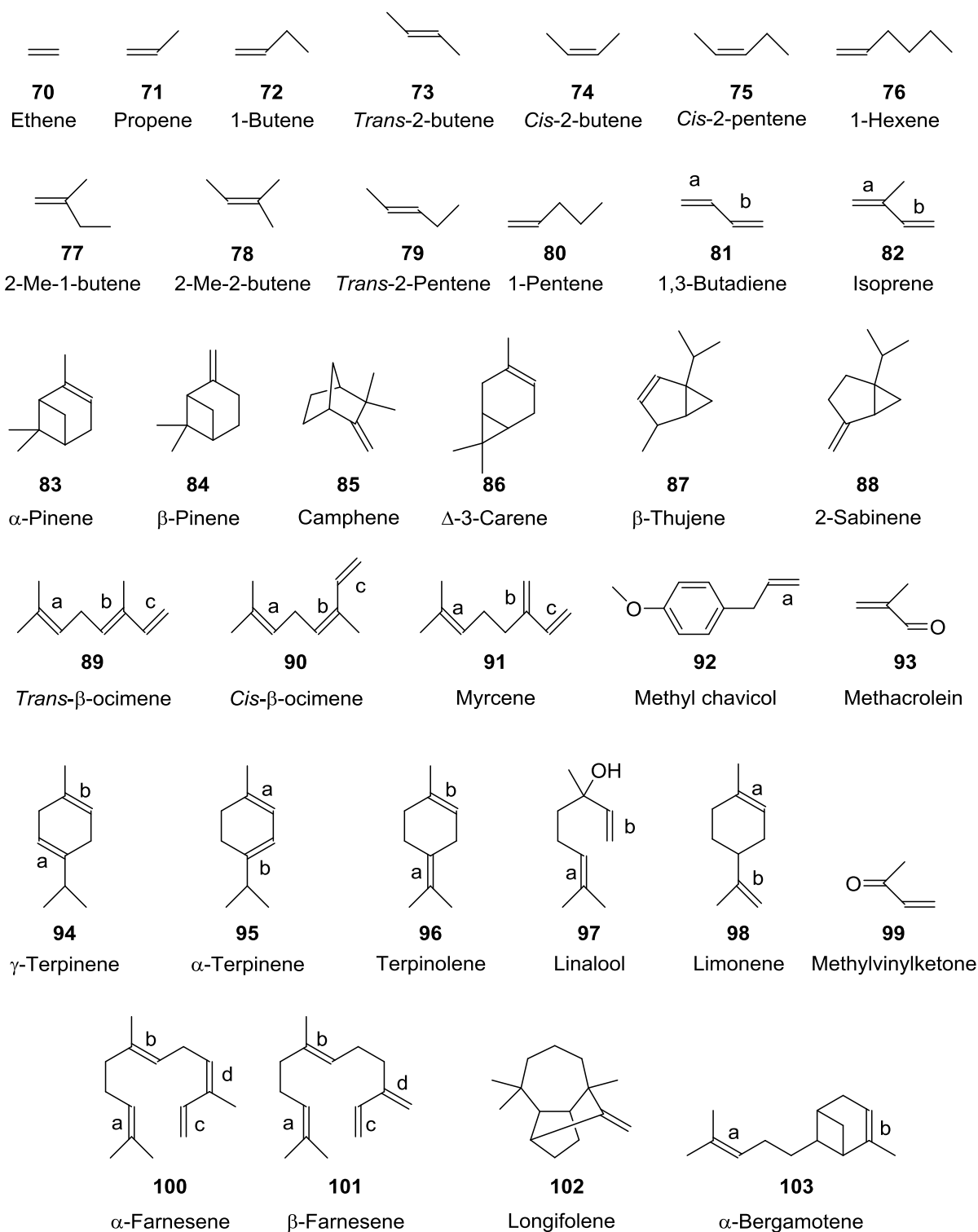


Figure 24: List of unsaturated volatile organic compounds considered in the field data analysis as CI sources. For poly-unsaturated VOC, double bonds are labeled *a* through *d*.

Table 42: Concentrations (molecule cm⁻³) of the trace gasses at the four sites considered. See text for source literature.

	Rainforest	Megacity	Temperate forest	Rural area
Ethene		3.8×10^{11}		3.9×10^9
Propene		1.1×10^{11}		1.5×10^9
1-Butene		5.7×10^{10}		5.7×10^8
2-Methyl-1-butene		2.6×10^{10}		
2-Methyl-2-butene		1.7×10^{10}		
Trans-2-butene		2.0×10^{10}		2.0×10^8
Trans-2-pentene		1.4×10^{10}		2.0×10^7
Cis-2-butene		1.5×10^{10}		1.3×10^8
1,3-Butadiene		1.0×10^{10}		6.1×10^8
Trans-2-pentene		6.9×10^9		1.7×10^7
Cis-2-Pentene		6.9×10^9		1.7×10^7
1-Pentene		9.0×10^9		1.5×10^8
1-Hexene		3.0×10^9		8.4×10^7
1-Butene				6.9×10^7
Isoprene	2.4×10^{11}	6.2×10^9	3.0×10^9	7.6×10^9
α -Pinene	5.3×10^9		7.8×10^9	3.2×10^9
β -Pinene	1.3×10^9		2.3×10^{10}	1.5×10^9
Camphene	6.5×10^8		5.3×10^8	5.6×10^8
2-Sabinene	2.2×10^9			1.5×10^9
Myrcene	1.4×10^8		5.0×10^8	3.9×10^8
Δ -3-Carene	2.4×10^7		1.5×10^{10}	9.4×10^8
Terpinolene			1.2×10^8	7.3×10^7
γ -Terpinene	1.2×10^9		1.0×10^8	1.3×10^8
Limonene	1.4×10^{10}		5.6×10^9	5.9×10^8
β -Thujene	1.4×10^8			
<i>Cis</i> - β -ocimene	3.9×10^9			
<i>Trans</i> - β -ocimene	1.9×10^9			
α -Farnesene			3.1×10^8	
β -Farnesene			8.4×10^7	
Logifolene			3.7×10^8	
α -Bergamotene			3.3×10^8	
Methyl chavicol			5.3×10^9	
Linalool			1.9×10^7	
MVK	2.4×10^{10}		2.5×10^9	
MACR	2.4×10^{10}		2.6×10^9	
Organic acids	9.1×10^{10}	2.2×10^{11}	2.2×10^8	4.4×10^{10}
H ₂ O	6.1×10^{17}	2.4×10^{17}	2.1×10^{17}	3.9×10^{17}
H ₂ O--H ₂ O	5.5×10^{14}	8.5×10^{13}	1.3×10^{14}	2.1×10^{14}
O ₃	7.3×10^{11}	1.9×10^{12}	1.4×10^{12}	1.4×10^{12}
SO ₂	5.2×10^8	9.0×10^{10}	2.5×10^7	6.6×10^9
OH	5×10^6	6.0×10^6	5.4×10^6	4.0×10^6

b. SCI yield from ozonolysis of VOCs

Estimating the yield of stabilized Criegee intermediates is a complex problem, owing to the multiple reaction steps involved in the ozonolysis of alkenes. The ozonolysis process has been reviewed extensively,^{4,212} but it is instructive to briefly recapitulate the main features of the reaction system, where Figure 25 shows a scheme of an alkene ozonolysis reaction.

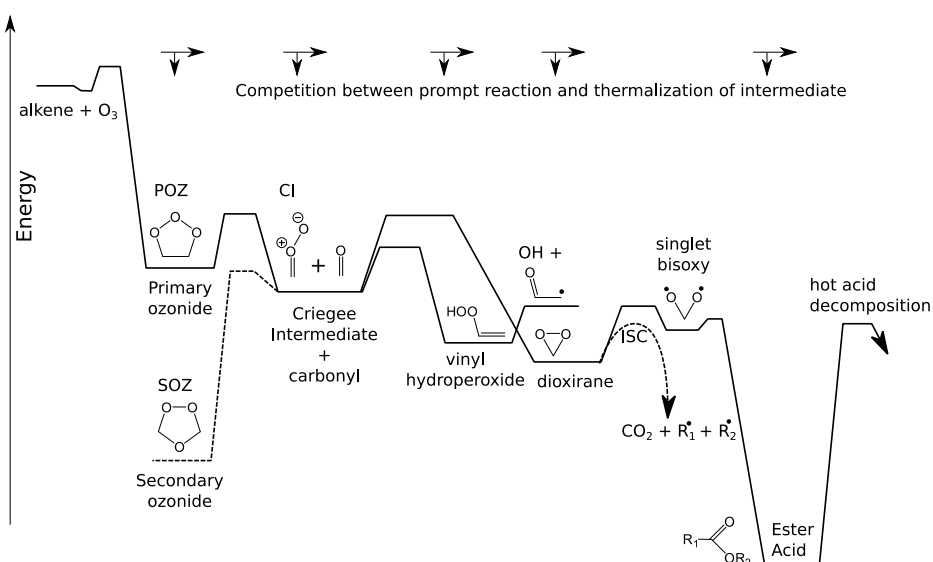
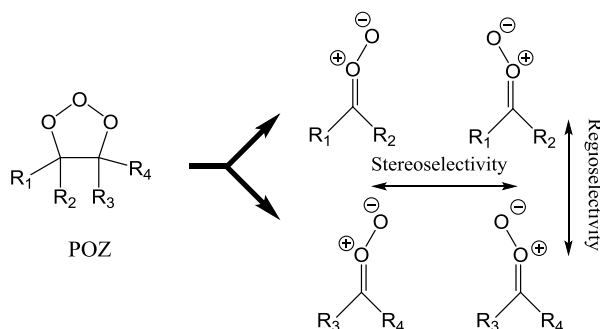


Figure 25: Schematic representation of the potential energy surface for the ozonolysis of alkenes. The yield of SCI depends on the chemical activation of the POZ at the moment of decomposition, the energy partition between the two fragments, and the rate of collisional stabilisation of the excited CI. The speciation of the SCI in asymmetric alkenes depends also on the relative properties of the 4 transition states for decomposition of the POZ.

For the formation of SCI, three steps are important. The first is the ozonolysis reaction, forming a chemically activated primary ozonide, POZ. With typical excitation energies around 50 to 60 kcal mol⁻¹, the POZ formed from small alkenes decomposes promptly to a Criegee intermediate and a carbonyl product. For larger POZ, such as those formed from monoterpenes, the POZ can lose (part of) its nascent energy in collisions with the bath gas; even when thermalized, the main fate of the POZ remains decomposition. The energy content at the time of POZ decomposition determines the amount of energy available to the dissociation fragments. The POZ decomposition can occur formally through four transition states, leaving the carbonyl oxide moiety on one or the other carbon in the double bond (regio-specificity), and for each case the outer oxide O-atom can point towards either of the two substituents on that carbon (stereo-specificity); for symmetric alkenes some or all of the transition states can be degenerate.



The energy present in the POZ at the time of decomposition is distributed among the CI product, the carbonyl product, and the relative motion (translation and rotation) of these two fragments. The nascent energy of the CI product can thus range from zero up to, and including, the total energy present in the dissociating POZ, with a statistical energy distribution that depends on the relative state densities of both fragments, the state density of the degrees of freedom for their relative motion, and the kinematic properties of the dissociation process. A special case is the dissociation of cyclic alkenes, where both dissociation fragments are tethered together into a single product, which thus retains the full energy of the dissociation POZ. For asymmetric alkenes, the regio- and stereo-specific speciation also induces further differences between the internal energy distributions of the different CI products.

The subsequent fate of the CI then depends strongly on its energy content. Those CI with low energy content will attain a thermal Boltzmann energy distribution, i.e. they become so-called "stabilized CI", SCI, with a comparatively long lifetime of micro- to milliseconds. This is sufficiently long for bimolecular reactions to compete with unimolecular reactions. CI borne with higher energy content, so-called "excited CI", can lose their enhanced internal energy in collisions with the bath gas, thus becoming SCI, but this occurs in competition with fast, chemically activated unimolecular reactions; bimolecular reactions are too slow to compete as the co-reactant concentrations in the atmosphere are too low. The different energy content in excited CI versus SCI also affects the contribution of the individual unimolecular reaction channels, i.e. one can't use rate constants derived for stabilized CI to determine the fate for excited CI.

The total yield of SCI, and the speciation of the SCI formed, is thus dependent on the subtle interplay between chemical activation, unimolecular reactions, and collisional energy loss at both the POZ and the CI stage, as well as on the statistical and dynamical energy redistribution in the POZ dissociation step. It is therefore specific to each individual VOC (where the number of non-hydrogen atoms has a strong impact on the state densities), and is dependent on temperature, pressure, and the bath gas (always air in the atmosphere).^{184,212–214} Measurements of the SCI yields are thus not straightforward, as the reaction conditions and potentially the concentration of co-reactants (e.g. SCI scavengers) could influence the observations. Table 43 lists experimental data of the SCI yields for a set of VOC; as one can see, there is significant scatter across the measurements though more recent measurement tend to converge to a specific value, as ameliorated detection methods and a better understanding of the VOC and CI chemistry allows for improved experimental design.

Table 43: Experimental data on the yield of stabilized CI from the ozonolysis of olefines and monoterpenes.

VOC	Y_{SCI}	Source reference
Ethene	0.38	Su et al., 1980 ⁸⁵
	0.35	Niki et al., 1981 ⁸⁶
	0.39	Hatakeyama et al., 1984 ²¹³
	0.40	Atkinson and Lloyd, 1984 ²¹⁵
	0.47	Horie and Moortgat, 1991 ²¹⁶
	0.44	Neeb et al., 1996 ¹⁰¹
	0.42	Neeb et al., 1997 ⁸⁹
	0.52	Horie et al., 1999 ¹³⁹
	0.39	Hasson et al., 2001 ²¹⁷
	0.54	Alam et al., 2011 ²¹⁸
	0.40	Berndt et al., 2014 ²¹⁹
	0.37	Newland et al., 2015 ⁴⁵
	0.10	Dodge and Arnts, 1979
Propene	0.40	Atkinson and Lloyd, 1984 ²¹⁵
	0.25	Hatakeyama et al., 1984 ²¹⁵
	0.44	Horie and Moortgat, 1991 ²¹⁶
	0.22	Rickard et al., 1999 ²²⁰
	0.16	Atkinson et al., 2006 ²²¹
<i>Trans</i> -2-butene	0.43	Cox and Penkett, 1972 ²²²
	0.40	Niki et al., 1977 ²²³
	0.40	Atkinson and Lloyd, 1984 ²¹⁵
	0.18	Hatakeyama et al., 1984 ²¹⁵
	0.42	Horie and Moortgat, 1991 ²¹⁶
	0.13	Rickard et al., 1999 ²²⁰
	0.24	Hasson et al., 2001 ²¹⁷
	0.53	Berndt et al., 2012 ⁷²
	0.40	Berndt et al., 2014 ²²⁴
	0.28	Newland et al., 2015 ⁴⁵
<i>Cis</i> -2-butene	0.19	Rickard et al., 1999 ²²⁰
	0.16	Atkinson et al., 2006 ²²¹
	0.38	Newland et al., 2015 ⁴⁵
2-Me-2-butene	0.10	Rickard et al., 1999 ²²⁰
2,3-diMe-2-butene	0.30	Niki et al., 1977 ²²³
	0.11	Rickard et al., 1999 ²²⁰
	0.10	Hasson et al., 2001 ²¹⁷
	0.65	Drozd and Donahue, 2011 ²²⁵
	0.62	Berndt et al., 2012 ⁷²
	0.49	Berndt et al., 2014 ²²⁴
	0.32	Newland et al., 2015 ⁴⁵
	0.30	Neeb et al., 1997 ⁸⁹
Isoprene	0.28 (0.53 ^a)	Rickard et al., 1999 ²²⁰
	0.26	Hasson et al., 2001 ²¹⁷
	0.58	Sipilä et al., 2014 ¹⁰³
	0.56	Newland et al., 2015 ²²⁶
	0.61	Nguyen et al., 2016 ¹⁰⁷
1-Me-cyclohexene	0.16	Berndt et al., 2012 ⁷²
α -pinene	0.15	Drozd and Donahue, 2011 ²²⁵
	0.15	Donahue et al., 2011 ¹⁸⁴
	0.15	Sipilä et al., 2014 ¹⁰³
β -pinene	0.25	Hatakeyama and Akimoto, 1994 ²²⁷
	0.14	Rickard et al., 1999 ²²⁰
	0.27	Hasson et al., 2001 ²¹⁷
	0.50	Ahrens et al., 2014 ⁷⁵
Limonene	0.30	Leungsakul et al., 2005 ²²⁸
	0.27	Sipilä et al., 2014 ¹⁰³
Camphene	0.31	Hasson et al., 2001 ²¹⁷

^a Newland et al.²²⁶ reanalyzed this data, finding 0.53 is likely to better represent the SCI yield.

c. Rate coefficients for ozonolysis of VOCs

Table 44: Rate coefficients k_{VOC+O_3} ($\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$) at room temperature (source Atkinson et al.²²¹ unless indicated otherwise), adopted yields Y_{SCI} of stabilized CI (see text section U.2.b how these numbers are derived, and Table 43 for literature data), and site-specificity factor α from the SAR by King et al.²²⁹, for the VOC considered in the field data. The structures, and the labeling of the double bonds (a, b, c, d) is shown in Figure 24.

#	VOC	$k_{VOC+O_3}(298 \text{ K})$	Y_{SCI}	α
70	Ethene	1.6×10^{-18}	0.37	1
71	Propene	1.0×10^{-17}	0.37	1
72	1-Butene	9.6×10^{-18}	0.40	1
73	Trans-2-butene	1.9×10^{-16}	0.40	1
74	Cis-2-butene	1.2×10^{-16}	0.38	1
75	Cis-2-pentene	1.1×10^{-17}	0.29	1
76	1-Hexene	1.1×10^{-17}	0.40	1
77	2-Methyl-1-butene	1.4×10^{-17}	0.40	1
78	2-Methyl-2-butene	4.0×10^{-16}	0.40	1
79	Trans-2-pentene	1.3×10^{-16}	0.40	1
80	1-Pentene	1.6×10^{-16}	0.29	1
81	1,3-Butadiene	6.8×10^{-18}	0.40	1
82	Isoprene	1.2×10^{-17}	0.58	0.72 (a) 0.28 (b)
83	α -Pinene	9.4×10^{-17}	0.10	1
84	β -Pinene	1.9×10^{-17}	0.50	1
85	Camphene	6.8×10^{-19}	0.50	1
86	Δ -3-Carene	9.4×10^{-17}	0.10	1
87	β -Thujene	1.7×10^{-16} ref.229	0.15	1
88	2-Sabinene	8.2×10^{-17}	0.30	1
89	Trans- β -ocimene	4.9×10^{-16}	0.40	0.6 (a) 0.2 (b) 0.2 (c)
90	Cis- β -ocimene	4.9×10^{-16}	0.40	0.6 (a) 0.2 (b) 0.2 (c)
91	Myrcene	4.6×10^{-16}	0.40	0.9 (a) 0.05 (b) 0.05 (c)
92	Methyl chavicol	9.8×10^{-18} ref. 229	0.40	1
93	MACR	1.2×10^{-18}	0.40	1
94	γ -Terpinene	1.5×10^{-16}	0.15	0.54 (a) 0.46 (b)
95	α -Terpinene	1.5×10^{-14}	0.15	0.5 (a) 0.5 (b)
96	Terpinolene	1.6×10^{-15}	0.27	0.3 (a) 0.7 (b)
97	Linalool	4.3×10^{-16}	0.40	0.9 (a) 0.1 (b)
98	Limonene	2.1×10^{-16}	0.27	0.78 (a) 0.22 (b)
99	MVK	5.2×10^{-18}	0.40	1
100	α -Farnesene	3.2×10^{-16} ref.229	0.40	0.36 (a) 0.4 (b) 0.12 (c) 0.12 (d)
101	β -Farnesene	3.2×10^{-16} ref.230	0.40	0.4 (a) 0.4 (b) 0.1 (c) 0.1 (d)
102	Longifolene	5.0×10^{-19}	0.50	1
103	α -Bergamotene	2.5×10^{-16} ref.229	0.40	0.44 (a) 0.66 (b)

2. Methodology

The four specific environments were chosen both for the availability of larger data sets, and to cover conditions where large differences in the amount of CI produced, and in their speciation, are expected. The rainforest site is dominated by isoprene emissions and with general large monoterpenes emissions but relatively low ozone and NO_x concentration, and where OH recycling becomes important.^{199,231} In contrast, the temperate forest chemistry is driven by monoterpenes emissions combined with a relatively high ozone concentration. The polluted mega-city is characterized by a plethora of anthropogenic unsaturated VOCs emission combined with a high ozone concentration enhancing the production of CI. This environment can be treated as an upper limit for the CI concentration in urban centers. The rural site represents a balanced mixture of anthropogenic and biogenic influences; the very extensive data set for this site allows for the comparison between the relative impacts of anthropogenic vs biogenic CI. Combined, these four sites cover a wide range of tropospheric conditions and are thus reasonable representative of the expected CI concentrations.

a. General approach

As discussed in extensive detail below, ozonolysis of VOC is assumed to be the sole source of SCI, whereas SCI loss processes include unimolecular decay, reaction with water vapor (H₂O and (H₂O)₂), SO₂, and acids. The speciated SCI concentrations at room temperature are then calculated assuming steady state, a reasonable assumption considering their short lifetime (< 1 sec) relative to the rate of change for the source and sinks. The total SCI concentration [SCI_{tot}] is then the sum of the speciated SCI, obtained by dividing their production rate SCI_{PR} by their summed loss rate SCI_{LR}:

$$[SCI_{tot}] = \sum \frac{SCI_{PR}}{SCI_{LR}}$$

b. SCI source strength

The production rate SCI_{PR} of one single stabilized CI stereoisomer in a specific VOC ozonolysis reaction is calculated using the following general formula:

$$SCI_{PR} = k_{VOC+O_3} \times [VOC] \times [O_3] \times \alpha \times Y_{SCI} \times Y_{Spec}$$

Here [VOC] and [O₃] are the average concentrations of the VOC and ozone, respectively, k_{VOC+O_3} is the rate coefficient between the VOC and O₃, α is the site-specific contribution of each double bond in the total ozonolysis reaction, Y_{SCI} the total yield of stabilized CI in the VOC+O₃ reaction, and Y_{Spec} the fractional yield of a given stereoisomer-specific SCI species in the ozonolysis. The rate coefficients are available in literature, and are listed in Table 44. This table also contains the site-specificities α calculated based on the SAR by King et al.²²⁹

Literature data on the SCI yield Y_{SCI} is fragmented, with no direct data available for most VOC, and sometimes large data scatter for the VOC where multiple studies are available, such as for small alkenes; Table 43 lists a selection of the available experimental data, while Table 45 summarizes our approach to determining Y_{SCI} . For ethene and *cis*-2-butene, we select the values by Newland et al.⁴⁵ obtained by elaborate fitting of highly detailed experiments, while for *trans*-2-butene and propene we use a weighted average over the literature data of 0.40 and 0.30, respectively. For other non-cyclic, non-conjugated VOC, we adopt a value of 0.40, of the same magnitude as the Y_{SCI} selected above. For isoprene, we adopt a value of 0.60, following the in-depth analysis by Nguyen et al.¹⁰⁷ The yield of stabilized CI from α -pinene is rather low, 0.15, as the endocyclic double bond makes formation of thermalized CI more difficult.¹⁸⁴ We adopt this same value for other VOC with endocyclic double bonds (Δ -3-carene, β -thujene, α - and γ -terpinene). For β -pinene, with an exocyclic double bond, we adopt the most direct measurement by Ahrens et al.⁷⁵ with an SCI yield of 0.50, in agreement with a recent theoretical study by Nguyen et al.³³ We assume the same yield for camphene, 2-sabinene and longifolene, based on the similarity in the structures, where we choose to neglect the Hasson et al.²¹⁷ value for camphene as this study appears to underestimate SCI yields (see Table 43). Finally, there is literature data available for limonene, where we adopt the most recent value of 0.27 by Sipilä et al.¹⁰³ Finally, for all other VOC we use $Y_{SCI} =$

0.4,^{217,232} as this seems a reasonable median value that ensures that CI concentrations are not under- or over-estimated by too large a factor.

Table 45: Summary of the procedure for assigning Y_{SCI} to a specific bond or VOC

Type of double bond	Y_{SCI} used	VOCs in current study with this type of bond
Literature data available	Use literature value Y_{SCI}	Isoprene, camphene, ethene, propene, trans-2-butene, cis-2-butene, 1-pentene, α -pinene, β -pinene, limonene
Endocyclic double bond	Treat as α -pinene: $Y_{SCI} = 0.15$	δ -3-Carene, γ -Terpinene, β -Thujene, α -Terpinene
Exocyclic double bond implanted on ring	Treat as β -pinene: $Y_{SCI} = 0.50$	Sabinene, Longifolene
All other double bonds	$Y_{SCI} = 0.40$	All other VOC

Very little information is available on the stereoisomer-specific yield, Y_{Spec} ; Table 46 summarizes our estimation procedure for this quantity. For isoprene, we adopt the CI yields as predicted in the theoretical study by Zhang et al.^{121,122}: 56% CH_2OO (**1**), 24% Z-MVK oxide (**31**), 13% E-MVK-oxide (**33**), 6% E-MACR oxide (**43**), and 1% Z-MACR oxide (**42**) (see Figure 3 for CI structures). For β -pinene, Ahrens et al.⁷⁵ provides specific yields for the 2 large SCI formed; we employ 10% CH_2OO (**1**), 13% E-nopinone oxide (**50**) and 77% Z-nopinone oxide (**51**). Propene-specific Y_{Spec} are used based on the study by Novelli et al.⁴⁹: 50% CH_2OO (**1**), 40% Z- CH_3CHOO (**2**) and 10% E- CH_3CHOO (**6**). For ozonolysis reactions that can form RCHOO CI (i.e. 2-methyl-2-butene, trans-2-butene, trans- and cis-2-pentene), there is some evidence that the lower-energy Z-RCHOO is formed in higher concentration: Taatjes et al.⁶² tentatively suggested a 90% dominance, whereas Sheps et al.⁶³ estimated a 70 % contribution. We adopt a ratio of 1:4 for E-RCHOO to Z-RCHOO, favoring the energetically more stable Z-CI. For the remaining VOCs, we assume all four stereo-specific CI formed for each double bond are generated in equal yields; if the double bond is symmetrically substituted, or if symmetric CI are formed, the yields of identical CI are summed.

Table 46: Summary of the procedure for assigning SCI speciation to a double bond or VOC

Type of double bond	Y_{Spec} used	VOCs in current study with this type of bond
Literature data available	Use literature values Y_{Spec}	Isoprene, β -pinene, propene
No literature data available	All 4 possible SCI in equal yields.	All other VOC
Formation of "RCHOO" SCI (per carbon in the double bond)	Adjust 1:1 SCI yields for that carbon to 80% Z-RCHOO, 20 % E-RCHOO	trans-2-butene, cis-2-butene, 2-methyl-2-butene, trans-2-pentene, cis-2-pentene
Symmetric double bonds / symmetric SCI	Sum yields for identical SCI.	All VOC, as applicable

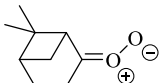
c. SCI loss processes

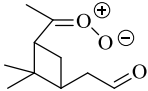
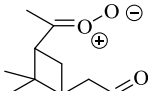
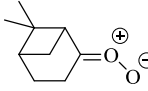
In the field data analysis, the loss rate SCI_{LR} for a SCI comprises unimolecular rate, reaction with water and water dimers, reaction with sulfur dioxide (SO_2) and reaction with organic acids:

$$SCI_{LR} = k_{decay} + k_{H_2O}[H_2O] + k_{(H_2O)_2}[(H_2O)_2] + k_{SO_2}[SO_2] + k_{acid}[acid]$$

For the rate coefficients for unimolecular decay k_{decay} , the reaction with water k_{H_2O} , and with water dimers $k_{(H_2O)_2}$ we rely on the structure-activity relationships proposed in this work in sections R, S.5, and T.4. Table 47 shows the most common SCI classes found in the atmosphere, and a list of VOCs that generate this type of SCI classes.

Table 47: List of SCI classes (defined by R₁ and R₂ substituents) with highest production rates in the atmosphere (roughly in order of decreasing source strength). Rate coefficients at 298 K for unimolecular decay (k_{uni} in units of s⁻¹), reaction with H₂O ($k_{\text{H}_2\text{O}}$, cm³ molecule⁻¹ s⁻¹) and with (H₂O)₂ ($k_{(\text{H}_2\text{O})_2}$, cm³ molecule⁻¹ s⁻¹) for that SCI class are reproduced from the SAR tables. The VOC represented in our field data that generate SCI of that class are listed.

SCI class	Rate coefficient	Source VOC
R ₁ -H R ₂ -H	$k_{\text{uni}} = 0.3$ $k_{\text{H}_2\text{O}} = 8.7 \times 10^{-16}$ $k_{(\text{H}_2\text{O})_2} = 1.4 \times 10^{-12}$	β -Pinene, Limonene, , Myrcene, Isoprene, Cis- β -ocimene, 2-Sabinene, Trans- β -ocimene, Camphene, Longifolene, β -Farnesene, α -Farnesene, Methyl chavicol, Linalool, Ehtylene, Propene, Isobutene, 2-Methyl-1-butene, 1-Pentene, 1-Hexene, 1,3-Butadiene, 1-Butene, MVK, MACR
R ₁ -CH ₃ R ₂ -H	$k_{\text{uni}} = 136$ $k_{\text{H}_2\text{O}} = 6.7 \times 10^{-19}$ $k_{(\text{H}_2\text{O})_2} = 2.1 \times 10^{-15}$	Propene, 2-Methyl-2-butene, Trans-2-butene, Trans-2-pentene, Cis-2-butene, Cis-2-pentene
R ₁ -H R ₂ -CH ₃	$k_{\text{uni}} = 53$ $k_{\text{H}_2\text{O}} = 2.3 \times 10^{-14}$ $k_{(\text{H}_2\text{O})_2} = 2.7 \times 10^{-11}$	Propene, 2-Methyl-2-butene, Trans-2-butene, Trans-2-pentene, Cis-2-butene, Cis-2-pentene
R ₁ -CH ₃ R ₂ -CH ₃	$k_{\text{uni}} = 478$ $k_{\text{H}_2\text{O}} = 7.5 \times 10^{-18}$ $k_{(\text{H}_2\text{O})_2} = 1.8 \times 10^{-14}$	Myrcene, Cis- β -ocimene, Trans- β -ocimene, Terpinolene, α -Bergamotene, β -Farnesene, α -Farnesene, Linalool, Isobutene, 2-Methyl-2-butene
R ₁ -CH ₃ R ₂ -C(R ₃)=CR ₄ R ₅	$k_{\text{uni}} = 50$ $k_{\text{H}_2\text{O}} = 8.1 \times 10^{-20}$ $k_{(\text{H}_2\text{O})_2} = 3.1 \times 10^{-16}$	Isoprene, Cis- β -ocimene, Trans- β -ocimene, α -Farnesene
R ₁ -H R ₂ -CH ₂ R _a	$k_{\text{uni}} = 74$ $k_{\text{H}_2\text{O}} = 1.6 \times 10^{-14}$ $k_{(\text{H}_2\text{O})_2} = 1.7 \times 10^{-11}$	Limonene, δ -3-Carene, Myrcene, α -Bergamotene, β -Farnesene, α -Farnesene, Linalool, Trans-2-pentene, Cis-2-pentene, 1-Pentene, 1-Hexene, 1-Butene
R ₁ -CH ₂ R _a R ₂ -H	$k_{\text{uni}} = 205$ $k_{\text{H}_2\text{O}} = 1.5 \times 10^{-18}$ $k_{(\text{H}_2\text{O})_2} = 4.3 \times 10^{-15}$	Limonene, δ -3-Carene, Myrcene, Trans- β -ocimene, α -Bergamotene, β -Farnesene, α -Farnesene, Linalool, Trans-2-pentene, Cis-2-pentene, 1-Pentene, 1-Hexene, 1-Butene, α -Pinene
R ₁ -H R ₂ -C(R ₃)=CR ₄ R ₅	$k_{\text{uni}} = 30$ $k_{\text{H}_2\text{O}} = 8.7 \times 10^{-16}$ $k_{(\text{H}_2\text{O})_2} = 2.7 \times 10^{-13}$	Cis- β -ocimene, γ -Terpinene, Trans- β -ocimene, Terpinolene, α -Farnesene, Methyl chavicol, Myrcene, Isoprene, β -Farnesene, 1,3-Butadiene
R ₁ -CH ₃ R ₂ -CH ₂ R _a	$k_{\text{uni}} = 433$ $k_{\text{H}_2\text{O}} = 9.1 \times 10^{-18}$ $k_{(\text{H}_2\text{O})_2} = 2.1 \times 10^{-14}$	Limonene, δ -3-Carene, Terpinolene, α -Terpinene, β -Farnesene, α -Farnesene, 2-Methyl-1-butene
R ₁ -CH ₂ R _a R ₂ -CH ₃	$k_{\text{uni}} = 689$ $k_{\text{H}_2\text{O}} = 1.5 \times 10^{-17}$ $k_{(\text{H}_2\text{O})_2} = 3.2 \times 10^{-14}$	Limonene, δ -3-Carene, Terpinolene, α -Terpinene, β -Farnesene, α -Farnesene, 2-Methyl-1-butene
R ₁ -CR ₃ =CR ₄ R' R ₂ -CH ₃	$k_{\text{uni}} = 13400$ $k_{\text{H}_2\text{O}} = 1.8 \times 10^{-18}$ $k_{(\text{H}_2\text{O})_2} = 4.8 \times 10^{-15}$	Isoprene, Cis- β -ocimene, Trans- β -ocimene, α -Farnesene
R ₁ -CH ₂ -CR ₃ =CR ₄ R ₅ R ₂ -H	$k_{\text{uni}} = 4180$ $k_{\text{H}_2\text{O}} = 1.5 \times 10^{-18}$ $k_{(\text{H}_2\text{O})_2} = 3.9 \times 10^{-15}$	Cis- β -ocimene, γ -Terpinene, Trans- β -ocimene, Terpinolene, α -Farnesene, Methyl chavicol
	$k_{\text{uni}} = 2.0$ $k_{\text{H}_2\text{O}} = 4.2 \times 10^{-16}$ $k_{(\text{H}_2\text{O})_2} = 6.0 \times 10^{-13}$	β -Pinene

	$k_{\text{uni}} = 60$ $k_{\text{H}_2\text{O}} = 2.4 \times 10^{-19}$ $k_{(\text{H}_2\text{O})_2} = 8.9 \times 10^{-16}$	α -Pinene
	$k_{\text{uni}} = 250$ $k_{\text{H}_2\text{O}} = 9.8 \times 10^{-18}$ $k_{(\text{H}_2\text{O})_2} = 3.2 \times 10^{-15}$	α -Pinene
$\text{R}_1 - \text{CH}_2\text{R}_a$ $\text{R}_2 - \text{C}(\text{R}_3)=\text{CR}_4\text{R}_5$	$k_{\text{uni}} = 39$ $k_{\text{H}_2\text{O}} = 2.1 \times 10^{-19}$ $k_{(\text{H}_2\text{O})_2} = 7.3 \times 10^{-16}$	Terpinolene
$\text{R}_1 - \text{CHR}_a\text{R}_b$ $\text{R}_2 - \text{CH}_3$	$k_{\text{uni}} = 14$ $k_{\text{H}_2\text{O}} = 9.8 \times 10^{-18}$ $k_{(\text{H}_2\text{O})_2} = 1.9 \times 10^{-14}$	Limonene, α -Bergamotene
$\text{R}_1 - \text{CH}_3$ $\text{R}_2 - \text{CHR}_a\text{R}_b$	$k_{\text{uni}} = 611$ $k_{\text{H}_2\text{O}} = 4.3 \times 10^{-18}$ $k_{(\text{H}_2\text{O})_2} = 1.1 \times 10^{-14}$	Limonene, α -Bergamotene
$\text{R}_1 - \text{CR}_3=\text{CR}_4\text{R}'$ $\text{R}_2 - \text{H}$	$k_{\text{uni}} = 14300$ $k_{\text{H}_2\text{O}} = 1.2 \times 10^{-19}$ $k_{(\text{H}_2\text{O})_2} = 4.3 \times 10^{-16}$	Myrcene, Isoprene, Cis- β -ocimene, β -Farnesene, α -Farnesene, 1,3-Butadiene
	$k_{\text{uni}} = 375$ $k_{\text{H}_2\text{O}} = 1.7 \times 10^{-18}$ $k_{(\text{H}_2\text{O})_2} = 3.7 \times 10^{-15}$	β -Pinene
$\text{R}_1 - \text{CR}_3=\text{CR}_4\text{CH}_2\text{R}_a$ $\text{R}_2 - \text{H}$	$k_{\text{uni}} = 5.7 \times 10^6$ $k_{\text{H}_2\text{O}} = 1.2 \times 10^{-19}$ $k_{(\text{H}_2\text{O})_2} = 4.3 \times 10^{-16}$	Trans- β -ocimene

3. Results

The steady state concentration for four environment is calculated as described before, explicitly speciating all CI formed from the unsaturated species measured at each site, and accounting for CI loss by unimolecular reactions, H_2O , $(\text{H}_2\text{O})_2$, SO_2 and acids. As the lifetime of the different CI species can differ by many orders of magnitude, one should consider that CI with high production rates are not necessarily those with the highest ambient concentration, and vice versa. At the same time, some CI species are formed by ozonolysis of multiple species, further complicating the CI apportionment analysis. Each site has between 100 and 150 distinct CI species formed, and as shown below the species distributions are characterized by a long tail, with no single or small set of CI exceedingly dominant over the others. As such, we will aim to describe 90-95% of the source VOC, CI production rate, or CI concentrations rather than describe the entire speciation. The most relevant CI are shown in Figure 3 and Figure 26, where the latter figure depicts those CI that were not considered explicitly in the theoretical kinetic analysis. These two figures do not show all CI that are formed from the VOCs considered in the field data analysis (Figure 24). The CI speciation at each of the sites is listed in Table 48.

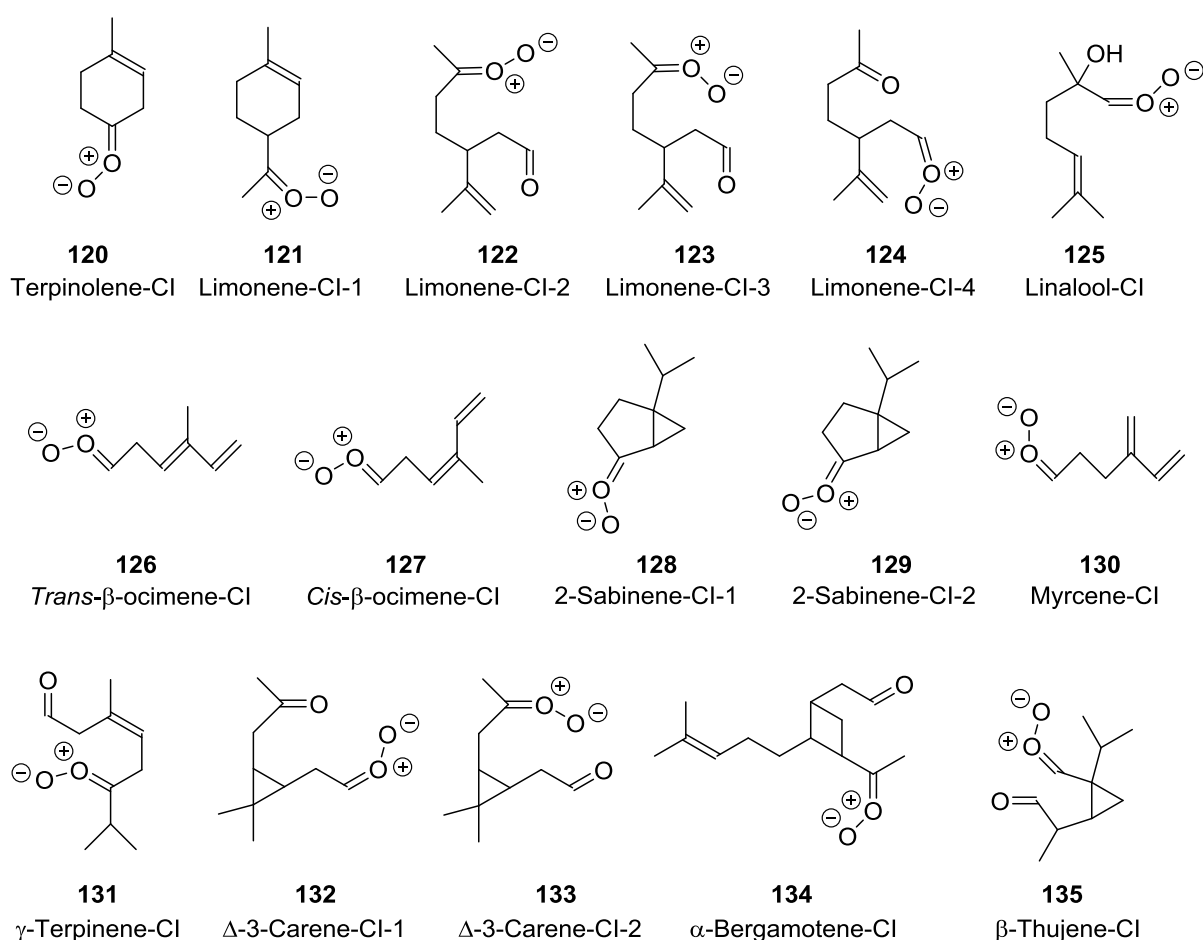


Figure 26: CI formed in ozonolysis of biogenic VOCs measured during field campaigns. The CI shown constitute a sizable fraction of the CI population at at least one measurement site, together with the CI shown in Figure 3, and do not represent an exhaustive list of all CI that are formed.

a. Amazonian rain forest

Isoprene dominates the formation of SCI (34%) in this environment, followed by limonene (15%), *cis*- and *trans*- β -ocimene (14% each), α -pinene (11%) and terpinolene (6%). These BVOCs together contribute up to 95% of the total CI production rate in the Amazonian forest. Accounting for CI losses, we find that an average concentration of SCI of $\sim 1.5 \times 10^4$ molecules cm^{-3} , where contributions of the VOCs to the ambient CI concentration parallels their contribution to the production rate, *i.e.* isoprene is still the dominant contributor (44%), followed by α -pinene (15%), limonene (11%), *cis*- and *trans*- β -ocimene and terpinolene all contributing up to 8% (see Figure 27). Unimolecular reaction is the major loss process for the SCI from the non-isoprene BVOC: for α -pinene it accounts for 62% of the total loss, 60% for limonene, 64% for *cis*- and *trans*-ocimene and 83% for terpinolene. The driving factor is the formation of β -unsaturated CI from the conjugated BVOCs, which leads to very fast unimolecular isomerization rates (up to $1 \times 10^6 \text{ s}^{-1}$). As these loss processes are independent of co-reactant concentrations, the loss of these CI is mostly independent of the reaction conditions. For the SCI generated from isoprene, the main loss is the reaction with water, owing mostly to the fast reaction of CH_2OO (**1**) with water dimer, combined with a 50% contribution of this species in the isoprene CI yield. The concentration of isoprene in the Amazonian forest exceeds that at the other sites by more than 1 order of magnitude, such that the concentration of isoprene-derived SCI is globally likely highest in the Amazonian forest (6×10^3 molecules cm^{-3}).

In this environment, the SCI with the largest production rate is CH_2OO (**1**) (23%) followed by $(\text{CH}_3)_2\text{COO}$ (**7**) (11%), *Z*-MVK oxide (**31**) (11%) and *E*-MVK oxide (**32**) (5%) accounting for 50% of the total SCI production rate. In the ambient CI concentration, the dominant contribution is *E*-MVK oxide (**31**) (42%) followed by *Z*-pinonaldehyde-K-oxide (**55**) (9%) with all the other SCI present in less than 5% each (Table 48). These two SCI have a large production rate (from isoprene and α -pinene, respectively) and a longer lifetime due to a slower reaction with water and water dimers, and a relatively slow unimolecular rate, $\sim 50 \text{ s}^{-1}$.

b. Mexico City

In Mexico City the large majority of VOCs measured is represented by short branched-chain unsaturated compounds with an extensive contribution from anthropogenic activities. Due to the high average concentration of both VOC and ozone, the predicted average CI concentration, 5.5×10^4 molecules cm^{-3} , is the largest of the environments analyzed within this study. Five short branched-chain hydrocarbons contribute up to 90% to both the formation rate and the concentration of CI: isobutene, 2-methyl-2-butene, *trans*-2-butene, *trans*-2-pentene and *cis*-2-butene (29%, 27%, 15%, 9%, 7%, respectively, to the production, and 19%, 28%, 22%, 10%, 10%, respectively, to the concentration, see Figure 27).

The similarity between the different VOC in this environment converts in smaller variety of relevant CI species (Table 48). *Z*- CH_3CHOO (**2**) constitutes 35% of CI formation, and contributes up to 64% of the ambient CI concentration as it is formed from many of the VOC in this environment, reacts slowly with water and water dimer ($k \leq 3 \times 10^{-14} \text{ cm}^3 \text{ molecules}^{-1} \text{ s}^{-1}$), and has a comparatively slow unimolecular loss rate ($\sim 130 \text{ s}^{-1}$). $(\text{CH}_3)_2\text{COO}$ (**7**) is formed in a similar amount, 28% of the total CI production, but contributes only 18% to the CI concentration, owing to its faster unimolecular loss rate ($\sim 480 \text{ s}^{-1}$). Finally, CH_2OO (**1**) also constitutes a large fraction of the production, 20%, but its fast reaction with water dimers ($k = 5 \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$) limits its contribution to the ambient CI concentration to 13% in this environment.

The source speciation and CI speciation agrees well with a recent study by Khan et al.²³³ for the London urban atmosphere, which likewise is dominated by short-chain smaller alkenes.

c. Sierra Nevada temperate forest

The chemistry in the temperate forest included in this study (Sierra Nevada, California, USA), is driven mostly by monoterpenes. Limonene, δ -3-carene and β -pinene dominate the production rate of SCI with 27%, 20%, and 20% contribution, respectively. Together with α -pinene and myrcene, each contributing 10%, these comprise 85% of the total production rate of SCI in this environment. Isoprene contributes less than 3%. The

SCI with the largest production rates are Z-nopinone oxide (**51**), 15% of the total production, followed by CH₂OO (**1**), 8 %, with all others each contributing less than 6%.

Limonene is also the BVOC that contribute the most to the ambient concentration of SCI (27%) followed by β -pinene (21%), α -pinene (13%), δ -3-carene and MVK (both 8%) and myrcene (4%) (see Figure 27). Again, isoprene contributes less than 3%. Combined the predicted average ambient concentration of SCI is $\sim 8 \times 10^3$ molecule cm⁻³. Unimolecular reactions are the major loss processes, destroying more than 75% of the SCI from all these BVOC excluding β -pinene. For β -pinene-derived CI, the main loss is the reaction with water and water dimers (86%) as both CH₂OO (**1**), and Z-nopinone oxide (**50**) formed with a yield of 77%, react fast with water dimers ($k > 6 \times 10^{-13}$ cm³ molecule⁻¹ s⁻¹). The largest contributions to the ambient SCI are Z-nopinone oxide (**51**), 19%, followed by limonene-CI-1 (**121**), 17%, Z-pinonaldehyde-K-oxide (**55**), and E-(CHO)CHOO (**57**), both contributing up to 8%. All other CI each contributes less than 5% (Table 48).

d. Hohenpeissenberg mid-latitude rural area

The mid-latitude rural area (Hohenpeissenberg, Germany) is characterized by the largest variety of VOC measured, with contributions from both natural and anthropogenic sources. It therefore represents an intermediate case between an environment dominated by biogenic emissions (e.g. Amazonia, Sierra Nevada) and a site dominated by anthropogenic sources (e.g. Mexico city). At the same time, average concentrations of the measured VOCs are smaller than the other environments so lower concentrations of SCI can be expected. This environment is characterized by a widely diversified contribution for the VOC to the production rate of the CI, with contributions by myrcene (20%), 2-sabinene (16%), isoprene (16%), α -pinene (12%), limonene (8%) and isobutene (8%), combined constituting still only 80% of the SCI production. Interestingly, in this environment, the SCI with the largest production rate are represented by smaller CI, specifically CH₂OO (**1**) (24%), (CH₃)₂COO (**7**) (13%) and Z-CH₃CHOO (**2**) (5%). The highest contribution of a more complex CI is 5% by E-MVK oxide (**31**), but all other CI contribute each less than 5%. Combined, the predicted average concentration of SCI is 2.3×10^3 molecules cm⁻³.

Table 48: Speciated contributions (%) of CI and total CI concentration at the four measurement sites, calculated as an average over the measurement periods indicated in Table 41. The CI Lewis structures can be found in Figure 3 and Figure 26.

#	CI	Amazonia	Mexico City	Temperate forest	Rural area
1	CH ₂ OO	2	13	2	4
2	Z-CH ₃ CHOO		64		8
7	(CH ₃) ₂ COO	5	18	2	6
33	E-MVK-Oxide	47		2	18
43	E-MACR-Oxide	1			
50	E-Nopinone-oxide			1	
51	Z-Nopinone-Oxide			19	2
52	E-Pinonaldehyde-A-oxide	3		2	3
53	Z-Pinonaldehyde-A-oxide	3		2	3
55	Z-Pinonaldehyde-K-oxide	9		8	10
57	E-(CHO)CHOO			8	
59	E-(C(=O)CH ₃)CHOO			2	
120	Terpinolene-CI	5			
121	Limonene-CI-1	4		17	3
122	Limonene-CI-2	2		3	
123	Limonene-CI-3			2	
124	Limonene-CI-4	4		5	
126	Trans- β -ocimene-CI	2			
127	Cis- β -ocimene-CI	2			
128	2-Sabinene-CI-1	2			25
129	2-Sabinene-CI-2				3
130	Myrcene-CI			2	4
131	γ -Terpinene-CI			4	2
132	Δ -3-Carene-CI-1			5	
133	Δ -3-Carene-CI-2			1	
134	α -Bergamotene-CI			4	
Total average CI concentration (molecule cm ⁻³)		1.5×10^4	5.5×10^4	7.7×10^3	2.3×10^3

The sources of the most important ambient CI are the same VOC, i.e. 2-Sabinene contributes up to 29%, followed by isoprene (20%), α -pinene (15%) and myrcene (9%) (see Figure 27). Despite their high fraction in the CI production, small CI constitute a minor part of the total concentration of CI (8%, 6% and 4% for Z-CH₃CHOO (2), (CH₃)₂COO (7) and CH₂OO (1), respectively). Here, CH₂OO (1) is quickly lost to reaction with water dimers, while unimolecular reactions rapidly decay (CH₃)₂COO (7) and Z-CH₃CHOO (2). Instead, the ambient CI consist of larger CI with the longer lifetime, such as 2-sabinene-CI-2 (129) (25%), *E*-MVK oxide (31) (18%) and Z-pinonaldehyde-K-oxide (55) (10%) (see Table 48).

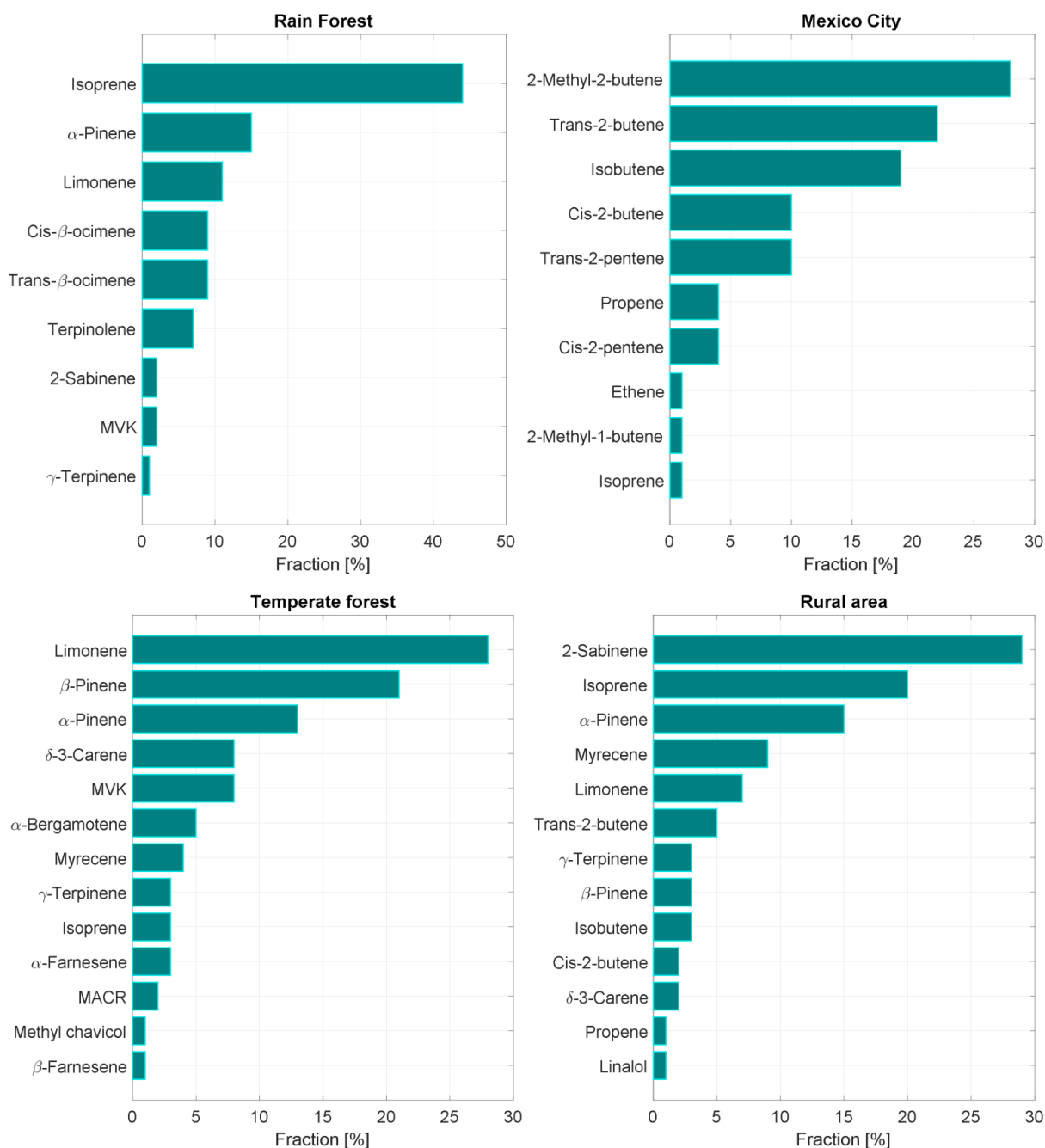


Figure 27: Contribution of the source VOC to the concentration of ambient CI for each of the four measurement sites.

4. Atmospheric SCI speciation

The CI species constituting most to the ambient concentration (Table 48) is variegated, with many found in all environments examined, though with different contributions. Furthermore, the results for Mexico City show that there is again a large difference in speciation between biogenic and anthropogenic environments. It is thus clear that, in the atmosphere, no single CI can be considered as the most critical species. This suggests in turn that the study of the CI chemistry and speciation will remain a complex topic as one cannot focus on a handful of CI, with each environment providing its own CI mixture. From this study, it is found that unimolecular decay is the major loss process, contributing at each measurement site for more than 50% of the total CI loss. The second major loss path is represented by reactions with water and water dimers, where especially the CH₂OO CI has a large impact. These two paths together contribute in all cases to more than 90% to the total loss. This is an important finding, as it indicates that the concentration of CI in the troposphere will be relative small everywhere. Indeed, unimolecular loss is mostly independent on the environment, barring its temperature dependence that will also affect the CI production rate through ozonolysis, and atmospheric humidity is not drastically different across most parts of the globe. The contribution of two important loss processes also makes the predictions more robust to uncertainties on the individual rate coefficients. For example, even if one were to completely neglect the loss of CI by reactions with H₂O and (H₂O)₂, the predicted ambient concentration of non-CH₂OO CI would still only increase by a factor of two in Amazonia or Mexico city.

The theoretical predictions described earlier predicted very slow decay rates for some CI substitution patterns. However, for most of these, no source paths are present from the VOC found at the measurement sites. It is interesting to examine in more detail some specific, slow-reacting CI known to be formed in the atmosphere, as these could accumulate to a higher concentration. For the CI generated at our measurement sites, the lowest unimolecular rate coefficients were predicted for β -thujene-CI (**135**), *E*-(CHO)CHOO (**57**), *E*-(C(O)CH₃)CHOO (**59**), linalool-CI (**125**), and CH₂OO (**1**), with $k(298\text{K})$ values of 0.01, 0.037, 0.17, and 0.3 s⁻¹, respectively. These originate from β -thujene, MVK, MACR, linalool, and any VOC with a terminal double bond, respectively. CH₂OO is formed in large amounts as many VOC present a terminal double bond, but its fast reaction with water dimers prevents the slow unimolecular rate to elongate the lifetime of this CI. β -Thujene-CI (**135**) has the slowest unimolecular loss rate among these CI, and furthermore reacts slowly with water and water dimers, so it has the potential to accumulate to higher concentrations. It is formed from the ozonolysis of β -thujene, a BVOC that reacts fast with ozone ($k = 1.7 \times 10^{-16}$ cm³ molecule⁻¹ s⁻¹) but was observed only in the rain forest, and only in a very low concentration (~ 6 ppt), limiting its contribution to the total CI production. *E*-(CHO)CHOO (**57**) and *E*-(C(O)CH₃)CHOO (**59**) originate from MVK and MACR ozonolysis, respectively, and react relatively slow with water ($k = 5.1 \times 10^{-18}$ cm³ molecule⁻¹ s⁻¹) and water dimers ($k = 1.4 \times 10^{-18}$ cm³ molecule⁻¹ s⁻¹). MVK and MACR are present in large concentrations in isoprene-rich environments such as the Amazonian forest, given that they are the most important secondary stable products from the oxidation of isoprene by the OH radical. However, the slow rate coefficient of MACR and MVK ozonolysis ($k < 5 \times 10^{-18}$ cm³ molecule⁻¹ s⁻¹) limits the production rate of these two long-lived SCI in the Amazonian forest, representing less than 1% of the total production rate and an ambient concentration of less than 250 molecule cm⁻³. In the temperate Sierra Nevada forest they contribute slightly more, due to a higher ozone concentration and a lower relative humidity, but still the predicted concentration remains below 500 molecule cm⁻³ so they are also not likely to accumulate in any environment. Finally, linalool-CI (**125**), is formed from linalool which, like β -thujene, reacts fast with ozone ($k = 4.3 \times 10^{-16}$ cm³ molecule⁻¹ s⁻¹), but is observed only in very small concentration (less than 1 ppt), strongly limiting the source strength of this CI, thus preventing higher concentration of the product CI. In summary, we found no evidence of a CI that benefitted from a slow unimolecular rate and a slow reaction with water, combined with a large production rate, to yield to high CI concentration. In general, the balancing between these three aspects of CI chemistry explains why no single CI was found accumulate to a dominant contribution to the concentration, and why the average concentration predicted remained low.

Two of the above CI (**125**, **135**) show a quaternary carbon in *syn*-position ($R_1 = -CR_aR_bR_c$ in Table 31), which in general yields low rate coefficients and hence a long lifetime; however, no VOC with a sufficiently high concentration in the atmosphere appears to have this functionality. Two of the above CI (**57**, **59**) show a carbonyl group in *syn*-position ($R_1 = -CHO$ or $-C(O)R_a$ in Table 31), which against yields low rate coefficients and hence a long lifetime. Carbonyl substitution in a CI is typically a result of ozonolysis in second- or later generation products, i.e. primary emitted multi-unsaturated VOCs that have already undergone oxidation processes initiated by OH, O₃, NO₃, or other oxidants. These compounds are usually not present in high concentrations due to their high reactivity to a variety of oxidants, deposition, photolysis, and other loss processes.

5. Uncertainty analysis

The complexity of the analysis makes a straightforward, direct estimate of the uncertainty interval of the predicted CI concentrations intractable. Several contributions to the uncertainty can be distinguished, and are discussed below.

The first source of uncertainty is the reliance on direct measurements for VOC concentrations and speciation, and of co-reactant concentrations such as O₃, OH, SO₂, and acids. These measurements show their own variability and uncertainty; however, we consider the ability to include these data directly, and propagate the speciation fully to the CI analysis, as a particular strength in this study. Our predictions rely on averaged values, strongly dampening the uncertainties caused by measurement variability.

The second source of error is the estimate of the CI source strength and speciation. We consider the uncertainties on the rate coefficients for ozonolysis as negligible compared to other sources of error. The site-specificity for ozonolysis of poly-unsaturated relies on the application of a structure-activity relationship, and is likewise not a determining source of uncertainty. The total yield of SCI from the ozonolysis carries a fairly large relative uncertainty. However, given that we typically use a yield of 0.4, our absolute SCI concentration can realistically not be underestimated by more than a factor of two due to this factor. A more important aspect of the ozonolysis step is the speciation of the CI, as combinatorically up to 4 distinct CI can be formed from each double bond, and the lifetimes of these can differ by many orders of magnitude. The impact of changing the CI speciation for a given VOC could thus dwarf all other uncertainties in the ozonolysis step. To probe the maximal impact this speciation uncertainty could have on our predictions, we have implemented the scenario where, for each bond, 100% of the CI formed is that with the longest lifetime, thus maximizing the predicted atmospheric CI concentration. For the Amazonian forest, the average concentration thus obtained was about 6×10^4 molecule cm⁻³, only a factor of 5 above our best-effort prediction, and a similar result was found for the temperate forest and the rural site where the increase in the CI observed is likewise around a factor of 5. In Mexico City, this biased speciation even only increases the [SCI] by 30%. The reason for this limited impact toward CI speciation was already discussed above (section U.4); briefly, it hinges on the fact that there appear to be no VOC that enjoy the combination of elevated concentration, fast ozonolysis, and formation of long-lived CI, all of which are necessary to accumulate notably high CI concentrations.

The third source of uncertainty are the decay rates used in this study; see sections R.4, S.6 and T.5 for a discussion of the uncertainty on the predicted unimolecular and water-driven loss rates. Given the large number of VOC and CI species that contribute, and their long-tail population distribution that prohibits any one CI to have a dominant impact, the uncertainty on any specific rate coefficient would have only a minor impact, averaging out across the population and reducing the overall uncertainty strongly relative to the per-species uncertainty. This leaves the analysis vulnerable to a systematic bias in the loss process rate coefficients. However, as the SARs used to predict the rate coefficients are specifically designed to match the best available experimental and theoretical data, this is unlikely to occur to a critical degree. It should also be noted that multiple loss processes are at play, and that a systematic error on one of them would merely shift the burden to one of the other loss processes (see also section U.5), still preventing the accumulation of higher concentrations of CI in the atmosphere.

Accounting for all the above factors, we estimate an uncertainty of an order of magnitude on the predicted CI concentration. This suggests that the CI concentration in the atmosphere will remain below 1×10^5 molecule cm^{-3} at all times in most places, and that earlier estimates of CI concentration as high as 1×10^6 molecule cm^{-3} are not compatible with our detailed analysis. These predictions also suggest that *in situ* observation of CI might be difficult, especially as these low concentrations are in turn summed across a large variety of different CI. Based on this analysis, we also find that contribution of CI on H_2SO_4 formation remains very small on a global scale, though some local impact cannot be excluded.

V. Global modeling

1. Methodology

The ECHAM/MESSy Atmospheric Chemistry (EMAC) model is a numerical chemistry and climate simulation system that includes sub-models describing tropospheric and middle atmosphere processes and their interaction with oceans, land and human influences.²³⁴ It uses the second version of the Modular Earth Submodel System (MESSy2) to link multi-institutional computer codes. The core atmospheric model is the 5th generation European Centre Hamburg general circulation model (ECHAM5).²³⁵ For the present study we applied EMAC (ECHAM5 version 5.3.02, MESSy version 2.53.0) in the T63L31ECMWF-resolution, i.e. with a spherical truncation of T63 (corresponding to a quadratic Gaussian grid of approx. 1.9 by 1.9 degrees in latitude and longitude) with 31 vertical hybrid pressure levels up to 0.1 hPa. The applied model setup comprised the submodels AEROPT, AIRSEA, BIOBURN, CLOUD, CLOUDOPT, CONVECT, CVTRANS, DDEP, E5VDIFF, GWAVE, JVAL, LNOX, MECCA, MEGAN, OFFEMIS, ONEMIS, ORBIT, PTRAC, QBO, RAD, S4D, SCAV, SEDI, SORBIT, SURFACE, TNUDGE, TROPOP. The global model has been run in the Quasi Chemical Transport Model (QCTM) mode for which the feedbacks between chemistry and dynamics are switched off.²³⁶

Biogenic emissions of about 30 VOCs are modelled with the MEGAN algorithm,²³⁷ while anthropogenic and biomass burning VOC emissions are modelled as in Cabrera-Perez et al.²³⁸

The chemical model used in the EMAC model is the Mainz Organics Mechanism (MOM) and was already used in the study of Lelieveld et al.²³⁹ It is integral part of the CAABA/MECCA atmospheric chemistry module²⁴⁰ and comprises the detailed chemistry of about 40 primarily emitted and 30 unsaturated organic compounds reacting with O₃. Altogether the model encodes the chemistry of a wide range of terpenes, aromatics, and linear alkenes, depicted in Figure 28. The chemical mechanism MOM includes recent OH-recycling reactions of VOC oxidation which have first been implemented for isoprene.^{241–243} The mechanism has been extended by addition of α - and β -pinene oxidation²⁴⁴ and of aromatics degradation.²³⁸

The MOM chemical model described above was then extended to incorporate the main CI formation pathways and loss processes. The chemical model contains ozonolysis reactions of the ~30 VOC shown in Figure 28, which are a good representation of the wide variety of primary emitted VOC as well secondary VOC formed *in situ*. Often these VOC represent a more extended class of VOC all thought to react similarly. Source and sinks were added for all CI formed from these VOCs, where care was taken to not influence the overall chemistry in the model which was shown earlier to describe the atmospheric processes well. Rather, we focus specifically on the expected CI concentrations, speciated per source VOC, and with explicit loss processes by unimolecular decay, and bimolecular reactions with H₂O, (H₂O)₂, SO₂, NO₂, and acids. Future work could extend this chemistry by incorporating detailed mechanisms for each of the reaction products formed in these reactions, where not already implicitly contained in the kinetic model. It should be noted that other loss processes may exist that are not included in the current model, but these will serve mainly to (further) reduce the concentration of CI. The explicit consideration of several distinct loss processes allows for the assessment of the impact of CI on atmospheric chemistry, without necessarily incorporating this impact explicitly.

The reaction kinetics used mostly follows the same methodology as described for the field data analysis. The ozonolysis rate coefficients were unchanged from the original kinetic model (see above), where the predicted yields of the CI, and their speciation, follows the methodology described in section U.2. Each of the CI species formed is assigned to a CI class, and its unimolecular decay rate is described using the SAR in section R.1. Several of the VOC in Figure 28 lead to CI with functionalization that is not described explicitly in the SAR; as described in section R.3, we typically treat these complex functionalities by replacement with an analogous alkyl, carbonyl, or alkoxy functionality that is handled directly by the SAR. The bimolecular reactions with H₂O and (H₂O)₂ follows the SARs in sections S.5 and T.4, respectively, where we use a similar strategy to handle complex functionalities as for unimolecular reactions. The reaction of CI with SO₂ and NO₂

uses the rate coefficients as discussed in section E.4 and E.5, building upon the scarce experimental data. Note that these rate coefficients vary only moderately as a function of functionalization, strongly reducing the expected uncertainty relative to e.g. the more diversified reaction with water. Finally, the fast loss process towards acids builds upon the generalized rate coefficient described in section E.6, where we include reactions with the organic acids HCOOH, HCOCO₂H, CH₃CO₂H, HOCH₂CO₂H, CH₃COCO₂H, MALDALCO₂H, C₅CO₁₄OH, PHCOOH, PINIC, PINONIC, HOOCH₂CO₂H, MACO₂H, LHC₄ACCO₂H, and C₈₉CO₂H (all represented by their model molecular identifiers), as well as with the inorganic acids HNO₃, HNO₄, HCl, HBr, and H₂SO₄. Again, we conclude from the literature data that all rate coefficients of CI with acids are of a similar order of magnitude, and the lack of speciation induces only a moderate uncertainty. It should be stressed here that our model extension only describes the CI as transient intermediates that do not influence the original model chemistry, and all of the reactions given above only regenerate the ozonolysis products already included in the model, with the same yield. Extending the model to include explicit secondary chemistry will be guided by the results described later in this work with regards to the importance of specific reaction channels.

The extended model thus created is the most explicit atmospheric CI model available to date. Compared to earlier efforts, it is mainly distinguished by a highly speciated description of the unimolecular decay and bimolecular reaction with water and water dimer, building upon an extensive set of literature data and new theory-based data. These three reactions are the main loss processes in the atmosphere, and as such the current model has a much better representation of the CI concentrations than earlier efforts that generalized to all CI a data set that contained only a small fraction of the information available in this work. Other sources of uncertainties, such as the yield and speciation of stabilized CI from the ozonolysis reactions are thought to have a smaller impact on the predicted concentrations. As such, while the CI concentration predictions likely still carry an uncertainty of about an order of magnitude, this is significantly reduced compared to other estimates that did not have access even to correct order-of-magnitude rate estimates for many classes of CI important in the atmosphere.

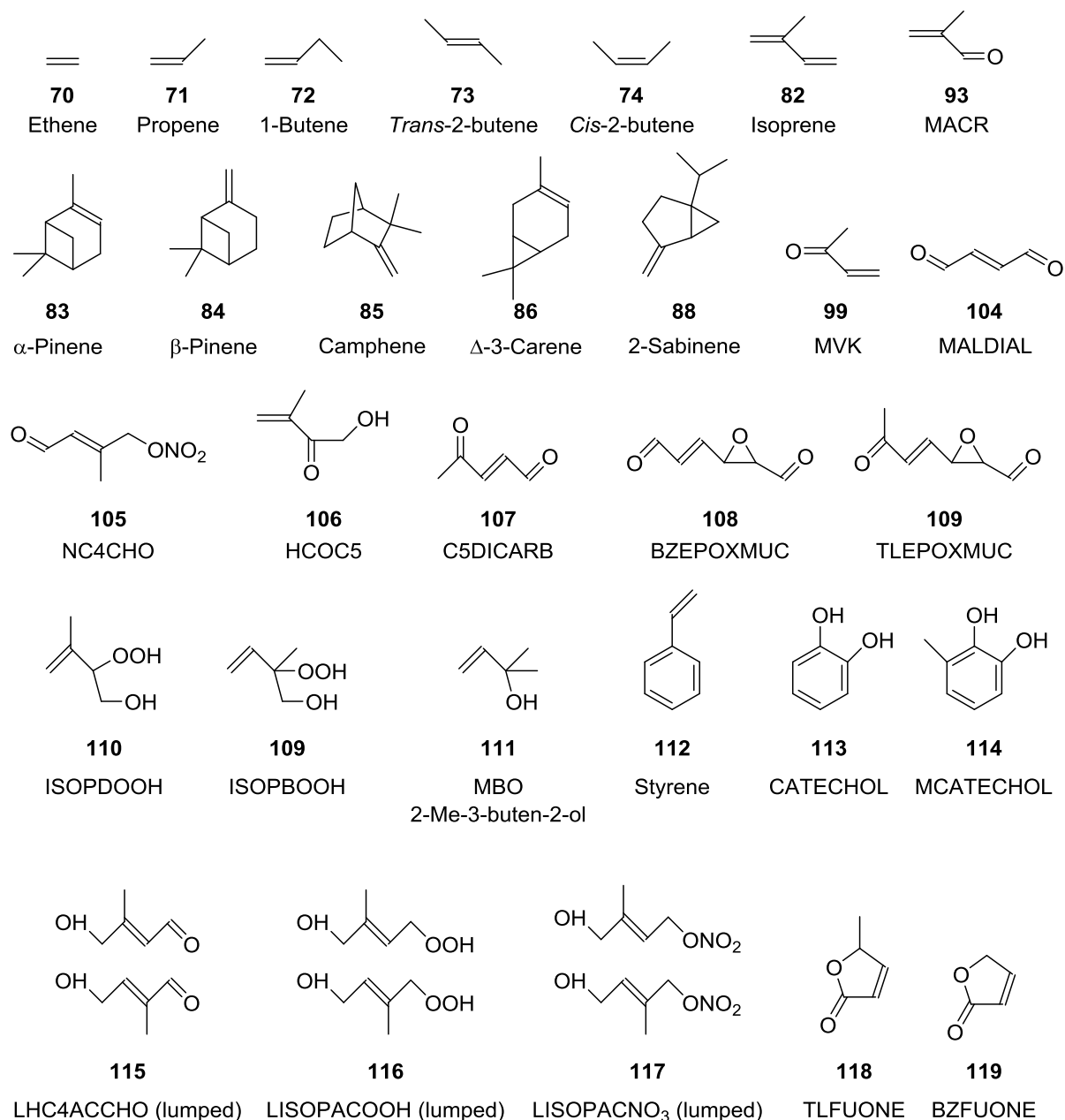


Figure 28: List of unsaturated organic compounds considered as CI sources in the global modeling. Species 104-118 are labeled using their MCM compound code. For lumped species 115 through 117 a 1:1 distribution is assumed.

2. Additional results

The bulk of the CI formation occurs at the surface, where VOC and O₃ are available in highest concentrations. Near the equator, updrafts can lead to increased concentrations of CI at higher altitudes (Figure 29), where the lifetime of these CI is extended due to the lower temperatures and lower absolute humidity. Even at altitudes exceeding 10 km, concentrations as high as 1×10^3 molecule cm⁻³ are predicted, which could affect chemistry locally provided the bimolecular reactions of interest remain sufficiently fast in these reaction conditions.

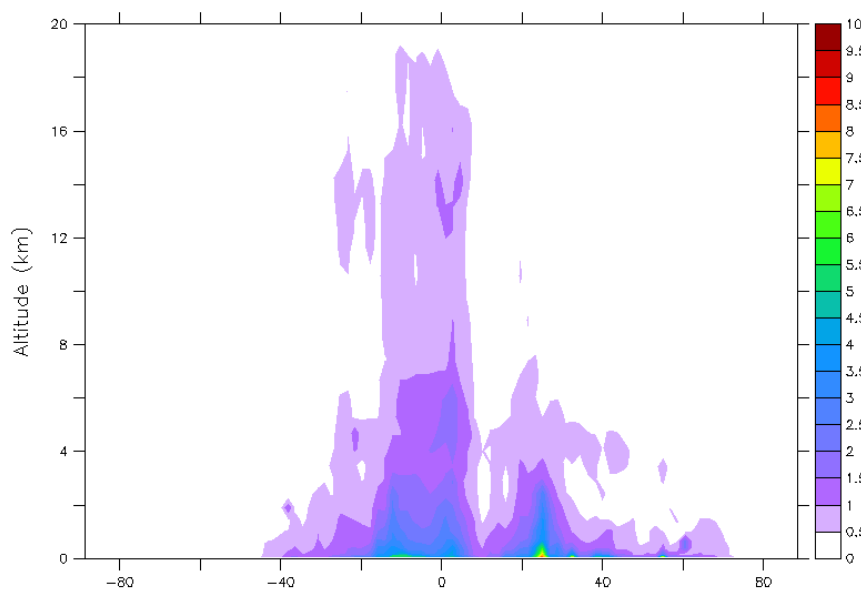


Figure 29: Annual maximum concentration of CI (10^4 molecule cm^{-3}) as a function of altitude and latitude.

Figure 30 and Figure 31 show the CI source VOC as a function of the season. Isoprene and the monoterpenes are a dominant source, as expected considering their emission strengths. Aromatic compounds have a negligible contribution to the CI formation; their impact is limited to a local enhancement along shipping routes in the oceans, areas where the CI concentration is predicted to be very low already. Over landmasses, the contribution of small, linear alkenes is highest in polluted areas.

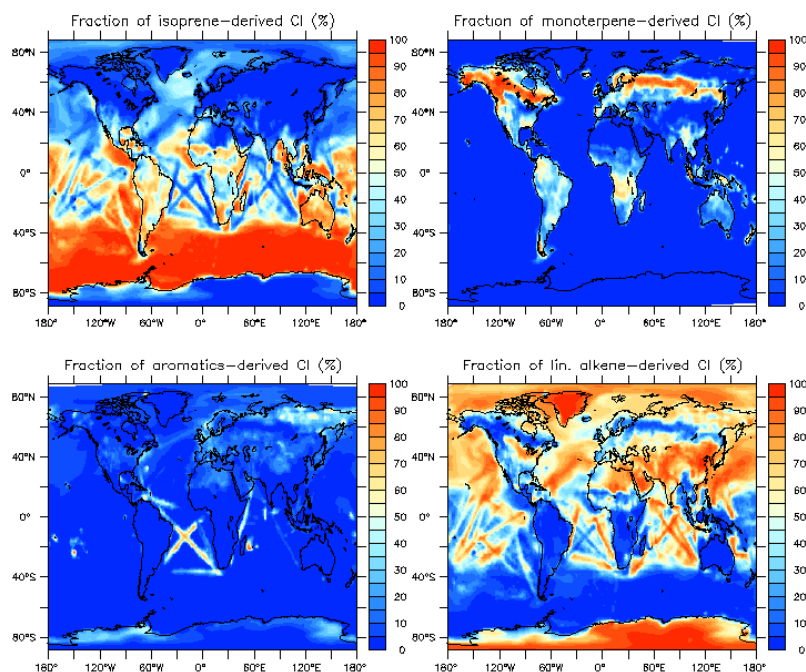


Figure 30: Contributions of the source VOC classes to the CI concentration (%) during winter (January).

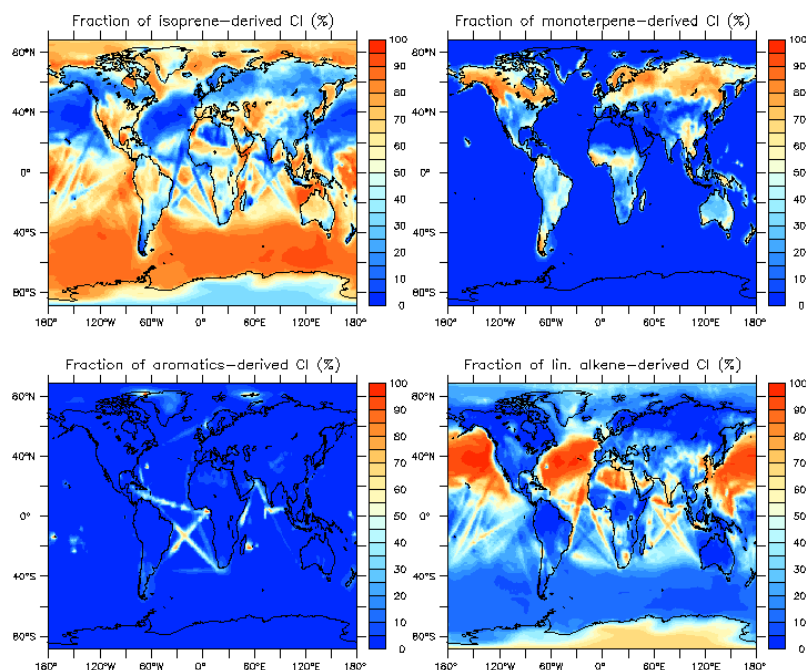


Figure 31: Contributions of the source VOC classes to the CI concentration (%) during summer (June).

The loss processes of CI (see Figure 32) are predicted to be roughly equally distributed across unimolecular decay, reaction with H_2O , and reaction with $(\text{H}_2\text{O})_2$. Combining these latter two channels then indicates that water is the main, but not dominant loss processes. It should be noted that about 20 to 25% of the CI formed is CH_2OO , a CI that is known to react fast with water dimer, while its unimolecular decay is very slow ($k \sim 0.3 \text{ s}^{-1}$). This CI thus increases the contribution of the water loss channel significantly. A second group of CI that is mainly lost to water are the E-RCHOO Criegee intermediates that are formed from terminal double bonds, such as *anti*- CH_3CHOO whose rate coefficients with water is among the few that have been measured. The loss of most of the remaining CI, i.e. all di-substituted, or E-RCHOO CI, tends to be dominated by unimolecular reactions (see Figure 33). The CI concentration is negligibly influenced by SO_2 and NO_2 , though loss by acids can contribute for a few percent, in agreement with earlier predictions by Vereecken et al.^{73,245}

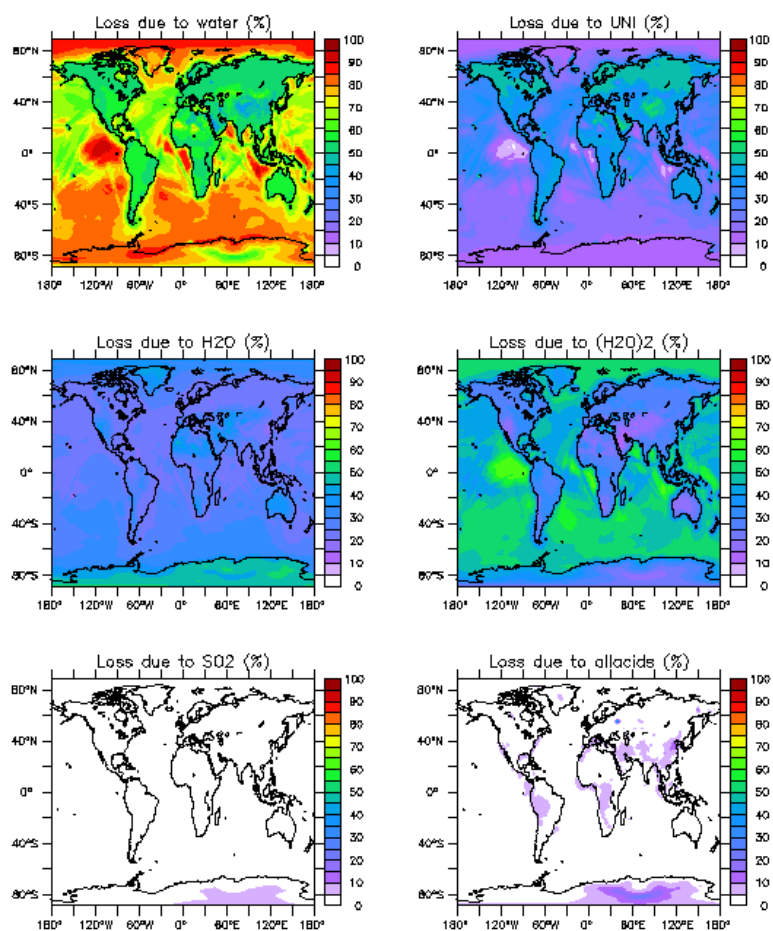


Figure 32: Loss processes of CI (%). Loss towards water is shown both combined and separately for H_2O and $(\text{H}_2\text{O})_2$. Loss to acids includes all organic and inorganic acids in the model. Loss to NO_2 is negligible everywhere.

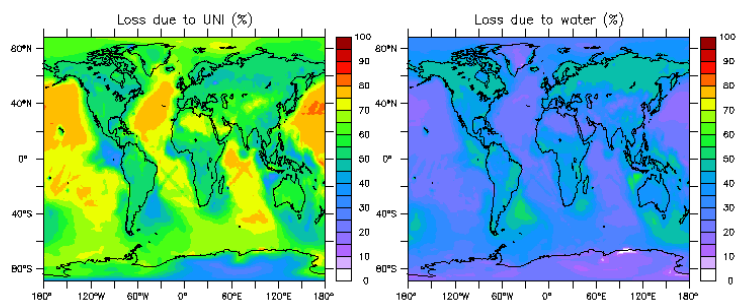


Figure 33: Loss processes of non- CH_2OO CI (%) by unimolecular processes or by reaction with water or water dimer.

W. Impact of CI on atmospheric chemistry

Several estimates of CI concentration are available in the literature,^{57,83,233,246–249} though most of these generalize upon of the limited available data on CI chemistry, thus sometimes using rate coefficients now known to not be the best representation of CI chemistry, or omitting loss processes due to lack of data. This implies large uncertainties on the SCI concentration, which are typically predicted to be $> 10^5$ molecule cm^{-3} . A recent study of field data by Novelli et al.²⁵⁰ used a reverse approach, looking at unexplained phenomena such as missing H_2SO_4 sources, unexplained OH reactivity, or unexplained OH sources, and estimated the CI concentration required to explain these phenomena, in the assumption that CI are the sole drivers in these phenomena, i.e. it estimates an upper limit to CI impact. Their predicted concentration, 5×10^4 molecules cm^{-3} , is lower than earlier estimates, and cannot be exceeded significantly without unreasonably perturbing the fairly well-defined budgets of various species. Our current estimates, based on a highly detailed analysis, are lower still, with predicted yearly peak concentrations never exceeding 1×10^5 molecules cm^{-3} , even in the regions with the most favourable conditions, and average CI concentrations that are over an order of magnitude lower. These low predictions are compatible with the most recent modeling studies.^{83,233,246}

A critical reaction of CI is their fast reaction with SO_2 , forming SO_3 that rapidly hydrates to H_2SO_4 ; this gas phase source of sulphuric acid is the main reason for the interest in atmospheric CI chemistry as it affects particle nucleation. SCI as a source of tropospheric H_2SO_4 , in competition with OH radicals, has been inferred experimentally by Mauldin III et al.¹⁰⁶ A more recent study by Percival et al.²⁴⁶ predicted that the $\text{CI} + \text{SO}_2$ reaction could have a global impact on the H_2SO_4 budget, with up to a 200% $[\text{H}_2\text{SO}_4]$ increase in tropical latitudes, and more moderate increases elsewhere. Khan et al.²³³ predicted an SO_2 oxidation increase of approximately 1/3 in UK urban areas. Our own modeling study finds CI contributing to about 2/3 of the gas phase H_2SO_4 formation in the equatorial belt, with negligible contributions across most of the globe (see Figure 4 in the main text). Our most detailed analysis based on extensive field measurements, finds even lower contributions (see Table 49).

Table 49: Contribution of CI to SO_2 oxidation, and formic acid lifetime towards CI, for 4 sites

	Amazonia	Mexico City	Sierra Nevada	Hohenpeissenberg
Contribution CI to total SO_2 oxidation				
Field data (time series average)	29 %	54 %	19 %	7 %
Modeling (yearly average)	62 %	N/A ^a	10 %	5 %
Gas phase lifetime of HCOOH to CI				
Field data (time series average)	3.5	1	7	27
Modeling (yearly average)	11	N/A ^a	70	79

^a The Mexico City region is not sufficiently resolved in the global model to capture the specific regional chemistry

It should be noted that a large part of the difference in predicted contribution of the CI between our two approaches, and against the literature, is related to the use of different OH concentrations in the analysis. E.g. in the Amazonian forest, our field data analysis uses the experimentally observed average OH concentration of 5×10^6 molecules cm^{-3} as measured by Lelieveld et al.¹⁹⁹ These comparatively high OH concentrations have been suspected to be influence by interferences in the measurement,^{49,250,251} but even using a concentration of 2.5×10^6 molecules cm^{-3} as observed by Whalley et al.²³¹ in a tropical rainforest in East Asia would allow a contribution of SCI of about 50%. The typically higher contributions for $\text{CI} + \text{SO}_2$ found in the modeling studies for this region is due to their lower average $[\text{OH}]$ predictions, i.e. $\sim 0.2 \times 10^6$ molecules cm^{-3} yearly average in our model study, and 1×10^6 molecules cm^{-3} for Percival et al.²⁴⁶ In other regions, the $[\text{OH}]$ are more directly comparable,

e.g. field measurements on Sierra Nevada find an average of 5.4×10^6 molecules cm^{-3} OH over the time period studied, compared to 1×10^6 molecules cm^{-3} yearly average predicted in our modeling study.

As second reaction of important is the fast reaction of SCI with organic acids, and CI could represent an additional loss path. Based on the concentrations estimated in this study from the field data, and adopting a rate coefficient of 2.4×10^{-10} $\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (see section E.6), a lifetime of organic acids towards SCI of ~ 4 days is obtained (see Table 49) in the Amazonian region, longer in Sierra Nevada and Hohenpeissenberg, but about 1 day in Mexico city; CI could thus represent an important gas phase loss processes in some regions. The global lifetime of organic acids in the troposphere is predicted²⁵² to be 2 to 4 days, with a loss dominated by wet and dry deposition rather than gas phase processes. A full assessment of the impact of CI on the atmospheric acid concentration is therefore not obvious, and cannot be done unambiguously based solely on our field data. The modeling study shows that CI does not affect the atmospheric lifetime across most of the globe (see Figure 5 in the main paper), but in the equatorial belt the loss processes becomes competitive against OH, as shown by the life-time of 11 days against CI, compared to 136 days against OH in Amazonia. Again, a more detailed study is required to assess the overall impact of the CI loss path in the total acid loss, i.e. across gas phase and heterogeneous phase.

Overall, we conclude that the impact of CI on atmospheric chemistry is highly limited globally, though there appears to be some regional contribution on SO_2 and carboxylic acid oxidation, e.g. near the equatorial belt, or in specific regions such as Mexico City.

X. References

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Y.Raw quantum chemical data

This section lists the geometries, vibrational wavenumbers, energies, and other data obtained from the quantum chemical characterization of the intermediates. Also included is a population analysis across the conformers for each structure, accounting for the M06-2X/aug-cc-pVTZ relative energy. Conformers that are non-unique (e.g. which are enantiomers of other conformers) are typically not all calculated explicitly, but are included by multiplying the thermochemical data of a single reference conformer.

```
#####
CH2O2
#####

Population analysis as 298K (%)
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)
Compound Qtot      Erel  Erel2  n*Q*MB      %
-----
CH2O2      2.856e+36  0.00   0.00   2.856e+36  100
Total                               2.856e+36  100

CH2O2
~~~~~
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -189.33059345
E(CCSD/Aug-CC-pVTZ) (Hartree): -189.29649234
  T1 diagnostic: 0.041942
E(MP2/Aug-CC-pVTZ) (Hartree): -189.28461281
E(MP3/Aug-CC-pVTZ) (Hartree): -189.28352075
E(RHF/Aug-CC-pVTZ) (Hartree): -188.63545474
E(CCSD(T)/Aug-CC-pVQZ) (Hartree): -189.37915913
E(CCSD/Aug-CC-pVQZ) (Hartree): -189.34290819
  T1 diagnostic: 0.040884
E(MP2/Aug-CC-pVQZ) (Hartree): -189.33750960
E(MP3/Aug-CC-pVQZ) (Hartree): -189.33168563
E(RHF/Aug-CC-pVQZ) (Hartree): -188.64753905
E(UM062X/Aug-CC-pVTZ) (Hartree): -189.57546372
Point group : CS
Electronic state : 1-A'
Cartesian coordinates (Angs):
  C      1.057192      -0.186724      0.000000
  O      0.000000      0.458901      0.000000
  O     -1.164431     -0.209976      0.000000
  H      1.006139     -1.269491      0.000000
  H      1.966157      0.398436      0.000000
Rotational constants (GHz):  81.1979300   12.6778000   10.9656800
Vibrational harmonic frequencies (cm-1):
  537.7503 ( A')      697.5723 ( A'')      930.1710 ( A')
 1022.3957 ( A'')     1261.0787 ( A')      1433.3936 ( A')
 1630.8711 ( A')     3141.7356 ( A')      3292.7088 ( A')
Zero-point correction (Hartree): 0.031775

Population analysis as 298K (%)
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)
Compound      Qtot      Erel  Erel2  n*Q*MB      %
-----
TS.CH2O2.13Hshift 2.788e+36  0.00   0.00   2.788e+36  100
Total                               2.788e+36  100

TS.CH2O2.13Hshift
~~~~~
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -189.27753712
E(CCSD/Aug-CC-pVTZ) (Hartree): -189.24345173
  T1 diagnostic: 0.029614
E(MP2/Aug-CC-pVTZ) (Hartree): -189.23474553
E(MP3/Aug-CC-pVTZ) (Hartree): -189.23307748
E(RHF/Aug-CC-pVTZ) (Hartree): -188.57615265
E(CCSD(T)/Aug-CC-pVQZ) (Hartree): -189.32578088
E(CCSD/Aug-CC-pVQZ) (Hartree): -189.28951437
  T1 diagnostic: 0.028783
E(MP2/Aug-CC-pVQZ) (Hartree): -189.28735507
E(MP3/Aug-CC-pVQZ) (Hartree): -189.28091953
E(RHF/Aug-CC-pVQZ) (Hartree): -188.58784039
E(UM062X/Aug-CC-pVTZ) (Hartree): -189.52234228
Electronic state : 1-A
Cartesian coordinates (Angs):
  C     -0.965828      0.361823      0.000043
  O     -0.141454     -0.569297     -0.000012
  O      1.099500      0.154828     -0.000032
  H      0.140901      1.111971      0.000027
  H     -2.010302      0.032845      0.000068
Rotational constants (GHz):  60.4695000   14.4937100   11.6914300
Vibrational harmonic frequencies (cm-1):
  i1784.7183           758.1734           766.2667
   942.8200           1191.5035          1290.6442
  1615.0177           2146.2743          3088.4891
Zero-point correction (Hartree): 0.026881

Population analysis as 298K (%)
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)
Compound      Qtot      Erel  Erel2  n*Q*MB      %
-----
```

```

-----
TS.CH2O2.isominv.C2v 2.370e+36 0.00 0.00 2.370e+36 100
Total 2.370e+36 100

TS.CH2O2.isominv.C2v
~~~~~
E(UM062X/Aug-CC-pVTZ) (Hartree): -189.51786719
Point group : C2v
Electronic state : 1-A1
Cartesian coordinates (Angs):
  C 0.000000 0.000000 -1.219154
  O 0.000000 0.000000 -0.007508
  H 0.000000 0.949213 -1.762881
  H 0.000000 -0.949213 -1.762881
  O 0.000000 0.000000 1.362595
Rotational constants (GHz): 278.2753300 9.4404600 9.1307000
Vibrational harmonic frequencies (cm-1):
  i626.7485 291.7360 727.7886
  1070.5400 1210.6255 1550.0482
  1739.9277 3015.4639 3129.7993
Zero-point correction (Hartree): 0.029015

Population analysis as 298K (%)
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)
Compound Qtot Erel Erel2 n*Q*MB %
-----
TS.CH2O2.isomrot 3.721e+36 0.00 0.00 7.441e+36 100
Total 7.441e+36 100

TS.CH2O2.isomrot
~~~~~
E(CCSO(T)/Aug-CC-pVTZ) (Hartree): -189.28011416
E(CCSO(Aug-CC-pVTZ) (Hartree): -189.25492429
T1 diagnostic: 0.029735
E(MP2/Aug-CC-pVTZ) (Hartree): -189.22705911
E(MP3/Aug-CC-pVTZ) (Hartree): -189.24278882
E(PMP2/Aug-CC-pVTZ) (Hartree): -189.25008523
E(PMP3/Aug-CC-pVTZ) (Hartree): -189.26570587
E(PUHF/Aug-CC-pVTZ) (Hartree): -188.66534182
E(UHF/Aug-CC-pVTZ) (Hartree): -188.64215189
E(UM062X/Aug-CC-pVTZ) (Hartree): -189.53171702
Electronic state : 1-A
Cartesian coordinates (Angs):
  C 1.121528 -0.126785 -0.000002
  O -0.099814 0.533913 -0.000559
  H 1.448503 -0.510327 -0.953024
  H 1.450248 -0.506132 0.954139
  O -1.103676 -0.311767 0.000421
Rotational constants (GHz): 58.9965800 12.4180500 11.0834500
Vibrational harmonic frequencies (cm-1):
  i533.9763 393.8856 607.0916
  1079.3881 1111.7427 1206.6285
  1448.0682 3160.8899 3311.4865
Zero-point correction (Hartree): 0.028065

Population analysis as 298K (%)
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)
Compound Qtot Erel Erel2 n*Q*MB %
-----
TS.CH2O2.ringclose 2.994e+36 0.00 0.00 5.988e+36 100
Total 5.988e+36 100

TS.CH2O2.ringclose
~~~~~
E(CCSO(T)/Aug-CC-pVTZ) (Hartree): -189.29947456
E(CCSO(Aug-CC-pVTZ) (Hartree): -189.26422265
T1 diagnostic: 0.049172
E(MP2/Aug-CC-pVTZ) (Hartree): -189.24813707
E(MP3/Aug-CC-pVTZ) (Hartree): -189.24792316
E(RHF/Aug-CC-pVTZ) (Hartree): -188.60530967
E(CCSO(T)/Aug-CC-pVQZ) (Hartree): -189.34730204
E(CCSO(Aug-CC-pVQZ) (Hartree): -189.30993237
T1 diagnostic: 0.047927
E(MP2/Aug-CC-pVQZ) (Hartree): -189.30041387
E(MP3/Aug-CC-pVQZ) (Hartree): -189.29553662
E(RHF/Aug-CC-pVQZ) (Hartree): -188.61693690
E(RM062X/Aug-CC-pVTZ) (Hartree): -189.53988647
Electronic state : 1-A
Cartesian coordinates (Angs):
  C -0.893544 -0.284853 0.003517
  O -0.065879 0.653979 -0.083513
  O 1.053666 -0.275495 0.075903
  H -1.779051 -0.132609 0.624007
  H -0.761982 -1.186141 -0.584227
Rotational constants (GHz): 44.7966700 15.7823200 12.1712600
Vibrational harmonic frequencies (cm-1):
  i837.4296 785.6104 801.1938
  1101.6583 1227.8193 1453.3583
  1618.7345 3079.0581 3229.2940
Zero-point correction (Hartree): 0.030292

Population analysis as 298K (%)
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)
Compound Qtot Erel Erel2 n*Q*MB %
-----
TS.CH2O2.ringclose 2.994e+36 0.00 0.00 5.988e+36 100
Total 5.988e+36 100

TS.CH2O2.ringclose

```

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~~~~~
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -189.29947456
E(CCSD/Aug-CC-pVTZ) (Hartree): -189.26422265
  T1 diagnostic: 0.049172
E(MP2/Aug-CC-pVTZ) (Hartree): -189.24813707
E(MP3/Aug-CC-pVTZ) (Hartree): -189.24792316
E(RHF/Aug-CC-pVTZ) (Hartree): -188.60530967
E(CCSD(T)/Aug-CC-pVQZ) (Hartree): -189.34730204
E(CCSD/Aug-CC-pVQZ) (Hartree): -189.30993237
  T1 diagnostic: 0.047927
E(MP2/Aug-CC-pVQZ) (Hartree): -189.30041387
E(MP3/Aug-CC-pVQZ) (Hartree): -189.29553662
E(RHF/Aug-CC-pVQZ) (Hartree): -188.61693690
E(RM062X/Aug-CC-pVTZ) (Hartree): -189.53988647
Electronic state : 1-A
Cartesian coordinates (Angs):
  C    -0.893544    -0.284853    0.003517
  O    -0.065879    0.653979   -0.083513
  O     1.053666   -0.275495    0.075903
  H    -1.779051   -0.132609    0.624007
  H    -0.761982   -1.186141   -0.584227
Rotational constants (GHz):  44.7966700  15.7823200  12.1712600
Vibrational harmonic frequencies (cm-1):
  i837.4296          785.6104          801.1938
 1101.6583          1227.8193          1453.3583
 1618.7345          3079.0581          3229.2940
Zero-point correction (Hartree): 0.030292

#####
Z- (CH3) CHOO
#####

Population analysis as 298K (%)
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)
Compound Qtot      Erel  Erel2  n*Q*MB      %
-----
CH3CHO2s 3.748e+37 0.00  0.00  3.748e+37 100
Total    3.748e+37 100

CH3CHO2s
~~~~~
E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -228.39106504
E(CCSD/Aug-CC-pVDZ) (Hartree): -228.36107891
  T1 diagnostic: 0.036890
E(MP2/Aug-CC-pVDZ) (Hartree): -228.32874469
E(MP3/Aug-CC-pVDZ) (Hartree): -228.34388514
E(RHF/Aug-CC-pVDZ) (Hartree): -227.64668973
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -228.59065161
E(CCSD/Aug-CC-pVTZ) (Hartree): -228.54908136
  T1 diagnostic: 0.035105
E(MP2/Aug-CC-pVTZ) (Hartree): -228.52797753
E(MP3/Aug-CC-pVTZ) (Hartree): -228.53654107
E(RHF/Aug-CC-pVTZ) (Hartree): -227.70288046
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -228.59065146
E(CCSD-T/AUG-CC-PVTZ) (Hartree): -228.58913737
E(CCSD/AUG-CC-PVTZ) (Hartree): -228.54908073
  T1 diagnostic: 0.035096
  D1 diagnostic: 0.160268
E(CCSD[T]/AUG-CC-PVTZ) (Hartree): -228.59576124
E(RHF/AUG-CC-PVTZ) (Hartree): -227.70288056
E(CCSD(T)/Aug-CC-pVQZ) (Hartree): -228.64894392
E(CCSD/Aug-CC-pVQZ) (Hartree): -228.60473056
  T1 diagnostic: 0.034234
E(MP2/Aug-CC-pVQZ) (Hartree): -228.59219321
E(MP3/Aug-CC-pVQZ) (Hartree): -228.59418876
E(RHF/Aug-CC-pVQZ) (Hartree): -227.71709662
E(RM062X/Aug-CC-pVTZ) (Hartree): -228.90272701
Electronic state : 1-A
Cartesian coordinates (Angs):
  C     0.471417    0.702258    0.000009
  O    -0.770016    0.584690    0.000003
  O    -1.269067   -0.677676    0.000002
  C     1.348246   -0.472175   -0.000015
  H     0.807438    1.732755    0.000032
  H     1.095834   -1.089417   -0.866318
  H     1.095907   -1.089400    0.866323
  H     2.395505   -0.190547   -0.000045
Rotational constants (GHz):  17.8489200  7.2532700  5.3217500
Vibrational harmonic frequencies (cm-1):
  216.1377          321.0560          471.8577
  683.1234          781.1765          928.5602
  998.9468          1068.7093          1112.1445
 1361.4043          1410.3805          1440.5155
 1464.6823          1647.0242          3053.7590
 3098.7604          3190.5974          3206.8169
Zero-point correction (Hartree): 0.060270

Population analysis as 298K (%)
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)
Compound Qtot      Erel  Erel2  n*Q*MB      %
-----
TS.CH3CHO2s.isominv 7.433e+37 0.00  0.00  7.433e+37 100
Total              7.433e+37 100

TS.CH3CHO2s.isominv
~~~~~
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -228.52211272
E(CCSD/Aug-CC-pVTZ) (Hartree): -228.48306069
  T1 diagnostic: 0.027111

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E(MP2/Aug-CC-pVTZ) (Hartree): -228.45694041
 E(MP3/Aug-CC-pVTZ) (Hartree): -228.47131856
 E(RHF/Aug-CC-pVTZ) (Hartree): -227.65040739
 E(RM062X/Aug-CC-pVTZ) (Hartree): -228.83969726
 Point group : CS
 Electronic state : 1-A'
 Cartesian coordinates (Angs):
 C 0.674650 -0.378855 0.000000
 O 0.000000 0.629316 0.000000
 C 0.086218 -1.748637 0.000000
 H 1.767485 -0.269365 0.000000
 H -0.998531 -1.699463 0.000000
 H 0.438115 -2.293311 0.877936
 H 0.438115 -2.293311 -0.877936
 O -0.776299 1.785734 0.000000
 Rotational constants (GHz): 37.8957200 4.2794200 3.9383100
 Vibrational harmonic frequencies (cm-1):
 i563.0603 (A') 112.8006 (A'') 236.4851 (A'')
 383.7108 (A') 677.8868 (A') 758.3476 (A'')
 928.7640 (A') 1085.7106 (A'') 1114.4369 (A')
 1388.9301 (A') 1430.6543 (A') 1470.4343 (A'')
 1471.5937 (A') 1776.8569 (A') 3034.3987 (A')
 3063.7274 (A') 3122.9966 (A'') 3184.6119 (A')
 Zero-point correction (Hartree): 0.057506

Population analysis as 298K (%)
 Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)
 Compound Qtot Erel Erel2 n*Q*MB %

 TS.CH3CHO2s.isomrot 5.467e+37 0.00 0.00 1.093e+38 100
 Total 1.093e+38 100

TS.CH3CHO2s.isomrot
 ~~~~~  
 E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -228.53294188  
 E(CCSD/Aug-CC-pVTZ) (Hartree): -228.49979550  
 T1 diagnostic: 0.026842  
 E(MP2/Aug-CC-pVTZ) (Hartree): -228.46161656  
 E(MP3/Aug-CC-pVTZ) (Hartree): -228.48724996  
 E(PMP2/Aug-CC-pVTZ) (Hartree): -228.48521978  
 E(PMP3/Aug-CC-pVTZ) (Hartree): -228.51073600  
 E(PUHF/Aug-CC-pVTZ) (Hartree): -227.72326430  
 E(UHF/Aug-CC-pVTZ) (Hartree): -227.69948578  
 E(UM062X/Aug-CC-pVTZ) (Hartree): -228.85041849  
 Electronic state : 1-A  
 Cartesian coordinates (Angs):  
 C -0.471427 0.646973 -0.186575  
 O 0.775942 0.411988 0.402731  
 C -1.511963 -0.369886 0.057617  
 H -0.421792 1.278770 -1.061449  
 H -1.636218 -0.544062 1.127388  
 H -1.233429 -1.323734 -0.403629  
 H -2.461484 -0.047493 -0.363158  
 O 1.430715 -0.540238 -0.218407  
 Rotational constants (GHz): 20.8790400 5.6869900 5.0349300  
 Vibrational harmonic frequencies (cm-1):  
 i343.6376 159.0343 255.9744  
 469.1424 573.5811 901.9797  
 1007.9786 1115.4176 1141.6749  
 1204.7110 1342.2499 1408.3872  
 1465.4410 1482.5991 3028.5608  
 3099.4755 3157.6795 3215.0032  
 Zero-point correction (Hartree): 0.057020

Population analysis as 298K (%)  
 Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)  
 Compound Qtot Erel Erel2 n\*Q\*MB %  
 -----  
 TS.CH3CHO2s.ringclose 3.037e+37 0.00 0.00 6.074e+37 100  
 Total 6.074e+37 100

TS.CH3CHO2s.ringclose  
 ~~~~~  
 E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -228.35361976
 E(CCSD/Aug-CC-pVDZ) (Hartree): -228.32293161
 T1 diagnostic: 0.042207
 E(MP2/Aug-CC-pVDZ) (Hartree): -228.28574577
 E(MP3/Aug-CC-pVDZ) (Hartree): -228.30311291
 E(RHF/Aug-CC-pVDZ) (Hartree): -227.61369114
 E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -228.55208420
 E(CCSD/Aug-CC-pVTZ) (Hartree): -228.51009697
 T1 diagnostic: 0.039780
 E(MP2/Aug-CC-pVTZ) (Hartree): -228.48421037
 E(MP3/Aug-CC-pVTZ) (Hartree): -228.49529104
 E(RHF/Aug-CC-pVTZ) (Hartree): -227.66928291
 E(CCSD(T)/Aug-CC-pVQZ) (Hartree): -228.60962646
 E(CCSD/Aug-CC-pVQZ) (Hartree): -228.56504334
 T1 diagnostic: 0.038761
 E(MP2/Aug-CC-pVQZ) (Hartree): -228.54774488
 E(MP3/Aug-CC-pVQZ) (Hartree): -228.55233197
 E(RHF/Aug-CC-pVQZ) (Hartree): -227.68306326
 E(RM062X/Aug-CC-pVTZ) (Hartree): -228.86079976
 Electronic state : 1-A
 Cartesian coordinates (Angs):
 C 0.287520 0.607623 0.213383
 O -0.874717 0.597442 -0.277355
 O -1.082288 -0.800965 0.152829
 C 1.395460 -0.316128 -0.106111
 H 0.522574 1.481602 0.833405
 H 1.100788 -1.016335 -0.879234

```

      H      1.672571      -0.872867      0.790675
      H      2.262228      0.286814     -0.392270
Rotational constants (GHz):  16.7248000    7.3453000    5.6098400
Vibrational harmonic frequencies (cm-1):
      i756.7567      258.0086      380.9343
      492.6234      762.4510      889.9869
      923.8059      1106.4819     1152.5744
      1378.6086     1404.9938     1442.4294
      1462.5684     1636.1606     3046.5125
      3065.6703     3111.8145     3203.0362
Zero-point correction (Hartree): 0.058591

Population analysis as 298K (%)
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)
Compound      Qtot      Erel      Erel2      n*Q*MB      %
-----
TS.CH3CHO2s.14Hshift 1.826e+37 0.00    0.00    3.651e+37 100
Total              3.651e+37 100

TS.CH3CHO2s.14Hshift
~~~~~
E(CCS(D)T)/Aug-CC-pVDZ) (Hartree): -228.36073497
E(CCS(D)Aug-CC-pVDZ) (Hartree): -228.32875776
  T1 diagnostic: 0.030049
E(MP2/Aug-CC-pVDZ) (Hartree): -228.30517910
E(MP3/Aug-CC-pVDZ) (Hartree): -228.31480758
E(RHF/Aug-CC-pVDZ) (Hartree): -227.60180227
E(CCS(D)T)/Aug-CC-pVTZ) (Hartree): -228.56091428
E(CCS(D)Aug-CC-pVTZ) (Hartree): -228.51704635
  T1 diagnostic: 0.028442
E(MP2/Aug-CC-pVTZ) (Hartree): -228.50501030
E(MP3/Aug-CC-pVTZ) (Hartree): -228.50773561
E(RHF/Aug-CC-pVTZ) (Hartree): -227.65739339
E(CCS(D)T)/AUG-CC-PVTZ) (Hartree): -228.56091534
E(CCS(D)-T/AUG-CC-PVTZ) (Hartree): -228.55981183
E(CCS(D)AUG-CC-PVTZ) (Hartree): -228.51704645
  T1 diagnostic: 0.028447
  D1 diagnostic: 0.124733
E(CCS(D)T)/AUG-CC-PVTZ) (Hartree): -228.56494259
E(RHF/AUG-CC-PVTZ) (Hartree): -227.65739350
E(CCS(D)T)/Aug-CC-pVQZ) (Hartree): -228.61944789
E(CCS(D)Aug-CC-pVQZ) (Hartree): -228.57284300
  T1 diagnostic: 0.027748
E(MP2/Aug-CC-pVQZ) (Hartree): -228.56945445
E(MP3/Aug-CC-pVQZ) (Hartree): -228.56552776
E(RHF/Aug-CC-pVQZ) (Hartree): -227.67142660
E(RM062X/Aug-CC-pVTZ) (Hartree): -228.87467857
Electronic state : 1-A
Cartesian coordinates (Angs):
      C      0.543227      0.707059      0.035157
      O     -0.737844      0.648862      0.025236
      O     -1.142477     -0.675663     -0.024712
      C      1.233637     -0.511019     -0.016049
      H      0.926954      1.712330     -0.096209
      H      1.072501     -1.172815      0.834400
      H      2.256272     -0.473202     -0.361738
      H      0.125658     -1.028142     -0.495290
Rotational constants (GHz):  16.9110200    8.5085600    5.8062300
Vibrational harmonic frequencies (cm-1):
      i1618.1972      503.4335      534.7613
      713.5631      756.1878      870.5213
      968.7228      989.7768     1056.4046
      1217.3921      1323.4907     1359.5181
      1493.5595      1593.7212     1880.7527
      3111.4342      3205.1557     3239.0718
Zero-point correction (Hartree): 0.056538

Population analysis as 298K (%)
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)
Compound      Qtot      Erel      Erel2      n*Q*MB      %
-----
TS.CH3CHO2s.14Hshift 1.826e+37 0.00    0.00    3.651e+37 100
Total              3.651e+37 100

TS.CH3CHO2s.14Hshift
~~~~~
E(CCS(D)T)/Aug-CC-pVDZ) (Hartree): -228.36073497
E(CCS(D)Aug-CC-pVDZ) (Hartree): -228.32875776
  T1 diagnostic: 0.030049
E(MP2/Aug-CC-pVDZ) (Hartree): -228.30517910
E(MP3/Aug-CC-pVDZ) (Hartree): -228.31480758
E(RHF/Aug-CC-pVDZ) (Hartree): -227.60180227
E(CCS(D)T)/Aug-CC-pVTZ) (Hartree): -228.56091428
E(CCS(D)Aug-CC-pVTZ) (Hartree): -228.51704635
  T1 diagnostic: 0.028442
E(MP2/Aug-CC-pVTZ) (Hartree): -228.50501030
E(MP3/Aug-CC-pVTZ) (Hartree): -228.50773561
E(RHF/Aug-CC-pVTZ) (Hartree): -227.65739339
E(CCS(D)T)/AUG-CC-PVTZ) (Hartree): -228.56091534
E(CCS(D)-T/AUG-CC-PVTZ) (Hartree): -228.55981183
E(CCS(D)AUG-CC-PVTZ) (Hartree): -228.51704645
  T1 diagnostic: 0.028447
  D1 diagnostic: 0.124733
E(CCS(D)T)/AUG-CC-PVTZ) (Hartree): -228.56494259
E(RHF/AUG-CC-PVTZ) (Hartree): -227.65739350
E(CCS(D)T)/Aug-CC-pVQZ) (Hartree): -228.61944789
E(CCS(D)Aug-CC-pVQZ) (Hartree): -228.57284300
  T1 diagnostic: 0.027748
E(MP2/Aug-CC-pVQZ) (Hartree): -228.56945445
E(MP3/Aug-CC-pVQZ) (Hartree): -228.56552776

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E(RHF/Aug-CC-pVQZ) (Hartree): -227.67142660
E(RM062X/Aug-CC-pVTZ) (Hartree): -228.87467857
Electronic state : 1-A
Cartesian coordinates (Angs):
  C    0.543227    0.707059    0.035157
  O   -0.737844    0.648862    0.025236
  O   -1.142477   -0.675663   -0.024712
  C    1.233637   -0.511019   -0.016049
  H    0.926954    1.712330   -0.096209
  H    1.072501   -1.172815    0.834400
  H    2.256272   -0.473202   -0.361738
  H    0.125658   -1.028142   -0.495290
Rotational constants (GHz): 16.9110200    8.5085600    5.8062300
Vibrational harmonic frequencies (cm-1):
  i1618.1972    503.4335    534.7613
  713.5631    756.1878    870.5213
  968.7228    989.7768    1056.4046
  1217.3921    1323.4907    1359.5181
  1493.5595    1593.7212    1880.7527
  3111.4342    3205.1557    3239.0718
Zero-point correction (Hartree): 0.056538

#####
Z- (C2H5)CHOO
#####

Population analysis as 298K (%)
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)
Compound      Qtot      Erel      Erel2  n*Q*MB      %
-----
C2H5CHO2s.t  4.707e+38  0.00    0.00  4.707e+38  74.6
C2H5CHO2s.m  3.703e+38  0.91    0.91  7.999e+37  12.7
C2H5CHO2s.p  3.701e+38  0.91    0.91  7.987e+37  12.7
Total                    6.305e+38  100

C2H5CHO2s.m
~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -268.20891076
Electronic state : 1-A
Cartesian coordinates (Angs):
  C    0.278488    0.954642   -0.135695
  O    1.314221    0.275612   -0.283081
  O    1.327618   -0.984289    0.228911
  C   -0.917895    0.438892    0.550898
  H    0.354777    1.942889   -0.577451
  C   -1.663293   -0.565823   -0.346569
  H   -0.570192   -0.077975    1.447288
  H   -1.561536    1.273088    0.822159
  H   -0.992569   -1.374567   -0.624064
  H   -2.040388   -0.082014   -1.245996
  H   -2.508603   -0.978277    0.199616
Rotational constants (GHz): 9.2619000    3.9974200    3.2413300
Vibrational harmonic frequencies (cm-1):
  144.7554    202.1935    241.0359
  347.4841    546.8786    661.1445
  816.7362    876.9389    916.8954
  920.6522    1030.0026    1092.8152
  1150.8714    1285.8789    1335.4185
  1386.9254    1403.7146    1466.2957
  1499.7696    1515.5925    1647.1204
  3075.2132    3081.2750    3138.6153
  3153.7830    3174.9335    3188.9435
Zero-point correction (Hartree): 0.089536

C2H5CHO2s.p
~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -268.20891080
Electronic state : 1-A
Cartesian coordinates (Angs):
  C   -0.278611    0.954607   -0.135735
  O   -1.314433    0.275605   -0.282925
  O   -1.327521   -0.984497    0.228739
  C    0.917796    0.438879    0.550736
  H   -0.355273    1.943045   -0.577040
  C    1.663601   -0.565645   -0.346462
  H    1.561334    1.273195    0.821986
  H    0.569918   -0.077892    1.447140
  H    2.042335   -0.081234   -1.244863
  H    0.992829   -1.373786   -0.625585
  H    2.507772   -0.979245    0.200617
Rotational constants (GHz): 9.2625200    3.9970400    3.2408500
Vibrational harmonic frequencies (cm-1):
  144.9025    202.1630    240.9850
  347.5326    546.9053    661.1894
  816.7920    876.9699    916.7529
  920.7489    1030.2455    1092.8723
  1150.8697    1285.9860    1335.5587
  1386.9916    1403.7525    1466.2754
  1499.7891    1515.6077    1646.9981
  3075.0210    3081.2855    3138.3958
  3153.8206    3174.9602    3188.7790
Zero-point correction (Hartree): 0.089537

C2H5CHO2s.t
~~~~~
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -267.83270092
E(CCSD/Aug-CC-pVTZ) (Hartree): -267.78343884
T1 diagnostic: 0.031771
E(MP2/Aug-CC-pVTZ) (Hartree): -267.75207093
E(MP3/Aug-CC-pVTZ) (Hartree): -267.77058857
E(RHF/Aug-CC-pVTZ) (Hartree): -266.75118583

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E(RM062X/Aug-CC-pVTZ) (Hartree): -268.20968191
Electronic state : 1-A
Cartesian coordinates (Angs):
  C    0.147992    0.707436   -0.000067
  O    1.387183    0.572657    0.000036
  O    1.866777   -0.699183    0.000063
  C   -0.762122   -0.445328   -0.000130
  H   -0.177877    1.743524   -0.000089
  C   -2.230974   -0.051801    0.000106
  H   -0.478329   -1.063590   -0.859144
  H   -0.478101   -1.063944    0.858541
  H   -2.482662    0.536676   -0.881796
  H   -2.482730    0.535469    0.882783
  H   -2.861356   -0.937773   -0.000541
Rotational constants (GHz):  16.1239500    2.8610300    2.5034300
Vibrational harmonic frequencies (cm-1):
  111.1714        204.5145        231.9078
  370.5662        476.2135        701.5065
  713.1797        858.5241        917.4724
  944.3001        1067.0259       1112.6771
  1146.7364       1252.3157       1321.5467
  1401.6998       1426.3424       1430.7653
  1508.0179       1509.9326       1648.5509
  3043.9019       3059.6485       3072.5721
  3137.5791       3156.1547       3180.5211
Zero-point correction (Hartree): 0.088861

Population analysis as 298K (%)
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)
Compound      Qtot      Erel  Erel2  n*Q*MB  %
-----
TS.C2H5CHO2s.isom.t 7.197e+38 0.00  0.00  2.159e+39 100
Total              2.159e+39 100

TS.C2H5CHO2s.isom.t
~~~~~
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -267.77510058
E(CCSD/Aug-CC-pVTZ) (Hartree): -267.73417998
T1 diagnostic: 0.024523
E(MP2/Aug-CC-pVTZ) (Hartree): -267.68585129
E(MP3/Aug-CC-pVTZ) (Hartree): -267.72140975
E(PMP2/Aug-CC-pVTZ) (Hartree): -267.70942834
E(PMP3/Aug-CC-pVTZ) (Hartree): -267.74487027
E(PUHF/Aug-CC-pVTZ) (Hartree): -266.77110716
E(UHF/Aug-CC-pVTZ) (Hartree): -266.74735529
E(UM062X/Aug-CC-pVTZ) (Hartree): -268.15747902
Electronic state : 1-A
Cartesian coordinates (Angs):
  C    0.116127    0.627706   -0.068250
  O    1.428124    0.414843    0.364359
  C   -0.880174   -0.407642    0.280933
  H    0.040839    1.274393   -0.932381
  C   -2.284711   -0.010327   -0.156412
  H   -0.584733   -1.352770   -0.191575
  H   -0.842440   -0.583913    1.359321
  H   -2.326370    0.143219   -1.234663
  H   -2.596415    0.913874    0.328847
  H   -3.002019   -0.787112    0.099762
  O    2.022336   -0.523108   -0.335226
Rotational constants (GHz):  17.5495700    2.5174500    2.3971400
Vibrational harmonic frequencies (cm-1):
  i347.0656        73.9701        196.4229
  242.2443        320.3713        475.9265
  596.1529        784.3369        908.5703
  1040.3347       1073.4394       1105.9862
  1158.3016       1202.6858       1264.4460
  1291.8472       1395.8852       1417.3187
  1473.9942       1504.4710       1509.4248
  3014.8607       3067.0664       3070.6663
  3137.2391       3150.6418       3197.9312
Zero-point correction (Hartree): 0.085829

Population analysis as 298K (%)
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)
Compound      Qtot      Erel  Erel2  n*Q*MB  %
-----
TS.C2H5CHO2s.ringclose.m 3.348e+38 0.00  0.00  6.696e+38 40.7
TS.C2H5CHO2s.ringclose.c 3.360e+38 0.17  0.17  5.040e+38 30.6
TS.C2H5CHO2s.ringclose.p 3.834e+38 0.29  0.29  4.708e+38 28.6
Total              1.644e+39 100

TS.C2H5CHO2s.ringclose.c
~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -268.16849221
Electronic state : 1-A
Cartesian coordinates (Angs):
  C   -0.494244    0.874532    0.022098
  O   -1.312215    0.088455   -0.530445
  O   -1.066805   -0.971255    0.466123
  C    0.947119    0.664785    0.282771
  H   -0.871570    1.890979    0.191606
  C    1.578392   -0.606045   -0.256174
  H    1.418129    1.560965   -0.144996
  H    1.096369    0.768732    1.362710
  H    1.223814   -0.812001   -1.265022
  H    1.317264   -1.456964    0.362349
  H    2.660559   -0.488943   -0.284243
Rotational constants (GHz):  8.8451700    4.3342000    3.4379200
Vibrational harmonic frequencies (cm-1):
  i723.3923        122.3789        205.9285

```

306.3177	338.0684	642.6742
706.4620	800.2317	874.9133
958.6883	1029.8116	1114.1781
1134.3300	1273.0215	1385.7983
1393.4538	1419.9476	1442.3718
1491.2205	1502.6908	1625.2200
3011.1481	3059.6258	3064.9275
3083.8522	3147.9909	3193.4979

Zero-point correction (Hartree): 0.087319

TS.C2H5CHO2s.ringclose.m

~~~~~

E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -267.79558425

E(CCSD/Aug-CC-pVTZ) (Hartree): -267.74562631

T1 diagnostic: 0.035831

E(MP2/Aug-CC-pVTZ) (Hartree): -267.70996201

E(MP3/Aug-CC-pVTZ) (Hartree): -267.73056482

E(RHF/Aug-CC-pVTZ) (Hartree): -266.71785884

E(RM062X/Aug-CC-pVTZ) (Hartree): -268.16905863

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.377359 | -0.713276 | -0.279257 |
| O | -1.560424 | -0.357330 | -0.022728 |
| O | -1.163063 | 1.063936  | 0.057104  |
| C | 0.835334  | -0.446536 | 0.525808  |
| H | -0.269645 | -1.402393 | -1.128042 |
| C | 1.860321  | 0.386700  | -0.249600 |
| H | 0.547319  | 0.046138  | 1.449107  |
| H | 1.265411  | -1.433753 | 0.735463  |
| H | 1.459518  | 1.383076  | -0.414798 |
| H | 2.089935  | -0.062738 | -1.216298 |
| H | 2.785583  | 0.455500  | 0.317858  |

Rotational constants (GHz): 10.6699200 3.6482100 3.0748900

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i738.5010 | 129.5666  | 224.6056  |
| 253.0654  | 417.3856  | 518.8957  |
| 793.3788  | 810.9441  | 903.8542  |
| 965.1401  | 1029.4709 | 1109.1428 |
| 1178.1046 | 1277.0484 | 1329.4942 |
| 1387.9042 | 1402.2484 | 1460.2594 |
| 1498.5962 | 1511.9251 | 1627.0168 |
| 3022.4868 | 3048.0177 | 3072.8142 |
| 3141.8649 | 3169.3493 | 3175.5707 |

Zero-point correction (Hartree): 0.087614

TS.C2H5CHO2s.ringclose.p

~~~~~

E(RM062X/Aug-CC-pVTZ) (Hartree): -268.16829041

Electronic state : 1-A

Cartesian coordinates (Angs):

C	0.238388	-0.499402	0.330512
O	1.321061	-0.694242	-0.287614
O	1.777742	0.675858	0.017419
C	-0.769221	0.557338	0.072032
H	-0.052407	-1.299151	1.026188
C	-2.140873	-0.089224	-0.143945
H	-0.800100	1.210260	0.947326
H	-0.433484	1.159935	-0.767083
H	-2.440386	-0.686297	0.717961
H	-2.141282	-0.733032	-1.022420
H	-2.892528	0.683081	-0.292005

Rotational constants (GHz): 14.4359900 3.0219500 2.6878400

Vibrational harmonic frequencies (cm-1):

i747.3359	116.7993	206.1050
273.6410	397.6511	488.1564
738.7993	815.2354	905.4423
966.1582	1025.6510	1109.3867
1168.5324	1262.3940	1314.6889
1390.5236	1411.9323	1455.4267
1502.4358	1508.0437	1627.5614
3042.3602	3068.2190	3074.9781
3133.7303	3153.3395	3165.5205

Zero-point correction (Hartree): 0.087306

Population analysis as 298K (%)

Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)

Compound	Qtot	Erel	Erel2	n*Q*MB	%
TS.C2H5CHO2s.14Hshift.t	2.945e+38	0.00	0.00	5.891e+38	99.8
TS.C2H5CHO2s.14Hshift.m	2.192e+38	3.53	3.53	1.139e+36	0.193
Total				5.902e+38	100

TS.C2H5CHO2s.14Hshift.m

~~~~~

E(RM062X/Aug-CC-pVTZ) (Hartree): -268.17670832

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.426836  | 0.988057  | -0.123553 |
| O | 1.374759  | 0.131836  | -0.282228 |
| O | 0.975095  | -1.099539 | 0.220349  |
| C | -0.768566 | 0.539390  | 0.459755  |
| H | 0.760560  | 2.009498  | -0.275872 |
| H | -0.004407 | -0.452906 | 0.926484  |
| C | -1.721385 | -0.402491 | -0.291654 |
| H | -1.290302 | 1.328699  | 0.989469  |
| H | -2.364501 | -0.918203 | 0.418454  |
| H | -1.169294 | -1.144405 | -0.859779 |
| H | -2.352194 | 0.169206  | -0.971017 |

Rotational constants (GHz): 9.2799700 4.4223300 3.3780800

Vibrational harmonic frequencies (cm-1):

|            |          |          |
|------------|----------|----------|
| i1627.8095 | 156.1936 | 245.0608 |
|------------|----------|----------|

```

281.0744      547.0428      657.8997
802.4903      876.7883      898.1621
963.8460     1008.4314     1076.2374
1101.4301     1183.5820     1314.4867
1349.7132     1396.0573     1421.4552
1506.0613     1507.3987     1587.4591
1862.3722     3076.6550     3141.2419
3161.5008     3181.4031     3191.3908
Zero-point correction (Hartree): 0.085421

TS.C2H5CHO2s.14Hshift.t
~~~~~
E (CCSD(T)/Aug-CC-pVTZ) (Hartree): -267.80308502
E (CCSD/Aug-CC-pVTZ) (Hartree): -267.75118803
T1 diagnostic: 0.025902
E (MP2/Aug-CC-pVTZ) (Hartree): -267.72982383
E (MP3/Aug-CC-pVTZ) (Hartree): -267.74150765
E (RHF/Aug-CC-pVTZ) (Hartree): -266.70457093
E (RM062X/Aug-CC-pVTZ) (Hartree): -268.18165092
Electronic state : 1-A
Cartesian coordinates (Angs):
C -0.160755 0.796944 0.107576
O -1.413817 0.559275 -0.044324
O -1.618378 -0.810900 -0.081040
C 0.704397 -0.302092 0.187505
H 0.100202 1.840748 -0.036798
H -0.258804 -0.977083 -0.409245
C 2.169673 -0.108940 -0.121010
H 0.480868 -0.964959 1.025489
H 2.735073 0.196244 0.759818
H 2.316235 0.641123 -0.897033
H 2.604099 -1.038543 -0.483745
Rotational constants (GHz): 14.4566400 3.1667100 2.7008900
Vibrational harmonic frequencies (cm-1):
i1612.2136 115.1344 258.7849
288.8298 507.8015 547.2847
731.7486 833.0714 921.4829
969.2671 990.4884 1076.8392
1148.0540 1198.9880 1302.5089
1358.7160 1419.4211 1425.9984
1498.6005 1508.0539 1613.7547
1858.6407 3067.6438 3095.7785
3130.9739 3144.5047 3186.8791
Zero-point correction (Hartree): 0.084746

Population analysis as 298K (%)
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)
Compound Qtot Erel Erel2 n*Q*MB %

TS.C2H5CHO2s.14Hshift.m 2.192e+38 0.00 0.00 4.384e+38 100
Total 4.384e+38 100

TS.C2H5CHO2s.14Hshift.m
~~~~~
E (RM062X/Aug-CC-pVTZ) (Hartree): -268.17670832
Electronic state : 1-A
Cartesian coordinates (Angs):
C       0.426836      0.988057     -0.123553
O       1.374759      0.131836     -0.282228
O       0.975095     -1.099539      0.220349
C      -0.768566      0.539390      0.459755
H       0.760560      2.009498     -0.275872
H      -0.004407     -0.452906      0.926484
C      -1.721385     -0.402491     -0.291654
H      -1.290302      1.328699      0.989469
H      -2.364501     -0.918203      0.418454
H      -1.169294     -1.144405     -0.859779
H      -2.352194      0.169206     -0.971017
Rotational constants (GHz): 9.2799700 4.4223300 3.3780800
Vibrational harmonic frequencies (cm-1):
i1627.8095      156.1936      245.0608
281.0744      547.0428      657.8997
802.4903      876.7883      898.1621
963.8460     1008.4314     1076.2374
1101.4301     1183.5820     1314.4867
1349.7132     1396.0573     1421.4552
1506.0613     1507.3987     1587.4591
1862.3722     3076.6550     3141.2419
3161.5008     3181.4031     3191.3908
Zero-point correction (Hartree): 0.085421

#####
Z- (nC3H7) CHOO
#####

Population analysis as 298K (%)
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)
Compound      Qtot      Erel      Erel2  n*Q*MB      %
-----
C3H7CHO2s.tt 5.470e+39 0.00 0.00 1.094e+40 46.5
C3H7CHO2s.tp 4.759e+39 0.11 0.11 7.862e+39 33.4
C3H7CHO2s.pt 4.465e+39 0.71 0.71 2.704e+39 11.5
C3H7CHO2s.pp 4.803e+39 1.07 1.07 1.588e+39 6.76
C3H7CHO2s.mp 3.131e+39 1.61 1.61 4.158e+38 1.77
Total 2.351e+40 100

C3H7CHO2s.mp
~~~~~
E (RM062X/Aug-CC-pVTZ) (Hartree): -307.51545190
Electronic state : 1-A

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```

Cartesian coordinates (Angs):
 C -0.752551 -0.896276 -0.413583
 O -1.598114 0.019611 -0.427369
 O -1.524053 0.997283 0.515710
 C 0.342626 -1.000004 0.567808
 H -0.896258 -1.610859 -1.218693
 C 1.640623 -0.381745 0.005940
 H 0.035287 -0.475865 1.471041
 H 0.506160 -2.057624 0.776919
 C 1.522383 1.113183 -0.257852
 H 2.430837 -0.578210 0.730745
 H 1.920519 -0.906747 -0.910049
 H 1.270854 1.648101 0.655967
 H 0.731576 1.329940 -0.976354
 H 2.459873 1.505168 -0.650180
Rotational constants (GHz): 5.5870400 2.7166100 2.1616600
Vibrational harmonic frequencies (cm-1):
 106.2476 122.8886 206.2518
 270.9319 312.1026 400.2984
 554.9757 647.5692 786.1926
 838.1904 902.3921 919.3761
 923.6792 982.7211 1069.0596
 1107.9991 1171.0214 1252.5588
 1277.2642 1346.9829 1370.3795
 1404.0852 1431.3077 1468.4708
 1486.7192 1501.1004 1504.4815
 1649.8053 3060.9349 3069.7539
 3080.4127 3104.2723 3138.2337
 3147.1250 3151.2330 3180.6346
Zero-point correction (Hartree): 0.118345

C3H7CHO2s.pp
~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -307.51621788
Electronic state : 1-A
Cartesian coordinates (Angs):
  C   -0.660642   0.951786   0.036628
  O   -1.613885   0.344252   -0.491285
  O   -1.810568   -0.956519   -0.147506
  C    0.251421   0.314203   1.001921
  H   -0.582951   1.981480   -0.296469
  C    1.225486   -0.656320   0.303054
  H    0.803690   1.089518   1.531953
  H   -0.373372   -0.251268   1.696761
  C    2.165110   0.050359   -0.665354
  H    1.798303   -1.158125   1.082428
  H    0.636512   -1.414379   -0.209226
  H    2.737160   0.832328   -0.163059
  H    1.615286   0.510990   -1.487748
  H    2.872752   -0.652572   -1.101796
Rotational constants (GHz):    6.6151900    2.2030800    2.1014600
Vibrational harmonic frequencies (cm-1):
  61.7662    139.2471    193.5023
  254.8351    346.1035    382.8695
  548.9583    678.1897    763.6282
  851.6034    898.3985    917.8537
  925.0406    994.6480    1069.7519
  1113.7011    1141.2709    1256.4963
  1281.1576    1352.5808    1362.9649
  1399.9378    1419.4976    1465.5062
  1498.7570    1507.4683    1508.6971
  1645.2234    3054.9527    3066.5386
  3088.6757    3111.5395    3128.2570
  3137.8520    3148.8891    3189.4125
Zero-point correction (Hartree): 0.118250

C3H7CHO2s.pt
~~~~~
E(CCSd(T)/Aug-CC-pVTZ) (Hartree): -307.07554699
E(CCSd/Aug-CC-pVTZ) (Hartree): -307.01815591
T1 diagnostic: 0.029332
E(MP2/Aug-CC-pVTZ) (Hartree): -306.97733459
E(MP3/Aug-CC-pVTZ) (Hartree): -307.00507890
E(RHF/Aug-CC-pVTZ) (Hartree): -305.79846173
E(RM062X/Aug-CC-pVTZ) (Hartree): -307.51682196
Electronic state : 1-A
Cartesian coordinates (Angs):
 C 1.064863 0.934673 0.058236
 O 1.901238 0.020809 0.206176
 O 1.549039 -1.234299 -0.183876
 C -0.275229 0.698149 -0.499596
 H 1.427922 1.898486 0.400110
 C -1.187830 0.009379 0.536419
 H -0.709535 1.643770 -0.821192
 H -0.153684 0.026726 -1.352791
 C -2.526672 -0.358343 -0.086334
 H -0.676862 -0.881360 0.897749
 H -1.338479 0.679314 1.384191
 H -2.386220 -1.060742 -0.907790
 H -3.034689 0.523641 -0.478833
 H -3.181462 -0.825064 0.647808
Rotational constants (GHz): 7.5993500 2.0376200 1.7725700
Vibrational harmonic frequencies (cm-1):
 74.1986 141.0959 191.0799
 255.2482 326.5885 379.0637
 541.0671 670.6475 762.2992
 850.8936 899.9266 915.8930
 936.0059 1022.7699 1057.3238
 1113.7647 1158.9546 1265.2047
 1299.4935 1334.7825 1371.4472
 1395.5102 1413.8965 1465.4103
 1497.7732 1504.3149 1507.6873

```

1645.1079                    3060.9441                    3063.1500  
 3076.1986                    3116.7828                    3130.1340  
 3141.9296                    3145.3634                    3188.2095  
 Zero-point correction (Hartree): 0.118283

C3H7CHO2s.tp

~~~~~  
 E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -307.07526782  
 E(CCSD/Aug-CC-pVTZ) (Hartree): -307.01809053  
 T1 diagnostic: 0.029218  
 E(MP2/Aug-CC-pVTZ) (Hartree): -306.97707548  
 E(MP3/Aug-CC-pVTZ) (Hartree): -307.00501073  
 E(RHF/Aug-CC-pVTZ) (Hartree): -305.79846069  
 E(RM062X/Aug-CC-pVTZ) (Hartree): -307.51708906  
 Electronic state : 1-A  
 Cartesian coordinates (Angs):  
 C    0.576944    -0.546664    -0.386847  
 O    1.796689    -0.630733    -0.143787  
 O    2.383073    0.447770    0.440529  
 C    -0.201667    0.658963    -0.073715  
 H    0.166460    -1.434501    -0.859104  
 C    -1.680498    0.525735    -0.412908  
 H    -0.026972    0.881238    0.985838  
 H    0.296003    1.486517    -0.592866  
 C    -2.395250    -0.473680    0.489318  
 H    -2.148355    1.504977    -0.318273  
 H    -1.791035    0.233303    -1.459696  
 H    -2.326200    -0.166022    1.533065  
 H    -1.955994    -1.469875    0.411607  
 H    -3.449182    -0.558061    0.230398  
 Rotational constants (GHz):    9.8285700    1.7148500    1.6201400  
 Vibrational harmonic frequencies (cm-1):  
 77.0275                    124.6840                    190.5135  
 261.0244                    307.9537                    442.7125  
 472.9629                    695.0244                    738.5580  
 790.8282                    901.5050                    913.3632  
 932.1647                    1011.2572                    1089.3374  
 1106.2829                    1150.3180                    1225.5957  
 1283.7600                    1339.9191                    1376.8731  
 1406.0100                    1419.1625                    1428.3337  
 1496.0148                    1505.8155                    1510.4913  
 1648.9329                    3037.5207                    3052.4661  
 3059.6720                    3067.9887                    3107.3192  
 3129.2963                    3142.9854                    3177.9593  
 Zero-point correction (Hartree): 0.117603

C3H7CHO2s.tt

~~~~~  
 E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -307.07552943  
 E(CCSD/Aug-CC-pVTZ) (Hartree): -307.01844358  
 T1 diagnostic: 0.029230  
 E(MP2/Aug-CC-pVTZ) (Hartree): -306.97720991  
 E(MP3/Aug-CC-pVTZ) (Hartree): -307.00538485  
 E(RHF/Aug-CC-pVTZ) (Hartree): -305.79946220  
 E(RM062X/Aug-CC-pVTZ) (Hartree): -307.51721940  
 Electronic state : 1-A  
 Cartesian coordinates (Angs):  
 C    -0.872604    0.783084    -0.000025  
 O    -2.056598    0.393134    0.000007  
 O    -2.261699    -0.950195    0.000111  
 C    0.258818    -0.152393    0.000032  
 H    -0.770357    1.864401    -0.000096  
 C    1.618141    0.532394    -0.000102  
 H    0.117353    -0.818762    0.859964  
 H    0.117270    -0.818963    -0.859728  
 C    2.754724    -0.479995    -0.000023  
 H    1.699839    1.179628    -0.876069  
 H    1.699906    1.179840    0.875702  
 H    2.701514    -1.121065    -0.880389  
 H    2.701577    -1.120854    0.880501  
 H    3.724798    0.013727    -0.000117  
 Rotational constants (GHz):    11.1165400    1.5789100    1.4182300  
 Vibrational harmonic frequencies (cm-1):  
 96.5582                    104.5550                    154.1549  
 256.1872                    334.8551                    400.5113  
 476.2550                    697.5631                    703.2927  
 795.0491                    902.7992                    919.0136  
 938.4752                    1059.0003                    1081.8028  
 1126.7734                    1158.6194                    1239.8959  
 1277.6164                    1322.0641                    1380.1140  
 1413.1403                    1419.9604                    1428.8101  
 1496.7501                    1505.2877                    1512.4844  
 1649.5720                    3031.6081                    3047.1044  
 3056.0089                    3064.7645                    3091.6839  
 3131.9689                    3144.8168                    3180.5292  
 Zero-point correction (Hartree): 0.117553

Population analysis as 298K (%)

Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)

| Compound                  | Qtot      | Erel | Erel2 | n*Q*MB    | %    |
|---------------------------|-----------|------|-------|-----------|------|
| TS.C3H7CHO2s.ringclose.mt | 3.793e+39 | 0.00 | 0.00  | 7.585e+39 | 22.7 |
| TS.C3H7CHO2s.ringclose.pt | 4.703e+39 | 0.33 | 0.33  | 5.400e+39 | 16.2 |
| TS.C3H7CHO2s.ringclose.pm | 4.018e+39 | 0.24 | 0.24  | 5.362e+39 | 16.1 |
| TS.C3H7CHO2s.ringclose.ct | 4.150e+39 | 0.38 | 0.38  | 4.349e+39 | 13   |
| TS.C3H7CHO2s.ringclose.mm | 3.452e+39 | 0.46 | 0.46  | 3.153e+39 | 9.45 |
| TS.C3H7CHO2s.ringclose.mp | 3.375e+39 | 0.48 | 0.48  | 2.980e+39 | 8.92 |
| TS.C3H7CHO2s.ringclose.cp | 2.164e+39 | 0.25 | 0.25  | 2.852e+39 | 8.54 |
| TS.C3H7CHO2s.ringclose.pp | 4.339e+39 | 1.22 | 1.22  | 1.110e+39 | 3.33 |
| TS.C3H7CHO2s.ringclose.cm | 2.483e+39 | 1.26 | 1.26  | 5.930e+38 | 1.78 |
| Total                     |           |      |       | 3.338e+40 | 100  |

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TS.C3H7CHO2s.ringclose.cm
~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -307.47451174
Electronic state : 1-A
Cartesian coordinates (Angs):
  C    1.254717    0.662470   -0.208845
  O    1.745165   -0.308474    0.430005
  O    0.871901   -1.281262   -0.259058
  C   -0.154925    1.105714   -0.275736
  H    1.992728    1.342780   -0.653203
  C   -1.183355    0.377764    0.591087
  H   -0.094349    2.175189   -0.030698
  H   -0.438151    1.091963   -1.335515
  C   -2.083760   -0.557274   -0.205228
  H   -0.663719   -0.181384    1.366911
  H   -1.794157    1.133163    1.087729
  H   -1.486324   -1.313803   -0.708524
  H   -2.654638   -0.003080   -0.952326
  H   -2.793983   -1.058989    0.450384
Rotational constants (GHz):    6.1702700    2.6513100    2.1198100
Vibrational harmonic frequencies (cm-1):
  i724.6333    111.5058    138.1274
  209.4140    284.7943    329.6392
  370.4487    635.2810    731.1725
  781.4086    807.7364    870.0756
  982.1489    1011.7667    1085.5979
  1114.7717    1149.0967    1242.1960
  1307.4010    1367.5111    1387.2278
  1405.3700    1409.4717    1436.5434
  1486.3510    1501.2961    1512.7884
  1625.1070    3010.2951    3041.8818
  3059.3078    3061.7281    3074.9653
  3121.7016    3137.3024    3160.3317
Zero-point correction (Hartree): 0.116099

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TS.C3H7CHO2s.ringclose.cp
~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -307.47621141
Electronic state : 1-A
Cartesian coordinates (Angs):
 C -1.029652 0.671714 -0.427307
 O -1.409325 -0.527108 -0.548878
 O -1.216088 -0.784147 0.889401
 C 0.251948 1.209045 0.084254
 H -1.689161 1.410793 -0.901163
 C 1.351607 0.258177 0.528977
 H 0.600271 1.851466 -0.739588
 H -0.012430 1.913804 0.880744
 C 1.678300 -0.817683 -0.499042
 H 2.236656 0.868535 0.719413
 H 1.057625 -0.205200 1.466699
 H 1.874968 -0.381347 -1.480809
 H 0.855677 -1.523744 -0.590903
 H 2.566479 -1.371793 -0.199866
Rotational constants (GHz): 5.4009800 2.8376400 2.4689000
Vibrational harmonic frequencies (cm-1):
 i725.2284 101.8026 149.3402
 246.7499 297.1993 328.1502
 369.5226 621.0629 750.1519
 797.7492 834.7190 850.6680
 958.6066 994.9147 1074.6050
 1116.8604 1141.9641 1255.3830
 1303.6257 1376.3239 1386.9592
 1409.6864 1417.7622 1433.7143
 1478.2684 1500.0386 1516.9897
 1621.6905 2992.1392 3050.6802
 3056.3297 3059.0623 3071.8702
 3125.7604 3149.5559 3160.3703
Zero-point correction (Hartree): 0.116187

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TS.C3H7CHO2s.ringclose.ct
~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -307.47561224
Electronic state : 1-A
Cartesian coordinates (Angs):
  C   -1.135718    0.843382    0.001242
  O   -1.846427   -0.021937   -0.580415
  O   -1.554228   -1.043080    0.443772
  C    0.303086    0.774956    0.337956
  H   -1.615395    1.821458    0.134752
  C    1.097398   -0.431303   -0.137479
  H    0.712551    1.704978   -0.085109
  H    0.391381    0.910753    1.422005
  C    2.593410   -0.142172   -0.106505
  H    0.850951   -1.284002    0.487493
  H    0.778533   -0.693729   -1.147268
  H    2.918881    0.128855    0.899126
  H    2.856051    0.679632   -0.774270
  H    3.163235   -1.016996   -0.414873
Rotational constants (GHz):    8.1817900    2.0151500    1.7937100
Vibrational harmonic frequencies (cm-1):
  i723.8371    75.8284    133.6567
  202.9863    250.2159    321.0346
  361.2619    666.6134    694.8228
  778.1606    829.7779    871.5169
  968.4339    1001.2385    1066.6929
  1127.5882    1150.6679    1248.3226
  1310.5722    1323.1634    1385.3369
  1413.3383    1415.3978    1437.2513
  1492.5355    1504.8968    1510.7548
  1622.0214    2995.9738    3050.7850

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3057.2646                    3059.7609                    3087.1252  
 3116.2479                    3140.0334                    3160.7168  
 Zero-point correction (Hartree): 0.115804

TS.C3H7CHO2s.ringclose.mm

~~~~~  
 E(RM062X/Aug-CC-pVTZ) (Hartree): -307.47614260
 Electronic state : 1-A
 Cartesian coordinates (Angs):
 C -0.728790 -0.751236 -0.070713
 O -1.929883 -0.388269 -0.221880
 O -1.530976 1.028415 -0.321666
 C 0.212057 -0.291259 0.976993
 H -0.417507 -1.594733 -0.699390
 C 1.388907 0.532017 0.432124
 H -0.346052 0.284224 1.710691
 H 0.609251 -1.209143 1.429291
 C 2.107902 -0.136723 -0.732747
 H 0.990963 1.496870 0.124225
 H 2.084250 0.700607 1.254278
 H 1.465847 -0.191634 -1.613209
 H 2.423544 -1.150584 -0.478250
 H 2.996114 0.426430 -1.013210
 Rotational constants (GHz): 6.9506700 2.1426000 2.0879200
 Vibrational harmonic frequencies (cm-1):
 i740.5223 65.6988 146.6776
 227.0601 278.2239 377.1914
 427.0707 521.9544 753.7786
 811.1290 855.0452 905.2267
 977.7804 1006.2786 1077.1032
 1128.0636 1152.6969 1258.1598
 1285.8698 1329.1962 1370.2051
 1392.0306 1417.6231 1459.0977
 1493.8015 1502.6745 1511.6866
 1620.4211 3016.3054 3052.9231
 3061.6733 3085.8501 3111.5838
 3140.7212 3143.9392 3156.8468
 Zero-point correction (Hartree): 0.116464

TS.C3H7CHO2s.ringclose.mp

~~~~~  
 E(RM062X/Aug-CC-pVTZ) (Hartree): -307.47590729  
 Electronic state : 1-A  
 Cartesian coordinates (Angs):  
 C    -0.900918    -0.663503    -0.397056  
 O    -1.965248    -0.035933    -0.138216  
 O    -1.216863    1.174398    0.259753  
 C    0.226767    -0.944754    0.516244  
 H    -0.888025    -1.183106    -1.365668  
 C    1.594071    -0.560861    -0.071724  
 H    0.051750    -0.466751    1.474893  
 H    0.208529    -2.038284    0.628376  
 C    1.816149    0.942695    -0.161050  
 H    2.356387    -1.015734    0.560677  
 H    1.702332    -1.019713    -1.058133  
 H    1.655429    1.412232    0.809131  
 H    1.119600    1.407625    -0.855341  
 H    2.834466    1.154549    -0.484717  
 Rotational constants (GHz):    6.3146800    2.5149400    2.0038900  
 Vibrational harmonic frequencies (cm-1):  
 i736.1134                    81.6720                    124.8974  
   218.5734                    287.9829                    315.5263  
   455.8970                    526.9459                    772.8022  
   802.7518                    819.3317                    909.1487  
   974.4435                    1007.4611                    1077.5235  
 1114.8545                    1178.3201                    1238.8300  
 1279.2731                    1352.4558                    1374.6956  
 1388.2583                    1426.3034                    1450.8534  
 1490.7525                    1496.3936                    1504.3726  
 1621.7216                    3002.9497                    3042.7675  
 3055.3482                    3071.3884                    3103.2003  
 3140.3359                    3153.9357                    3170.7540  
 Zero-point correction (Hartree): 0.116261

TS.C3H7CHO2s.ringclose.mt

~~~~~  
 E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -307.03860433
 E(CCSD/Aug-CC-pVTZ) (Hartree): -306.98071879
 T1 diagnostic: 0.032992
 E(MP2/Aug-CC-pVTZ) (Hartree): -306.93535007
 E(MP3/Aug-CC-pVTZ) (Hartree): -306.96541714
 E(RHF/Aug-CC-pVTZ) (Hartree): -305.76593199
 E(RM062X/Aug-CC-pVTZ) (Hartree): -307.47671114
 Electronic state : 1-A
 Cartesian coordinates (Angs):
 C 1.040528 -0.727704 0.235513
 O 2.152714 -0.235977 -0.104471
 O 1.616462 1.138837 -0.033324
 C -0.266825 -0.532447 -0.426250
 H 1.087452 -1.479582 1.034848
 C -1.293138 0.145180 0.491615
 H -0.126697 0.044008 -1.336552
 H -0.629584 -1.541570 -0.663394
 C -2.670900 0.182901 -0.153819
 H -1.342523 -0.385833 1.445444
 H -0.930968 1.150110 0.700581
 H -3.041507 -0.823330 -0.352740
 H -2.638093 0.721811 -1.100869
 H -3.389474 0.683926 0.492688
 Rotational constants (GHz): 9.4498400 1.8045600 1.6510400
 Vibrational harmonic frequencies (cm-1):
 i737.5831 90.4922 120.7117

195.6683	255.5398	335.9875
437.3136	513.7346	759.7168
801.3776	854.1528	913.1476
983.5206	1027.7283	1066.0209
1125.8711	1178.1259	1259.2392
1289.9114	1319.0179	1371.8512
1390.2424	1415.9198	1456.8384
1498.7557	1504.4585	1510.5759
1623.7634	3011.0126	3050.8491
3060.1280	3063.3818	3119.5615
3139.0953	3142.2050	3160.7553

Zero-point correction (Hartree): 0.116293

TS.C3H7CHO2s.ringclose.pm

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E(RM062X/Aug-CC-pVTZ) (Hartree): -307.47602233

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.657272  | -0.096169 | 0.612958  |
| O | 1.535740  | -0.861269 | 0.127267  |
| O | 2.259728  | 0.287901  | -0.451122 |
| C | -0.201117 | 0.873262  | -0.109517 |
| H | 0.400059  | -0.290023 | 1.664463  |
| C | -1.674548 | 0.582901  | 0.203256  |
| H | 0.066491  | 1.875065  | 0.234984  |
| H | 0.029823  | 0.821044  | -1.171106 |
| C | -2.122486 | -0.771205 | -0.333650 |
| H | -1.836651 | 0.633208  | 1.283063  |
| H | -2.276367 | 1.378586  | -0.234932 |
| H | -1.553802 | -1.587381 | 0.116423  |
| H | -1.971588 | -0.826236 | -1.412011 |
| H | -3.176436 | -0.950047 | -0.128325 |

Rotational constants (GHz): 8.1057800 1.9826100 1.7962800

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i745.1769 | 82.3521   | 110.1734  |
| 207.2303  | 297.1400  | 322.9772  |
| 446.0966  | 484.0380  | 754.4387  |
| 771.7391  | 849.6313  | 905.0589  |
| 968.1619  | 1003.6129 | 1071.1460 |
| 1113.9224 | 1167.1319 | 1230.2385 |
| 1271.5696 | 1340.6780 | 1369.4336 |
| 1389.7445 | 1422.3784 | 1451.0172 |
| 1491.8295 | 1503.0539 | 1506.0610 |
| 1625.1445 | 3037.4518 | 3057.4041 |
| 3060.0653 | 3072.8580 | 3105.2113 |
| 3126.9821 | 3143.7817 | 3152.3557 |

Zero-point correction (Hartree): 0.115986

TS.C3H7CHO2s.ringclose.pp

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E(RM062X/Aug-CC-pVTZ) (Hartree): -307.47454973

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-0.653258	-0.520139	-0.038612
O	-1.820002	-0.637214	0.430778
O	-2.308834	0.448812	-0.440551
C	0.192335	0.697526	-0.026622
H	-0.174016	-1.465539	-0.324730
C	1.574514	0.372836	0.563294
H	0.309431	1.051433	-1.054131
H	-0.345901	1.469676	0.517547
C	2.483187	-0.378065	-0.403012
H	2.041297	1.317702	0.841367
H	1.458100	-0.190782	1.491873
H	2.647422	0.208323	-1.307419
H	2.060487	-1.336992	-0.705011
H	3.453205	-0.579554	0.048405

Rotational constants (GHz): 10.0830300 1.7166600 1.6416400

Vibrational harmonic frequencies (cm-1):

i758.4241	78.6423	115.2995
197.5576	277.9196	316.4151
451.8207	483.3761	738.8848
781.8337	867.2679	890.4434
983.5784	1001.5686	1073.6810
1123.5521	1147.7704	1242.8831
1276.8312	1341.8278	1364.7007
1393.3384	1424.3422	1452.1595
1495.2872	1507.5614	1509.2899
1624.0811	3056.1213	3062.7829
3066.0768	3071.3119	3105.4283
3131.6653	3141.7404	3152.5414

Zero-point correction (Hartree): 0.116072

TS.C3H7CHO2s.ringclose.pt

~~~~~

E(RM062X/Aug-CC-pVTZ) (Hartree): -307.47588748

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.921993 | 0.573371  | 0.296329  |
| O | -1.983170 | 0.520463  | -0.385090 |
| O | -2.223873 | -0.872787 | 0.038793  |
| C | 0.261295  | -0.311015 | 0.188035  |
| H | -0.812409 | 1.472273  | 0.918991  |
| C | 1.522858  | 0.529874  | -0.043299 |
| H | 0.361242  | -0.862871 | 1.127116  |
| H | 0.084184  | -1.042030 | -0.597286 |
| C | 2.761849  | -0.352761 | -0.118425 |
| H | 1.417447  | 1.100108  | -0.968148 |
| H | 1.633864  | 1.256819  | 0.764884  |
| H | 2.675125  | -1.072788 | -0.932013 |
| H | 2.894737  | -0.911285 | 0.808502  |
| H | 3.658095  | 0.241552  | -0.287506 |

Rotational constants (GHz): 11.2184900 1.6035900 1.4824200  
 Vibrational harmonic frequencies (cm-1):  
 i749.4375 90.9734 103.7938  
 183.1133 248.6139 366.7648  
 380.0151 506.1816 733.7650  
 778.6666 864.1867 911.0542  
 979.3439 1035.4660 1063.3961  
 1122.7452 1173.6720 1247.7514  
 1276.5743 1322.4520 1378.9896  
 1391.8674 1416.5550 1452.2013  
 1496.3357 1503.1847 1510.9896  
 1625.6108 3043.2301 3055.3598  
 3062.7378 3065.4459 3092.7812  
 3134.1705 3144.3033 3152.8717  
 Zero-point correction (Hartree): 0.115993

Population analysis as 298K (%)  
 Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)  
 Compound Qtot Erel Erel2 n\*Q\*MB %  
 -----  
 TS.C3H7CHO2s.14Hshift.tt 2.920e+39 0.00 0.00 5.840e+39 38.4  
 TS.C3H7CHO2s.14Hshift.tm 3.574e+39 0.16 0.16 5.487e+39 36.1  
 TS.C3H7CHO2s.14Hshift.tp 3.991e+39 0.44 0.44 3.793e+39 25  
 TS.C3H7CHO2s.14Hshift.mp 2.409e+39 2.78 2.78 4.379e+37 0.288  
 TS.C3H7CHO2s.14Hshift.mt 2.760e+39 3.21 3.21 2.463e+37 0.162  
 TS.C3H7CHO2s.14Hshift.mm 1.384e+39 4.32 4.32 1.882e+36 0.0124  
 Total 1.519e+40 100

TS.C3H7CHO2s.14Hshift.mm  
 ~~~~~  
 E(RM062X/Aug-CC-pVTZ) (Hartree): -307.48325362
 Electronic state : 1-A
 Cartesian coordinates (Angs):
 C -0.858141 0.767537 0.592789
 O -1.516056 -0.329763 0.453979
 O -1.126355 -0.945755 -0.729151
 C 0.096670 1.077201 -0.387311
 H -1.270761 1.411272 1.362399
 H -0.628240 0.276776 -1.147823
 C 1.380936 0.220200 -0.557933
 H 0.271524 2.142293 -0.473253
 C 1.700623 -0.650651 0.649512
 H 1.302441 -0.411821 -1.441014
 H 2.195017 0.921698 -0.735381
 H 0.894771 -1.361876 0.828980
 H 1.838078 -0.042955 1.544829
 H 2.615923 -1.216973 0.480300

Rotational constants (GHz): 5.6418400 2.8249300 2.5699800
 Vibrational harmonic frequencies (cm-1):
 i1614.6150 103.1012 198.5989
 238.8911 307.8416 397.6556
 563.7363 672.1470 776.8856
 826.0802 839.6231 923.8524
 964.9587 981.0291 1042.4272
 1108.8964 1122.6831 1182.8279
 1295.9286 1307.5584 1351.8865
 1360.3284 1406.1760 1421.0427
 1494.3530 1500.5947 1514.9896
 1586.4834 1870.6600 3061.3951
 3084.5491 3116.7575 3134.5666
 3144.7658 3181.2279 3197.9000
 Zero-point correction (Hartree): 0.114552

TS.C3H7CHO2s.14Hshift.mp
 ~~~~~  
 E(RM062X/Aug-CC-pVTZ) (Hartree): -307.48532924  
 Electronic state : 1-A  
 Cartesian coordinates (Angs):  
 C 1.238857 -0.884845 -0.007936  
 O 1.851958 0.232256 0.181419  
 O 0.995760 1.287214 -0.111341  
 C -0.104748 -0.825821 -0.403417  
 H 1.915809 -1.732848 -0.025142  
 H 0.208654 0.406508 -0.805809  
 C -1.194959 -0.326299 0.566261  
 H -0.419881 -1.687031 -0.982497  
 C -2.326401 0.375981 -0.168313  
 H -1.577464 -1.192096 1.108800  
 H -0.748450 0.346044 1.294421  
 H -2.756823 -0.270854 -0.933699  
 H -1.959280 1.279205 -0.656446  
 H -3.120798 0.661216 0.520189

Rotational constants (GHz): 7.1679300 2.3835000 1.9700400  
 Vibrational harmonic frequencies (cm-1):  
 i1618.6182 63.8351 196.9505  
 227.8440 295.0925 394.2256  
 548.7157 650.4447 784.3402  
 826.8793 845.6504 919.7482  
 961.7230 988.7479 1052.7777  
 1094.8639 1111.2306 1182.0940  
 1293.6881 1318.0613 1336.6442  
 1351.5786 1414.9705 1425.5232  
 1487.9464 1501.2357 1503.6798  
 1581.0842 1862.0805 3060.2077  
 3073.5087 3121.9926 3137.9756  
 3145.8931 3166.7207 3191.7313  
 Zero-point correction (Hartree): 0.114181

TS.C3H7CHO2s.14Hshift.mt  
 ~~~~~  
 E(RM062X/Aug-CC-pVTZ) (Hartree): -307.48452767

Electronic state : 1-A
 Cartesian coordinates (Angs):

C	0.787938	0.999557	0.002149
O	1.754506	0.291193	-0.468862
O	1.620164	-1.022852	-0.038834
C	-0.175890	0.347165	0.787098
H	0.965537	2.064938	-0.103711
H	0.771828	-0.578896	0.942019
C	-1.192884	-0.626674	0.164003
H	-0.638199	1.011554	1.510640
C	-2.385321	0.112062	-0.433079
H	-0.697726	-1.228600	-0.593226
H	-1.532445	-1.308261	0.944088
H	-2.068502	0.768488	-1.243986
H	-2.886479	0.723988	0.317639
H	-3.114435	-0.592603	-0.832927

 Rotational constants (GHz): 7.5353300 2.1866200 1.9622000
 Vibrational harmonic frequencies (cm-1):

i1623.0841	64.3957	186.6563
209.3178	273.6697	379.8179
565.3554	668.2216	757.6435
826.7878	851.8781	926.3301
965.7741	992.7661	1037.3782
1085.4787	1120.8718	1184.2785
1291.1375	1309.5231	1333.0376
1362.7185	1410.1737	1424.5293
1496.2893	1499.0495	1506.7556
1579.9407	1863.0978	3057.5566
3084.1593	3120.9846	3132.0250
3146.1412	3159.1604	3189.8795

 Zero-point correction (Hartree): 0.114051

TS.C3H7CHO2s.14Hshift.tm
 ~~~~~  
 E(RM062X/Aug-CC-pVTZ) (Hartree): -307.48893281  
 Electronic state : 1-A  
 Cartesian coordinates (Angs):  

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.909332 | 0.877408  | 0.012869  |
| O | -2.040628 | 0.295645  | -0.165677 |
| O | -1.884223 | -1.071169 | 0.000561  |
| C | 0.196913  | 0.070851  | 0.308087  |
| H | -0.912960 | 1.923103  | -0.278467 |
| H | -0.503762 | -0.914241 | -0.225673 |
| C | 1.593636  | 0.586159  | 0.045946  |
| H | 0.080311  | -0.509402 | 1.226694  |
| C | 2.576365  | -0.560828 | -0.166042 |
| H | 1.589506  | 1.228431  | -0.836214 |
| H | 1.931995  | 1.201605  | 0.882679  |
| H | 2.280931  | -1.166927 | -1.022048 |
| H | 2.602488  | -1.211408 | 0.708597  |
| H | 3.584797  | -0.188510 | -0.339800 |

 Rotational constants (GHz): 9.3019000 1.7929600 1.5659800  
 Vibrational harmonic frequencies (cm-1):  

|            |           |           |
|------------|-----------|-----------|
| i1601.7497 | 57.5076   | 169.9207  |
| 206.7796   | 304.1680  | 417.1105  |
| 514.6237   | 532.0691  | 727.9454  |
| 793.0545   | 837.2200  | 943.1132  |
| 961.0475   | 977.4691  | 1061.1332 |
| 1110.0092  | 1171.2750 | 1196.8026 |
| 1273.6414  | 1312.8312 | 1337.4072 |
| 1378.6434  | 1414.7288 | 1431.8311 |
| 1495.2558  | 1502.7604 | 1511.1883 |
| 1610.7286  | 1851.0016 | 3054.2679 |
| 3064.1627  | 3082.8993 | 3096.0040 |
| 3133.9900  | 3142.5451 | 3188.4785 |

 Zero-point correction (Hartree): 0.113598

TS.C3H7CHO2s.14Hshift.tp  
 ~~~~~  
 E(RM062X/Aug-CC-pVTZ) (Hartree): -307.48839514
 Electronic state : 1-A
 Cartesian coordinates (Angs):

C	0.588235	0.575963	-0.560406
O	1.782575	0.642913	-0.091755
O	2.076034	-0.530109	0.586528
C	-0.144880	-0.590577	-0.304308
H	0.228983	1.522506	-0.952381
H	0.707027	-0.787349	0.692732
C	-1.656520	-0.546044	-0.373222
H	0.326389	-1.484674	-0.717439
C	-2.263437	0.477425	0.581520
H	-1.984553	-0.338449	-1.395322
H	-2.037665	-1.537132	-0.129732
H	-1.928501	1.488967	0.347442
H	-1.969955	0.262906	1.608948
H	-3.350980	0.470193	0.526064

 Rotational constants (GHz): 8.5805800 1.8833000 1.7976200
 Vibrational harmonic frequencies (cm-1):

i1622.4340	49.4173	155.7722
211.3967	307.4824	413.9069
508.0845	583.9748	729.1029
777.9191	834.6953	936.7143
959.6160	977.8385	1045.2923
1101.4282	1134.1922	1199.8561
1289.2648	1306.3823	1363.3609
1370.0417	1410.0459	1423.5596
1493.8923	1503.4016	1507.7585
1607.5012	1854.0939	3051.6242
3062.2112	3093.6602	3105.1224
3130.6255	3141.9748	3185.4253

 Zero-point correction (Hartree): 0.113513

```

TS.C3H7CHO2s.14Hshift.tt
~~~~~
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -307.04605344
E(CCSD/Aug-CC-pVTZ) (Hartree): -306.98622582
T1 diagnostic: 0.023911
E(MP2/Aug-CC-pVTZ) (Hartree): -306.95530493
E(MP3/Aug-CC-pVTZ) (Hartree): -306.97628852
E(RHF/Aug-CC-pVTZ) (Hartree): -305.75254931
E(RM062X/Aug-CC-pVTZ) (Hartree): -307.48920132
Electronic state : 1-A
Cartesian coordinates (Angs):
  C    0.628691    0.760632    0.094435
  O    1.901726    0.621103   -0.000042
  O    2.201358   -0.718222   -0.194589
  C   -0.161183   -0.393863    0.009017
  H    0.326735    1.749087    0.427760
  H    0.937355   -1.049522    0.328815
  C   -1.563626   -0.353812    0.570614
  H   -0.058896   -0.919513   -0.943772
  C   -2.584438    0.179671   -0.430806
  H   -1.844706   -1.360987    0.879442
  H   -1.577736    0.252922    1.477941
  H   -2.598015   -0.435565   -1.330895
  H   -2.337074    1.198648   -0.732020
  H   -3.589002    0.186113   -0.009786
Rotational constants (GHz):  10.7305800    1.7178800    1.6063200
Vibrational harmonic frequencies (cm-1):
  i1602.7807    67.1652    160.4612
  218.3742    316.9195    391.7803
  524.3518    558.2030    746.3899
  778.8602    834.6487    942.6232
  964.3144    980.5468    1036.7953
  1094.8160    1168.2301    1192.1706
  1268.5820    1314.5943    1351.5669
  1376.7692    1414.0924    1428.7024
  1494.7494    1503.6465    1510.1134
  1609.3341    1858.2358    3058.3866
  3069.1560    3083.7143    3102.4563
  3129.5823    3137.4398    3184.5417
Zero-point correction (Hartree): 0.113617

Population analysis as 298K (%)
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)
Compound      Qtot      Erel      Erel2  n*Q*MB      %
-----
TS.C3H7CHO2s.14Hshift.mp 2.409e+39 0.00    0.00  4.817e+39 62.3
TS.C3H7CHO2s.14Hshift.mt 2.760e+39 0.42    0.42  2.709e+39 35
TS.C3H7CHO2s.14Hshift.mm 1.384e+39 1.54    1.54  2.071e+38 2.68
Total                                7.734e+39 100

TS.C3H7CHO2s.14Hshift.mm
~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -307.48325362
Electronic state : 1-A
Cartesian coordinates (Angs):
  C   -0.858141    0.767537    0.592789
  O   -1.516056   -0.329763    0.453979
  O   -1.126355   -0.945755   -0.729151
  C    0.096670    1.077201   -0.387311
  H   -1.270761    1.411272    1.362399
  H   -0.628240    0.276776   -1.147823
  C    1.380936    0.220200   -0.557933
  H    0.271524    2.142293   -0.473253
  C    1.700623   -0.650651    0.649512
  H    1.302441   -0.411821   -1.441014
  H    2.195017    0.921698   -0.735381
  H    0.894771   -1.361876    0.828980
  H    1.838078   -0.042955    1.544829
  H    2.615923   -1.216973    0.480300
Rotational constants (GHz):  5.6418400    2.8249300    2.5699800
Vibrational harmonic frequencies (cm-1):
  i1614.6150    103.1012    198.5989
  238.8911    307.8416    397.6556
  563.7363    672.1470    776.8856
  826.0802    839.6231    923.8524
  964.9587    981.0291    1042.4272
  1108.8964    1122.6831    1182.8279
  1295.9286    1307.5584    1351.8865
  1360.3284    1406.1760    1421.0427
  1494.3530    1500.5947    1514.9896
  1586.4834    1870.6600    3061.3951
  3084.5491    3116.7575    3134.5666
  3144.7658    3181.2279    3197.9000
Zero-point correction (Hartree): 0.114552

TS.C3H7CHO2s.14Hshift.mp
~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -307.48532924
Electronic state : 1-A
Cartesian coordinates (Angs):
  C    1.238857   -0.884845   -0.007936
  O    1.851958    0.232256    0.181419
  O    0.995760    1.287214   -0.111341
  C   -0.104748   -0.825821   -0.403417
  H    1.915809   -1.732848   -0.025142
  H    0.208654    0.406508   -0.805809
  C   -1.194959   -0.326299    0.566261
  H   -0.419881   -1.687031   -0.982497
  C   -2.326401    0.375981   -0.168313
  H   -1.577464   -1.192096    1.108800
  H   -0.748450    0.346044    1.294421

```

```

      H      -2.756823      -0.270854      -0.933699
      H      -1.959280      1.279205      -0.656446
      H      -3.120798      0.661216      0.520189
Rotational constants (GHz):      7.1679300      2.3835000      1.9700400
Vibrational harmonic frequencies (cm-1):
  i1618.6182      63.8351      196.9505
    227.8440      295.0925      394.2256
    548.7157      650.4447      784.3402
    826.8793      845.6504      919.7482
    961.7230      988.7479      1052.7777
   1094.8639      1111.2306      1182.0940
   1293.6881      1318.0613      1336.6442
   1351.5786      1414.9705      1425.5232
   1487.9464      1501.2357      1503.6798
   1581.0842      1862.0805      3060.2077
   3073.5087      3121.9926      3137.9756
   3145.8931      3166.7207      3191.7313
Zero-point correction (Hartree): 0.114181

```

TS.C3H7CHO2s.14Hshift.mt

```

~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -307.48452767
Electronic state : 1-A
Cartesian coordinates (Angs):
  C      0.787938      0.999557      0.002149
  O      1.754506      0.291193      -0.468862
  O      1.620164      -1.022852      -0.038834
  C     -0.175890      0.347165      0.787098
  H      0.965537      2.064938      -0.103711
  H      0.771828      -0.578896      0.942019
  C     -1.192884      -0.626674      0.164003
  H     -0.638199      1.011554      1.510640
  C     -2.385321      0.112062      -0.433079
  H     -0.697726      -1.228600      -0.593226
  H     -1.532445      -1.308261      0.944088
  H     -2.068502      0.768488      -1.243986
  H     -2.886479      0.723988      0.317639
  H     -3.114435      -0.592603      -0.832927
Rotational constants (GHz):      7.5353300      2.1866200      1.9622000
Vibrational harmonic frequencies (cm-1):
  i1623.0841      64.3957      186.6563
    209.3178      273.6697      379.8179
    565.3554      668.2216      757.6435
    826.7878      851.8781      926.3301
    965.7741      992.7661      1037.3782
   1085.4787      1120.8718      1184.2785
   1291.1375      1309.5231      1333.0376
   1362.7185      1410.1737      1424.5293
   1496.2893      1499.0495      1506.7556
   1579.9407      1863.0978      3057.5566
   3084.1593      3120.9846      3132.0250
   3146.1412      3159.1604      3189.8795
Zero-point correction (Hartree): 0.114051

```

```

#####
Z-(iC3H7)CHOO
#####

```

Population analysis as 298K (%)
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)

Compound	Qtot	Erel	Erel2	n*Q*MB	%
iC3H7CHO2s.t	2.650e+39	0.00	0.00	2.650e+39	93.6
iC3H7CHO2s.m	3.209e+39	2.11	2.11	9.145e+37	3.23
iC3H7CHO2s.c	3.206e+39	2.11	2.11	9.127e+37	3.22
Total				2.833e+39	100

```

iC3H7CHO2s.c
~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -307.51496510
Electronic state : 1-A
Cartesian coordinates (Angs):
  C      0.521703      0.000137      1.016222
  O      1.559999      0.000034      0.327644
  O      1.461651      -0.000254      -1.028817
  C     -0.869232      0.000075      0.494987
  H      0.742744      0.000394      2.079794
  C     -1.157470      1.270870      -0.318396
  C     -1.157652      -1.270864      -0.318059
  H     -1.510213      0.000193      1.378266
  H     -0.532176      1.294551      -1.206116
  H     -0.975759      2.170397      0.268642
  H     -2.206596      1.262140      -0.611760
  H     -0.976448      -2.170255      0.269354
  H     -0.532146      -1.295095      -1.205616
  H     -2.206702      -1.261873      -0.611702
Rotational constants (GHz):      4.9906800      2.8310200      2.7033800
Vibrational harmonic frequencies (cm-1):
   99.4432      199.6116      204.3940
  226.4760      251.0397      342.2697
  420.9683      548.6053      752.4216
  821.4036      889.8866      914.2444
  942.9628      980.1257      985.1088
 1125.0896      1129.1166      1204.3309
 1339.1299      1383.7156      1385.2498
 1399.7165      1429.1207      1482.6747
 1497.6901      1503.8895      1526.6920
 1651.4178      3073.4505      3073.9861
 3078.2666      3139.7847      3140.4492
 3173.5634      3180.7545      3182.5407
Zero-point correction (Hartree): 0.117735

```

```

iC3H7CHO2s.m
~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -307.51496508
Electronic state : 1-A
Cartesian coordinates (Angs):
  C    0.521667   -0.002150    1.016218
  O    1.559985   -0.000903    0.327668
  O    1.461807    0.002161   -1.028755
  C   -0.869303   -0.000695    0.494885
  H    0.742735   -0.004741    2.079776
  C   -1.157380    1.271550   -0.316191
  C   -1.157796   -1.270260   -0.320274
  H   -1.510295   -0.001966    1.378146
  H   -0.532721    1.296499   -1.204311
  H   -0.974733    2.170006    0.272228
  H   -2.206744    1.263953   -0.608763
  H   -0.976884   -2.170642    0.265722
  H   -0.532066   -1.293169   -1.207710
  H   -2.206759   -1.260669   -0.614224
Rotational constants (GHz):   4.9906300   2.8309200   2.7031900
Vibrational harmonic frequencies (cm-1):
  99.3796      199.6273      204.4134
 226.4434     250.9143     342.2097
 420.9461     548.6237     752.3711
 821.3981     889.8558     914.3610
 942.9459     980.0594     985.1293
1125.1525    1129.1020    1204.3469
1339.1566    1383.6873    1385.2783
1399.7266    1429.1177    1482.6850
1497.6897    1503.8838    1526.6815
1651.3536    3073.4009    3073.9280
3078.3192    3139.6952    3140.3555
3173.6209    3180.7353    3182.5305
Zero-point correction (Hartree): 0.117734

iC3H7CHO2s.t
~~~~~
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -307.07697078
E(CCSD/Aug-CC-pVTZ) (Hartree): -307.01940505
  T1 diagnostic: 0.029382
E(MP2/Aug-CC-pVTZ) (Hartree): -306.97898582
E(MP3/Aug-CC-pVTZ) (Hartree): -307.00626413
E(RHF/Aug-CC-pVTZ) (Hartree): -305.79867876
E(RM062X/Aug-CC-pVTZ) (Hartree): -307.51813880
Electronic state : 1-A
Cartesian coordinates (Angs):
  C    0.337625   -0.765206    0.428195
  O    1.564703   -0.588737    0.298645
  O    1.983293    0.390805   -0.548464
  C   -0.679327    0.036375   -0.281586
  H    0.092692   -1.561833    1.126306
  C   -2.029439   -0.669311   -0.275099
  C   -0.749161    1.430318    0.367298
  H   -0.293570    0.165784   -1.296230
  H   -2.393261   -0.801910    0.745432
  H   -1.977334   -1.648150   -0.751006
  H   -2.762847   -0.070871   -0.812930
  H    0.233894    1.894469    0.374160
  H   -1.129133    1.358747    1.386869
  H   -1.432599    2.054164   -0.206895
Rotational constants (GHz):   6.3708600   2.4797700   2.0579200
Vibrational harmonic frequencies (cm-1):
 119.3031      202.9556      220.6715
 236.1397      288.8686      336.7730
 415.2870      555.1039      684.6954
 870.1370      881.4629      913.4543
 942.3843      965.2037      988.3559
1134.4663     1181.8777     1201.2091
1309.4997     1324.6475     1386.6071
1405.4209     1423.3022     1489.1319
1497.7940     1507.1766     1519.0504
1647.4393     3060.4722     3065.7584
3073.1340     3129.8496     3138.5193
3145.6230     3167.4727     3169.0248
Zero-point correction (Hartree): 0.117550

Population analysis as 298K (%)
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)
Compound      Qtot      Erel      Erel2  n*Q*MB      %
-----
TS.iC3H7CHO2s.ringclose.c 2.450e+39 0.00   0.00  4.901e+39 52.8
TS.iC3H7CHO2s.ringclose.p 2.197e+39 0.19   0.19  3.184e+39 34.3
TS.iC3H7CHO2s.ringclose.m 5.412e+39 1.31   1.31  1.189e+39 12.8
Total                                9.273e+39 100

TS.iC3H7CHO2s.ringclose.c
~~~~~
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -307.04087110
E(CCSD/Aug-CC-pVTZ) (Hartree): -306.98264916
  T1 diagnostic: 0.032789
E(MP2/Aug-CC-pVTZ) (Hartree): -306.93818118
E(MP3/Aug-CC-pVTZ) (Hartree): -306.96739562
E(RHF/Aug-CC-pVTZ) (Hartree): -305.76621993
E(RM062X/Aug-CC-pVTZ) (Hartree): -307.47875144
Electronic state : 1-A
Cartesian coordinates (Angs):
  C    0.486912   -0.468981    0.505156
  O    1.656322   -0.739520    0.118460
  O    1.855736    0.636616   -0.382620
  C   -0.643715    0.051113   -0.305691

```

H	0.239362	-0.799501	1.525377
H	-0.290292	0.169036	-1.326694
C	-1.769228	-0.988529	-0.215542
C	-1.104831	1.402470	0.243875
H	-2.110383	-1.108593	0.814592
H	-1.457067	-1.961344	-0.593638
H	-2.616615	-0.648464	-0.809308
H	-0.317189	2.142120	0.129074
H	-1.365445	1.324889	1.301726
H	-1.993668	1.728651	-0.294633
Rotational constants (GHz):	5.9834600	2.6161900	2.0509800
Vibrational harmonic frequencies (cm-1):			
i725.3703	108.8151		208.8430
228.1326	247.5049		312.0976
347.9171	437.0778		537.4756
803.6384	863.0093		933.1330
942.7904	975.0838		1011.7195
1122.2523	1179.8948		1202.8357
1311.6900	1335.9333		1385.7664
1392.5166	1413.4844		1487.9447
1493.6598	1502.1919		1516.2441
1626.2753	3030.7981		3057.7538
3059.4485	3123.1400		3127.9694
3143.5016	3149.3146		3170.5585
Zero-point correction (Hartree):	0.115709		

TS.iC3H7CHO2s.ringclose.m

E(RM062X/Aug-CC-pVTZ) (Hartree): -307.47639889

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-0.395811	-0.849801	-0.037409
O	-1.480145	-0.602959	0.558007
O	-1.887584	0.389394	-0.453816
C	0.713211	0.085791	-0.380422
H	-0.181464	-1.918147	-0.177256
H	0.697759	0.188404	-1.470364
C	0.598219	1.458000	0.271251
C	2.021764	-0.622187	0.008020
H	0.433025	1.351032	1.344202
H	-0.229238	2.022249	-0.141669
H	1.530234	2.002050	0.123704
H	2.112475	-1.601850	-0.461274
H	2.086677	-0.749578	1.089580
H	2.868076	-0.016465	-0.309091
Rotational constants (GHz):	6.2779400	2.6721300	2.1343100
Vibrational harmonic frequencies (cm-1):			
i732.4655	42.6152		164.7081
223.9864	285.9276		309.1557
379.1340	411.0603		628.8665
785.2846	824.0558		929.4089
949.2716	970.5596		977.6401
1127.0005	1153.5839		1196.8753
1282.1057	1346.9169		1398.4535
1400.5223	1421.0558		1484.9902
1491.1590	1507.4593		1514.0548
1614.6113	3044.6825		3051.6536
3062.8883	3073.7426		3131.8379
3135.5686	3151.1818		3200.7320
Zero-point correction (Hartree):	0.115441		

TS.iC3H7CHO2s.ringclose.p

E(RM062X/Aug-CC-pVTZ) (Hartree): -307.47857842

Electronic state : 1-A

Cartesian coordinates (Angs):

C	0.579214	-0.619673	-0.635925
O	1.698863	-0.100204	-0.373347
O	1.336808	0.137528	1.036498
C	-0.775397	-0.034217	-0.483692
H	0.626064	-1.576306	-1.174002
H	-1.195567	-0.182299	-1.490973
C	-1.609786	-0.897442	0.472258
C	-0.821087	1.441290	-0.127305
H	-1.214778	-0.786355	1.479906
H	-1.586416	-1.953096	0.200070
H	-2.645043	-0.561556	0.448668
H	-0.078931	2.008085	-0.687712
H	-0.617091	1.581366	0.929485
H	-1.811267	1.831819	-0.362669
Rotational constants (GHz):	5.3522300	2.8317400	2.5526600
Vibrational harmonic frequencies (cm-1):			
i706.6446	98.7066		203.0631
245.5516	255.0331		312.3422
348.2857	482.7434		616.6870
804.0242	820.4833		933.4492
962.2987	979.6651		1004.3553
1107.4274	1155.3824		1220.5958
1290.1166	1384.0454		1392.2105
1401.4328	1424.5243		1483.1158
1492.5861	1499.8164		1514.8751
1617.0729	2979.9705		3050.4576
3068.0406	3074.4152		3139.8349
3141.0253	3162.7629		3181.5477
Zero-point correction (Hartree):	0.115840		

Population analysis as 298K (%)

Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)

Compound	Qtot	Erel	Erel2	n*Q*MB	%
TS.iC3H7CHO2s.14Hshift	1.878e+39	0.00	0.00	3.755e+39	100

```

Total                                     3.755e+39 100

TS.iC3H7CHO2s.14Hshift
~~~~~
E (CCSD(T)/Aug-CC-pVTZ) (Hartree): -307.04317461
E (CCSD/Aug-CC-pVTZ) (Hartree): -306.98246202
  T1 diagnostic: 0.024245
E (MP2/Aug-CC-pVTZ) (Hartree): -306.95312966
E (MP3/Aug-CC-pVTZ) (Hartree): -306.97228847
E (RHF/Aug-CC-pVTZ) (Hartree): -305.74566046
E (RM062X/Aug-CC-pVTZ) (Hartree): -307.48567137
Electronic state : 1-A
Cartesian coordinates (Angs):
  C   -0.371284   -0.840617   -0.491111
  O   -1.608740   -0.578572   -0.246110
  O   -1.689134   0.511108   0.611045
  C    0.612863   -0.020230   0.085759
  H   -0.234914   -1.819007   -0.944293
  H   -0.373617   0.291483   0.943506
  C    0.759924   1.430441   -0.393547
  C    1.943370   -0.691501   0.351840
  H    1.234436   2.025751   0.385833
  H   -0.197468   1.878067   -0.638832
  H    1.404250   1.452407   -1.274150
  H    2.611046   -0.612139   -0.509239
  H    1.832145   -1.743891   0.609247
  H    2.437887   -0.201516   1.190799
Rotational constants (GHz):    5.9936100    2.7482000    2.2005600
Vibrational harmonic frequencies (cm-1):
  i1629.5059      138.3801      183.7703
   218.9224      257.8829      339.2498
   358.0914      534.7917      577.0732
   745.3889      871.6362      955.1345
   973.8175      985.6809     1011.1785
  1060.1664     1117.5137     1219.2109
  1304.7721     1333.8212     1371.2929
  1392.8204     1419.8353     1489.0109
  1494.5820     1505.0451     1509.0452
  1602.7570     1847.6458     3049.9982
  3060.8065     3113.9908     3123.5591
  3137.3487     3170.2801     3182.9106
Zero-point correction (Hartree): 0.113128

#####
Z-(tC4H9)CHOO
#####

Population analysis as 298K (%)
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)
Compound  Qtot      Erel  Erel2  n*Q*MB      %
-----
tC4H9CHO2s 1.170e+40 0.00  0.00  1.170e+40 100
Total      1.170e+40 100

tC4H9CHO2s
~~~~~
E (CCSD(T)/Aug-CC-pVTZ) (Hartree): -346.32023078
E (CCSD/Aug-CC-pVTZ) (Hartree): -346.25386480
  T1 diagnostic: 0.027653
E (MP2/Aug-CC-pVTZ) (Hartree): -346.20522408
E (MP3/Aug-CC-pVTZ) (Hartree): -346.24035910
E (RHF/Aug-CC-pVTZ) (Hartree): -344.84199111
E (RM062X/Aug-CC-pVTZ) (Hartree): -346.82522964
Electronic state : 1-A
Cartesian coordinates (Angs):
  C    0.426558   0.996580   -0.003134
  O    1.653302   0.778924   -0.002421
  O    2.117431   -0.498728   0.000760
  C   -0.664523   -0.020453   -0.000222
  H    0.207010   2.062064   -0.005285
  C   -0.556197   -0.885766   1.266488
  C   -1.995910   0.733805   -0.002138
  C   -0.557662   -0.894999   -1.260328
  H   -0.654987   -0.275634   2.164911
  H    0.393470   -1.411540   1.293299
  H   -1.373841   -1.607448   1.255766
  H   -2.096869   1.359250   -0.890577
  H   -2.095012   1.366940   0.881038
  H   -2.817968   0.019129   0.001816
  H    0.389818   -1.424821   -1.282750
  H   -0.652939   -0.291096   -2.163347
  H   -1.378135   -1.613417   -1.245578
Rotational constants (GHz):    4.0641900    1.9824900    1.8884600
Vibrational harmonic frequencies (cm-1):
   112.5856      193.7028      218.8954
   232.4876      247.0955      284.5343
   323.2931      379.4093      393.9062
   397.5285      556.4888      678.5064
   809.6136      891.6524      913.1765
   947.4868      960.3936      961.6559
   976.2856     1056.0855     1064.3813
  1236.7929     1254.9597     1291.6554
  1385.6873     1391.8488     1413.8328
  1434.0357     1475.8512     1492.0555
  1497.7729     1499.9253     1510.5909
  1532.3783     1643.0225     3054.6211
  3063.1286     3064.5057     3123.4981
  3128.7654     3129.3533     3141.2584
  3157.8190     3179.7406     3180.7937
Zero-point correction (Hartree): 0.145536

```


Population analysis as 298K (%)
 Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)
 Compound Qtot Erel Erel2 n*Q*MB %

 TS.tC4H9CHO2s.isom 2.698e+40 0.00 0.00 5.397e+40 100
 Total 5.397e+40 100

TS.tC4H9CHO2s.isom

~~~~~

E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -346.26483731

E(CCSD/Aug-CC-pVTZ) (Hartree): -346.20708463

T1 diagnostic: 0.021322

E(MP2/Aug-CC-pVTZ) (Hartree): -346.14170467

E(MP3/Aug-CC-pVTZ) (Hartree): -346.19386085

E(PMP2/Aug-CC-pVTZ) (Hartree): -346.16598420

E(PMP3/Aug-CC-pVTZ) (Hartree): -346.21801434

E(PUHF/Aug-CC-pVTZ) (Hartree): -344.86521048

E(UHF/Aug-CC-pVTZ) (Hartree): -344.84074069

E(UM062X/Aug-CC-pVTZ) (Hartree): -346.77631923

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.486757  | -0.394008 | 0.755705  |
| O | 1.645039  | -0.612508 | 0.004660  |
| C | -0.733807 | 0.027596  | 0.010421  |
| H | 0.476672  | -0.925700 | 1.697630  |
| C | -0.439804 | 1.305462  | -0.783373 |
| C | -1.159275 | -1.090822 | -0.956657 |
| C | -1.842558 | 0.283558  | 1.030647  |
| H | 0.355157  | 1.142428  | -1.510556 |
| H | -0.132092 | 2.112559  | -0.118690 |
| H | -1.337024 | 1.615996  | -1.320353 |
| H | -1.395648 | -2.006470 | -0.413568 |
| H | -0.365798 | -1.306857 | -1.671630 |
| H | -2.046667 | -0.780459 | -1.510691 |
| H | -1.561076 | 1.080493  | 1.719571  |
| H | -2.057002 | -0.615415 | 1.610739  |
| H | -2.757305 | 0.580715  | 0.517326  |
| O | 2.474074  | 0.401507  | 0.077811  |

Rotational constants (GHz): 4.2151800 1.7573100 1.7120300

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i334.8937 | 55.6802   | 160.5460  |
| 209.8035  | 226.7728  | 277.9532  |
| 284.1537  | 306.2184  | 347.5315  |
| 386.6655  | 417.6629  | 512.5223  |
| 629.4783  | 767.9924  | 930.4560  |
| 948.3826  | 959.9057  | 968.2606  |
| 1037.3257 | 1051.2873 | 1083.8796 |
| 1207.7057 | 1228.0104 | 1243.5651 |
| 1287.3106 | 1359.0674 | 1392.9860 |
| 1399.8997 | 1430.5350 | 1479.3228 |
| 1487.6781 | 1488.7949 | 1503.8975 |
| 1505.0953 | 1523.4333 | 3053.2473 |
| 3055.0631 | 3060.2955 | 3124.6271 |
| 3127.5958 | 3131.4570 | 3134.4933 |
| 3137.6496 | 3141.1040 | 3202.9108 |

Zero-point correction (Hartree): 0.141857

Population analysis as 298K (%)

Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)

| Compound                | Qtot      | Erel | Erel2 | n*Q*MB    | %   |
|-------------------------|-----------|------|-------|-----------|-----|
| TS.tC4H9CHO2s.ringclose | 1.253e+40 | 0.00 | 0.00  | 2.507e+40 | 100 |
| Total                   |           |      |       | 2.507e+40 | 100 |

TS.tC4H9CHO2s.ringclose

~~~~~

E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -346.28570366

E(CCSD/Aug-CC-pVTZ) (Hartree): -346.21867658

T1 diagnostic: 0.031500

E(MP2/Aug-CC-pVTZ) (Hartree): -346.16600719

E(MP3/Aug-CC-pVTZ) (Hartree): -346.20304462

E(RHF/Aug-CC-pVTZ) (Hartree): -344.81101807

E(RM062X/Aug-CC-pVTZ) (Hartree): -346.78789297

Electronic state : 1-A

Cartesian coordinates (Angs):

C	0.562442	0.769151	-0.409167
O	1.721608	0.814423	0.084807
O	1.952284	-0.628034	-0.118385
C	-0.620031	-0.036917	0.017419
H	0.351828	1.541413	-1.162970
C	-0.409510	-0.802598	1.317865
C	-1.738208	1.012538	0.200493
C	-1.003911	-0.979436	-1.131299
H	0.036574	-0.161204	2.078381
H	0.247698	-1.651739	1.169043
H	-1.378735	-1.146338	1.681416
H	-1.912811	1.582357	-0.713087
H	-1.503743	1.707609	1.007614
H	-2.661800	0.494859	0.456096
H	-0.224974	-1.724939	-1.271348
H	-1.146493	-0.436415	-2.067507
H	-1.943368	-1.473137	-0.880880

Rotational constants (GHz): 3.8706800 2.0715200 1.9457600

Vibrational harmonic frequencies (cm-1):

i700.8879	78.3950	180.6831
229.1726	247.5073	285.6340
301.5667	335.8468	362.7120
409.5999	441.8731	589.1857
776.5472	806.4454	905.5677
948.7502	967.8927	976.0347

994.2147	1055.5444	1068.2122
1215.5921	1242.4673	1316.2594
1389.4589	1399.6015	1402.0748
1427.7728	1474.5637	1486.3890
1491.2634	1495.4272	1507.3103
1522.5749	1613.2695	3036.8647
3055.9383	3058.0702	3068.4610
3124.6228	3129.8001	3130.9606
3141.4224	3163.5641	3191.5538

Zero-point correction (Hartree): 0.143631

E- (CH3) CHOO
#####

Population analysis as 298K (%)
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)
Compound Qtot Erel Erel2 n*Q*MB %

CH3CHO2a 4.701e+37 0.00 0.00 4.701e+37 100
Total 4.701e+37 100

CH3CHO2a
~~~~~  
E (CCSD(T)/Aug-CC-pVDZ) (Hartree): -228.38520144  
E (CCSD/Aug-CC-pVDZ) (Hartree): -228.35603813  
Tl diagnostic: 0.036580  
E (MP2/Aug-CC-pVDZ) (Hartree): -228.32228608  
E (MP3/Aug-CC-pVDZ) (Hartree): -228.33886122  
E (RHF/Aug-CC-pVDZ) (Hartree): -227.64577921  
E (CCSD(T)/Aug-CC-pVTZ) (Hartree): -228.58475567  
E (CCSD/Aug-CC-pVTZ) (Hartree): -228.54410235  
Tl diagnostic: 0.034770  
E (MP2/Aug-CC-pVTZ) (Hartree): -228.52150934  
E (MP3/Aug-CC-pVTZ) (Hartree): -228.53160724  
E (RHF/Aug-CC-pVTZ) (Hartree): -227.70219095  
E (CCSD(T)/Aug-CC-pVQZ) (Hartree): -228.64303436  
E (CCSD/Aug-CC-pVQZ) (Hartree): -228.59976593  
Tl diagnostic: 0.033892  
E (MP2/Aug-CC-pVQZ) (Hartree): -228.58568930  
E (MP3/Aug-CC-pVQZ) (Hartree): -228.58925132  
E (RHF/Aug-CC-pVQZ) (Hartree): -227.71641816  
E (RM062X/Aug-CC-pVTZ) (Hartree): -228.89710572  
Electronic state : 1-A  
Cartesian coordinates (Angs):  
C -0.370039 0.399961 -0.000016  
O 0.566461 -0.412338 -0.000016  
O 1.839494 0.076289 0.000014  
H -0.096126 1.452422 -0.000002  
C -1.762517 -0.093270 0.000005  
H -2.286708 0.287505 0.878116  
H -1.782679 -1.179231 0.000001  
H -2.286786 0.287547 -0.878036  
Rotational constants (GHz): 50.1860100 4.4801100 4.2196900  
Vibrational harmonic frequencies (cm-1):  
167.6530 268.3336 329.1509  
566.4967 883.5010 901.6039  
986.5165 1094.5197 1168.6110  
1362.4820 1421.7142 1467.7291  
1469.4722 1672.6658 3064.4357  
3120.6224 3166.0899 3183.3546  
Zero-point correction (Hartree): 0.059904

Population analysis as 298K (%)  
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)  
Compound Qtot Erel Erel2 n\*Q\*MB %  
-----  
TS.CH3CHO2s.isominv 7.433e+37 0.00 0.00 7.433e+37 100  
Total 7.433e+37 100

TS.CH3CHO2s.isominv  
~~~~~  
E (CCSD(T)/Aug-CC-pVTZ) (Hartree): -228.52211272
E (CCSD/Aug-CC-pVTZ) (Hartree): -228.48306069
Tl diagnostic: 0.027111
E (MP2/Aug-CC-pVTZ) (Hartree): -228.45694041
E (MP3/Aug-CC-pVTZ) (Hartree): -228.47131856
E (RHF/Aug-CC-pVTZ) (Hartree): -227.65040739
E (RM062X/Aug-CC-pVTZ) (Hartree): -228.83969726
Point group : CS
Electronic state : 1-A'
Cartesian coordinates (Angs):
C 0.674650 -0.378855 0.000000
O 0.000000 0.629316 0.000000
C 0.086218 -1.748637 0.000000
H 1.767485 -0.269365 0.000000
H -0.998531 -1.699463 0.000000
H 0.438115 -2.293311 0.877936
H 0.438115 -2.293311 -0.877936
O -0.776299 1.785734 0.000000
Rotational constants (GHz): 37.8957200 4.2794200 3.9383100
Vibrational harmonic frequencies (cm-1):
i563.0603 (A') 112.8006 (A'') 236.4851 (A'')
383.7108 (A') 677.8868 (A') 758.3476 (A'')
928.7640 (A') 1085.7106 (A'') 1114.4369 (A')
1388.9301 (A') 1430.6543 (A') 1470.4343 (A'')
1471.5937 (A') 1776.8569 (A') 3034.3987 (A')
3063.7274 (A') 3122.9966 (A'') 3184.6119 (A')
Zero-point correction (Hartree): 0.057506

Population analysis as 298K (%)
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)
Compound Qtot Erel Erel2 n*Q*MB %

TS.CH3CHO2s.isomrot 5.467e+37 0.00 0.00 1.093e+38 100
Total 1.093e+38 100

TS.CH3CHO2s.isomrot
~~~~~  
E (CCSD(T)/Aug-CC-pVTZ) (Hartree): -228.53294188  
E (CCSD/Aug-CC-pVTZ) (Hartree): -228.49979550  
T1 diagnostic: 0.026842  
E (MP2/Aug-CC-pVTZ) (Hartree): -228.46161656  
E (MP3/Aug-CC-pVTZ) (Hartree): -228.48724996  
E (PMP2/Aug-CC-pVTZ) (Hartree): -228.48521978  
E (PMP3/Aug-CC-pVTZ) (Hartree): -228.51073600  
E (PUHF/Aug-CC-pVTZ) (Hartree): -227.72326430  
E (UHF/Aug-CC-pVTZ) (Hartree): -227.69948578  
E (UM062X/Aug-CC-pVTZ) (Hartree): -228.85041849  
Electronic state : 1-A  
Cartesian coordinates (Angs):  
C -0.471427 0.646973 -0.186575  
O 0.775942 0.411988 0.402731  
C -1.511963 -0.369886 0.057617  
H -0.421792 1.278770 -1.061449  
H -1.636218 -0.544062 1.127388  
H -1.233429 -1.323734 -0.403629  
H -2.461484 -0.047493 -0.363158  
O 1.430715 -0.540238 -0.218407  
Rotational constants (GHz): 20.8790400 5.6869900 5.0349300  
Vibrational harmonic frequencies (cm-1):  
i343.6376 159.0343 255.9744  
469.1424 573.5811 901.9797  
1007.9786 1115.4176 1141.6749  
1204.7110 1342.2499 1408.3872  
1465.4410 1482.5991 3028.5608  
3099.4755 3157.6795 3215.0032  
Zero-point correction (Hartree): 0.057020

Population analysis as 298K (%)  
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)  
Compound Qtot Erel Erel2 n\*Q\*MB %  
-----  
TS.CH3CHO2a.ringclose 4.359e+37 0.00 0.00 8.719e+37 100  
Total 8.719e+37 100

TS.CH3CHO2a.ringclose  
~~~~~  
E (CCSD(T)/Aug-CC-pVDZ) (Hartree): -228.36015008
E (CCSD/Aug-CC-pVDZ) (Hartree): -228.32943770
T1 diagnostic: 0.041528
E (MP2/Aug-CC-pVDZ) (Hartree): -228.29288172
E (MP3/Aug-CC-pVDZ) (Hartree): -228.30941000
E (RHF/Aug-CC-pVDZ) (Hartree): -227.61934776
E (CCSD(T)/Aug-CC-pVTZ) (Hartree): -228.55883238
E (CCSD/Aug-CC-pVTZ) (Hartree): -228.51677434
T1 diagnostic: 0.039281
E (MP2/Aug-CC-pVTZ) (Hartree): -228.49149604
E (MP3/Aug-CC-pVTZ) (Hartree): -228.50173632
E (RHF/Aug-CC-pVTZ) (Hartree): -227.67511427
E (CCSD(T)/Aug-CC-pVQZ) (Hartree): -228.61654079
E (CCSD/Aug-CC-pVQZ) (Hartree): -228.57187914
T1 diagnostic: 0.038300
E (MP2/Aug-CC-pVQZ) (Hartree): -228.55519338
E (MP3/Aug-CC-pVQZ) (Hartree): -228.55894706
E (RHF/Aug-CC-pVQZ) (Hartree): -227.68893711
E (RM062X/Aug-CC-pVTZ) (Hartree): -228.86696485
Electronic state : 1-A
Cartesian coordinates (Angs):
C -0.280243 -0.199951 -0.361640
O 0.596233 0.674675 -0.123573
O 1.583401 -0.344927 0.253147
C -1.641971 -0.048993 0.179340
H -0.002910 -1.044282 -0.986394
H -1.667699 -0.623318 1.112493
H -2.388685 -0.468438 -0.490392
H -1.844491 0.991722 0.421500
Rotational constants (GHz): 27.7373800 5.2516700 4.9049300
Vibrational harmonic frequencies (cm-1):
i576.5907 148.6440 356.5845
460.3716 780.9087 830.9782
983.4914 1052.7939 1137.8264
1366.0593 1390.2772 1446.2163
1468.6372 1615.3091 3045.8735
3128.1652 3163.3739 3186.2878
Zero-point correction (Hartree): 0.058234

Population analysis as 298K (%)
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)
Compound Qtot Erel Erel2 n*Q*MB %

TS.CH3CHO2a.13Hshift 4.913e+37 0.00 0.00 4.913e+37 100
Total 4.913e+37 100

TS.CH3CHO2a.13Hshift
~~~~~  
E (CCSD(T)/Aug-CC-pVTZ) (Hartree): -228.53546057  
E (CCSD/Aug-CC-pVTZ) (Hartree): -228.49385732

```

T1 diagnostic: 0.024176
E(MP2/Aug-CC-pVTZ) (Hartree): -228.47611680
E(MP3/Aug-CC-pVTZ) (Hartree): -228.48407824
E(RHF/Aug-CC-pVTZ) (Hartree): -227.64271619
E(UM062X/Aug-CC-pVTZ) (Hartree): -228.84705605
Electronic state : 1-A
Cartesian coordinates (Angs):
  C   -0.324875   -0.361343   -0.000237
  O    0.511029    0.571639   -0.000113
  O    1.751707   -0.167472    0.000155
  H    0.794757   -1.105603   -0.000203
  C   -1.761205   -0.012263    0.000084
  H   -2.223693   -0.474298   -0.873362
  H   -1.933479    1.062199    0.000067
  H   -2.222996   -0.473996    0.874082
Rotational constants (GHz):  43.6302900   4.7166200   4.3697400
Vibrational harmonic frequencies (cm-1):
  11733.8939      146.3916      261.9447
  370.6842       688.5270      877.3991
  933.6765      1018.9566     1180.0328
  1232.5786     1387.1019     1450.5259
  1459.3673     1612.2635     2143.8090
  3062.1052     3128.7999     3161.7366
Zero-point correction (Hartree): 0.054940

#####
E-(C2H5)CHOO
#####

Population analysis as 298K (%)
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)
Compound  Qtot      Erel  Erel2  n*Q*MB  %
-----
C2H5CHO2a.c 4.994e+38 0.00  0.00  4.994e+38 54.5
C2H5CHO2a.m 7.402e+38 0.75  0.75  2.089e+38 22.8
C2H5CHO2a.p 7.408e+38 0.75  0.75  2.086e+38 22.8
Total                  9.169e+38 100

C2H5CHO2a.c
~~~~~
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -267.82748523
E(CCSD/Aug-CC-pVTZ) (Hartree): -267.77922090
T1 diagnostic: 0.030813
E(MP2/Aug-CC-pVTZ) (Hartree): -267.74667682
E(MP3/Aug-CC-pVTZ) (Hartree): -267.76665599
E(RHF/Aug-CC-pVTZ) (Hartree): -266.75123025
E(RM062X/Aug-CC-pVTZ) (Hartree): -268.20515143
Electronic state : 1-A
Cartesian coordinates (Angs):
 C -0.244360 0.711254 -0.000617
 O -0.890709 -0.345570 0.000447
 O -2.255931 -0.263470 -0.000024
 C 1.236710 0.675493 0.000529
 H -0.823760 1.632123 -0.001950
 C 1.828282 -0.725076 -0.000370
 H 1.571526 1.252884 -0.867091
 H 1.569971 1.250775 0.870249
 H 1.509050 -1.280527 -0.879987
 H 1.508182 -1.282089 0.877924
 H 2.914359 -0.670880 0.000219
Rotational constants (GHz): 15.0947500 2.8991000 2.5062600
Vibrational harmonic frequencies (cm-1):
 143.2808 200.1924 210.6227
 282.9865 427.2043 631.4122
 739.3799 919.4567 941.2833
 948.4146 1027.9771 1121.2055
 1134.1050 1279.6150 1354.0790
 1402.2046 1425.8909 1454.5141
 1502.4651 1507.0105 1669.7369
 3046.5982 3069.5775 3084.4426
 3157.1257 3161.0085 3162.5956
Zero-point correction (Hartree): 0.088859

C2H5CHO2a.m
~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -268.20402959
Electronic state : 1-A
Cartesian coordinates (Angs):
  C   -0.187673   -0.003791    0.395785
  O   -1.165655    0.276907   -0.312373
  O   -2.359279   -0.318689   -0.025363
  C    1.131557    0.606004    0.112813
  H   -0.359882   -0.719930    1.197707
  C    2.182349   -0.470661   -0.178273
  H    1.026404    1.298886   -0.719748
  H    1.431305    1.178386    0.994683
  H    1.922532   -1.032312   -1.073524
  H    2.266314   -1.170691    0.652272
  H    3.155402   -0.009394   -0.331454
Rotational constants (GHz):  20.5307500   2.3686600   2.2896400
Vibrational harmonic frequencies (cm-1):
  79.7521      200.0389      211.3336
  332.9275     417.8564      549.9181
  779.1640     926.8661      940.6521
  958.8758     1041.1719     1107.7357
  1186.7225     1281.6784     1324.1954
  1388.2442     1416.0107     1475.0222
  1505.0924     1509.8947     1667.7291
  3061.9740     3075.3944     3132.1995
  3150.1421     3156.5168     3159.0405
Zero-point correction (Hartree): 0.088931

```

```

C2H5CHO2a.p
~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -268.20402949
Electronic state : 1-A
Cartesian coordinates (Angs):
 C 0.187688 -0.002659 0.396502
 O 1.165315 0.275799 -0.313101
 O 2.358944 -0.318523 -0.025076
 C -1.131711 0.606371 0.112060
 H 0.360245 -0.716251 1.200608
 C -2.181677 -0.471191 -0.177871
 H -1.431973 1.180046 0.992886
 H -1.026241 1.298003 -0.721523
 H -2.265426 -1.170281 0.653535
 H -1.921359 -1.033879 -1.072355
 H -3.155120 -0.010972 -0.331884
Rotational constants (GHz): 20.5192100 2.3693500 2.2904500
Vibrational harmonic frequencies (cm-1):
 79.6281 199.8424 211.6180
 333.0314 417.8733 550.0523
 779.3343 926.9401 941.4437
 959.0261 1041.3235 1107.7260
 1186.6703 1281.6864 1324.2141
 1388.2458 1416.1701 1475.0537
 1505.1514 1509.9277 1667.4956
 3062.1244 3075.1663 3131.9991
 3150.0028 3156.5970 3158.7975
Zero-point correction (Hartree): 0.088933

Population analysis as 298K (%)
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)
Compound Qtot Erel Erel2 n*Q*MB %

TS.C2H5CHO2s.isom.t 7.197e+38 0.00 0.00 2.159e+39 100
Total 2.159e+39 100

TS.C2H5CHO2s.isom.t
~~~~~
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -267.77510058
E(CCSD/Aug-CC-pVTZ) (Hartree): -267.73417998
T1 diagnostic: 0.024523
E(MP2/Aug-CC-pVTZ) (Hartree): -267.68585129
E(MP3/Aug-CC-pVTZ) (Hartree): -267.72140975
E(PMP2/Aug-CC-pVTZ) (Hartree): -267.70942834
E(PMP3/Aug-CC-pVTZ) (Hartree): -267.74487027
E(PUHF/Aug-CC-pVTZ) (Hartree): -266.77110716
E(UHF/Aug-CC-pVTZ) (Hartree): -266.74735529
E(UM062X/Aug-CC-pVTZ) (Hartree): -268.15747902
Electronic state : 1-A
Cartesian coordinates (Angs):
  C    0.116127    0.627706   -0.068250
  O    1.428124    0.414843    0.364359
  C   -0.880174   -0.407642    0.280933
  H    0.040839    1.274393   -0.932381
  C   -2.284711   -0.010327   -0.156412
  H   -0.584733   -1.352770   -0.191575
  H   -0.842440   -0.583913    1.359321
  H   -2.326370    0.143219   -1.234663
  H   -2.596415    0.913874    0.328847
  H   -3.002019   -0.787112    0.099762
  O    2.022336   -0.523108   -0.335226
Rotational constants (GHz): 17.5495700 2.5174500 2.3971400
Vibrational harmonic frequencies (cm-1):
  i347.0656      73.9701      196.4229
  242.2443     320.3713     475.9265
  596.1529     784.3369     908.5703
  1040.3347     1073.4394    1105.9862
  1158.3016     1202.6858    1264.4460
  1291.8472     1395.8852    1417.3187
  1473.9942     1504.4710    1509.4248
  3014.8607     3067.0664    3070.6663
  3137.2391     3150.6418    3197.9312
Zero-point correction (Hartree): 0.085829

Population analysis as 298K (%)
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)
Compound      Qtot      Erel      Erel2  n*Q*MB      %
-----
TS.C2H5CHO2a.ringclose.c 5.015e+38 0.00 0.00 1.003e+39 48.4
TS.C2H5CHO2a.ringclose.p 5.788e+38 0.29 0.29 7.086e+38 34.2
TS.C2H5CHO2a.ringclose.m 5.938e+38 0.71 0.71 3.595e+38 17.4
Total                2.071e+39 100

TS.C2H5CHO2a.ringclose.c
~~~~~
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -267.80171700
E(CCSD/Aug-CC-pVTZ) (Hartree): -267.75203454
T1 diagnostic: 0.034478
E(MP2/Aug-CC-pVTZ) (Hartree): -267.71687057
E(MP3/Aug-CC-pVTZ) (Hartree): -267.73699231
E(RHF/Aug-CC-pVTZ) (Hartree): -266.72425934
E(RM062X/Aug-CC-pVTZ) (Hartree): -268.17505878
Electronic state : 1-A
Cartesian coordinates (Angs):
 C -0.341166 0.589416 -0.263390
 O -0.881985 -0.538956 -0.416424
 O -2.037964 -0.147336 0.408637
 C 1.085075 0.709957 0.101903
 H -0.946068 1.474948 -0.441032

```

```

C 1.851094 -0.602811 0.102377
H 1.531808 1.467633 -0.547704
H 1.075614 1.168530 1.099790
H 1.856702 -1.049268 -0.890219
H 1.390968 -1.313597 0.785081
H 2.880550 -0.437290 0.411047
Rotational constants (GHz): 13.2690900 3.1039900 2.7877000
Vibrational harmonic frequencies (cm-1):
i564.6614 91.9854 204.6825
239.3957 352.4090 630.9623
728.4668 819.1978 831.3997
954.5184 1023.6401 1099.2599
1125.6163 1267.7743 1375.2091
1383.9847 1418.3956 1433.8427
1502.1554 1507.3092 1606.5917
3029.6661 3077.7167 3084.4686
3156.4831 3163.9667 3164.8795
Zero-point correction (Hartree): 0.087195

```

TS.C2H5CHO2a.ringclose.m

```

~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -268.17435688
Electronic state : 1-A
Cartesian coordinates (Angs):
C      0.277306      -0.546086      0.393429
O      1.155900      -0.434666      -0.505616
O      1.754988      0.739748      0.143491
C      -1.142646      -0.677691      0.021076
H      0.603011      -0.515934      1.430389
C      -1.709917      0.755251      -0.085024
H      -1.208763      -1.171510      -0.948025
H      -1.683893      -1.246431      0.774884
H      -1.146312      1.326134      -0.819547
H      -1.646556      1.271511      0.870771
H      -2.753048      0.706728      -0.388361
Rotational constants (GHz): 10.9182500  3.3819200  2.9252900
Vibrational harmonic frequencies (cm-1):
i561.9256      91.3205      162.0894
212.1087      469.8403      545.3693
809.9925      837.1445      864.9975
948.1692      1021.5299      1083.3353
1156.6319      1264.6923      1311.5445
1376.9757      1408.0691      1483.0113
1498.6238      1508.5793      1604.4918
3080.5941      3087.6202      3141.6286
3159.1964      3164.0603      3169.7195
Zero-point correction (Hartree): 0.087621

```

TS.C2H5CHO2a.ringclose.p

```

~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -268.17440671
Electronic state : 1-A
Cartesian coordinates (Angs):
C 0.248161 -0.156598 -0.204031
O 1.278307 0.553152 -0.361160
O 2.132893 -0.449319 0.285792
C -0.990928 0.434186 0.338810
H 0.294856 -1.202553 -0.501545
C -2.255819 -0.290699 -0.100544
H -0.865375 0.374375 1.428278
H -0.992728 1.499278 0.100744
H -2.209470 -1.346794 0.162927
H -2.396310 -0.214876 -1.177548
H -3.129054 0.138571 0.384673
Rotational constants (GHz): 18.9134700 2.4917500 2.3904200
Vibrational harmonic frequencies (cm-1):
i568.9104 85.4242 182.7133
237.0351 405.7768 491.0714
714.6502 828.6149 846.8047
956.3582 1064.8703 1101.1221
1151.9306 1263.3607 1332.9939
1385.7010 1423.7237 1432.8064
1505.6836 1509.5997 1608.2283
3027.5078 3077.0488 3102.4245
3146.7135 3150.2003 3158.7777
Zero-point correction (Hartree): 0.087006

```

```

Population analysis as 298K (%)
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)
Compound Qtot Erel Erel2 n*Q*MB %

TS.C2H5CHO2a.13Hshift.c 5.057e+38 0.00 0.00 5.057e+38 50.4
TS.C2H5CHO2a.13Hshift.t 1.054e+39 0.85 0.85 2.498e+38 24.9
TS.C2H5CHO2a.13Hshift.p 1.049e+39 0.85 0.85 2.484e+38 24.7
Total 1.004e+39 100

```

TS.C2H5CHO2a.13Hshift.c

```

~~~~~
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -267.77831565
E(CCSD/Aug-CC-pVTZ) (Hartree): -267.72883575
T1 diagnostic: 0.021825
E(MP2/Aug-CC-pVTZ) (Hartree): -267.70145632
E(MP3/Aug-CC-pVTZ) (Hartree): -267.71885701
E(RHF/Aug-CC-pVTZ) (Hartree): -266.69082292
E(UM062X/Aug-CC-pVTZ) (Hartree): -268.15498192
Electronic state : 1-A
Cartesian coordinates (Angs):
C      -0.298233      0.630376      0.000004
O      -0.828461      -0.505965      0.000084
O      -2.230819      -0.156656      -0.000049
H      -1.588630      1.015779      -0.000108

```

```

C      1.180067      0.718635      0.000019
C      1.925662     -0.608768     -0.000038
H      1.438959      1.337769     -0.864573
H      1.438962      1.337699      0.864661
H      1.669844     -1.196688     -0.879495
H      1.669990     -1.196698      0.879455
H      3.000141     -0.438356     -0.000125
Rotational constants (GHz):  16.5030600      2.8614200      2.5129500
Vibrational harmonic frequencies (cm-1):
i1724.4453      122.6698      198.5409
208.2263      286.6141      503.2201
690.8565      724.4985      904.3297
978.4659      1020.7193      1082.5153
1160.9728      1175.4624      1275.3482
1380.8248      1417.1816      1431.2997
1504.1598      1505.5443      1591.6407
2141.0508      3054.4900      3077.9164
3080.6558      3154.5238      3156.5288
Zero-point correction (Hartree): 0.083901

```

TS.C2H5CHO2a.13Hshift.p

```

~~~~~
E(UM062X/Aug-CC-pVT2) (Hartree): -268.15373891
Electronic state : 1-A
Cartesian coordinates (Angs):
C 0.211976 -0.030880 0.320698
O 1.146391 0.452533 -0.359454
O 2.243168 -0.405543 0.024943
H 1.191708 -0.865288 0.715762
C -1.135084 0.577769 0.207764
C -2.166065 -0.486921 -0.180330
H -1.375975 0.968525 1.200052
H -1.123612 1.409843 -0.496953
H -2.159373 -1.308019 0.534017
H -1.952632 -0.891358 -1.167883
H -3.161548 -0.049434 -0.197696
Rotational constants (GHz): 18.6421600 2.4750200 2.3498900
Vibrational harmonic frequencies (cm-1):
i1729.3026 53.5900 174.2493
211.3127 353.8045 452.0857
667.2627 784.2444 899.6744
975.2174 1028.6774 1068.6832
1176.7275 1225.6446 1273.6719
1332.5791 1413.1024 1463.3445
1502.7308 1510.5496 1600.6154
2142.3889 3059.4557 3079.6486
3114.9489 3155.0366 3160.1577
Zero-point correction (Hartree): 0.084017

```

TS.C2H5CHO2a.13Hshift.t

```

~~~~~
E(UM062X/Aug-CC-pVT2) (Hartree): -268.15373887
Electronic state : 1-A
Cartesian coordinates (Angs):
C      0.212031     -0.030036      0.321471
O      1.145923      0.451704     -0.360552
O      2.243044     -0.405324      0.025249
H      1.192168     -0.863364      0.718004
C     -1.135224      0.578061      0.207845
C     -2.165470     -0.487340     -0.180377
H     -1.376807      0.968913      1.199920
H     -1.123907      1.409845     -0.497212
H     -2.159019     -1.308021      0.534454
H     -1.951077     -0.892276     -1.167526
H     -3.161110     -0.050254     -0.198851
Rotational constants (GHz):  18.6316500      2.4754600      2.3506200
Vibrational harmonic frequencies (cm-1):
i1729.1906      53.2586      174.2031
211.2563      354.0028      451.9959
667.3185      784.4233      899.6250
975.1779      1028.8095      1068.6001
1176.6999      1225.6599      1273.6599
1332.4833      1413.0629      1463.4773
1502.7061      1510.5465      1600.6419
2142.4105      3059.4844      3079.6202
3115.0073      3154.9881      3160.1539
Zero-point correction (Hartree): 0.084017

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#####
E-(nC3H7)CHOO
#####

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```

Population analysis as 298K (%)
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)
Compound      Qtot      Erel      Erel2  n*Q*MB      %
-----
C3H7CHO2a.ct  5.766e+39  0.00      0.00  1.153e+40  31
C3H7CHO2a.pm  8.603e+39  0.31      0.31  1.021e+40  27.4
C3H7CHO2a.pt  8.658e+39  0.51      0.51  7.312e+39  19.6
C3H7CHO2a.cm  4.436e+39  0.33      0.33  5.105e+39  13.7
C3H7CHO2a.pp  1.058e+40  1.14      1.14  3.073e+39  8.25
Total                  3.723e+40  100

```

C3H7CHO2a.cm

```

~~~~~
E(RM062X/Aug-CC-pVT2) (Hartree): -307.51220488
Electronic state : 1-A
Cartesian coordinates (Angs):
C 0.753037 0.761858 -0.288914
O 1.170096 -0.287017 0.221186
O 2.489646 -0.606833 0.047653

```

```

C -0.660652 1.172134 -0.110031
H 1.482384 1.350499 -0.841977
C -1.558583 0.129609 0.547729
H -0.640866 2.102504 0.468631
H -1.044246 1.454921 -1.095796
C -1.828342 -1.070642 -0.352913
H -1.103461 -0.197955 1.482655
H -2.499663 0.614493 0.806814
H -0.907960 -1.597458 -0.599781
H -2.302003 -0.756101 -1.283953
H -2.494871 -1.777853 0.137479
Rotational constants (GHz): 6.8552400 2.1117700 1.7743800
Vibrational harmonic frequencies (cm-1):
109.1106 141.8602 172.6616
242.1162 271.4118 342.8626
445.4126 631.3076 785.1453
815.3188 870.0783 954.1457
973.3061 993.1935 1069.1117
1114.5688 1151.2605 1248.8524
1301.0494 1354.5639 1383.6145
1408.6915 1423.2889 1450.4903
1494.3741 1506.2767 1512.6346
1669.8253 3037.3130 3063.3163
3066.2256 3083.5763 3115.8655
3137.7701 3150.2729 3160.1080
Zero-point correction (Hartree): 0.117670

```

```

C3H7CHO2a.ct
~~~~~
E (CCSD(T)/Aug-CC-pVTZ) (Hartree): -307.07017805
E (CCSD/Aug-CC-pVTZ) (Hartree): -307.01406073
T1 diagnostic: 0.028410
E (MP2/Aug-CC-pVTZ) (Hartree): -306.97165728
E (MP3/Aug-CC-pVTZ) (Hartree): -307.00129997
E (RHF/Aug-CC-pVTZ) (Hartree): -305.79922609
E (RM062X/Aug-CC-pVTZ) (Hartree): -307.51255151
Electronic state : 1-A
Cartesian coordinates (Angs):
C      0.916410      0.731973      0.000509
O      1.456814     -0.382990     -0.000621
O      2.823564     -0.433878      0.000066
C     -0.560374      0.841763     -0.000445
H      1.583977      1.591234      0.002177
C     -1.303151     -0.486966      0.000686
H     -0.841881      1.448794      0.867586
H     -0.840693      1.446335     -0.870668
C     -2.811037     -0.278081     -0.000152
H     -0.999759     -1.067538     -0.870956
H     -1.000431     -1.065642      0.873839
H     -3.128708      0.279224     -0.882253
H     -3.129438      0.281157      0.880460
H     -3.337182     -1.230750      0.000674
Rotational constants (GHz):   12.8452800   1.5286400   1.4010800
Vibrational harmonic frequencies (cm-1):
85.8642      146.3566      151.6083
245.5381      262.8847      331.4369
411.2676      678.6194      717.9762
834.8948      878.5938      959.9942
967.7245     1009.1755     1068.7775
1135.9401     1152.0283     1255.6249
1319.5141     1328.0286     1374.2949
1417.8532     1422.6759     1451.9824
1495.3828     1505.9815     1511.5609
1667.6939     3032.3921     3055.6212
3061.9332     3081.4211     3110.7397
3133.8331     3145.5494     3163.6797
Zero-point correction (Hartree): 0.117495

```

```

C3H7CHO2a.pm
~~~~~
E (CCSD(T)/Aug-CC-pVTZ) (Hartree): -307.07053238
E (CCSD/Aug-CC-pVTZ) (Hartree): -307.01403443
T1 diagnostic: 0.029125
E (MP2/Aug-CC-pVTZ) (Hartree): -306.97205797
E (MP3/Aug-CC-pVTZ) (Hartree): -307.00092835
E (RHF/Aug-CC-pVTZ) (Hartree): -305.79817009
E (RM062X/Aug-CC-pVTZ) (Hartree): -307.51220556
Electronic state : 1-A
Cartesian coordinates (Angs):
C -0.631286 -0.511696 0.306285
O -1.483242 0.030858 -0.412888
O -2.601435 0.535641 0.185854
C 0.613747 -1.046983 -0.288022
H -0.845351 -0.536325 1.373908
C 1.843811 -0.318047 0.275551
H 0.673891 -2.111136 -0.046230
H 0.560749 -0.941834 -1.371223
C 1.858188 1.158780 -0.095758
H 1.864678 -0.435019 1.360991
H 2.734646 -0.814547 -0.108363
H 0.989438 1.679901 0.308796
H 1.841993 1.285491 -1.178691
H 2.750607 1.649151 0.288747
Rotational constants (GHz): 7.7027700 1.8577600 1.6286400
Vibrational harmonic frequencies (cm-1):
60.8906 103.5683 180.3716
257.8733 287.6064 363.0223
456.2882 550.6609 779.1609
838.5668 895.6889 954.7105
975.3304 1003.0564 1075.3496
1109.7784 1183.1614 1247.5803
1280.8007 1337.7049 1370.8366

```



1392.4474                    1425.9059                    1473.5366  
 1494.5519                    1505.0791                    1506.8979  
 1666.2043                    3062.1824                    3063.7226  
 3069.4844                    3107.3883                    3128.6740  
 3134.1096                    3144.8239                    3152.0367  
 Zero-point correction (Hartree): 0.117642

C3H7CHO2a.pp

~~~~~  
 E(RM062X/Aug-CC-pVTZ) (Hartree): -307.51096861

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.614571  | -0.015377 | 0.364458  |
| O | 1.687742  | 0.309664  | -0.166648 |
| O | 2.711304  | -0.591300 | -0.151150 |
| C | -0.524945 | 0.930251  | 0.346068  |
| H | 0.580747  | -1.008522 | 0.806851  |
| C | -1.706795 | 0.398627  | -0.482579 |
| H | -0.855500 | 1.079105  | 1.378248  |
| H | -0.173799 | 1.884393  | -0.042856 |
| C | -2.302004 | -0.890957 | 0.069296  |
| H | -2.468813 | 1.177716  | -0.501020 |
| H | -1.379820 | 0.253467  | -1.512871 |
| H | -2.601643 | -0.767471 | 1.110996  |
| H | -1.594958 | -1.718841 | 0.018531  |
| H | -3.183538 | -1.182025 | -0.498952 |

Rotational constants (GHz): 9.2853500                    1.6296000                    1.4953600

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| 54.7666   | 88.5728   | 187.6604  |
| 247.8070  | 310.2532  | 343.0973  |
| 465.1300  | 557.4663  | 761.4762  |
| 859.5613  | 878.7915  | 957.2528  |
| 977.3557  | 1013.6432 | 1077.2020 |
| 1125.4832 | 1162.4092 | 1258.5731 |
| 1289.6479 | 1335.0637 | 1365.8971 |
| 1398.9394 | 1422.6720 | 1475.6456 |
| 1496.0395 | 1506.0906 | 1512.7346 |
| 1662.1026 | 3054.3336 | 3063.5790 |
| 3076.4862 | 3110.8928 | 3133.4474 |
| 3137.0745 | 3143.7368 | 3168.1071 |

Zero-point correction (Hartree): 0.117733

C3H7CHO2a.pt

~~~~~  
 E(RM062X/Aug-CC-pVTZ) (Hartree): -307.51186096

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.837409 | 0.029161  | 0.435214  |
| O | -1.759819 | -0.296678 | -0.326722 |
| O | -2.984686 | 0.273006  | -0.133357 |
| C | 0.513642  | -0.543766 | 0.249056  |
| H | -1.081691 | 0.759348  | 1.204966  |
| C | 1.549431  | 0.548363  | -0.051820 |
| H | 0.797222  | -1.057143 | 1.172982  |
| H | 0.480205  | -1.281830 | -0.551596 |
| C | 2.948742  | -0.037161 | -0.179166 |
| H | 1.268902  | 1.059443  | -0.973564 |
| H | 1.527425  | 1.296232  | 0.743189  |
| H | 2.989163  | -0.774641 | -0.980994 |
| H | 3.249374  | -0.530951 | 0.745381  |
| H | 3.678994  | 0.739340  | -0.399436 |

Rotational constants (GHz): 17.3265500                    1.3094000                    1.2903300

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| 65.8720   | 89.3796   | 172.3493  |
| 250.1531  | 308.0581  | 340.6973  |
| 394.7977  | 589.4165  | 746.1763  |
| 852.4166  | 900.8095  | 953.3093  |
| 978.4734  | 1043.4843 | 1067.7416 |
| 1123.0288 | 1186.8652 | 1262.4423 |
| 1289.6853 | 1330.3384 | 1371.6970 |
| 1393.5838 | 1418.1228 | 1473.9735 |
| 1496.9345 | 1504.2428 | 1511.3547 |
| 1666.1201 | 3049.8675 | 3063.2332 |
| 3068.0873 | 3100.9685 | 3127.5882 |
| 3136.2699 | 3145.1025 | 3155.5729 |

Zero-point correction (Hartree): 0.117618

Population analysis as 298K (%)

Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)

| Compound                  | Qtot      | Erel | Erel2 | n*Q*MB    | %    |
|---------------------------|-----------|------|-------|-----------|------|
| TS.C3H7CHO2a.ringclose.ct | 6.501e+39 | 0.24 | 0.24  | 8.729e+39 | 16.4 |
| TS.C3H7CHO2a.ringclose.cp | 4.029e+39 | 0.09 | 0.09  | 6.931e+39 | 13   |
| TS.C3H7CHO2a.ringclose.cm | 3.871e+39 | 0.07 | 0.07  | 6.902e+39 | 13   |
| TS.C3H7CHO2a.ringclose.mp | 3.445e+39 | 0.00 | 0.00  | 6.890e+39 | 12.9 |
| TS.C3H7CHO2a.ringclose.pm | 5.347e+39 | 0.31 | 0.31  | 6.335e+39 | 11.9 |
| TS.C3H7CHO2a.ringclose.pt | 6.570e+39 | 0.50 | 0.50  | 5.658e+39 | 10.6 |
| TS.C3H7CHO2a.ringclose.mm | 4.805e+39 | 0.43 | 0.43  | 4.623e+39 | 8.68 |
| TS.C3H7CHO2a.ringclose.mt | 6.347e+39 | 0.65 | 0.65  | 4.217e+39 | 7.92 |
| TS.C3H7CHO2a.ringclose.pp | 6.593e+39 | 0.88 | 0.88  | 2.978e+39 | 5.59 |
| Total                     |           |      |       | 5.326e+40 | 100  |

TS.C3H7CHO2a.ringclose.cm

~~~~~  
 E(RM062X/Aug-CC-pVTZ) (Hartree): -307.48302093

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.830203  | 0.764119  | -0.177277 |
| O | 1.210561  | -0.060822 | 0.695233  |
| O | 2.050494  | -0.794145 | -0.269124 |
| C | -0.592704 | 1.153002  | -0.299880 |

```

H 1.590198 1.229171 -0.800465
C -1.562427 0.219610 0.412856
H -0.650721 2.186509 0.066424
H -0.808945 1.223025 -1.371026
C -1.602251 -1.152683 -0.251819
H -1.262521 0.122271 1.456188
H -2.552906 0.674476 0.406812
H -0.609941 -1.604643 -0.272046
H -1.958255 -1.071079 -1.279843
H -2.272271 -1.824283 0.281799
Rotational constants (GHz): 5.9714500 2.4812700 2.0313700
Vibrational harmonic frequencies (cm-1):
i554.6112 72.5111 132.1346
200.9631 285.3569 352.7422
369.9912 629.4949 744.4816
813.1036 841.6972 861.3592
926.5425 977.2162 1054.7769
1102.7507 1140.3728 1239.0386
1296.0437 1363.1203 1382.1284
1397.1088 1419.2629 1429.6568
1496.5494 1508.0292 1513.8939
1608.4915 3028.0523 3060.2893
3065.2869 3083.4260 3113.6808
3135.2978 3145.1710 3158.0495
Zero-point correction (Hartree): 0.116068

```

TS.C3H7CHO2a.ringclose.cp

~~~~~

E(RM062X/Aug-CC-pVTZ) (Hartree): -307.48291690

Electronic state : 1-A

Cartesian coordinates (Angs):

```

C -0.801562 0.441714 -0.487245
O -1.086926 -0.704942 -0.045148
O -2.450914 -0.283724 0.311094
C 0.447345 1.127625 -0.095119
H -1.497996 0.906822 -1.180240
C 1.463643 0.252465 0.625964
H 0.864076 1.611216 -0.983469
H 0.103036 1.952260 0.545124
C 2.053880 -0.816833 -0.285593
H 2.255428 0.894368 1.011307
H 0.981408 -0.213498 1.485158
H 2.540666 -0.365204 -1.151329
H 1.279745 -1.494705 -0.645031
H 2.796525 -1.411762 0.242871
Rotational constants (GHz): 7.6647600 2.0739100 1.8463200
Vibrational harmonic frequencies (cm-1):
i558.2084 81.7112 121.3276
197.1239 268.7904 340.7868
360.1141 634.7279 749.4715
788.7289 835.2558 874.9785
913.8900 1006.2676 1062.0938
1098.3952 1144.8337 1233.3887
1295.6690 1368.1133 1383.1925
1403.5040 1416.7730 1427.0437
1491.9891 1505.4106 1510.1106
1600.7105 3019.2397 3061.9435
3072.1837 3085.4484 3116.1661
3137.0806 3145.1225 3165.8628
Zero-point correction (Hartree): 0.115998

```

TS.C3H7CHO2a.ringclose.ct

~~~~~

E(RM062X/Aug-CC-pVTZ) (Hartree): -307.48243421

Electronic state : 1-A

Cartesian coordinates (Angs):

```

C -0.987717 0.610009 -0.241176
O -1.476081 -0.537268 -0.428374
O -2.578275 -0.271571 0.512090
C 0.454800 0.794657 0.013970
H -1.654678 1.465879 -0.307935
C 1.304122 -0.460083 -0.125536
H 0.807081 1.613173 -0.622291
H 0.511502 1.194842 1.036467
C 2.767004 -0.179082 0.188242
H 0.910665 -1.227962 0.539977
H 1.203102 -0.850483 -1.138954
H 2.882713 0.189029 1.208417
H 3.176717 0.573762 -0.486310
H 3.368495 -1.080537 0.087897
Rotational constants (GHz): 11.4820800 1.6014000 1.5178100
Vibrational harmonic frequencies (cm-1):
i565.9116 71.7538 91.0275
180.2297 245.2525 325.3650
361.4471 644.4113 712.6526
790.7858 832.1396 869.3271
927.3770 1012.5339 1067.3825
1114.4654 1144.5671 1245.3593
1314.1553 1333.6682 1375.6819
1408.5142 1419.7125 1429.8398
1495.3657 1505.8132 1511.1817
1603.3219 3016.7669 3061.5477
3063.0370 3081.7719 3112.6157
3134.8974 3144.9238 3158.9743
Zero-point correction (Hartree): 0.115749

```

TS.C3H7CHO2a.ringclose.mm

~~~~~

E(RM062X/Aug-CC-pVTZ) (Hartree): -307.48280367

Electronic state : 1-A

Cartesian coordinates (Angs):

```

C 0.741059 -0.473022 0.542894

```

```

O 1.650542 -0.351450 -0.325001
O 1.760116 1.095529 -0.101720
C -0.495323 -1.199086 0.200977
H 0.905078 -0.012493 1.513463
C -1.414701 -0.232346 -0.586619
H -0.232112 -2.044313 -0.436905
H -0.996053 -1.546619 1.103474
C -1.828655 0.984792 0.229566
H -0.882430 0.081966 -1.484372
H -2.288211 -0.801826 -0.902337
H -0.961998 1.602553 0.467321
H -2.311297 0.687589 1.161973
H -2.532524 1.598478 -0.329755
Rotational constants (GHz): 5.9251600 2.4565200 1.9983500
Vibrational harmonic frequencies (cm-1):
i553.9960 73.8011 119.4898
154.5761 270.8224 342.5065
470.0450 562.1736 752.8728
826.8191 865.9290 898.8369
931.2950 1013.3773 1058.9450
1114.8921 1131.9583 1227.6560
1271.7979 1338.0641 1363.8643
1384.9926 1422.4574 1480.4141
1491.5901 1503.7317 1514.1041
1600.8283 3058.4732 3075.0798
3082.8142 3116.3218 3133.4213
3142.0497 3144.1298 3168.1568
Zero-point correction (Hartree): 0.116433

TS.C3H7CHO2a.ringclose.mp
~~~~~
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -307.04583936
E(CCSD/Aug-CC-pVTZ) (Hartree): -306.98755727
T1 diagnostic: 0.032126
E(MP2/Aug-CC-pVTZ) (Hartree): -306.94346446
E(MP3/Aug-CC-pVTZ) (Hartree): -306.97214576
E(RHF/Aug-CC-pVTZ) (Hartree): -305.77011121
E(RM062X/Aug-CC-pVTZ) (Hartree): -307.48367617
Electronic state : 1-A
Cartesian coordinates (Angs):
C      -0.772067      -0.780068      -0.169224
O     -1.450317      -0.068118      0.625085
O     -1.788603      0.882855     -0.445198
C      0.590883     -1.211044      0.181714
H     -1.229434     -1.059925     -1.115326
C      1.592494     -0.181603     -0.406876
H      0.693587     -1.233153      1.266960
H      0.782996     -2.196323     -0.241373
C      1.472818      1.185506      0.251585
H      2.590716     -0.596136     -0.267080
H      1.428999     -0.100945     -1.482454
H      1.635733      1.110778      1.327351
H      0.485079      1.614554      0.084804
H      2.218922      1.866510     -0.155175
Rotational constants (GHz):      5.6302200      2.6441200      2.0953900
Vibrational harmonic frequencies (cm-1):
i563.0356      90.2716      125.1611
172.8851      279.0934      351.1483
470.7935      549.8526      772.2840
832.9414      861.5727      902.0675
932.3639      1005.5515      1055.6208
1105.2747      1159.7353      1233.7691
1265.6744      1330.9901      1362.4190
1383.9180      1430.5452      1481.1539
1495.2110      1504.6684      1517.7519
1600.9476      3063.3465      3074.3934
3078.7910      3112.0048      3136.2563
3140.3911      3147.5365      3161.6005
Zero-point correction (Hartree): 0.116615

TS.C3H7CHO2a.ringclose.mt
~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -307.48237912
Electronic state : 1-A
Cartesian coordinates (Angs):
C -0.953986 0.590251 0.356890
O -1.733247 0.287081 -0.589115
O -2.233957 -0.896302 -0.123908
C 0.463725 0.871207 0.079640
H -1.361059 0.606942 1.364926
C 1.221860 -0.476913 0.151374
H 0.558602 1.281790 -0.926406
H 0.871575 1.565516 0.813678
C 2.699336 -0.283971 -0.156595
H 1.092179 -0.909905 1.143705
H 0.761187 -1.166940 -0.555190
H 3.162121 0.400545 0.554765
H 2.837711 0.125717 -1.157215
H 3.229711 -1.233345 -0.104467
Rotational constants (GHz): 9.3294600 1.7221500 1.5872800
Vibrational harmonic frequencies (cm-1):
i557.2465 89.4013 92.0711
129.8478 256.1622 332.0311
479.7002 529.9118 755.9700
827.2471 876.2463 899.2620
937.0568 1024.9131 1050.9882
1104.6280 1160.5295 1243.0741
1279.5388 1326.2957 1367.0980
1381.9346 1416.4402 1479.6720
1496.9439 1503.6424 1510.6832
1602.2895 3063.4925 3072.8399
3084.1522 3113.3719 3133.1494

```

```

3143.7445 3144.7732 3166.1599
Zero-point correction (Hartree): 0.116358

TS.C3H7CHO2a.ringclose.pm
~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -307.48236409
Electronic state : 1-A
Cartesian coordinates (Angs):
  C   -0.670216   -0.056815   -0.151227
  O   -1.635856   -0.405492    0.580561
  O   -2.615145   -0.041651   -0.451047
  C    0.406151    0.804114    0.377822
  H   -0.643111   -0.425459   -1.175500
  C    1.749696    0.568051   -0.303632
  H    0.046562    1.827376    0.204064
  H    0.448590    0.677802    1.462008
  C    2.304755   -0.816815    0.005555
  H    1.629929    0.693490   -1.381810
  H    2.450658    1.335602    0.021995
  H    1.620147   -1.599392   -0.327535
  H    2.452509   -0.943400    1.078510
  H    3.260403   -0.980076   -0.488947
Rotational constants (GHz):  9.7558600  1.6507700  1.5767200
Vibrational harmonic frequencies (cm-1):
  i562.0913      73.8010      104.3953
  186.2191      287.4678      331.3547
  405.5346      511.1169      751.8703
  778.0722      831.7734      910.0045
  916.1050      1020.5371     1084.7473
  1100.0459      1161.1626     1227.6226
  1282.3915      1349.3941     1378.4853
  1387.8755      1419.4059     1431.7026
  1494.8319      1505.1729     1507.9344
  1608.4022      3026.6769     3057.5631
  3069.7405      3096.9442     3109.1804
  3129.7829      3145.5523     3145.9763
Zero-point correction (Hartree): 0.115797

TS.C3H7CHO2a.ringclose.pp
~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -307.48143119
Electronic state : 1-A
Cartesian coordinates (Angs):
 C -0.695703 -0.105975 -0.283013
 O -1.881311 -0.501130 -0.114597
 O -2.362328 0.859902 0.146406
 C 0.422303 -0.823869 0.362404
 H -0.531140 0.739828 -0.947349
 C 1.787154 -0.504520 -0.238860
 H 0.385384 -0.536127 1.421362
 H 0.172843 -1.888348 0.342068
 C 2.247358 0.911129 0.089191
 H 2.511784 -1.224635 0.139753
 H 1.747060 -0.647950 -1.320596
 H 2.352999 1.040136 1.166723
 H 1.534799 1.658362 -0.262041
 H 3.208701 1.127968 -0.372717
Rotational constants (GHz): 8.5821400 1.7435800 1.5397400
Vibrational harmonic frequencies (cm-1):
 i565.5649 57.3437 115.5823
 188.8056 269.6013 343.4173
 390.4651 512.3372 712.3460
 805.6384 830.6099 899.3268
 933.2632 1015.3747 1089.7033
 1111.7630 1140.0230 1236.3257
 1288.4276 1349.0967 1375.8047
 1393.1806 1419.6297 1430.2147
 1496.2385 1507.1490 1510.1181
 1606.0551 3028.0275 3063.8310
 3069.9536 3086.1150 3108.7241
 3133.0800 3145.9904 3155.3435
Zero-point correction (Hartree): 0.115774

TS.C3H7CHO2a.ringclose.pt
~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -307.48199608
Electronic state : 1-A
Cartesian coordinates (Angs):
  C   -0.890518    0.217587   -0.203025
  O   -1.892408   -0.519647   -0.411080
  O   -2.744305    0.304773    0.454241
  C    0.415856   -0.373782    0.143080
  H   -1.013907    1.293224   -0.313793
  C    1.611549    0.480246   -0.263394
  H    0.387653   -0.493180    1.235803
  H    0.455364   -1.387403   -0.262802
  C    2.924828   -0.137438    0.195918
  H    1.616257    0.601577   -1.347876
  H    1.499171    1.478831    0.163306
  H    3.059146   -1.130166   -0.234458
  H    2.946469   -0.239031    1.281402
  H    3.773264    0.475454   -0.102348
Rotational constants (GHz):  15.6160500  1.3541000  1.3316500
Vibrational harmonic frequencies (cm-1):
  i564.9088      77.4619      86.6772
  160.1725      250.1667      353.8085
  420.8005      470.7639      720.2729
  790.4823      832.0151      904.0933
  932.6047      1059.4974     1080.5703
  1121.0970      1159.5885     1245.3226
  1284.2898      1328.8929     1378.8574
  1399.9439      1419.7685     1432.0628

```

|           |           |           |
|-----------|-----------|-----------|
| 1496.7240 | 1505.2009 | 1511.7064 |
| 1607.5683 | 3015.4751 | 3062.7885 |
| 3067.2849 | 3088.0293 | 3105.0361 |
| 3133.3667 | 3145.8368 | 3151.2662 |

Zero-point correction (Hartree): 0.115730

#####  
E-(iC3H7)CHOO  
#####

Population analysis as 298K (%)  
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)

| Compound     | Qtot      | Erel | Erel2 | n*Q*MB    | %    |
|--------------|-----------|------|-------|-----------|------|
| iC3H7CHO2a.m | 4.169e+39 | 0.00 | 0.00  | 8.338e+39 | 71.7 |
| iC3H7CHO2a.p | 6.010e+39 | 0.36 | 0.36  | 3.285e+39 | 28.3 |
| Total        |           |      |       | 1.162e+40 | 100  |

iC3H7CHO2a.m  
~~~~~  
E (CCSD(T)/Aug-CC-pVTZ) (Hartree): -307.07212719
E (CCSD/Aug-CC-pVTZ) (Hartree): -307.01560303
T1 diagnostic: 0.028644
E (MP2/Aug-CC-pVTZ) (Hartree): -306.97408624
E (MP3/Aug-CC-pVTZ) (Hartree): -307.00267445
E (RHF/Aug-CC-pVTZ) (Hartree): -305.79932025
E (RM062X/Aug-CC-pVTZ) (Hartree): -307.51392051
Electronic state : 1-A
Cartesian coordinates (Angs):

C	-0.451505	-0.460847	0.353614
O	-1.321322	0.287587	-0.113021
O	-2.607045	-0.176424	-0.168824
C	0.966028	-0.021968	0.427888
H	-0.785176	-1.444075	0.682243
C	1.835942	-1.040606	-0.321943
C	1.170377	1.396890	-0.082410
H	1.235397	-0.075155	1.489192
H	1.608185	-1.020301	-1.387575
H	1.678626	-2.054301	0.045182
H	2.886952	-0.789009	-0.191072
H	0.559162	2.111192	0.465424
H	0.901886	1.464556	-1.136332
H	2.216851	1.676975	0.024803

Rotational constants (GHz): 7.2015700 2.1060500 1.7645200
Vibrational harmonic frequencies (cm-1):

92.9167	196.4211	202.4685
226.9421	271.7561	338.5909
443.6600	449.9325	612.4572
850.8171	934.4358	943.0167
968.0989	980.2483	991.6915
1122.6943	1159.1462	1210.9917
1306.2381	1355.7340	1391.6941
1408.7207	1428.8072	1489.8859
1494.7259	1507.5107	1515.4263
1663.6011	3031.8321	3067.0628
3074.5320	3140.8103	3146.3605
3149.6163	3154.0867	3155.9754

Zero-point correction (Hartree): 0.117278

iC3H7CHO2a.p
~~~~~  
E (RM062X/Aug-CC-pVTZ) (Hartree): -307.51329147  
Electronic state : 1-A  
Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.461448  | -0.000371 | 0.279024  |
| O | 1.478313  | 0.000055  | -0.428641 |
| O | 2.695348  | -0.000109 | 0.193460  |
| C | -0.887468 | -0.000026 | -0.340141 |
| H | 0.617586  | -0.000837 | 1.358019  |
| C | -1.640471 | -1.262583 | 0.091895  |
| C | -1.639750 | 1.262954  | 0.092033  |
| H | -0.751784 | 0.000037  | -1.421639 |
| H | -1.747989 | -1.292698 | 1.177215  |
| H | -1.123896 | -2.165482 | -0.228716 |
| H | -2.638295 | -1.260200 | -0.344643 |
| H | -1.122716 | 2.165564  | -0.228641 |
| H | -1.747110 | 1.293116  | 1.177368  |
| H | -2.637633 | 1.261098  | -0.344375 |

Rotational constants (GHz): 7.5007200 1.9208700 1.6607300  
Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| 66.1594   | 191.2034  | 210.8061  |
| 222.8955  | 279.7851  | 320.7729  |
| 424.4977  | 482.5595  | 535.7381  |
| 874.4516  | 940.2854  | 941.7673  |
| 964.4342  | 973.7375  | 998.4812  |
| 1126.9792 | 1189.6829 | 1212.6207 |
| 1324.9702 | 1336.3154 | 1388.7803 |
| 1400.9854 | 1424.7258 | 1490.4244 |
| 1494.3648 | 1507.1554 | 1516.1146 |
| 1668.4877 | 3063.3674 | 3063.7559 |
| 3101.4606 | 3134.2152 | 3138.8483 |
| 3142.9943 | 3149.5317 | 3150.0010 |

Zero-point correction (Hartree): 0.117219

Population analysis as 298K (%)  
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)

| Compound                  | Qtot      | Erel | Erel2 | n*Q*MB    | %    |
|---------------------------|-----------|------|-------|-----------|------|
| TS.iC3H7CHO2a.ringclose.p | 5.024e+39 | 0.08 | 0.08  | 8.799e+39 | 36.1 |
| TS.iC3H7CHO2a.ringclose.c | 4.239e+39 | 0.00 | 0.00  | 8.477e+39 | 34.8 |

```

TS.iC3H7CHO2a.ringclose.m 5.014e+39 0.20 0.20 7.117e+39 29.2
Total 2.439e+40 100

TS.iC3H7CHO2a.ringclose.c
~~~~~
E (CCSD(T)/Aug-CC-pVTZ) (Hartree): -307.04672225
E (CCSD/Aug-CC-pVTZ) (Hartree): -306.98856754
T1 diagnostic: 0.032547
E (MP2/Aug-CC-pVTZ) (Hartree): -306.94446593
E (MP3/Aug-CC-pVTZ) (Hartree): -306.97306323
E (RHF/Aug-CC-pVTZ) (Hartree): -305.77208574
E (RM062X/Aug-CC-pVTZ) (Hartree): -307.48425038
Electronic state : 1-A
Cartesian coordinates (Angs):
C 0.451602 -0.520909 0.115005
O 1.479480 -0.428882 -0.610362
O 2.259739 0.185378 0.473385
C -0.856149 -0.036073 -0.371657
H 0.561514 -0.951346 1.109722
H -0.844105 -0.105569 -1.461334
C -2.018877 -0.811226 0.232921
C -0.898171 1.459029 0.015195
H -1.997911 -0.742996 1.321585
H -1.991339 -1.863618 -0.045879
H -2.963740 -0.392399 -0.109530
H -0.046536 1.992679 -0.401076
H -0.880388 1.573497 1.098807
H -1.821671 1.892854 -0.365261
Rotational constants (GHz): 6.8203100 2.2354900 1.9220500
Vibrational harmonic frequencies (cm-1):
i551.8523 84.7404 146.1384
206.9650 226.7165 307.8846
333.0016 519.8631 566.1588
821.1711 836.4661 887.7904
943.5073 979.1326 1001.2832
1121.9363 1179.4419 1197.0368
1294.1348 1334.2529 1383.7569
1397.6993 1424.7223 1488.9260
1489.7805 1505.3475 1512.7488
1603.9863 3065.5214 3069.5970
3081.6788 3135.8901 3138.6084
3145.9487 3148.1290 3161.8978
Zero-point correction (Hartree): 0.115598

TS.iC3H7CHO2a.ringclose.m
~~~~~
E (RM062X/Aug-CC-pVTZ) (Hartree): -307.48378574
Electronic state : 1-A
Cartesian coordinates (Angs):
C 0.510712 -0.459443 -0.126608
O 1.375508 0.388724 -0.477159
O 2.417513 -0.279274 0.318736
C -0.827252 -0.047116 0.358406
H 0.762630 -1.514437 -0.217623
H -0.726405 -0.164090 1.448752
C -1.144411 1.409507 0.043273
C -1.900108 -1.023374 -0.125318
H -1.217365 1.557585 -1.034290
H -0.373222 2.073988 0.425360
H -2.098553 1.682966 0.489762
H -1.640060 -2.054840 0.110389
H -2.033232 -0.939354 -1.204024
H -2.851600 -0.794864 0.350541
Rotational constants (GHz): 6.9364700 2.2195500 1.8335100
Vibrational harmonic frequencies (cm-1):
i557.8967 59.4190 184.6705
203.3330 235.8509 282.8298
342.7675 525.4512 622.8160
746.4019 832.5961 903.1773
931.8071 980.4285 999.4264
1101.6128 1168.4674 1210.0761
1289.2033 1348.1342 1381.0066
1406.9602 1427.3000 1490.5034
1496.6220 1509.6094 1513.3021
1597.9046 2993.7254 3068.3896
3075.3969 3138.6800 3145.1143
3149.4543 3152.8634 3164.2645
Zero-point correction (Hartree): 0.115457

TS.iC3H7CHO2a.ringclose.p
~~~~~
E (RM062X/Aug-CC-pVTZ) (Hartree): -307.48431306
Electronic state : 1-A
Cartesian coordinates (Angs):
C 0.531474 -0.031152 0.662282
O 1.241944 -0.748838 -0.094422
O 2.178424 0.358918 -0.349169
C -0.933337 0.051165 0.480182
H 1.032400 0.539414 1.441430
H -1.387196 0.142521 1.469526
C -1.159202 1.381607 -0.275428
C -1.504553 -1.132446 -0.287240
H -0.667384 1.342752 -1.246297
H -0.764514 2.232966 0.276236
H -2.229133 1.521585 -0.421030
H -1.317516 -2.072652 0.228976
H -1.055653 -1.193656 -1.277271
H -2.580238 -1.008611 -0.401622
Rotational constants (GHz): 5.9086900 2.5861100 2.0957100
Vibrational harmonic frequencies (cm-1):
i549.8296 58.0109 166.4112
200.4526 244.8574 267.7246

```

```

355.3774 562.5985 633.1736
807.9360 831.9319 881.7267
945.9883 981.9285 998.8038
1108.1160 1128.5545 1198.1705
1290.9912 1375.1410 1385.2348
1405.6953 1423.4027 1488.2053
1490.3987 1503.1403 1514.4814
1594.9330 3070.0450 3072.6071
3075.1216 3149.4487 3151.7122
3152.5714 3153.1052 3156.2659
Zero-point correction (Hartree): 0.115786

```

Population analysis as 298K (%)

Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)

| Compound                 | Qtot      | Erel | Erel2 | n*Q*MB    | %   |
|--------------------------|-----------|------|-------|-----------|-----|
| TS.iC3H7CHO2a.13Hshift.p | 5.581e+39 | 0.00 | 0.00  | 1.116e+40 | 100 |
| Total                    |           |      |       | 1.116e+40 | 100 |

```

TS.iC3H7CHO2a.13Hshift.p
~~~~~
E (CCSD(T)/Aug-CC-pVTZ) (Hartree): -307.02268505
E (CCSD/Aug-CC-pVTZ) (Hartree): -306.96492377
  T1 diagnostic: 0.020423
E (MP2/Aug-CC-pVTZ) (Hartree): -306.92870650
E (MP3/Aug-CC-pVTZ) (Hartree): -306.95457472
E (RHF/Aug-CC-pVTZ) (Hartree): -305.73852835
E (UM062X/Aug-CC-pVTZ) (Hartree): -307.46340471
Electronic state : 1-A
Cartesian coordinates (Angs):
  C      -0.500089      -0.366496      0.340961
  O      -1.269824      0.464152     -0.197161
  O      -2.534708     -0.228952     -0.104116
  H      -1.651217     -1.060417      0.453996
  C       0.948640     -0.046016      0.435786
  H       1.174906     -0.122075      1.505042
  C       1.721393     -1.165602     -0.277450
  C       1.316621      1.337745     -0.085014
  H       1.510831     -1.148923     -1.346680
  H       1.452777     -2.145518      0.112305
  H       2.790037     -1.012483     -0.137921
  H       0.763061      2.119621      0.431671
  H       1.094528      1.414982     -1.149241
  H       2.381940      1.515426      0.055345
Rotational constants (GHz):      7.0153900      2.1691600      1.7898400
Vibrational harmonic frequencies (cm-1):
  i1720.0202      67.1576      169.1288
    204.2583      220.2193      268.4049
    341.5212      470.6148      519.2800
    660.8193      886.1564      906.3534
    934.0508      979.2870      1051.1484
   1098.2339     1150.8993     1181.8186
   1218.6974     1293.4588     1370.8418
   1403.6558     1423.3881     1489.4703
   1494.1824     1506.6553     1513.6589
   1583.7342     2144.8939     3043.6688
   3069.6082     3070.9552     3141.6388
   3144.4665     3150.0228     3155.1513
Zero-point correction (Hartree): 0.112376

```

```

#####
E-(tC4H9)CHOO
#####

```

Population analysis as 298K (%)

Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)

| Compound   | Qtot      | Erel | Erel2 | n*Q*MB    | %   |
|------------|-----------|------|-------|-----------|-----|
| tC4H9CHO2a | 2.204e+40 | 0.00 | 0.00  | 2.204e+40 | 100 |
| Total      |           |      |       | 2.204e+40 | 100 |

```

tC4H9CHO2a
~~~~~
E (CCSD(T)/Aug-CC-pVTZ) (Hartree): -346.31858490
E (CCSD/Aug-CC-pVTZ) (Hartree): -346.25353491
 T1 diagnostic: 0.026673
E (MP2/Aug-CC-pVTZ) (Hartree): -346.20404049
E (MP3/Aug-CC-pVTZ) (Hartree): -346.24028324
E (RHF/Aug-CC-pVTZ) (Hartree): -344.84726418
E (RM062X/Aug-CC-pVTZ) (Hartree): -346.82428033
Electronic state : 1-A
Cartesian coordinates (Angs):
 C 0.622306 -0.483075 -0.001016
 O 1.572810 0.310043 -0.000069
 O 2.841843 -0.205926 -0.000249
 C -0.788052 -0.000786 -0.000131
 H 0.874706 -1.543640 -0.001852
 C -0.857077 -1.521886 -0.001715
 C -1.465274 -0.578703 -1.252543
 C -1.462226 -0.575795 1.255402
 H -0.371803 1.936606 -0.884172
 H -0.370029 1.938579 0.878818
 H -1.901435 1.833309 -0.001006
 H -1.401188 -1.667250 -1.272168
 H -1.008562 -0.187042 -2.160942
 H -2.519362 -0.300690 -1.248071
 H -1.002794 -0.182433 2.161683
 H -1.398651 -1.664329 1.277129
 H -2.516177 -0.297211 1.253146
Rotational constants (GHz): 4.3887700 1.5872900 1.5634500

```

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| 75.0277   | 191.6239  | 194.2685  |
| 217.6971  | 281.3063  | 281.5230  |
| 331.2522  | 342.5914  | 355.1545  |
| 457.5295  | 468.8302  | 567.2023  |
| 798.6399  | 935.4400  | 947.9488  |
| 955.1149  | 969.0596  | 972.5532  |
| 984.8689  | 1057.6287 | 1068.1914 |
| 1235.9574 | 1246.6989 | 1314.9920 |
| 1379.0517 | 1397.3873 | 1407.0366 |
| 1435.5417 | 1480.8754 | 1488.0179 |
| 1488.2077 | 1504.0511 | 1507.9699 |
| 1524.9153 | 1662.9076 | 3058.7361 |
| 3060.2349 | 3069.2604 | 3132.6528 |
| 3135.1230 | 3140.3216 | 3140.5807 |
| 3142.0965 | 3145.1970 | 3148.0605 |

Zero-point correction (Hartree): 0.145118

Population analysis as 298K (%)

Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)

| Compound           | Qtot      | Erel | Erel2 | n*Q*MB    | %   |
|--------------------|-----------|------|-------|-----------|-----|
| TS.tC4H9CHO2s.isom | 2.698e+40 | 0.00 | 0.00  | 5.397e+40 | 100 |
| Total              |           |      |       | 5.397e+40 | 100 |

TS.tC4H9CHO2s.isom

~~~~~

E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -346.26483731  
E(CCSD/Aug-CC-pVTZ) (Hartree): -346.20708463  
T1 diagnostic: 0.021322  
E(MP2/Aug-CC-pVTZ) (Hartree): -346.14170467  
E(MP3/Aug-CC-pVTZ) (Hartree): -346.19386085  
E(PMP2/Aug-CC-pVTZ) (Hartree): -346.16598420  
E(PMP3/Aug-CC-pVTZ) (Hartree): -346.21801434  
E(PUHF/Aug-CC-pVTZ) (Hartree): -344.86521048  
E(UHF/Aug-CC-pVTZ) (Hartree): -344.84074069  
E(UM062X/Aug-CC-pVTZ) (Hartree): -346.77631923  
Electronic state : 1-A  
Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.486757  | -0.394008 | 0.755705  |
| O | 1.645039  | -0.612508 | 0.004660  |
| C | -0.733807 | 0.027596  | 0.010421  |
| H | 0.476672  | -0.925700 | 1.697630  |
| C | -0.439804 | 1.305462  | -0.783373 |
| C | -1.159275 | -1.090822 | -0.956657 |
| C | -1.842558 | 0.283558  | 1.030647  |
| H | 0.355157  | 1.142428  | -1.510556 |
| H | -0.132092 | 2.112559  | -0.118690 |
| H | -1.337024 | 1.615996  | -1.320353 |
| H | -1.395648 | -2.006470 | -0.413568 |
| H | -0.365798 | -1.306857 | -1.671630 |
| H | -2.046667 | -0.780459 | -1.510691 |
| H | -1.561076 | 1.080493  | 1.719571  |
| H | -2.057002 | -0.615415 | 1.610739  |
| H | -2.757305 | 0.580715  | 0.517326  |
| O | 2.474074  | 0.401507  | 0.077811  |

Rotational constants (GHz): 4.2151800 1.7573100 1.7120300

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i334.8937 | 55.6802   | 160.5460  |
| 209.8035  | 226.7728  | 277.9532  |
| 284.1537  | 306.2184  | 347.5315  |
| 386.6655  | 417.6629  | 512.5223  |
| 629.4783  | 767.9924  | 930.4560  |
| 948.3826  | 959.9057  | 968.2606  |
| 1037.3257 | 1051.2873 | 1083.8796 |
| 1207.7057 | 1228.0104 | 1243.5651 |
| 1287.3106 | 1359.0674 | 1392.9860 |
| 1399.8997 | 1430.5350 | 1479.3228 |
| 1487.6781 | 1488.7949 | 1503.8975 |
| 1505.0953 | 1523.4333 | 3053.2473 |
| 3055.0631 | 3060.2955 | 3124.6271 |
| 3127.5958 | 3131.4570 | 3134.4933 |
| 3137.6496 | 3141.1040 | 3202.9108 |

Zero-point correction (Hartree): 0.141857

Population analysis as 298K (%)

Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)

| Compound                | Qtot      | Erel | Erel2 | n*Q*MB    | %   |
|-------------------------|-----------|------|-------|-----------|-----|
| TS.tC4H9CHO2a.ringclose | 2.196e+40 | 0.00 | 0.00  | 4.393e+40 | 100 |
| Total                   |           |      |       | 4.393e+40 | 100 |

TS.tC4H9CHO2a.ringclose

~~~~~

E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -346.29342533  
E(CCSD/Aug-CC-pVTZ) (Hartree): -346.22672108  
T1 diagnostic: 0.029909  
E(MP2/Aug-CC-pVTZ) (Hartree): -346.17481332  
E(MP3/Aug-CC-pVTZ) (Hartree): -346.21100437  
E(RHF/Aug-CC-pVTZ) (Hartree): -344.81973392  
E(RM062X/Aug-CC-pVTZ) (Hartree): -346.79515580  
Electronic state : 1-A  
Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.632083  | -0.124931 | -0.566937 |
| O | 1.545520  | 0.685384  | -0.249560 |
| O | 2.478366  | -0.410686 | 0.060689  |
| C | -0.736448 | -0.008402 | -0.007260 |
| H | 0.879738  | -0.929563 | -1.258357 |
| C | -1.029452 | 1.414073  | 0.461110  |
| C | -1.761414 | -0.495744 | -1.029836 |



```

C -0.698214 -0.970559 1.205298
H -1.021764 2.112038 -0.375996
H -0.293652 1.745219 1.191136
H -2.016589 1.442168 0.922187
H -1.525168 -1.502382 -1.376703
H -1.803598 0.167725 -1.893783
H -2.749704 -0.519685 -0.571291
H 0.062219 -0.659686 1.919764
H -0.484273 -1.992989 0.895393
H -1.677625 -0.947046 1.684361
Rotational constants (GHz): 4.1439500 1.8077200 1.7307100
Vibrational harmonic frequencies (cm-1):
i537.9881 64.9178 147.6939
193.0944 241.7166 264.3497
273.5863 338.7748 354.5148
374.3315 570.7850 589.2753
748.9893 833.4165 855.2570
957.9831 967.6406 975.9895
990.6466 1039.2962 1064.2748
1219.1827 1257.6477 1318.3654
1377.3457 1393.9411 1405.8068
1431.8582 1477.4912 1486.5125
1489.0935 1502.3671 1507.0333
1521.5353 1593.3537 3059.6046
3061.2320 3067.8283 3132.9488
3136.4722 3138.7490 3139.4470
3140.5160 3152.2069 3155.2212
Zero-point correction (Hartree): 0.143553

```

```

Population analysis as 298K (%)
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)
Compound Qtot Erel Erel2 n*Q*MB %

TS.tC4H9CHO2a.13Hshift 3.082e+40 0.00 0.00 3.082e+40 100
Total 3.082e+40 100

```

```

TS.tC4H9CHO2a.13Hshift
~~~~~
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -346.26937986
E(CCSD/Aug-CC-pVTZ) (Hartree): -346.20297403
T1 diagnostic: 0.019250
E(MP2/Aug-CC-pVTZ) (Hartree): -346.15897534
E(MP3/Aug-CC-pVTZ) (Hartree): -346.19221979
E(RHF/Aug-CC-pVTZ) (Hartree): -344.78624738
E(UM062X/Aug-CC-pVTZ) (Hartree): -346.77386103
Electronic state : 1-A
Cartesian coordinates (Angs):
C      0.661003      -0.393428      -0.000028
O      1.531507      0.508439      -0.000011
O      2.745234      -0.278090      -0.000014
H      1.758844      -1.178206      -0.000028
C      -0.782797      -0.016961      -0.000010
C      -0.997967      1.494082      -0.000128
C      -1.395300      -0.658997      -1.254003
C      -1.395166      -0.658763      1.254175
H      -0.554047      1.954074      -0.882335
H      -0.554028      1.954205      0.882002
H      -2.066867      1.709060      -0.000132
H      -1.230099      -1.735664      -1.263605
H      -0.969180      -0.233128      -2.162085
H      -2.469205      -0.470413      -1.256406
H      -0.968943      -0.232716      2.162126
H      -1.229969      -1.735428      1.263966
H      -2.469069      -0.470172      1.256656
Rotational constants (GHz): 4.2741800 1.6374900 1.5963100
Vibrational harmonic frequencies (cm-1):
i1721.0653 52.3622 160.5528
201.8172 210.9621 272.5887
283.5996 331.3769 347.8357
357.2569 490.9008 524.3271
612.3280 832.5032 903.8595
959.8176 960.8320 972.4587
1022.9149 1040.6234 1101.6319
1158.1203 1235.0503 1255.0158
1323.8918 1393.1676 1403.9601
1430.1593 1479.0477 1488.5539
1489.6392 1503.2353 1504.9628
1522.8885 1583.2054 2133.5501
3060.5255 3060.6730 3064.5378
3135.0181 3135.9122 3138.7522
3142.4395 3143.6315 3144.6193
Zero-point correction (Hartree): 0.140269

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#####
(CH3)2COO
#####

```

```

Population analysis as 298K (%)
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)
Compound Qtot Erel Erel2 n*Q*MB %
-----
diMeCO2 3.903e+38 0.00 0.00 3.903e+38 100
Total 3.903e+38 100

```

```

diMeCO2
~~~~~
E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -267.60813750
E(CCSD/Aug-CC-pVDZ) (Hartree): -267.57299562
E(MP2/Aug-CC-pVDZ) (Hartree): -267.52824241

```

```

E(MP3/Aug-CC-pVDZ) (Hartree): -267.55502588
E(PMP2/Aug-CC-pVDZ) (Hartree): -267.52824241
E(PMP3/Aug-CC-pVDZ) (Hartree): -267.55502588
E(PUHF/Aug-CC-pVDZ) (Hartree): -266.70129407
E(RHF/Aug-CC-pVDZ) (Hartree): -266.70129407
E(UHF/Aug-CC-pVDZ) (Hartree): -266.70129407
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -267.84500760
E(CCSD/Aug-CC-pVTZ) (Hartree): -267.79627238
E(MP2/Aug-CC-pVTZ) (Hartree): -267.76526815
E(MP3/Aug-CC-pVTZ) (Hartree): -267.78404314
E(PMP2/Aug-CC-pVTZ) (Hartree): -267.76526815
E(PMP3/Aug-CC-pVTZ) (Hartree): -267.78404314
E(PUHF/Aug-CC-pVTZ) (Hartree): -266.76658097
E(RHF/Aug-CC-pVTZ) (Hartree): -266.76658097
E(UHF/Aug-CC-pVTZ) (Hartree): -266.76658097
E(CCSD(T)/Aug-CC-pVQZ) (Hartree): -267.91298307
E(CCSD/Aug-CC-pVQZ) (Hartree): -267.86112935
T1 diagnostic: 0.029500
E(MP2/Aug-CC-pVQZ) (Hartree): -267.84075451
E(MP3/Aug-CC-pVQZ) (Hartree): -267.85113872
E(RHF/Aug-CC-pVQZ) (Hartree): -266.78298926
E(UM062X/Aug-CC-pVTZ) (Hartree): -268.22346276
Electronic state : 1-A
Cartesian coordinates (Angs):
 C -0.371023 0.018452 -0.000027
 O 0.558598 -0.817600 -0.000024
 O 1.839016 -0.328582 0.000021
 C -0.054287 1.456041 -0.000027
 C -1.752455 -0.524533 0.000001
 H 0.577833 1.668419 -0.865255
 H 0.577302 1.668413 0.865633
 H -0.955030 2.062056 -0.000193
 H -1.739071 -1.610392 -0.000038
 H -2.287778 -0.159336 -0.877977
 H -2.287572 -0.159472 0.878172
Rotational constants (GHz): 8.9511500 4.3735300 3.0465400
Vibrational harmonic frequencies (cm-1):
 161.9172 207.9974 291.0495
 329.8759 366.4004 493.5235
 609.7892 827.3699 925.0897
 952.8532 989.4152 1085.5994
 1102.0385 1316.0865 1393.9572
 1411.7332 1442.1692 1466.9932
 1474.3193 1486.7857 1653.9848
 3059.3253 3065.3016 3110.0182
 3121.6808 3182.2182 3183.6520
Zero-point correction (Hartree): 0.088190

Population analysis as 298K (%)
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)
Compound Qtot Erel Erel2 n*Q*MB %

TS.diMeCO2.isom 4.956e+38 0.00 0.00 9.913e+38 100
Total 9.913e+38 100

TS.diMeCO2.isom
~~~~~
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -267.78556120
E(CCSD/Aug-CC-pVTZ) (Hartree): -267.74425739
T1 diagnostic: 0.024775
E(MP2/Aug-CC-pVTZ) (Hartree): -267.69640255
E(MP3/Aug-CC-pVTZ) (Hartree): -267.73133960
E(PMP2/Aug-CC-pVTZ) (Hartree): -267.72029545
E(PMP3/Aug-CC-pVTZ) (Hartree): -267.75511071
E(PUHF/Aug-CC-pVTZ) (Hartree): -266.77970063
E(UHF/Aug-CC-pVTZ) (Hartree): -266.75562543
E(UM062X/Aug-CC-pVTZ) (Hartree): -268.13198734
E(UM062X/Aug-CC-pVTZ) (Hartree): -268.16825267
Electronic state : 1-A
Cartesian coordinates (Angs):
  C -0.442119 0.000012 -0.331191
  O 0.941415 -0.000066 -0.611985
  C -0.962960 1.309603 0.124108
  C -0.963130 -1.309505 0.124124
  H -0.598744 1.536823 1.133234
  H -2.050727 1.296407 0.149132
  H -0.630047 2.109440 -0.536778
  H -0.598958 -1.536758 1.133257
  H -0.630299 -2.109389 -0.536748
  H -2.050895 -1.296184 0.149131
  O 1.654701 -0.000059 0.487801
Rotational constants (GHz): 6.9309700 4.7376500 3.3623300
Vibrational harmonic frequencies (cm-1):
  i205.7831 157.8320 160.0238
  227.7967 337.5068 380.4836
  563.3004 786.8929 925.7269
  978.8307 979.4352 1088.0265
  1202.1731 1235.5949 1298.0466
  1403.8080 1408.6064 1462.8788
  1478.1633 1478.6889 1490.6895
  3017.0215 3019.4137 3106.1471
  3107.0397 3153.4287 3156.9765
Zero-point correction (Hartree): 0.085669

Population analysis as 298K (%)
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)
Compound Qtot Erel Erel2 n*Q*MB %
-----
TS.diMeCO2.ringclose 2.906e+38 0.00 0.00 5.811e+38 100
Total 5.811e+38 100

```

```

TS.diMeCO2.ringclose
~~~~~
E (CCSD(T)/Aug-CC-pVDZ) (Hartree): -267.57495605
E (CCSD/Aug-CC-pVDZ) (Hartree): -267.53890892
 T1 diagnostic: 0.036259
E (MP2/Aug-CC-pVDZ) (Hartree): -267.49028828
E (MP3/Aug-CC-pVDZ) (Hartree): -267.51880414
E (RHF/Aug-CC-pVDZ) (Hartree): -266.67067274
E (CCSD(T)/Aug-CC-pVTZ) (Hartree): -267.81074125
E (CCSD/Aug-CC-pVTZ) (Hartree): -267.76133516
 T1 diagnostic: 0.034142
E (MP2/Aug-CC-pVTZ) (Hartree): -267.72650856
E (MP3/Aug-CC-pVTZ) (Hartree): -267.74725742
E (RHF/Aug-CC-pVTZ) (Hartree): -266.73529977
E (CCSD(T)/Aug-CC-pVQZ) (Hartree): -267.87808689
E (CCSD/Aug-CC-pVQZ) (Hartree): -267.82559361
 T1 diagnostic: 0.033269
E (MP2/Aug-CC-pVQZ) (Hartree): -267.80142355
E (MP3/Aug-CC-pVQZ) (Hartree): -267.81384327
E (RHF/Aug-CC-pVQZ) (Hartree): -266.75131657
E (RM062X/Aug-CC-pVTZ) (Hartree): -268.18587953
Electronic state : 1-A
Cartesian coordinates (Angs):
 C 0.276871 0.014079 -0.133273
 O -0.624310 -0.781141 -0.543012
 O -1.602043 -0.298570 0.451520
 C 0.116460 1.489595 -0.079565
 C 1.584519 -0.600303 0.201864
 H -0.855639 1.780536 -0.458400
 H 0.935916 1.938421 -0.648243
 H 0.213106 1.830965 0.951973
 H 1.767608 -1.455313 -0.446946
 H 1.478059 -0.988205 1.220402
 H 2.404672 0.111060 0.178995
Rotational constants (GHz): 7.5118100 4.9016300 3.4517400
Vibrational harmonic frequencies (cm-1):
 i525.6732 151.8074 241.4630
 342.8285 396.6357 409.6866
 492.2899 795.7689 831.9238
 901.0121 976.6161 1061.5109
 1082.4080 1276.1206 1379.6895
 1402.2399 1441.9423 1453.2832
 1466.6160 1482.6182 1608.1167
 3050.0807 3054.2249 3115.3790
 3128.2888 3185.5422 3209.5611
Zero-point correction (Hartree): 0.086428

Population analysis as 298K (%)
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)
Compound Qtot Erel Erel2 n*Q*MB %

TS.diMeCO2.14Hshift 2.542e+38 0.00 0.00 5.084e+38 100
Total 5.084e+38 100

TS.diMeCO2.14Hshift
~~~~~
E (CCSD(T)/Aug-CC-pVDZ) (Hartree): -267.57868962
E (CCSD/Aug-CC-pVDZ) (Hartree): -267.54130689
  T1 diagnostic: 0.026368
E (MP2/Aug-CC-pVDZ) (Hartree): -267.50537290
E (MP3/Aug-CC-pVDZ) (Hartree): -267.52630341
E (RHF/Aug-CC-pVDZ) (Hartree): -266.65599751
E (CCSD(T)/Aug-CC-pVTZ) (Hartree): -267.81616846
E (CCSD/Aug-CC-pVTZ) (Hartree): -267.76484428
  T1 diagnostic: 0.024972
E (MP2/Aug-CC-pVTZ) (Hartree): -267.74299454
E (MP3/Aug-CC-pVTZ) (Hartree): -267.75555360
E (RHF/Aug-CC-pVTZ) (Hartree): -266.72071529
E (CCSD(T)/Aug-CC-pVQZ) (Hartree): -267.88436394
E (CCSD/Aug-CC-pVQZ) (Hartree): -267.82982275
  T1 diagnostic: 0.024392
E (MP2/Aug-CC-pVQZ) (Hartree): -267.81869500
E (MP3/Aug-CC-pVQZ) (Hartree): -267.82276401
E (RHF/Aug-CC-pVQZ) (Hartree): -266.73694829
E (RM062X/Aug-CC-pVTZ) (Hartree): -268.19575670
Electronic state : 1-A
Cartesian coordinates (Angs):
  C     -0.403187      0.075375      0.069477
  O      0.462908     -0.878805      0.054743
  O      1.749346     -0.360213     -0.053552
  C      0.127055      1.377611     -0.013644
  C     -1.820165     -0.354047     -0.027392
  H      0.747321      1.676272      0.830131
  H     -0.550455      2.146769     -0.357171
  H      1.218039      0.827135     -0.503225
  H     -2.308403      0.211025     -0.821040
  H     -2.337657     -0.123705      0.903873
  H     -1.889088     -1.418994     -0.232742
Rotational constants (GHz):      9.8122500      4.4433200      3.1654700
Vibrational harmonic frequencies (cm-1):
  i1600.2526      112.4382      279.5460
  365.3802      522.9059      546.1012
  670.8825      745.1908      856.5118
  947.0117      988.2277      999.6685
 1057.6460     1096.8264     1337.0938
 1380.9006     1420.9607     1464.8077
 1475.1740     1530.9559     1569.7390
 1889.9489     3074.7348     3116.8576
 3139.2765     3175.9222     3228.4203
Zero-point correction (Hartree): 0.084277

```

Population analysis as 298K (%)  
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)

| Compound            | Qtot      | Erel | Erel2 | n*Q*MB    | %   |
|---------------------|-----------|------|-------|-----------|-----|
| TS.diMeCO2.14Hshift | 2.542e+38 | 0.00 | 0.00  | 5.084e+38 | 100 |
| Total               |           |      |       | 5.084e+38 | 100 |

TS.diMeCO2.14Hshift  
~~~~~  
E(CCSD(T)/Aug-CC-pVDZ) (Hartree): -267.57868962
E(CCSD/Aug-CC-pVDZ) (Hartree): -267.54130689
Tl diagnostic: 0.026368
E(MP2/Aug-CC-pVDZ) (Hartree): -267.50537290
E(MP3/Aug-CC-pVDZ) (Hartree): -267.52630341
E(RHF/Aug-CC-pVDZ) (Hartree): -266.65599751
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -267.81616846
E(CCSD/Aug-CC-pVTZ) (Hartree): -267.76484428
Tl diagnostic: 0.024972
E(MP2/Aug-CC-pVTZ) (Hartree): -267.74299454
E(MP3/Aug-CC-pVTZ) (Hartree): -267.7555360
E(RHF/Aug-CC-pVTZ) (Hartree): -266.72071529
E(CCSD(T)/Aug-CC-pVQZ) (Hartree): -267.88436394
E(CCSD/Aug-CC-pVQZ) (Hartree): -267.82982275
Tl diagnostic: 0.024392
E(MP2/Aug-CC-pVQZ) (Hartree): -267.81869500
E(MP3/Aug-CC-pVQZ) (Hartree): -267.82276401
E(RHF/Aug-CC-pVQZ) (Hartree): -266.73694829
E(RM062X/Aug-CC-pVTZ) (Hartree): -268.19575670
Electronic state : 1-A
Cartesian coordinates (Angs):
C -0.403187 0.075375 0.069477
O 0.462908 -0.878805 0.054743
O 1.749346 -0.360213 -0.053552
C 0.127055 1.377611 -0.013644
C -1.820165 -0.354047 -0.027392
H 0.747321 1.676272 0.830131
H -0.550455 2.146769 -0.357171
H 1.218039 0.827135 -0.503225
H -2.308403 0.211025 -0.821040
H -2.337657 -0.123705 0.903873
H -1.889088 -1.418994 -0.232742
Rotational constants (GHz): 9.8122500 4.4433200 3.1654700
Vibrational harmonic frequencies (cm-1):
i1600.2526 112.4382 279.5460
365.3802 522.9059 546.1012
670.8825 745.1908 856.5118
947.0117 988.2277 999.6685
1057.6460 1096.8264 1337.0938
1380.9006 1420.9607 1464.8077
1475.1740 1530.9559 1569.7390
1889.9489 3074.7348 3116.8576
3139.2765 3175.9222 3228.4203
Zero-point correction (Hartree): 0.084277

E-(CH3)(C2H5)COO
#####

Population analysis as 298K (%)
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)

Compound	Qtot	Erel	Erel2	n*Q*MB	%
CH3_C2H5_COO.c	3.595e+39	0.00	0.00	3.595e+39	57.9
CH3_C2H5_COO.p	4.281e+39	0.70	0.70	1.309e+39	21.1
CH3_C2H5_COO.t	4.275e+39	0.70	0.70	1.307e+39	21
Total				6.210e+39	100

CH3_C2H5_COO.c
~~~~~  
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -307.08780693  
E(CCSD/Aug-CC-pVTZ) (Hartree): -307.03135032  
Tl diagnostic: 0.027445  
E(MP2/Aug-CC-pVTZ) (Hartree): -306.99047584  
E(MP3/Aug-CC-pVTZ) (Hartree): -307.01901915  
E(RHF/Aug-CC-pVTZ) (Hartree): -305.81513629  
E(RM062X/Aug-CC-pVTZ) (Hartree): -307.53134221  
Electronic state : 1-A  
Cartesian coordinates (Angs):  
C 0.165767 0.350629 -0.000113  
O 0.479833 -0.858422 0.000046  
O 1.820437 -1.159498 0.000026  
C 1.222878 1.375847 -0.000067  
H 1.867111 1.205990 -0.865495  
H 1.866609 1.206577 0.865848  
H 0.803580 2.377473 -0.000511  
C -1.288247 0.676005 0.000120  
C -2.211571 -0.531230 -0.000099  
H -1.469255 1.316086 0.869357  
H -1.469624 1.316901 -0.868368  
H -2.042120 -1.150556 0.878329  
H -2.041846 -1.150498 -0.878522  
H -3.249585 -0.206116 -0.000257  
Rotational constants (GHz): 5.9485000 2.6681300 1.9056700  
Vibrational harmonic frequencies (cm-1):  
97.6539 190.0470 213.1410  
225.4136 289.6452 336.2052  
448.3801 495.1192 617.4933  
759.8615 803.8719 950.3711  
975.7987 1012.0773 1040.1430

|           |           |           |
|-----------|-----------|-----------|
| 1113.1655 | 1123.9644 | 1248.5358 |
| 1284.8834 | 1387.6940 | 1403.8605 |
| 1424.1421 | 1443.3698 | 1458.8818 |
| 1483.7292 | 1499.7967 | 1508.8594 |
| 1651.4923 | 3047.2445 | 3061.2674 |
| 3072.1832 | 3084.2815 | 3112.4987 |
| 3157.7490 | 3160.1310 | 3180.8150 |

Zero-point correction (Hartree): 0.117015

CH3\_C2H5\_COO.p  
~~~~~  
E(RM062X/Aug-CC-pVTZ) (Hartree): -307.53046474
Electronic state : 1-A
Cartesian coordinates (Angs):

C	-0.118207	0.053191	0.235526
O	-0.982826	-0.829541	0.042104
O	-2.238269	-0.410257	-0.314013
C	-0.484139	1.470983	0.080301
H	-1.341099	1.672872	0.726853
H	-0.857701	1.624999	-0.934732
H	0.352954	2.125891	0.302553
C	1.248794	-0.419160	0.588185
C	2.246066	-0.106891	-0.532935
H	1.556371	0.088669	1.505166
H	1.207511	-1.488505	0.785213
H	2.284544	0.961413	-0.742175
H	1.967147	-0.624914	-1.448933
H	3.243947	-0.430780	-0.245130

Rotational constants (GHz): 6.9759000 2.2912500 1.9515000
Vibrational harmonic frequencies (cm-1):

75.1746	167.3705	212.3743
243.5456	332.4057	350.8176
397.1129	540.1087	614.0372
796.4259	807.4762	944.2018
990.2177	1002.3397	1029.8968
1091.9679	1122.4306	1269.6545
1311.3482	1361.0339	1392.3160
1414.0384	1441.9363	1479.7482
1481.5226	1504.0771	1513.7103
1646.1586	3059.2969	3068.3663
3075.4767	3109.8638	3133.6943
3153.0484	3155.8338	3180.4326

Zero-point correction (Hartree): 0.117256

CH3_C2H5_COO.t
~~~~~  
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -307.08757923  
E(CCSD/Aug-CC-pVTZ) (Hartree): -307.03081414  
T1 diagnostic: 0.028099  
E(MP2/Aug-CC-pVTZ) (Hartree): -306.99024509  
E(MP3/Aug-CC-pVTZ) (Hartree): -307.01820920  
E(RHF/Aug-CC-pVTZ) (Hartree): -305.81379637  
E(RM062X/Aug-CC-pVTZ) (Hartree): -307.53046473  
Electronic state : 1-A  
Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.118212  | 0.053242  | 0.235651  |
| O | 0.982768  | -0.829530 | 0.042166  |
| O | 2.238231  | -0.410282 | -0.314069 |
| C | 0.484028  | 1.470988  | 0.080288  |
| H | 0.857553  | 1.624943  | -0.934799 |
| H | 1.341152  | 1.672980  | 0.726608  |
| H | -0.353018 | 2.125942  | 0.302527  |
| C | -1.248762 | -0.419112 | 0.588290  |
| C | -2.245903 | -0.106987 | -0.533053 |
| H | -1.207498 | -1.488427 | 0.785418  |
| H | -1.556531 | 0.088910  | 1.505099  |
| H | -1.966768 | -0.624907 | -1.449043 |
| H | -2.284572 | 0.961314  | -0.742283 |
| H | -3.243757 | -0.431050 | -0.245358 |

Rotational constants (GHz): 6.9754200 2.2913800 1.9516300  
Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| 75.2624   | 167.4231  | 212.3723  |
| 243.6093  | 332.3860  | 350.8353  |
| 397.1229  | 540.1429  | 614.0402  |
| 796.4291  | 807.5420  | 944.1347  |
| 990.1982  | 1002.2899 | 1029.8899 |
| 1091.9241 | 1122.4291 | 1269.6377 |
| 1311.3498 | 1361.0098 | 1392.3614 |
| 1414.0242 | 1441.8961 | 1479.7675 |
| 1481.5429 | 1504.0701 | 1513.7275 |
| 1646.2130 | 3059.2038 | 3068.3797 |
| 3075.4828 | 3109.6551 | 3133.7616 |
| 3153.0824 | 3155.8514 | 3180.4991 |

Zero-point correction (Hartree): 0.117256

Population analysis as 298K (%)  
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)  
Compound Qtot Erel Erel2 n\*Q\*MB %  
-----  
TS.C2H5\_CH3\_COO.isom.t 5.470e+39 0.00 0.00 1.094e+40 100  
Total 1.094e+40 100

TS.C2H5\_CH3\_COO.isom.t  
~~~~~  
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -307.02756767
E(CCSD/Aug-CC-pVTZ) (Hartree): -306.97827175
T1 diagnostic: 0.023108
E(MP2/Aug-CC-pVTZ) (Hartree): -306.92061252
E(MP3/Aug-CC-pVTZ) (Hartree): -306.96510934
E(PMP2/Aug-CC-pVTZ) (Hartree): -306.94458524
E(PMP3/Aug-CC-pVTZ) (Hartree): -306.98895926

```

E(PUHF/Aug-CC-pVTZ) (Hartree): -305.82597615
E(UHF/Aug-CC-pVTZ) (Hartree): -305.80181962
E(UM062X/Aug-CC-pVTZ) (Hartree): -307.47512710
Electronic state : 1-A
Cartesian coordinates (Angs):
C      0.108994      0.225448     -0.359238
O      1.396190     -0.307242     -0.586536
O      1.987080     -0.636114      0.536664
C      0.119803      1.628913      0.114710
C     -0.899190     -0.800647      0.015553
H      0.428472      1.678913      1.166464
H     -0.869252      2.073694      0.028592
H      0.826019      2.220175     -0.466939
C     -2.320859     -0.256326      0.078907
H     -0.834333     -1.621066     -0.702831
H     -0.615146     -1.226261      0.987266
H     -2.602881      0.209441     -0.865481
H     -2.425780      0.487145      0.868144
H     -3.025750     -1.059515      0.284163
Rotational constants (GHz):      6.0918000      2.4132200      1.9487600
Vibrational harmonic frequencies (cm-1):
1202.2863      72.8607      133.3182
193.0871      257.6745      274.5989
370.5836      400.4749      600.8603
760.3845      774.1396      949.4953
968.2232      1012.8489      1074.5237
1104.2248      1183.9435      1212.8065
1268.6251      1305.4293      1373.1260
1405.0501      1415.2272      1470.3942
1474.1705      1483.1671      1504.0968
1511.4071      3002.9251      3012.0305
3069.2766      3077.2329      3110.3104
3137.0588      3147.5234      3158.6652
Zero-point correction (Hartree): 0.114523

Population analysis as 298K (%)
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)
Compound      Qtot      Erel      Erel2      n*Q*MB      %
-----
TS.CH3_C2H5_COO.ringclose.c 5.609e+39 0.00 0.00 1.122e+40 78.3
TS.CH3_C2H5_COO.ringclose.t 2.130e+39 0.19 0.19 3.101e+39 21.7
Total      1.432e+40 100

TS.CH3_C2H5_COO.ringclose.c
~~~~~
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -307.05338215
E(CCSD/Aug-CC-pVTZ) (Hartree): -306.99611252
T1 diagnostic: 0.031037
E(MP2/Aug-CC-pVTZ) (Hartree): -306.95146567
E(MP3/Aug-CC-pVTZ) (Hartree): -306.98185758
E(RHF/Aug-CC-pVTZ) (Hartree): -305.78313310
E(UM062X/Aug-CC-pVTZ) (Hartree): -307.49322104
Electronic state : 1-A
Cartesian coordinates (Angs):
C     -0.251025      0.257299     -0.100564
O     -0.418922     -0.940191     -0.487353
O     -1.551797     -1.151239      0.440444
C     -1.314053      1.296704     -0.165160
C      1.116659      0.649162      0.339940
H     -2.217138      0.885241     -0.599203
H     -0.930002      2.143259     -0.740407
H     -1.537871      1.658167      0.838997
C      2.218475     -0.312314     -0.080082
H      1.310592      1.677897      0.033867
H      1.033366      0.679778      1.435108
H      2.289710     -0.373073     -1.164698
H      2.020354     -1.311636      0.298913
H      3.176405      0.026700      0.307890
Rotational constants (GHz):      5.6683700      2.7820600      2.0822800
Vibrational harmonic frequencies (cm-1):
1529.2746      39.9939      195.5108
222.8116      242.6457      346.1106
400.2104      427.5597      557.1729
742.6143      787.0731      839.8035
956.8387      977.1766      1016.1391
1108.9174      1110.9300      1221.3576
1270.1526      1388.1677      1417.2375
1418.3474      1436.1304      1447.0290
1466.4988      1501.7035      1508.6525
1600.8893      3024.7148      3055.9527
3083.9344      3103.8955      3121.0518
3153.9050      3168.2338      3208.0339
Zero-point correction (Hartree): 0.115201

TS.CH3_C2H5_COO.ringclose.t
~~~~~
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -307.05273503
E(CCSD/Aug-CC-pVTZ) (Hartree): -306.99537843
T1 diagnostic: 0.031441
E(MP2/Aug-CC-pVTZ) (Hartree): -306.95084383
E(MP3/Aug-CC-pVTZ) (Hartree): -306.98115058
E(RHF/Aug-CC-pVTZ) (Hartree): -305.78174060
E(UM062X/Aug-CC-pVTZ) (Hartree): -307.49307407
Electronic state : 1-A
Cartesian coordinates (Angs):
C     -0.222528     -0.022574     -0.169997
O     -1.215933     -0.731046     -0.526208
O     -2.090534     -0.173640      0.523482
C     -0.256058      1.460640     -0.118434
C      1.030259     -0.777749      0.102703
H     -1.223270      1.821692     -0.445639

```

H	0.560620	1.843971	-0.736384
H	-0.075097	1.801848	0.901890
C	2.331437	0.007919	0.100965
H	0.840025	-1.220298	1.089705
H	1.044865	-1.626654	-0.584517
H	2.307429	0.821898	0.823792
H	2.537955	0.431441	-0.881146
H	3.160540	-0.645828	0.362683
Rotational constants (GHz): 7.0683400 2.3855900 1.9831500			
Vibrational harmonic frequencies (cm-1):			
i506.6540	92.8035		234.6967
252.9398	266.1637		371.3945
397.2978	468.0287		478.5927
733.5821	763.2838		843.7562
952.9738	971.5698		1025.7993
1106.0517	1110.2543		1266.2245
1278.1393	1363.6331		1402.4687
1422.0423	1435.0714		1442.2538
1463.2658	1506.8586		1510.5992
1596.4834	3029.7946		3054.6917
3076.3443	3092.7554		3115.8667
3145.6485	3153.8065		3209.4198
Zero-point correction (Hartree): 0.115354			
Population analysis as 298K (%)			
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)			
Compound	Qtot	Erel	Erel2 n*Q*MB %

TS.CH3_C2H5_COO.14Hshift.p	3.575e+39	0.13	0.13 5.698e+39 42.9
TS.CH3_C2H5_COO.14Hshift.c	2.269e+39	0.00	0.00 4.538e+39 34.1
TS.CH3_C2H5_COO.14Hshift.t	3.576e+39	0.50	0.50 3.059e+39 23
Total			1.329e+40 100
TS.CH3_C2H5_COO.14Hshift.c			
~~			
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -307.05848986			
E(CCSD/Aug-CC-pVTZ) (Hartree): -306.99932071			
T1 diagnostic: 0.022893			
E(MP2/Aug-CC-pVTZ) (Hartree): -306.96769410			
E(MP3/Aug-CC-pVTZ) (Hartree): -306.98981387			
E(RHF/Aug-CC-pVTZ) (Hartree): -305.76829060			
E(UM062X/Aug-CC-pVTZ) (Hartree): -307.50299970			
Electronic state : 1-A			
Cartesian coordinates (Angs):			
C	-0.146974	0.389046	-0.102813
O	-0.471275	-0.857788	-0.130575
O	-1.842832	-1.005265	0.062815
C	-1.214244	1.287960	0.093880
C	1.314064	0.681967	-0.088649
H	-1.953786	1.306059	-0.705074
H	-0.949678	2.265580	0.472041
H	-1.893271	0.264876	0.576003
C	2.210390	-0.532321	0.107496
H	1.546132	1.194107	-1.026211
H	1.470986	1.426820	0.695177
H	2.070611	-1.255104	-0.693475
H	1.988450	-1.032471	1.048146
H	3.253991	-0.225363	0.115984
Rotational constants (GHz): 6.6242400 2.6304100 1.9558100			
Vibrational harmonic frequencies (cm-1):			
i1591.5019	72.4703		201.2825
223.7428	289.2340		443.0283
532.9395	556.7713		653.2635
741.8003	759.8951		877.2902
923.2437	996.5905		1013.2684
1047.4412	1102.3967		1121.0136
1285.6669	1299.5046		1353.5871
1415.4672	1421.8922		1458.0116
1500.3353	1505.2761		1527.4418
1559.7042	1888.6982		3062.0882
3083.9609	3091.6123		3118.1566
3157.7771	3159.5121		3228.6381
Zero-point correction (Hartree): 0.113163			
TS.CH3_C2H5_COO.14Hshift.p			
~~			
E(UM062X/Aug-CC-pVTZ) (Hartree): -307.50286253			
Electronic state : 1-A			
Cartesian coordinates (Angs):			
C	-0.084051	0.063254	0.153095
O	-0.941777	-0.878592	-0.041156
O	-2.211509	-0.342363	-0.235388
C	-0.601013	1.373402	0.112568
C	1.273988	-0.380026	0.567210
H	-0.998985	1.683970	-0.852340
H	-0.011843	2.131424	0.610682
H	-1.784394	0.836355	0.328357
C	2.326546	-0.018120	-0.483276
H	1.503842	0.124414	1.508347
H	1.253054	-1.452443	0.754545
H	2.344125	1.056371	-0.658251
H	2.113846	-0.514560	-1.428714
H	3.313823	-0.328950	-0.147862
Rotational constants (GHz): 7.8023700 2.2512200 1.9430700			
Vibrational harmonic frequencies (cm-1):			
i1588.5854	44.9258		180.6228
216.7087	348.6966		388.4067
519.8224	552.5650		717.0770
741.1295	786.0772		878.4765
932.0377	990.8829		1012.3208
1034.9013	1088.2074		1116.5719

```

1268.4796      1326.8688      1348.8809
1401.4142      1420.5985      1476.5254
1501.9896      1504.5918      1531.1486
1563.6030      1890.1342      3071.5296
3076.2714      3116.1198      3128.6814
3152.6268      3155.1722      3222.6791
Zero-point correction (Hartree): 0.113240

```

TS.CH3_C2H5_COO.14Hshift.t

~~~~~

E(UM062X/Aug-CC-pVTZ) (Hartree): -307.50243734

Electronic state : 1-A

Cartesian coordinates (Angs):

```

C      -0.097488      0.060965      -0.332204
O      -0.944096      -0.876401      -0.072312
O      -2.142005      -0.334442      0.384100
C      -0.565828      1.372529      -0.120687
C      1.295064      -0.403082      -0.581598
H      -1.388931      1.670848      -0.768521
H      0.187311      2.136549      0.012037
H      -1.489719      0.844873      0.655815
C      2.217916      0.000568      0.573594
H      1.279817      -1.485870      -0.696631
H      1.649245      0.039577      -1.512823
H      1.874404      -0.438025      1.508906
H      2.249147      1.082042      0.693056
H      3.229551      -0.349127      0.379214

```

Rotational constants (GHz): 7.3304500 2.3322800 2.0353600

Vibrational harmonic frequencies (cm-1):

```

i1598.1722      41.8343      182.7024
229.8494      346.9815      393.2748
540.2866      583.4190      658.4196
745.4165      801.9974      887.1264
926.6407      987.3947      1022.4471
1037.1120      1095.1289      1107.4111
1271.5785      1325.8442      1346.1443
1395.7790      1422.3787      1485.2243
1500.8852      1507.2487      1531.0030
1562.1633      1890.2217      3077.3663
3084.9785      3115.6930      3133.1048
3156.1839      3157.2116      3227.4131

```

Zero-point correction (Hartree): 0.113402

```

#####
E- (CH3) (iC3H7) COO
#####

```

Population analysis as 298K (%)

Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)

| Compound        | Qtot      | Erel | Erel2 | n*Q*MB    | %    |
|-----------------|-----------|------|-------|-----------|------|
| CH3_ic3H7_COO.p | 2.152e+40 | 0.00 | 0.00  | 4.305e+40 | 69.9 |
| CH3_ic3H7_COO.c | 2.665e+40 | 0.22 | 0.22  | 1.853e+40 | 30.1 |
| Total           |           |      |       | 6.158e+40 | 100  |

CH3\_ic3H7\_COO.c

~~~~~

E(RM062X/Aug-CC-pVTZ) (Hartree): -346.83955725

Electronic state : 1-A

Cartesian coordinates (Angs):

```

C      -0.370860      -0.000177      0.028203
O      -1.287037      0.001560      -0.823658
O      -2.577795      0.000654      -0.360761
C      -0.721193      -0.002757      1.458713
H      -1.358054      -0.868928      1.652462
H      -1.359341      0.861867      1.655102
H      0.159740      -0.003134      2.092625
C      1.026635      0.000883      -0.502829
H      0.944056      0.002944      -1.589853
C      1.764343      1.263481      -0.048342
C      1.764559      -1.263129      -0.053030
H      1.859627      1.291028      1.037619
H      1.247692      2.165475      -0.372791
H      2.767930      1.270604      -0.471719
H      1.247734      -2.164056      -0.380167
H      1.860464      -1.294333      1.032788
H      2.767904      -1.268993      -0.476999

```

Rotational constants (GHz): 4.4909400 1.6133500 1.6093400

Vibrational harmonic frequencies (cm-1):

```

62.2640      147.7844      208.4747
236.3395      261.9841      267.2220
305.4760      353.5946      369.4652
495.2145      575.2015      603.5377
785.7017      902.2118      942.7889
961.0587      978.0836      1022.1021
1033.9870      1087.5534      1129.6923
1194.7057      1315.9498      1343.0936
1361.5175      1391.7224      1400.9466
1425.7827      1441.3874      1478.2774
1490.5754      1495.9371      1508.4190
1520.1160      1640.8001      3060.5086
3065.4398      3066.1146      3097.4629
3108.9845      3136.2851      3141.3372
3145.6606      3146.2234      3187.5380

```

Zero-point correction (Hartree): 0.145562

CH3_ic3H7_COO.p

~~~~~

E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -346.33239342

E(CCSD/Aug-CC-pVTZ) (Hartree): -346.26744742

T1 diagnostic: 0.025958



```

E(MP2/Aug-CC-pVTZ) (Hartree): -346.21802261
E(MP3/Aug-CC-pVTZ) (Hartree): -346.25469877
E(RHF/Aug-CC-pVTZ) (Hartree): -344.86170911
E(RM062X/Aug-CC-pVTZ) (Hartree): -346.83988244
Electronic state : 1-A
Cartesian coordinates (Angs):
  C      -0.371767      0.200172     -0.197054
  O      -0.984386     -0.817632      0.190819
  O      -2.338621     -0.701883      0.388068
  C      -1.121698      1.446289     -0.432839
  H      -1.615516      1.738074      0.496885
  H      -1.936787      1.224426     -1.124970
  H      -0.476966      2.235641     -0.807091
  C       1.109152      0.082788     -0.373460
  H       1.325599      0.500621     -1.362101
  C       1.802873      0.968166      0.673006
  C       1.604608     -1.354500     -0.302811
  H       1.607188      0.585042      1.674706
  H       1.462291      2.001533      0.626326
  H       2.878727      0.955312      0.505851
  H       1.110409     -1.984656     -1.039595
  H       1.412123     -1.777978      0.682128
  H       2.677974     -1.379381     -0.484283
Rotational constants (GHz):   4.0633500   1.9490400   1.4981000
Vibrational harmonic frequencies (cm-1):
  70.9410      163.9138      213.1773
  231.0921      247.5368      275.9793
  326.0779      354.7060      390.1463
  477.0614      553.2129      622.9472
  779.1167      908.1902      937.2110
  951.8039      980.6176     1006.2006
 1043.0803     1126.4092     1145.3872
 1181.8528     1260.9908     1316.0813
 1382.9877     1395.4651     1410.4268
 1426.5213     1443.3003     1477.7934
 1490.2747     1494.5823     1507.6505
 1520.5542     1642.6681     3043.8867
 3060.9067     3067.1883     3074.4772
 3111.3553     3141.0783     3146.9963
 3148.4767     3153.8950     3182.0698
Zero-point correction (Hartree): 0.145544

Population analysis as 298K (%)
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)
Compound      Qtot      Erel      Erel2  n*Q*MB      %
-----
TS.CH3_iC3H7_COO.ringclose.t 2.250e+40 0.00   0.00  4.500e+40 64
TS.CH3_iC3H7_COO.ringclose.p 1.269e+40 0.16   0.16  1.935e+40 27.5
TS.CH3_iC3H7_COO.ringclose.m 2.292e+40 1.21   1.21  5.939e+39 8.45
Total              7.028e+40 100

TS.CH3_iC3H7_COO.ringclose.m
~~~~~
E(UM062X/Aug-CC-pVTZ) (Hartree): -346.80117970
Electronic state : 1-A
Cartesian coordinates (Angs):
 C 0.445555 0.112820 0.119002
 O 1.171338 -0.916510 0.297677
 O 2.251774 -0.404727 -0.568378
 C 0.907761 1.484176 0.455010
 C -0.947659 -0.147780 -0.362392
 H 1.902072 1.443040 0.882425
 H 0.181245 1.933502 1.137672
 H 0.932684 2.103796 -0.442027
 H -0.764707 -0.386417 -1.420838
 C -1.535135 -1.398556 0.299662
 C -1.892311 1.043771 -0.279667
 H -0.868716 -2.250740 0.201545
 H -1.715333 -1.216231 1.359512
 H -2.487740 -1.640147 -0.168120
 H -2.105095 1.300529 0.758922
 H -1.490860 1.925164 -0.776486
 H -2.837715 0.790815 -0.756688
Rotational constants (GHz): 4.0189700 2.0417900 1.5239500
Vibrational harmonic frequencies (cm-1):
 i495.8558 36.3311 188.9801
 246.2122 262.6066 276.9427
 294.9496 357.2070 397.9729
 448.4742 491.1357 577.2937
 718.7739 842.0900 906.8352
 932.6738 971.4786 984.5238
 993.1817 1096.5522 1157.8292
1187.6902 1254.5108 1298.2419
1353.1992 1399.3008 1406.5934
1428.1651 1440.3665 1462.9971
1494.2652 1498.3594 1512.8390
1517.0868 1582.8654 3002.0917
3055.0668 3068.4026 3073.3339
3118.7105 3137.1103 3142.6733
3150.6169 3173.5669 3209.2040
Zero-point correction (Hartree): 0.143865

TS.CH3_iC3H7_COO.ringclose.p
~~~~~
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -346.29827353
E(CCSD/Aug-CC-pVTZ) (Hartree): -346.23238905
T1 diagnostic: 0.029319
E(MP2/Aug-CC-pVTZ) (Hartree): -346.17937142
E(MP3/Aug-CC-pVTZ) (Hartree): -346.21788561
E(RHF/Aug-CC-pVTZ) (Hartree): -344.82917492
E(UM062X/Aug-CC-pVTZ) (Hartree): -346.80298928

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Electronic state : 1-A  
 Cartesian coordinates (Angs):  

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.398291 | 0.286603  | -0.260669 |
| O | -1.321986 | -0.323083 | -0.888228 |
| O | -2.141317 | -0.504910 | 0.328037  |
| C | -0.628616 | 1.530906  | 0.516349  |
| C | 0.965683  | -0.297067 | -0.406815 |
| H | -1.671655 | 1.816635  | 0.463614  |
| H | 0.033360  | 2.307301  | 0.123515  |
| H | -0.353467 | 1.372225  | 1.560466  |
| H | 0.998838  | -0.732503 | -1.408558 |
| C | 2.119991  | 0.670000  | -0.191290 |
| C | 1.003467  | -1.462951 | 0.606164  |
| H | 2.106187  | 1.079674  | 0.819072  |
| H | 2.096986  | 1.498028  | -0.899041 |
| H | 3.063636  | 0.142082  | -0.321088 |
| H | 0.157927  | -2.131297 | 0.459744  |
| H | 0.967107  | -1.080335 | 1.626337  |
| H | 1.934101  | -2.012809 | 0.475027  |

 Rotational constants (GHz): 4.0187500 2.0548400 1.6694400  
 Vibrational harmonic frequencies (cm-1):  

|           |           |           |
|-----------|-----------|-----------|
| i488.4483 | 78.5827   | 182.3546  |
| 217.7637  | 249.4449  | 271.3216  |
| 290.9836  | 340.2688  | 393.9090  |
| 469.6720  | 497.8175  | 583.4407  |
| 744.0803  | 836.3301  | 901.7622  |
| 940.0864  | 961.2804  | 982.4711  |
| 1002.8174 | 1104.6624 | 1127.1190 |
| 1189.9472 | 1281.9944 | 1289.7984 |
| 1368.7854 | 1396.2306 | 1408.1186 |
| 1426.0102 | 1439.7336 | 1462.4963 |
| 1489.4200 | 1492.4745 | 1508.1127 |
| 1514.7493 | 1591.9042 | 3055.9109 |
| 3066.1755 | 3067.1087 | 3072.8424 |
| 3114.0513 | 3137.4323 | 3141.8768 |
| 3143.4099 | 3162.8982 | 3211.9726 |

 Zero-point correction (Hartree): 0.144002

TS.CH3\_iC3H7\_COO.ringclose.t  
 ~~~~~  
 E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -346.29886886
 E(CCSD/Aug-CC-pVTZ) (Hartree): -346.23312523
 T1 diagnostic: 0.029025
 E(MP2/Aug-CC-pVTZ) (Hartree): -346.18007014
 E(MP3/Aug-CC-pVTZ) (Hartree): -346.21860016
 E(RHF/Aug-CC-pVTZ) (Hartree): -344.83079860
 E(UM062X/Aug-CC-pVTZ) (Hartree): -346.80314221
 Electronic state : 1-A
 Cartesian coordinates (Angs):

C	-0.439652	0.194912	-0.311596
O	-0.767228	-1.025170	-0.451943
O	-1.782606	-0.957581	0.621625
C	-1.399893	1.321045	-0.438459
C	1.006059	0.478603	-0.081180
H	-2.393738	0.955101	-0.664490
H	-1.020609	1.996740	-1.210809
H	-1.429477	1.884238	0.495631
H	1.201214	1.523994	-0.323019
C	1.220955	0.265287	1.431481
C	1.909710	-0.443855	-0.895294
H	0.964273	-0.758996	1.698019
H	0.603956	0.936505	2.026519
H	2.268465	0.448362	1.666746
H	1.754386	-0.317182	-1.965826
H	1.716073	-1.483912	-0.640098
H	2.951044	-0.218791	-0.669838

 Rotational constants (GHz): 3.6877200 1.9764300 1.9095300
 Vibrational harmonic frequencies (cm-1):

i492.5294	55.1795	164.1755
203.6057	229.5860	239.7618
265.3429	320.3654	387.7510
439.9259	565.5182	593.6641
757.9123	841.3139	898.3334
942.4331	974.0490	984.6184
1010.1027	1113.2495	1118.0345
1182.0925	1229.2070	1319.5871
1382.4542	1397.2809	1410.1443
1426.9202	1443.2249	1463.7225
1487.1568	1490.0386	1502.9475
1518.6584	1594.8152	3048.8287
3069.4376	3073.6048	3089.4540
3113.1728	3145.0948	3149.2480
3153.0740	3158.6778	3210.3854

 Zero-point correction (Hartree): 0.143899

Population analysis as 298K (%)
 Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)

Compound	Qtot	Erel	Erel2	n*Q*MB	%
TS.CH3_iC3H7_COO.14Hshift.c	2.084e+40	0.00	0.00	4.169e+40	45.5
TS.CH3_iC3H7_COO.14Hshift.m	1.779e+40	0.01	0.01	3.504e+40	38.2
TS.CH3_iC3H7_COO.14Hshift.p	1.839e+40	0.53	0.53	1.498e+40	16.3
Total				9.170e+40	100

TS.CH3_iC3H7_COO.14Hshift.c
 ~~~~~  
 E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -346.30367497  
 E(CCSD/Aug-CC-pVTZ) (Hartree): -346.23599365  
 T1 diagnostic: 0.021831  
 E(MP2/Aug-CC-pVTZ) (Hartree): -346.19590825  
 E(MP3/Aug-CC-pVTZ) (Hartree): -346.22597223

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E(RHF/Aug-CC-pVTZ) (Hartree): -344.81558107
E(UM062X/Aug-CC-pVTZ) (Hartree): -346.81189859
Electronic state : 1-A
Cartesian coordinates (Angs):
  C    0.342456   -0.125661   -0.015064
  O    1.256490   0.274487   -0.831473
  O    2.514821   0.161793   -0.245289
  C    0.807988   -0.589327   1.231643
  C   -1.058792   0.170397   -0.439612
  H    1.424549   -1.485789   1.182761
  H    0.091474   -0.594638   2.041410
  H    1.917028   0.079247   0.987549
  H   -1.000554   0.562543   -1.455944
  C   -1.910415   -1.098275   -0.420289
  C   -1.648450   1.249726   0.475200
  H   -1.973863   -1.499327   0.591521
  H   -1.494336   -1.868419   -1.068131
  H   -2.919696   -0.870089   -0.760914
  H   -1.042919   2.154492   0.462665
  H   -1.714854   0.891098   1.502406
  H   -2.654042   1.499486   0.139507
Rotational constants (GHz):    4.7140700    1.6413300    1.6083900
Vibrational harmonic frequencies (cm-1):
  i1589.1898           40.1626           162.5414
    223.7970           239.4735           271.3764
    314.2121           369.8260           484.8878
    544.2124           570.3643           688.2421
    743.7414           880.1438           902.7569
    940.7453           948.4346           981.0493
   1005.8560          1045.6007          1100.0856
   1131.4703          1197.5033          1325.9908
   1338.0561          1343.3950          1397.5421
   1405.3802          1430.3942          1489.7823
   1492.4199          1504.0659          1506.9960
   1532.8680          1560.1396          1889.3888
   3066.0748          3068.1813          3089.2603
   3116.2140          3138.7434          3143.8107
   3145.0415          3149.2409          3226.2629
Zero-point correction (Hartree): 0.141578

TS.CH3_iC3H7_COO.14Hshift.m
~~~~~
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -346.30328370
E(CCSD/Aug-CC-pVTZ) (Hartree): -346.23573221
 T1 diagnostic: 0.021626
E(MP2/Aug-CC-pVTZ) (Hartree): -346.19549429
E(MP3/Aug-CC-pVTZ) (Hartree): -346.22581599
E(RHF/Aug-CC-pVTZ) (Hartree): -344.81567170
E(UM062X/Aug-CC-pVTZ) (Hartree): -346.81181142
Electronic state : 1-A
Cartesian coordinates (Angs):
 C 0.350200 0.242504 -0.130208
 O 0.959959 -0.802808 0.311767
 O 2.337498 -0.594263 0.315811
 C 1.181972 1.325264 -0.480587
 C -1.118777 0.101730 -0.369835
 H 1.736169 1.768794 0.345204
 H 0.757493 2.047713 -1.164349
 H 2.167850 0.451024 -0.553003
 H -1.283266 0.509968 -1.371677
 C -1.873852 0.989291 0.628647
 C -1.601814 -1.342058 -0.316970
 H -1.713970 0.631139 1.646036
 H -1.542198 2.024536 0.570852
 H -2.941651 0.952565 0.417895
 H -1.064662 -1.970767 -1.024295
 H -1.457558 -1.759250 0.679032
 H -2.664243 -1.379549 -0.552608
Rotational constants (GHz): 4.3739700 1.9077800 1.5056500
Vibrational harmonic frequencies (cm-1):
 i1588.9840 46.0056 174.2652
 216.5058 226.1186 275.2490
 328.6659 389.1945 479.6274
 531.6244 567.7878 699.4404
 742.9579 861.1122 902.6414
 935.6343 951.3388 981.6949
 1004.9459 1030.4864 1128.0811
 1144.8300 1193.4835 1299.4145
 1316.0163 1353.9301 1396.7988
 1415.8220 1427.9105 1489.7899
 1493.3726 1504.2517 1506.4036
 1528.9304 1556.7405 1888.5432
 3053.8762 3066.7146 3074.2998
 3115.7918 3139.9038 3146.5452
 3150.2706 3153.8501 3222.6112
Zero-point correction (Hartree): 0.141505

TS.CH3_iC3H7_COO.14Hshift.p
~~~~~
E(UM062X/Aug-CC-pVTZ) (Hartree): -346.81115971
Electronic state : 1-A
Cartesian coordinates (Angs):
  C   -0.359094   0.185127   -0.304019
  O   -0.933037   -0.866166   0.173205
  O   -2.275194   -0.607441   0.444007
  C   -1.197771   1.306503   -0.463112
  C    1.134422   0.126419   -0.393623
  H   -2.000027   1.171436   -1.187196
  H   -0.708840   2.268462   -0.526122
  H   -2.012277   0.734841   0.404455
  H    1.400942   0.537271   -1.369907
  C    1.723726   1.043704   0.688299

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C      1.679656      -1.291515      -0.267379
H      1.453097      0.675251      1.677928
H      1.368900      2.067971      0.591884
H      2.809740      1.046808      0.607404
H      1.251755      -1.954738      -1.016840
H      1.456015      -1.705189      0.714842
H      2.760910      -1.274684      -0.395140
Rotational constants (GHz):      4.2801000      1.9526500      1.5428800
Vibrational harmonic frequencies (cm-1):
  11592.1793      39.7623      179.5280
    222.2907      240.1280      272.4397
    342.3282      392.5023      471.4659
    541.2095      608.8227      651.9558
    745.1507      866.3630      893.6572
    940.0295      948.9641      983.1625
   1000.2518      1048.2458      1124.6605
   1141.0853      1191.3902      1302.1027
   1323.7837      1355.6965      1394.1543
   1413.8930      1431.0308      1489.8070
   1493.0561      1503.9563      1510.4830
   1528.8838      1554.1366      1890.0971
   3066.9701      3071.1636      3075.2468
   3116.4671      3142.5256      3149.8286
   3152.0683      3153.1589      3229.6969
Zero-point correction (Hartree): 0.141687

#####
E- (CH3) (tC4H9) COO
#####

Population analysis as 298K (%)
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)
Compound      Qtot      Erel      Erel2      n*Q*MB      %
-----
CH3_tc4H9_COO 9.124e+40 0.00      0.00      9.124e+40 100
Total          9.124e+40 100

CH3_tc4H9_COO
~~~~~
E (CCSD(T)/Aug-CC-pVTZ) (Hartree): -385.57828543
E (CCSD/Aug-CC-pVTZ) (Hartree): -385.50447808
T1 diagnostic: 0.024595
E (MP2/Aug-CC-pVTZ) (Hartree): -385.44754672
E (MP3/Aug-CC-pVTZ) (Hartree): -385.49131407
E (RHF/Aug-CC-pVTZ) (Hartree): -383.90697728
E (RM062X/Aug-CC-pVTZ) (Hartree): -386.14945515
Electronic state : 1-A
Cartesian coordinates (Angs):
C 0.539158 0.190075 -0.000210
O 1.304309 -0.799163 -0.000150
O 2.655419 -0.556110 0.000010
C -0.939981 -0.088761 -0.000032
C 1.132844 1.539878 -0.000149
C -1.215652 -1.590182 0.000295
C -1.549093 0.552978 1.255976
C -1.549687 0.552553 -1.255902
H -0.791541 -2.069640 0.881108
H -0.791751 -2.069988 -0.880433
H -2.293265 -1.752979 0.000441
H -1.390458 1.630595 1.279878
H -1.124014 0.118694 2.160863
H -2.623872 0.370411 1.261183
H -1.125119 0.117945 -2.160875
H -1.391066 1.630154 -1.280341
H -2.624476 0.370029 -1.260502
H 1.796102 1.618157 -0.864570
H 1.795106 1.618443 0.865045
H 0.381002 2.321124 -0.000543
Rotational constants (GHz): 3.0377700 1.5103000 1.3049100
Vibrational harmonic frequencies (cm-1):
 66.0561 146.5057 198.1974
 227.0837 262.3940 266.6766
 298.5566 313.4049 339.8490
 358.6342 372.6277 402.4757
 479.9369 577.9114 583.4912
 747.0821 860.3371 948.4543
 954.5303 964.8041 971.9541
 1007.1902 1033.3839 1060.7447
 1063.8957 1190.2202 1237.9961
 1258.9687 1346.9885 1391.0847
 1397.4973 1408.1656 1435.7921
 1441.7725 1473.0713 1482.2853
 1488.6346 1488.6597 1505.1483
 1508.8538 1529.4311 1628.2750
 3061.0523 3061.3133 3063.1147
 3070.2946 3107.9964 3134.6837
 3135.7660 3140.2229 3141.7222
 3144.2951 3150.2544 3197.0050
Zero-point correction (Hartree): 0.173429

Population analysis as 298K (%)
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)
Compound Qtot Erel Erel2 n*Q*MB %

TS.CH3_tc4H9_COO.ringclose 6.203e+40 0.00 0.00 1.241e+41 100
Total 1.241e+41 100

TS.CH3_tc4H9_COO.ringclose
~~~~~
E (CCSD(T)/Aug-CC-pVTZ) (Hartree): -385.54410726

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E (CCSD/Aug-CC-pVTZ) (Hartree): -385.46945894
  T1 diagnostic: 0.027631
E (MP2/Aug-CC-pVTZ) (Hartree): -385.40874253
E (MP3/Aug-CC-pVTZ) (Hartree): -385.45461538
E (RHF/Aug-CC-pVTZ) (Hartree): -383.87495790
E (RM062X/Aug-CC-pVTZ) (Hartree): -386.11263735
Electronic state : 1-A
Cartesian coordinates (Angs):
  C -0.574075 0.218777 -0.271428
  O -1.271778 -0.779236 -0.642423
  O -2.266999 -0.588833 0.433927
  C 0.872354 -0.057937 0.018984
  C -1.134207 1.593492 -0.190293
  C 1.411977 -1.121885 -0.941809
  C 1.749637 1.190141 -0.013918
  C 0.832353 -0.635792 1.454282
  H 1.418389 -0.756540 -1.969050
  H 0.815529 -2.029665 -0.899767
  H 2.436848 -1.362050 -0.659114
  H 1.404167 1.950607 0.685476
  H 1.787385 1.627166 -1.012424
  H 2.765678 0.914939 0.268321
  H 0.175946 -1.502739 1.500472
  H 0.473966 0.104542 2.169230
  H 1.846206 -0.927500 1.730169
  H -1.055121 1.972029 0.829703
  H -2.176088 1.585190 -0.484915
  H -0.530919 2.247793 -0.825042
Rotational constants (GHz): 2.8577900 1.6738300 1.4517500
Vibrational harmonic frequencies (cm-1):
  i478.0986 56.5159 171.8123
  206.3794 260.5004 269.3309
  273.0816 305.7561 333.3133
  360.4103 370.6658 403.0436
  464.3736 527.0354 592.6554
  686.3637 836.4820 853.0197
  950.9813 967.1022 973.7315
  977.7294 998.8097 1050.3585
  1060.9119 1183.5762 1217.4960
  1265.0380 1335.1926 1394.3048
  1399.4973 1406.6688 1433.4251
  1440.6910 1462.8679 1478.1452
  1486.9439 1493.1220 1501.9918
  1511.0277 1525.6900 1577.3980
  3057.2398 3060.5488 3063.0434
  3068.2265 3118.1703 3131.7514
  3135.4592 3136.4726 3141.8180
  3155.4870 3165.7696 3212.5680
Zero-point correction (Hartree): 0.172024

Population analysis as 298K (%)
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)
Compound Qtot Erel Erel2 n*Q*MB %
-----
TS.CH3_tC4H9_COO.14Hshift 6.925e+40 0.00 0.00 1.385e+41 100
Total 1.385e+41 100

TS.CH3_tC4H9_COO.14Hshift
~~~~~
E (CCSD(T)/Aug-CC-pVTZ) (Hartree): -385.54914587
E (CCSD/Aug-CC-pVTZ) (Hartree): -385.47271840
 T1 diagnostic: 0.020583
E (MP2/Aug-CC-pVTZ) (Hartree): -385.42500739
E (MP3/Aug-CC-pVTZ) (Hartree): -385.46236040
E (RHF/Aug-CC-pVTZ) (Hartree): -383.86086442
E (RM062X/Aug-CC-pVTZ) (Hartree): -386.12140060
Electronic state : 1-A
Cartesian coordinates (Angs):
 C 0.520558 -0.199955 -0.103026
 O 1.280841 0.841559 -0.089348
 O 2.617359 0.470482 0.042235
 C -0.957935 0.061992 -0.004315
 C 1.198314 -1.433493 -0.014133
 C -1.263263 1.556365 -0.093777
 C -1.663045 -0.690342 -1.138948
 C -1.434738 -0.482850 1.351796
 H -0.915719 1.974948 -1.037461
 H -0.789355 2.108549 0.715733
 H -2.341508 1.700899 -0.028168
 H -1.465513 -1.760304 -1.084917
 H -1.332887 -0.327581 -2.112540
 H -2.739190 -0.533014 -1.061615
 H -0.926703 0.020416 2.174147
 H -1.260648 -1.554457 1.438078
 H -2.506035 -0.303435 1.445779
 H 2.220138 -0.758443 0.481149
 H 1.852680 -1.650804 -0.857328
 H 0.619783 -2.283404 0.318459
Rotational constants (GHz): 3.1660900 1.5030000 1.3188500
Vibrational harmonic frequencies (cm-1):
 i1589.3600 41.1344 166.8846
 224.5907 235.1806 277.3618
 295.6807 326.4401 335.8764
 363.1345 406.2058 479.6793
 541.6115 567.6255 655.4125
 746.5751 830.9012 893.0735
 931.9469 956.8838 963.7536
 972.4264 1004.0761 1032.9575
 1054.1251 1067.3826 1235.9023
 1240.3016 1259.2865 1340.0476
 1389.4455 1398.5580 1409.3381

```

|           |           |           |
|-----------|-----------|-----------|
| 1439.1023 | 1480.9141 | 1488.1691 |
| 1488.4357 | 1500.8535 | 1505.3960 |
| 1510.3205 | 1530.0992 | 1546.1506 |
| 1889.7822 | 3060.9885 | 3064.1402 |
| 3070.7658 | 3114.5539 | 3134.2467 |
| 3137.4324 | 3142.0763 | 3143.5057 |
| 3147.0740 | 3151.6528 | 3231.8376 |

Zero-point correction (Hartree): 0.169544

#####  
Z-(C2H5)(CH3)COO  
#####

Population analysis as 298K (%)  
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)  
Compound Qtot Erel Erel2 n\*Q\*MB %  
-----  
C2H5\_CH3\_COO.t 3.946e+39 0.00 0.00 3.946e+39 55.4  
C2H5\_CH3\_COO.p 3.357e+39 0.44 0.44 3.173e+39 44.6  
Total 7.119e+39 100

C2H5\_CH3\_COO.p  
~~~~~  
E(RM062X/Aug-CC-pVTZ) (Hartree): -307.53002821  
Electronic state : 1-A  
Cartesian coordinates (Angs):  
C 0.574484 -0.097757 0.124102  
O 0.589349 1.116371 -0.174222  
O -0.550027 1.850038 0.047494  
C -0.644507 -0.726133 0.677441  
C 1.820717 -0.857345 -0.147139  
C -1.665641 -0.953920 -0.449594  
H -0.375429 -1.666692 1.155923  
H -1.065351 -0.032345 1.405497  
H -1.275933 -1.645348 -1.196424  
H -1.900222 -0.003477 -0.922224  
H -2.577341 -1.379119 -0.035957  
H 2.568397 -0.224119 -0.615325  
H 1.591612 -1.705849 -0.794870  
H 2.209366 -1.263390 0.788340  
Rotational constants (GHz): 3.9369400 3.7166700 2.1784500  
Vibrational harmonic frequencies (cm-1):  
119.9771 166.1772 205.4782  
218.0198 302.3043 344.3617  
373.7525 585.5516 621.5532  
780.8789 820.3026 941.5354  
989.2434 1004.0137 1019.9169  
1100.7138 1118.7958 1263.2281  
1303.2700 1365.7865 1395.6432  
1420.2297 1465.2333 1470.8582  
1476.3430 1500.6197 1517.2337  
1655.0328 3061.7186 3073.1701  
3081.7098 3118.5286 3136.3227  
3149.4187 3172.5034 3180.4569  
Zero-point correction (Hartree): 0.117371

C2H5\_CH3\_COO.t  
~~~~~  
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -307.08680070  
E(CCSD/Aug-CC-pVTZ) (Hartree): -307.02999899  
T1 diagnostic: 0.027961  
E(MP2/Aug-CC-pVTZ) (Hartree): -306.98938365  
E(MP3/Aug-CC-pVTZ) (Hartree): -307.01750903  
E(RHF/Aug-CC-pVTZ) (Hartree): -305.81224000  
E(RM062X/Aug-CC-pVTZ) (Hartree): -307.53022449  
Electronic state : 1-A  
Cartesian coordinates (Angs):  
C -0.176152 0.384123 -0.000010  
O -1.426999 0.330357 -0.000012  
O -2.000966 -0.914470 0.000008  
C 0.600415 -0.872253 0.000004  
C 0.416889 1.745547 0.000003  
C 2.110633 -0.701783 -0.000004  
H 0.233860 -1.450843 0.854935  
H 0.233852 -1.450870 -0.854905  
H 2.456471 -0.163209 0.881875  
H 2.456465 -0.163247 -0.881909  
H 2.592852 -1.676716 0.000016  
H -0.366715 2.497176 -0.000312  
H 1.053384 1.873305 -0.876852  
H 1.052845 1.873501 0.877223  
Rotational constants (GHz): 5.4064300 2.7784700 1.8985900  
Vibrational harmonic frequencies (cm-1):  
90.3079 160.9234 244.0701  
251.6068 283.3474 323.8682  
446.1919 497.3397 624.7666  
750.4670 777.9141 954.4531  
974.9659 988.2145 1040.8710  
1109.6631 1121.0925 1256.0300  
1293.9257 1379.8010 1409.8085  
1425.5828 1443.7538 1463.8284  
1470.1220 1508.3366 1513.1352  
1642.2173 3049.7233 3063.4000  
3067.1253 3073.4756 3123.5442  
3137.8877 3152.0989 3181.7767  
Zero-point correction (Hartree): 0.116860

Population analysis as 298K (%)  
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)  
Compound Qtot Erel Erel2 n\*Q\*MB %

```

TS.C2H5_CH3_COO.isom.t 5.470e+39 0.00 0.00 1.094e+40 100
Total 1.094e+40 100

TS.C2H5_CH3_COO.isom.t
~~~~~
E (CCSD(T)/Aug-CC-pVTZ) (Hartree): -307.02756767
E (CCSD/Aug-CC-pVTZ) (Hartree): -306.97827175
T1 diagnostic: 0.023108
E (MP2/Aug-CC-pVTZ) (Hartree): -306.92061252
E (MP3/Aug-CC-pVTZ) (Hartree): -306.96510934
E (PMP2/Aug-CC-pVTZ) (Hartree): -306.94458524
E (PMP3/Aug-CC-pVTZ) (Hartree): -306.98895926
E (PUHF/Aug-CC-pVTZ) (Hartree): -305.82597615
E (UHF/Aug-CC-pVTZ) (Hartree): -305.80181962
E (UM062X/Aug-CC-pVTZ) (Hartree): -307.47512710
Electronic state : 1-A
Cartesian coordinates (Angs):
C 0.108994 0.225448 -0.359238
O 1.396190 -0.307242 -0.586536
O 1.987080 -0.636114 0.536664
C 0.119803 1.628913 0.114710
C -0.899190 -0.800647 0.015553
H 0.428472 1.678913 1.166464
H -0.869252 2.073694 0.028592
H 0.826019 2.220175 -0.466939
C -2.320859 -0.256326 0.078907
H -0.834333 -1.621066 -0.702831
H -0.615146 -1.226261 0.987266
H -2.602881 0.209441 -0.865481
H -2.425780 0.487145 0.868144
H -3.025750 -1.059515 0.284163
Rotational constants (GHz): 6.0918000 2.4132200 1.9487600
Vibrational harmonic frequencies (cm-1):
i202.2863 72.8607 133.3182
193.0871 257.6745 274.5989
370.5836 400.4749 600.8603
760.3845 774.1396 949.4953
968.2232 1012.8489 1074.5237
1104.2248 1183.9435 1212.8065
1268.6251 1305.4293 1373.1260
1405.0501 1415.2272 1470.3942
1474.1705 1483.1671 1504.0968
1511.4071 3002.9251 3012.0305
3069.2766 3077.2329 3110.3104
3137.0588 3147.5234 3158.6652
Zero-point correction (Hartree): 0.114523

Population analysis as 298K (%)
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)
Compound Qtot Erel Erel2 n*Q*MB %
-----
TS.C2H5_CH3_COO.ringclose.m 2.289e+39 0.00 0.00 4.578e+39 65.7
TS.C2H5_CH3_COO.ringclose.c 2.736e+39 0.74 0.74 1.570e+39 22.5
TS.C2H5_CH3_COO.ringclose.p 4.732e+39 1.45 1.45 8.248e+38 11.8
Total 6.972e+39 100

TS.C2H5_CH3_COO.ringclose.c
~~~~~
E (RM062X/Aug-CC-pVTZ) (Hartree): -307.49282957
Electronic state : 1-A
Cartesian coordinates (Angs):
C 0.563246 -0.154645 -0.090684
O 0.524114 1.015920 -0.580706
O -0.279672 1.572821 0.520951
C -0.627314 -0.992726 0.218781
C 1.920513 -0.736245 0.064442
C -1.987659 -0.457217 -0.191089
H -0.414083 -1.944636 -0.285264
H -0.588688 -1.231803 1.286190
H -1.932952 0.015485 -1.170576
H -2.336852 0.290098 0.511506
H -2.700029 -1.279714 -0.240548
H 2.350492 -0.262257 0.952263
H 2.539983 -0.438541 -0.781171
H 1.913890 -1.813566 0.196942
Rotational constants (GHz): 4.8952500 3.2680100 2.2349600
Vibrational harmonic frequencies (cm-1):
i486.5216 106.9138 158.3552
200.1256 289.2109 328.4238
381.9575 409.9383 564.3097
731.1065 779.1848 840.3965
952.6085 1015.8943 1027.3329
1094.2527 1113.0333 1203.3362
1278.3127 1375.6247 1407.4789
1417.1266 1439.3949 1460.9220
1480.0169 1488.2845 1502.9716
1594.9775 3020.6839 3055.5272
3066.5550 3082.2031 3125.2883
3145.6442 3186.4229 3195.4614
Zero-point correction (Hartree): 0.115091

TS.C2H5_CH3_COO.ringclose.m
~~~~~
E (CCSD(T)/Aug-CC-pVTZ) (Hartree): -307.05461675
E (CCSD/Aug-CC-pVTZ) (Hartree): -306.99704949
T1 diagnostic: 0.031541
E (MP2/Aug-CC-pVTZ) (Hartree): -306.95274091
E (MP3/Aug-CC-pVTZ) (Hartree): -306.98266218
E (RHF/Aug-CC-pVTZ) (Hartree): -305.78288801
E (RM062X/Aug-CC-pVTZ) (Hartree): -307.49444880

```

Electronic state : 1-A  
 Cartesian coordinates (Angs):  
 C 0.402909 0.317755 0.235354  
 O 1.457457 -0.389005 0.288702  
 O 0.847253 -1.497744 -0.469203  
 C -0.923866 -0.130130 0.740270  
 C 0.570517 1.699343 -0.277084  
 C -1.978471 -0.195063 -0.366665  
 H -0.803200 -1.097738 1.215989  
 H -1.226330 0.621023 1.479827  
 H -1.692600 -0.957613 -1.086713  
 H -2.075970 0.759696 -0.884673  
 H -2.947948 -0.445309 0.058653  
 H 0.559208 1.618154 -1.369206  
 H 1.551570 2.078802 0.004194  
 H -0.228947 2.365545 0.034681  
 Rotational constants (GHz): 4.5066600 3.3330200 2.3022200  
 Vibrational harmonic frequencies (cm-1):  
 i508.1342 122.1932 171.0685  
 223.7848 235.0787 344.9358  
 416.1627 473.0309 522.9113  
 760.2686 809.6292 845.9656  
 956.0200 1001.0408 1017.4227  
 1089.8971 1093.6856 1253.9333  
 1297.3081 1346.6645 1378.6684  
 1402.4905 1452.3821 1463.7537  
 1477.5788 1499.2713 1513.9427  
 1597.5428 3028.0806 3052.3591  
 3071.6770 3127.3101 3139.7873  
 3168.4840 3176.0218 3182.3492  
 Zero-point correction (Hartree): 0.115532

TS.C2H5\_CH3\_COO.ringclose.p  
 ~~~~~  
 E(RM062X/Aug-CC-pVTZ) (Hartree): -307.49176202
 Electronic state : 1-A
 Cartesian coordinates (Angs):
 C 0.243732 0.278747 0.029357
 O 1.287066 -0.008470 0.695268
 O 1.767648 -0.980733 -0.304275
 C -0.776412 -0.732753 -0.373583
 C 0.035350 1.724351 -0.231709
 C -2.137933 -0.412814 0.258617
 H -0.858235 -0.725600 -1.462408
 H -0.409706 -1.710349 -0.080078
 H -2.571330 0.509729 -0.122992
 H -2.058945 -0.333401 1.342512
 H -2.831170 -1.221110 0.034845
 H 0.742074 1.977349 -1.028736
 H 0.331953 2.300450 0.644377
 H -0.970772 1.971374 -0.551563
 Rotational constants (GHz): 5.2186800 2.8343400 2.1148000
 Vibrational harmonic frequencies (cm-1):
 i510.7214 71.4337 133.1399
 186.1424 279.8261 337.0602
 386.0652 452.0801 509.0563
 774.3267 781.9533 839.9943
 951.0042 986.2560 1024.3597
 1064.4085 1104.7635 1237.5750
 1286.6950 1332.1925 1375.9792
 1412.4413 1456.9515 1466.6678
 1477.9880 1506.4523 1508.3432
 1591.6824 3054.7806 3074.0620
 3081.5255 3125.6692 3143.0864
 3151.0357 3180.1421 3199.0370
 Zero-point correction (Hartree): 0.115148

Population analysis as 298K (%)
 Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)
 Compound Qtot Erel Erel2 n*Q*MB %

 TS.C2H5_CH3_COO.14Hshift.t 2.930e+39 0.00 0.00 5.860e+39 99.8
 TS.C2H5_CH3_COO.14Hshift.m 2.580e+39 3.62 3.62 1.146e+37 0.195
 Total 5.871e+39 100

TS.C2H5_CH3_COO.14Hshift.m
 ~~~~~  
 E(RM062X/Aug-CC-pVTZ) (Hartree): -307.49763326  
 Electronic state : 1-A  
 Cartesian coordinates (Angs):  
 C -0.619713 -0.141481 0.010270  
 O -0.546809 1.125086 -0.244496  
 O 0.695451 1.622474 0.146007  
 C 0.542859 -0.738640 0.541380  
 C -1.985023 -0.716102 -0.086893  
 H 0.873926 0.517631 0.886814  
 C 1.779734 -0.946463 -0.343326  
 H 0.316773 -1.602045 1.158341  
 H 2.663000 -1.078229 0.278737  
 H 1.943265 -0.090651 -0.991435  
 H 1.661783 -1.838505 -0.958509  
 H -2.024268 -1.436265 -0.904593  
 H -2.727933 0.061591 -0.243657  
 H -2.202821 -1.257890 0.833630  
 Rotational constants (GHz): 4.6499000 3.3887300 2.1620500  
 Vibrational harmonic frequencies (cm-1):  
 i1604.3251 123.4763 154.9661  
 189.4394 257.6241 306.5157  
 362.5360 614.0647 644.3663  
 696.5736 855.2359 889.4336  
 970.1830 1020.9041 1055.9143



|           |           |           |
|-----------|-----------|-----------|
| 1064.5317 | 1094.1936 | 1111.6934 |
| 1278.2261 | 1347.5543 | 1391.7171 |
| 1401.6489 | 1448.6613 | 1474.9266 |
| 1493.8459 | 1506.6440 | 1515.9025 |
| 1567.2554 | 1874.7758 | 3069.8784 |
| 3071.3750 | 3133.6989 | 3135.1468 |
| 3155.9902 | 3172.2215 | 3175.7268 |

Zero-point correction (Hartree): 0.113058

TS.C2H5\_CH3\_COO.14Hshift.t

~~~~~  
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -307.05835076
E(CCSD/Aug-CC-pVTZ) (Hartree): -306.99880247

T1 diagnostic: 0.023211
E(MP2/Aug-CC-pVTZ) (Hartree): -306.96799558
E(MP3/Aug-CC-pVTZ) (Hartree): -306.98914760
E(RHF/Aug-CC-pVTZ) (Hartree): -305.76647537
E(RM062X/Aug-CC-pVTZ) (Hartree): -307.50285123
Electronic state : 1-A

Cartesian coordinates (Angs):

C	0.150043	0.431777	-0.125197
O	1.430178	0.331815	0.015138
O	1.796307	-1.008154	0.100477
C	-0.562455	-0.781219	-0.180786
C	-0.396324	1.804410	0.012835
H	0.490837	-1.326085	0.410760
C	-2.042663	-0.776575	0.115171
H	-0.257687	-1.404023	-1.023760
H	-2.621103	-0.273520	-0.662916
H	-2.258325	-0.283404	1.062684
H	-2.413471	-1.796517	0.189735
H	0.408130	2.527575	0.114538
H	-1.032317	1.846302	0.898507
H	-1.019555	2.050032	-0.846611

Rotational constants (GHz): 5.0356800 3.0552500 1.9804100

Vibrational harmonic frequencies (cm-1):

i1601.5943	104.2313	146.2772
240.4421	265.7943	280.2096
406.2556	537.4926	571.4376
696.1581	793.1526	850.9037
970.4196	991.9274	1055.3238
1067.1770	1080.8281	1154.7795
1285.7422	1382.3693	1403.4012
1421.6919	1446.4131	1472.5415
1488.0903	1505.2788	1508.6621
1590.3501	1873.2274	3054.7286
3070.7712	3095.9608	3117.3124
3132.3513	3147.5587	3177.0799

Zero-point correction (Hartree): 0.112510

Population analysis as 298K (%)
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)

Compound	Qtot	Erel	Erel2	n*Q*MB	%
TS.C2H5_CH3_COO.14Hshift.m	2.580e+39	0.00	0.00	5.160e+39	100
Total				5.160e+39	100

TS.C2H5_CH3_COO.14Hshift.m

~~~~~  
E(RM062X/Aug-CC-pVTZ) (Hartree): -307.49763326  
Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.619713 | -0.141481 | 0.010270  |
| O | -0.546809 | 1.125086  | -0.244496 |
| O | 0.695451  | 1.622474  | 0.146007  |
| C | 0.542859  | -0.738640 | 0.541380  |
| C | -1.985023 | -0.716102 | -0.086893 |
| H | 0.873926  | 0.517631  | 0.886814  |
| C | 1.779734  | -0.946463 | -0.343326 |
| H | 0.316773  | -1.602045 | 1.158341  |
| H | 2.663000  | -1.078229 | 0.278737  |
| H | 1.943265  | -0.090651 | -0.991435 |
| H | 1.661783  | -1.838505 | -0.958509 |
| H | -2.024268 | -1.436265 | -0.904593 |
| H | -2.727933 | 0.061591  | -0.243657 |
| H | -2.202821 | -1.257890 | 0.833630  |

Rotational constants (GHz): 4.6499000 3.3887300 2.1620500

Vibrational harmonic frequencies (cm-1):

|            |           |           |
|------------|-----------|-----------|
| i1604.3251 | 123.4763  | 154.9661  |
| 189.4394   | 257.6241  | 306.5157  |
| 362.5360   | 614.0647  | 644.3663  |
| 696.5736   | 855.2359  | 889.4336  |
| 970.1830   | 1020.9041 | 1055.9143 |
| 1064.5317  | 1094.1936 | 1111.6934 |
| 1278.2261  | 1347.5543 | 1391.7171 |
| 1401.6489  | 1448.6613 | 1474.9266 |
| 1493.8459  | 1506.6440 | 1515.9025 |
| 1567.2554  | 1874.7758 | 3069.8784 |
| 3071.3750  | 3133.6989 | 3135.1468 |
| 3155.9902  | 3172.2215 | 3175.7268 |

Zero-point correction (Hartree): 0.113058

#####  
(C2H5)2COO  
#####

Population analysis as 298K (%)  
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)

| Compound | Qtot | Erel | Erel2 | n*Q*MB | % |
|----------|------|------|-------|--------|---|
| -----    |      |      |       |        |   |

```

C2H5_C2H5_COO.pc 2.704e+40 0.27 0.27 3.438e+40 36.6
C2H5_C2H5_COO.tc 2.971e+40 0.00 0.00 2.971e+40 31.6
C2H5_C2H5_COO.pp 3.553e+40 1.08 1.08 1.144e+40 12.2
C2H5_C2H5_COO.pm 2.363e+40 0.87 0.87 1.096e+40 11.7
C2H5_C2H5_COO.tp 2.624e+40 1.15 1.15 7.570e+39 8.05
Total 9.407e+40 100

C2H5_C2H5_COO.pc
~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -346.83793877
Electronic state : 1-A
Cartesian coordinates (Angs):
C -0.099664 -0.097373 -0.264474
O -0.149720 1.115922 0.028964
O 1.015373 1.846558 -0.026727
C 1.183210 -0.733935 -0.635883
C -1.374792 -0.863652 -0.181621
C 2.033665 -0.960201 0.624553
C -2.573439 -0.065588 0.303797
H 0.979190 -1.676261 -1.142604
H 1.706161 -0.047155 -1.301673
H -1.553400 -1.287510 -1.174907
H -1.179352 -1.726113 0.464525
H 1.537968 -1.645195 1.312294
H 2.204953 -0.008369 1.120948
H 2.992195 -1.392908 0.346682
H -2.774944 0.773886 -0.358376
H -2.395931 0.334959 1.299853
H -3.455936 -0.700687 0.337131
Rotational constants (GHz): 3.7327700 1.9670900 1.4475900
Vibrational harmonic frequencies (cm-1):
81.5756 128.6830 199.3341
205.2842 221.3392 246.6973
298.2540 361.8968 442.8903
583.0589 624.2774 757.5767
799.6721 822.8652 953.0085
974.7788 1024.6502 1038.5825
1076.6142 1118.5205 1126.4472
1231.1879 1277.9549 1294.5967
1344.4921 1392.9590 1418.3265
1426.5567 1457.0526 1473.5431
1500.7826 1501.6529 1508.5751
1517.5315 1652.6853 3043.7674
3068.7169 3071.9247 3081.7182
3082.8528 3135.3264 3148.4479
3156.6292 3158.6868 3171.6799
Zero-point correction (Hartree): 0.146267

C2H5_C2H5_COO.pm
~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -346.83724605
Electronic state : 1-A
Cartesian coordinates (Angs):
C -0.037121 -0.405315 0.290741
O 0.741265 -1.240673 -0.220748
O 2.077880 -0.934150 -0.275627
C 0.474647 0.885973 0.801229
C -1.476990 -0.785715 0.325620
C 0.827106 1.828321 -0.361406
C -2.345092 0.214777 -0.442933
H -0.273632 1.332786 1.455019
H 1.383426 0.663854 1.362743
H -1.582420 -1.790766 -0.077836
H -1.787580 -0.805345 1.373785
H -0.059966 2.091142 -0.936300
H 1.550745 1.344341 -1.012177
H 1.262386 2.744406 0.032007
H -2.059215 0.248483 -1.493184
H -2.250922 1.218760 -0.030469
H -3.391286 -0.077324 -0.382093
Rotational constants (GHz): 3.4923200 2.1076500 1.5206900
Vibrational harmonic frequencies (cm-1):
83.0699 130.8659 194.2561
200.2909 241.8771 263.9598
342.7039 349.2992 404.7801
589.0945 650.6933 781.5172
797.3740 821.6047 945.2480
974.9501 1015.3458 1044.3582
1068.3066 1110.2050 1125.5223
1254.8050 1274.1399 1302.7419
1349.6454 1378.9280 1400.3610
1417.5260 1468.5951 1476.8915
1499.8524 1505.3979 1510.3825
1519.8347 1644.8065 3060.7032
3073.5206 3074.1794 3079.1366
3130.8891 3132.4683 3150.0955
3151.7867 3153.8609 3171.6930
Zero-point correction (Hartree): 0.146526

C2H5_C2H5_COO.pp
~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -346.83680872
Electronic state : 1-A
Cartesian coordinates (Angs):
C 0.133850 0.143291 -0.102878
O -0.355481 1.284495 -0.252886
O -1.594975 1.534236 0.283918
C -0.619435 -0.913404 0.606888
C 1.487437 -0.072981 -0.685565
C -1.726933 -1.457300 -0.311380
C 2.552872 -0.164547 0.413085
H 0.065597 -1.707429 0.900543

```

```

H -1.075338 -0.457681 1.486018
H 1.462835 -1.005632 -1.254327
H 1.709819 0.743224 -1.370016
H -1.302710 -1.922572 -1.200889
H -2.384779 -0.643567 -0.605788
H -2.306804 -2.207906 0.221142
H 2.334232 -0.970357 1.112390
H 2.606082 0.768487 0.971235
H 3.527980 -0.356773 -0.029466
Rotational constants (GHz): 3.5875900 1.9543700 1.4569000
Vibrational harmonic frequencies (cm-1):
72.4285 111.2236 176.6237
206.8191 221.3353 241.4652
343.8800 355.8660 399.1377
576.3029 702.5231 769.9750
798.2685 822.8757 942.6011
973.8656 1010.7435 1045.0049
1063.7789 1102.7383 1131.4664
1255.3655 1279.7586 1303.5360
1342.0252 1381.4673 1399.8229
1416.6927 1470.3350 1480.8479
1500.4700 1505.3529 1511.8658
1518.0781 1648.0160 3066.0873
3071.9979 3075.8910 3082.6173
3133.3285 3136.1989 3148.2621
3153.7707 3155.5023 3170.4523
Zero-point correction (Hartree): 0.146433

C2H5_C2H5_COO.tc
~~~~~
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -346.32950528
E(CCSD/Aug-CC-pVTZ) (Hartree): -346.26490170
T1 diagnostic: 0.025746
E(MP2/Aug-CC-pVTZ) (Hartree): -346.21452335
E(MP3/Aug-CC-pVTZ) (Hartree): -346.25231967
E(RHF/Aug-CC-pVTZ) (Hartree): -344.86024836
E(RM062X/Aug-CC-pVTZ) (Hartree): -346.83788718
Electronic state : 1-A
Cartesian coordinates (Angs):
C      -0.003176      0.090577      0.000048
O      -0.605395      1.187323      0.000284
O      0.160660      2.327750      0.000017
C      1.474963      0.082640      -0.000393
C      -0.851244      -1.135123      0.000270
C      2.124455      -1.291483      0.000119
C      -2.347671      -0.867322      -0.000288
H      1.776385      0.697062      -0.855591
H      1.776917      0.698053      0.853882
H      -0.555475      -1.733227      -0.866954
H      -0.556071      -1.732445      0.868260
H      1.849926      -1.869947      -0.881494
H      1.849876      -1.869301      0.882145
H      3.207125      -1.186567      0.000106
H      -2.640427      -0.296075      -0.878776
H      -2.641008      -0.295541      0.877654
H      -2.893334      -1.808325      -0.000175
Rotational constants (GHz):      2.8371300      2.3591700      1.3295100
Vibrational harmonic frequencies (cm-1):
80.2646      117.5481      202.0842
212.4143      246.2779      248.9596
290.5936      366.1860      499.4706
506.1172      617.4953      728.4265
770.3829      796.6479      957.2329
991.6973      1022.4540      1030.1964
1087.4371      1120.7515      1131.9065
1242.3172      1249.7168      1293.5059
1353.3726      1408.8286      1423.2061
1426.8275      1444.0687      1454.3384
1500.8302      1507.2280      1509.4537
1512.4049      1638.3155      3048.7491
3051.3539      3063.3627      3073.9324
3074.8898      3084.0390      3138.3901
3151.7498      3158.3954      3159.5533
Zero-point correction (Hartree): 0.145788

C2H5_C2H5_COO.tp
~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -346.83635687
Electronic state : 1-A
Cartesian coordinates (Angs):
C -0.231934 -0.171032 0.241640
O -1.253151 -0.895140 0.200466
O -2.412948 -0.328036 -0.261281
C -0.336117 1.242206 -0.180114
C 1.023717 -0.856775 0.658859
C 0.902355 2.093189 0.051345
C 1.825462 -1.293621 -0.575495
H -0.649226 1.221767 -1.230509
H -1.223570 1.635579 0.325687
H 1.617730 -0.179004 1.271150
H 0.759258 -1.725536 1.258762
H 1.776682 1.699327 -0.465497
H 1.141995 2.166736 1.111718
H 0.729029 3.102101 -0.316560
H 2.066846 -0.445814 -1.215153
H 1.251904 -2.009208 -1.161834
H 2.757250 -1.764343 -0.268655
Rotational constants (GHz): 3.0127600 2.2260400 1.4355800
Vibrational harmonic frequencies (cm-1):
95.7536 118.1404 170.8859
201.0809 249.2349 254.7365
334.9259 364.0042 452.7760

```

|           |           |           |
|-----------|-----------|-----------|
| 545.5091  | 624.1115  | 758.9692  |
| 777.4136  | 801.9932  | 944.7367  |
| 985.5762  | 1006.5101 | 1037.4832 |
| 1085.2079 | 1117.8835 | 1126.6019 |
| 1253.1458 | 1263.4657 | 1299.5390 |
| 1346.5017 | 1386.2510 | 1410.1545 |
| 1425.9193 | 1437.9138 | 1486.6641 |
| 1501.3216 | 1507.8039 | 1510.2287 |
| 1517.2640 | 1631.4585 | 3045.2012 |
| 3064.7934 | 3073.4889 | 3076.5670 |
| 3092.6854 | 3135.6624 | 3140.8516 |
| 3150.8125 | 3154.4196 | 3158.0689 |

Zero-point correction (Hartree): 0.146085

Population analysis as 298K (%)

Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)

| Compound                      | Qtot      | Erel | Erel2 | n*Q*MB    | %    |
|-------------------------------|-----------|------|-------|-----------|------|
| TS.C2H5_C2H5_COO.ringclose.mc | 3.304e+40 | 0.07 | 0.07  | 5.896e+40 | 35.8 |
| TS.C2H5_C2H5_COO.ringclose.mp | 1.677e+40 | 0.00 | 0.00  | 3.354e+40 | 20.4 |
| TS.C2H5_C2H5_COO.ringclose.cc | 4.316e+40 | 0.91 | 0.91  | 1.872e+40 | 11.4 |
| TS.C2H5_C2H5_COO.ringclose.cp | 2.842e+40 | 0.68 | 0.68  | 1.810e+40 | 11   |
| TS.C2H5_C2H5_COO.ringclose.mm | 1.354e+40 | 0.53 | 0.53  | 1.101e+40 | 6.69 |
| TS.C2H5_C2H5_COO.ringclose.pp | 5.053e+40 | 1.50 | 1.50  | 8.045e+39 | 4.89 |
| TS.C2H5_C2H5_COO.ringclose.cm | 1.848e+40 | 1.04 | 1.04  | 6.398e+39 | 3.89 |
| TS.C2H5_C2H5_COO.ringclose.pm | 5.444e+40 | 1.78 | 1.78  | 5.419e+39 | 3.29 |
| TS.C2H5_C2H5_COO.ringclose.pc | 3.003e+40 | 1.56 | 1.56  | 4.284e+39 | 2.6  |
| Total                         |           |      |       | 1.645e+41 | 100  |

TS.C2H5\_C2H5\_COO.ringclose.cc

~~~~~

E(RM062X/Aug-CC-pVTZ) (Hartree): -346.79990680

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.087709  | -0.166778 | -0.008233 |
| O | 0.110548  | 0.978034  | -0.552407 |
| O | -0.632837 | 1.625015  | 0.558077  |
| C | -1.162829 | -0.897122 | 0.367288  |
| C | 1.387176  | -0.888236 | 0.133692  |
| C | -2.411975 | -0.440160 | -0.373603 |
| H | -0.960424 | -1.956945 | 0.182248  |
| H | -1.289798 | -0.799152 | 1.447091  |
| H | -2.266220 | -0.508036 | -1.451197 |
| H | -2.638897 | 0.590084  | -0.121355 |
| H | -3.251119 | -1.078883 | -0.104501 |
| C | 2.615244  | -0.033236 | -0.124789 |
| H | 1.388131  | -1.317982 | 1.140674  |
| H | 1.338993  | -1.753800 | -0.536280 |
| H | 2.615141  | 0.837052  | 0.528489  |
| H | 2.629792  | 0.325318  | -1.151489 |
| H | 3.520770  | -0.608857 | 0.054822  |

Rotational constants (GHz): 4.5001200 1.8408500 1.4659200

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i523.5692 | 53.8691   | 86.8427   |
| 180.1045  | 201.3438  | 221.8645  |
| 282.0155  | 354.7143  | 388.8947  |
| 427.8700  | 601.9287  | 717.1566  |
| 784.4614  | 800.6434  | 834.7764  |
| 977.9959  | 1011.9391 | 1026.4338 |
| 1056.2087 | 1120.4448 | 1124.4001 |
| 1162.5135 | 1258.7782 | 1296.8562 |
| 1368.6969 | 1403.9766 | 1419.2420 |
| 1422.7939 | 1436.4969 | 1452.9565 |
| 1492.9127 | 1499.1160 | 1505.7696 |
| 1517.1674 | 1596.7991 | 3041.8303 |
| 3052.4382 | 3071.4814 | 3080.2030 |
| 3084.2228 | 3096.1027 | 3144.9754 |
| 3159.1569 | 3161.1281 | 3190.4340 |

Zero-point correction (Hartree): 0.143912

TS.C2H5\_C2H5\_COO.ringclose.cm

~~~~~

E(RM062X/Aug-CC-pVTZ) (Hartree): -346.79978916

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.111890 | -0.290725 | -0.131535 |
| O | 0.594834  | -1.255303 | -0.563151 |
| O | 1.508184  | -1.261828 | 0.591919  |
| C | 0.411420  | 1.068148  | 0.170240  |
| C | -1.568983 | -0.586758 | -0.037955 |
| C | 1.861378  | 1.347804  | -0.185163 |
| H | -0.259555 | 1.741107  | -0.378895 |
| H | 0.204669  | 1.277059  | 1.224621  |
| H | 2.114290  | 0.895531  | -1.142921 |
| H | 2.529015  | 0.928261  | 0.557921  |
| H | 2.015229  | 2.423777  | -0.256037 |
| C | -2.531375 | 0.582165  | 0.090031  |
| H | -1.808517 | -1.240522 | -0.880157 |
| H | -1.626319 | -1.240217 | 0.842837  |
| H | -2.510963 | 1.214609  | -0.796646 |
| H | -2.297896 | 1.201341  | 0.954673  |
| H | -3.547389 | 0.212289  | 0.210753  |

Rotational constants (GHz): 3.8544800 1.9743800 1.4410700

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i464.9925 | 95.7827   | 110.2991  |
| 196.8087  | 222.9498  | 258.2694  |
| 319.9492  | 337.4773  | 380.9289  |
| 461.8328  | 552.9284  | 700.1525  |
| 750.4609  | 801.2510  | 845.0041  |
| 968.2693  | 1011.8167 | 1032.1989 |
| 1085.4134 | 1110.8327 | 1125.9220 |

|           |           |           |
|-----------|-----------|-----------|
| 1202.9366 | 1262.9681 | 1292.5751 |
| 1355.0887 | 1410.3197 | 1417.6435 |
| 1423.1099 | 1434.1711 | 1441.6355 |
| 1489.0408 | 1502.1726 | 1508.3244 |
| 1510.2361 | 1582.5160 | 3027.8403 |
| 3028.1168 | 3066.9984 | 3076.4496 |
| 3082.5640 | 3087.2571 | 3145.5204 |
| 3146.0022 | 3153.0928 | 3196.5285 |

Zero-point correction (Hartree): 0.144007

TS.C2H5\_C2H5\_COO.ringclose.cp

E(RM062X/Aug-CC-pVTZ) (Hartree): -346.80062231

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.115777  | -0.150336 | -0.354072 |
| O | -0.039671 | 1.030975  | -0.795334 |
| O | -0.570516 | 1.565154  | 0.472978  |
| C | -0.968004 | -1.003638 | 0.203311  |
| C | 1.485785  | -0.710498 | -0.498104 |
| C | -2.388374 | -0.471058 | 0.142441  |
| H | -0.876882 | -1.939687 | -0.363781 |
| H | -0.676441 | -1.272590 | 1.223969  |
| H | -2.568305 | 0.027610  | -0.808752 |
| H | -2.563443 | 0.254689  | 0.927783  |
| H | -3.090086 | -1.298424 | 0.240408  |
| C | 2.355531  | -0.087000 | 0.609761  |
| H | 1.480589  | -1.796088 | -0.427339 |
| H | 1.870922  | -0.404408 | -1.472241 |
| H | 2.004435  | -0.389792 | 1.594713  |
| H | 2.310182  | 0.998311  | 0.552807  |
| H | 3.386226  | -0.413471 | 0.491262  |

Rotational constants (GHz): 4.1795200 1.9356300 1.5896400

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i466.3870 | 67.2194   | 111.5862  |
| 173.9016  | 197.1839  | 214.8226  |
| 292.9175  | 330.1153  | 402.2446  |
| 502.6147  | 603.0956  | 764.5233  |
| 776.8747  | 818.6161  | 844.1306  |
| 963.7456  | 1008.1778 | 1023.3457 |
| 1072.1199 | 1099.4940 | 1124.4629 |
| 1193.8952 | 1258.8547 | 1273.8819 |
| 1332.8644 | 1401.6492 | 1414.6759 |
| 1421.7040 | 1438.3528 | 1483.3569 |
| 1488.3804 | 1497.2316 | 1501.3939 |
| 1511.2317 | 1589.5915 | 3019.9663 |
| 3061.4518 | 3077.1509 | 3080.9233 |
| 3081.5501 | 3140.0983 | 3145.2423 |
| 3157.1497 | 3168.2058 | 3194.8436 |

Zero-point correction (Hartree): 0.144265

TS.C2H5\_C2H5\_COO.ringclose.mc

E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -346.29717046

E(CCSD/Aug-CC-pVTZ) (Hartree): -346.23170026

T1 diagnostic: 0.029176

E(MP2/Aug-CC-pVTZ) (Hartree): -346.17763465

E(MP3/Aug-CC-pVTZ) (Hartree): -346.21714232

E(RHF/Aug-CC-pVTZ) (Hartree): -344.83044365

E(RM062X/Aug-CC-pVTZ) (Hartree): -346.80164045

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.063941 | 0.085868  | 0.252505  |
| O | -0.430586 | 1.301359  | 0.309771  |
| O | 0.719269  | 1.766235  | -0.493897 |
| C | 1.264066  | -0.394218 | 0.730420  |
| C | -1.066374 | -0.901113 | -0.233475 |
| C | 2.093284  | -1.041481 | -0.380505 |
| H | 1.794486  | 0.445958  | 1.166085  |
| H | 1.048563  | -1.143937 | 1.500886  |
| H | 2.313185  | -0.296753 | -1.141630 |
| H | 1.564778  | -1.875276 | -0.843396 |
| H | 3.026487  | -1.423456 | 0.027862  |
| C | -2.515386 | -0.465946 | -0.053738 |
| H | -0.832516 | -0.990404 | -1.303825 |
| H | -0.858782 | -1.879108 | 0.201280  |
| H | -2.693739 | 0.485649  | -0.547554 |
| H | -2.759012 | -0.350149 | 1.001088  |
| H | -3.182814 | -1.211941 | -0.479017 |

Rotational constants (GHz): 3.5797600 2.0651400 1.4953700

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i505.2933 | 56.1347   | 110.7409  |
| 180.5454  | 207.3613  | 225.1932  |
| 284.1828  | 348.8182  | 411.0602  |
| 497.0332  | 583.6189  | 750.5216  |
| 783.9699  | 811.2696  | 845.2744  |
| 963.9267  | 999.3272  | 1046.1199 |
| 1052.1129 | 1106.9369 | 1114.4348 |
| 1224.3439 | 1258.2030 | 1282.1218 |
| 1342.3415 | 1396.3607 | 1411.2945 |
| 1416.1580 | 1439.8435 | 1464.5714 |
| 1499.3004 | 1501.9479 | 1508.8494 |
| 1513.2075 | 1588.6573 | 3020.1885 |
| 3028.1708 | 3072.5459 | 3084.2248 |
| 3109.5911 | 3139.9746 | 3154.0458 |
| 3165.9113 | 3170.4894 | 3174.4525 |

Zero-point correction (Hartree): 0.144311

TS.C2H5\_C2H5\_COO.ringclose.mm

E(RM062X/Aug-CC-pVTZ) (Hartree): -346.80116715

Electronic state : 1-A

```

Cartesian coordinates (Angs):
C -0.147972 -0.442648 0.207365
O -1.029149 -1.355174 0.313801
O -2.042540 -0.557261 -0.399329
C -0.333931 0.940319 0.728634
C 1.144674 -0.871384 -0.395711
C -0.375942 1.995156 -0.380569
H -1.255443 0.960344 1.302163
H 0.519361 1.137955 1.386368
H -1.273081 1.844398 -0.974583
H 0.490258 1.927513 -1.039248
H -0.390179 2.992286 0.054778
C 2.398468 -0.127203 0.042907
H 1.225291 -1.948754 -0.245149
H 0.972686 -0.744459 -1.473753
H 2.569436 -0.246371 1.112113
H 2.338289 0.937316 -0.174422
H 3.265110 -0.526194 -0.479802
Rotational constants (GHz): 3.3324200 2.2474000 1.5391800
Vibrational harmonic frequencies (cm-1):
i505.1923 100.0371 162.8100
190.8198 217.2777 237.1435
282.3096 381.0347 456.1674
483.0401 509.9765 726.1474
778.9203 815.2840 850.4817
957.2669 1002.2918 1034.6247
1069.9032 1105.9352 1118.2953
1249.0732 1260.8585 1303.3689
1344.8392 1367.6588 1401.5938
1421.9548 1438.1908 1468.3964
1496.6203 1506.0553 1509.1697
1516.7086 1584.6286 3022.7489
3043.7273 3074.1505 3079.6205
3106.5535 3139.3081 3148.1554
3158.2215 3166.2529 3175.5663
Zero-point correction (Hartree): 0.144580

```

```

TS.C2H5_C2H5_COO.ringclose.mp
~~~~~
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -346.29764219
E(CCSD/Aug-CC-pVTZ) (Hartree): -346.23197184
T1 diagnostic: 0.029492
E(MP2/Aug-CC-pVTZ) (Hartree): -346.17813527
E(MP3/Aug-CC-pVTZ) (Hartree): -346.21734281
E(RHF/Aug-CC-pVTZ) (Hartree): -344.83007262
E(RM062X/Aug-CC-pVTZ) (Hartree): -346.80227807
Electronic state : 1-A
Cartesian coordinates (Angs):
C      0.042742      0.267690     -0.537329
O      0.290460      1.506258     -0.395074
O      -0.504980      1.619637      0.844376
C      -1.332225     -0.292221     -0.631479
C      1.228425     -0.613645     -0.699540
C      -1.644230     -1.283856      0.491423
H      -2.041098      0.529115     -0.630495
H      -1.364984     -0.820365     -1.592533
H      -1.616801     -0.764036      1.446094
H      -0.925954     -2.104320      0.514082
H      -2.633744     -1.710958      0.343006
C      1.908273     -0.756098      0.674870
H      0.942762     -1.583536     -1.102778
H      1.915363     -0.117250     -1.388078
H      1.254120     -1.261016      1.383050
H      2.144470      0.227535      1.074559
H      2.824115     -1.333544      0.571017
Rotational constants (GHz): 2.9074200 2.4675500 1.7923100
Vibrational harmonic frequencies (cm-1):
i487.3619      93.5409      138.0463
178.9424      197.0656      240.7588
250.3773      398.3429      434.7782
473.6260      636.9393      772.1559
804.9415      819.6180      845.3984
958.1208      999.3006     1032.4483
1058.5064     1095.6721     1114.7137
1234.3061     1255.2218     1288.0476
1340.6217     1354.6336     1401.4734
1411.6937     1461.4967     1481.8956
1494.3562     1502.4908     1509.6504
1516.6189     1591.7710     3023.5789
3070.7277     3072.2339     3081.7229
3135.4085     3138.4427     3159.1017
3166.4652     3167.4714     3175.2452
Zero-point correction (Hartree): 0.144841

```

```

TS.C2H5_C2H5_COO.ringclose.pc
~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -346.79912816
Electronic state : 1-A
Cartesian coordinates (Angs):
C 0.016212 0.148686 0.059287
O -0.606628 1.068264 0.673405
O -0.249994 2.088764 -0.339862
C 1.472106 0.230449 -0.275167
C -0.723701 -1.123757 -0.198572
C 2.242710 -1.008311 0.193231
H 1.561067 0.333310 -1.358109
H 1.856113 1.148466 0.159474
H 1.936800 -1.908314 -0.338270
H 2.111521 -1.178645 1.261962
H 3.304713 -0.860239 0.008586
C -2.231805 -1.004060 -0.052856
H -0.429881 -1.465051 -1.195419

```

```

H -0.310720 -1.871757 0.486973
H -2.614506 -0.218404 -0.701404
H -2.503615 -0.749444 0.968752
H -2.711649 -1.944195 -0.316429
Rotational constants (GHz): 3.1049400 2.2633900 1.4422500
Vibrational harmonic frequencies (cm-1):
i536.8618 57.6401 115.7840
188.9259 230.3506 241.2591
278.5980 355.6352 408.4308
444.0223 572.4923 739.1321
762.6755 804.6290 838.0796
964.8890 1009.4962 1024.6519
1050.1739 1110.2470 1122.2844
1212.5290 1262.0660 1281.7181
1328.0126 1400.4942 1413.1028
1420.1444 1435.7525 1460.7322
1499.5993 1506.1751 1508.4072
1510.6480 1593.8704 3048.1178
3068.9592 3078.3680 3083.5850
3084.8544 3135.7242 3148.6249
3158.6975 3161.3233 3168.0818
Zero-point correction (Hartree): 0.144183

```

```

TS.C2H5_C2H5_COO.ringclose.pm
~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -346.79895658
Electronic state : 1-A
Cartesian coordinates (Angs):
C      0.106503      -0.241582      0.133541
O      0.078724      -1.276784      -0.602662
O      1.193282      -1.935633      0.107468
C      1.310287      0.625599      0.277883
C      -1.194270      0.158208      0.740139
C      1.020025      2.009141      -0.323469
H      1.545728      0.720597      1.339732
H      2.147132      0.137635      -0.208561
H      0.210820      2.527149      0.189306
H      0.761114      1.927036      -1.378713
H      1.912286      2.627136      -0.246335
C      -2.318363      0.215968      -0.298687
H      -1.407433      -0.633243      1.466477
H      -1.096226      1.094363      1.284322
H      -2.386327      -0.725707      -0.838144
H      -2.138985      1.015063      -1.016714
H      -3.269249      0.405296      0.193738
Rotational constants (GHz):      2.7463500      2.5119800      1.5121000
Vibrational harmonic frequencies (cm-1):
i490.7675      41.1054      87.9452
181.1427      202.5123      233.3094
273.8746      349.8322      401.7225
519.2740      564.6732      760.3290
797.6378      810.1920      844.3610
957.1942      1002.5268      1030.9474
1046.9511      1101.1597      1102.5587
1217.1454      1254.7246      1273.3268
1320.8862      1382.1918      1407.1447
1412.6679      1469.8418      1475.5218
1502.8400      1504.7334      1507.8052
1513.8487      1587.0496      3052.1053
3071.6915      3079.9542      3083.1922
3135.7229      3142.6869      3150.4838
3153.4457      3168.4298      3185.8975
Zero-point correction (Hartree): 0.144351

```

```

TS.C2H5_C2H5_COO.ringclose.pp
~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -346.79943577
Electronic state : 1-A
Cartesian coordinates (Angs):
C -0.015614 0.117175 -0.234085
O 0.473899 1.123487 -0.837812
O 0.589739 1.931786 0.393516
C -1.272862 0.173537 0.566646
C 0.708108 -1.163988 -0.439171
C -2.355091 -0.707706 -0.074138
H -1.053579 -0.179389 1.576871
H -1.583185 1.209835 0.638629
H -2.096197 -1.764722 -0.063495
H -2.541583 -0.409369 -1.105281
H -3.283943 -0.587765 0.479890
C 1.960460 -1.113461 0.459227
H 0.089228 -2.022155 -0.191269
H 1.017034 -1.217855 -1.484115
H 1.682098 -1.065452 1.510528
H 2.552207 -0.231593 0.224968
H 2.558810 -2.007070 0.296779
Rotational constants (GHz): 3.0656800 2.2748400 1.5661700
Vibrational harmonic frequencies (cm-1):
i491.0318 54.6277 81.9310
167.7742 198.7037 206.0964
260.4744 360.3395 399.7803
476.6276 651.5127 760.3575
788.7807 821.6160 841.1580
955.6228 991.6915 1014.6236
1048.4826 1090.2682 1120.9814
1228.4165 1256.6514 1273.3577
1314.6759 1356.0953 1407.2396
1414.4195 1468.5032 1483.0085
1496.6216 1505.0473 1505.9711
1514.3972 1586.8044 3073.5488
3078.0149 3079.5696 3085.0359
3142.7418 3148.4501 3152.6243

```

3160.1914                      3171.8790                      3183.7204  
Zero-point correction (Hartree): 0.144387

Population analysis as 298K (%)  
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)

| Compound                      | Qtot      | Erel | Erel2 | n*Q*MB    | %      |
|-------------------------------|-----------|------|-------|-----------|--------|
| TS.C2H5_C2H5_COO.14Hshift.t.c | 2.354e+40 | 0.00 | 0.00  | 4.708e+40 | 46.4   |
| TS.C2H5_C2H5_COO.14Hshift.t.p | 2.767e+40 | 0.18 | 0.18  | 4.096e+40 | 40.3   |
| TS.C2H5_C2H5_COO.14Hshift.t.m | 2.005e+40 | 0.66 | 0.66  | 1.313e+40 | 12.9   |
| TS.C2H5_C2H5_COO.14Hshift.m.p | 3.311e+40 | 3.50 | 3.50  | 1.810e+38 | 0.178  |
| TS.C2H5_C2H5_COO.14Hshift.m.c | 2.217e+40 | 3.48 | 3.48  | 1.235e+38 | 0.122  |
| TS.C2H5_C2H5_COO.14Hshift.m.m | 3.380e+40 | 4.09 | 4.09  | 6.825e+37 | 0.0672 |
| Total                         |           |      |       | 1.015e+41 | 100    |

TS.C2H5\_C2H5\_COO.14Hshift.m.c  
~~~~~  
E(RM062X/Aug-CC-pVTZ) (Hartree): -346.80487366  
Electronic state : 1-A  
Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.137941  | -0.205215 | -0.057533 |
| O | 0.170693  | 1.063297  | 0.195059  |
| O | -1.045339 | 1.654907  | -0.149687 |
| C | -1.089433 | -0.712417 | -0.535343 |
| C | 1.456058  | -0.899840 | -0.012253 |
| H | -1.338049 | 0.568383  | -0.871476 |
| C | -2.296864 | -0.823156 | 0.405169  |
| H | -0.958143 | -1.591351 | -1.157714 |
| H | -3.215358 | -0.890048 | -0.174992 |
| H | -2.366089 | 0.044919  | 1.054070  |
| H | -2.219065 | -1.719221 | 1.021165  |
| C | 2.667497  | 0.013552  | 0.107706  |
| H | 1.415070  | -1.609220 | 0.819346  |
| H | 1.505999  | -1.515852 | -0.913532 |
| H | 2.626248  | 0.600104  | 1.023051  |
| H | 2.715394  | 0.707940  | -0.728859 |
| H | 3.579967  | -0.578836 | 0.119500  |

Rotational constants (GHz): 4.4854300 1.8312600 1.4012600  
Vibrational harmonic frequencies (cm-1):

|            |           |           |
|------------|-----------|-----------|
| i1600.4979 | 64.8537   | 155.8143  |
| 165.5786   | 219.9616  | 242.0913  |
| 268.9183   | 304.6437  | 430.2632  |
| 623.0067   | 637.4292  | 681.4876  |
| 795.3045   | 857.4533  | 887.0730  |
| 982.2243   | 1008.2178 | 1045.4607 |
| 1079.1233  | 1096.3919 | 1105.6810 |
| 1121.9765  | 1246.3578 | 1288.7197 |
| 1345.4728  | 1355.7639 | 1397.2344 |
| 1419.9163  | 1446.4917 | 1484.0989 |
| 1501.0457  | 1505.2239 | 1507.9052 |
| 1513.0471  | 1560.4416 | 1875.9507 |
| 3056.7334  | 3068.8205 | 3082.6368 |
| 3088.4792  | 3132.1144 | 3156.4378 |
| 3157.0004  | 3158.1985 | 3175.2605 |

Zero-point correction (Hartree): 0.141921

TS.C2H5\_C2H5\_COO.14Hshift.m.m  
~~~~~  
E(RM062X/Aug-CC-pVTZ) (Hartree): -346.80416287  
Electronic state : 1-A  
Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.179205 | -0.065592 | 0.265578  |
| O | 0.233382  | -1.291986 | 0.317875  |
| O | 1.417804  | -1.433370 | -0.405080 |
| C | 0.659244  | 0.842692  | -0.413494 |
| C | -1.594647 | 0.119569  | 0.692492  |
| H | 1.162649  | -0.257922 | -0.999316 |
| C | 1.997144  | 1.268123  | 0.208034  |
| H | 0.109715  | 1.677488  | -0.836158 |
| H | 2.654717  | 1.665451  | -0.562853 |
| H | 2.493287  | 0.424569  | 0.678539  |
| H | 1.839462  | 2.046778  | 0.954233  |
| C | -2.501948 | 0.321167  | -0.527525 |
| H | -1.904207 | -0.764735 | 1.247964  |
| H | -1.656404 | 0.985559  | 1.351388  |
| H | -2.448862 | -0.542858 | -1.187691 |
| H | -2.209908 | 1.204133  | -1.093099 |
| H | -3.533467 | 0.448633  | -0.205871 |

Rotational constants (GHz): 3.9483900 1.8956500 1.4770200  
Vibrational harmonic frequencies (cm-1):

|            |           |           |
|------------|-----------|-----------|
| i1612.2118 | 43.7064   | 146.2273  |
| 156.9228   | 222.6214  | 235.6577  |
| 260.1992   | 356.0276  | 389.0246  |
| 623.8656   | 673.3229  | 733.3086  |
| 803.5560   | 855.1108  | 889.7491  |
| 973.6176   | 1004.1925 | 1039.1648 |
| 1078.4608  | 1099.2069 | 1105.6281 |
| 1107.1093  | 1268.1585 | 1273.3345 |
| 1334.8548  | 1353.7719 | 1395.4153 |
| 1410.3898  | 1469.1931 | 1490.2412 |
| 1503.0129  | 1505.4577 | 1508.2696 |
| 1518.3762  | 1563.0022 | 1874.7161 |
| 3069.9566  | 3076.1854 | 3084.1442 |
| 3131.5976  | 3133.0332 | 3154.3410 |
| 3154.9988  | 3158.6235 | 3176.7222 |

Zero-point correction (Hartree): 0.142168

TS.C2H5\_C2H5\_COO.14Hshift.m.p  
~~~~~  
E(RM062X/Aug-CC-pVTZ) (Hartree): -346.80485293  
Electronic state : 1-A



```

Cartesian coordinates (Angs):
C 0.162427 -0.315761 0.200519
O -0.486479 -1.315703 -0.302168
O -1.859883 -1.113391 -0.166970
C -0.618164 0.752180 0.691236
C 1.623777 -0.535968 0.376161
H -1.603250 -0.164816 0.741887
C -1.363610 1.676602 -0.281168
H -0.114921 1.295099 1.485450
H -2.159630 2.202817 0.242312
H -1.806580 1.109513 -1.094595
H -0.682844 2.418855 -0.698686
C 2.443316 0.480952 -0.420167
H 1.834253 -0.424388 1.442765
H 1.868017 -1.558538 0.092396
H 2.192211 1.497703 -0.120795
H 2.250403 0.382601 -1.487402
H 3.506754 0.325880 -0.249706
Rotational constants (GHz): 3.7336900 2.0072100 1.4709700
Vibrational harmonic frequencies (cm-1):
i1602.1730 52.4323 125.0724
 149.6131 208.2730 250.6896
 282.6459 339.4179 386.6513
 591.2076 662.9207 751.2608
 789.9946 855.8941 890.8662
 979.8388 1002.4902 1041.7657
 1078.1702 1085.7931 1101.1828
 1118.5399 1258.7947 1277.0962
 1342.6342 1357.6555 1394.5796
 1411.7029 1468.1896 1482.2452
 1501.5531 1505.8863 1507.9844
 1514.8182 1563.6580 1874.1090
 3067.2037 3067.7124 3073.3365
 3125.8425 3131.0953 3148.8705
 3149.5816 3152.0766 3173.5278
Zero-point correction (Hartree): 0.141918

```

```

TS.C2H5_C2H5_COO.14Hshift.t.c
~~~~~
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -346.30055551
E(CCSD/Aug-CC-pVTZ) (Hartree): -346.23311872
T1 diagnostic: 0.021547
E(MP2/Aug-CC-pVTZ) (Hartree): -346.19262836
E(MP3/Aug-CC-pVTZ) (Hartree): -346.22326902
E(RHF/Aug-CC-pVTZ) (Hartree): -344.81361749
E(RM062X/Aug-CC-pVTZ) (Hartree): -346.80992779
Electronic state : 1-A
Cartesian coordinates (Angs):
C     -0.012407      0.043828     -0.158958
O     -0.441781      1.255033     -0.027525
O      0.632595      2.130199      0.116242
C      1.387135     -0.116400     -0.156162
C     -1.047435     -1.025566     -0.088193
H      1.432895      1.066965      0.447038
C      1.974548     -1.473480      0.147096
H      1.865782      0.422718     -0.975684
H      1.756196     -2.206664     -0.632838
H      1.599267     -1.869285      1.090595
H      3.056518     -1.402108      0.234205
C     -2.473536     -0.524468      0.087260
H     -0.947050     -1.636378     -0.989497
H     -0.758629     -1.683067      0.736752
H     -2.765988      0.119209     -0.739968
H     -2.574834      0.050237      1.005406
H     -3.160496     -1.366965      0.127994
Rotational constants (GHz):   3.0525700   2.2983400   1.3620500
Vibrational harmonic frequencies (cm-1):
i1596.6104      61.5339      153.8195
  192.8684      214.8521      256.2689
  276.3806      294.4105      489.3777
  541.5550      563.6893      675.6657
  751.7132      824.8217      845.3809
  983.4843      1004.3432     1030.7730
 1069.7777      1104.7526     1112.2018
 1154.9130      1256.4458     1282.3806
 1353.2819      1394.4108     1420.0421
 1422.3981      1446.1566     1478.0252
 1501.7973      1502.1025     1504.5702
 1512.4379      1580.0225     1873.1974
 3052.6652      3057.0685     3082.6038
 3083.1449      3095.5433     3114.9641
 3146.8601      3156.1160     3158.5188
Zero-point correction (Hartree): 0.141423

```

```

TS.C2H5_C2H5_COO.14Hshift.t.m
~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -346.80913591
Electronic state : 1-A
Cartesian coordinates (Angs):
C 0.116637 -0.188584 0.386277
O 0.755123 -1.292220 0.179061
O 2.013983 -1.025210 -0.354287
C 0.813939 0.994022 0.072815
C -1.335630 -0.359966 0.676063
H 1.567742 0.244326 -0.707866
C 0.041510 2.272656 -0.144542
H 1.734258 1.100883 0.650054
H -0.295192 2.715749 0.794836
H -0.834746 2.111636 -0.771311
H 0.667111 3.008295 -0.646089
C -2.119005 -0.674925 -0.604377
H -1.441953 -1.182573 1.383514

```

```

H -1.712350 0.546528 1.146872
H -1.743673 -1.589352 -1.059199
H -2.023974 0.131086 -1.330451
H -3.174776 -0.806350 -0.375975
Rotational constants (GHz): 2.9102200 2.3969800 1.4962300
Vibrational harmonic frequencies (cm-1):
i1596.3441 85.1341 144.4415
162.1755 199.1174 259.0849
261.2000 362.0729 421.0476
539.3727 624.6029 681.3787
786.7837 828.9466 840.7032
968.8133 996.7378 1022.9693
1066.0681 1101.7217 1110.4830
1155.9065 1259.6842 1282.1686
1348.0623 1389.4763 1407.4147
1421.9339 1460.8003 1486.4660
1499.9241 1501.9689 1508.1755
1515.4291 1585.5893 1873.4325
3058.9951 3076.7642 3088.5880
3095.0659 3121.9904 3133.3574
3145.3786 3152.6798 3160.5749
Zero-point correction (Hartree): 0.141685

```

```

TS.C2H5_C2H5_COO.14Hshift.t.p
~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -346.80977482
Electronic state : 1-A
Cartesian coordinates (Angs):
C      -0.137179      -0.273274      0.108462
O      -1.061536      -1.175455      0.134982
O      -2.292618      -0.610508      -0.183413
C      -0.555879      1.026665      -0.240428
C      1.191192      -0.710035      0.615466
H      -1.773250      0.632090      0.103273
C      0.289135      2.216143      0.148429
H      -0.987646      1.070955      -1.241982
H      1.205447      2.294330      -0.440204
H      0.569080      2.179296      1.200751
H      -0.272709      3.135607      -0.002698
C      2.222039      -0.762644      -0.516044
H      1.510898      0.008304      1.372635
H      1.084086      -1.681656      1.094999
H      2.322355      0.209133      -0.996924
H      1.924098      -1.487373      -1.271862
H      3.195020      -1.054115      -0.125851
Rotational constants (GHz):      3.1741100      2.1908000      1.4331600
Vibrational harmonic frequencies (cm-1):
i1596.2489      58.3560      135.8300
178.0520      198.7819      256.0339
273.1701      364.4740      405.3134
545.4613      579.8447      731.4880
776.8299      820.8521      842.3485
980.5593      999.5222      1026.0420
1062.8590      1087.7868      1106.7283
1153.2765      1263.9873      1293.9083
1339.1767      1390.6123      1409.7718
1420.8611      1457.6213      1486.0016
1500.1794      1500.7585      1504.7365
1517.0844      1583.1173      1873.9334
3058.1655      3074.7544      3079.7848
3095.2577      3119.2696      3130.2611
3144.5365      3152.8929      3154.5550
Zero-point correction (Hartree): 0.141554

```

```

Population analysis as 298K (%)
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)
Compound      Qtot      Erel      Erel2      n*Q*MB      %
-----
TS.C2H5_C2H5_COO.14Hshift.m.p 3.311e+40 0.01 0.01 6.499e+40 48.6
TS.C2H5_C2H5_COO.14Hshift.m.c 2.217e+40 0.00 0.00 4.434e+40 33.1
TS.C2H5_C2H5_COO.14Hshift.m.m 3.380e+40 0.60 0.60 2.450e+40 18.3
Total      1.338e+41 100

```

```

TS.C2H5_C2H5_COO.14Hshift.m.c
~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -346.80487366
Electronic state : 1-A
Cartesian coordinates (Angs):
C 0.137941 -0.205215 -0.057533
O 0.170693 1.063297 0.195059
O -1.045339 1.654907 -0.149687
C -1.089433 -0.712417 -0.535343
C 1.456058 -0.899840 -0.012253
H -1.338049 0.568383 -0.871476
C -2.296864 -0.823156 0.405169
H -0.958143 -1.591351 -1.157714
H -3.215358 -0.890048 -0.174992
H -2.366089 0.044919 1.054070
H -2.219065 -1.719221 1.021165
C 2.667497 0.013552 0.107706
H 1.415070 -1.609220 0.819346
H 1.505999 -1.515852 -0.913532
H 2.626248 0.600104 1.023051
H 2.715394 0.707940 -0.728859
H 3.579967 -0.578836 0.119500
Rotational constants (GHz): 4.4854300 1.8312600 1.4012600
Vibrational harmonic frequencies (cm-1):
i1600.4979 64.8537 155.8143
165.5786 219.9616 242.0913
268.9183 304.6437 430.2632
623.0067 637.4292 681.4876

```

|           |           |           |
|-----------|-----------|-----------|
| 795.3045  | 857.4533  | 887.0730  |
| 982.2243  | 1008.2178 | 1045.4607 |
| 1079.1233 | 1096.3919 | 1105.6810 |
| 1121.9765 | 1246.3578 | 1288.7197 |
| 1345.4728 | 1355.7639 | 1397.2344 |
| 1419.9163 | 1446.4917 | 1484.0989 |
| 1501.0457 | 1505.2239 | 1507.9052 |
| 1513.0471 | 1560.4416 | 1875.9507 |
| 3056.7334 | 3068.8205 | 3082.6368 |
| 3088.4792 | 3132.1144 | 3156.4378 |
| 3157.0004 | 3158.1985 | 3175.2605 |

Zero-point correction (Hartree): 0.141921

TS.C2H5\_C2H5\_COO.14Hshift.m.m

~~~~~

E(RM062X/Aug-CC-pVTZ) (Hartree): -346.80416287

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.179205 | -0.065592 | 0.265578  |
| O | 0.233382  | -1.291986 | 0.317875  |
| O | 1.417804  | -1.433370 | -0.405080 |
| C | 0.659244  | 0.842692  | -0.413494 |
| C | -1.594647 | 0.119569  | 0.692492  |
| H | 1.162649  | -0.257922 | -0.999316 |
| C | 1.997144  | 1.268123  | 0.208034  |
| H | 0.109715  | 1.677488  | -0.836158 |
| H | 2.654717  | 1.665451  | -0.562853 |
| H | 2.493287  | 0.424569  | 0.678539  |
| H | 1.839462  | 2.046778  | 0.954233  |
| C | -2.501948 | 0.321167  | -0.527525 |
| H | -1.904207 | -0.764735 | 1.247964  |
| H | -1.656404 | 0.985559  | 1.351388  |
| H | -2.448862 | -0.542858 | -1.187691 |
| H | -2.209908 | 1.204133  | -1.093099 |
| H | -3.533467 | 0.448633  | -0.205871 |

Rotational constants (GHz): 3.9483900 1.8956500 1.4770200

Vibrational harmonic frequencies (cm-1):

|            |           |           |
|------------|-----------|-----------|
| i1612.2118 | 43.7064   | 146.2273  |
| 156.9228   | 222.6214  | 235.6577  |
| 260.1992   | 356.0276  | 389.0246  |
| 623.8656   | 673.3229  | 733.3086  |
| 803.5560   | 855.1108  | 889.7491  |
| 973.6176   | 1004.1925 | 1039.1648 |
| 1078.4608  | 1099.2069 | 1105.6281 |
| 1107.1093  | 1268.1585 | 1273.3345 |
| 1334.8548  | 1353.7719 | 1395.4153 |
| 1410.3898  | 1469.1931 | 1490.2412 |
| 1503.0129  | 1505.4577 | 1508.2696 |
| 1518.3762  | 1563.0022 | 1874.7161 |
| 3069.9566  | 3076.1854 | 3084.1442 |
| 3131.5976  | 3133.0332 | 3154.3410 |
| 3154.9988  | 3158.6235 | 3176.7222 |

Zero-point correction (Hartree): 0.142168

TS.C2H5\_C2H5\_COO.14Hshift.m.p

~~~~~

E(RM062X/Aug-CC-pVTZ) (Hartree): -346.80485293

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.162427  | -0.315761 | 0.200519  |
| O | -0.486479 | -1.315703 | -0.302168 |
| O | -1.859883 | -1.113391 | -0.166970 |
| C | -0.618164 | 0.752180  | 0.691236  |
| C | 1.623777  | -0.535968 | 0.376161  |
| H | -1.603250 | -0.164816 | 0.741887  |
| C | -1.363610 | 1.676602  | -0.281168 |
| H | -0.114921 | 1.295099  | 1.485450  |
| H | -2.159630 | 2.202817  | 0.242312  |
| H | -1.806580 | 1.109513  | -1.094595 |
| H | -0.682844 | 2.418855  | -0.698686 |
| C | 2.443316  | 0.480952  | -0.420167 |
| H | 1.834253  | -0.424388 | 1.442765  |
| H | 1.868017  | -1.558538 | 0.092396  |
| H | 2.192211  | 1.497703  | -0.120795 |
| H | 2.250403  | 0.382601  | -1.487402 |
| H | 3.506754  | 0.325880  | -0.249706 |

Rotational constants (GHz): 3.7336900 2.0072100 1.4709700

Vibrational harmonic frequencies (cm-1):

|            |           |           |
|------------|-----------|-----------|
| i1602.1730 | 52.4323   | 125.0724  |
| 149.6131   | 208.2730  | 250.6896  |
| 282.6459   | 339.4179  | 386.6513  |
| 591.2076   | 662.9207  | 751.2608  |
| 789.9946   | 855.8941  | 890.8662  |
| 979.8388   | 1002.4902 | 1041.7657 |
| 1078.1702  | 1085.7931 | 1101.1828 |
| 1118.5399  | 1258.7947 | 1277.0962 |
| 1342.6342  | 1357.6555 | 1394.5796 |
| 1411.7029  | 1468.1896 | 1482.2452 |
| 1501.5531  | 1505.8863 | 1507.9844 |
| 1514.8182  | 1563.6580 | 1874.1090 |
| 3067.2037  | 3067.7124 | 3073.3365 |
| 3125.8425  | 3131.0953 | 3148.8705 |
| 3149.5816  | 3152.0766 | 3173.5278 |

Zero-point correction (Hartree): 0.141918

#####  
E- (C2H5) (iC3H7) COO  
#####

Population analysis as 298K (%)  
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)

| Compound          | Qtot      | Erel | Erel2 | n*Q*MB    | %     |
|-------------------|-----------|------|-------|-----------|-------|
| C2H5_ic3H7_COO.pp | 1.240e+41 | 0.00 | 0.00  | 2.481e+41 | 33.2  |
| C2H5_ic3H7_COO.pm | 1.704e+41 | 0.29 | 0.29  | 2.081e+41 | 27.8  |
| C2H5_ic3H7_COO.cp | 1.441e+41 | 0.30 | 0.30  | 1.731e+41 | 23.1  |
| C2H5_ic3H7_COO.pt | 1.437e+41 | 0.53 | 0.53  | 1.181e+41 | 15.8  |
| C2H5_ic3H7_COO.ct | 1.419e+41 | 3.07 | 3.07  | 7.944e+38 | 0.106 |
| Total             |           |      |       | 7.482e+41 | 100   |

C2H5\_ic3H7\_COO.cp  
~~~~~  
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -385.57471219  
E(CCSD/Aug-CC-pVTZ) (Hartree): -385.50138686  
T1 diagnostic: 0.024852  
E(MP2/Aug-CC-pVTZ) (Hartree): -385.44263524  
E(MP3/Aug-CC-pVTZ) (Hartree): -385.48822339  
E(RHF/Aug-CC-pVTZ) (Hartree): -383.90682139  
E(RM062X/Aug-CC-pVTZ) (Hartree): -386.14624896  
Electronic state : 1-A  
Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.134555  | -0.318361 | 0.005538  |
| O | 0.832384  | -1.214461 | -0.519929 |
| O | 2.172437  | -1.256701 | -0.222626 |
| C | 0.755288  | 0.681020  | 0.903435  |
| C | 1.570025  | 1.699148  | 0.088116  |
| H | -0.018824 | 1.179038  | 1.484837  |
| H | 1.430980  | 0.135309  | 1.563487  |
| C | -1.320878 | -0.341459 | -0.341258 |
| H | -1.447977 | -1.115013 | -1.098850 |
| C | -2.145308 | -0.713754 | 0.895811  |
| C | -1.759864 | 1.009407  | -0.910312 |
| H | -2.042601 | 0.039943  | 1.676971  |
| H | -1.839712 | -1.676919 | 1.301423  |
| H | -3.198740 | -0.772534 | 0.624737  |
| H | -1.194497 | 1.270202  | -1.803988 |
| H | -1.629066 | 1.804411  | -0.174743 |
| H | -2.816280 | 0.967844  | -1.172566 |
| H | 0.923067  | 2.286921  | -0.561842 |
| H | 2.309333  | 1.174503  | -0.511578 |
| H | 2.082836  | 2.379579  | 0.764574  |

Rotational constants (GHz): 2.7185900 1.5130700 1.2181900  
Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| 66.9091   | 120.4841  | 175.2602  |
| 204.2316  | 224.0281  | 231.1741  |
| 268.6193  | 283.0530  | 309.4457  |
| 359.9778  | 373.3480  | 493.7096  |
| 590.9257  | 688.9156  | 777.9274  |
| 818.4816  | 893.3463  | 941.8994  |
| 967.5553  | 979.4787  | 987.0068  |
| 1047.1656 | 1075.1906 | 1115.6008 |
| 1131.1191 | 1194.9119 | 1264.5623 |
| 1303.6055 | 1341.0773 | 1355.8781 |
| 1377.2414 | 1398.5543 | 1401.0913 |
| 1425.8593 | 1467.4465 | 1489.6648 |
| 1494.9296 | 1501.9988 | 1507.5278 |
| 1514.9675 | 1520.9608 | 1640.4531 |
| 3063.6911 | 3065.8204 | 3075.1613 |
| 3080.8012 | 3095.6610 | 3134.4568 |
| 3135.5760 | 3141.5497 | 3144.7397 |
| 3147.0455 | 3149.9988 | 3170.4314 |

Zero-point correction (Hartree): 0.174805

C2H5\_ic3H7\_COO.ct  
~~~~~  
E(RM062X/Aug-CC-pVTZ) (Hartree): -386.14150938  
Electronic state : 1-A  
Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.423269  | -0.216552 | 0.087925  |
| O | 1.369819  | -1.033742 | 0.209877  |
| O | 2.647825  | -0.562579 | 0.081543  |
| C | 0.774779  | 1.197795  | -0.171675 |
| C | -0.327409 | 2.244884  | -0.170383 |
| H | 1.566852  | 1.430156  | 0.547661  |
| H | 1.329047  | 1.178466  | -1.118567 |
| C | -0.932194 | -0.858306 | 0.153589  |
| H | -0.736417 | -1.880507 | 0.479666  |
| C | -1.885452 | -0.206244 | 1.157386  |
| C | -1.547207 | -0.920820 | -1.250370 |
| H | -2.290636 | 0.729943  | 0.780614  |
| H | -1.398577 | -0.015959 | 2.113382  |
| H | -2.722360 | -0.880781 | 1.334715  |
| H | -0.894856 | -1.452799 | -1.941092 |
| H | -1.733969 | 0.075543  | -1.648927 |
| H | -2.500655 | -1.446343 | -1.202919 |
| H | -0.756276 | 2.375967  | 0.820844  |
| H | -1.133746 | 2.011428  | -0.863032 |
| H | 0.095734  | 3.200916  | -0.472539 |

Rotational constants (GHz): 2.4405900 1.5767400 1.2105200  
Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| 75.0516   | 112.7262  | 159.7816  |
| 200.9480  | 219.9624  | 247.8186  |
| 278.7522  | 301.3656  | 314.7826  |
| 370.5544  | 376.5459  | 510.1076  |
| 564.4925  | 637.7209  | 726.1670  |
| 779.2469  | 898.5212  | 940.8126  |
| 978.0824  | 979.8454  | 1004.5328 |
| 1070.5542 | 1083.8489 | 1119.1359 |
| 1141.0223 | 1195.8240 | 1262.8818 |
| 1304.7217 | 1341.3246 | 1367.3173 |
| 1385.6677 | 1400.1915 | 1416.9091 |
| 1429.0973 | 1436.5152 | 1490.6339 |
| 1493.6636 | 1501.3361 | 1510.9144 |

|           |           |           |
|-----------|-----------|-----------|
| 1518.5019 | 1525.0218 | 1608.8715 |
| 3033.9866 | 3058.2238 | 3068.7727 |
| 3073.0890 | 3084.1860 | 3088.0017 |
| 3139.4214 | 3141.7487 | 3146.3898 |
| 3149.9650 | 3158.8799 | 3162.5988 |

Zero-point correction (Hartree): 0.174478

C2H5\_iC3H7\_COO.pm

~~~~~

E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -385.57448535

E(CCSD/Aug-CC-pVTZ) (Hartree): -385.50148312

T1 diagnostic: 0.024509

E(MP2/Aug-CC-pVTZ) (Hartree): -385.44235653

E(MP3/Aug-CC-pVTZ) (Hartree): -385.48847406

E(RHF/Aug-CC-pVTZ) (Hartree): -383.90833164

E(RM062X/Aug-CC-pVTZ) (Hartree): -386.14616526

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.122027 | 0.002690  | -0.099108 |
| O | -0.373437 | 1.222702  | -0.198733 |
| O | -1.634490 | 1.598230  | -0.602827 |
| C | -1.171333 | -1.005227 | -0.370422 |
| C | -2.152919 | -1.049828 | 0.812637  |
| H | -1.705307 | -0.692536 | -1.267722 |
| H | -0.706000 | -1.977711 | -0.522788 |
| C | 1.266290  | -0.369253 | 0.318683  |
| H | 1.147859  | -1.167509 | 1.059112  |
| C | 2.008236  | -0.954512 | -0.893158 |
| C | 2.037787  | 0.791966  | 0.930233  |
| H | 2.144038  | -0.184662 | -1.652773 |
| H | 1.471864  | -1.789921 | -1.340408 |
| H | 2.990648  | -1.306808 | -0.582585 |
| H | 1.510081  | 1.217377  | 1.781782  |
| H | 2.182629  | 1.583903  | 0.196790  |
| H | 3.015956  | 0.446574  | 1.261423  |
| H | -2.588812 | -0.064867 | 0.959002  |
| H | -1.648093 | -1.364359 | 1.725952  |
| H | -2.947646 | -1.761953 | 0.601495  |

Rotational constants (GHz): 2.7515900 1.4682600 1.2043700

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| 64.8475   | 103.5461  | 178.0748  |
| 204.5576  | 218.3311  | 228.8557  |
| 250.9173  | 277.2802  | 328.7064  |
| 366.4944  | 396.3279  | 472.2270  |
| 586.5139  | 708.2117  | 763.4204  |
| 821.9077  | 897.6645  | 938.2918  |
| 953.4476  | 981.5699  | 987.2783  |
| 1054.2007 | 1093.6966 | 1114.7723 |
| 1146.3939 | 1184.1523 | 1245.4170 |
| 1293.4938 | 1314.7847 | 1341.1217 |
| 1391.5142 | 1399.3028 | 1418.7755 |
| 1426.0819 | 1470.5655 | 1489.7513 |
| 1494.3104 | 1499.2124 | 1507.2856 |
| 1516.0172 | 1520.7116 | 1645.9004 |
| 3042.6838 | 3067.7010 | 3071.9975 |
| 3074.4354 | 3084.6435 | 3137.0920 |
| 3142.0221 | 3147.1359 | 3148.9392 |
| 3150.0325 | 3152.3925 | 3172.1105 |

Zero-point correction (Hartree): 0.174706

C2H5\_iC3H7\_COO.pp

~~~~~

E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -385.57467972

E(CCSD/Aug-CC-pVTZ) (Hartree): -385.50151044

T1 diagnostic: 0.024550

E(MP2/Aug-CC-pVTZ) (Hartree): -385.44255839

E(MP3/Aug-CC-pVTZ) (Hartree): -385.48852189

E(RHF/Aug-CC-pVTZ) (Hartree): -383.90726065

E(RM062X/Aug-CC-pVTZ) (Hartree): -386.14665272

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.106996  | -0.182393 | 0.316047  |
| O | 0.369915  | -1.302279 | -0.173657 |
| O | 1.687148  | -1.687533 | -0.254053 |
| C | 1.198038  | 0.705528  | 0.779380  |
| C | 1.950797  | 1.318979  | -0.412087 |
| H | 0.779871  | 1.480010  | 1.421221  |
| H | 1.889414  | 0.079664  | 1.346021  |
| C | -1.339253 | 0.197890  | 0.391756  |
| H | -1.522878 | 0.425535  | 1.448053  |
| C | -1.570886 | 1.488409  | -0.406639 |
| C | -2.274043 | -0.914996 | -0.059130 |
| H | -1.370959 | 1.318777  | -1.465125 |
| H | -0.935977 | 2.303291  | -0.061569 |
| H | -2.609321 | 1.798457  | -0.301268 |
| H | -2.116835 | -1.826981 | 0.512828  |
| H | -2.111582 | -1.148516 | -1.110886 |
| H | -3.307542 | -0.595988 | 0.066721  |
| H | 1.300031  | 1.967803  | -0.996752 |
| H | 2.333038  | 0.523074  | -1.045856 |
| H | 2.786342  | 1.912878  | -0.047679 |

Rotational constants (GHz): 2.6715400 1.6656800 1.1561100

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| 65.4537   | 133.8324  | 193.5514  |
| 202.4997  | 222.4706  | 232.0168  |
| 258.0404  | 283.2853  | 331.9427  |
| 370.1523  | 393.0359  | 470.0751  |
| 598.8495  | 659.9757  | 779.1218  |
| 819.1935  | 896.0486  | 935.9214  |
| 958.2909  | 981.2726  | 990.4138  |
| 1053.1328 | 1090.8534 | 1128.9429 |
| 1152.6177 | 1178.3479 | 1238.4064 |

|           |           |           |
|-----------|-----------|-----------|
| 1283.1225 | 1317.9741 | 1347.7132 |
| 1387.1340 | 1399.9078 | 1418.0180 |
| 1426.4995 | 1468.7056 | 1488.6200 |
| 1492.7916 | 1500.9938 | 1507.0885 |
| 1514.7660 | 1521.7171 | 1639.5477 |
| 3033.4820 | 3065.4867 | 3073.1749 |
| 3074.6122 | 3078.6232 | 3130.8226 |
| 3138.8986 | 3145.3491 | 3146.7122 |
| 3149.3670 | 3156.2233 | 3171.4508 |

Zero-point correction (Hartree): 0.174728

C2H5\_iC3H7\_COO.pt

~~~~~  
E(RM062X/Aug-CC-pVTZ) (Hartree): -386.14538069

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.246321 | -0.220056 | -0.083416 |
| O | -0.265546 | -1.462545 | 0.066898  |
| O | -1.479401 | -2.056563 | 0.313269  |
| C | -1.523347 | 0.525413  | -0.020243 |
| C | -1.463255 | 1.994107  | -0.409346 |
| H | -2.223662 | -0.046441 | -0.636837 |
| H | -1.914838 | 0.369970  | 0.991828  |
| C | 1.104946  | 0.403847  | -0.246243 |
| H | 0.989466  | 1.239206  | -0.939615 |
| C | 1.533679  | 0.967230  | 1.119583  |
| C | 2.145909  | -0.570137 | -0.784736 |
| H | 1.681981  | 0.148341  | 1.823556  |
| H | 0.792296  | 1.646765  | 1.537381  |
| H | 2.473760  | 1.506966  | 1.014191  |
| H | 1.841688  | -0.989134 | -1.742287 |
| H | 2.297156  | -1.394552 | -0.090054 |
| H | 3.094668  | -0.051896 | -0.916538 |
| H | -1.150432 | 2.118193  | -1.445702 |
| H | -0.780883 | 2.564562  | 0.219213  |
| H | -2.451295 | 2.438463  | -0.310079 |

Rotational constants (GHz): 2.1363100 1.8158200 1.1733500

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| 76.9305   | 115.4333  | 166.7452  |
| 194.0055  | 229.7387  | 242.5749  |
| 249.7925  | 270.4300  | 340.3095  |
| 356.3525  | 410.2817  | 520.3812  |
| 558.2708  | 619.2582  | 750.0513  |
| 779.5424  | 898.5496  | 939.8748  |
| 955.6074  | 979.7307  | 996.9052  |
| 1065.6116 | 1096.5789 | 1136.2214 |
| 1140.9146 | 1182.5245 | 1251.6867 |
| 1259.4405 | 1319.8317 | 1355.4025 |
| 1395.0860 | 1412.0282 | 1422.3662 |
| 1426.1028 | 1443.0029 | 1489.3333 |
| 1493.9504 | 1505.6223 | 1507.3387 |
| 1511.4538 | 1520.2805 | 1629.1413 |
| 3046.5113 | 3065.9133 | 3067.4357 |
| 3074.3748 | 3075.3355 | 3079.9775 |
| 3139.3495 | 3142.0764 | 3146.5685 |
| 3148.8684 | 3151.8880 | 3153.6204 |

Zero-point correction (Hartree): 0.174295

Population analysis as 298K (%)

Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)

| Compound                       | Qtot      | Erel | Erel2 | n*Q*MB    | %      |
|--------------------------------|-----------|------|-------|-----------|--------|
| TS.C2H5_iC3H7_COO.ringclose.tp | 1.111e+41 | 0.00 | 0.00  | 2.221e+41 | 45.3   |
| TS.C2H5_iC3H7_COO.ringclose.tc | 1.904e+41 | 0.73 | 0.73  | 1.109e+41 | 22.6   |
| TS.C2H5_iC3H7_COO.ringclose.tm | 3.073e+41 | 1.32 | 1.32  | 6.613e+40 | 13.5   |
| TS.C2H5_iC3H7_COO.ringclose.pp | 6.614e+40 | 0.73 | 0.73  | 3.875e+40 | 7.91   |
| TS.C2H5_iC3H7_COO.ringclose.pc | 1.002e+41 | 1.07 | 1.07  | 3.274e+40 | 6.68   |
| TS.C2H5_iC3H7_COO.ringclose.mc | 2.542e+41 | 2.02 | 2.02  | 1.678e+40 | 3.42   |
| TS.C2H5_iC3H7_COO.ringclose.mp | 1.129e+41 | 2.93 | 2.93  | 1.591e+39 | 0.325  |
| TS.C2H5_iC3H7_COO.ringclose.pm | 1.344e+41 | 3.48 | 3.48  | 7.553e+38 | 0.154  |
| TS.C2H5_iC3H7_COO.ringclose.mm | 1.206e+41 | 4.01 | 4.01  | 2.782e+38 | 0.0568 |
| Total                          |           |      |       | 4.900e+41 | 100    |

TS.C2H5\_iC3H7\_COO.ringclose.mc

~~~~~  
E(UM062X/Aug-CC-pVTZ) (Hartree): -386.10780823

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.115468  | -0.148287 | -0.051139 |
| O | 0.551831  | -1.319719 | 0.183784  |
| O | 1.586625  | -1.283303 | -0.864203 |
| C | 0.951955  | 1.078727  | 0.036915  |
| C | -1.359139 | -0.066086 | -0.308313 |
| C | 2.357298  | 0.917504  | 0.590547  |
| H | 0.958792  | 1.554295  | -0.948104 |
| H | 0.361873  | 1.758541  | 0.665303  |
| H | -1.455343 | -0.617740 | -1.252760 |
| C | -2.119478 | -0.855695 | 0.766902  |
| C | -1.926020 | 1.334826  | -0.488300 |
| H | -2.039313 | -0.353424 | 1.731588  |
| H | -1.732864 | -1.866457 | 0.864252  |
| H | -3.173173 | -0.905418 | 0.498230  |
| H | -1.387970 | 1.904849  | -1.243765 |
| H | -1.902751 | 1.894216  | 0.447605  |
| H | -2.966747 | 1.263263  | -0.800956 |
| H | 3.025630  | 0.518682  | -0.163242 |
| H | 2.361067  | 0.223551  | 1.429837  |
| H | 2.722638  | 1.883882  | 0.935691  |

Rotational constants (GHz): 2.9510700 1.4828400 1.1695000

Vibrational harmonic frequencies (cm-1):

|           |         |          |
|-----------|---------|----------|
| i452.1817 | 27.4738 | 105.2957 |
|-----------|---------|----------|

|           |           |           |
|-----------|-----------|-----------|
| 183.4403  | 203.3002  | 236.4189  |
| 253.6728  | 285.8961  | 317.0482  |
| 339.6719  | 354.0177  | 475.3149  |
| 509.1882  | 585.7272  | 723.0329  |
| 794.0810  | 845.1791  | 897.9722  |
| 937.4614  | 981.7203  | 1005.1126 |
| 1047.0903 | 1060.1709 | 1110.0927 |
| 1153.6883 | 1165.7290 | 1224.1493 |
| 1278.0479 | 1295.0870 | 1352.2458 |
| 1397.0877 | 1412.0169 | 1415.5033 |
| 1428.4671 | 1434.6947 | 1487.2986 |
| 1493.7644 | 1497.9221 | 1501.9123 |
| 1512.5405 | 1517.1027 | 1570.0899 |
| 3023.6920 | 3026.0374 | 3067.4153 |
| 3071.3326 | 3073.0542 | 3080.7850 |
| 3135.2092 | 3141.2802 | 3143.8234 |
| 3147.4434 | 3171.8040 | 3195.5938 |

Zero-point correction (Hartree): 0.172442

TS.C2H5\_iC3H7\_COO.ringclose.mm  
 ~~~~~  
 E (UM062X/Aug-CC-pVT2) (Hartree): -386.10521800  
 Electronic state : 1-A  
 Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.426899 | -0.217280 | 0.068528  |
| O | -1.190242 | -1.037949 | -0.528781 |
| O | -2.265443 | -0.993304 | 0.488332  |
| C | -0.847302 | 1.182527  | 0.366808  |
| C | 0.981393  | -0.695034 | 0.264882  |
| C | -0.208104 | 2.111640  | -0.682742 |
| H | -1.927449 | 1.235958  | 0.320852  |
| H | -0.522995 | 1.465095  | 1.367676  |
| H | 0.848645  | -1.695720 | 0.685612  |
| C | 1.642578  | -0.865060 | -1.114568 |
| C | 1.829015  | 0.133844  | 1.220371  |
| H | 1.811533  | 0.103955  | -1.583583 |
| H | 1.023686  | -1.471810 | -1.772209 |
| H | 2.606092  | -1.356728 | -0.990412 |
| H | 1.359921  | 0.217524  | 2.199567  |
| H | 2.015751  | 1.137369  | 0.840990  |
| H | 2.794813  | -0.352119 | 1.353231  |
| H | -0.525743 | 1.826574  | -1.685048 |
| H | 0.879356  | 2.105030  | -0.652828 |
| H | -0.542219 | 3.131076  | -0.499920 |

Rotational constants (GHz): 2.3304100 1.6815600 1.3340400  
 Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i469.8963 | 56.3818   | 130.5860  |
| 183.5317  | 218.4148  | 227.4034  |
| 239.5055  | 257.0480  | 295.2805  |
| 326.8049  | 369.2183  | 487.4641  |
| 505.2793  | 616.4974  | 738.5102  |
| 809.6490  | 831.4665  | 899.5604  |
| 939.4592  | 968.6881  | 983.0518  |
| 1006.7421 | 1067.5237 | 1115.5795 |
| 1142.4661 | 1184.5255 | 1238.3213 |
| 1281.7444 | 1302.6205 | 1331.0555 |
| 1369.1265 | 1397.0403 | 1405.1263 |
| 1428.8246 | 1480.0336 | 1494.1850 |
| 1495.7941 | 1500.0113 | 1509.8295 |
| 1514.7136 | 1517.3612 | 1576.9240 |
| 3060.6583 | 3072.3935 | 3074.0600 |
| 3079.0787 | 3107.6700 | 3143.0615 |
| 3145.0294 | 3147.6713 | 3149.9465 |
| 3158.0688 | 3161.5144 | 3202.9910 |

Zero-point correction (Hartree): 0.173017

TS.C2H5\_iC3H7\_COO.ringclose.mp  
 ~~~~~  
 E (UM062X/Aug-CC-pVT2) (Hartree): -386.10721997  
 Electronic state : 1-A  
 Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.157597  | -0.402574 | 0.068975  |
| O | 0.494570  | -1.624592 | -0.046911 |
| O | 1.813724  | -1.300203 | -0.619953 |
| C | 0.954281  | 0.565003  | 0.879817  |
| C | -1.222435 | -0.083158 | -0.422592 |
| C | 1.711991  | 1.635625  | 0.091102  |
| H | 0.238582  | 1.048735  | 1.555290  |
| H | 1.661218  | -0.023781 | 1.458701  |
| H | -1.345023 | -0.642739 | -1.350582 |
| C | -2.181205 | -0.685536 | 0.625801  |
| C | -1.523544 | 1.390024  | -0.661180 |
| H | -2.075765 | -0.169674 | 1.581170  |
| H | -1.989099 | -1.745970 | 0.774281  |
| H | -3.206555 | -0.558262 | 0.282192  |
| H | -0.918976 | 1.799930  | -1.467268 |
| H | -1.357998 | 1.987701  | 0.235524  |
| H | -2.571219 | 1.497099  | -0.940087 |
| H | 1.050731  | 2.247067  | -0.518533 |
| H | 2.437416  | 1.148148  | -0.553562 |
| H | 2.230221  | 2.293810  | 0.786244  |

Rotational constants (GHz): 2.4970400 1.7266600 1.2267200  
 Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i496.7246 | 49.5525   | 137.9716  |
| 187.5956  | 204.0220  | 230.5085  |
| 247.8529  | 296.4585  | 305.8993  |
| 338.1240  | 385.6424  | 489.2445  |
| 518.9669  | 675.1625  | 701.3834  |
| 809.8982  | 851.4793  | 898.3264  |
| 939.7502  | 974.0931  | 987.0546  |
| 1036.7920 | 1068.7274 | 1119.1039 |
| 1127.7494 | 1188.9729 | 1260.2703 |

|           |           |           |
|-----------|-----------|-----------|
| 1300.0243 | 1314.2803 | 1345.7809 |
| 1369.1764 | 1394.4683 | 1403.4179 |
| 1426.4137 | 1463.4350 | 1490.6599 |
| 1495.2826 | 1501.1902 | 1507.2016 |
| 1514.6419 | 1522.9943 | 1575.3091 |
| 3030.5743 | 3065.1439 | 3070.4816 |
| 3086.0917 | 3092.1924 | 3136.4273 |
| 3140.6747 | 3145.0127 | 3152.8363 |
| 3158.6947 | 3160.7254 | 3181.1647 |

Zero-point correction (Hartree): 0.173311

TS.C2H5\_iC3H7\_COO.ringclose.pc

E(UM062X/Aug-CC-pVT2) (Hartree): -386.10953574

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.109515 | -0.059046 | -0.315980 |
| O | -0.638115 | -1.054657 | -0.906511 |
| O | -1.375021 | -1.526312 | 0.280205  |
| C | -0.877202 | 1.040434  | 0.327370  |
| C | 1.382598  | -0.024696 | -0.371344 |
| C | -2.389153 | 1.014719  | 0.186686  |
| H | -0.566643 | 1.091505  | 1.376217  |
| H | -0.463991 | 1.951290  | -0.124042 |
| H | 1.649163  | -0.462498 | -1.336876 |
| C | 2.035662  | 1.337464  | -0.194619 |
| C | 1.837140  | -1.016523 | 0.722810  |
| H | 1.799174  | 1.765773  | 0.779707  |
| H | 1.727652  | 2.043073  | -0.965543 |
| H | 3.117757  | 1.227905  | -0.252477 |
| H | 1.340014  | -1.977064 | 0.607370  |
| H | 1.600117  | -0.623487 | 1.711739  |
| H | 2.915536  | -1.149287 | 0.651873  |
| H | -2.830996 | 0.310810  | 0.881850  |
| H | -2.673751 | 0.702815  | -0.816990 |
| H | -2.786127 | 2.012811  | 0.368095  |

Rotational constants (GHz): 2.8985100 1.5812700 1.1992700

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i446.4869 | 70.0403   | 115.3803  |
| 185.5987  | 200.2867  | 220.5729  |
| 260.4094  | 285.4728  | 325.3034  |
| 337.2923  | 346.6448  | 487.1892  |
| 517.6918  | 591.5040  | 742.6695  |
| 785.2308  | 837.8411  | 900.6987  |
| 941.2408  | 980.8711  | 995.3296  |
| 1023.8280 | 1072.6182 | 1125.9813 |
| 1129.7080 | 1184.1660 | 1230.2960 |
| 1272.5358 | 1288.8832 | 1361.3582 |
| 1396.6374 | 1414.9840 | 1420.2453 |
| 1426.7375 | 1437.3542 | 1489.3908 |
| 1490.8012 | 1492.1289 | 1502.1710 |
| 1507.7894 | 1515.1286 | 1577.1256 |
| 3030.7793 | 3062.6925 | 3064.6591 |
| 3066.5386 | 3070.6286 | 3080.7611 |
| 3137.2474 | 3141.1953 | 3142.9382 |
| 3144.9656 | 3164.4744 | 3194.8647 |

Zero-point correction (Hartree): 0.172660

TS.C2H5\_iC3H7\_COO.ringclose.pm

E(UM062X/Aug-CC-pVT2) (Hartree): -386.10598667

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.273778  | 0.240470  | -0.207627 |
| O | 0.714806  | 1.213818  | -0.900230 |
| O | 1.158874  | 2.001230  | 0.273102  |
| C | 1.154490  | -0.564293 | 0.691757  |
| C | -1.171423 | -0.065856 | -0.413574 |
| C | 1.604823  | -1.838557 | -0.044534 |
| H | 2.011246  | 0.039131  | 0.961708  |
| H | 0.608526  | -0.823179 | 1.599772  |
| H | -1.404336 | 0.240786  | -1.435304 |
| C | -1.642582 | -1.488009 | -0.149654 |
| C | -1.873838 | 0.936000  | 0.537673  |
| H | -1.326924 | -1.839672 | 0.833008  |
| H | -1.280995 | -2.186112 | -0.901636 |
| H | -2.731560 | -1.509330 | -0.171468 |
| H | -1.512673 | 1.948817  | 0.374447  |
| H | -1.685740 | 0.666276  | 1.577150  |
| H | -2.946233 | 0.889839  | 0.354871  |
| H | 2.117382  | -1.579536 | -0.969929 |
| H | 0.782627  | -2.509262 | -0.278404 |
| H | 2.307752  | -2.376659 | 0.588557  |

Rotational constants (GHz): 2.1717300 2.0034200 1.2323900

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i466.4194 | 72.5658   | 89.1247   |
| 166.7702  | 202.3595  | 222.8338  |
| 238.3816  | 283.4245  | 302.5245  |
| 344.5112  | 367.3234  | 465.3720  |
| 503.6283  | 672.8202  | 727.1488  |
| 805.9003  | 830.9505  | 897.6578  |
| 943.0266  | 964.9066  | 990.9117  |
| 1014.3257 | 1045.6035 | 1113.3576 |
| 1122.0823 | 1187.6590 | 1241.0817 |
| 1283.3531 | 1293.0483 | 1327.7920 |
| 1376.3902 | 1394.9664 | 1408.9697 |
| 1426.0970 | 1480.9649 | 1489.0166 |
| 1489.7285 | 1502.6871 | 1505.0415 |
| 1514.5383 | 1521.7120 | 1572.8136 |
| 3067.6281 | 3070.1077 | 3079.8927 |
| 3080.8644 | 3093.7312 | 3137.5789 |
| 3143.1995 | 3148.6741 | 3150.1746 |



3166.1698 3169.7049 3202.9038  
 Zero-point correction (Hartree): 0.172945

TS.C2H5\_iC3H7\_COO.ringclose.pp

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E(UM062X/Aug-CC-pVTZ) (Hartree): -386.11062164

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.265006 | -0.261722 | -0.505370 |
| O | -0.941005 | -1.317603 | -0.735934 |
| O | -1.920706 | -1.019573 | 0.323736  |
| C | -0.857318 | 1.104296  | -0.581004 |
| C | 1.187709  | -0.496250 | -0.254174 |
| C | -0.922532 | 1.837951  | 0.761512  |
| H | -0.226119 | 1.672666  | -1.272613 |
| H | -1.856683 | 1.000941  | -0.993319 |
| H | 1.441959  | -1.372451 | -0.856847 |
| C | 2.116403  | 0.663421  | -0.583733 |
| C | 1.292188  | -0.923070 | 1.226536  |
| H | 1.893846  | 1.540804  | 0.022542  |
| H | 2.053861  | 0.946566  | -1.633910 |
| H | 3.144739  | 0.370648  | -0.375830 |
| H | 0.593873  | -1.728101 | 1.445672  |
| H | 1.069275  | -0.085020 | 1.885664  |
| H | 2.309081  | -1.258783 | 1.424220  |
| H | 0.060282  | 1.953024  | 1.216669  |
| H | -1.559919 | 1.277023  | 1.439857  |
| H | -1.339163 | 2.832336  | 0.612881  |

Rotational constants (GHz): 2.4045400 1.7812400 1.3896100

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i484.6443 | 90.7043   | 154.4310  |
| 180.7037  | 206.7754  | 220.3118  |
| 236.4339  | 254.7369  | 321.9994  |
| 341.8742  | 404.2159  | 472.0974  |
| 502.0886  | 652.2322  | 728.2399  |
| 807.9382  | 845.1906  | 902.7306  |
| 942.2673  | 969.3917  | 985.6607  |
| 1038.7544 | 1063.9884 | 1124.7088 |
| 1132.1057 | 1189.0122 | 1250.0056 |
| 1292.1796 | 1309.1231 | 1346.5086 |
| 1371.5141 | 1396.3222 | 1403.1182 |
| 1426.9834 | 1462.9168 | 1488.4636 |
| 1491.9053 | 1497.8662 | 1507.4128 |
| 1514.0809 | 1516.3048 | 1575.6790 |
| 3042.8027 | 3062.2525 | 3070.6020 |
| 3072.3546 | 3079.9961 | 3140.5936 |
| 3141.5819 | 3145.9607 | 3150.7015 |
| 3160.9572 | 3163.3983 | 3173.7277 |

Zero-point correction (Hartree): 0.173195

TS.C2H5\_iC3H7\_COO.ringclose.tc

~~~~~

E(UM062X/Aug-CC-pVTZ) (Hartree): -386.11000078

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.115161  | -0.149105 | -0.089580 |
| O | 0.235872  | 0.794149  | -0.932341 |
| O | 1.072317  | 1.636711  | -0.055133 |
| C | 1.249557  | -0.912467 | 0.497612  |
| C | -1.282656 | -0.553023 | 0.248313  |
| C | 2.647648  | -0.610105 | -0.010464 |
| H | 1.179131  | -0.813792 | 1.585844  |
| H | 0.981327  | -1.959362 | 0.300109  |
| H | -1.260062 | -1.517849 | 0.755419  |
| C | -1.799112 | 0.520917  | 1.224566  |
| C | -2.162380 | -0.625133 | -0.999151 |
| H | -1.767587 | 1.498878  | 0.746508  |
| H | -1.195505 | 0.566645  | 2.129631  |
| H | -2.826725 | 0.285086  | 1.498059  |
| H | -1.804803 | -1.377548 | -1.700939 |
| H | -2.179593 | 0.338720  | -1.504314 |
| H | -3.179472 | -0.882814 | -0.707585 |
| H | 3.036749  | 0.294591  | 0.441498  |
| H | 2.636860  | -0.457132 | -1.088534 |
| H | 3.304851  | -1.448812 | 0.216323  |

Rotational constants (GHz): 3.1777100 1.3866600 1.2857300

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i451.6188 | 45.5380   | 107.9724  |
| 168.1463  | 194.9854  | 212.0296  |
| 239.9718  | 262.3624  | 288.7801  |
| 336.0246  | 342.7398  | 464.9874  |
| 559.0655  | 613.5473  | 763.4437  |
| 793.9412  | 843.4183  | 890.9007  |
| 944.0069  | 984.0422  | 1011.0353 |
| 1040.0571 | 1074.9654 | 1114.0973 |
| 1123.9284 | 1159.7024 | 1199.0925 |
| 1274.5214 | 1327.1123 | 1371.7715 |
| 1395.7164 | 1406.7720 | 1418.6656 |
| 1429.3264 | 1438.9072 | 1486.7750 |
| 1489.9592 | 1490.6105 | 1502.0598 |
| 1503.4794 | 1519.0115 | 1584.8448 |
| 3014.9864 | 3062.6359 | 3069.3374 |
| 3072.0661 | 3080.3926 | 3092.7619 |
| 3143.4529 | 3144.2769 | 3147.3793 |
| 3154.1297 | 3158.4032 | 3195.5729 |

Zero-point correction (Hartree): 0.172580

TS.C2H5\_iC3H7\_COO.ringclose.tm

~~~~~

E(UM062X/Aug-CC-pVTZ) (Hartree): -386.10912168

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.246716  | 0.199588  | -0.074121 |
| O | 0.021543  | 1.073953  | -0.968634 |
| O | 0.505215  | 2.201222  | -0.142065 |
| C | 1.597427  | -0.042206 | 0.508210  |
| C | -0.906930 | -0.670398 | 0.300244  |
| C | 2.105238  | -1.420115 | 0.054346  |
| H | 2.260486  | 0.755651  | 0.195175  |
| H | 1.517109  | -0.012828 | 1.596971  |
| H | -0.547375 | -1.496994 | 0.911949  |
| C | -1.833193 | 0.218664  | 1.151411  |
| C | -1.632475 | -1.198024 | -0.937215 |
| H | -2.166097 | 1.072706  | 0.563904  |
| H | -1.326033 | 0.595451  | 2.038274  |
| H | -2.697227 | -0.367556 | 1.461501  |
| H | -0.986698 | -1.839805 | -1.535769 |
| H | -1.969921 | -0.369609 | -1.557564 |
| H | -2.501817 | -1.776279 | -0.627592 |
| H | 2.167917  | -1.469752 | -1.032272 |
| H | 1.470736  | -2.234906 | 0.399589  |
| H | 3.104158  | -1.582531 | 0.454174  |

Rotational constants (GHz): 2.2298500 1.7853900 1.3142600

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i471.4244 | 42.1295   | 80.9639   |
| 159.2612  | 192.2781  | 207.8999  |
| 230.9476  | 238.2887  | 265.8966  |
| 334.9180  | 376.9781  | 439.4214  |
| 559.8490  | 668.8349  | 743.7476  |
| 806.2272  | 839.8799  | 894.0264  |
| 945.5409  | 970.8039  | 985.2820  |
| 1035.6925 | 1050.5436 | 1115.7026 |
| 1118.0256 | 1185.5968 | 1217.8631 |
| 1264.6878 | 1316.2208 | 1330.7207 |
| 1391.9174 | 1401.1393 | 1408.6677 |
| 1424.6640 | 1471.4273 | 1485.9156 |
| 1489.4938 | 1501.3388 | 1503.8621 |
| 1506.7307 | 1518.6366 | 1584.6368 |
| 3069.7188 | 3069.9366 | 3071.4318 |
| 3080.0029 | 3101.5158 | 3141.0146 |
| 3141.9508 | 3147.5097 | 3150.0553 |
| 3153.6536 | 3157.7766 | 3189.0145 |

Zero-point correction (Hartree): 0.172640

TS.C2H5\_iC3H7\_COO.ringclose.tp

~~~~~

E (CCSD(T)/Aug-CC-pVTZ) (Hartree): -385.54286610

E (CCSD/Aug-CC-pVTZ) (Hartree): -385.46884059

T1 diagnostic: 0.027639

E (MP2/Aug-CC-pVTZ) (Hartree): -385.40644196

E (MP3/Aug-CC-pVTZ) (Hartree): -385.45397497

E (RHF/Aug-CC-pVTZ) (Hartree): -383.87771356

E (UM062X/Aug-CC-pVTZ) (Hartree): -386.11167337

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.130575  | 0.263192  | -0.370111 |
| O | -0.062450 | 1.502910  | -0.162715 |
| O | 1.080768  | 1.621281  | 0.766158  |
| C | 1.410164  | -0.287766 | -0.893524 |
| C | -1.042074 | -0.634112 | -0.153997 |
| C | 2.076744  | -1.270232 | 0.071667  |
| H | 1.139471  | -0.820684 | -1.813871 |
| H | 2.074508  | 0.539359  | -1.121169 |
| H | -0.816324 | -1.613721 | -0.577426 |
| C | -1.211835 | -0.761726 | 1.371213  |
| C | -2.303094 | -0.053212 | -0.795397 |
| H | -1.383872 | 0.223033  | 1.803169  |
| H | -0.328547 | -1.188100 | 1.843404  |
| H | -2.068102 | -1.401843 | 1.579878  |
| H | -2.198202 | 0.041859  | -1.875417 |
| H | -2.517898 | 0.929763  | -0.380190 |
| H | -3.146884 | -0.709771 | -0.588196 |
| H | 1.414943  | -2.099709 | 0.322847  |
| H | 2.348242  | -0.745497 | 0.984567  |
| H | 2.973243  | -1.685081 | -0.384249 |

Rotational constants (GHz): 2.5583300 1.6289400 1.3799300

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i472.7553 | 71.0810   | 122.0499  |
| 166.8036  | 197.8884  | 212.3373  |
| 242.1750  | 250.3380  | 283.9238  |
| 341.3706  | 396.7542  | 462.1463  |
| 556.5950  | 683.3403  | 743.4237  |
| 811.4837  | 845.6207  | 895.6125  |
| 945.1924  | 977.7985  | 986.3375  |
| 1052.6708 | 1063.1941 | 1110.6235 |
| 1120.1540 | 1187.3301 | 1225.4571 |
| 1278.8252 | 1326.8406 | 1343.7265 |
| 1390.3478 | 1400.5128 | 1402.3974 |
| 1424.3354 | 1462.0274 | 1486.2742 |
| 1489.3894 | 1499.5514 | 1503.3725 |
| 1512.6718 | 1519.9679 | 1585.4485 |
| 3020.9458 | 3069.6156 | 3071.0376 |
| 3071.5269 | 3087.4611 | 3138.6442 |
| 3143.4292 | 3149.2078 | 3153.2060 |
| 3156.3475 | 3165.0052 | 3173.0571 |

Zero-point correction (Hartree): 0.173088

Population analysis as 298K (%)

Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)

| Compound                      | Qtot      | Erel | Erel2 | n*Q*MB    | %    |
|-------------------------------|-----------|------|-------|-----------|------|
| TS.C2H5_iC3H7_COO.14Hshift.mp | 1.098e+41 | 0.00 | 0.00  | 2.196e+41 | 68.5 |
| TS.C2H5_iC3H7_COO.14Hshift.tp | 1.031e+41 | 0.58 | 0.58  | 7.727e+40 | 24.1 |

TS.C2H5\_ic3H7\_COO.14Hshift.pp 7.810e+40 1.58 1.58 1.090e+40 3.4  
 TS.C2H5\_ic3H7\_COO.14Hshift.cp 1.013e+41 1.83 1.83 9.296e+39 2.9  
 TS.C2H5\_ic3H7\_COO.14Hshift.cm 2.008e+41 3.24 3.24 1.680e+39 0.524  
 TS.C2H5\_ic3H7\_COO.14Hshift.mm 1.645e+41 3.23 3.23 1.411e+39 0.44  
 TS.C2H5\_ic3H7\_COO.14Hshift.tm 1.962e+41 3.98 3.98 4.718e+38 0.147  
 Total 3.206e+41 100

TS.C2H5\_ic3H7\_COO.14Hshift.cm

~~~~~  
 E(UM062X/Aug-CC-pVTZ) (Hartree): -386.11380899

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.076905 | -0.213857 | -0.118765 |
| O | -0.717141 | -1.206946 | -0.647619 |
| O | -2.022452 | -1.257682 | -0.155744 |
| C | -0.823886 | 0.617659  | 0.741866  |
| C | 1.404196  | -0.258443 | -0.317072 |
| H | -1.652167 | -0.441108 | 0.834335  |
| C | -1.890411 | 1.557068  | 0.160961  |
| H | -0.206706 | 1.100472  | 1.492818  |
| H | 1.597169  | -1.030728 | -1.063346 |
| C | 1.926024  | 1.089020  | -0.811458 |
| C | 2.077550  | -0.669944 | 0.997843  |
| H | 1.737061  | 1.866111  | -0.069967 |
| H | 1.448674  | 1.384445  | -1.744981 |
| H | 3.001129  | 1.032646  | -0.978380 |
| H | 1.706070  | -1.631807 | 1.347454  |
| H | 1.897644  | 0.074564  | 1.773332  |
| H | 3.153519  | -0.746030 | 0.845968  |
| H | -2.451018 | 1.066999  | -0.629654 |
| H | -1.425461 | 2.457271  | -0.241806 |
| H | -2.588582 | 1.855169  | 0.940882  |

Rotational constants (GHz): 2.8754700 1.4602900 1.1994100

Vibrational harmonic frequencies (cm-1):

|            |           |           |
|------------|-----------|-----------|
| i1612.6264 | 38.8189   | 118.4212  |
| 153.4426   | 207.9493  | 228.9872  |
| 248.1692   | 259.4318  | 282.6887  |
| 318.3055   | 368.0361  | 487.9424  |
| 614.9439   | 667.9794  | 768.5473  |
| 845.1231   | 884.6936  | 913.1317  |
| 940.9222   | 981.5776  | 1007.6645 |
| 1020.1321  | 1076.1241 | 1095.1064 |
| 1113.4579  | 1132.7003 | 1197.0600 |
| 1269.3560  | 1323.7236 | 1338.8957 |
| 1362.6654  | 1393.8912 | 1399.8050 |
| 1420.8066  | 1474.6310 | 1489.7499 |
| 1492.4492  | 1504.8640 | 1505.7331 |
| 1507.8824  | 1521.4015 | 1559.1847 |
| 1875.3500  | 3063.2088 | 3066.9078 |
| 3067.3264  | 3084.5637 | 3131.3951 |
| 3135.2752  | 3141.2455 | 3142.9303 |
| 3147.9902  | 3154.1594 | 3174.1305 |

Zero-point correction (Hartree): 0.170227

TS.C2H5\_ic3H7\_COO.14Hshift.cp

~~~~~  
 E(UM062X/Aug-CC-pVTZ) (Hartree): -386.11600586

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.353866 | -0.287730 | -0.078414 |
| O | -1.245466 | -1.208179 | 0.109080  |
| O | -2.524767 | -0.664003 | 0.113108  |
| C | -0.870192 | 1.012167  | -0.267193 |
| C | 1.050105  | -0.781857 | 0.087091  |
| H | -1.978723 | 0.571538  | 0.314770  |
| C | -0.045497 | 2.257482  | -0.039829 |
| H | -1.515437 | 1.048288  | -1.148102 |
| H | 0.960635  | -1.849357 | 0.294835  |
| C | 1.837714  | -0.590097 | -1.210470 |
| C | 1.758374  | -0.120430 | 1.273646  |
| H | 1.923959  | 0.467110  | -1.460001 |
| H | 1.358797  | -1.101488 | -2.044043 |
| H | 2.843220  | -0.992835 | -1.091687 |
| H | 1.147253  | -0.152067 | 2.174881  |
| H | 2.007548  | 0.916197  | 1.057023  |
| H | 2.687636  | -0.653260 | 1.471907  |
| H | 0.848327  | 2.305563  | -0.664801 |
| H | 0.266210  | 2.346478  | 0.998974  |
| H | -0.647387 | 3.134075  | -0.270247 |

Rotational constants (GHz): 2.4969800 1.5803300 1.2390000

Vibrational harmonic frequencies (cm-1):

|            |           |           |
|------------|-----------|-----------|
| i1585.8556 | 56.4390   | 158.7017  |
| 183.5215   | 195.8958  | 230.9255  |
| 256.9441   | 289.5589  | 304.4812  |
| 329.5501   | 371.2054  | 466.9525  |
| 561.3668   | 631.1415  | 686.7292  |
| 825.6255   | 829.8441  | 912.6930  |
| 938.9372   | 979.6568  | 1015.8225 |
| 1024.8792  | 1058.0820 | 1110.0547 |
| 1132.1528  | 1157.5575 | 1199.2963 |
| 1298.5942  | 1332.9525 | 1343.2770 |
| 1391.1273  | 1399.3718 | 1415.2288 |
| 1425.4071  | 1461.9367 | 1489.4137 |
| 1492.0400  | 1498.7628 | 1507.9882 |
| 1516.6798  | 1523.6274 | 1575.1199 |
| 1878.3084  | 3061.2175 | 3069.2047 |
| 3073.0123  | 3083.5429 | 3084.0832 |
| 3125.1435  | 3141.5005 | 3143.0198 |
| 3146.2055  | 3147.9233 | 3160.6642 |

Zero-point correction (Hartree): 0.170164

TS.C2H5\_ic3H7\_COO.14Hshift.mm

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~~~~~
E(UM062X/Aug-CC-pVTZ) (Hartree): -386.11379354
Electronic state : 1-A
Cartesian coordinates (Angs):
C      -0.070614      -0.091982      0.203346
O      -0.308893      -1.239765     -0.343154
O      -1.660551      -1.563916     -0.213658
C      -1.189740      0.593378      0.723307
C       1.372263      0.259283      0.380890
H      -1.768468      -0.625867      0.727692
C      -2.224639      1.212004     -0.226200
H      -0.922170      1.254430      1.541680
H       1.458728      0.562982      1.429033
C       2.321590      -0.898484      0.101631
C       1.692999      1.482281     -0.488403
H       2.254777      -1.207148     -0.941160
H       2.092429      -1.762950      0.721465
H       3.345995      -0.587156      0.300583
H       1.024176      2.313103     -0.267925
H       1.594551      1.230604     -1.544886
H       2.717804      1.804352     -0.309234
H      -2.425790      0.553301     -1.065984
H      -1.867963      2.169366     -0.607497
H      -3.159666      1.385550      0.303303
Rotational constants (GHz):   2.9461400      1.5461200      1.1288200
Vibrational harmonic frequencies (cm-1):
i1592.2925      43.9395      125.1482
153.4597      210.2824      225.4207
250.0991      270.9102      281.9546
325.9992      386.0389      469.6922
604.6875      665.3729      765.2966
845.1641      884.0828      906.3285
936.8031      979.1855      1005.9605
1037.6362      1075.4917      1086.1583
1130.9613      1146.9933      1190.7605
1248.9108      1311.2999      1347.9234
1357.4328      1394.8598      1402.4972
1423.8366      1471.8387      1488.6604
1493.7042      1504.4712      1505.6246
1508.0347      1518.4418      1557.6339
1876.2877      3049.8237      3064.3308
3065.5388      3073.4068      3129.4307
3137.2642      3144.3384      3146.6116
3151.3716      3153.6711      3172.7345
Zero-point correction (Hartree): 0.170188

```

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TS.C2H5_iC3H7_COO.14Hshift.mp
~~~~~
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -385.54555898
E(CCSD/Aug-CC-pVTZ) (Hartree): -385.46960700
T1 diagnostic: 0.020644
E(MP2/Aug-CC-pVTZ) (Hartree): -385.42072035
E(MP3/Aug-CC-pVTZ) (Hartree): -385.45930387
E(RHF/Aug-CC-pVTZ) (Hartree): -383.86038545
E(UM062X/Aug-CC-pVTZ) (Hartree): -386.11865933
Electronic state : 1-A
Cartesian coordinates (Angs):
C 0.222442 -0.173164 0.041272
O 0.373387 -1.451597 0.147635
O 1.724997 -1.770277 0.253965
C 1.408864 0.588422 0.077506
C -1.162527 0.300380 -0.262162
H 2.036182 -0.534928 -0.251220
C 1.425741 1.986025 -0.493979
H 1.950742 0.466788 1.017278
H -1.052708 1.042077 -1.058040
C -2.092758 -0.813437 -0.726051
C -1.714959 1.018808 0.977275
H -2.228735 -1.553723 0.061390
H -1.698223 -1.325362 -1.601605
H -3.066969 -0.395132 -0.974865
H -1.054967 1.821116 1.303511
H -1.829016 0.311482 1.799050
H -2.692570 1.442958 0.752715
H 0.848174 2.694985 0.103228
H 1.032166 2.006497 -1.509778
H 2.448022 2.356028 -0.537632
Rotational constants (GHz): 2.2895700 1.7623500 1.1653000
Vibrational harmonic frequencies (cm-1):
i1588.5359 59.6597 148.4930
176.0154 191.7809 228.2566
256.6720 265.6071 287.9443
344.2642 402.0389 502.2631
552.4893 584.3890 710.5493
813.6636 835.4070 910.1619
936.4105 980.2376 1009.6118
1014.2472 1060.8754 1115.7026
1143.5436 1155.5756 1193.8332
1266.6945 1314.0270 1352.6923
1390.6415 1402.3129 1420.9544
1423.2674 1461.5180 1489.5218
1493.4299 1502.0957 1503.8528
1506.4357 1519.1643 1576.4003
1873.7867 3055.9210 3063.6115
3067.7744 3074.0179 3094.0479
3117.5241 3139.4389 3145.1551
3146.4133 3148.1559 3152.6718
Zero-point correction (Hartree): 0.169909

```

```

TS.C2H5_iC3H7_COO.14Hshift.pp
~~~~~
E(UM062X/Aug-CC-pVTZ) (Hartree): -386.11643576

```

Electronic state : 1-A  
 Cartesian coordinates (Angs):  

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.355085 | -0.219377 | -0.252031 |
| O | -1.250070 | -1.155029 | -0.259893 |
| O | -2.514876 | -0.631682 | -0.012790 |
| C | -0.856103 | 1.084249  | -0.053819 |
| C | 1.044064  | -0.757405 | -0.235213 |
| H | -1.912906 | 0.511767  | 0.486716  |
| C | 0.012344  | 2.224705  | 0.419598  |
| H | -1.572984 | 1.356986  | -0.831776 |
| H | 0.974493  | -1.736054 | -0.714536 |
| C | 2.031145  | 0.109231  | -1.010769 |
| C | 1.495720  | -0.985650 | 1.213860  |
| H | 2.232979  | 1.043501  | -0.489962 |
| H | 1.659733  | 0.344927  | -2.007478 |
| H | 2.975735  | -0.423182 | -1.116207 |
| H | 0.796306  | -1.631191 | 1.742026  |
| H | 1.575212  | -0.043365 | 1.754500  |
| H | 2.477158  | -1.458914 | 1.216863  |
| H | 0.576076  | 2.685005  | -0.392727 |
| H | 0.719701  | 1.911030  | 1.184788  |
| H | -0.614448 | 2.998658  | 0.859495  |

 Rotational constants (GHz): 2.4923900 1.6227600 1.2292500  
 Vibrational harmonic frequencies (cm-1):  

|            |           |           |
|------------|-----------|-----------|
| i1596.1968 | 72.4948   | 157.4300  |
| 191.5139   | 209.3037  | 229.8268  |
| 255.0787   | 274.9178  | 311.4549  |
| 323.5398   | 381.0180  | 466.4128  |
| 557.6926   | 630.6988  | 679.2454  |
| 822.2878   | 828.3829  | 911.6029  |
| 939.1207   | 980.4869  | 1003.1615 |
| 1020.9227  | 1065.2763 | 1114.2083 |
| 1143.3757  | 1155.8273 | 1200.2886 |
| 1294.8514  | 1324.9504 | 1339.7137 |
| 1394.5039  | 1401.0814 | 1418.3956 |
| 1426.4566  | 1462.3264 | 1489.2493 |
| 1492.7447  | 1497.2397 | 1510.9193 |
| 1513.6448  | 1522.4203 | 1578.7750 |
| 1877.0437  | 3066.4660 | 3070.5900 |
| 3072.6583  | 3077.0745 | 3084.9872 |
| 3126.7756  | 3140.3196 | 3141.8526 |
| 3148.7654  | 3152.6936 | 3156.1143 |

 Zero-point correction (Hartree): 0.170198

TS.C2H5\_iC3H7\_COO.14Hshift.tm  
 ~~~~~  
 E(UM062X/Aug-CC-pVTZ) (Hartree): -386.11275647
 Electronic state : 1-A
 Cartesian coordinates (Angs):

C	-0.088663	-0.038454	0.089550
O	-0.286702	1.220501	-0.138801
O	-1.542431	1.416305	-0.717597
C	-1.172035	-0.895264	-0.198389
C	1.334779	-0.414984	0.368242
H	-1.590635	0.111246	-0.991991
C	-2.423333	-0.871781	0.690973
H	-0.851998	-1.903050	-0.441490
H	1.309098	-1.170696	1.156142
C	1.921950	-1.059076	-0.897218
C	2.183603	0.768681	0.820190
H	1.937103	-0.333257	-1.710425
H	1.347345	-1.925881	-1.217803
H	2.944695	-1.377560	-0.699874
H	1.763324	1.251049	1.700945
H	2.257858	1.514664	0.030571
H	3.187330	0.421378	1.060674
H	-2.681584	0.144330	0.973941
H	-2.259540	-1.459122	1.594567
H	-3.267733	-1.302277	0.155845

 Rotational constants (GHz): 3.0684600 1.4056800 1.1858800
 Vibrational harmonic frequencies (cm-1):

i1608.6451	34.9858	134.7662
153.1429	208.4514	223.3222
241.6865	266.9079	276.6134
343.7774	388.2367	463.5419
632.1052	672.2951	749.0362
842.4515	885.3584	911.8645
939.2636	982.3833	1001.9539
1028.1304	1079.1667	1095.6126
1127.2638	1136.0585	1188.9582
1261.1035	1322.5133	1343.9990
1355.3462	1396.5051	1401.5538
1422.6032	1470.9819	1489.1359
1494.3060	1504.9186	1506.8314
1508.6891	1518.8789	1556.7579
1875.5104	3066.3075	3068.8525
3070.6470	3074.2827	3131.7587
3141.8119	3148.3785	3150.7374
3151.6955	3158.5495	3175.4506

 Zero-point correction (Hartree): 0.170351

TS.C2H5_iC3H7_COO.14Hshift.tp
 ~~~~~  
 E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -385.54506350  
 E(CCSD/Aug-CC-pVTZ) (Hartree): -385.46904190  
 T1 diagnostic: 0.021022  
 E(MP2/Aug-CC-pVTZ) (Hartree): -385.41989948  
 E(MP3/Aug-CC-pVTZ) (Hartree): -385.45854190  
 E(RHF/Aug-CC-pVTZ) (Hartree): -383.86002419  
 E(UM062X/Aug-CC-pVTZ) (Hartree): -386.11789441  
 Electronic state : 1-A  
 Cartesian coordinates (Angs):

```

C      -0.214027      -0.184505      -0.207313
O      -0.205123      -1.434394      0.119301
O      -1.504027      -1.879441      0.358753
C      -1.484609      0.419586      -0.282238
C      1.129431      0.477533      -0.204076
H      -1.904776      -0.558478      0.498743
C      -1.600547      1.923096      -0.214764
H      -2.130597      -0.061492      -1.019100
H      1.016071      1.427174      -0.728539
C      1.551359      0.755228      1.245077
C      2.171379      -0.379861      -0.922442
H      1.663764      -0.185172      1.783753
H      0.817585      1.365143      1.770461
H      2.506439      1.279180      1.255895
H      1.878451      -0.586388      -1.950770
H      2.302997      -1.330030      -0.407372
H      3.127051      0.142365      -0.933530
H      -1.305668      2.403317      -1.149978
H      -0.985520      2.338859      0.582407
H      -2.630517      2.209741      -0.011860
Rotational constants (GHz):      2.2926000      1.7219900      1.2203900
Vibrational harmonic frequencies (cm-1):
i1599.4971      68.6278      149.9252
162.7619      193.7604      224.4274
258.5882      264.3692      274.7364
355.2492      376.2880      510.9717
547.1276      617.2596      696.0758
820.4295      836.5363      911.5459
944.6581      981.0338      1001.0396
1011.6071      1064.1857      1127.8106
1135.5623      1157.8902      1191.9867
1256.8152      1342.1892      1366.7718
1388.4459      1398.8310      1418.8416
1422.7369      1461.6988      1490.0606
1493.7959      1502.1759      1505.3734
1509.8652      1521.8647      1581.5091
1872.3841      3058.9319      3066.7610
3071.8914      3087.7809      3094.0865
3121.5766      3142.7043      3144.7023
3146.1010      3146.9702      3152.7522
Zero-point correction (Hartree): 0.170070

Population analysis as 298K (%)
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)
Compound      Qtot      Erel      Erel2      n*Q*MB      %
-----
TS.C2H5_ic3H7_COO.14Hshift.cm 2.008e+41 0.01 0.01 3.918e+41 47.2
TS.C2H5_ic3H7_COO.14Hshift.mm 1.645e+41 0.00 0.00 3.290e+41 39.6
TS.C2H5_ic3H7_COO.14Hshift.tm 1.962e+41 0.75 0.75 1.100e+41 13.2
Total      8.308e+41 100

TS.C2H5_ic3H7_COO.14Hshift.cm
~~~~~
E(UM062X/Aug-CC-pVTZ) (Hartree): -386.11380899
Electronic state : 1-A
Cartesian coordinates (Angs):
C -0.076905 -0.213857 -0.118765
O -0.717141 -1.206946 -0.647619
O -2.022452 -1.257682 -0.155744
C -0.823886 0.617659 0.741866
C 1.404196 -0.258443 -0.317072
H -1.652167 -0.441108 0.834335
C -1.890411 1.557068 0.160961
H -0.206706 1.100472 1.492818
H 1.597169 -1.030728 -1.063346
C 1.926024 1.089020 -0.811458
C 2.077550 -0.669944 0.997843
H 1.737061 1.866111 -0.069967
H 1.448674 1.384445 -1.744981
H 3.001129 1.032646 -0.978380
H 1.706070 -1.631807 1.347454
H 1.897644 0.074564 1.773332
H 3.153519 -0.746030 0.845968
H -2.451018 1.066999 -0.629654
H -1.425461 2.457271 -0.241806
H -2.588582 1.855169 0.940882
Rotational constants (GHz): 2.8754700 1.4602900 1.1994100
Vibrational harmonic frequencies (cm-1):
i1612.6264 38.8189 118.4212
153.4426 207.9493 228.9872
248.1692 259.4318 282.6887
318.3055 368.0361 487.9424
614.9439 667.9794 768.5473
845.1231 884.6936 913.1317
940.9222 981.5776 1007.6645
1020.1321 1076.1241 1095.1064
1113.4579 1132.7003 1197.0600
1269.3560 1323.7236 1338.8957
1362.6654 1393.8912 1399.8050
1420.8066 1474.6310 1489.7499
1492.4492 1504.8640 1505.7331
1507.8824 1521.4015 1559.1847
1875.3500 3063.2088 3066.9078
3067.3264 3084.5637 3131.3951
3135.2752 3141.2455 3142.9303
3147.9902 3154.1594 3174.1305
Zero-point correction (Hartree): 0.170227

TS.C2H5_ic3H7_COO.14Hshift.mm
~~~~~
E(UM062X/Aug-CC-pVTZ) (Hartree): -386.11379354

```

Electronic state : 1-A  
 Cartesian coordinates (Angs):  

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.070614 | -0.091982 | 0.203346  |
| O | -0.308893 | -1.239765 | -0.343154 |
| O | -1.660551 | -1.563916 | -0.213658 |
| C | -1.189740 | 0.593378  | 0.723307  |
| C | 1.372263  | 0.259283  | 0.380890  |
| H | -1.768468 | -0.625867 | 0.727692  |
| C | -2.224639 | 1.212004  | -0.226200 |
| H | -0.922170 | 1.254430  | 1.541680  |
| H | 1.458728  | 0.562982  | 1.429033  |
| C | 2.321590  | -0.898484 | 0.101631  |
| C | 1.692999  | 1.482281  | -0.488403 |
| H | 2.254777  | -1.207148 | -0.941160 |
| H | 2.092429  | -1.762950 | 0.721465  |
| H | 3.345995  | -0.587156 | 0.300583  |
| H | 1.024176  | 2.313103  | -0.267925 |
| H | 1.594551  | 1.230604  | -1.544886 |
| H | 2.717804  | 1.804352  | -0.309234 |
| H | -2.425790 | 0.553301  | -1.065984 |
| H | -1.867963 | 2.169366  | -0.607497 |
| H | -3.159666 | 1.385550  | 0.303303  |

 Rotational constants (GHz): 2.9461400 1.5461200 1.1288200  
 Vibrational harmonic frequencies (cm-1):  

|            |           |           |
|------------|-----------|-----------|
| i1592.2925 | 43.9395   | 125.1482  |
| 153.4597   | 210.2824  | 225.4207  |
| 250.0991   | 270.9102  | 281.9546  |
| 325.9992   | 386.0389  | 469.6922  |
| 604.6875   | 665.3729  | 765.2966  |
| 845.1641   | 884.0828  | 906.3285  |
| 936.8031   | 979.1855  | 1005.9605 |
| 1037.6362  | 1075.4917 | 1086.1583 |
| 1130.9613  | 1146.9933 | 1190.7605 |
| 1248.9108  | 1311.2999 | 1347.9234 |
| 1357.4328  | 1394.8598 | 1402.4972 |
| 1423.8366  | 1471.8387 | 1488.6604 |
| 1493.7042  | 1504.4712 | 1505.6246 |
| 1508.0347  | 1518.4418 | 1557.6339 |
| 1876.2877  | 3049.8237 | 3064.3308 |
| 3065.5388  | 3073.4068 | 3129.4307 |
| 3137.2642  | 3144.3384 | 3146.6116 |
| 3151.3716  | 3153.6711 | 3172.7345 |

 Zero-point correction (Hartree): 0.170188

TS.C2H5\_iC3H7\_COO.14Hshift.tm  
 ~~~~~  
 E(UM062X/Aug-CC-pVTZ) (Hartree): -386.11275647
 Electronic state : 1-A
 Cartesian coordinates (Angs):

C	-0.088663	-0.038454	0.089550
O	-0.286702	1.220501	-0.138801
O	-1.542431	1.416305	-0.717597
C	-1.172035	-0.895264	-0.198389
C	1.334779	-0.414984	0.368242
H	-1.590635	0.111246	-0.991991
C	-2.423333	-0.871781	0.690973
H	-0.851998	-1.903050	-0.441490
H	1.309098	-1.170696	1.156142
C	1.921950	-1.059076	-0.897218
C	2.183603	0.768681	0.820190
H	1.937103	-0.333257	-1.710425
H	1.347345	-1.925881	-1.217803
H	2.944695	-1.377560	-0.699874
H	1.763324	1.251049	1.700945
H	2.257858	1.514664	0.030571
H	3.187330	0.421378	1.060674
H	-2.681584	0.144330	0.973941
H	-2.259540	-1.459122	1.594567
H	-3.267733	-1.302277	0.155845

 Rotational constants (GHz): 3.0684600 1.4056800 1.1858800
 Vibrational harmonic frequencies (cm-1):

i1608.6451	34.9858	134.7662
153.1429	208.4514	223.3222
241.6865	266.9079	276.6134
343.7774	388.2367	463.5419
632.1052	672.2951	749.0362
842.4515	885.3584	911.8645
939.2636	982.3833	1001.9539
1028.1304	1079.1667	1095.6126
1127.2638	1136.0585	1188.9582
1261.1035	1322.5133	1343.9990
1355.3462	1396.5051	1401.5538
1422.6032	1470.9819	1489.1359
1494.3060	1504.9186	1506.8314
1508.6891	1518.8789	1556.7579
1875.5104	3066.3075	3068.8525
3070.6470	3074.2827	3131.7587
3141.8119	3148.3785	3150.7374
3151.6955	3158.5495	3175.4506

 Zero-point correction (Hartree): 0.170351

 E-(C2H5)(tC4H9)COO
 #####

Population analysis as 298K (%)
 Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)

Compound	Qtot	Erel	Erel2	n*Q*MB	%

C2H5_tC4H9_COO.p	4.638e+41	0.00	0.00	9.275e+41	99.9
C2H5_tC4H9_COO.t	4.722e+41	3.85	3.85	7.069e+38	0.0762

Total 9.282e+41 100

C2H5_tC4H9_COO.p
~~~~~  
E (CCSD(T)/Aug-CC-pVTZ) (Hartree): -424.82059732  
E (CCSD/Aug-CC-pVTZ) (Hartree): -424.73853008  
T1 diagnostic: 0.023464  
E (MP2/Aug-CC-pVTZ) (Hartree): -424.67215243  
E (MP3/Aug-CC-pVTZ) (Hartree): -424.72510193  
E (RHF/Aug-CC-pVTZ) (Hartree): -422.95244655  
E (RM062X/Aug-CC-pVTZ) (Hartree): -425.45610740  
Electronic state : 1-A  
Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.292887  | -0.183753 | 0.173008  |
| O | 0.725039  | -1.318304 | -0.128470 |
| O | 2.060007  | -1.585956 | 0.061086  |
| C | 1.226928  | 0.841387  | 0.695948  |
| C | -1.182163 | 0.048445  | -0.028886 |
| C | 2.105876  | 1.393006  | -0.438609 |
| H | 0.667670  | 1.640761  | 1.176920  |
| H | 1.866107  | 0.339070  | 1.423331  |
| H | 1.506527  | 1.931866  | -1.171301 |
| H | 2.626583  | 0.572801  | -0.925947 |
| H | 2.840975  | 2.081287  | -0.026842 |
| C | -1.839226 | -1.142341 | -0.722370 |
| C | -1.820289 | 0.256635  | 1.354683  |
| C | -1.367343 | 1.314723  | -0.876871 |
| H | -1.737455 | -2.050717 | -0.131286 |
| H | -1.393317 | -1.324983 | -1.699055 |
| H | -2.900145 | -0.932769 | -0.858191 |
| H | -1.397958 | 1.116486  | 1.873277  |
| H | -1.689657 | -0.626359 | 1.980045  |
| H | -2.888889 | 0.431376  | 1.227282  |
| H | -0.926499 | 1.191500  | -1.866389 |
| H | -0.920763 | 2.189505  | -0.404287 |
| H | -2.433570 | 1.505635  | -0.999904 |

Rotational constants (GHz): 2.1589200 1.2836500 1.0333500  
Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| 64.1642   | 126.2940  | 177.9653  |
| 204.8907  | 214.1228  | 230.1599  |
| 260.7281  | 280.1175  | 300.2788  |
| 320.4896  | 337.6710  | 363.8248  |
| 385.5856  | 409.0054  | 476.7248  |
| 573.0337  | 677.6842  | 764.7779  |
| 816.9383  | 849.8496  | 951.1893  |
| 955.1649  | 966.9211  | 971.6686  |
| 986.8241  | 1032.6166 | 1045.9714 |
| 1077.7145 | 1102.3917 | 1185.8571 |
| 1236.4763 | 1259.6836 | 1279.2448 |
| 1322.5057 | 1375.2887 | 1396.0431 |
| 1398.8200 | 1409.2252 | 1436.0645 |
| 1467.0591 | 1482.5170 | 1487.8857 |
| 1488.7109 | 1500.7433 | 1505.8293 |
| 1509.2621 | 1516.8480 | 1528.7275 |
| 1629.0850 | 3060.5053 | 3062.5793 |
| 3070.6536 | 3076.2547 | 3083.5608 |
| 3134.4161 | 3135.8948 | 3137.2153 |
| 3139.3700 | 3143.8700 | 3145.6027 |
| 3151.7631 | 3152.5859 | 3171.7409 |

Zero-point correction (Hartree): 0.202772

C2H5\_tC4H9\_COO.t  
~~~~~  
E (RM062X/Aug-CC-pVTZ) (Hartree): -425.44978227
Electronic state : 1-A
Cartesian coordinates (Angs):

C	-0.444865	-0.235467	-0.030644
O	-0.857305	-1.420764	-0.079801
O	-2.206604	-1.647687	-0.019774
C	-1.483298	0.820292	0.074671
C	1.061036	-0.094894	-0.000399
C	-1.121558	2.290726	-0.063527
H	-2.247685	0.524661	-0.650936
H	-1.988769	0.610889	1.026131
H	-0.792492	2.531127	-1.072076
H	-0.352359	2.614774	0.633977
H	-2.012446	2.883113	0.137289
C	1.727150	-1.449328	-0.253878
C	1.548832	0.900875	-1.062739
C	1.452046	0.395707	1.404566
H	1.475707	-1.833594	-1.241663
H	1.424636	-2.190266	0.482746
H	2.807827	-1.321425	-0.196075
H	1.290982	1.927661	-0.821338
H	1.145714	0.658935	-2.046774
H	2.635514	0.836594	-1.120891
H	1.167965	-0.337051	2.159780
H	0.986674	1.347299	1.654100
H	2.533941	0.527418	1.444036

Rotational constants (GHz): 1.8074100 1.4747300 1.0015600
Vibrational harmonic frequencies (cm-1):

66.9435	115.3554	155.5513
197.7176	229.2870	249.7854
269.3323	299.0960	302.0694
317.5811	352.7855	373.7460
388.0484	417.3977	519.1602
572.0883	600.9141	710.3013
787.7075	846.9108	952.3623
956.3470	970.8653	974.0683
1011.0387	1030.9168	1056.3030
1099.0490	1112.6557	1189.8633
1235.1569	1256.4684	1277.5674

1327.7517	1384.8797	1397.3426
1405.8698	1422.9641	1432.3542
1440.4192	1480.7624	1489.0064
1490.4918	1502.8362	1504.3942
1514.3328	1521.6311	1531.8142
1594.3247	3032.4470	3061.7326
3064.7522	3067.6841	3072.6134
3084.7888	3131.3878	3134.6104
3144.0329	3146.5206	3151.6074
3156.9645	3163.5475	3176.2915

Zero-point correction (Hartree): 0.202585

Population analysis as 298K (%)

Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)

Compound	Qtot	Erel	Erel2	n*Q*MB	%
TS.tC4H9_C2H5_COO.isom.p	1.139e+42	0.00	0.00	3.418e+42	100
Total				3.418e+42	100

TS.tC4H9_C2H5_COO.isom.p

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E (CCSD(T)/Aug-CC-pVTZ) (Hartree): -424.75835418

E (CCSD/Aug-CC-pVTZ) (Hartree): -424.68336714

T1 diagnostic: 0.020633

E (MP2/Aug-CC-pVTZ) (Hartree): -424.59899373

E (MP3/Aug-CC-pVTZ) (Hartree): -424.66896735

E (PMP2/Aug-CC-pVTZ) (Hartree): -424.62406750

E (PMP3/Aug-CC-pVTZ) (Hartree): -424.69389982

E (PUHF/Aug-CC-pVTZ) (Hartree): -422.96095713

E (UHF/Aug-CC-pVTZ) (Hartree): -422.93568118

E (UM062X/Aug-CC-pVTZ) (Hartree): -425.39900418

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.244257  | 0.014211  | -0.570893 |
| O | 0.712130  | 1.328916  | -0.706493 |
| O | 1.350209  | 1.753194  | 0.362480  |
| C | -1.117776 | -0.143789 | 0.050120  |
| C | 1.286148  | -1.045772 | -0.663187 |
| C | -1.909682 | 1.161426  | -0.052159 |
| C | -1.889102 | -1.253429 | -0.675558 |
| C | -0.953640 | -0.527248 | 1.532150  |
| C | 2.394573  | -0.989848 | 0.398688  |
| H | 0.780355  | -2.009669 | -0.607647 |
| H | 1.748631  | -0.993969 | -1.653423 |
| H | 3.052993  | -1.850559 | 0.284342  |
| H | 1.977627  | -1.000535 | 1.404377  |
| H | 2.989902  | -0.085960 | 0.295364  |
| H | -2.004995 | 1.481884  | -1.090007 |
| H | -1.431545 | 1.962921  | 0.508905  |
| H | -2.909377 | 1.007199  | 0.354367  |
| H | -1.377525 | -2.213331 | -0.611416 |
| H | -2.025128 | -1.004782 | -1.728364 |
| H | -2.872756 | -1.371474 | -0.219032 |
| H | -0.387601 | 0.235059  | 2.067844  |
| H | -0.432560 | -1.480604 | 1.632681  |
| H | -1.935397 | -0.626371 | 1.999140  |

Rotational constants (GHz): 2.0781800 1.3481300 1.0851000

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i212.8417 | 30.0146   | 79.7549   |
| 138.0179  | 209.4418  | 245.5756  |
| 253.8290  | 268.8639  | 292.6684  |
| 308.7729  | 313.6099  | 350.4770  |
| 370.3164  | 386.7266  | 453.2113  |
| 495.0736  | 623.0921  | 694.8138  |
| 783.8811  | 834.9613  | 942.6917  |
| 958.5481  | 963.0052  | 968.2393  |
| 1015.3853 | 1031.2690 | 1047.9677 |
| 1065.1172 | 1157.0099 | 1178.7857 |
| 1199.3187 | 1224.0467 | 1263.6513 |
| 1294.3514 | 1321.2567 | 1370.4457 |
| 1391.8062 | 1400.4145 | 1409.8878 |
| 1429.4128 | 1470.8072 | 1480.5705 |
| 1487.2865 | 1490.5022 | 1498.8592 |
| 1504.5810 | 1506.8563 | 1510.3522 |
| 1524.5627 | 3044.1793 | 3048.9355 |
| 3058.3562 | 3063.0514 | 3072.6231 |
| 3112.5837 | 3120.1123 | 3128.6309 |
| 3132.8485 | 3134.4224 | 3138.9767 |
| 3143.0804 | 3144.3617 | 3160.8590 |

Zero-point correction (Hartree): 0.199894

Population analysis as 298K (%)

Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)

| Compound                      | Qtot      | Erel | Erel2 | n*Q*MB    | %    |
|-------------------------------|-----------|------|-------|-----------|------|
| TS.C2H5_tC4H9_COO.ringclose.c | 4.816e+41 | 0.25 | 0.25  | 6.347e+41 | 51.9 |
| TS.C2H5_tC4H9_COO.ringclose.m | 2.864e+41 | 0.00 | 0.00  | 5.729e+41 | 46.8 |
| TS.C2H5_tC4H9_COO.ringclose.p | 6.602e+41 | 2.63 | 2.63  | 1.555e+40 | 1.27 |
| Total                         |           |      |       | 1.223e+42 | 100  |

TS.C2H5\_tC4H9\_COO.ringclose.c

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E (RM062X/Aug-CC-pVTZ) (Hartree): -425.41898628

Electronic state : 1-A

Cartesian coordinates (Angs):

C	0.291815	-0.047301	-0.160395
O	0.649453	-1.174020	-0.632479
O	1.518271	-1.520121	0.508097
C	1.246610	1.050401	0.157366
C	-1.192619	0.143404	-0.007317

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C      2.704344      0.833901     -0.210933
H      0.841125      1.918681     -0.376727
H      1.129571      1.301809      1.216024
H      2.785048      0.328946     -1.172286
H      3.202246      0.212503      0.523757
H      3.205792      1.798556     -0.280217
C     -1.517439     -0.657709      1.275972
C     -1.625207      1.595829      0.168461
C     -1.922903     -0.489308     -1.197762
H     -1.037402     -0.215777      2.149005
H     -1.176627     -1.687102      1.183214
H     -2.597730     -0.640053      1.423402
H     -1.420352      2.188366     -0.723851
H     -1.137761      2.069032      1.020036
H     -2.700470      1.622214      0.344893
H     -1.659968     -1.538016     -1.309550
H     -1.685830      0.031518     -2.125920
H     -2.997035     -0.412853     -1.029068
Rotational constants (GHz):    2.3550800    1.2436000    1.0476000
Vibrational harmonic frequencies (cm-1):
i435.0079      47.6033      121.3966
173.7895      203.9690      211.8984
255.6638      267.2422      295.9722
315.2682      337.3928      349.6434
363.8460      370.0913      474.4862
560.4455      570.5797      718.6818
794.8238      834.8913      853.8673
951.6071      966.7185      977.2516
1001.7981     1017.4983      1049.5247
1073.1414     1082.5704      1146.1991
1215.4443     1261.4315      1277.8318
1310.6658     1394.4291      1399.3142
1411.7807     1417.1874      1432.5335
1438.3953     1478.3155      1487.4032
1489.3710     1493.1489      1501.2908
1502.4951     1511.0149      1525.8952
1562.8779     3032.1779      3060.9761
3063.0740     3067.5391      3069.3160
3081.4330     3131.1279      3134.7582
3136.2803     3141.5874      3145.0751
3157.0785     3166.3541      3196.5047
Zero-point correction (Hartree): 0.200665

TS.C2H5_tC4H9_COO.ringclose.m
~~~~~
E (CCSD(T)/Aug-CC-pVTZ) (Hartree): -424.78733647
E (CCSD/Aug-CC-pVTZ) (Hartree): -424.70401771
T1 diagnostic: 0.026742
E (MP2/Aug-CC-pVTZ) (Hartree): -424.63435417
E (MP3/Aug-CC-pVTZ) (Hartree): -424.68868102
E (RHF/Aug-CC-pVTZ) (Hartree): -422.91891059
E (RM062X/Aug-CC-pVTZ) (Hartree): -425.41989679
Electronic state : 1-A
Cartesian coordinates (Angs):
C      0.290314     -0.325373     -0.396110
O      0.399467     -1.594151     -0.471391
O      1.568842     -1.625208      0.424572
C      1.403533      0.582323     -0.807434
C     -1.058609      0.183432      0.028869
C      2.057459      1.369994      0.330936
H      2.151497     -0.039419     -1.291318
H      0.977229      1.280795     -1.534865
H      2.492435      0.669440      1.038680
H      1.348819      2.007189      0.857490
H      2.841267      2.007652     -0.073874
C     -2.156727     -0.745624     -0.501811
C     -1.016863      0.080954      1.572492
C     -1.338111      1.621303     -0.401537
H     -2.011231     -1.766634     -0.158897
H     -2.179993     -0.745049     -1.591855
H     -3.120506     -0.387632     -0.139772
H     -0.281536      0.760669      2.000360
H     -0.767178     -0.933013      1.880534
H     -2.003167      0.345368      1.955606
H     -1.387509      1.707280     -1.487628
H     -0.588674      2.319177     -0.033062
H     -2.303897      1.926995      0.000714
Rotational constants (GHz):    2.0212100    1.4509800    1.1234700
Vibrational harmonic frequencies (cm-1):
i478.3894      67.5177      157.7727
181.0573      197.2721      213.4580
234.7553      263.4257      284.6683
298.3843      350.1061      358.9372
372.2466      406.2939      490.6279
514.6684      663.4247      686.2434
810.0564      835.1763      862.4282
951.7185      965.2770      972.4058
976.3580      1029.0354      1044.8301
1070.1539      1077.2826      1187.8281
1217.5902      1259.5292      1281.4342
1334.4630      1351.0398      1394.1571
1396.6742      1406.0525      1432.4204
1463.0798      1476.7206      1488.4935
1492.6920      1495.4522      1503.5912
1507.3642      1517.6996      1525.2018
1558.3112      3047.2114      3062.6935
3065.4745      3068.8272      3080.0943
3131.0313      3135.5497      3139.7514
3143.0471      3153.6795      3154.7002
3160.3271      3167.6128      3173.1911
Zero-point correction (Hartree): 0.201182

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TS.C2H5_tC4H9_COO.ringclose.p
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E(RM062X/Aug-CC-pVTZ) (Hartree): -425.41536836
Electronic state : 1-A
Cartesian coordinates (Angs):
  C    0.422716    0.254609   -0.000434
  O    0.677931    1.254424    0.741367
  O    1.355510    2.052873   -0.308321
  C    1.513501   -0.541366   -0.634817
  C   -1.023957   -0.164743   -0.032176
  C    1.856310   -1.681610    0.346243
  H    1.186687   -0.947218   -1.589582
  H    2.375821    0.093427   -0.788364
  H    0.999663   -2.308918    0.586143
  H    2.246765   -1.266789    1.274007
  H    2.623196   -2.313696   -0.097097
  C   -1.774122    1.047722   -0.622993
  C   -1.305296   -1.394341   -0.891117
  C   -1.486706   -0.395500    1.415650
  H   -1.436849    1.262034   -1.636818
  H   -1.608525    1.934837   -0.016528
  H   -2.838705    0.813813   -0.649583
  H   -0.777067   -2.281022   -0.544849
  H   -1.044831   -1.219723   -1.934736
  H   -2.373097   -1.609549   -0.850338
  H   -1.278857    0.475453    2.033643
  H   -0.994382   -1.264775    1.852924
  H   -2.562031   -0.574872    1.414674
Rotational constants (GHz):    1.8339400    1.5144800    1.1127700
Vibrational harmonic frequencies (cm-1):
  i448.2100          41.0738          124.7526
  161.5496          181.2083          224.3679
  228.3099          261.5797          273.4480
  290.4961          331.4906          358.0621
  376.7465          381.1753          469.6099
  522.0280          656.4617          708.8306
  816.4279          830.8212          851.7662
  951.8540          963.6594          966.4127
  976.6986          1007.3913         1034.1030
  1053.6607         1078.9567         1177.5453
  1219.6569         1246.1611         1264.0175
  1300.6805         1340.8302         1392.1124
  1395.8058         1408.4711         1433.9534
  1476.6313         1482.2189         1489.7188
  1494.7128         1499.7810         1500.3341
  1506.8399         1518.0151         1524.8205
  1566.1272         3062.2872         3065.6649
  3070.9773         3078.3271         3122.1556
  3131.7284         3135.8296         3140.1017
  3145.8278         3154.1087         3157.3106
  3158.6977         3166.6762         3209.8030
Zero-point correction (Hartree): 0.200845

Population analysis as 298K (%)
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)
Compound      Qtot      Erel      Erel2  n*Q*MB      %
-----
TS.C2H5_tC4H9_COO.14Hshift.t  2.804e+41  0.00    0.00  5.609e+41  66.8
TS.C2H5_tC4H9_COO.14Hshift.m  6.064e+41  0.87    0.87  2.791e+41  33.2
Total                                8.400e+41 100

TS.C2H5_tC4H9_COO.14Hshift.m
~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -425.42320278
Electronic state : 1-A
Cartesian coordinates (Angs):
  C   -0.261875   -0.118664    0.039219
  O   -0.667526   -1.314934   -0.245408
  O   -2.000782   -1.481331    0.134475
  C   -1.241875    0.750168    0.566706
  C    1.228174    0.090162   -0.026291
  H   -1.901098   -0.388889    0.877685
  C   -2.351615    1.282721   -0.351405
  H   -0.822460    1.523115    1.201225
  H   -3.191680    1.634896    0.244448
  H   -2.710804    0.506274   -1.020550
  H   -1.983439    2.118532   -0.947416
  C    1.930451   -1.102228   -0.674820
  C    1.502648    1.366550   -0.829160
  C    1.736318    0.263641    1.414532
  H    1.569626   -1.269424   -1.689074
  H    1.772408   -2.015769   -0.104769
  H    3.000771   -0.900881   -0.718285
  H    1.016441    2.229702   -0.375005
  H    1.143226    1.268527   -1.854046
  H    2.576634    1.552420   -0.860233
  H    1.524231   -0.623714    2.010525
  H    1.283244    1.126726    1.899969
  H    2.816011    0.414512    1.390310
Rotational constants (GHz):    2.2986200    1.2299700    1.0132700
Vibrational harmonic frequencies (cm-1):
  i1596.5959          40.4593          121.1031
  154.3702          210.7293          220.5587
  247.5856          270.4140          282.6080
  294.5426          326.7707          337.3994
  362.6576          406.5658          471.0933
  585.5882          671.1804          767.0733
  818.0667          873.6162          890.9433
  956.1031          962.1952          972.8446
  1006.6949         1020.6368         1052.1038
  1058.3501         1080.9399         1098.6515

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1209.5224	1238.6857	1258.5219
1308.4183	1343.0480	1393.3862
1398.0786	1404.5546	1430.2223
1465.3020	1481.7686	1487.1715
1488.7969	1503.7994	1505.1462
1506.4062	1507.3359	1525.9136
1546.2785	1877.2746	3058.2096
3062.6582	3064.9847	3069.8515
3128.8402	3132.0504	3135.6050
3137.1818	3141.7338	3144.7408
3152.7594	3161.9700	3175.9301

Zero-point correction (Hartree): 0.198219

TS.C2H5_tC4H9_COO.14Hshift.t

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E (CCSD(T)/Aug-CC-pVTZ) (Hartree): -424.78785876

E (CCSD/Aug-CC-pVTZ) (Hartree): -424.70279246

T1 diagnostic: 0.019873

E (MP2/Aug-CC-pVTZ) (Hartree): -424.64668939

E (MP3/Aug-CC-pVTZ) (Hartree): -424.69204365

E (RHF/Aug-CC-pVTZ) (Hartree): -422.90049445

E (RM062X/Aug-CC-pVTZ) (Hartree): -425.42459818

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.401570  | -0.241883 | 0.106271  |
| O | 0.786016  | -1.473434 | -0.013132 |
| O | 2.172223  | -1.564402 | -0.073564 |
| C | 1.458544  | 0.692732  | 0.196198  |
| C | -1.092005 | -0.045309 | 0.005656  |
| H | 2.230048  | -0.240167 | -0.355666 |
| C | 1.318752  | 2.165143  | -0.110018 |
| H | 2.078192  | 0.474788  | 1.069663  |
| H | 0.571612  | 2.672734  | 0.503014  |
| H | 1.067423  | 2.335595  | -1.154852 |
| H | 2.272175  | 2.656575  | 0.073337  |
| C | -1.806547 | -1.385271 | -0.181535 |
| C | -1.569817 | 0.612588  | 1.307658  |
| C | -1.418957 | 0.864218  | -1.188786 |
| H | -1.589695 | -2.071237 | 0.635465  |
| H | -1.511974 | -1.865982 | -1.113000 |
| H | -2.881363 | -1.206503 | -0.207987 |
| H | -1.068802 | 1.563081  | 1.484013  |
| H | -1.384181 | -0.039170 | 2.161451  |
| H | -2.642805 | 0.796840  | 1.244101  |
| H | -0.967918 | 0.487252  | -2.107127 |
| H | -1.086904 | 1.886236  | -1.028509 |
| H | -2.500960 | 0.879336  | -1.322992 |

Rotational constants (GHz): 1.8911500 1.4484300 1.0148400

Vibrational harmonic frequencies (cm-1):

|            |           |           |
|------------|-----------|-----------|
| i1600.2340 | 57.6042   | 161.1386  |
| 200.2558   | 202.3421  | 246.0701  |
| 256.9698   | 275.6549  | 295.0766  |
| 308.8432   | 325.9078  | 351.9138  |
| 378.9665   | 411.6475  | 481.1547  |
| 566.6373   | 602.3510  | 659.7709  |
| 811.6424   | 831.3738  | 863.5491  |
| 958.1807   | 961.1589  | 971.6626  |
| 1011.7632  | 1022.8615 | 1048.8267 |
| 1061.2623  | 1067.7987 | 1154.9784 |
| 1226.6016  | 1241.2006 | 1255.5507 |
| 1311.1846  | 1378.6508 | 1397.5240 |
| 1402.9893  | 1421.9588 | 1426.4476 |
| 1452.6529  | 1480.8967 | 1488.3717 |
| 1488.6943  | 1499.7827 | 1504.4792 |
| 1508.1995  | 1516.2905 | 1528.5352 |
| 1556.2763  | 1878.2858 | 3060.9656 |
| 3064.7682  | 3066.6826 | 3071.2088 |
| 3079.2710  | 3125.7409 | 3132.3840 |
| 3133.7540  | 3143.8886 | 3148.0346 |
| 3149.0897  | 3152.2526 | 3171.9616 |

Zero-point correction (Hartree): 0.198228

Population analysis as 298K (%)

Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)

| Compound                     | Qtot      | Erel | Erel2 | n*Q*MB    | %   |
|------------------------------|-----------|------|-------|-----------|-----|
| TS.C2H5_tC4H9_COO.14Hshift.m | 6.064e+41 | 0.00 | 0.00  | 1.213e+42 | 100 |
| Total                        |           |      |       | 1.213e+42 | 100 |

TS.C2H5\_tC4H9\_COO.14Hshift.m

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E (RM062X/Aug-CC-pVTZ) (Hartree): -425.42320278

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-0.261875	-0.118664	0.039219
O	-0.667526	-1.314934	-0.245408
O	-2.000782	-1.481331	0.134475
C	-1.241875	0.750168	0.566706
C	1.228174	0.090162	-0.026291
H	-1.901098	-0.388889	0.877685
C	-2.351615	1.282721	-0.351405
H	-0.822460	1.523115	1.201225
H	-3.191680	1.634896	0.244448
H	-2.710804	0.506274	-1.020550
H	-1.983439	2.118532	-0.947416
C	1.930451	-1.102228	-0.674820
C	1.502648	1.366550	-0.829160
C	1.736318	0.263641	1.414532
H	1.569626	-1.269424	-1.689074
H	1.772408	-2.015769	-0.104769
H	3.000771	-0.900881	-0.718285

H	1.016441	2.229702	-0.375005
H	1.143226	1.268527	-1.854046
H	2.576634	1.552420	-0.860233
H	1.524231	-0.623714	2.010525
H	1.283244	1.126726	1.899969
H	2.816011	0.414512	1.390310

Rotational constants (GHz): 2.2986200 1.2299700 1.0132700

Vibrational harmonic frequencies (cm-1):

i1596.5959	40.4593	121.1031
154.3702	210.7293	220.5587
247.5856	270.4140	282.6080
294.5426	326.7707	337.3994
362.6576	406.5658	471.0933
585.5882	671.1804	767.0733
818.0667	873.6162	890.9433
956.1031	962.1952	972.8446
1006.6949	1020.6368	1052.1038
1058.3501	1080.9399	1098.6515
1209.5224	1238.6857	1258.5219
1308.4183	1343.0480	1393.3862
1398.0786	1404.5546	1430.2223
1465.3020	1481.7686	1487.1715
1488.7969	1503.7994	1505.1462
1506.4062	1507.3359	1525.9136
1546.2785	1877.2746	3058.2096
3062.6582	3064.9847	3069.8515
3128.8402	3132.0504	3135.6050
3137.1818	3141.7338	3144.7408
3152.7594	3161.9700	3175.9301

Zero-point correction (Hartree): 0.198219

Z-(iC3H7)(CH3)COO
#####

Population analysis as 298K (%)
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)
Compound Qtot Erel Erel2 n*Q*MB %

iC3H7_CH3_COO.t 1.458e+40 0.00 0.00 2.916e+40 96.9
iC3H7_CH3_COO.c 2.612e+40 1.98 1.98 9.286e+38 3.09
Total 3.009e+40 100

iC3H7_CH3_COO.c
~~~~~  
E(RM062X/Aug-CC-pVTZ) (Hartree): -346.83552231  
Electronic state : 1-A  
Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.752227 | -0.168525 | -0.000243 |
| O | -0.976230 | 1.060287  | 0.000251  |
| O | 0.074038  | 1.944571  | 0.000574  |
| C | 0.615986  | -0.766564 | -0.000342 |
| C | -1.962632 | -1.032585 | -0.000425 |
| C | 1.386094  | -0.392748 | -1.273517 |
| C | 1.385366  | -0.394187 | 1.273691  |
| H | 0.459346  | -1.847480 | -0.001022 |
| H | 1.557720  | 0.678932  | -1.304494 |
| H | 0.840333  | -0.690998 | -2.168951 |
| H | 2.340999  | -0.917400 | -1.268799 |
| H | 0.839249  | -0.693703 | 2.168481  |
| H | 1.556812  | 0.677487  | 1.306056  |
| H | 2.340412  | -0.918609 | 1.268830  |
| H | -2.869751 | -0.436047 | 0.000282  |
| H | -1.941242 | -1.682404 | 0.876631  |
| H | -1.941869 | -1.680984 | -0.878594 |

Rotational constants (GHz): 2.9537200 2.4148100 1.8921000

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| 75.2673   | 177.9920  | 188.8446  |
| 203.6315  | 228.2607  | 258.4622  |
| 293.5974  | 302.7730  | 366.0634  |
| 437.2505  | 626.3266  | 627.7188  |
| 757.0701  | 908.3109  | 938.1561  |
| 951.3880  | 982.9405  | 1029.3225 |
| 1035.3631 | 1131.0679 | 1138.9984 |
| 1186.6017 | 1262.6668 | 1342.8528 |
| 1383.3973 | 1396.1321 | 1403.2522 |
| 1441.0833 | 1468.1169 | 1473.3109 |
| 1481.9691 | 1497.5728 | 1504.7919 |
| 1528.6891 | 1659.2136 | 3059.3484 |
| 3066.1121 | 3068.5493 | 3070.6245 |
| 3116.0589 | 3133.0712 | 3133.9960 |
| 3180.1127 | 3181.4555 | 3182.6968 |

Zero-point correction (Hartree): 0.145530

iC3H7\_CH3\_COO.t  
~~~~~  
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -346.33139485
E(CCSD/Aug-CC-pVTZ) (Hartree): -346.26618048
T1 diagnostic: 0.026123
E(MP2/Aug-CC-pVTZ) (Hartree): -346.21682427
E(MP3/Aug-CC-pVTZ) (Hartree): -346.25340626
E(RHF/Aug-CC-pVTZ) (Hartree): -344.85924541
E(RM062X/Aug-CC-pVTZ) (Hartree): -346.83884222
Electronic state : 1-A
Cartesian coordinates (Angs):

C	-0.344626	0.560344	-0.006804
O	-1.570551	0.315388	-0.072895
O	-1.966731	-0.945693	-0.443613
C	0.653901	-0.497753	-0.306966
C	0.012355	1.932603	0.436683
C	2.026535	0.059261	-0.660589

C	0.711767	-1.433685	0.913601
H	0.228699	-1.068573	-1.134834
H	2.463034	0.611170	0.173260
H	1.989089	0.718681	-1.527541
H	2.698678	-0.764450	-0.896313
H	-0.280473	-1.816252	1.140892
H	1.113017	-0.906459	1.781016
H	1.372155	-2.270695	0.691519
H	-0.883604	2.503434	0.660983
H	0.592228	2.437503	-0.336697
H	0.645838	1.873463	1.324225
Rotational constants (GHz): 3.2919600 2.3148100 1.6591800			
Vibrational harmonic frequencies (cm-1):			
102.9474	194.6174	216.7117	
224.4457	257.8142	278.3658	
309.1014	313.1309	379.5371	
468.9877	613.2181	628.9942	
742.7296	910.5998	937.2737	
952.6627	982.3887	1000.9283	
1035.8907	1105.3431	1139.7536	
1192.5389	1307.5098	1320.0543	
1365.9858	1389.2236	1421.1018	
1425.2109	1463.3475	1471.7400	
1490.4764	1500.0796	1509.6178	
1519.4210	1642.5111	3059.0445	
3061.0700	3065.0199	3083.6362	
3121.9588	3129.5385	3133.2771	
3141.1511	3164.3962	3182.0551	
Zero-point correction (Hartree): 0.145701			

Population analysis as 298K (%)

Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)

Compound	Qtot	Erel	Erel2	n*Q*MB	%
TS.iC3H7_CH3_COO.ringclose.p	1.411e+40	0.00	0.00	2.822e+40	56.9
TS.iC3H7_CH3_COO.ringclose.c	1.674e+40	0.27	0.27	2.119e+40	42.7
TS.iC3H7_CH3_COO.ringclose.m	1.785e+40	3.18	3.18	1.659e+38	0.335
Total				4.958e+40	100

TS.iC3H7_CH3_COO.ringclose.c

~~~~~

E(RM062X/Aug-CC-pVT2) (Hartree): -346.80254199

Electronic state : 1-A

Cartesian coordinates (Angs):

|                                                           |           |           |           |
|-----------------------------------------------------------|-----------|-----------|-----------|
| C                                                         | -0.495694 | 0.383664  | -0.049087 |
| O                                                         | -1.609572 | 0.155607  | -0.616873 |
| O                                                         | -1.691519 | -1.229282 | -0.113433 |
| C                                                         | 0.736197  | -0.427809 | -0.300355 |
| C                                                         | -0.457792 | 1.590260  | 0.813737  |
| H                                                         | 0.445424  | -1.212717 | -0.992600 |
| C                                                         | 1.800405  | 0.476175  | -0.941471 |
| C                                                         | 1.254831  | -1.059284 | 0.990947  |
| H                                                         | 2.202032  | 1.200660  | -0.233192 |
| H                                                         | 1.412117  | 1.012154  | -1.807527 |
| H                                                         | 2.626817  | -0.148647 | -1.277854 |
| H                                                         | 0.508918  | -1.735241 | 1.401860  |
| H                                                         | 1.493816  | -0.296867 | 1.735323  |
| H                                                         | 2.167995  | -1.615605 | 0.782370  |
| H                                                         | -0.953698 | 1.294712  | 1.744482  |
| H                                                         | -1.067029 | 2.375433  | 0.367746  |
| H                                                         | 0.544651  | 1.937486  | 1.039205  |
| Rotational constants (GHz): 3.3869500 2.1636100 1.8328300 |           |           |           |
| Vibrational harmonic frequencies (cm-1):                  |           |           |           |
| i498.2812                                                 | 87.8371   | 155.8287  |           |
| 191.4444                                                  | 233.2168  | 252.3344  |           |
| 287.3143                                                  | 304.8213  | 362.2360  |           |
| 466.6320                                                  | 495.0863  | 541.0765  |           |
| 736.8946                                                  | 839.9097  | 911.2493  |           |
| 942.3681                                                  | 967.9953  | 985.6640  |           |
| 1018.2604                                                 | 1077.7934 | 1116.0513 |           |
| 1184.0644                                                 | 1291.6684 | 1320.5873 |           |
| 1348.2813                                                 | 1376.4307 | 1391.0964 |           |
| 1415.0870                                                 | 1453.2719 | 1476.1362 |           |
| 1489.7091                                                 | 1495.0172 | 1505.5580 |           |
| 1518.0246                                                 | 1588.8062 | 3052.7358 |           |
| 3059.3467                                                 | 3063.8747 | 3123.4470 |           |
| 3126.6346                                                 | 3132.9866 | 3138.8238 |           |
| 3153.2136                                                 | 3163.7880 | 3197.4332 |           |
| Zero-point correction (Hartree): 0.143616                 |           |           |           |

TS.iC3H7\_CH3\_COO.ringclose.m

~~~~~

E(RM062X/Aug-CC-pVT2) (Hartree): -346.79800840

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-0.469846	0.443475	-0.082138
O	-1.494614	-0.129757	-0.566475
O	-1.701701	-0.978459	0.631179
C	0.778513	-0.292857	0.344325
C	-0.502307	1.931714	-0.071691
H	0.670927	-0.473013	1.415601
C	0.902598	-1.634797	-0.377094
C	2.034090	0.559245	0.128811
H	1.027675	-1.474496	-1.449065
H	0.021280	-2.243972	-0.209067
H	1.784818	-2.158140	-0.011522
H	2.022539	1.482252	0.706445
H	2.167192	0.810091	-0.925036
H	2.904015	-0.015640	0.441382
H	-1.467689	2.289303	-0.412638
H	0.303756	2.341241	-0.679898

H -0.322286 2.267422 0.952894
 Rotational constants (GHz): 3.3147900 2.5184400 1.6373400
 Vibrational harmonic frequencies (cm-1):
 i543.6742 73.1557 118.2905
 196.4229 280.5223 286.4787
 321.3263 353.9164 384.3815
 423.7707 469.0015 570.2774
 735.7388 823.8672 905.3984
 932.7201 968.3280 978.3024
 996.6020 1110.5836 1155.1246
 1178.9688 1239.0865 1302.6533
 1339.2356 1387.0696 1395.6700
 1420.5822 1446.9854 1470.5090
 1488.8497 1501.4922 1511.3467
 1523.3066 1584.9292 3061.7862
 3065.8826 3068.4366 3079.9133
 3129.1706 3132.2160 3137.1826
 3147.6937 3194.1323 3194.3638
 Zero-point correction (Hartree): 0.143720

TS.iC3H7_CH3_COO.ringclose.p
 ~~~~~  
 E (CCSD(T)/Aug-CC-pVTZ) (Hartree): -346.29857519  
 E (CCSD/Aug-CC-pVTZ) (Hartree): -346.23252837  
 T1 diagnostic: 0.030301  
 E (MP2/Aug-CC-pVTZ) (Hartree): -346.17917834  
 E (MP3/Aug-CC-pVTZ) (Hartree): -346.21779876  
 E (RHF/Aug-CC-pVTZ) (Hartree): -344.82872114  
 E (RM062X/Aug-CC-pVTZ) (Hartree): -346.80303761  
 Electronic state : 1-A  
 Cartesian coordinates (Angs):  
 C -0.694771 0.091839 -0.254287  
 O -1.145228 -1.094595 -0.194795  
 O -0.344089 -1.461654 0.983990  
 C 0.745644 0.460112 -0.402796  
 C -1.726412 1.159969 -0.281987  
 H 0.720910 1.158583 -1.251834  
 C 1.227219 1.256783 0.816413  
 C 1.680810 -0.690400 -0.739622  
 H 1.240074 0.596359 1.681082  
 H 0.584379 2.110186 1.033513  
 H 2.233638 1.628167 0.629419  
 H 1.230268 -1.368670 -1.462820  
 H 1.915197 -1.263950 0.151006  
 H 2.598855 -0.284942 -1.165793  
 H -2.070645 1.274372 0.750954  
 H -2.582679 0.817744 -0.862370  
 H -1.350397 2.112315 -0.643044  
 Rotational constants (GHz): 3.1521600 2.5100000 1.8645600  
 Vibrational harmonic frequencies (cm-1):  
 i477.1332 86.8341 175.8907  
 189.8969 237.3691 250.9616  
 300.5571 329.0893 351.4055  
 440.4289 534.4239 561.7656  
 716.1499 846.0483 921.0848  
 938.1308 975.1076 996.8535  
 1024.1902 1105.4120 1137.0582  
 1172.7914 1245.3284 1300.6261  
 1373.9332 1390.2877 1414.4065  
 1420.1352 1458.3296 1476.5377  
 1480.8934 1492.8761 1499.5698  
 1518.4300 1584.7585 2996.5002  
 3053.4108 3067.0684 3073.7890  
 3124.5831 3138.0244 3140.0429  
 3160.1827 3183.4638 3183.6073  
 Zero-point correction (Hartree): 0.143680

Population analysis as 298K (%)  
 Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)  
 Compound Qtot Erel Erel2 n\*Q\*MB %  
 -----  
 TS.iC3H7\_CH3\_COO.14Hshift 1.641e+40 0.00 0.00 3.281e+40 100  
 Total 3.281e+40 100

TS.iC3H7\_CH3\_COO.14Hshift  
 ~~~~~  
 E (CCSD(T)/Aug-CC-pVTZ) (Hartree): -346.29817231
 E (CCSD/Aug-CC-pVTZ) (Hartree): -346.22972735
 T1 diagnostic: 0.022050
 E (MP2/Aug-CC-pVTZ) (Hartree): -346.19115552
 E (MP3/Aug-CC-pVTZ) (Hartree): -346.21956911
 E (RHF/Aug-CC-pVTZ) (Hartree): -344.80669897
 E (RM062X/Aug-CC-pVTZ) (Hartree): -346.80640816
 Electronic state : 1-A
 Cartesian coordinates (Angs):
 C -0.468497 0.505876 0.135801
 O -1.598214 -0.113837 -0.007703
 O -1.384968 -1.390397 -0.527776
 C 0.697496 -0.230254 -0.166655
 C -0.597775 1.967426 0.365900
 H -0.150756 -1.008988 -0.879343
 C 1.078204 -1.374928 0.784883
 C 1.897575 0.577373 -0.609720
 H 1.693068 -2.104203 0.258212
 H 0.204797 -1.883467 1.180532
 H 1.666514 -0.975031 1.613881
 H 2.375812 1.092945 0.228812
 H 1.645063 1.319601 -1.366059
 H 2.642684 -0.090269 -1.041996
 H -1.633497 2.232533 0.560632
 H -0.258700 2.498061 -0.525435

```

H          0.038456      2.279728      1.193341
Rotational constants (GHz):      3.0637700      2.6058500      1.6721500
Vibrational harmonic frequencies (cm-1):
i1620.8057      106.7655      164.4446
183.6721      184.4484      261.9752
272.1287      307.0423      350.8970
416.9400      566.1884      618.6678
703.2243      752.1480      957.3875
983.0517      988.3744      1005.4248
1034.7684      1063.2718      1107.6364
1177.2227      1238.0573      1331.6933
1390.1283      1390.9141      1418.6046
1431.9867      1466.3491      1483.1200
1489.2180      1497.4926      1506.7994
1508.7724      1580.8433      1867.3884
3037.1976      3051.9269      3069.9041
3106.3727      3116.9293      3131.5909
3134.8823      3175.1936      3176.8721
Zero-point correction (Hartree): 0.140809

```

```

#####
Z-(iC3H7) (C2H5) COO
#####

```

```

Population analysis as 298K (%)
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)
Compound      Qtot      Erel      Erel2 n*Q*MB      %
-----
iC3H7_C2H5_COO.pc 1.221e+41 0.00 0.00 1.221e+41 39.1
iC3H7_C2H5_COO.tc 1.217e+41 0.00 0.00 1.217e+41 39
iC3H7_C2H5_COO.tp 8.945e+40 1.08 1.08 1.443e+40 4.63
iC3H7_C2H5_COO.pm 8.946e+40 1.08 1.08 1.442e+40 4.62
iC3H7_C2H5_COO.mc 2.092e+41 1.73 1.73 1.118e+40 3.59
iC3H7_C2H5_COO.tm 1.774e+41 1.69 1.69 1.016e+40 3.26
iC3H7_C2H5_COO.pp 1.754e+41 1.70 1.70 9.998e+39 3.21
iC3H7_C2H5_COO.mp 2.117e+41 2.36 2.36 3.916e+39 1.26
iC3H7_C2H5_COO.mm 2.113e+41 2.36 2.36 3.905e+39 1.25
Total          3.118e+41 100

```

```

iC3H7_C2H5_COO.mc
~~~~~
E(RM062X/Aug-CC-pVT2) (Hartree): -386.14355811
Electronic state : 1-A
Cartesian coordinates (Angs):
C      -0.328925      -0.118461      -0.000229
O      -0.481300      1.120128      0.000196
O       0.619196      1.946483      0.000550
C       1.003178      -0.793629      -0.000369
C      -1.583614      -0.927179      -0.000468
C       1.793028      -0.464552      -1.273386
C       1.791948      -0.465867      1.273690
H       0.784395      -1.863974      -0.001036
H       2.024377      0.595954      -1.304692
H       1.230840      -0.732042      -2.168482
H       2.717024      -1.042006      -1.269386
H       1.229320      -0.735028      2.168010
H       2.022562      0.594765      1.306604
H       2.716364      -1.042642      1.269515
C      -2.872691      -0.123944      -0.000086
H      -1.526063      -1.591544      -0.869266
H      -1.525941      -1.592193      0.867826
H      -2.931913      0.516063      -0.878071
H      -2.931812      0.515392      0.878395
H      -3.729871      -0.793832      -0.000292
Rotational constants (GHz):      2.8784900      1.4420200      1.2334900
Vibrational harmonic frequencies (cm-1):
59.0923      115.8548      176.2214
194.0465      217.8727      225.9449
239.9298      258.8550      297.3296
298.0372      418.1569      454.1849
608.9973      633.5066      770.1990
798.6014      900.6930      938.5079
956.0477      985.6586      1012.3815
1076.8915      1093.2473      1137.1462
1140.3310      1168.3641      1225.7460
1282.6679      1341.9418      1370.1627
1384.8378      1402.7405      1423.5819
1441.1396      1455.7393      1482.5595
1498.2104      1500.9729      1505.0022
1506.6268      1528.6553      1658.6808
3039.3370      3062.8649      3064.1360
3067.5787      3068.9704      3082.3319
3132.0788      3133.0440      3156.9517
3157.3350      3178.4886      3179.8641
Zero-point correction (Hartree): 0.174299

```

```

iC3H7_C2H5_COO.mm
~~~~~
E(RM062X/Aug-CC-pVT2) (Hartree): -386.14281915
Electronic state : 1-A
Cartesian coordinates (Angs):
C       0.316196      0.350913      0.244168
O      -0.085969      1.481764      -0.103780
O      -1.374236      1.642467      -0.549982
C      -0.531993      -0.877709      0.213681
C       1.743371      0.293740      0.675824
C      -1.732190      -0.747187      1.160856
C      -0.959194      -1.224748      -1.218448
H       0.107334      -1.682140      0.584486
H      -2.392777      0.044031      0.819396
H      -1.411138      -0.527019      2.179176

```



```

H      -2.269494      -1.695063      1.172959
H      -0.093893      -1.354795      -1.869029
H      -1.588754      -0.436289      -1.620178
H      -1.514072      -2.162376      -1.199631
C       2.586752      -0.497120      -0.330733
H       2.120407      1.308477      0.783824
H       1.781025      -0.196326      1.651752
H       2.574533      -0.010853      -1.304966
H       2.212847      -1.513409      -0.450903
H       3.617968      -0.555420      0.011123
Rotational constants (GHz): 2.5133300 1.5978800 1.3181200
Vibrational harmonic frequencies (cm-1):
73.7938      87.4924      164.1911
200.7669      210.5620      220.6018
237.3800      258.4166      308.9164
359.0227      383.9619      437.0238
605.3552      716.7310      754.7141
805.8845      904.5965      939.2848
944.6331      985.9458      995.1541
1062.4702      1088.1400      1129.7939
1141.3599      1188.8234      1249.5890
1283.4188      1344.2640      1347.9255
1381.9724      1399.9967      1412.3120
1435.5713      1480.7717      1481.5003
1496.4549      1502.6904      1506.1285
1510.2957      1528.7412      1652.2293
3063.7854      3067.0732      3067.5091
3069.7448      3073.9735      3131.9478
3133.1280      3134.0789      3152.7367
3154.2314      3177.7160      3179.1459
Zero-point correction (Hartree): 0.174562

```

```

iC3H7_C2H5_COO.mp
~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -386.14281908
Electronic state : 1-A
Cartesian coordinates (Angs):
C      -0.316343      0.350655      0.243877
O       0.085772      1.481711      -0.103495
O       1.374002      1.642761      -0.549412
C       0.532070      -0.877817      0.213093
C      -1.743453      0.293168      0.675672
C       0.960798      -1.224051      -1.218723
C       1.731221      -0.747294      1.161625
H      -0.107388      -1.682627      0.582843
H       1.591644      -0.435947      -1.619089
H       0.096227      -1.352596      -1.870595
H       1.514598      -2.162319      -1.199971
H       1.408903      -0.528922      2.179937
H       2.391259      0.045134      0.821855
H       2.269687      -1.694524      1.172960
C      -2.586916      -0.497146      -0.331194
H      -1.780953      -0.197438      1.651336
H      -2.120528      1.307828      0.784330
H      -2.212715      -1.513225      -0.452324
H      -2.575177      -0.010131      -1.305059
H      -3.618004      -0.556098      0.010937
Rotational constants (GHz): 2.5132000 1.5977400 1.3181600
Vibrational harmonic frequencies (cm-1):
73.7343      87.4816      164.1100
200.6895      210.5296      220.4991
237.3763      258.3635      308.8716
359.0052      383.9598      437.0292
605.3632      716.7512      754.7013
805.9314      904.6118      939.2777
944.8116      985.9542      995.2264
1062.5513      1088.1117      1129.8556
1141.3374      1188.8201      1249.6078
1283.4330      1344.2510      1347.9708
1381.9906      1400.0250      1412.3661
1435.5587      1480.7812      1481.4922
1496.4452      1502.7115      1506.1124
1510.3006      1528.7277      1652.1995
3063.7650      3067.0412      3067.4639
3069.7075      3073.9494      3131.8645
3133.0791      3134.0181      3152.6724
3154.2285      3177.6973      3179.0237
Zero-point correction (Hartree): 0.174561

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iC3H7_C2H5_COO.pc
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E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -385.57418305
E(CCSD/Aug-CC-pVTZ) (Hartree): -385.50113156
T1 diagnostic: 0.024300
E(MP2/Aug-CC-pVTZ) (Hartree): -385.44208625
E(MP3/Aug-CC-pVTZ) (Hartree): -385.48826371
E(RHF/Aug-CC-pVTZ) (Hartree): -383.90712194
E(RM062X/Aug-CC-pVTZ) (Hartree): -386.14649342
Electronic state : 1-A
Cartesian coordinates (Angs):
C      -0.247870      0.048635      -0.143741
O      -0.721828      1.203851      -0.220951
O       0.139371      2.257594      -0.421921
C       1.219060      -0.169471      -0.248672
C      -1.226760      -1.046891      0.111523
C       1.840562      0.246189      1.096428
C       1.593726      -1.596169      -0.628133
H       1.561913      0.544747      -0.999788
H       1.514626      -0.426532      1.891868
H       1.560545      1.268380      1.339941
H       2.925464      0.183944      1.024470
H       1.161646      -1.892305      -1.583810

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H	1.275388	-2.312554	0.130585
H	2.676787	-1.670323	-0.714353
C	-2.665764	-0.586685	0.278891
H	-1.133331	-1.766819	-0.706359
H	-0.875172	-1.581655	1.000533
H	-3.017658	-0.078242	-0.616325
H	-2.758242	0.108732	1.110585
H	-3.310027	-1.442588	0.467852
Rotational constants (GHz):	2.3682700	1.7054600	1.1686100
Vibrational harmonic frequencies (cm-1):			
83.2437	111.9785		199.7183
202.9687	226.2807		243.1640
257.8207	281.9388		303.3891
327.9079	410.9804		515.8160
602.6019	620.3989		740.4100
796.4899	907.3459		938.9992
958.9187	984.6344		1006.9136
1043.7814	1086.1711		1121.8313
1143.2272	1191.4268		1261.0998
1281.9616	1317.8143		1349.8427
1385.7992	1417.1613		1423.8451
1426.1617	1452.7428		1489.6215
1499.3842	1500.9266		1507.1844
1509.6238	1519.4296		1638.0435
3045.6253	3058.7524		3062.6532
3076.6183	3082.8463		3084.0239
3130.0473	3133.6766		3141.3841
3157.5096	3158.0080		3163.5453
Zero-point correction (Hartree):	0.174470		

iC3H7_C2H5_COO.pm

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E(RM062X/Aug-CC-pVTZ) (Hartree): -386.14521482

Electronic state : 1-A

Cartesian coordinates (Angs):

|                                          |           |           |           |
|------------------------------------------|-----------|-----------|-----------|
| C                                        | -0.055336 | -0.465336 | -0.348828 |
| O                                        | -0.905864 | -1.380073 | -0.244920 |
| O                                        | -2.218066 | -1.040156 | -0.035588 |
| C                                        | -0.476981 | 0.957386  | -0.247913 |
| C                                        | 1.351640  | -0.932528 | -0.515149 |
| C                                        | -0.755276 | 1.283449  | 1.230657  |
| C                                        | 0.515179  | 1.929862  | -0.872616 |
| H                                        | -1.438852 | 0.993770  | -0.765336 |
| H                                        | 0.169871  | 1.283296  | 1.807716  |
| H                                        | -1.451676 | 0.561144  | 1.649860  |
| H                                        | -1.196954 | 2.276759  | 1.298140  |
| H                                        | 0.687731  | 1.714474  | -1.926912 |
| H                                        | 1.476588  | 1.917675  | -0.357579 |
| H                                        | 0.117927  | 2.941327  | -0.799874 |
| C                                        | 2.154593  | -0.748155 | 0.779273  |
| H                                        | 1.327978  | -1.983599 | -0.796221 |
| H                                        | 1.819387  | -0.369803 | -1.323683 |
| H                                        | 1.688392  | -1.294067 | 1.598094  |
| H                                        | 2.222724  | 0.300432  | 1.063530  |
| H                                        | 3.165411  | -1.127640 | 0.643781  |
| Rotational constants (GHz):              | 2.1786700 | 1.8379800 | 1.3080600 |
| Vibrational harmonic frequencies (cm-1): |           |           |           |
| 101.6447                                 | 121.5790  |           | 181.2715  |
| 211.8049                                 | 224.2384  |           | 247.3364  |
| 259.2429                                 | 298.4875  |           | 321.5358  |
| 364.6810                                 | 383.4135  |           | 471.2879  |
| 611.3806                                 | 678.5525  |           | 750.3303  |
| 800.4061                                 | 908.1142  |           | 938.9071  |
| 948.2061                                 | 983.4565  |           | 991.1787  |
| 1041.7099                                | 1093.3950 |           | 1122.9662 |
| 1144.8277                                | 1192.0398 |           | 1265.0560 |
| 1307.1273                                | 1317.4866 |           | 1355.4437 |
| 1374.1508                                | 1391.1223 |           | 1413.8652 |
| 1424.4708                                | 1480.2649 |           | 1492.7485 |
| 1498.8074                                | 1501.0626 |           | 1509.9990 |
| 1514.0023                                | 1520.2676 |           | 1628.1854 |
| 3064.1622                                | 3066.4429 |           | 3074.0824 |
| 3076.4025                                | 3086.8767 |           | 3132.9519 |
| 3135.8139                                | 3139.2932 |           | 3141.1238 |
| 3153.3513                                | 3158.0357 |           | 3163.8944 |
| Zero-point correction (Hartree):         | 0.174914  |           |           |

iC3H7\_C2H5\_COO.pp

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E(RM062X/Aug-CC-pVTZ) (Hartree): -386.14401319

Electronic state : 1-A

Cartesian coordinates (Angs):

C	0.116902	-0.393370	0.125961
O	-0.277966	-1.575884	0.000606
O	-1.499965	-1.807924	-0.580347
C	-0.750361	0.730110	-0.317695
C	1.445927	-0.247683	0.791065
C	-1.810080	0.918139	0.784810
C	-0.005017	2.025651	-0.609442
H	-1.268372	0.364155	-1.205280
H	-1.345418	1.271780	1.706960
H	-2.330557	-0.018985	0.969672
H	-2.533332	1.665254	0.461145
H	0.667896	1.927953	-1.459561
H	0.570385	2.370976	0.250764
H	-0.729530	2.802913	-0.849357
C	2.590747	-0.121708	-0.221736
H	1.417259	0.630250	1.437909
H	1.603153	-1.125479	1.415434
H	2.487084	0.768182	-0.838058
H	2.614754	-0.993093	-0.873817
H	3.541416	-0.060279	0.304335

Rotational constants (GHz): 2.2485100 1.8190600 1.2004700
Vibrational harmonic frequencies (cm-1):
66.1529 94.4647 175.1294
197.5748 226.5429 239.4891
266.7100 281.9691 312.2909
357.9992 392.4503 474.1459
606.1536 722.3494 729.7038
797.9703 903.9455 935.2668
948.7629 985.3243 992.1332
1056.3376 1067.9363 1124.0240
1137.4231 1189.4584 1267.1418
1310.5855 1322.6585 1345.8001
1377.3654 1388.4491 1415.1794
1422.3074 1480.7486 1489.1332
1497.7379 1506.8280 1507.9592
1512.6843 1521.8012 1627.8752
3058.3981 3065.1058 3079.9709
3084.0258 3091.1935 3130.2198
3133.2447 3136.0054 3144.7460
3153.4098 3160.5995 3168.4019
Zero-point correction (Hartree): 0.174693

iC3H7_C2H5_COO.tc

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E(RM062X/Aug-CC-pVTZ) (Hartree): -386.14649344

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.247863  | 0.048638  | -0.143967 |
| O | 0.721762  | 1.203903  | -0.221030 |
| O | -0.139554 | 2.257574  | -0.421883 |
| C | -1.219063 | -0.169488 | -0.248686 |
| C | 1.226729  | -1.046867 | 0.111561  |
| C | -1.593697 | -1.596159 | -0.628197 |
| C | -1.840324 | 0.246086  | 1.096618  |
| H | -1.562052 | 0.544818  | -0.999657 |
| H | -1.275086 | -2.312610 | 0.130355  |
| H | -1.161852 | -1.892163 | -1.584036 |
| H | -2.676780 | -1.670399 | -0.714116 |
| H | -1.560227 | 1.268256  | 1.340195  |
| H | -1.514298 | -0.426774 | 1.891912  |
| H | -2.925250 | 0.183958  | 1.024866  |
| C | 2.665748  | -0.586638 | 0.278875  |
| H | 0.875118  | -1.581441 | 1.000671  |
| H | 1.133295  | -1.767028 | -0.706152 |
| H | 2.758193  | 0.108982  | 1.110414  |
| H | 3.017683  | -0.078387 | -0.616437 |
| H | 3.310057  | -1.442450 | 0.468070  |

Rotational constants (GHz): 2.3682000 1.7055200 1.1686600

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| 83.3523   | 112.1259  | 199.7661  |
| 202.9910  | 226.3524  | 243.2098  |
| 257.8979  | 281.9910  | 303.4198  |
| 327.9131  | 411.0046  | 515.8431  |
| 602.5994  | 620.4365  | 740.4188  |
| 796.5148  | 907.2926  | 939.0196  |
| 958.9138  | 984.6380  | 1006.8895 |
| 1043.7557 | 1086.1820 | 1121.8094 |
| 1143.2003 | 1191.4351 | 1261.1226 |
| 1281.9567 | 1317.8005 | 1349.8639 |
| 1385.7948 | 1417.1724 | 1423.8636 |
| 1426.1711 | 1452.7694 | 1489.6204 |
| 1499.3947 | 1500.9322 | 1507.1873 |
| 1509.6337 | 1519.4325 | 1637.9900 |
| 3045.6200 | 3058.7008 | 3062.5749 |
| 3076.4411 | 3082.8340 | 3084.0122 |
| 3129.9786 | 3133.6158 | 3141.3139 |
| 3157.4691 | 3157.9955 | 3163.4372 |

Zero-point correction (Hartree): 0.174470

iC3H7\_C2H5\_COO.tm

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E(RM062X/Aug-CC-pVTZ) (Hartree): -386.14401299

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-0.117518	-0.392692	0.126456
O	0.275188	-1.575947	0.001193
O	1.496452	-1.810338	-0.580334
C	0.751487	0.729099	-0.317861
C	-1.446505	-0.244915	0.791160
C	0.008331	2.026123	-0.608746
C	1.812466	0.915236	0.783822
H	1.268054	0.362291	-1.205933
H	-0.565517	2.372458	0.252068
H	-0.665641	1.929960	-1.458199
H	0.734057	2.802042	-0.849316
H	2.331487	-0.022741	0.968298
H	1.349102	1.269671	1.706298
H	2.536628	1.661172	0.459498
C	-2.590911	-0.119239	-0.222176
H	-1.604606	-1.121939	1.416459
H	-1.417401	0.633643	1.437076
H	-2.615629	-0.991580	-0.872915
H	-2.486148	0.769624	-0.839789
H	-3.541602	-0.055991	0.303646

Rotational constants (GHz): 2.2483800 1.8192800 1.2003600

Vibrational harmonic frequencies (cm-1):

65.5755	94.3207	175.0508
197.2711	226.3371	239.3955
266.4548	281.6956	312.4049
357.9832	392.4702	474.1153
606.1977	722.3382	729.7305
797.9755	903.8704	935.1933

948.7264	985.2882	992.1425
1056.3236	1067.8555	1124.0300
1137.2975	1189.4025	1267.0884
1310.5320	1322.5804	1345.7615
1377.3359	1388.3887	1415.1370
1422.2929	1480.7809	1489.1508
1497.7171	1506.7843	1507.9857
1512.5982	1521.8150	1627.7865
3058.5349	3065.2159	3080.0730
3084.1437	3091.1973	3130.2747
3133.1947	3136.0349	3144.7507
3153.5145	3160.8172	3168.3828

Zero-point correction (Hartree): 0.174688

iC3H7_C2H5_COO.tp

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E(RM062X/Aug-CC-pVTZ) (Hartree): -386.14521476

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.055170  | -0.465269 | -0.348859 |
| O | 0.905446  | -1.380277 | -0.244943 |
| O | 2.217781  | -1.040631 | -0.035681 |
| C | 0.477174  | 0.957285  | -0.248024 |
| C | -1.351885 | -0.932133 | -0.515228 |
| C | -0.514941 | 1.930067  | -0.872333 |
| C | 0.755869  | 1.283285  | 1.230514  |
| H | 1.438887  | 0.993415  | -0.765794 |
| H | -1.476161 | 1.918093  | -0.356887 |
| H | -0.687977 | 1.714917  | -1.926584 |
| H | -0.117478 | 2.941455  | -0.799620 |
| H | 1.451719  | 0.560571  | 1.649867  |
| H | -0.169400 | 1.283917  | 1.807390  |
| H | 1.198265  | 2.276275  | 1.297882  |
| C | -2.154618 | -0.747932 | 0.779432  |
| H | -1.819575 | -0.369154 | -1.323587 |
| H | -1.328401 | -1.983166 | -0.796466 |
| H | -2.222533 | 0.300618  | 1.063913  |
| H | -1.688302 | -1.294192 | 1.597933  |
| H | -3.165482 | -1.127292 | 0.643932  |

Rotational constants (GHz): 2.1786400 1.8380900 1.3080500

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| 101.6876  | 121.5458  | 181.2818  |
| 211.6813  | 224.2507  | 247.3153  |
| 259.2684  | 298.5581  | 321.5746  |
| 364.6936  | 383.4386  | 471.2965  |
| 611.3979  | 678.5717  | 750.3824  |
| 800.4011  | 908.1124  | 938.8693  |
| 948.1341  | 983.4035  | 991.1435  |
| 1041.6112 | 1093.3882 | 1122.9610 |
| 1144.7692 | 1192.0408 | 1265.0184 |
| 1307.1019 | 1317.4302 | 1355.4264 |
| 1374.1510 | 1391.0944 | 1413.8215 |
| 1424.4895 | 1480.2495 | 1492.7343 |
| 1498.8028 | 1501.0611 | 1510.0058 |
| 1513.9775 | 1520.2498 | 1628.1000 |
| 3064.0920 | 3066.4214 | 3073.9793 |
| 3076.4099 | 3087.0224 | 3132.8974 |
| 3135.8389 | 3139.3132 | 3141.1047 |
| 3153.4242 | 3158.0353 | 3164.0550 |

Zero-point correction (Hartree): 0.174913

Population analysis as 298K (%)

Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)

| Compound                       | Qtot      | Erel | Erel2 | n*Q*MB    | %      |
|--------------------------------|-----------|------|-------|-----------|--------|
| TS.iC3H7_C2H5_COO.ringclose.cm | 4.308e+41 | 0.54 | 0.54  | 3.434e+41 | 35.5   |
| TS.iC3H7_C2H5_COO.ringclose.pm | 1.884e+41 | 0.34 | 0.34  | 2.120e+41 | 21.9   |
| TS.iC3H7_C2H5_COO.ringclose.pp | 1.060e+41 | 0.00 | 0.00  | 2.120e+41 | 21.9   |
| TS.iC3H7_C2H5_COO.ringclose.cp | 1.179e+41 | 0.29 | 0.29  | 1.438e+41 | 14.9   |
| TS.iC3H7_C2H5_COO.ringclose.pt | 8.270e+40 | 0.67 | 0.67  | 5.312e+40 | 5.49   |
| TS.iC3H7_C2H5_COO.ringclose.mt | 1.825e+41 | 3.21 | 3.21  | 1.626e+39 | 0.168  |
| TS.iC3H7_C2H5_COO.ringclose.mp | 1.900e+41 | 3.43 | 3.43  | 1.163e+39 | 0.12   |
| TS.iC3H7_C2H5_COO.ringclose.mm | 1.588e+41 | 3.65 | 3.65  | 6.738e+38 | 0.0696 |
| TS.iC3H7_C2H5_COO.ringclose.ct | 7.422e+40 | 3.55 | 3.55  | 3.681e+38 | 0.038  |
| Total                          |           |      |       | 9.682e+41 | 100    |

TS.iC3H7\_C2H5\_COO.ringclose.cm

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E(RM062X/Aug-CC-pVTZ) (Hartree): -386.10960057

Electronic state : 1-A

Cartesian coordinates (Angs):

C	0.236973	0.232985	-0.069899
O	0.800441	1.218566	-0.642493
O	-0.130223	2.211085	-0.067244
C	-1.206463	-0.107435	-0.273465
C	1.125724	-0.647125	0.738347
H	-1.611747	0.665645	-0.919829
C	-1.288604	-1.474313	-0.971179
C	-1.972287	-0.112125	1.048311
H	-0.998519	-2.290349	-0.309502
H	-0.666567	-1.512012	-1.865858
H	-2.320469	-1.646450	-1.275003
H	-1.942946	0.876859	1.499476
H	-1.550800	-0.835949	1.748668
H	-3.009351	-0.392555	0.867017
C	2.497046	-0.867636	0.101238
H	1.240858	-0.088751	1.676987
H	0.629574	-1.582846	0.983546
H	2.976149	0.083382	-0.116262
H	2.404248	-1.426673	-0.828859
H	3.133496	-1.433608	0.777392

Rotational constants (GHz): 2.3250600 1.7261200 1.2694400
 Vibrational harmonic frequencies (cm-1):
 i485.1427 25.0855 84.8239
 168.1543 197.5082 204.8799
 237.6067 274.6417 283.0454
 305.8330 373.9473 494.7624
 512.6714 593.2890 748.6124
 796.0571 845.5120 905.5269
 944.2822 976.5015 979.7049
 1030.4710 1071.2139 1101.5253
 1119.3566 1184.5215 1249.5564
 1256.2487 1317.1903 1350.7963
 1391.9562 1395.6870 1409.5575
 1416.5404 1457.5692 1489.5561
 1494.7430 1502.8539 1504.2337
 1509.7250 1516.9642 1580.3580
 3028.9107 3060.7044 3062.6326
 3081.0581 3123.6848 3131.0012
 3137.5869 3143.2616 3151.8885
 3154.5419 3162.3284 3172.2934
 Zero-point correction (Hartree): 0.172487

TS.iC3H7_C2H5_COO.ringclose.cp

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E(RM062X/Aug-CC-pVTZ) (Hartree): -386.11043354

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.214102  | 0.188165  | -0.433895 |
| O | 0.871287  | 1.208784  | -0.812386 |
| O | 0.750917  | 1.902521  | 0.487164  |
| C | -1.189420 | 0.264838  | 0.077811  |
| C | 0.904909  | -1.115378 | -0.619029 |
| H | -1.449329 | 1.319082  | 0.100581  |
| C | -2.105133 | -0.484256 | -0.903276 |
| C | -1.300832 | -0.315272 | 1.486972  |
| H | -1.938942 | -1.561028 | -0.877104 |
| H | -1.974841 | -0.135380 | -1.927575 |
| H | -3.140290 | -0.302371 | -0.616690 |
| H | -0.678485 | 0.251454  | 2.175893  |
| H | -0.994935 | -1.363549 | 1.508363  |
| H | -2.337351 | -0.266698 | 1.819039  |
| C | 2.000866  | -1.214707 | 0.459828  |
| H | 0.213928  | -1.951688 | -0.551461 |
| H | 1.373064  | -1.105318 | -1.605229 |
| H | 1.563547  | -1.245097 | 1.456038  |
| H | 2.657083  | -0.349175 | 0.404643  |
| H | 2.581970  | -2.121018 | 0.304814  |

Rotational constants (GHz): 2.3353600 1.7072500 1.4396500

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i479.1635 | 81.8693   | 101.7192  |
| 174.8883  | 195.8162  | 205.6942  |
| 247.3774  | 257.3640  | 278.8881  |
| 307.5577  | 397.1502  | 470.7448  |
| 516.4624  | 668.8406  | 745.4922  |
| 811.6402  | 841.6767  | 907.0308  |
| 942.9872  | 967.0145  | 977.9481  |
| 1015.9755 | 1069.6861 | 1101.3367 |
| 1124.3021 | 1183.8653 | 1247.5199 |
| 1273.5343 | 1318.4693 | 1349.3498 |
| 1351.7526 | 1391.8482 | 1408.3155 |
| 1416.5779 | 1479.0843 | 1488.9515 |
| 1494.3017 | 1496.7672 | 1505.3888 |
| 1509.2757 | 1519.6533 | 1584.2662 |
| 3058.6802 | 3064.4739 | 3078.2216 |
| 3081.8780 | 3123.4914 | 3133.1931 |
| 3139.6856 | 3149.0595 | 3155.3638 |
| 3159.1959 | 3160.0590 | 3170.3965 |

Zero-point correction (Hartree): 0.172918

TS.iC3H7\_C2H5\_COO.ringclose.ct

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E(RM062X/Aug-CC-pVTZ) (Hartree): -386.10514281

Electronic state : 1-A

Cartesian coordinates (Angs):

C	0.363226	0.464761	0.212877
O	1.416492	1.021269	0.668546
O	2.310196	0.330182	-0.276899
C	0.206012	-1.027557	0.203857
C	-0.667401	1.440725	-0.242278
H	1.140465	-1.403525	0.611174
C	-0.951836	-1.456019	1.121184
C	0.043149	-1.582433	-1.211074
H	-1.922883	-1.357002	0.642753
H	-0.963713	-0.896963	2.057629
H	-0.811346	-2.507495	1.369128
H	0.927473	-1.353354	-1.800356
H	-0.832941	-1.168281	-1.711576
H	-0.084924	-2.663547	-1.161451
C	-2.143431	1.077250	-0.297347
H	-0.495409	2.353107	0.331681
H	-0.295135	1.680069	-1.250522
H	-2.541974	0.878805	0.695194
H	-2.335497	0.209920	-0.923866
H	-2.695935	1.916299	-0.716281

Rotational constants (GHz): 2.2603800 1.8037700 1.3299700

Vibrational harmonic frequencies (cm-1):

i486.2837	96.0748	131.1594
180.6287	205.0163	221.4577
282.1971	285.3128	295.1565
306.1229	391.1954	448.8999
501.9976	562.6644	697.3650
777.0625	844.6996	910.0558

945.0533	973.5707	980.8909
1044.5019	1085.8716	1113.9359
1132.4499	1183.1186	1268.1813
1307.9479	1324.0814	1354.8178
1373.3196	1391.6406	1413.0177
1425.0947	1430.8462	1487.3117
1495.1461	1502.7027	1507.4637
1519.8215	1521.2192	1566.2433
3003.8745	3067.7650	3068.7426
3085.8010	3096.3680	3126.4006
3133.3588	3142.3284	3150.3635
3164.5553	3165.4488	3170.3343

Zero-point correction (Hartree): 0.172823

TS.iC3H7_C2H5_COO.ringclose.mmm

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E(RM062X/Aug-CC-pVTZ) (Hartree): -386.10523732

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.216063 | -0.260944 | 0.178053  |
| O | -0.217069 | -1.284449 | -0.572438 |
| O | 0.820582  | -2.037752 | 0.151141  |
| C | 0.958545  | 0.638254  | 0.409514  |
| C | -1.552989 | 0.116516  | 0.723480  |
| H | 1.016805  | 0.807434  | 1.489083  |
| C | 2.302045  | 0.181355  | -0.134733 |
| C | 0.564614  | 1.982850  | -0.254188 |
| H | 2.192742  | -0.179207 | -1.156846 |
| H | 2.713940  | -0.629372 | 0.453619  |
| H | 2.989612  | 1.027851  | -0.134412 |
| H | -0.383112 | 2.383377  | 0.099550  |
| H | 0.507757  | 1.858554  | -1.336351 |
| H | 1.340623  | 2.714698  | -0.040324 |
| C | -2.605485 | 0.250015  | -0.381523 |
| H | -1.817922 | -0.719536 | 1.378731  |
| H | -1.489586 | 1.014502  | 1.332569  |
| H | -2.639755 | -0.654550 | -0.984067 |
| H | -2.376619 | 1.092467  | -1.033099 |
| H | -3.586593 | 0.413109  | 0.058300  |

Rotational constants (GHz): 2.5684800 1.7722100 1.1886800

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i435.8125 | 42.5649   | 91.3515   |
| 191.9526  | 210.5419  | 230.4292  |
| 256.7476  | 305.1013  | 322.8288  |
| 347.7203  | 405.8878  | 437.1896  |
| 571.0812  | 606.4827  | 769.0009  |
| 806.3680  | 846.5024  | 889.4097  |
| 935.3662  | 977.5960  | 983.9688  |
| 1052.4489 | 1079.2658 | 1114.2796 |
| 1120.7420 | 1147.4771 | 1208.0516 |
| 1257.5253 | 1275.3075 | 1351.4918 |
| 1388.4655 | 1404.3405 | 1417.5512 |
| 1426.9477 | 1479.7132 | 1484.4293 |
| 1488.1814 | 1503.7346 | 1507.9985 |
| 1511.9015 | 1516.8228 | 1574.6146 |
| 3053.3716 | 3054.8753 | 3069.3336 |
| 3073.1670 | 3078.4788 | 3137.7631 |
| 3139.5296 | 3145.6573 | 3151.6495 |
| 3158.1550 | 3168.4361 | 3197.1549 |

Zero-point correction (Hartree): 0.173065

TS.iC3H7\_C2H5\_COO.ringclose.mp

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E(RM062X/Aug-CC-pVTZ) (Hartree): -386.10542481

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-0.256386	-0.053064	0.265227
O	-0.444515	0.961980	1.004135
O	-0.200750	1.988161	-0.025458
C	1.019351	-0.391390	-0.440768
C	-1.400821	-1.004585	0.217820
H	0.739351	-0.733995	-1.442033
C	2.089786	0.683988	-0.521956
C	1.581402	-1.613830	0.331162
H	2.239566	1.142684	0.454259
H	1.809614	1.471109	-1.211533
H	3.026363	0.225248	-0.841369
H	0.873663	-2.433992	0.425985
H	1.893321	-1.305720	1.329416
H	2.457814	-1.982170	-0.197871
C	-2.488087	-0.343412	-0.651100
H	-1.114087	-1.968984	-0.192234
H	-1.779125	-1.132160	1.233695
H	-2.139504	-0.212578	-1.674253
H	-2.741427	0.636412	-0.253153
H	-3.374899	-0.973217	-0.662630

Rotational constants (GHz): 2.6183500 1.7140200 1.2439300

Vibrational harmonic frequencies (cm-1):

i428.2638	50.5544	77.8816
177.3906	192.8355	203.8339
257.9763	287.2455	312.6004
349.2251	393.0570	439.5295
532.4883	695.9113	738.8169
814.9296	844.1974	892.2375
935.0688	970.2198	981.5942
1024.0344	1084.4746	1095.2192
1131.1686	1166.7360	1217.7181
1259.6124	1272.4302	1328.8791
1391.8653	1404.4535	1418.4747
1426.8523	1479.0541	1481.8503
1486.1339	1496.4116	1504.3731
1507.5571	1516.0816	1576.3533

3049.9547	3070.8114	3074.7411
3078.4172	3082.3900	3139.8074
3145.7826	3149.4781	3156.8589
3163.0288	3172.5759	3195.6579

Zero-point correction (Hartree): 0.172906

TS.iC3H7_C2H5_COO.ringclose.mt

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E(RM062X/Aug-CC-pVTZ) (Hartree): -386.10591144

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.231328  | -0.218741 | 0.348883  |
| O | 0.225103  | -1.435384 | 0.725438  |
| O | -0.003556 | -1.950525 | -0.644638 |
| C | -0.938141 | 0.442240  | -0.345012 |
| C | 1.466064  | 0.537218  | 0.688276  |
| H | -0.762181 | 0.329178  | -1.415849 |
| C | -2.247975 | -0.259960 | 0.015827  |
| C | -1.011933 | 1.939024  | -0.028506 |
| H | -2.461339 | -0.135969 | 1.078593  |
| H | -2.190154 | -1.318241 | -0.215542 |
| H | -3.064398 | 0.191936  | -0.545373 |
| H | -0.150771 | 2.489399  | -0.405796 |
| H | -1.094791 | 2.117018  | 1.045048  |
| H | -1.901414 | 2.353027  | -0.500522 |
| C | 2.331650  | 0.539714  | -0.590740 |
| H | 1.255079  | 1.556233  | 0.999360  |
| H | 1.984071  | 0.002280  | 1.481618  |
| H | 1.841740  | 1.096769  | -1.388327 |
| H | 2.496084  | -0.479200 | -0.935067 |
| H | 3.289743  | 1.007871  | -0.376909 |

Rotational constants (GHz): 2.3940400 1.8921700 1.2632200

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i518.2541 | 43.6320   | 80.7841   |
| 165.8552  | 206.1654  | 219.7240  |
| 276.7174  | 299.6169  | 323.0162  |
| 376.5464  | 400.6279  | 447.2563  |
| 499.0705  | 675.8335  | 726.9916  |
| 821.0463  | 834.0521  | 903.4206  |
| 934.3711  | 968.7774  | 979.8724  |
| 1012.2540 | 1063.1659 | 1110.0742 |
| 1159.8557 | 1181.9975 | 1230.4590 |
| 1271.8821 | 1303.1775 | 1308.9968 |
| 1346.5519 | 1393.5237 | 1404.7524 |
| 1418.9164 | 1484.4946 | 1489.5959 |
| 1496.0278 | 1502.2398 | 1510.4358 |
| 1514.2933 | 1522.4678 | 1566.2287 |
| 3060.9632 | 3068.6437 | 3075.4144 |
| 3083.4874 | 3106.3373 | 3131.2161 |
| 3136.6809 | 3142.9919 | 3148.0656 |
| 3162.6300 | 3174.3886 | 3189.6838 |

Zero-point correction (Hartree): 0.173039

TS.iC3H7\_C2H5\_COO.ringclose.pm

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E(RM062X/Aug-CC-pVTZ) (Hartree): -386.10998113

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-0.313852	0.054166	0.070734
O	-0.526247	1.306314	0.023002
O	0.517215	1.559648	-0.986332
C	0.993719	-0.576168	0.431374
C	-1.500372	-0.819501	-0.156301
H	0.702044	-1.278939	1.225226
C	1.531218	-1.416441	-0.733846
C	2.046361	0.373084	0.982245
H	1.798175	-0.748733	-1.550650
H	0.800846	-2.141351	-1.093568
H	2.416851	-1.959815	-0.407840
H	1.604570	1.108728	1.652800
H	2.534272	0.911146	0.176345
H	2.786401	-0.205114	1.536397
C	-2.807895	-0.223732	0.359334
H	-1.544644	-0.908075	-1.250408
H	-1.315611	-1.819349	0.232962
H	-2.982705	0.755122	-0.079193
H	-2.784450	-0.113351	1.442359
H	-3.638558	-0.876419	0.100974

Rotational constants (GHz): 2.8969100 1.5093700 1.2446400

Vibrational harmonic frequencies (cm-1):

i469.0681	50.4269	91.0895
176.4603	193.0345	204.1706
246.2164	288.5220	302.4549
322.0712	361.6229	459.7354
530.7489	620.1803	735.2949
797.9945	849.6708	909.9059
942.8544	984.5528	993.9499
1045.3924	1081.4023	1111.1099
1125.5319	1161.9449	1229.9452
1260.2518	1300.3591	1374.5991
1392.2984	1411.6951	1417.2597
1422.8807	1453.8860	1480.7073
1491.5097	1499.3535	1502.5662
1510.5091	1516.9118	1576.9550
2995.5362	3023.6952	3067.6544
3072.3380	3082.9758	3123.3788
3138.6351	3139.4455	3153.0279
3158.9747	3170.9138	3182.4041

Zero-point correction (Hartree): 0.172542

TS.iC3H7_C2H5_COO.ringclose.pp

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E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -385.54167319  
 E(CCSD/Aug-CC-pVTZ) (Hartree): -385.46749188  
 T1 diagnostic: 0.028639  
 E(MP2/Aug-CC-pVTZ) (Hartree): -385.40465207  
 E(MP3/Aug-CC-pVTZ) (Hartree): -385.45251357  
 E(RHF/Aug-CC-pVTZ) (Hartree): -383.87578813  
 E(RM062X/Aug-CC-pVTZ) (Hartree): -386.11087073  
 Electronic state : 1-A  
 Cartesian coordinates (Angs):  

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.247535 | -0.230820 | -0.463851 |
| O | -0.291177 | -1.490320 | -0.299757 |
| O | 0.309433  | -1.466321 | 1.045654  |
| C | 0.994694  | 0.596039  | -0.414988 |
| C | -1.545273 | 0.402894  | -0.826502 |
| H | 0.933652  | 1.153584  | -1.361676 |
| C | 0.915917  | 1.631239  | 0.714376  |
| C | 2.299411  | -0.183628 | -0.385306 |
| H | 0.923017  | 1.109331  | 1.669464  |
| H | 0.017104  | 2.245133  | 0.651629  |
| H | 1.780911  | 2.290404  | 0.657515  |
| H | 2.260620  | -1.046476 | -1.048516 |
| H | 2.502899  | -0.546326 | 0.616863  |
| H | 3.108950  | 0.471114  | -0.709334 |
| C | -2.456928 | 0.388467  | 0.412892  |
| H | -1.399356 | 1.413786  | -1.201789 |
| H | -1.997217 | -0.212310 | -1.608089 |
| H | -2.044478 | 1.006842  | 1.207952  |
| H | -2.553216 | -0.626836 | 0.790865  |
| H | -3.440653 | 0.769733  | 0.148210  |

 Rotational constants (GHz): 2.7399400 1.6830900 1.3508700  
 Vibrational harmonic frequencies (cm-1):  

|           |           |           |
|-----------|-----------|-----------|
| i455.3856 | 72.1773   | 116.6274  |
| 175.1634  | 195.5862  | 198.1453  |
| 246.6653  | 268.3224  | 298.3686  |
| 327.1856  | 415.9566  | 441.9033  |
| 547.4786  | 647.6817  | 744.5888  |
| 813.7641  | 848.2781  | 911.1004  |
| 942.9649  | 977.7968  | 985.2042  |
| 1035.3355 | 1087.6447 | 1106.7846 |
| 1145.2006 | 1162.2121 | 1231.8051 |
| 1255.4538 | 1300.6650 | 1338.6374 |
| 1387.5577 | 1404.2214 | 1417.2153 |
| 1423.0381 | 1478.6169 | 1481.1736 |
| 1490.3978 | 1497.1033 | 1501.9703 |
| 1508.9412 | 1519.0480 | 1579.9544 |
| 2990.3249 | 3067.0277 | 3069.3607 |
| 3072.5948 | 3081.2978 | 3137.0054 |
| 3138.4259 | 3140.1385 | 3157.1027 |
| 3157.8718 | 3168.4476 | 3182.0226 |

 Zero-point correction (Hartree): 0.172889

TS.iC3H7\_C2H5\_COO.ringclose.pt  
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 E(RM062X/Aug-CC-pVTZ) (Hartree): -386.10957388
 Electronic state : 1-A
 Cartesian coordinates (Angs):

C	-0.198012	-0.521867	-0.146951
O	0.405009	-1.632694	-0.299496
O	1.387589	-1.367806	0.763386
C	0.446735	0.819252	-0.288507
C	-1.663747	-0.647534	0.097994
H	-0.260426	1.371854	-0.920347
C	0.510410	1.544946	1.062164
C	1.801922	0.796216	-0.981279
H	1.240993	1.040007	1.689718
H	-0.448478	1.545518	1.580936
H	0.814257	2.578896	0.903957
H	1.779728	0.171826	-1.873623
H	2.561129	0.401314	-0.314191
H	2.064322	1.812154	-1.276756
C	-2.563055	0.521289	-0.274946
H	-1.977781	-1.579501	-0.375819
H	-1.714098	-0.853080	1.176644
H	-2.520783	0.723467	-1.344563
H	-2.290551	1.432509	0.253810
H	-3.594612	0.285212	-0.021731

 Rotational constants (GHz): 2.4919600 1.7266400 1.3031700
 Vibrational harmonic frequencies (cm-1):

i471.7062	83.1138	127.9985
183.3340	199.3369	228.7309
248.7578	273.0487	304.5031
335.8226	406.6614	464.5707
509.9118	565.5787	702.4372
777.0363	849.1607	911.3089
945.4141	980.8731	986.0579
1040.4491	1094.3233	1113.9701
1146.2652	1176.7561	1242.3956
1268.4762	1306.4759	1358.8793
1388.9147	1415.4710	1420.9289
1423.8896	1438.3715	1480.6079
1495.7429	1497.5180	1509.4292
1509.9360	1520.2765	1570.7031
3020.4242	3020.9740	3069.0884
3073.8219	3078.0507	3096.6789
3137.8619	3138.7327	3146.3503
3155.3251	3165.0975	3184.7209

 Zero-point correction (Hartree): 0.172664

Population analysis as 298K (%)
 Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)

Compound	Qtot	Erel	Erel2	n*Q*MB	%


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TS.iC3H7_C2H5_COO.14Hshift.c 1.697e+41 0.00 0.00 3.394e+41 54.2
TS.iC3H7_C2H5_COO.14Hshift.p 1.246e+41 0.07 0.07 2.209e+41 35.3
TS.iC3H7_C2H5_COO.14Hshift.m 1.029e+41 0.67 0.67 6.618e+40 10.6
Total 6.265e+41 100

TS.iC3H7_C2H5_COO.14Hshift.c
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E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -385.54032494
E(CCSD/Aug-CC-pVTZ) (Hartree): -385.46396144
T1 diagnostic: 0.020653
E(MP2/Aug-CC-pVTZ) (Hartree): -385.41578844
E(MP3/Aug-CC-pVTZ) (Hartree): -385.45361885
E(RHF/Aug-CC-pVTZ) (Hartree): -383.85359568
E(RM062X/Aug-CC-pVTZ) (Hartree): -386.11333719
Electronic state : 1-A
Cartesian coordinates (Angs):
  C -0.278420 -0.011654 0.038365
  O -0.600837 -1.258626 -0.110896
  O 0.506905 -1.999318 -0.527496
  C 1.084161 0.309746 -0.150458
  C -1.428808 0.926901 0.175756
  H 1.117160 -0.861645 -0.840776
  C 2.073384 -0.196984 0.910851
  C 1.389336 1.724643 -0.590606
  H 3.070806 -0.277717 0.479471
  H 1.789553 -1.168625 1.302726
  H 2.120154 0.520866 1.733246
  H 1.250828 2.446662 0.220349
  H 0.778194 2.040619 -1.435264
  H 2.432415 1.787997 -0.900197
  C -2.799709 0.266413 0.200182
  H -1.256085 1.523094 1.076388
  H -1.352624 1.635177 -0.653695
  H -2.882778 -0.432233 1.030408
  H -2.981819 -0.288029 -0.717881
  H -3.574013 1.022996 0.307816
Rotational constants (GHz): 2.6417100 1.6288100 1.1535000
Vibrational harmonic frequencies (cm-1):
i1608.1982 46.4466 144.4532
167.7238 182.6476 227.5503
228.5930 269.5618 288.1215
305.4774 353.5866 485.3052
561.4123 608.1314 678.6725
761.3469 801.3177 952.8572
983.9809 991.2928 1017.3958
1028.2626 1082.5774 1101.1991
1111.6649 1164.9346 1221.7021
1282.1097 1328.9368 1346.0008
1390.7815 1413.6033 1421.7793
1431.7757 1467.7838 1488.9626
1496.8037 1500.7978 1501.5951
1507.2529 1509.5671 1571.3872
1868.9421 3034.8812 3050.1586
3055.7865 3082.2141 3084.0948
3105.1288 3115.4445 3133.9937
3155.2397 3158.6223 3176.0971
Zero-point correction (Hartree): 0.169600

TS.iC3H7_C2H5_COO.14Hshift.m
~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -386.11267441
Electronic state : 1-A
Cartesian coordinates (Angs):
  C -0.234943 -0.225778 0.320903
  O -0.204427 -1.508558 0.135222
  O 0.920257 -1.865225 -0.611283
  C 0.872466 0.505423 -0.162388
  C -1.564400 0.279394 0.775085
  H 1.055212 -0.563585 -0.958048
  C 2.224537 0.312267 0.541291
  C 0.612026 1.950557 -0.526780
  H 3.035623 0.558175 -0.143627
  H 2.362003 -0.707835 0.884921
  H 2.286684 0.991014 1.394510
  H 0.622020 2.599144 0.354034
  H -0.337697 2.089254 -1.041541
  H 1.399390 2.303233 -1.193149
  C -2.610108 0.210151 -0.343996
  H -1.883976 -0.345354 1.610489
  H -1.450381 1.298428 1.140002
  H -2.721007 -0.814663 -0.691922
  H -2.318379 0.828498 -1.191549
  H -3.573598 0.561876 0.019679
Rotational constants (GHz): 2.5154400 1.7442000 1.2037700
Vibrational harmonic frequencies (cm-1):
i1618.7336 90.8411 123.3868
169.6895 193.9376 211.9331
214.6697 262.9368 296.8940
338.3791 367.7987 422.6279
563.6196 663.1444 730.5848
750.0768 799.1885 950.4765
979.1696 984.1672 1012.9466
1018.1358 1070.6660 1105.4866
1111.8775 1178.7662 1227.4917
1273.1007 1330.6152 1344.6645
1390.7548 1402.5298 1420.2187
1441.7174 1482.6960 1490.2954
1494.5860 1502.4196 1504.4983
1507.2411 1514.3839 1577.9084
1862.2722 3041.7423 3054.4234
3076.3220 3083.6107 3108.4526

```

3118.0578 3133.3457 3138.1157
3150.7203 3161.4536 3179.6917
Zero-point correction (Hartree): 0.170008

TS.iC3H7_C2H5_COO.14Hshift.p

E(RM062X/Aug-CC-pVT2) (Hartree): -386.11351386

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-0.164785	-0.470996	-0.196010
O	0.464645	-1.602380	-0.125838
O	1.843180	-1.393579	-0.149759
C	0.636472	0.693392	-0.200496
C	-1.627557	-0.591748	-0.443137
H	1.618729	-0.156843	-0.591896
C	1.360352	1.054098	1.105872
C	0.071810	1.909043	-0.902728
H	2.236533	1.664640	0.888582
H	1.683145	0.171824	1.649781
H	0.690478	1.640069	1.739856
H	-0.681742	2.425514	-0.300635
H	-0.369648	1.665921	-1.868314
H	0.876457	2.621973	-1.083636
C	-2.426457	-0.042699	0.742124
H	-1.861181	-0.018887	-1.342389
H	-1.871676	-1.634908	-0.637672
H	-2.168476	0.997587	0.936630
H	-2.220523	-0.618019	1.643344
H	-3.493712	-0.097741	0.537370

Rotational constants (GHz): 2.3125700 1.7892200 1.2781700

Vibrational harmonic frequencies (cm-1):

i1612.7068	68.5353	120.8648
180.8747	182.5952	215.6716
217.8597	264.1380	321.4032
347.7887	365.9201	413.4450
567.6922	620.0738	743.7757
757.7228	801.6055	955.1422
983.9221	985.9352	1015.1500
1020.1382	1076.1700	1084.0265
1110.4811	1176.5527	1234.1774
1272.2635	1328.1567	1340.2035
1390.8735	1406.0851	1420.1365
1442.9689	1479.0915	1488.6881
1495.8456	1499.7157	1502.4303
1508.6583	1512.6394	1574.9859
1870.3825	3039.4836	3049.0074
3074.1204	3081.0601	3105.9616
3114.4923	3129.1153	3135.6796
3151.2530	3153.5572	3174.5613

Zero-point correction (Hartree): 0.169890

(iC3H7)2COO
#####

Population analysis as 298K (%)

Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)

Compound	Qtot	Erel	Erel2	n*Q*MB	%
iC3H7_iC3H7_COO.pp	4.733e+41	0.00	0.00	4.733e+41	22.2
iC3H7_iC3H7_COO.tm	4.731e+41	0.00	0.00	4.731e+41	22.2
iC3H7_iC3H7_COO.tp	1.131e+42	0.76	0.76	3.120e+41	14.7
iC3H7_iC3H7_COO.pm	1.129e+42	0.76	0.76	3.116e+41	14.6
iC3H7_iC3H7_COO.mp	1.038e+42	0.97	0.97	2.021e+41	9.5
iC3H7_iC3H7_COO.mm	1.034e+42	0.97	0.97	2.010e+41	9.44
iC3H7_iC3H7_COO.mc	1.025e+42	1.18	1.18	1.409e+41	6.62
iC3H7_iC3H7_COO.pc	4.443e+41	2.44	2.44	7.268e+39	0.341
iC3H7_iC3H7_COO.tc	4.442e+41	2.44	2.44	7.260e+39	0.341
Total				2.129e+42	100

iC3H7_iC3H7_COO.mc

E(RM062X/Aug-CC-pVT2) (Hartree): -425.45202119

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-0.081068	0.389381	0.000678
O	0.465582	1.513838	0.003149
O	1.834763	1.614092	0.003319
C	0.680236	-0.895278	-0.002021
C	-1.580250	0.426323	0.000874
C	1.522239	-1.037743	-1.276828
C	1.520722	-1.043107	1.273229
H	-0.070377	-1.687454	-0.004171
H	2.277568	-0.258549	-1.315476
H	0.899090	-0.974441	-2.169409
H	2.003966	-2.015187	-1.268571
H	0.896247	-0.985332	2.165250
H	2.274921	-0.263048	1.316781
H	2.003997	-2.019744	1.260670
H	-1.863461	1.478873	0.003401
C	-2.128439	-0.237408	-1.265502
C	-2.128459	-0.243491	1.264017
H	-1.860449	-1.293764	-1.305855
H	-1.751127	0.248926	-2.164109
H	-3.215664	-0.169079	-1.269463
H	-1.751219	0.238529	2.164975
H	-1.860452	-1.300020	1.299310
H	-3.215687	-0.175212	1.268252

Rotational constants (GHz): 2.0466900 1.1898800 1.1174600

Vibrational harmonic frequencies (cm-1):

69.3995	81.4816	163.9165

199.4711	202.9312	207.8434
225.6832	250.1222	250.4095
257.8510	317.5709	347.7224
363.0879	427.0976	493.4890
607.7725	742.9963	758.5735
880.1287	912.7818	939.2326
942.9797	973.1830	979.2416
990.3319	1047.9307	1102.9106
1133.1141	1142.1229	1192.5774
1197.0475	1267.2471	1341.2663
1345.4995	1359.9152	1383.3583
1400.5259	1401.0689	1422.8087
1432.8655	1482.2271	1489.1301
1495.0387	1498.5594	1506.5672
1506.7197	1513.8954	1529.9533
1645.0415	3064.5957	3064.8198
3066.9384	3067.0861	3080.3346
3097.7032	3131.4456	3132.4448
3135.5549	3141.1107	3143.5131
3144.1323	3177.4506	3179.1886

Zero-point correction (Hartree): 0.202869

iC3H7_iC3H7_COO.mm
 ~~~~~  
 E(RM062X/Aug-CC-pVTZ) (Hartree): -425.45223910  
 Electronic state : 1-A  
 Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.110702 | 0.150946  | 0.102282  |
| O | -0.015402 | 1.283238  | -0.414855 |
| O | 1.215297  | 1.767668  | -0.792160 |
| C | 1.060649  | -0.739971 | 0.361701  |
| C | -1.501846 | -0.293203 | 0.444569  |
| C | 1.760855  | -1.145188 | -0.941209 |
| C | 2.027752  | -0.097020 | 1.364469  |
| H | 0.646408  | -1.639560 | 0.822035  |
| H | 2.182774  | -0.269474 | -1.425255 |
| H | 1.067509  | -1.630473 | -1.628839 |
| H | 2.555879  | -1.852188 | -0.705361 |
| H | 1.521197  | 0.156160  | 2.296195  |
| H | 2.461105  | 0.803915  | 0.941006  |
| H | 2.817944  | -0.811727 | 1.592864  |
| H | -1.445161 | -0.678198 | 1.468411  |
| C | -2.528903 | 0.826962  | 0.372821  |
| C | -1.884828 | -1.461903 | -0.476928 |
| H | -2.614741 | 1.204198  | -0.645340 |
| H | -2.255773 | 1.661462  | 1.015703  |
| H | -3.502166 | 0.449654  | 0.683336  |
| H | -1.167379 | -2.279805 | -0.425504 |
| H | -1.942691 | -1.117939 | -1.509990 |
| H | -2.861927 | -1.847011 | -0.189361 |

Rotational constants (GHz): 2.1614500 1.2184900 1.0138000  
 Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| 60.2629   | 88.8954   | 161.5456  |
| 191.9650  | 209.5868  | 217.8180  |
| 232.3739  | 244.0610  | 256.2665  |
| 278.6266  | 291.2491  | 353.8523  |
| 391.7964  | 424.0148  | 474.5610  |
| 612.8911  | 731.9468  | 766.2339  |
| 875.7666  | 918.2439  | 937.5725  |
| 942.1424  | 958.6832  | 981.2198  |
| 987.9367  | 1091.2433 | 1115.4143 |
| 1127.6107 | 1147.6542 | 1158.7451 |
| 1206.3868 | 1234.5686 | 1311.5203 |
| 1343.6799 | 1369.2490 | 1383.7524 |
| 1401.3161 | 1403.7490 | 1425.9886 |
| 1436.7027 | 1481.4520 | 1489.2235 |
| 1493.3915 | 1497.4588 | 1503.9660 |
| 1507.9050 | 1515.9066 | 1528.9518 |
| 1650.4290 | 3040.0473 | 3065.0814 |
| 3065.7088 | 3066.3988 | 3070.5172 |
| 3074.3962 | 3130.4499 | 3131.7238 |
| 3139.7563 | 3145.9150 | 3148.0054 |
| 3153.0449 | 3176.5075 | 3178.0525 |

Zero-point correction (Hartree): 0.202760

iC3H7\_iC3H7\_COO.mp  
 ~~~~~  
 E(RM062X/Aug-CC-pVTZ) (Hartree): -425.45223915
 Electronic state : 1-A
 Cartesian coordinates (Angs):

C	0.110728	0.150729	0.101904
O	0.015460	1.283192	-0.414909
O	-1.215287	1.767736	-0.792019
C	-1.060627	-0.740124	0.361343
C	1.501843	-0.293449	0.444282
C	-2.026623	-0.097251	1.365337
C	-1.762144	-1.144469	-0.941071
H	-0.646336	-1.640090	0.820933
H	-2.459019	0.804723	0.943094
H	-1.519376	0.154024	2.297196
H	-2.817631	-0.811267	1.593063
H	-1.069328	-1.628594	-1.630059
H	-2.185231	-0.268593	-1.423779
H	-2.556335	-1.852295	-0.704890
H	1.444951	-0.678767	1.468011
C	1.884980	-1.461798	-0.477540
C	2.528839	0.826813	0.373077
H	1.943367	-1.117355	-1.510418
H	1.167319	-2.279559	-0.426827
H	2.861880	-1.847257	-0.189761
H	2.255574	1.661027	1.016269
H	2.614715	1.204444	-0.644930

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H          3.502088      0.449427      0.683526
Rotational constants (GHz): 2.1613900 1.2183900 1.0138500
Vibrational harmonic frequencies (cm-1):
  60.2002      88.7139      161.5091
 191.9338      209.6376      217.6177
 232.3109      244.0799      256.2736
 278.6262      291.1588      353.8768
 391.7992      423.9926      474.5633
 612.8716      731.9709      766.2448
 875.7749      918.2335      937.5846
 942.1288      958.6276      981.2198
 987.9280     1091.2926     1115.3585
1127.6283     1147.6372     1158.7696
1206.3850     1234.5895     1311.5533
1343.6927     1369.2699     1383.7214
1401.2947     1403.7623     1425.9754
1436.7370     1481.4468     1489.2098
1493.3908     1497.4489     1503.9546
1507.8857     1515.8944     1528.9276
1650.3579     3039.8769     3065.0229
3065.6809     3066.4178     3070.4299
3074.4203     3130.4041     3131.7649
3139.7172     3145.9091     3148.0333
3153.0751     3176.5641     3178.1062
Zero-point correction (Hartree): 0.202758

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iC3H7_iC3H7_COO.pc
~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -425.45055752
Electronic state : 1-A
Cartesian coordinates (Angs):
  C      -0.153776      -0.475795      -0.130580
  O      -0.838529     -1.529371      -0.128580
  O      -2.189658     -1.452671      -0.338159
  C      -0.848777      0.823672      -0.348561
  C      1.296811      -0.715328      0.181725
  C      -1.544210      1.202399      0.973397
  C      0.006777      1.964211      -0.883712
  H      -1.642570      0.581739      -1.058573
  H      -0.810147      1.483035      1.729336
  H      -2.148791      0.372607      1.333083
  H      -2.196307      2.057044      0.797942
  H      0.451817      1.725182      -1.847976
  H      0.801851      2.249295      -0.195465
  H      -0.632317      2.836173      -1.020052
  H      1.370053      -1.793452      0.329104
  C      2.241098      -0.330880      -0.962180
  C      1.692983      -0.026686      1.492039
  H      2.362656      0.746645      -1.042836
  H      1.890114      -0.715479      -1.919151
  H      3.221971      -0.762255      -0.764776
  H      1.053666      -0.342853      2.315331
  H      1.636092      1.057811      1.408266
  H      2.721976      -0.288723      1.736912
Rotational constants (GHz): 1.8672400 1.3387100 1.0779900
Vibrational harmonic frequencies (cm-1):
  82.1936      113.2830      165.2723
 212.4699      230.1584      238.1708
 251.6742      255.2906      286.9494
 303.3412      323.8584      358.9104
 367.9189      422.0775      513.6732
 639.2937      687.1996      743.0324
 886.1076      918.0257      939.7356
 944.7920      978.2994      981.4766
 993.2490     1031.0167     1106.1380
1139.1994     1148.2919     1190.6896
1202.4006     1310.0293     1334.2665
1347.8437     1366.5218     1372.1601
1390.4428     1400.4451     1421.5434
1429.2277     1484.4814     1492.9730
1493.1154     1501.2788     1504.1261
1515.0663     1518.6616     1524.4512
1609.2665     3062.8870     3067.5605
3072.0112     3073.7389     3077.5603
3088.9651     3135.1878     3136.9469
3138.9774     3140.7487     3146.1259
3154.9774     3158.2052     3164.5217
Zero-point correction (Hartree): 0.203414

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iC3H7_iC3H7_COO.pm
~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -425.45271301
Electronic state : 1-A
Cartesian coordinates (Angs):
  C      0.003729      -0.225953      -0.112438
  O      0.075608     -1.436596     -0.422682
  O      -1.061032     -2.086509     -0.844576
  C      -1.311186      0.470022     -0.164633
  C      1.286321      0.393186      0.361047
  C      -2.060186      0.049196      1.114782
  C      -1.237508      1.985194     -0.298438
  H      -1.840062      0.027174     -1.009355
  H      -1.562297      0.449829      1.999859
  H      -2.113305     -1.035454      1.179794
  H      -3.072347      0.450113      1.084754
  H      -0.807837      2.292876     -1.249950
  H      -0.663092      2.444952      0.506719
  H      -2.247811      2.389640     -0.247872
  H      1.008901      1.146452      1.102277
  C      2.217955     -0.628707      1.005742
  C      1.984705      1.099848     -0.810780
  H      2.540645     -1.369198      0.276023

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H      1.727651      -1.154114      1.823646
H      3.099298      -0.121108      1.395212
H      1.359384      1.862988      -1.268000
H      2.253910      0.368748      -1.573097
H      2.897375      1.575229      -0.453635
Rotational constants (GHz):      1.8357100      1.3712500      1.0123000
Vibrational harmonic frequencies (cm-1):
49.9969      78.5818      168.3536
191.7635      216.7371      228.1375
244.6018      247.5690      262.7880
280.3035      334.3279      346.0503
388.0563      433.3640      536.5067
602.4643      719.8466      739.0950
884.9577      917.2065      937.0885
940.6282      956.9310      981.9659
988.1015      1048.5616      1108.1043
1132.0513      1146.9428      1188.4179
1193.5814      1271.1798      1318.6810
1321.2794      1351.6672      1385.8015
1394.3024      1416.2854      1423.4361
1427.5589      1486.1177      1489.5109
1492.6002      1500.9585      1506.3784
1508.6804      1516.4358      1522.6092
1627.8578      3057.2035      3063.9795
3070.3622      3072.4634      3074.0180
3093.7929      3130.5559      3135.6069
3141.1715      3145.3813      3147.7919
3152.5353      3160.1928      3164.4854
Zero-point correction (Hartree): 0.202903

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iC3H7_iC3H7_COO.pp
~~~~~
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -424.81815518
E(CCSD/Aug-CC-pVTZ) (Hartree): -424.73624372
T1 diagnostic: 0.023610
E(MP2/Aug-CC-pVTZ) (Hartree): -424.66901137
E(MP3/Aug-CC-pVTZ) (Hartree): -424.72288530
E(RHF/Aug-CC-pVTZ) (Hartree): -422.95097434
E(RM062X/Aug-CC-pVTZ) (Hartree): -425.45411290
Electronic state : 1-A
Cartesian coordinates (Angs):
C      -0.055947      0.295230      -0.216896
O      -0.202397      1.525738      -0.034610
O      0.912434      2.325948      0.028890
C      1.314961      -0.266437      -0.369634
C      -1.319278      -0.512736      -0.221220
C      1.997218      -0.304358      1.009635
C      1.355947      -1.619868      -1.067514
H      1.844836      0.487592      -0.957630
H      1.541581      -1.061254      1.648302
H      1.932320      0.670082      1.487782
H      3.047824      -0.560145      0.878522
H      0.907214      -1.580719      -2.059892
H      0.848696      -2.394490      -0.491534
H      2.394482      -1.926806      -1.184237
H      -1.236401      -1.218042      -1.051581
C      -1.397274      -1.322908      1.083193
C      -2.566554      0.342984      -0.403664
H      -1.441379      -0.648305      1.938716
H      -0.543672      -1.985376      1.212093
H      -2.301817      -1.929606      1.077488
H      -2.513106      0.938785      -1.312854
H      -2.692655      1.024894      0.435860
H      -3.442665      -0.301524      -0.458685
Rotational constants (GHz):      1.8338100      1.4172700      1.0146800
Vibrational harmonic frequencies (cm-1):
76.7765      123.0787      181.5765
197.6026      207.3262      242.2333
244.4344      261.5643      281.3229
287.5133      325.2110      346.7313
395.6862      421.2649      529.2693
606.9846      689.0202      751.6056
886.3893      919.1209      936.2564
940.7698      959.9710      980.4118
986.9873      1046.9369      1115.2452
1142.2534      1149.0152      1185.7268
1196.3517      1262.7486      1311.4223
1322.0029      1354.1321      1384.8855
1394.0549      1417.1497      1423.3709
1426.6022      1483.8743      1492.3568
1493.5520      1501.2313      1505.0137
1509.8352      1518.9162      1520.1497
1622.5583      3062.1759      3065.7813
3066.9511      3071.8458      3072.3663
3075.0025      3133.7444      3137.8679
3138.7999      3140.3066      3148.5704
3153.4507      3154.3757      3165.6144
Zero-point correction (Hartree): 0.203088

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iC3H7_iC3H7_COO.tc
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E(RM062X/Aug-CC-pVTZ) (Hartree): -425.45055749
Electronic state : 1-A
Cartesian coordinates (Angs):
C      0.153829      -0.475845      -0.130428
O      0.838569      -1.529411      -0.128274
O      2.189638      -1.452481      -0.337785
C      0.848836      0.823503      -0.348709
C      -1.296653      -0.715205      0.182075
C      -0.006613      1.963725      -0.884602
C      1.543395      1.202752      0.973625
H      1.643185      0.581360      -1.057983

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H	-0.801954	2.248880	-0.196704
H	-0.451295	1.724273	-1.848925
H	0.632341	2.835756	-1.021033
H	2.147465	0.372991	1.334286
H	0.808841	1.484187	1.728753
H	2.196188	2.056833	0.797983
H	-1.369832	-1.793262	0.330102
C	-1.692983	-0.025890	1.491937
C	-2.240704	-0.331564	-0.962291
H	-1.636690	1.058593	1.407560
H	-1.053440	-0.341221	2.315381
H	-2.721806	-0.288389	1.736985
H	-1.889865	-0.717510	-1.918793
H	-2.361618	0.745935	-1.044352
H	-3.221819	-0.762151	-0.764430
Rotational constants (GHz):		1.8672200	1.3388600 1.0782100
Vibrational harmonic frequencies (cm-1):			
82.1675	113.3331	165.1297	
212.5485	230.1814	238.1984	
251.6794	255.2650	286.9735	
303.3694	323.8380	358.8998	
367.8862	422.1098	513.7404	
639.3460	687.2922	743.0580	
886.1263	917.9769	939.7144	
944.7780	978.3417	981.5141	
993.3135	1031.0092	1106.1457	
1139.2043	1148.2410	1190.6881	
1202.3468	1309.8935	1334.2326	
1347.8928	1366.4781	1372.2235	
1390.4241	1400.4594	1421.5521	
1429.2333	1484.4365	1492.9603	
1493.1100	1501.3065	1504.1075	
1515.0703	1518.6862	1524.4599	
1609.3859	3062.9565	3067.5887	
3072.0272	3073.7860	3077.7254	
3088.8088	3135.3267	3137.0474	
3138.9769	3140.7819	3146.1262	
3155.0059	3158.0697	3164.4635	
Zero-point correction (Hartree): 0.203415			
iC3H7_iC3H7_COO.tm			
~~			
E(RM062X/Aug-CC-pVTZ) (Hartree): -425.45411288			
Electronic state : 1-A			
Cartesian coordinates (Angs):			
C	0.055913	0.295225	-0.216991
O	0.202462	1.525716	-0.034604
O	-0.912325	2.326064	0.028964
C	-1.314961	-0.266362	-0.369743
C	1.319133	-0.512893	-0.221108
C	-1.355878	-1.619804	-1.067664
C	-1.997151	-0.304506	1.009589
H	-1.844838	0.487632	-0.957792
H	-0.848233	-2.394320	-0.491877
H	-0.907554	-1.580532	-2.060216
H	-2.394381	-1.927000	-1.183947
H	-1.932053	0.669722	1.488119
H	-1.541535	-1.061772	1.647836
H	-3.047808	-0.560017	0.878453
H	1.236091	-1.218631	-1.051084
C	2.566562	0.342521	-0.404121
C	1.397093	-1.322340	1.083810
H	2.693196	1.024413	0.435344
H	2.512913	0.938365	-1.313266
H	3.442470	-0.302232	-0.459503
H	0.543823	-1.985239	1.212753
H	1.440539	-0.647205	1.938930
H	2.302019	-1.928474	1.078728
Rotational constants (GHz):		1.8337400	1.4172400 1.0147600
Vibrational harmonic frequencies (cm-1):			
76.8318	123.0957	181.5324	
197.5775	207.3370	242.1696	
244.3435	261.6870	281.2596	
287.5427	325.2073	346.7488	
395.6772	421.2516	529.2752	
606.9954	689.0762	751.6203	
886.3349	919.1099	936.2500	
940.7185	959.8720	980.4004	
986.9605	1046.9055	1115.2372	
1142.1719	1148.9894	1185.7200	
1196.3402	1262.7934	1311.4045	
1322.0092	1354.1674	1384.8446	
1394.0340	1417.1847	1423.3585	
1426.5873	1483.8549	1492.3437	
1493.5485	1501.2211	1505.0022	
1509.8418	1518.9136	1520.1455	
1622.5305	3062.1699	3065.7900	
3066.9712	3071.8671	3072.3893	
3075.0071	3133.7289	3137.9296	
3138.8491	3140.3508	3148.5616	
3153.4555	3154.3430	3165.6912	
Zero-point correction (Hartree): 0.203088			
iC3H7_iC3H7_COO.tp			
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E(RM062X/Aug-CC-pVTZ) (Hartree): -425.45271301			
Electronic state : 1-A			
Cartesian coordinates (Angs):			
C	-0.003688	-0.225936	-0.112416
O	-0.075716	-1.436561	-0.422662
O	1.060831	-2.086546	-0.844674
C	1.311259	0.469900	-0.164652

C	-1.286243	0.393330	0.360970
C	1.237679	1.985104	-0.298589
C	2.060123	0.049203	1.114882
H	1.840202	0.026993	-1.009286
H	0.663101	2.444927	0.506403
H	0.808235	2.292694	-1.250231
H	2.247993	2.389484	-0.247877
H	2.113494	-1.035440	1.179834
H	1.561925	0.449555	1.999909
H	3.072147	0.450478	1.085090
H	-1.008828	1.146676	1.102121
C	-1.984864	1.099713	-0.810878
C	-2.217758	-0.628502	1.005975
H	-2.253939	0.368473	-1.573091
H	-1.359794	1.863006	-1.268156
H	-2.897624	1.574857	-0.453648
H	-1.727251	-1.153815	1.823826
H	-2.540636	-1.369081	0.276437
H	-3.098990	-0.120824	1.395606
Rotational constants (GHz):			
	1.8356900	1.3712200	1.0123400
Vibrational harmonic frequencies (cm-1):			
49.9623	78.5457		168.3341
191.7347	216.7188		228.0727
244.6154	247.5653		262.8163
280.2285	334.3024		346.0430
388.0732	433.3692		536.5043
602.4892	719.8687		739.0993
884.9538	917.2111		937.0813
940.6234	956.9375		981.9734
988.0969	1048.5502		1108.1024
1132.0485	1146.9212		1188.4088
1193.5676	1271.2029		1318.6920
1321.2751	1351.6540		1385.8114
1394.2892	1416.2816		1423.4009
1427.5613	1486.1242		1489.5127
1492.5948	1500.9446		1506.3789
1508.6741	1516.4265		1522.5973
1627.9051	3057.2245		3064.0167
3070.4095	3072.4687		3074.0168
3093.9095	3130.5807		3135.6828
3141.2191	3145.4218		3147.7467
3152.5506	3160.2061		3164.5744
Zero-point correction (Hartree): 0.202903			
Population analysis as 298K (%)			
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)			
Compound	Qtot	Erel	Erel2 n*Q*MB %

TS.iC3H7_iC3H7_COO.ringclose.pt	7.442e+41	0.00	0.00 1.488e+42 50.4
TS.iC3H7_iC3H7_COO.ringclose.ct	8.257e+41	0.11	0.11 1.378e+42 46.6
TS.iC3H7_iC3H7_COO.ringclose.pp	7.765e+41	1.86	1.86 6.665e+40 2.26
TS.iC3H7_iC3H7_COO.ringclose.mt	1.055e+42	3.07	3.07 1.173e+40 0.397
TS.iC3H7_iC3H7_COO.ringclose.pm	6.767e+41	2.94	2.94 9.394e+39 0.318
TS.iC3H7_iC3H7_COO.ringclose.cm	2.833e+41	3.78	3.78 9.607e+38 0.0325
TS.iC3H7_iC3H7_COO.ringclose.cp	4.174e+41	5.38	5.38 9.477e+37 0.00321
TS.iC3H7_iC3H7_COO.ringclose.mm	6.741e+41	5.95	5.95 5.840e+37 0.00198
TS.iC3H7_iC3H7_COO.ringclose.mp	4.243e+41	6.21	6.21 2.379e+37 0.000805
Total			2.955e+42 100
TS.iC3H7_iC3H7_COO.ringclose.cm			
~~			
E(RM062X/Aug-CC-pVTZ) (Hartree): -425.41478029			
Electronic state : 1-A			
Cartesian coordinates (Angs):			
C	0.039439	0.391494	-0.459677
O	0.205969	1.503288	-1.065886
O	-0.281092	2.312783	0.066071
C	-1.318141	-0.020170	0.035108
C	1.293102	-0.418247	-0.368854
H	-1.958583	0.823444	-0.206846
C	-1.818489	-1.260794	-0.724727
C	-1.364809	-0.231845	1.547845
H	-1.409614	-2.186387	-0.327502
H	-1.596018	-1.208092	-1.791148
H	-2.901841	-1.303697	-0.617541
H	-1.071721	0.681638	2.060143
H	-0.712347	-1.045380	1.866329
H	-2.382084	-0.492620	1.839558
H	1.861471	-0.146971	-1.262300
C	2.047866	0.191609	0.838232
C	1.200432	-1.932318	-0.251285
H	1.550535	-0.070955	1.771328
H	2.091549	1.275964	0.763070
H	3.057136	-0.217116	0.855586
H	0.726153	-2.384741	-1.119515
H	0.658750	-2.239641	0.641701
H	2.211187	-2.332396	-0.174194
Rotational constants (GHz):			
	1.6463300	1.6189900	1.1464000
Vibrational harmonic frequencies (cm-1):			
i468.5818	94.5787		119.7927
179.8639	206.0075		222.2953
228.9184	252.2678		279.8564
301.2992	302.2827		359.7125
361.6383	400.3693		485.3804
570.9565	671.9460		702.0410
836.0574	897.4036		916.6187
944.1853	946.5118		978.5599
985.1228	1000.4664		1096.0578
1128.9283	1144.2069		1178.6872
1198.8659	1285.3513		1309.0180
1324.2522	1356.9141		1378.3005

1392.0887	1397.5588	1416.6579
1427.9238	1486.2732	1489.4465
1492.7502	1494.9153	1506.7252
1511.2133	1519.3194	1522.3027
1560.8410	3064.5935	3066.2460
3068.9657	3071.3462	3076.4962
3124.7534	3133.3258	3140.5040
3141.6021	3146.8632	3157.7474
3161.2886	3163.5338	3167.7632

Zero-point correction (Hartree): 0.201727

TS.iC3H7_iC3H7_COO.ringclose.cp

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E(RM062X/Aug-CC-pVTZ) (Hartree): -425.41213254

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.108756  | 0.544647  | 0.044016  |
| O | 0.338351  | 1.761544  | 0.340478  |
| O | 1.592898  | 1.846879  | -0.434824 |
| C | 1.105943  | -0.523052 | 0.399057  |
| C | -1.288066 | 0.306364  | -0.460724 |
| H | 1.926262  | 0.024199  | 0.855615  |
| C | 0.493787  | -1.467148 | 1.445785  |
| C | 1.670335  | -1.293561 | -0.795133 |
| H | -0.315444 | -2.074984 | 1.045091  |
| H | 0.123046  | -0.920439 | 2.312676  |
| H | 1.276079  | -2.144139 | 1.788376  |
| H | 2.024309  | -0.600674 | -1.555130 |
| H | 0.940049  | -1.971931 | -1.232108 |
| H | 2.513723  | -1.892976 | -0.453099 |
| H | -1.482841 | 1.176154  | -1.090649 |
| C | -1.531282 | -0.949240 | -1.289017 |
| C | -2.248436 | 0.394948  | 0.741890  |
| H | -1.384874 | -1.863859 | -0.718281 |
| H | -0.888421 | -0.980705 | -2.166207 |
| H | -2.565557 | -0.938616 | -1.632398 |
| H | -2.070855 | 1.297965  | 1.323054  |
| H | -2.139380 | -0.472495 | 1.391149  |
| H | -3.272314 | 0.417372  | 0.371434  |

Rotational constants (GHz): 1.7346900 1.4531600 1.1312000

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i482.9108 | 70.7739   | 115.0982  |
| 170.0575  | 217.9695  | 231.7832  |
| 232.4390  | 247.9423  | 257.1244  |
| 286.9998  | 296.8562  | 339.7424  |
| 342.9693  | 411.7673  | 493.2839  |
| 575.5272  | 655.6252  | 706.4883  |
| 832.3338  | 890.8683  | 920.3395  |
| 937.8656  | 941.9757  | 977.4694  |
| 982.3997  | 1004.7321 | 1100.4013 |
| 1131.6121 | 1141.6285 | 1179.9620 |
| 1199.5795 | 1306.1975 | 1311.2962 |
| 1322.3926 | 1362.2724 | 1377.2043 |
| 1390.9849 | 1395.4408 | 1412.9005 |
| 1427.3851 | 1486.2891 | 1490.3195 |
| 1494.3249 | 1498.7586 | 1508.2586 |
| 1510.0254 | 1519.9224 | 1520.5792 |
| 1563.8791 | 3066.9963 | 3072.5534 |
| 3074.9691 | 3078.7035 | 3081.0081 |
| 3126.9641 | 3135.6652 | 3142.2144 |
| 3143.4014 | 3148.1079 | 3153.1191 |
| 3156.4322 | 3166.3370 | 3167.3128 |

Zero-point correction (Hartree): 0.201631

TS.iC3H7\_iC3H7\_COO.ringclose.ct

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E(RM062X/Aug-CC-pVTZ) (Hartree): -425.42003197

Electronic state : 1-A

Cartesian coordinates (Angs):

C	0.016857	0.171000	-0.331335
O	0.460227	1.027313	-1.160563
O	-0.292545	2.153593	-0.567759
C	-1.442869	-0.110589	-0.162922
C	1.049697	-0.625491	0.395883
H	-1.965280	0.583883	-0.814398
C	-1.704439	-1.556305	-0.615460
C	-1.897840	0.110548	1.278504
H	-1.263576	-2.284883	0.064886
H	-1.323246	-1.741183	-1.619930
H	-2.780583	-1.725413	-0.629944
H	-1.744931	1.149223	1.562951
H	-1.352302	-0.533446	1.971351
H	-2.956533	-0.131334	1.366311
H	0.566396	-1.442240	0.930017
C	2.097818	-1.175470	-0.573104
C	1.687756	0.336804	1.414595
H	2.567141	-0.361651	-1.122972
H	1.656386	-1.869396	-1.287752
H	2.866689	-1.703266	-0.010629
H	0.952720	0.722253	2.119359
H	2.132712	1.182850	0.893374
H	2.461079	-0.195637	1.966980

Rotational constants (GHz): 1.8447600 1.3558600 1.1641900

Vibrational harmonic frequencies (cm-1):

i463.7464	58.1698	88.5391
162.7906	196.7515	199.0245
218.3398	242.1385	248.5374
253.2066	280.3199	311.8554
366.0083	418.7456	511.1647
564.3495	707.5406	731.7997
841.5451	884.2677	913.8718
942.4552	946.1631	978.7666

987.5829	1011.4435	1086.1159
1114.9654	1126.7959	1183.5535
1190.6897	1247.2334	1317.4892
1329.5768	1349.9070	1389.4516
1393.6002	1399.1456	1413.9831
1424.5970	1485.7553	1486.6999
1492.2504	1495.6207	1502.3856
1504.4168	1512.7706	1520.9502
1579.3122	3059.6977	3062.2006
3068.9191	3069.0188	3107.5219
3123.7159	3132.6222	3137.1829
3140.9290	3146.7161	3152.9694
3153.5556	3157.7659	3160.0220

Zero-point correction (Hartree): 0.201129

TS.ic3H7_ic3H7_COO.ringclose.mm
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E(RM062X/Aug-CC-pVTZ) (Hartree): -425.41096047

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.029205  | -0.217162 | 0.328318  |
| O | -0.319214 | -1.149139 | 1.122140  |
| O | -0.962945 | -2.012730 | 0.111992  |
| C | -0.919504 | 0.657587  | -0.432653 |
| C | 1.507099  | 0.015236  | 0.288328  |
| H | -0.388561 | 1.008222  | -1.320126 |
| C | -2.280251 | 0.110288  | -0.832674 |
| C | -1.125347 | 1.871936  | 0.511121  |
| H | -2.800687 | -0.292917 | 0.032425  |
| H | -2.185128 | -0.688526 | -1.559710 |
| H | -2.868680 | 0.926580  | -1.255610 |
| H | -0.198830 | 2.316957  | 0.862853  |
| H | -1.710031 | 1.556756  | 1.374816  |
| H | -1.686063 | 2.634842  | -0.025860 |
| H | 1.884752  | -0.306687 | 1.260648  |
| C | 1.969956  | -1.037890 | -0.752160 |
| C | 2.043295  | 1.394433  | -0.066770 |
| H | 1.641342  | -0.750447 | -1.751521 |
| H | 1.562096  | -2.020349 | -0.524327 |
| H | 3.058109  | -1.075609 | -0.742090 |
| H | 1.888596  | 2.116909  | 0.731490  |
| H | 1.596849  | 1.785603  | -0.980570 |
| H | 3.116787  | 1.317046  | -0.236539 |

Rotational constants (GHz): 1.9395200 1.4522600 1.0278700

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i414.1440 | 59.3244   | 67.8706   |
| 179.8346  | 187.1814  | 222.5819  |
| 229.1878  | 256.0968  | 278.6464  |
| 312.3536  | 326.1984  | 349.4976  |
| 361.8242  | 413.0207  | 500.3926  |
| 556.8136  | 689.1707  | 733.6199  |
| 832.4142  | 879.6676  | 903.8443  |
| 939.2206  | 942.6843  | 979.0595  |
| 985.2247  | 1000.4773 | 1097.6277 |
| 1114.7781 | 1126.6834 | 1178.7581 |
| 1192.2706 | 1245.1768 | 1279.1418 |
| 1286.8018 | 1368.6801 | 1389.0849 |
| 1394.9300 | 1422.1368 | 1426.3641 |
| 1428.9615 | 1481.0800 | 1483.4811 |
| 1489.0766 | 1490.4128 | 1499.5330 |
| 1505.4975 | 1512.5455 | 1524.2735 |
| 1564.1300 | 3065.1209 | 3066.6796 |
| 3071.1850 | 3077.6292 | 3079.7031 |
| 3082.1268 | 3138.2084 | 3141.6664 |
| 3147.1294 | 3151.9499 | 3152.6922 |
| 3162.9560 | 3176.8621 | 3188.7749 |

Zero-point correction (Hartree): 0.201368

TS.ic3H7\_ic3H7\_COO.ringclose.mp  
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E(RM062X/Aug-CC-pVTZ) (Hartree): -425.41073696

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-0.041514	-0.377068	-0.060607
O	-0.402153	-1.453599	0.507569
O	-1.457922	-1.855198	-0.439887
C	-0.924984	0.816573	-0.242612
C	1.431350	-0.318580	-0.361265
H	-0.625431	1.318296	-1.163622
C	-2.431799	0.626018	-0.213566
C	-0.511892	1.729171	0.946728
H	-2.729004	0.055438	0.663462
H	-2.777389	0.085629	-1.087251
H	-2.903942	1.609215	-0.175342
H	0.557568	1.912814	1.011544
H	-0.842490	1.274810	1.880718
H	-1.014443	2.687797	0.833090
H	1.562065	-1.227857	-0.959606
C	1.924144	0.865590	-1.181910
C	2.239562	-0.515690	0.931085
H	1.824299	1.811768	-0.652094
H	1.397429	0.945218	-2.131517
H	2.981860	0.724222	-1.401362
H	1.875130	-1.371652	1.494073
H	2.180600	0.371940	1.560814
H	3.285155	-0.683347	0.678514

Rotational constants (GHz): 2.0493600 1.3229400 1.0318000

Vibrational harmonic frequencies (cm-1):

i405.0043	60.4742	101.6135
184.0804	209.2092	227.0826
253.4539	262.6697	281.4155
296.8231	320.7632	353.6940

368.5830	404.7803	496.6782
554.9374	652.8330	749.1547
835.5764	871.0459	908.7102
934.9371	944.9329	976.9817
982.7345	1026.0649	1104.1882
1125.9011	1138.5941	1159.6446
1198.6422	1240.9502	1277.8271
1296.4311	1366.6224	1386.7896
1397.0509	1422.4125	1424.7954
1430.0771	1482.0937	1484.1285
1492.9342	1497.5491	1499.3170
1511.0766	1516.6845	1519.4654
1561.1007	3035.2185	3068.7336
3072.9174	3073.7078	3077.0922
3093.6495	3140.8674	3143.9035
3145.7917	3148.6217	3151.3521
3164.2761	3169.9435	3192.7043

Zero-point correction (Hartree): 0.201555

TS.iC3H7_iC3H7_COO.ringclose.mt

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E(RM062X/Aug-CC-pVT2) (Hartree): -425.41538459

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.023425 | -0.099519 | -0.070487 |
| O | -0.093672 | -0.964161 | -0.997111 |
| O | 0.589645  | -2.059354 | -0.283150 |
| C | 1.244780  | 0.444775  | 0.508115  |
| C | -1.332828 | 0.485382  | 0.355868  |
| H | 1.095856  | 0.503685  | 1.590804  |
| C | 2.541495  | -0.276492 | 0.182347  |
| C | 1.315377  | 1.896917  | -0.033891 |
| H | 2.601590  | -0.483073 | -0.885145 |
| H | 2.608591  | -1.225089 | 0.701310  |
| H | 3.380128  | 0.361614  | 0.464073  |
| H | 0.421715  | 2.482734  | 0.170927  |
| H | 1.480780  | 1.878959  | -1.111668 |
| H | 2.162551  | 2.398224  | 0.429526  |
| H | -1.153334 | 1.322019  | 1.029538  |
| C | -2.157505 | 0.938996  | -0.848622 |
| C | -2.049933 | -0.635717 | 1.129733  |
| H | -2.314335 | 0.106253  | -1.531909 |
| H | -1.663371 | 1.744849  | -1.390880 |
| H | -3.128458 | 1.296217  | -0.508468 |
| H | -1.469985 | -0.964442 | 1.990941  |
| H | -2.203235 | -1.495186 | 0.479319  |
| H | -3.014048 | -0.264704 | 1.475345  |

Rotational constants (GHz): 2.1208700 1.3199000 1.0228300

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i414.0082 | 39.1857   | 78.2587   |
| 161.4310  | 196.9741  | 209.1083  |
| 226.0958  | 251.3752  | 265.5979  |
| 270.9062  | 312.1684  | 342.3846  |
| 367.5271  | 416.3654  | 476.8908  |
| 601.5374  | 694.5698  | 761.5338  |
| 841.1563  | 874.1923  | 903.7392  |
| 934.3895  | 949.3363  | 980.5653  |
| 986.5116  | 1049.2765 | 1082.6567 |
| 1117.5999 | 1123.8853 | 1147.4628 |
| 1197.6344 | 1209.2731 | 1271.4884 |
| 1334.4353 | 1365.0503 | 1395.6722 |
| 1397.4433 | 1407.0865 | 1426.1333 |
| 1428.5495 | 1483.0836 | 1485.1842 |
| 1486.0173 | 1489.8249 | 1501.8466 |
| 1505.8232 | 1510.0608 | 1519.3025 |
| 1574.2354 | 3052.8422 | 3068.6177 |
| 3068.7786 | 3069.2461 | 3072.4613 |
| 3103.5849 | 3139.2778 | 3140.5707 |
| 3145.0642 | 3145.2810 | 3153.3958 |
| 3156.5754 | 3158.5391 | 3196.3148 |

Zero-point correction (Hartree): 0.201211

TS.iC3H7\_iC3H7\_COO.ringclose.pm

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E(RM062X/Aug-CC-pVT2) (Hartree): -425.41580534

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-0.093874	-0.284919	-0.180682
O	-0.066767	-1.511405	0.154495
O	0.751395	-1.250871	1.354720
C	1.143663	0.522117	-0.490403
C	-1.442201	0.294199	-0.503755
H	0.815395	1.222434	-1.266701
C	1.693131	1.353716	0.674584
C	2.232612	-0.384050	-1.064165
H	2.200490	0.691233	1.369459
H	0.912366	1.878737	1.220305
H	2.397017	2.089198	0.284269
H	1.886419	-0.922759	-1.945633
H	2.536727	-1.104544	-0.308837
H	3.090500	0.224350	-1.348523
H	-1.392481	0.549936	-1.569120
C	-2.574479	-0.691556	-0.257821
C	-1.654846	1.605878	0.269223
H	-2.619573	-0.957698	0.797718
H	-2.438932	-1.609219	-0.825708
H	-3.522828	-0.239339	-0.544842
H	-0.922098	2.364264	0.001859
H	-1.598021	1.427229	1.342774
H	-2.646041	1.992078	0.037368

Rotational constants (GHz): 2.2171400 1.2656400 1.0503400

Vibrational harmonic frequencies (cm-1):

i531.8626	37.5204	115.1019
178.1741	197.1764	214.3780
240.8986	259.5083	284.1465
288.6433	299.9329	331.5254
366.4461	425.8764	482.4867
575.6823	681.3973	737.2706
845.2477	881.9029	926.8951
937.7009	951.1936	981.9960
985.9625	1060.6893	1081.4690
1129.4147	1137.5360	1159.1384
1208.2813	1217.2310	1294.7667
1326.1541	1369.6377	1386.7613
1401.6077	1405.7505	1418.9111
1425.6137	1482.6300	1489.0108
1491.8234	1497.7666	1501.1479
1508.4356	1514.2033	1524.6760
1565.1168	3024.0200	3036.9790
3070.0435	3070.9506	3074.4204
3074.9457	3138.9844	3144.6124
3147.9358	3148.9062	3156.8526
3157.1988	3166.0349	3177.3822

Zero-point correction (Hartree): 0.201422

TS.iC3H7_iC3H7_COO.ringclose.pp
 ~~~~~  
 E(RM062X/Aug-CC-pVTZ) (Hartree): -425.41710061  
 Electronic state : 1-A  
 Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.077580  | -0.296291 | 0.074593  |
| O | -0.038756 | -1.559441 | 0.182789  |
| O | -1.103222 | -1.658803 | -0.831437 |
| C | -1.043120 | 0.663442  | 0.332703  |
| C | 1.455591  | 0.199010  | -0.257354 |
| H | -0.585613 | 1.414649  | 0.987965  |
| C | -1.474986 | 1.379525  | -0.953443 |
| C | -2.234366 | 0.056821  | 1.062194  |
| H | -1.972881 | 0.658223  | -1.597418 |
| H | -0.632844 | 1.805623  | -1.498620 |
| H | -2.164700 | 2.185414  | -0.705567 |
| H | -1.912697 | -0.565476 | 1.896388  |
| H | -2.818620 | -0.561394 | 0.388852  |
| H | -2.855029 | 0.863733  | 1.452344  |
| H | 1.412115  | 0.191606  | -1.358976 |
| C | 1.780957  | 1.616342  | 0.206215  |
| C | 2.536562  | -0.795546 | 0.169104  |
| H | 1.794074  | 1.669048  | 1.295784  |
| H | 1.076196  | 2.356575  | -0.165286 |
| H | 2.772675  | 1.890414  | -0.149745 |
| H | 2.351086  | -1.786202 | -0.234755 |
| H | 2.577021  | -0.870027 | 1.256251  |
| H | 3.505740  | -0.446053 | -0.182102 |

Rotational constants (GHz): 2.1455900 1.3159500 0.9975400  
 Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i470.4659 | 36.5771   | 114.5764  |
| 171.3358  | 194.5159  | 199.2131  |
| 228.2844  | 250.8052  | 286.5178  |
| 307.2292  | 312.7430  | 321.9107  |
| 378.2210  | 457.1378  | 473.4976  |
| 524.4353  | 652.9327  | 715.0276  |
| 844.3168  | 880.7133  | 928.0221  |
| 934.7635  | 947.1567  | 981.2917  |
| 985.5822  | 1059.0449 | 1062.6318 |
| 1108.0938 | 1158.3504 | 1170.3146 |
| 1206.0653 | 1240.9297 | 1291.9564 |
| 1306.4104 | 1334.4835 | 1388.9977 |
| 1404.1803 | 1414.1820 | 1423.5028 |
| 1426.7433 | 1479.4037 | 1491.7587 |
| 1495.5253 | 1497.2062 | 1498.3515 |
| 1511.9798 | 1518.3204 | 1520.5901 |
| 1556.9776 | 2982.6868 | 3028.4178 |
| 3069.2030 | 3070.4311 | 3072.5846 |
| 3073.9739 | 3136.7467 | 3137.2335 |
| 3138.8496 | 3141.7923 | 3159.1298 |
| 3163.8392 | 3174.9427 | 3185.1698 |

Zero-point correction (Hartree): 0.200998

TS.iC3H7\_iC3H7\_COO.ringclose.pt  
 ~~~~~  
 E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -424.78696083
 E(CCSD/Aug-CC-pVTZ) (Hartree): -424.70441877
 T1 diagnostic: 0.027019
 E(MP2/Aug-CC-pVTZ) (Hartree): -424.63307379
 E(MP3/Aug-CC-pVTZ) (Hartree): -424.68920326
 E(RHF/Aug-CC-pVTZ) (Hartree): -422.92348385
 E(RM062X/Aug-CC-pVTZ) (Hartree): -425.42021290
 Electronic state : 1-A
 Cartesian coordinates (Angs):

C	-0.069534	-0.218372	-0.171642
O	-0.149250	-1.409783	0.264410
O	0.779985	-1.198120	1.389426
C	1.196733	0.444893	-0.604524
C	-1.372924	0.491916	-0.352210
H	0.925196	0.821045	-1.602710
C	1.498810	1.671764	0.265401
C	2.403078	-0.471363	-0.734902
H	1.728665	1.335854	1.274800
H	0.661509	2.368714	0.305188
H	2.359418	2.198703	-0.144106
H	2.128017	-1.428182	-1.176256
H	2.837067	-0.669424	0.239616
H	3.143627	0.009313	-1.374906
H	-1.195484	1.425671	-0.886388

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C      -2.353619      -0.383560      -1.136570
C      -1.913965      0.796648      1.054547
H      -2.517378      -1.325001      -0.615237
H      -1.986268      -0.600214      -2.139060
H      -3.307035      0.135397      -1.224350
H      -1.231026      1.425960      1.622926
H      -2.051532      -0.133213      1.604225
H      -2.872133      1.307043      0.964971
Rotational constants (GHz):      2.2483100      1.2016900      1.1070400
Vibrational harmonic frequencies (cm-1):
i442.6634      52.8383      96.7665
163.1165      191.1082      199.6168
215.3398      248.2203      261.0413
278.5666      298.8977      316.7111
360.5880      434.4948      482.9577
595.8460      694.9423      737.7417
847.0698      877.7001      925.8465
942.5023      946.2382      983.9869
987.1971      1056.2229      1095.6856
1106.4360      1128.4351      1156.9928
1197.2766      1227.8243      1295.4718
1332.2235      1369.9650      1389.3437
1396.1993      1406.4927      1419.7513
1429.3041      1481.1514      1486.1797
1490.4599      1493.8958      1499.6496
1503.4749      1514.1928      1521.1993
1575.9954      2984.3390      3067.7186
3069.7782      3070.0116      3073.1316
3091.2500      3138.5938      3140.5053
3142.4569      3147.8851      3153.0444
3156.4123      3158.2808      3183.1452
Zero-point correction (Hartree): 0.201139

Population analysis as 298K (%)
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)
Compound      Qtot      Erel      Erel2      n*Q*MB      %
-----
TS.iC3H7_iC3H7_COO.14Hshift.m 5.656e+41 0.00 0.00 1.131e+42 71.7
TS.iC3H7_iC3H7_COO.14Hshift.p 6.866e+41 0.72 0.72 4.095e+41 25.9
TS.iC3H7_iC3H7_COO.14Hshift.c 6.489e+41 2.10 2.10 3.757e+40 2.38
Total 1.578e+42 100

TS.iC3H7_iC3H7_COO.14Hshift.c
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E(RM062X/Aug-CC-pVTZ) (Hartree): -425.41917183
Electronic state : 1-A
Cartesian coordinates (Angs):
C      0.049849      -0.454190      0.022989
O      0.648824      -1.608099      -0.002377
O      1.979418      -1.471270      -0.393606
C      0.875585      0.663392      -0.242137
C      -1.433180      -0.581412      0.202312
H      1.706259      -0.255447      -0.811134
C      1.896314      1.006537      0.858142
C      0.268316      1.901657      -0.864672
H      2.756213      1.516494      0.424347
H      2.251122      0.121982      1.378396
H      1.430391      1.681920      1.580031
H      -0.407182      2.434891      -0.189083
H      -0.266998      1.685267      -1.786210
H      1.074256      2.592475      -1.113944
H      -1.613459      -1.643361      0.377986
C      -1.880134      0.214480      1.429737
C      -2.220990      -0.171331      -1.046884
H      -1.686528      1.278337      1.292810
H      -1.360218      -0.115569      2.328192
H      -2.950709      0.082929      1.584933
H      -1.812799      -0.627852      -1.947781
H      -2.227566      0.908938      -1.173314
H      -3.253275      -0.500851      -0.934295
Rotational constants (GHz):      1.9847000      1.3016900      1.0678200
Vibrational harmonic frequencies (cm-1):
i1611.7575      50.1762      118.4993
177.9335      192.7292      208.0586
211.6851      239.6007      262.3116
298.3485      299.8095      342.2636
361.0890      379.0732      480.3967
592.7728      644.7633      748.5696
767.7457      903.3203      941.5249
961.0021      981.8080      987.1825
1008.9884      1027.0999      1075.8282
1095.8198      1133.0449      1177.0635
1194.8689      1248.6164      1310.4681
1339.3691      1343.2677      1391.6428
1398.2873      1408.6577      1422.4228
1444.5881      1485.9625      1490.5579
1491.7362      1497.4058      1497.9557
1507.1351      1513.9062      1522.9840
1567.1866      1877.8401      3039.8548
3047.0330      3065.9789      3072.2066
3079.5985      3106.4634      3113.2914
3139.3378      3141.1062      3142.3797
3146.7984      3162.3106      3171.5856
Zero-point correction (Hartree): 0.198317

TS.iC3H7_iC3H7_COO.14Hshift.m
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E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -424.78561561
E(CCSD/Aug-CC-pVTZ) (Hartree): -424.70066990
T1 diagnostic: 0.019899
E(MP2/Aug-CC-pVTZ) (Hartree): -424.64426914

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E(MP3/Aug-CC-pVTZ) (Hartree): -424.68987265
E(RHF/Aug-CC-pVTZ) (Hartree): -422.90009517
E(RM062X/Aug-CC-pVTZ) (Hartree): -425.42233952
Electronic state : 1-A
Cartesian coordinates (Angs):
C      -0.072574      -0.243241      -0.092160
O      -0.090017      -1.528488       0.076012
O       1.194986      -2.056179      -0.060367
C       1.199934       0.343353      -0.282947
C      -1.415080       0.403838      -0.220262
H       1.572552      -0.920113      -0.626334
C       2.140951       0.373301       0.931550
C       1.254562       1.625935      -1.083875
H       3.177431       0.426141       0.598871
H       2.026587      -0.505703       1.558321
H       1.933085       1.265833       1.527209
H       0.906436       2.490959      -0.510780
H       0.673317       1.569173      -2.003307
H       2.288581       1.826643      -1.364840
H      -1.350910       1.041875      -1.105592
C      -2.559184      -0.587419      -0.389208
C      -1.625476       1.313486       0.998690
H      -2.650943      -1.223265       0.490619
H      -2.405918      -1.231956      -1.252485
H      -3.495139      -0.045823      -0.518912
H      -0.808939       2.025545       1.113217
H      -1.688441       0.713915       1.907273
H      -2.556252       1.868589       0.890849
Rotational constants (GHz):      1.9854300      1.3513700      0.9972300
Vibrational harmonic frequencies (cm-1):
i1609.5560      60.7688      119.0469
172.7442      180.7922      218.2314
225.1861      238.2840      266.7734
275.4235      293.4970      351.9478
354.6878      400.0820      502.2127
561.7981      624.9976      754.4573
771.1344      893.9814      936.7263
966.6532      979.6917      988.1391
1003.8409      1021.3268      1087.0139
1121.6872      1129.6516      1152.2794
1205.0659      1227.8473      1310.0578
1328.0758      1346.5017      1390.6520
1397.9222      1418.2070      1421.9759
1443.5158      1485.5807      1489.6440
1493.7880      1497.9000      1498.9479
1505.2562      1508.5564      1516.6624
1568.4368      1872.1587      3036.9108
3047.3626      3063.1664      3068.3765
3073.1074      3104.7880      3113.1804
3134.0812      3137.1198      3143.9733
3145.7444      3152.3638      3174.4715
Zero-point correction (Hartree): 0.198142

TS.iC3H7_iC3H7_COO.14Hshift.p
~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -425.42129666
Electronic state : 1-A
Cartesian coordinates (Angs):
C      -0.041338      -0.163766       0.057338
O      -0.105179      -1.413837      -0.281172
O       1.117123      -1.841543      -0.804509
C       1.222335       0.454932      -0.073131
C      -1.380357       0.474036       0.279787
H       1.469119      -0.545236      -0.939949
C       2.341686       0.008257       0.880226
C       1.221125       1.950594      -0.300869
H       3.313291       0.202332       0.426450
H       2.277679      -1.049199       1.115566
H       2.280278       0.586881       1.804392
H       1.096761       2.504727       0.634046
H       0.442243       2.269562      -0.992161
H       2.178892       2.251125      -0.726170
H      -1.195500       1.460287       0.706098
C      -2.114131       0.632306      -1.057323
C      -2.212104      -0.352027       1.264071
H      -2.302076      -0.347447      -1.494961
H      -1.534383       1.219044      -1.768800
H      -3.069218       1.131350      -0.896612
H      -1.699775      -0.473156       2.217553
H      -2.413201      -1.340833       0.854916
H      -3.162951       0.147605       1.444496
Rotational constants (GHz):      2.0528600      1.2575800      1.0242400
Vibrational harmonic frequencies (cm-1):
i1617.8573      58.1129      115.5002
168.9382      184.5437      207.4598
215.4606      234.1403      264.2673
266.3371      274.9800      345.6151
359.1920      382.2905      506.4120
561.1550      657.9831      749.9741
774.6669      893.3638      942.1896
967.2501      980.8494      986.5901
994.8152      1019.9115      1095.8759
1116.1152      1131.9474      1153.3407
1203.7580      1223.6370      1329.2797
1343.1925      1355.6510      1391.9554
1397.1973      1408.6545      1420.1456
1442.6565      1487.8582      1490.4491
1491.8913      1496.8596      1503.9472
1506.4852      1508.2794      1519.3366
1574.6176      1863.5324      3040.8447
3054.2262      3066.5816      3069.9842
3092.0117      3107.5606      3117.6538

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3136.9359 3142.4254 3144.0976
3145.8371 3151.8258 3179.1522
Zero-point correction (Hartree): 0.198241

E-(iC3H7)(tC4H9)COO
#####

Population analysis as 298K (%)
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)
Compound Qtot Erel Erel2 n*Q*MB %

iC3H7_tC4H9_COO.c 3.083e+42 0.00 0.00 3.083e+42 97.9
iC3H7_tC4H9_COO.t 1.312e+42 2.19 2.19 6.534e+40 2.08
Total 3.149e+42 100

iC3H7_tC4H9_COO.c
~~~~~

E(RM062X/Aug-CC-pVTZ) (Hartree): -464.76161067

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.073733 | -0.228599 | -0.000027 |
| O | -0.342205 | -1.448956 | 0.000042  |
| O | -1.648737 | -1.874825 | 0.000014  |
| C | -1.128546 | 0.832035  | -0.000056 |
| C | 1.399239  | 0.108251  | -0.000052 |
| C | -1.978984 | 0.767186  | -1.275459 |
| C | -1.978713 | 0.767229  | 1.275574  |
| H | -0.600916 | 1.785524  | -0.000112 |
| H | -2.518934 | -0.173630 | -1.320124 |
| H | -1.358689 | 0.864852  | -2.167047 |
| H | -2.687223 | 1.595395  | -1.263776 |
| H | -1.358243 | 0.865371  | 2.166988  |
| H | -2.518320 | -0.173767 | 1.320583  |
| H | -2.687239 | 1.595190  | 1.263831  |
| C | 1.704945  | 0.936042  | -1.258206 |
| C | 1.704924  | 0.936217  | 1.258045  |
| C | 2.258059  | -1.154154 | 0.000084  |
| H | 1.130993  | 1.861408  | -1.292244 |
| H | 1.493184  | 0.362714  | -2.161051 |
| H | 2.763567  | 1.196759  | -1.260570 |
| H | 1.493025  | 0.363024  | 2.160943  |
| H | 1.131061  | 1.861644  | 1.291903  |
| H | 2.763574  | 1.196817  | 1.260447  |
| H | 2.064512  | -1.764637 | -0.880403 |
| H | 2.064472  | -1.764458 | 0.880689  |
| H | 3.309564  | -0.867198 | 0.000078  |

Rotational constants (GHz): 1.7611400 1.0237000 0.9039400

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| 64.1297   | 87.5252   | 164.9552  |
| 196.8955  | 197.7759  | 213.0744  |
| 231.1511  | 251.4932  | 259.6603  |
| 267.1691  | 297.1761  | 303.5861  |
| 325.6957  | 341.3427  | 389.9011  |
| 407.9087  | 430.7774  | 474.5928  |
| 582.0964  | 746.3577  | 761.3884  |
| 829.6862  | 905.8869  | 942.4297  |
| 952.5638  | 954.1686  | 968.2167  |
| 971.9188  | 991.0745  | 1037.6124 |
| 1045.1611 | 1120.6478 | 1129.3272 |
| 1132.6457 | 1214.4339 | 1237.0496 |
| 1259.3261 | 1313.2835 | 1345.9042 |
| 1383.1661 | 1399.1605 | 1399.6973 |
| 1407.3137 | 1428.1732 | 1435.4333 |
| 1479.9531 | 1484.4219 | 1487.9113 |
| 1488.3898 | 1498.4625 | 1505.3742 |
| 1508.0455 | 1508.1485 | 1522.3082 |
| 1532.3246 | 1635.3154 | 3060.9045 |
| 3061.5419 | 3067.0847 | 3067.3849 |
| 3071.0737 | 3096.6944 | 3130.6779 |
| 3131.6945 | 3134.0440 | 3134.8110 |
| 3139.3811 | 3142.2828 | 3144.6705 |
| 3152.2286 | 3180.5139 | 3182.2723 |

Zero-point correction (Hartree): 0.230885

iC3H7\_tC4H9\_COO.t

~~~~~

E(RM062X/Aug-CC-pVTZ) (Hartree): -464.75874451

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-0.153960	0.358978	-0.179137
O	-0.300565	1.604088	-0.254378
O	-1.552749	2.135073	-0.425091
C	-1.383709	-0.485501	-0.269145
C	1.272977	-0.082121	0.077164
C	-1.232520	-1.920558	-0.756506
C	-2.088874	-0.418462	1.099605
C	-2.017314	0.069947	-0.963900
H	-0.625382	-2.536488	-0.094778
H	-0.814166	-1.970542	-1.759968
H	-2.226052	-2.367314	-0.791557
H	-2.196748	0.616003	1.418994
H	-1.536446	-0.983912	1.850211
H	-3.082271	-0.855484	1.006558
C	2.189634	1.135786	0.216370
C	1.310978	-0.882314	1.388569
C	1.788964	-0.949723	-1.082825
H	1.864406	1.790453	1.022703
H	2.215740	1.720436	-0.701690
H	3.198808	0.787598	0.435398
H	0.687730	-1.773230	1.349225

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H      0.984081      -0.268103      2.228046
H      2.337875      -1.197709      1.576069
H      1.651402      -0.446927      -2.040585
H      1.306459      -1.921619      -1.124222
H      2.857440      -1.112904      -0.939313
Rotational constants (GHz):      1.5470300      1.1781700      0.8868200
Vibrational harmonic frequencies (cm-1):
73.6404      123.4756      163.4711
215.4089      230.1540      242.4343
244.1894      258.9249      281.2586
297.6470      316.1443      325.9660
341.5613      365.3693      388.7445
417.6549      427.4088      529.4088
598.4457      684.4501      743.6940
838.4893      912.7772      940.1009
954.2320      958.2201      972.0612
973.7242      991.9221      1029.0470
1047.2029      1075.0819      1139.3725
1187.4324      1220.2590      1238.6208
1256.1458      1315.3369      1348.1839
1367.7918      1389.9341      1398.3324
1406.6898      1424.1451      1437.1518
1481.1218      1484.0037      1489.1881
1493.9293      1502.9200      1504.1207
1506.8504      1515.9200      1523.5692
1530.0978      1593.7830      3063.8837
3065.8207      3067.1549      3071.2611
3072.6701      3075.7248      3131.1409
3132.5287      3135.2769      3139.5264
3145.6360      3149.1605      3154.1086
3157.8421      3162.6483      3177.0043
Zero-point correction (Hartree): 0.231504

Population analysis as 298K (%)
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)
Compound      Qtot      Erel      Erel2      n*Q*MB      %
-----
TS.tC4H9_iC3H7_COO.isom.t 7.214e+42 0.00      0.00      1.443e+43 99
TS.tC4H9_iC3H7_COO.isom.c 2.751e+42 2.45      2.45      8.758e+40 0.601
TS.tC4H9_iC3H7_COO.isom.p 2.449e+42 2.57      2.57      6.426e+40 0.441
Total      1.458e+43 100

TS.tC4H9_iC3H7_COO.isom.c
~~~~~
E(UM062X/Aug-CC-pVT2) (Hartree): -464.70466901
Electronic state : 1-A
Cartesian coordinates (Angs):
C      0.110652      0.279825      -0.459150
O      -0.321645      1.544339      -0.909802
O      -0.597725      2.369993      0.072625
C      -0.985920      -0.606860      0.071681
C      1.593634      0.241600      -0.224461
C      -2.176140      -0.555901      -0.897362
C      -0.494835      -2.054204      0.164456
C      -1.468805      -0.161446      1.465967
H      1.965624      1.147645      -0.707620
C      1.954569      0.340152      1.265496
C      2.313775      -0.941049      -0.882169
H      1.649446      -0.559257      1.801169
H      1.472785      1.199349      1.730326
H      3.034534      0.443879      1.376332
H      3.388846      -0.760701      -0.864232
H      2.004926      -1.063948      -1.919808
H      2.128217      -1.874514      -0.355236
H      -1.878245      -0.877591      -1.896105
H      -2.586407      0.450131      -0.968293
H      -2.962595      -1.221570      -0.539945
H      0.307733      -2.164730      0.893003
H      -0.142693      -2.417213      -0.801185
H      -1.322746      -2.686804      0.485985
H      -1.891584      0.840119      1.436223
H      -0.655076      -0.167916      2.190029
H      -2.239387      -0.854238      1.810031
Rotational constants (GHz):      1.4818100      1.1902400      0.9285700
Vibrational harmonic frequencies (cm-1):
i218.7716      42.8644      81.2838
154.2769      196.6056      222.4758
250.2362      252.4171      271.1499
282.1946      295.8496      316.9371
334.5478      354.7390      372.9416
395.6105      403.1751      476.4487
554.3265      641.3383      683.3132
831.7230      900.3523      932.4351
942.3833      960.1841      968.2902
969.0389      1022.1794      1035.8919
1041.5063      1101.0698      1113.9240
1175.8638      1201.8149      1214.2387
1228.7733      1260.3560      1330.8696
1332.7675      1390.2981      1393.7134
1396.6224      1399.6738      1416.4100
1431.6606      1478.1203      1486.1866
1487.2333      1490.5569      1495.2459
1502.2279      1505.6978      1512.5466
1516.5907      1528.5199      3057.5183
3058.6325      3059.3551      3063.6079
3066.4432      3068.2972      3127.1757
3128.2124      3130.2844      3133.3569
3134.7899      3140.5576      3143.6281
3146.1760      3156.9644      3160.1125
Zero-point correction (Hartree): 0.228621

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TS.tc4H9_iC3H7_COO.isom.p
~~~~~
E(UM062X/Aug-CC-pVTZ) (Hartree): -464.70456047
Electronic state : 1-A
Cartesian coordinates (Angs):
C      -0.077628      0.432942     -0.072601
O       0.417569      1.620235      0.520635
O       0.876723      2.463465     -0.368885
C       0.932307     -0.683435     -0.030504
C      -1.577325      0.391306     -0.029393
C       1.276086     -1.016215      1.434550
C       0.400984     -1.939989     -0.719428
C       2.213983     -0.234571     -0.747228
H      -1.872373      1.442927     -0.007298
C      -2.226052     -0.225098     -1.272395
C      -2.117838     -0.261188      1.252342
H      -2.132473     -1.308769     -1.287522
H      -1.783469      0.172825     -2.184913
H      -3.289882      0.013112     -1.275532
H      -1.892525     -1.327966      1.272312
H      -3.201449     -0.147923      1.298204
H     -1.686645      0.198008      2.141625
H       0.405745     -1.395099      1.969975
H       1.648041     -0.134885      1.955973
H       2.052768     -1.782442      1.460778
H       0.150400     -1.744520     -1.762020
H      -0.479855     -2.338297     -0.216968
H       1.173501     -2.709273     -0.693949
H       2.661743      0.630826     -0.261326
H       2.005702      0.028715     -1.784272
H       2.939333     -1.049358     -0.731124
Rotational constants (GHz):   1.4381000   1.1672800   0.9146500
Vibrational harmonic frequencies (cm-1):
i155.6007      52.0092      80.3132
140.9528      195.7969      226.3157
261.3390      263.7426      275.6335
283.9097      293.2791      309.5128
327.0181      352.7989      382.3498
394.5549      417.3409      478.2226
535.8619      610.4625      715.7430
832.9530      899.8295      931.3978
942.2341      960.6838      967.3160
970.8642      1012.8071     1034.3709
1040.9035      1098.2595     1116.2770
1174.6090      1216.4638     1225.7147
1238.4354      1267.1347     1332.7951
1335.6447      1389.6431     1391.5295
1397.4598      1400.9937     1417.1778
1430.8786      1479.2409     1485.7220
1488.1909      1491.3239     1496.4890
1503.7100      1506.5598     1513.1513
1516.8977      1528.8773     3056.4825
3057.5976      3059.4014     3063.7120
3064.8449      3069.8465     3126.5232
3128.2568      3129.7140     3133.3121
3135.2999      3136.4214     3142.0940
3144.3052      3146.3813     3157.7564
Zero-point correction (Hartree): 0.228695

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TS.tc4H9_iC3H7_COO.isom.t
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E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -464.00317523
E(CCSD/Aug-CC-pVTZ) (Hartree): -463.91977636
T1 diagnostic: 0.019919
E(MP2/Aug-CC-pVTZ) (Hartree): -463.82664275
E(MP3/Aug-CC-pVTZ) (Hartree): -463.90507313
E(PMP2/Aug-CC-pVTZ) (Hartree): -463.85171271
E(PMP3/Aug-CC-pVTZ) (Hartree): -463.93000193
E(PUHF/Aug-CC-pVTZ) (Hartree): -462.00777995
E(UHF/Aug-CC-pVTZ) (Hartree): -461.98250820
E(UM062X/Aug-CC-pVTZ) (Hartree): -464.70795641
Electronic state : 1-A
Cartesian coordinates (Angs):
C       0.111200      0.003931     -0.341377
O       0.373764      1.258388     -0.909392
O       0.648265      2.177526     -0.008867
C      -1.317941     -0.264049      0.047114
C       1.305150     -0.742801      0.162224
C      -2.263270      0.693913     -0.680468
C      -1.687019     -1.706308     -0.323820
C      -1.469231     -0.074168      1.567369
H       0.918051     -1.663202      0.603638
C       2.229647     -1.117877     -1.002020
C       2.096604     -0.000564      1.248356
H       2.600578     -0.216740     -1.491362
H       1.705100     -1.718316     -1.744758
H       3.087322     -1.683940     -0.638298
H       1.455133      0.320668      2.067160
H       2.581288      0.883182      0.835785
H       2.869599     -0.659978      1.644663
H      -2.148247      0.612209     -1.761653
H      -2.078698      1.728757     -0.396012
H      -3.293303      0.445957     -0.423424
H      -1.601450     -1.861025     -1.399839
H      -2.717366     -1.907667     -0.027292
H      -1.049289     -2.432285      0.179916
H      -1.197261      0.940903      1.857637
H      -0.833832     -0.772576      2.114135
H      -2.504701     -0.255719      1.861504
Rotational constants (GHz):   1.6581200   1.0664700   0.9130000
Vibrational harmonic frequencies (cm-1):
i213.7207      35.2237      46.4910

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129.4681	183.8038	215.9049
235.5197	258.9108	268.2746
278.0275	292.7032	305.5354
310.3399	333.0697	366.2887
391.6103	412.7430	475.1089
542.1654	642.3621	712.5158
824.9619	895.2292	931.7865
943.1199	957.8856	967.7049
968.7227	1026.8738	1037.0704
1053.9465	1094.4573	1111.3918
1172.4284	1186.8242	1222.9297
1225.7942	1272.8876	1300.0438
1322.9022	1387.7958	1393.5144
1395.3785	1402.6782	1417.4574
1430.0065	1479.9650	1484.8510
1485.2372	1489.6601	1491.3996
1502.5735	1504.7989	1507.3547
1511.1792	1523.6153	3048.8923
3057.1858	3058.9290	3063.0303
3063.9902	3078.8261	3119.7497
3127.7887	3131.7236	3132.0913
3134.3537	3135.2486	3135.9806
3138.2158	3144.8051	3149.4247

Zero-point correction (Hartree): 0.228001

Population analysis as 298K (%)

Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)

Compound	Qtot	Erel	Erel2	n*Q*MB	%
TS.iC3H7_tC4H9_COO.ringclose.p	1.706e+42	0.00	0.00	3.413e+42	99.9
TS.iC3H7_tC4H9_COO.ringclose.c	2.296e+42	4.35	4.35	2.968e+39	0.0868
TS.iC3H7_tC4H9_COO.ringclose.m	2.033e+42	4.50	4.50	2.037e+39	0.0596
Total				3.418e+42	100

TS.iC3H7_tC4H9_COO.ringclose.c

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E(RM062X/Aug-CC-pVTZ) (Hartree): -464.72113143

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.118819 | 0.430375  | -0.229354 |
| O | 0.084881  | 1.558794  | -0.781809 |
| O | -0.791799 | 2.330953  | 0.124652  |
| C | -1.521946 | -0.112787 | -0.166852 |
| C | 1.149115  | -0.318534 | 0.121445  |
| H | -2.124913 | 0.692842  | -0.575689 |
| C | -1.643878 | -1.326604 | -1.103600 |
| C | -2.047393 | -0.412064 | 1.236884  |
| H | -1.104857 | -2.202026 | -0.748069 |
| H | -1.299071 | -1.089809 | -2.110089 |
| H | -2.698754 | -1.593153 | -1.168075 |
| H | -1.860519 | 0.432987  | 1.896591  |
| H | -1.609305 | -1.311071 | 1.664925  |
| H | -3.124467 | -0.566643 | 1.176246  |
| C | 2.110877  | 0.687256  | 0.776878  |
| C | 0.965385  | -1.500598 | 1.071653  |
| C | 1.750325  | -0.798417 | -1.215960 |
| H | 1.656566  | 1.138194  | 1.659006  |
| H | 2.372883  | 1.485864  | 0.088511  |
| H | 3.016105  | 0.160293  | 1.078738  |
| H | 0.281993  | -2.256376 | 0.694267  |
| H | 0.615434  | -1.168820 | 2.048090  |
| H | 1.936867  | -1.975593 | 1.211566  |
| H | 1.861117  | 0.031442  | -1.912532 |
| H | 1.136719  | -1.571532 | -1.677043 |
| H | 2.737557  | -1.216335 | -1.015743 |

Rotational constants (GHz): 1.5032000 1.2077500 0.9635600

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i460.6976 | 43.3069   | 111.7219  |
| 168.2351  | 185.4233  | 221.5516  |
| 236.3145  | 243.8577  | 256.2886  |
| 266.1840  | 277.2335  | 301.8331  |
| 327.5408  | 351.9784  | 378.9012  |
| 392.6482  | 419.4326  | 511.1771  |
| 570.4925  | 642.7677  | 711.7641  |
| 822.5740  | 847.4150  | 909.7951  |
| 941.1576  | 954.9032  | 966.2981  |
| 977.9827  | 979.6649  | 1010.2982 |
| 1039.3709 | 1062.7864 | 1116.0543 |
| 1178.4509 | 1217.3795 | 1225.6996 |
| 1257.6071 | 1322.8942 | 1325.1657 |
| 1371.0837 | 1391.4532 | 1394.1983 |
| 1402.9747 | 1417.3906 | 1435.7127 |
| 1479.0189 | 1484.3304 | 1491.1297 |
| 1494.2623 | 1495.9279 | 1502.8906 |
| 1508.1546 | 1510.8369 | 1520.4058 |
| 1527.8725 | 1555.3471 | 3062.4924 |
| 3067.6744 | 3068.9131 | 3074.2658 |
| 3076.7983 | 3130.1409 | 3134.6106 |
| 3136.2468 | 3137.3133 | 3140.8563 |
| 3144.6651 | 3150.4270 | 3154.9073 |
| 3164.4776 | 3170.2995 | 3178.9412 |

Zero-point correction (Hartree): 0.229526

TS.iC3H7\_tC4H9\_COO.ringclose.m

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E(RM062X/Aug-CC-pVTZ) (Hartree): -464.72081439

Electronic state : 1-A

Cartesian coordinates (Angs):

C	0.149591	0.223220	0.115306
O	0.323440	1.209830	0.896549
O	1.120641	2.064898	-0.005981

C	1.261488	-0.644032	-0.385839
C	-1.301055	-0.133843	-0.114156
H	0.935738	-1.102960	-1.318508
C	2.654299	-0.061060	-0.554516
C	1.311290	-1.757254	0.700301
H	2.978862	0.431946	0.358043
H	2.677273	0.675247	-1.350428
H	3.342028	-0.876553	-0.786606
H	0.340456	-2.186375	0.938573
H	1.736025	-1.340983	1.613065
H	1.959333	-2.556693	0.345660
C	-1.859352	1.098935	-0.862537
C	-1.549601	-1.375920	-0.966401
C	-2.006213	-0.261788	1.244197
H	-1.351622	1.244201	-1.816051
H	-1.728892	2.001202	-0.269995
H	-2.919714	0.930838	-1.052752
H	-1.139059	-2.284100	-0.528601
H	-1.145735	-1.260880	-1.971797
H	-2.626639	-1.514866	-1.061965
H	-1.827607	0.615941	1.861043
H	-1.666926	-1.146884	1.783329
H	-3.078848	-0.356458	1.074309
Rotational constants (GHz): 1.7191600 1.1273300 0.8950100			
Vibrational harmonic frequencies (cm-1):			
i387.6248	47.3711	94.2946	
166.6475	187.8958	232.9479	
240.5206	252.7739	268.2965	
286.8793	299.9791	322.0233	
331.9168	357.4537	374.4166	
386.7902	411.5704	485.8751	
568.8745	690.6121	735.9343	
822.0752	849.2481	883.2859	
940.8334	953.5003	966.3258	
976.5052	977.5366	1023.9781	
1037.8420	1060.5014	1112.6382	
1130.0178	1206.9534	1218.8844	
1251.3352	1277.3697	1305.9054	
1386.3083	1395.1005	1399.0577	
1423.0406	1427.1380	1435.0343	
1475.7584	1482.0387	1484.7815	
1486.7397	1492.7732	1496.4710	
1501.3430	1508.9486	1520.5714	
1524.8204	1555.6446	3063.8591	
3064.7241	3066.2247	3070.5414	
3075.4616	3107.2060	3132.3369	
3133.9703	3138.0446	3148.1798	
3149.0240	3154.3149	3161.0449	
3162.3352	3167.0335	3188.7282	
Zero-point correction (Hartree): 0.229449			
TS.iC3H7_tC4H9_COO.ringclose.p			
~~			
E (CCSD(T)/Aug-CC-pVTZ) (Hartree): -464.03099424			
E (CCSD/Aug-CC-pVTZ) (Hartree): -463.93914045			
T1 diagnostic: 0.026381			
E (MP2/Aug-CC-pVTZ) (Hartree): -463.86049214			
E (MP3/Aug-CC-pVTZ) (Hartree): -463.92351200			
E (RHF/Aug-CC-pVTZ) (Hartree): -461.96437901			
E (RM062X/Aug-CC-pVTZ) (Hartree): -464.72785152			
Electronic state : 1-A			
Cartesian coordinates (Angs):			
C	0.100696	-0.292454	-0.201790
O	0.244653	-1.559244	-0.229592
O	1.176115	-1.600329	0.909748
C	1.244662	0.660873	-0.380003
C	-1.328736	0.171094	-0.086608
H	0.846129	1.411077	-1.072775
C	1.617660	1.391839	0.916580
C	2.470470	0.017553	-1.018543
H	2.046743	0.670227	1.607482
H	0.762823	1.865911	1.396387
H	2.351255	2.165026	0.690309
H	2.201075	-0.558764	-1.902741
H	2.956781	-0.649197	-0.313763
H	3.163072	0.804019	-1.318296
C	-1.675383	-0.057371	1.403510
C	-1.559780	1.631853	-0.462782
C	-2.222087	-0.733467	-0.947807
H	-1.102910	0.603209	2.053196
H	-1.465900	-1.085914	1.691551
H	-2.736948	0.151197	1.540999
H	-1.360114	1.809041	-1.520124
H	-0.949187	2.315076	0.124796
H	-2.605381	1.878163	-0.277491
H	-2.124310	-1.776664	-0.659235
H	-1.975104	-0.638343	-2.005574
H	-3.259187	-0.427006	-0.811302
Rotational constants (GHz): 1.7928100 1.0774600 0.9327300			
Vibrational harmonic frequencies (cm-1):			
i442.6780	59.0764	113.7537	
166.0610	190.7291	199.8322	
229.6053	246.1566	261.9061	
283.5835	290.8241	311.4985	
313.6005	354.6354	366.4080	
382.0846	445.4674	489.6963	
563.1439	688.4091	700.2940	
822.6937	859.5385	911.6029	
945.5276	953.2597	965.7348	
976.1624	984.2564	1022.0925	
1048.2048	1076.1918	1102.8453	
1146.9573	1214.5819	1220.3913	

1256.1603	1304.7885	1311.9139
1384.8816	1394.7235	1399.1525
1412.7191	1418.9835	1433.4380
1475.6978	1481.7067	1488.2140
1492.3596	1495.8721	1497.9407
1504.4537	1510.8981	1520.5537
1526.0106	1547.7476	3035.6455
3064.0985	3064.9611	3067.9976
3072.7117	3074.2155	3130.4728
3134.9117	3138.6154	3139.3565
3143.0010	3152.8548	3157.3031
3166.6894	3167.9946	3181.6072

Zero-point correction (Hartree): 0.229315

Population analysis as 298K (%)

Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)

Compound	Qtot	Erel	Erel2	n*Q*MB	%
TS.iC3H7_tC4H9_COO.14Hshift	1.535e+42	0.00	0.00	3.070e+42	100
Total				3.070e+42	100

TS.iC3H7_tC4H9_COO.14Hshift

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E(CCS(D)/Aug-CC-pVTZ) (Hartree): -464.02722220

E(CCS(D)/Aug-CC-pVTZ) (Hartree): -463.93307468

T1 diagnostic: 0.019331

E(MP2/Aug-CC-pVTZ) (Hartree): -463.86961828

E(MP3/Aug-CC-pVTZ) (Hartree): -463.92176120

E(RHF/Aug-CC-pVTZ) (Hartree): -461.93907200

E(RM062X/Aug-CC-pVTZ) (Hartree): -464.72753015

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.126859 | 0.315213  | -0.058063 |
| O | -0.323297 | 1.596483  | -0.168109 |
| O | -1.646274 | 1.880234  | -0.503855 |
| C | -1.295566 | -0.476429 | -0.183220 |
| C | 1.329503  | -0.064029 | 0.084712  |
| H | -1.817656 | 0.627634  | -0.802893 |
| C | -2.279466 | -0.355227 | 0.996153  |
| C | -1.220288 | -1.892046 | -0.710025 |
| H | -3.296377 | -0.555216 | 0.658835  |
| H | -2.259827 | 0.631382  | 1.449406  |
| H | -2.021047 | -1.099585 | 1.753883  |
| H | -0.720849 | -2.585097 | -0.026050 |
| H | -0.730728 | -1.952288 | -1.678972 |
| H | -2.238620 | -2.259886 | -0.840362 |
| C | 2.213927  | 1.182545  | 0.166260  |
| C | 1.463190  | -0.875579 | 1.380912  |
| C | 1.787351  | -0.915167 | -1.110541 |
| H | 1.916151  | 1.831220  | 0.988293  |
| H | 2.169702  | 1.762052  | -0.754378 |
| H | 3.244673  | 0.867915  | 0.329023  |
| H | 0.828185  | -1.760575 | 1.364475  |
| H | 1.190940  | -0.271709 | 2.247074  |
| H | 2.498133  | -1.198241 | 1.500325  |
| H | 1.544512  | -0.432385 | -2.057524 |
| H | 1.347936  | -1.908357 | -1.098364 |
| H | 2.870683  | -1.026288 | -1.054174 |

Rotational constants (GHz): 1.6631800 1.1282000 0.8784000

Vibrational harmonic frequencies (cm-1):

|            |           |           |
|------------|-----------|-----------|
| i1592.1148 | 54.4552   | 119.8878  |
| 178.8125   | 209.7283  | 217.0853  |
| 225.4789   | 257.0982  | 265.8446  |
| 283.0577   | 301.2157  | 308.6461  |
| 330.2936   | 339.4785  | 382.0658  |
| 386.5001   | 411.5011  | 491.4836  |
| 587.5045   | 612.9109  | 750.7978  |
| 769.4355   | 843.3751  | 955.6756  |
| 957.6990   | 961.5908  | 972.7258  |
| 988.7910   | 1007.5124 | 1028.0454 |
| 1045.5355  | 1055.7287 | 1097.0199 |
| 1136.1019  | 1206.5551 | 1239.3782 |
| 1252.6021  | 1284.0136 | 1315.9384 |
| 1387.4990  | 1396.0101 | 1398.3879 |
| 1407.1373  | 1419.4543 | 1442.3816 |
| 1479.9317  | 1484.0987 | 1486.1460 |
| 1490.7831  | 1494.6576 | 1499.7507 |
| 1504.0573  | 1506.2803 | 1516.7987 |
| 1528.3390  | 1551.5921 | 1886.1931 |
| 3038.3973  | 3044.5541 | 3060.0609 |
| 3066.3962  | 3070.8852 | 3105.0873 |
| 3111.9164  | 3130.7752 | 3132.1420 |
| 3142.7168  | 3143.9561 | 3148.7371 |
| 3152.0067  | 3170.3795 | 3173.6017 |

Zero-point correction (Hartree): 0.226456

#####

Z-(tC4H9) (CH3)COO

#####

Population analysis as 298K (%)

Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)

| Compound      | Qtot      | Erel | Erel2 | n*Q*MB    | %   |
|---------------|-----------|------|-------|-----------|-----|
| tC4H9_CH3_COO | 8.521e+40 | 0.00 | 0.00  | 8.521e+40 | 100 |
| Total         |           |      |       | 8.521e+40 | 100 |

tC4H9\_CH3\_COO

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E(CCS(D)/Aug-CC-pVTZ) (Hartree): -385.57253564

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E(CCSD/Aug-CC-pVTZ) (Hartree): -385.49825393
  T1 diagnostic: 0.024954
E(MP2/Aug-CC-pVTZ) (Hartree): -385.44095093
E(MP3/Aug-CC-pVTZ) (Hartree): -385.48512047
E(RHF/Aug-CC-pVTZ) (Hartree): -383.89906497
E(RM062X/Aug-CC-pVTZ) (Hartree): -386.14339321
Electronic state : 1-A
Cartesian coordinates (Angs):
  C    0.493184    0.654163   -0.000003
  O    1.675766    0.241143   -0.000011
  O    1.963064   -1.097869    0.000026
  C   -0.707567   -0.254540   -0.000002
  C    0.391003    2.141576    0.000025
  C   -0.673550   -1.126452    1.267675
  C   -2.003639    0.560923   -0.000340
  C   -0.673136   -1.126870   -1.267389
  H   -0.736546   -0.506163    2.163271
  H    0.233089   -1.721616    1.305156
  H   -1.543955   -1.783446    1.251859
  H   -2.094132    1.189700   -0.886194
  H   -2.094965    1.189047    0.885899
  H   -2.844288   -0.132175   -0.001012
  H    0.234550   -1.720439   -1.305249
  H   -0.738029   -0.506963   -2.163103
  H   -1.542315   -1.785466   -1.250600
  H    1.383499    2.581333    0.000256
  H   -0.162880    2.478544    0.876862
  H   -0.162439    2.478652   -0.877055
Rotational constants (GHz):    2.4329000    1.9554600    1.4408700
Vibrational harmonic frequencies (cm-1):
  62.9754      170.6419      187.5065
  222.5580      252.6144      263.2802
  302.3849      316.7374      335.5852
  351.4367      392.2054      401.8511
  444.8379      619.5377      631.9448
  679.0776      862.0276      957.2226
  959.2261      961.9446      976.3216
 1007.7982     1033.6828     1065.3111
 1070.3495     1203.2374     1231.7645
 1257.8648     1341.0585     1383.8254
 1392.3025     1413.1051     1431.1746
 1463.3917     1471.9751     1477.2462
 1495.4013     1498.3964     1503.7802
 1516.9771     1534.8680     1629.3387
 3058.5476     3059.0070     3063.7051
 3073.3756     3122.4699     3123.6658
 3127.2813     3138.8120     3139.5164
 3182.3593     3183.0399     3183.3918
Zero-point correction (Hartree): 0.173665

Population analysis as 298K (%)
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)
Compound      Qtot      Erel      Erel2  n*Q*MB      %
-----
TS.tC4H9_CH3_COO.ringclose 9.135e+40 0.00  0.00  1.827e+41 100
Total                  1.827e+41 100

TS.tC4H9_CH3_COO.ringclose
~~~~~
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -385.54080939
E(CCSD/Aug-CC-pVTZ) (Hartree): -385.46584880
  T1 diagnostic: 0.029801
E(MP2/Aug-CC-pVTZ) (Hartree): -385.40442106
E(MP3/Aug-CC-pVTZ) (Hartree): -385.45068847
E(RHF/Aug-CC-pVTZ) (Hartree): -383.87070961
E(RM062X/Aug-CC-pVTZ) (Hartree): -386.10903814
Electronic state : 1-A
Cartesian coordinates (Angs):
  C   -0.661815    0.412237   -0.154253
  O   -1.640240   -0.263084   -0.602236
  O   -1.588920   -1.324377    0.413702
  C    0.745682   -0.104237   -0.001713
  C   -1.003501    1.829149    0.138210
  C    0.936918   -1.519887   -0.542340
  C    1.636727    0.850671   -0.832647
  C    1.155830   -0.027080    1.474047
  H    0.460574   -1.632133   -1.516326
  H    0.504725   -2.257155    0.123086
  H    2.005630   -1.705834   -0.655488
  H    1.650875    1.866643   -0.444640
  H    1.323361    0.876925   -1.877393
  H    2.656810    0.471284   -0.799529
  H    0.535414   -0.699656    2.062767
  H    1.060955    0.984821    1.871192
  H    2.200005   -0.328006    1.565311
  H   -1.630620    1.786856    1.034829
  H   -1.636719    2.212067   -0.662554
  H   -0.156767    2.478757    0.319199
Rotational constants (GHz):    2.4746700    1.9433100    1.5208400
Vibrational harmonic frequencies (cm-1):
  i450.3362      56.9319      143.9620
  166.0241      215.2284      251.6223
  266.2407      312.5023      325.2666
  348.2477      378.0358      420.8653
  456.8572      522.1253      558.7465
  679.4631      840.1581      856.1414
  947.3729      963.2648      974.5869
  981.0901      1025.6931     1043.7573
 1059.4537      1160.6364     1214.3095
 1249.0869      1327.3086     1375.0824
 1391.1000      1403.8422     1428.6836

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1458.0731      1472.7535      1478.6664
1486.1217      1490.9387      1497.2135
1514.2943      1524.2849      1567.9105
3053.4348      3058.8471      3065.6976
3071.5832      3120.5281      3126.7908
3132.9220      3140.2263      3155.0284
3156.4144      3197.2044      3213.8176
Zero-point correction (Hartree): 0.171606
```

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#####
Z-(tC4H9)(C2H5)COO
#####
```

```
Population analysis as 298K (%)
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)
Compound      Qtot      Erel      Erel2      n*Q*MB      %
-----
tC4H9_C2H5_COO.c 6.757e+41 0.00      0.00      6.757e+41 88
tC4H9_C2H5_COO.p 4.253e+41 1.31      1.31      9.234e+40 12
Total              7.680e+41 100
```

```
tC4H9_C2H5_COO.c
~~~~~
E(CCSDT)/Aug-CC-pVTZ) (Hartree): -424.81521960
E(CCSDT)/Aug-CC-pVTZ) (Hartree): -424.73306769
T1 diagnostic: 0.023329
E(MP2)/Aug-CC-pVTZ) (Hartree): -424.66616467
E(MP3)/Aug-CC-pVTZ) (Hartree): -424.71987849
E(RHF)/Aug-CC-pVTZ) (Hartree): -422.94660880
E(RM062X)/Aug-CC-pVTZ) (Hartree): -425.45085600
Electronic state : 1-A
Cartesian coordinates (Angs):
  C      0.434390      0.024462      0.000024
  O      0.838750      1.208668      0.000012
  O     -0.033976      2.268317     -0.000009
  C     -1.024852     -0.353653     -0.000008
  C      1.535139     -0.990187      0.000039
  C     -1.684961      0.216501     -1.267985
  C     -1.202907     -1.874779     -0.000011
  C     -1.684973      0.216511      1.267983
  H     -1.240942     -0.223025     -2.162813
  H     -1.581455      1.296012     -1.307310
  H     -2.742179     -0.050903     -1.251464
  H     -0.773038     -2.341822      0.886015
  H     -0.773093     -2.341810     -0.886075
  H     -2.270795     -2.091310      0.000019
  H     -1.581469      1.296023      1.307297
  H     -1.240961     -0.223039      2.162799
  H     -2.742188     -0.050897      1.251433
  C      2.939313     -0.408835     -0.000028
  H      1.379422     -1.637566      0.867500
  H      1.379365     -1.637630     -0.867370
  H      3.105492      0.211904      0.877865
  H      3.105422      0.211855     -0.877970
  H      3.671326     -1.213792     -0.000034
Rotational constants (GHz):      2.0311000      1.3679800      1.0113300
Vibrational harmonic frequencies (cm-1):
  61.7652      85.6398      178.7700
  210.7255      230.8473      232.1791
  252.4114      263.9659      296.5454
  303.6649      323.0848      362.0533
  392.6956      401.4808      493.2183
  611.4579      613.2541      698.6101
  799.4589      857.5075      957.4153
  959.1731      964.7655      973.7770
 1012.7458      1032.9166      1050.2143
 1097.8114      1100.9339      1171.4003
 1229.9004      1255.2656      1288.3712
 1303.6455      1381.9083      1387.3059
 1406.4934      1422.0284      1430.4451
 1450.2414      1474.4359      1494.3234
 1498.6806      1498.8793      1503.0752
 1506.4097      1516.3583      1535.1883
 1626.7504      3054.2057      3057.7767
 3059.0905      3066.4191      3082.0065
 3083.1095      3121.7843      3122.9819
 3136.8690      3137.2338      3157.4602
 3158.6245      3181.7624      3182.6712
Zero-point correction (Hartree): 0.202306
```

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tC4H9_C2H5_COO.p
~~~~~
E(RM062X)/Aug-CC-pVTZ) (Hartree): -425.44929253
Electronic state : 1-A
Cartesian coordinates (Angs):
  C     -0.349009     -0.388335     -0.333844
  O     -0.172036     -1.625310     -0.236555
  O      1.010540     -2.149417      0.213605
  C      0.708970      0.628874      0.009318
  C     -1.749555     -0.044728     -0.739808
  C      1.969795      0.371763     -0.834815
  C      0.221750      2.050974     -0.282239
  C      1.024738      0.502957      1.511420
  H      1.744694      0.457494     -1.898885
  H      2.381669     -0.611185     -0.634932
  H      2.704432      1.138268     -0.584391
  H     -0.688954      2.302142      0.260818
  H      0.048761      2.209212     -1.347053
  H      0.997132      2.748687      0.032825
  H      1.340519     -0.507475      1.754152
  H      0.153315      0.766613      2.112898
```

H	1.826295	1.202061	1.752915
C	-2.623765	0.182572	0.501818
H	-1.749482	0.841457	-1.370248
H	-2.146463	-0.878858	-1.315263
H	-2.244460	0.994578	1.120261
H	-2.653377	-0.721076	1.108385
H	-3.639651	0.431430	0.201016
Rotational constants (GHz): 1.8380800 1.5216800 1.0933400			
Vibrational harmonic frequencies (cm-1):			
76.4188	118.9781	165.8335	
201.4543	216.8122	227.2536	
251.3399	265.8421	315.1132	
325.6088	358.6400	371.0938	
391.3794	403.8531	452.1558	
609.0520	671.7057	733.5116	
802.5878	858.4321	947.0721	
956.9448	959.4951	973.5523	
993.7605	1035.1407	1048.2897	
1075.3089	1116.6314	1198.5434	
1230.5318	1255.2558	1277.9657	
1326.5080	1358.9305	1383.5426	
1392.4569	1412.8380	1429.3628	
1473.0020	1485.4641	1494.7411	
1500.0501	1501.6592	1502.4139	
1512.0259	1519.1538	1535.2149	
1616.4407	3058.3062	3060.2600	
3065.1152	3074.4121	3103.5632	
3122.6563	3123.9112	3134.1437	
3139.2429	3144.2555	3152.7089	
3162.7096	3175.0613	3189.7227	
Zero-point correction (Hartree): 0.202838			
Population analysis as 298K (%)			
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)			
Compound	Qtot	Erel	Erel2 n*Q*MB %

TS.tC4H9_C2H5_COO.isom.p	1.139e+42	0.00	0.00 3.418e+42 100
Total			3.418e+42 100
TS.tC4H9_C2H5_COO.isom.p			
~~			
E (CCSD(T)/Aug-CC-pVTZ) (Hartree): -424.75835418			
E (CCSD/Aug-CC-pVTZ) (Hartree): -424.68336714			
T1 diagnostic: 0.020633			
E (MP2/Aug-CC-pVTZ) (Hartree): -424.59899373			
E (MP3/Aug-CC-pVTZ) (Hartree): -424.66896735			
E (PMP2/Aug-CC-pVTZ) (Hartree): -424.62406750			
E (PMP3/Aug-CC-pVTZ) (Hartree): -424.69389982			
E (PUHF/Aug-CC-pVTZ) (Hartree): -422.96095713			
E (UHF/Aug-CC-pVTZ) (Hartree): -422.93568118			
E (UM062X/Aug-CC-pVTZ) (Hartree): -425.39900418			
Electronic state : 1-A			
Cartesian coordinates (Angs):			
C	0.244257	0.014211	-0.570893
O	0.712130	1.328916	-0.706493
O	1.350209	1.753194	0.362480
C	-1.117776	-0.143789	0.050120
C	1.286148	-1.045772	-0.663187
C	-1.909682	1.161426	-0.052159
C	-1.889102	-1.253429	-0.675558
C	-0.953640	-0.527248	1.532150
C	2.394573	-0.989848	0.398688
H	0.780355	-2.009669	-0.607647
H	1.748631	-0.993969	-1.653423
H	3.052993	-1.850559	0.284342
H	1.977627	-1.000535	1.404377
H	2.989902	-0.085960	0.295364
H	-2.004995	1.481884	-1.090007
H	-1.431545	1.962921	0.508905
H	-2.909377	1.007199	0.354367
H	-1.377525	-2.213331	-0.611416
H	-2.025128	-1.004782	-1.728364
H	-2.872756	-1.371474	-0.219032
H	-0.387601	0.235059	2.067844
H	-0.432560	-1.480604	1.632681
H	-1.935397	-0.626371	1.999140
Rotational constants (GHz): 2.0781800 1.3481300 1.0851000			
Vibrational harmonic frequencies (cm-1):			
i212.8417	30.0146	79.7549	
138.0179	209.4418	245.5756	
253.8290	268.8639	292.6684	
308.7729	313.6099	350.4770	
370.3164	386.7266	453.2113	
495.0736	623.0921	694.8138	
783.8811	834.9613	942.6917	
958.5481	963.0052	968.2393	
1015.3853	1031.2690	1047.9677	
1065.1172	1157.0099	1178.7857	
1199.3187	1224.0467	1263.6513	
1294.3514	1321.2567	1370.4457	
1391.8062	1400.4145	1409.8878	
1429.4128	1470.8072	1480.5705	
1487.2865	1490.5022	1498.8592	
1504.5810	1506.8563	1510.3522	
1524.5627	3044.1793	3048.9355	
3058.3562	3063.0514	3072.6231	
3112.5837	3120.1123	3128.6309	
3132.8485	3134.4224	3138.9767	
3143.0804	3144.3617	3160.8590	
Zero-point correction (Hartree): 0.199894			

Population analysis as 298K (%)
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)

Compound	Qtot	Erel	Erel2	n*Q*MB	%
TS.tC4H9_C2H5_COO.ringclose.p	5.167e+41	0.00	0.00	1.033e+42	63.2
TS.tC4H9_C2H5_COO.ringclose.m	6.533e+41	0.46	0.46	6.015e+41	36.8
TS.tC4H9_C2H5_COO.ringclose.t	4.272e+41	4.38	4.38	5.271e+38	0.0322
Total				1.635e+42	100

TS.tC4H9_C2H5_COO.ringclose.m
~~~~~  
E(RM062X/Aug-CC-pVTZ) (Hartree): -425.41620783  
Electronic state : 1-A  
Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.397989  | 0.299903  | 0.077102  |
| O | 0.626556  | 1.439396  | -0.435983 |
| O | -0.432644 | 2.166191  | 0.282025  |
| C | -0.909982 | -0.440248 | -0.030913 |
| C | 1.597526  | -0.336811 | 0.698965  |
| C | -1.944282 | 0.264575  | -0.905969 |
| C | -0.557809 | -1.790674 | -0.701863 |
| C | -1.476710 | -0.694678 | 1.371020  |
| H | -1.487619 | 0.644580  | -1.819632 |
| H | -2.392270 | 1.103728  | -0.387713 |
| H | -2.716723 | -0.456532 | -1.177178 |
| H | 0.147130  | -2.386466 | -0.125240 |
| H | -0.151370 | -1.636319 | -1.702659 |
| H | -1.476643 | -2.367124 | -0.799939 |
| H | -1.712871 | 0.254542  | 1.847702  |
| H | -0.780566 | -1.247340 | 2.003053  |
| H | -2.388628 | -1.285498 | 1.278312  |
| C | 2.740300  | -0.470845 | -0.315470 |
| H | 1.894958  | 0.354733  | 1.492380  |
| H | 1.358610  | -1.292634 | 1.154041  |
| H | 2.956344  | 0.490913  | -0.774762 |
| H | 2.478420  | -1.181141 | -1.098586 |
| H | 3.637741  | -0.827465 | 0.184648  |

Rotational constants (GHz): 1.9726600 1.4408900 1.0955200  
Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i438.5681 | 52.3803   | 78.1533   |
| 178.2138  | 191.4334  | 212.5908  |
| 238.9786  | 257.6837  | 275.4347  |
| 307.9904  | 326.3244  | 345.8490  |
| 397.8947  | 423.5971  | 463.6981  |
| 553.7143  | 622.4689  | 724.8631  |
| 805.7551  | 847.8620  | 851.9520  |
| 947.4859  | 965.4467  | 974.5333  |
| 977.2160  | 1024.5304 | 1042.4776 |
| 1075.3421 | 1091.3241 | 1139.0743 |
| 1213.8440 | 1247.0953 | 1261.4652 |
| 1307.5569 | 1367.6103 | 1390.9041 |
| 1402.3658 | 1408.3834 | 1428.7481 |
| 1472.4751 | 1484.0962 | 1486.0872 |
| 1490.1568 | 1497.8149 | 1503.9629 |
| 1509.4900 | 1517.3969 | 1522.6300 |
| 1564.5223 | 3061.0131 | 3062.3983 |
| 3064.9614 | 3069.3120 | 3079.4517 |
| 3128.7929 | 3131.6435 | 3136.6207 |
| 3146.8893 | 3151.6840 | 3156.5165 |
| 3160.8149 | 3174.2820 | 3196.9417 |

Zero-point correction (Hartree): 0.200917

TS.tC4H9\_C2H5\_COO.ringclose.p  
~~~~~  
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -424.78402533
E(CCSD/Aug-CC-pVTZ) (Hartree): -424.70083428
T1 diagnostic: 0.028329
E(MP2/Aug-CC-pVTZ) (Hartree): -424.63012507
E(MP3/Aug-CC-pVTZ) (Hartree): -424.68541995
E(RHF/Aug-CC-pVTZ) (Hartree): -422.91733900
E(RM062X/Aug-CC-pVTZ) (Hartree): -425.41692496
Electronic state : 1-A
Cartesian coordinates (Angs):

C	0.376126	0.110351	-0.431622
O	0.716267	1.265542	-0.837674
O	0.424913	1.988461	0.411182
C	-0.997988	-0.255167	0.065791
C	1.455844	-0.909544	-0.562801
C	-2.003947	0.892062	0.007691
C	-1.493477	-1.371491	-0.887151
C	-0.893254	-0.811385	1.490947
H	-1.926957	1.430387	-0.936617
H	-1.835513	1.604057	0.806514
H	-3.008862	0.475604	0.090664
H	-0.880506	-2.269045	-0.851228
H	-1.538945	-1.016881	-1.917800
H	-2.502313	-1.647034	-0.583275
H	-0.528843	-0.036413	2.163191
H	-0.227664	-1.674443	1.545343
H	-1.883755	-1.129550	1.817806
C	2.530993	-0.579411	0.489947
H	1.092836	-1.924352	-0.438995
H	1.887508	-0.797292	-1.559892
H	2.137372	-0.700287	1.497670
H	2.861906	0.450339	0.378084
H	3.378509	-1.249608	0.363655

Rotational constants (GHz): 2.0335300 1.4378900 1.1533600
Vibrational harmonic frequencies (cm-1):

i429.0024	58.1455	98.6736
169.6649	185.6403	200.8132
231.4732	266.1759	283.8205

309.7217	321.1535	344.7341
394.0200	419.8070	468.2634
525.6130	655.9361	718.4470
809.0188	845.4820	853.2145
946.6097	965.5789	970.3218
976.7888	1012.7244	1038.2562
1068.0069	1095.8947	1156.2361
1211.6876	1246.6870	1257.0880
1306.6936	1357.0768	1391.9615
1403.6179	1411.8615	1430.0866
1473.6237	1477.2616	1484.5273
1489.3331	1496.6794	1498.8413
1507.3158	1512.1045	1524.5019
1564.1356	3057.1206	3065.3481
3070.6399	3075.9429	3081.2328
3126.1289	3132.9747	3139.5146
3149.9109	3151.3458	3155.8982
3165.2562	3181.8198	3197.5490

Zero-point correction (Hartree): 0.200902

TS.tC4H9_C2H5_COO.ringclose.t

~~~~~  
E(RM062X/Aug-CC-pVTZ) (Hartree): -425.40978625

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.139433 | -0.617425 | -0.222272 |
| O | 0.488269  | -1.652047 | -0.623684 |
| O | 1.439125  | -1.739877 | 0.491438  |
| C | 0.528696  | 0.720050  | -0.004748 |
| C | -1.588691 | -0.923812 | -0.017551 |
| C | 1.966665  | 0.741186  | -0.528855 |
| C | -0.271489 | 1.770718  | -0.810905 |
| C | 0.500279  | 1.080086  | 1.486066  |
| H | 2.003748  | 0.410012  | -1.567367 |
| H | 2.610577  | 0.095186  | 0.054259  |
| H | 2.330355  | 1.768016  | -0.484839 |
| H | -1.211932 | 2.040114  | -0.343128 |
| H | -0.466494 | 1.435988  | -1.831574 |
| H | 0.335513  | 2.672482  | -0.872291 |
| H | 1.129668  | 0.386946  | 2.039100  |
| H | -0.509131 | 1.044637  | 1.897549  |
| H | 0.878769  | 2.095638  | 1.609711  |
| C | -2.694650 | 0.111695  | 0.100097  |
| H | -1.828476 | -1.679542 | -0.769522 |
| H | -1.519631 | -1.505961 | 0.915508  |
| H | -2.849558 | 0.648892  | -0.832406 |
| H | -2.509630 | 0.834947  | 0.890625  |
| H | -3.621195 | -0.406948 | 0.341348  |

Rotational constants (GHz): 1.8868300 1.5230700 1.0946500

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i413.0554 | 49.8392   | 133.3872  |
| 159.1104  | 192.9311  | 217.0768  |
| 251.1044  | 289.1011  | 304.9333  |
| 316.6803  | 331.7205  | 349.1196  |
| 385.9909  | 423.5771  | 497.7204  |
| 503.2607  | 561.0015  | 655.0150  |
| 778.1761  | 838.1086  | 851.9484  |
| 953.2960  | 959.8091  | 973.3895  |
| 981.9387  | 1023.2482 | 1050.9105 |
| 1078.4837 | 1115.5510 | 1171.6036 |
| 1217.2392 | 1246.7783 | 1294.5750 |
| 1316.4364 | 1373.4123 | 1389.8205 |
| 1399.2283 | 1420.8268 | 1422.6031 |
| 1433.4017 | 1473.4309 | 1488.6300 |
| 1494.9208 | 1496.4185 | 1503.3812 |
| 1512.6388 | 1523.0783 | 1525.4142 |
| 1546.1185 | 2995.2987 | 3062.6474 |
| 3066.2294 | 3071.6346 | 3083.0779 |
| 3084.1333 | 3129.5590 | 3129.9163 |
| 3138.3503 | 3147.9845 | 3163.0139 |
| 3166.5905 | 3191.9970 | 3207.1314 |

Zero-point correction (Hartree): 0.200738

#####  
Z-(tC4H9)(iC3H7)COO  
#####

Population analysis as 298K (%)

Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)

| Compound          | Qtot      | Erel | Erel2 | n*Q*MB    | %     |
|-------------------|-----------|------|-------|-----------|-------|
| tC4H9_iC3H7_COO.p | 2.261e+42 | 0.00 | 0.00  | 4.522e+42 | 99.9  |
| tC4H9_iC3H7_COO.c | 2.087e+42 | 3.51 | 3.51  | 5.544e+39 | 0.122 |
| Total             |           |      |       | 4.527e+42 | 100   |

tC4H9\_iC3H7\_COO.c

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E(RM062X/Aug-CC-pVTZ) (Hartree): -464.75248535

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-0.079511	-0.491891	-0.168688
O	0.402983	-1.644893	-0.304495
O	1.743732	-1.894569	-0.224315
C	0.796460	0.712981	0.081360
C	-1.590252	-0.554001	-0.186052
C	1.840404	0.843740	-1.043150
C	0.017108	2.029713	0.133376
C	1.479658	0.497722	1.447266
H	1.347107	0.981993	-2.006735
H	2.483654	-0.026868	-1.092316
H	2.437708	1.734352	-0.842855

H	-0.791638	2.019753	0.861253
H	-0.385806	2.303991	-0.839663
H	0.715307	2.811753	0.431750
H	2.013299	-0.447908	1.470740
H	0.742065	0.524602	2.251217
H	2.185086	1.313788	1.608147
H	-1.800020	-1.562812	-0.541778
C	-2.139595	-0.460775	1.244034
C	-2.290652	0.424482	-1.132300
H	-1.953994	0.514629	1.690535
H	-1.695569	-1.223271	1.882649
H	-3.218066	-0.617280	1.221664
H	-1.762435	0.522174	-2.080654
H	-2.403418	1.412363	-0.693889
H	-3.288723	0.042613	-1.344649
Rotational constants (GHz): 1.5980800 1.1298000 0.9223200			
Vibrational harmonic frequencies (cm-1):			
73.4806	93.8291	161.1661	
194.5682	210.1062	224.0150	
230.7416	255.3662	265.7962	
279.3287	304.5807	336.4551	
357.9137	374.2236	390.2329	
399.7626	414.2700	511.3051	
613.3808	669.9850	742.8762	
847.3818	896.8027	944.3211	
957.8376	960.6315	973.9708	
982.8048	992.5055	1039.0331	
1045.9445	1075.9194	1131.6688	
1186.1293	1222.8351	1230.9063	
1261.2083	1334.8655	1343.5031	
1379.2924	1382.0828	1390.8636	
1402.6950	1424.1850	1431.1529	
1472.6913	1486.2413	1493.8692	
1494.8290	1496.9078	1503.8610	
1508.9424	1518.8846	1524.0596	
1537.7085	1593.8407	3056.8630	
3059.6946	3068.1285	3072.1768	
3077.5030	3090.0991	3121.0593	
3123.4518	3136.2014	3138.8862	
3140.8880	3149.0553	3166.3151	
3167.5174	3170.5602	3194.9233	
Zero-point correction (Hartree): 0.231250			
tC4H9_iC3H7_COO.p			
~~			
E (CCSD(T)/Aug-CC-pVTZ) (Hartree): -464.05872166			
E (CCSD/Aug-CC-pVTZ) (Hartree): -463.96771311			
T1 diagnostic: 0.022918			
E (MP2/Aug-CC-pVTZ) (Hartree): -463.89256902			
E (MP3/Aug-CC-pVTZ) (Hartree): -463.95393916			
E (RHF/Aug-CC-pVTZ) (Hartree): -461.99030061			
E (RM062X/Aug-CC-pVTZ) (Hartree): -464.75780538			
Electronic state : 1-A			
Cartesian coordinates (Angs):			
C	0.210518	0.241036	0.094829
O	0.341653	1.457972	-0.168438
O	-0.731708	2.255905	-0.474968
C	-1.130101	-0.451898	0.125602
C	1.527595	-0.462749	0.293856
C	-1.741653	-0.388269	-1.286438
C	-0.999760	-1.918997	0.545371
C	-2.042898	0.253153	1.145696
H	-1.141413	-0.962569	-1.993821
H	-1.818258	0.640086	-1.626976
H	-2.736627	-0.833470	-1.248942
H	-0.640621	-2.018290	1.569970
H	-0.344774	-2.490138	-0.111571
H	-1.989528	-2.372491	0.499166
H	-2.205104	1.290619	0.875225
H	-1.610336	0.205128	2.146269
H	-2.996236	-0.276489	1.167057
H	1.365302	-1.272909	1.003413
C	1.950533	-1.072178	-1.053916
C	2.617665	0.461025	0.827453
H	2.132653	-0.274330	-1.774108
H	1.195075	-1.738574	-1.466833
H	2.872180	-1.638279	-0.924300
H	2.317627	0.932539	1.761848
H	2.845133	1.247993	0.111172
H	3.523972	-0.116583	1.004966
Rotational constants (GHz): 1.6376800 1.1195300 0.8870300			
Vibrational harmonic frequencies (cm-1):			
69.9480	98.1654	163.4255	
192.2708	209.5034	223.9417	
239.3785	249.3611	260.4219	
278.1771	284.5512	330.3313	
345.6648	359.9933	395.0015	
404.0448	414.9396	509.6843	
612.8455	691.5010	740.8235	
848.7130	899.3672	941.2330	
957.1029	958.0611	961.3912	
973.1258	981.0295	1042.1491	
1049.2418	1104.1270	1137.6946	
1147.4045	1215.8891	1230.0418	
1254.0528	1304.4468	1320.5999	
1381.0292	1386.9686	1392.1492	
1411.0125	1424.3413	1429.4637	
1473.1337	1487.4010	1491.8458	
1494.1826	1498.1836	1503.1172	
1504.6443	1514.5017	1520.4666	
1535.1902	1617.4898	3059.2011	
3059.9892	3064.9756	3068.1928	

3074.3467	3106.7692	3122.1902
3124.5577	3135.4792	3140.6422
3142.0271	3146.9014	3151.6879
3156.7225	3176.3851	3190.5011

Zero-point correction (Hartree): 0.230973

Population analysis as 298K (%)

Compound	Qtot	Erel	Erel2	n*Q*MB	%
TS.tc4H9_iC3H7_COO.isom.t	7.214e+42	0.00	0.00	1.443e+43	99
TS.tc4H9_iC3H7_COO.isom.c	2.751e+42	2.45	2.45	8.758e+40	0.601
TS.tc4H9_iC3H7_COO.isom.p	2.449e+42	2.57	2.57	6.426e+40	0.441
Total				1.458e+43	100

TS.tc4H9_iC3H7_COO.isom.c

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E(UM062X/Aug-CC-pVTZ) (Hartree): -464.70466901

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.110652  | 0.279825  | -0.459150 |
| O | -0.321645 | 1.544339  | -0.909802 |
| O | -0.597725 | 2.369993  | 0.072625  |
| C | -0.985920 | -0.606860 | 0.071681  |
| C | 1.593634  | 0.241600  | -0.224461 |
| C | -2.176140 | -0.555901 | -0.897362 |
| C | -0.494835 | -2.054204 | 0.164456  |
| C | -1.468805 | -0.161446 | 1.465967  |
| H | 1.965624  | 1.147645  | -0.707620 |
| C | 1.954569  | 0.340152  | 1.265496  |
| C | 2.313775  | -0.941049 | -0.882169 |
| H | 1.649446  | -0.559257 | 1.801169  |
| H | 1.472785  | 1.199349  | 1.730326  |
| H | 3.034534  | 0.443879  | 1.376332  |
| H | 3.388846  | -0.760701 | -0.864232 |
| H | 2.004926  | -1.063948 | -1.919808 |
| H | 2.128217  | -1.874514 | -0.355236 |
| H | -1.878245 | -0.877591 | -1.896105 |
| H | -2.586407 | 0.450131  | -0.968293 |
| H | -2.962595 | -1.221570 | -0.539945 |
| H | 0.307733  | -2.164730 | 0.893003  |
| H | -0.142693 | -2.417213 | -0.801185 |
| H | -1.322746 | -2.686804 | 0.485985  |
| H | -1.891584 | 0.840119  | 1.436223  |
| H | -0.655076 | -0.167916 | 2.190029  |
| H | -2.239387 | -0.854238 | 1.810031  |

Rotational constants (GHz): 1.4818100 1.1902400 0.9285700

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i218.7716 | 42.8644   | 81.2838   |
| 154.2769  | 196.6056  | 222.4758  |
| 250.2362  | 252.4171  | 271.1499  |
| 282.1946  | 295.8496  | 316.9371  |
| 334.5478  | 354.7390  | 372.9416  |
| 395.6105  | 403.1751  | 476.4487  |
| 554.3265  | 641.3383  | 683.3132  |
| 831.7230  | 900.3523  | 932.4351  |
| 942.3833  | 960.1841  | 968.2902  |
| 969.0389  | 1022.1794 | 1035.8919 |
| 1041.5063 | 1101.0698 | 1113.9240 |
| 1175.8638 | 1201.8149 | 1214.2387 |
| 1228.7733 | 1260.3560 | 1330.8696 |
| 1332.7675 | 1390.2981 | 1393.7134 |
| 1396.6224 | 1399.6738 | 1416.4100 |
| 1431.6606 | 1478.1203 | 1486.1866 |
| 1487.2333 | 1490.5569 | 1495.2459 |
| 1502.2279 | 1505.6978 | 1512.5466 |
| 1516.5907 | 1528.5199 | 3057.5183 |
| 3058.6325 | 3059.3551 | 3063.6079 |
| 3066.4432 | 3068.2972 | 3127.1757 |
| 3128.2124 | 3130.2844 | 3133.3569 |
| 3134.7899 | 3140.5576 | 3143.6281 |
| 3146.1760 | 3156.9644 | 3160.1125 |

Zero-point correction (Hartree): 0.228621

TS.tc4H9\_iC3H7\_COO.isom.p

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E(UM062X/Aug-CC-pVTZ) (Hartree): -464.70456047

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-0.077628	0.432942	-0.072601
O	0.417569	1.620235	0.520635
O	0.876723	2.463465	-0.368885
C	0.932307	-0.683435	-0.030504
C	-1.577325	0.391306	-0.029393
C	1.276086	-1.016215	1.434550
C	0.400984	-1.939989	-0.719428
C	2.213983	-0.234571	-0.747228
H	-1.872373	1.442927	-0.007298
C	-2.226052	-0.225098	-1.272395
C	-2.117838	-0.261188	1.252342
H	-2.132473	-1.308769	-1.287522
H	-1.783469	0.172825	-2.184913
H	-3.289882	0.013112	-1.275532
H	-1.892525	-1.327966	1.272312
H	-3.201449	-0.147923	1.298204
H	-1.686645	0.198008	2.141625
H	0.405745	-1.395099	1.969975
H	1.648041	-0.134885	1.955973
H	2.052768	-1.782442	1.460778
H	0.150400	-1.744520	-1.762020
H	-0.479855	-2.338297	-0.216968

H	1.173501	-2.709273	-0.693949
H	2.661743	0.630826	-0.261326
H	2.005702	0.028715	-1.784272
H	2.939333	-1.049358	-0.731124
Rotational constants (GHz):	1.4381000	1.1672800	0.9146500
Vibrational harmonic frequencies (cm-1):			
i155.6007	52.0092		80.3132
140.9528	195.7969		226.3157
261.3390	263.7426		275.6335
283.9097	293.2791		309.5128
327.0181	352.7989		382.3498
394.5549	417.3409		478.2226
535.8619	610.4625		715.7430
832.9530	899.8295		931.3978
942.2341	960.6838		967.3160
970.8642	1012.8071		1034.3709
1040.9035	1098.2595		1116.2770
1174.6090	1216.4638		1225.7147
1238.4354	1267.1347		1332.7951
1335.6447	1389.6431		1391.5295
1397.4598	1400.9937		1417.1778
1430.8786	1479.2409		1485.7220
1488.1909	1491.3239		1496.4890
1503.7100	1506.5598		1513.1513
1516.8977	1528.8773		3056.4825
3057.5976	3059.4014		3063.7120
3064.8449	3069.8465		3126.5232
3128.2568	3129.7140		3133.3121
3135.2999	3136.4214		3142.0940
3144.3052	3146.3813		3157.7564
Zero-point correction (Hartree):	0.228695		

TS.tC4H9_iC3H7_COO.isom.t

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E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -464.00317523  
E(CCSD/Aug-CC-pVTZ) (Hartree): -463.91977636  
T1 diagnostic: 0.019919  
E(MP2/Aug-CC-pVTZ) (Hartree): -463.82664275  
E(MP3/Aug-CC-pVTZ) (Hartree): -463.90507313  
E(PMP2/Aug-CC-pVTZ) (Hartree): -463.85171271  
E(PMP3/Aug-CC-pVTZ) (Hartree): -463.93000193  
E(PUHF/Aug-CC-pVTZ) (Hartree): -462.00777995  
E(UHF/Aug-CC-pVTZ) (Hartree): -461.98250820  
E(UM062X/Aug-CC-pVTZ) (Hartree): -464.70795641  
Electronic state : 1-A

Cartesian coordinates (Angs):

|                                          |           |           |           |
|------------------------------------------|-----------|-----------|-----------|
| C                                        | 0.111200  | 0.003931  | -0.341377 |
| O                                        | 0.373764  | 1.258388  | -0.909392 |
| O                                        | 0.648265  | 2.177526  | -0.008867 |
| C                                        | -1.317941 | -0.264049 | 0.047114  |
| C                                        | 1.305150  | -0.742801 | 0.162224  |
| C                                        | -2.263270 | 0.693913  | -0.680468 |
| C                                        | -1.687019 | -1.706308 | -0.323820 |
| C                                        | -1.469231 | -0.074168 | 1.567369  |
| H                                        | 0.918051  | -1.663202 | 0.603638  |
| C                                        | 2.229647  | -1.117877 | -1.002020 |
| C                                        | 2.096604  | -0.000564 | 1.248356  |
| H                                        | 2.600578  | -0.216740 | -1.491362 |
| H                                        | 1.705100  | -1.718316 | -1.744758 |
| H                                        | 3.087322  | -1.683940 | -0.638298 |
| H                                        | 1.455133  | 0.320668  | 2.067160  |
| H                                        | 2.581288  | 0.883182  | 0.835785  |
| H                                        | 2.869599  | -0.659978 | 1.644663  |
| H                                        | -2.148247 | 0.612209  | -1.761653 |
| H                                        | -2.078698 | 1.728757  | -0.396012 |
| H                                        | -3.293303 | 0.445957  | -0.423424 |
| H                                        | -1.601450 | -1.861025 | -1.399839 |
| H                                        | -2.717366 | -1.907667 | -0.027292 |
| H                                        | -1.049289 | -2.432285 | 0.179916  |
| H                                        | -1.197261 | 0.940903  | 1.857637  |
| H                                        | -0.833832 | -0.772576 | 2.114135  |
| H                                        | -2.504701 | -0.255719 | 1.861504  |
| Rotational constants (GHz):              | 1.6581200 | 1.0664700 | 0.9130000 |
| Vibrational harmonic frequencies (cm-1): |           |           |           |
| i213.7207                                | 35.2237   |           | 46.4910   |
| 129.4681                                 | 183.8038  |           | 215.9049  |
| 235.5197                                 | 258.9108  |           | 268.2746  |
| 278.0275                                 | 292.7032  |           | 305.5354  |
| 310.3399                                 | 333.0697  |           | 366.2887  |
| 391.6103                                 | 412.7430  |           | 475.1089  |
| 542.1654                                 | 642.3621  |           | 712.5158  |
| 824.9619                                 | 895.2292  |           | 931.7865  |
| 943.1199                                 | 957.8856  |           | 967.7049  |
| 968.7227                                 | 1026.8738 |           | 1037.0704 |
| 1053.9465                                | 1094.4573 |           | 1111.3918 |
| 1172.4284                                | 1186.8242 |           | 1222.9297 |
| 1225.7942                                | 1272.8876 |           | 1300.0438 |
| 1322.9022                                | 1387.7958 |           | 1393.5144 |
| 1395.3785                                | 1402.6782 |           | 1417.4574 |
| 1430.0065                                | 1479.9650 |           | 1484.8510 |
| 1485.2372                                | 1489.6601 |           | 1491.3996 |
| 1502.5735                                | 1504.7989 |           | 1507.3547 |
| 1511.1792                                | 1523.6153 |           | 3048.8923 |
| 3057.1858                                | 3058.9290 |           | 3063.0303 |
| 3063.9902                                | 3078.8261 |           | 3119.7497 |
| 3127.7887                                | 3131.7236 |           | 3132.0913 |
| 3134.3537                                | 3135.2486 |           | 3135.9806 |
| 3138.2158                                | 3144.8051 |           | 3149.4247 |
| Zero-point correction (Hartree):         | 0.228001  |           |           |

Population analysis as 298K (%)

Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)

| Compound                       | Qtot      | Erel | Erel2 | n*Q*MB    | %       |
|--------------------------------|-----------|------|-------|-----------|---------|
| TS.tc4H9_iC3H7_COO.ringclose.t | 2.972e+42 | 0.00 | 0.00  | 5.944e+42 | 100     |
| TS.tc4H9_iC3H7_COO.ringclose.m | 1.555e+42 | 5.21 | 5.21  | 4.678e+38 | 0.00787 |
| TS.tc4H9_iC3H7_COO.ringclose.p | 1.990e+42 | 6.35 | 6.35  | 8.712e+37 | 0.00147 |
| Total                          |           |      |       | 5.945e+42 | 100     |

TS.tc4H9\_iC3H7\_COO.ringclose.m

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E(RM062X/Aug-CC-pVTZ) (Hartree): -464.71869388

Electronic state : 1-A

Cartesian coordinates (Angs):

C	0.112768	0.349868	-0.428623
O	-0.089221	1.476007	-0.996068
O	-0.715258	2.147816	0.150520
C	-1.013988	-0.506601	0.107114
C	1.579381	0.018473	-0.409863
C	-2.396768	0.083108	-0.183617
C	-0.932308	-1.866266	-0.630845
C	-0.847119	-0.727466	1.615004
H	-2.473786	0.402466	-1.222989
H	-2.601910	0.942115	0.442242
H	-3.142556	-0.691707	-0.003749
H	-0.109421	-2.485673	-0.293589
H	-0.857444	-1.733769	-1.711800
H	-1.855542	-2.406708	-0.429076
H	-0.916799	0.226039	2.135363
H	0.103938	-1.199461	1.861014
H	-1.646656	-1.383402	1.961905
H	1.955290	0.478336	-1.327936
C	2.130299	0.876994	0.758560
C	2.099477	-1.407886	-0.313030
H	1.844530	0.444172	1.716679
H	1.750863	1.895281	0.711764
H	3.217266	0.884693	0.693101
H	1.805673	-2.018452	-1.163308
H	1.783452	-1.903376	0.603572
H	3.188478	-1.362491	-0.297016

Rotational constants (GHz): 1.5908600 1.2513300 0.9311900

Vibrational harmonic frequencies (cm-1):

i406.4967	57.3594	104.5586
152.8286	198.9317	213.5859
221.2883	242.2877	282.6341
286.8172	302.0699	334.6636
350.4691	366.8615	384.4530
395.5908	456.1174	519.0266
554.0135	652.9465	705.1804
826.3142	850.9169	903.7443
943.6428	951.7689	961.3163
974.1758	986.1842	1000.9205
1032.8786	1070.4918	1125.1044
1168.8637	1212.6657	1220.4081
1249.0546	1276.8878	1319.1254
1377.4606	1390.4537	1396.1853
1404.7798	1426.3652	1432.0764
1474.7553	1485.7699	1487.4781
1492.2906	1495.0126	1498.1499
1508.4066	1514.3942	1522.9101
1524.6124	1543.8018	3059.0382
3063.3577	3066.9741	3071.3460
3072.5645	3075.2390	3131.1041
3132.5506	3138.3117	3139.8650
3146.1425	3155.2528	3161.7512
3165.9543	3196.9869	3205.7793

Zero-point correction (Hartree): 0.229670

TS.tc4H9_iC3H7_COO.ringclose.p

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E(RM062X/Aug-CC-pVTZ) (Hartree): -464.71671490

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.134108  | 0.459241  | 0.017996  |
| O | -0.012736 | 1.706248  | -0.206149 |
| O | -1.047092 | 1.962759  | 0.806509  |
| C | -1.011507 | -0.520296 | -0.143700 |
| C | 1.568974  | 0.131348  | 0.342897  |
| C | -2.133301 | 0.108723  | -0.979939 |
| C | -0.492532 | -1.752119 | -0.919030 |
| C | -1.562700 | -0.969371 | 1.216774  |
| H | -1.770566 | 0.365583  | -1.976153 |
| H | -2.522381 | 1.002104  | -0.506022 |
| H | -2.928877 | -0.628523 | -1.089427 |
| H | 0.023394  | -2.463553 | -0.282663 |
| H | 0.165137  | -1.473416 | -1.745151 |
| H | -1.355446 | -2.259756 | -1.347750 |
| H | -2.069772 | -0.136917 | 1.695647  |
| H | -0.777386 | -1.327336 | 1.882261  |
| H | -2.264639 | -1.788551 | 1.052342  |
| H | 1.721031  | 0.784556  | 1.211573  |
| C | 1.989283  | -1.278895 | 0.737171  |
| C | 2.471461  | 0.669671  | -0.782553 |
| H | 2.097831  | -1.927089 | -0.129627 |
| H | 1.306064  | -1.746449 | 1.442074  |
| H | 2.965210  | -1.212432 | 1.217722  |
| H | 2.248927  | 1.707561  | -1.013034 |
| H | 2.346241  | 0.068957  | -1.684034 |
| H | 3.511145  | 0.593398  | -0.468334 |

Rotational constants (GHz): 1.6200600 1.1709100 0.9066200

Vibrational harmonic frequencies (cm-1):

|           |          |          |
|-----------|----------|----------|
| i420.9214 | 41.1981  | 98.2977  |
| 181.4733  | 199.9124 | 224.5561 |

|           |           |           |
|-----------|-----------|-----------|
| 242.4479  | 246.9595  | 271.0690  |
| 296.4351  | 303.6505  | 315.1750  |
| 337.3802  | 356.3856  | 375.5610  |
| 409.3915  | 431.7127  | 518.2682  |
| 557.1058  | 621.3206  | 709.2556  |
| 831.4713  | 847.4899  | 903.7396  |
| 941.3176  | 957.8900  | 961.0015  |
| 978.2020  | 984.8133  | 1031.0554 |
| 1038.2136 | 1070.3717 | 1132.7925 |
| 1146.5574 | 1222.2628 | 1225.6501 |
| 1244.5949 | 1281.0821 | 1308.7442 |
| 1374.7144 | 1388.2183 | 1394.8372 |
| 1399.3283 | 1422.8214 | 1429.5014 |
| 1473.4843 | 1487.2065 | 1492.6795 |
| 1494.6828 | 1496.9675 | 1502.0325 |
| 1504.5979 | 1514.1096 | 1522.9527 |
| 1526.3156 | 1540.9214 | 3021.6557 |
| 3061.9734 | 3063.6930 | 3067.3725 |
| 3070.2547 | 3078.9463 | 3127.1506 |
| 3130.4477 | 3133.5025 | 3138.4312 |
| 3142.2521 | 3166.0907 | 3173.5732 |
| 3177.2822 | 3182.5837 | 3197.6704 |

Zero-point correction (Hartree): 0.229510

TS.tC4H9\_iC3H7\_COO.ringclose.t  
 ~~~~~  
 E (CCSD(T)/Aug-CC-pVTZ) (Hartree): -464.02957160
 E (CCSD/Aug-CC-pVTZ) (Hartree): -463.93797156
 T1 diagnostic: 0.026866
 E (MP2/Aug-CC-pVTZ) (Hartree): -463.85887828
 E (MP3/Aug-CC-pVTZ) (Hartree): -463.92231400
 E (RHF/Aug-CC-pVTZ) (Hartree): -461.96486377
 E (RM062X/Aug-CC-pVTZ) (Hartree): -464.72654942
 Electronic state : 1-A

Cartesian coordinates (Angs):

C	0.184361	0.166713	-0.222451
O	0.421183	1.190643	-0.936600
O	-0.315486	2.163719	-0.111568
C	-1.194083	-0.360220	0.080612
C	1.411339	-0.563033	0.232097
C	-2.321566	0.427882	-0.582047
C	-1.210482	-1.794158	-0.506759
C	-1.401730	-0.421406	1.598503
H	-2.076201	0.663728	-1.617172
H	-2.504600	1.362810	-0.066355
H	-3.224940	-0.183883	-0.568401
H	-0.469295	-2.452290	-0.058423
H	-1.056147	-1.774963	-1.586720
H	-2.193638	-2.222886	-0.317303
H	-1.376421	0.585146	2.012666
H	-0.644920	-1.030571	2.094657
H	-2.376986	-0.864870	1.802028
H	1.132265	-1.483002	0.739058
C	2.319753	-0.879256	-0.958580
C	2.115169	0.366762	1.235446
H	2.583154	0.035919	-1.485791
H	1.837126	-1.559938	-1.659431
H	3.234556	-1.347591	-0.598058
H	1.477392	0.591174	2.089350
H	2.374468	1.307206	0.752567
H	3.022035	-0.120583	1.591746

Rotational constants (GHz): 1.6994300 1.1044600 0.9561700

Vibrational harmonic frequencies (cm-1):

i414.8036	53.0332	75.3523
166.1593	183.7426	200.2789
220.0271	243.7963	249.7274
268.8391	275.9351	297.0175
316.2140	342.2040	365.3231
416.0890	431.8883	489.0623
577.6404	706.0893	720.6224
841.3449	844.0389	894.4021
946.8831	949.1080	966.0307
976.3843	988.0621	1024.0838
1029.6504	1085.4035	1109.9888
1129.1386	1197.1781	1211.5596
1249.5820	1308.5415	1338.9224
1385.8839	1392.0873	1395.8133
1404.9094	1422.3901	1430.6601
1475.8201	1484.1432	1484.5234
1489.2398	1493.0275	1498.5182
1502.8891	1509.3580	1514.4137
1523.9268	1563.2343	3058.7441
3063.2979	3068.4315	3069.0731
3069.5034	3123.5305	3128.8712
3132.3376	3137.9694	3140.6469
3144.4432	3150.6483	3153.1702
3155.0232	3162.4942	3197.2528

Zero-point correction (Hartree): 0.229219

 (tC4H9)2COO
 #####

Population analysis as 298K (%)
 Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)
 Compound Qtot Erel Erel2 n*Q*MB %

 tC4H9_tC4H9_COO 6.116e+42 0.00 0.00 6.116e+42 100
 Total 6.116e+42 100

tC4H9_tC4H9_COO

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E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -503.29644158
E(CCSD/Aug-CC-pVTZ) (Hartree): -503.19591881
T1 diagnostic: 0.022170
E(MP2/Aug-CC-pVTZ) (Hartree): -503.11392499
E(MP3/Aug-CC-pVTZ) (Hartree): -503.18167146
E(RHF/Aug-CC-pVTZ) (Hartree): -501.02362217
E(RM062X/Aug-CC-pVTZ) (Hartree): -504.05886409
Electronic state : 1-A
Cartesian coordinates (Angs):
  C    0.023313    0.345887   -0.068343
  O   -0.076795    1.597644   -0.080858
  O   -1.272679    2.258679   -0.025022
  C   -1.216077   -0.527325   -0.007137
  C    1.484792   -0.092890   -0.015573
  C   -2.140744   -0.180281   -1.191012
  C   -0.961658   -2.036280   -0.082790
  C   -1.902827   -0.229881    1.342404
  H   -1.640117   -0.393613   -2.137079
  H   -2.444266    0.859411   -1.171752
  H   -3.020067   -0.822640   -1.127380
  H   -0.266152   -2.401274    0.668967
  H   -0.616613   -2.345612   -1.066873
  H   -1.917875   -2.528427    0.095732
  H   -2.075774    0.834641    1.468737
  H   -1.295960   -0.606423    2.167680
  H   -2.859695   -0.752812    1.360844
  C    2.404709    1.100943   -0.301613
  C    1.775915   -0.583210    1.414563
  C    1.809622   -1.193008   -1.039611
  H    2.254591    1.909936    0.408534
  H    2.237998    1.495206   -1.303523
  H    3.437905    0.762490   -0.229931
  H    1.152447   -1.424570    1.707777
  H    1.625789    0.223779    2.131981
  H    2.818005   -0.900878    1.469345
  H    1.370420   -0.974075   -2.013966
  H    1.481554   -2.176773   -0.721662
  H    2.891334   -1.232688   -1.165726
Rotational constants (GHz):    1.3932400    0.9685900    0.7656900
Vibrational harmonic frequencies (cm-1):
  73.4900      87.9905      164.8101
 182.9709     208.8050     225.8277
 233.0197     257.3560     269.7535
 279.5095     292.2655     312.7541
 323.6137     344.1031     349.7892
 395.3914     404.3785     415.9672
 422.0111     438.6955     525.5494
 589.8936     674.4603     747.5174
 818.3427     864.6241     948.4041
 956.1132     958.8155     961.3690
 973.0366     978.0457     981.1858
1032.2132    1043.2063    1055.4108
1061.7605    1118.1874    1220.2632
1237.0600    1244.0013    1251.5710
1277.9898    1328.6585    1381.3870
1390.4799    1400.2698    1407.4143
1430.8167    1438.1322    1472.7594
1480.8692    1488.1868    1489.7520
1493.1864    1497.1129    1505.9497
1507.3693    1515.6769    1520.7444
1532.6217    1541.4162    1580.6698
3056.7288    3059.4867    3064.0422
3068.4871    3073.3304    3079.2711
3120.2971    3122.9949    3131.2701
3132.3367    3139.8029    3142.9773
3155.2240    3163.6573    3173.2105
3176.2334    3184.9413    3199.4335
Zero-point correction (Hartree): 0.259366

Population analysis as 298K (%)
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)
Compound      Qtot      Erel      Erel2  n*Q*MB      %
-----
TS.tC4H9_tC4H9_COO.ringclose 9.937e+42 0.00    0.00  1.987e+43 100
Total                  1.987e+43 100

TS.tC4H9_tC4H9_COO.ringclose
~~~~~
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -503.26405360
E(CCSD/Aug-CC-pVTZ) (Hartree): -503.16307630
T1 diagnostic: 0.027168
E(MP2/Aug-CC-pVTZ) (Hartree): -503.07583317
E(MP3/Aug-CC-pVTZ) (Hartree): -503.14694352
E(RHF/Aug-CC-pVTZ) (Hartree): -500.99629002
E(RM062X/Aug-CC-pVTZ) (Hartree): -504.02437034
Electronic state : 1-A
Cartesian coordinates (Angs):
  C    0.006679    0.369097   -0.152083
  O   -0.003302    1.551938   -0.616358
  O   -0.846124    2.188818    0.409732
  C   -1.279687   -0.422924    0.007667
  C    1.424410   -0.168032    0.025759
  C   -2.503148    0.330989   -0.527358
  C   -1.129453   -1.684927   -0.877815
  C   -1.545501   -0.821161    1.465869
  H   -2.278818    0.832566   -1.467704
  H   -2.845187    1.081179    0.174441
  H   -3.296326   -0.397740   -0.701277
  H   -0.289103   -2.317967   -0.615749
  H   -1.042181   -1.407831   -1.929383

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H	-2.037794	-2.275182	-0.762867
H	-1.552678	0.068854	2.092906
H	-0.822660	-1.533253	1.854282
H	-2.530878	-1.286491	1.512495
C	2.276607	0.996639	0.566189
C	1.595394	-1.338790	0.997584
C	1.944561	-0.548387	-1.375831
H	1.833214	1.412956	1.470564
H	2.359628	1.797380	-0.162845
H	3.272529	0.621604	0.801101
H	1.023857	-2.225415	0.743459
H	1.340398	-1.039999	2.013448
H	2.649489	-1.617855	0.992321
H	1.799979	0.272185	-2.077776
H	1.458463	-1.439988	-1.766951
H	3.014310	-0.746083	-1.297337
Rotational constants (GHz):			
	1.4195000	0.9764000	0.8006300
Vibrational harmonic frequencies (cm-1):			
i418.8158	23.6370		108.0347
177.0039	193.7974		221.2954
234.3248	241.3282		259.0751
274.9903	285.7214		302.2867
316.2775	328.0867		352.7382
364.4152	384.7731		392.7680
429.2532	439.0859		536.9244
555.7853	645.8316		720.7987
804.4049	836.2412		863.6667
946.7804	953.8669		963.6535
964.9483	977.7019		982.6706
1011.2959	1029.1377		1051.1675
1059.3931	1086.9751		1207.3998
1222.1462	1240.0079		1248.0846
1267.4763	1316.9105		1389.6850
1393.3600	1398.7789		1409.7740
1428.9819	1437.2340		1475.5788
1478.6543	1487.0178		1490.6195
1492.7292	1496.4509		1499.2845
1504.6334	1506.8568		1515.2102
1523.4249	1532.3832		1538.2605
3065.3733	3066.9601		3069.8578
3071.3120	3072.9832		3077.6727
3133.1202	3134.6152		3137.0249
3139.9311	3142.1231		3143.2173
3156.4206	3171.6392		3172.6949
3176.9741	3201.6825		3204.5907
Zero-point correction (Hartree): 0.257796			

(R-CH(CH3)(C2H5))(R-CH(CH3)(C2H5))COO
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Population analysis as 298K (%)
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)

Compound	Qtot	Erel	Erel2	n*Q*MB	%
dic2H5CH3CH_COO.cmptrRR	8.203e+43	0.22	0.22	5.655e+43	16
dic2H5CH3CH_COO.mpptRR	4.431e+43	0.00	0.00	4.431e+43	12.5
dic2H5CH3CH_COO.cmmnRR	4.606e+43	0.13	0.13	3.671e+43	10.4
dic2H5CH3CH_COO.cmmtRR	2.749e+44	1.43	1.43	2.472e+43	6.99
dic2H5CH3CH_COO.cmtmRR	3.212e+43	0.17	0.17	2.394e+43	6.77
dic2H5CH3CH_COO.mppmRR	3.255e+43	0.25	0.25	2.133e+43	6.03
dic2H5CH3CH_COO.ctptRR	1.697e+44	1.37	1.37	1.672e+43	4.73
dic2H5CH3CH_COO.mtmnRR	4.862e+43	0.69	0.69	1.526e+43	4.32
dic2H5CH3CH_COO.cmttRR	3.412e+43	0.62	0.62	1.206e+43	3.41
dic2H5CH3CH_COO.ctpmRR	1.231e+44	1.45	1.45	1.061e+43	3
dic2H5CH3CH_COO.mtttRR	1.675e+44	1.72	1.72	9.107e+42	2.58
dic2H5CH3CH_COO.pmmnRR	7.776e+43	1.27	1.27	9.031e+42	2.56
dic2H5CH3CH_COO.cttmRR	4.568e+43	1.00	1.00	8.439e+42	2.39
dic2H5CH3CH_COO.ptmtRR	2.497e+44	2.06	2.06	7.713e+42	2.18
dic2H5CH3CH_COO.ctmmRR	3.944e+43	1.02	1.02	7.047e+42	1.99
dic2H5CH3CH_COO.mppmRR	8.285e+43	1.57	1.57	5.873e+42	1.66
dic2H5CH3CH_COO.ctppRR	8.972e+43	1.62	1.62	5.831e+42	1.65
dic2H5CH3CH_COO.ctttRR	4.468e+43	1.23	1.23	5.599e+42	1.58
dic2H5CH3CH_COO.ptmnRR	2.907e+43	1.02	1.02	5.213e+42	1.48
dic2H5CH3CH_COO.mtmnRR	1.056e+44	1.87	1.87	4.472e+42	1.27
dic2H5CH3CH_COO.pmmnRR	1.340e+43	0.75	0.75	3.802e+42	1.08
dic2H5CH3CH_COO.ctmtRR	1.164e+44	2.09	2.09	3.406e+42	0.964
dic2H5CH3CH_COO.pmptrRR	3.367e+43	1.69	1.69	1.934e+42	0.547
dic2H5CH3CH_COO.mmmnRR	7.243e+43	2.18	2.18	1.814e+42	0.513
dic2H5CH3CH_COO.mpttRR	4.426e+43	1.96	1.96	1.611e+42	0.456
dic2H5CH3CH_COO.mttmRR	8.604e+43	2.57	2.57	1.117e+42	0.316
dic2H5CH3CH_COO.pppmRR	4.851e+43	2.27	2.27	1.050e+42	0.297
dic2H5CH3CH_COO.cpmnRR	2.403e+43	1.87	1.87	1.021e+42	0.289
dic2H5CH3CH_COO.cmptrRR	3.242e+43	2.22	2.22	7.613e+41	0.215
dic2H5CH3CH_COO.cmpmRR	2.355e+43	2.18	2.18	5.908e+41	0.167
dic2H5CH3CH_COO.mptmRR	8.380e+43	2.94	2.94	5.894e+41	0.167
dic2H5CH3CH_COO.mppmRR	1.138e+43	1.79	1.79	5.494e+41	0.155
dic2H5CH3CH_COO.cptmRR	1.929e+43	2.17	2.17	4.981e+41	0.141
dic2H5CH3CH_COO.mpppRR	1.881e+43	2.16	2.16	4.895e+41	0.139
dic2H5CH3CH_COO.cpttRR	2.371e+43	2.31	2.31	4.803e+41	0.136
dic2H5CH3CH_COO.mmmnRR	5.136e+43	2.85	2.85	4.149e+41	0.117
dic2H5CH3CH_COO.ptptRR	5.214e+43	2.88	2.88	4.060e+41	0.115
dic2H5CH3CH_COO.cpptRR	6.682e+43	3.02	3.02	4.045e+41	0.114
dic2H5CH3CH_COO.cpmnRR	6.164e+43	3.00	3.00	3.915e+41	0.111
dic2H5CH3CH_COO.mtppRR	2.596e+43	2.58	2.58	3.309e+41	0.0936
dic2H5CH3CH_COO.pmpmRR	2.053e+43	2.66	2.66	2.316e+41	0.0655
dic2H5CH3CH_COO.ctptRR	3.987e+43	3.16	3.16	1.904e+41	0.0539
dic2H5CH3CH_COO.cpppRR	3.313e+43	3.17	3.17	1.561e+41	0.0442
dic2H5CH3CH_COO.ppmnRR	3.436e+43	3.40	3.40	1.110e+41	0.0314
dic2H5CH3CH_COO.ptttRR	2.983e+43	3.36	3.36	1.020e+41	0.0289
dic2H5CH3CH_COO.ptpmRR	4.531e+43	3.65	3.65	9.594e+40	0.0271

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dic2H5CH3CH_COO.mtmpRR 7.944e+43 4.11 4.11 7.718e+40 0.0218
dic2H5CH3CH_COO.mmpRR 5.671e+43 4.00 4.00 6.640e+40 0.0188
dic2H5CH3CH_COO.mptpRR 2.175e+43 3.84 3.84 3.328e+40 0.00942
dic2H5CH3CH_COO.mttpRR 3.449e+43 4.12 4.12 3.302e+40 0.00934
dic2H5CH3CH_COO.pmpRR 2.044e+43 3.93 3.93 2.661e+40 0.00753
dic2H5CH3CH_COO.ptmRR 1.960e+43 4.00 4.00 2.273e+40 0.00643
dic2H5CH3CH_COO.pmttRR 3.697e+43 4.57 4.57 1.641e+40 0.00464
dic2H5CH3CH_COO.cmpRR 5.788e+43 4.99 4.99 1.258e+40 0.00356
dic2H5CH3CH_COO.ptmpRR 4.979e+43 4.91 4.91 1.239e+40 0.00351
dic2H5CH3CH_COO.cptpRR 2.535e+43 4.78 4.78 7.851e+39 0.00222
dic2H5CH3CH_COO.ctmpRR 5.984e+43 5.31 5.31 7.625e+39 0.00216
dic2H5CH3CH_COO.ptppRR 2.371e+43 4.85 4.85 6.564e+39 0.00186
dic2H5CH3CH_COO.pptpRR 2.763e+43 5.18 5.18 4.397e+39 0.00124
dic2H5CH3CH_COO.mmpRR 3.227e+43 5.59 5.59 2.585e+39 0.000731
dic2H5CH3CH_COO.cmpRR 2.781e+43 5.52 5.52 2.484e+39 0.000703
dic2H5CH3CH_COO.cpmRR 4.873e+43 5.97 5.97 2.024e+39 0.000573
dic2H5CH3CH_COO.pppRR 1.404e+43 5.76 5.76 8.352e+38 0.000236
dic2H5CH3CH_COO.ppttRR 3.310e+43 6.59 6.59 4.876e+38 0.000138
dic2H5CH3CH_COO.pttpRR 2.049e+43 6.57 6.57 3.117e+38 8.82e-05
dic2H5CH3CH_COO.pmtmRR 2.308e+43 6.78 6.78 2.474e+38 7e-05
dic2H5CH3CH_COO.pppRR 3.083e+43 7.13 7.13 1.818e+38 5.14e-05
dic2H5CH3CH_COO.pptmRR 1.346e+43 6.94 6.94 1.093e+38 3.09e-05
dic2H5CH3CH_COO.pmtpRR 9.627e+42 7.41 7.41 3.549e+37 1e-05
dic2H5CH3CH_COO.pptpRR 1.054e+43 9.93 9.93 5.516e+35 1.56e-07
Total 3.534e+44 100

dic2H5CH3CH_COO.cmmRR
~~~~~
E (RM062X/Aug-CC-pVTZ) (Hartree): -504.06898948
Electronic state : 1-A
Cartesian coordinates (Angs):
C 0.067974 -0.036167 0.003119
O 0.162479 -0.500041 -1.151489
O -0.876594 -1.236931 -1.673245
C 1.257384 0.739757 0.492362
C 2.556704 0.380972 -0.224033
C 0.936254 2.237098 0.381057
H 1.357236 0.490695 1.554692
C 2.990981 -1.060998 0.009688
H 2.441128 0.572641 -1.291727
H 3.328767 1.062992 0.136909
H 0.026726 2.499457 0.919814
H 0.806337 2.514789 -0.665196
H 1.758820 2.818613 0.794737
H 2.260844 -1.764808 -0.388473
H 3.111516 -1.260625 1.075928
H 3.944279 -1.263287 -0.475691
C -1.109023 -0.267787 0.893599
C -2.482694 0.039379 0.281488
C -1.018779 -1.719961 1.392610
H -0.958812 0.401892 1.745023
C -2.504188 1.319971 -0.539919
H -2.785254 -0.797128 -0.340986
H -3.183668 0.113827 1.116520
H -0.086409 -1.905082 1.927265
H -1.088144 -2.396985 0.543283
H -1.847483 -1.913887 2.072672
H -1.852929 1.217981 -1.409632
H -2.179039 2.181230 0.047074
H -3.508677 1.529870 -0.904159
Rotational constants (GHz): 1.4425400 0.7982800 0.7002900
Vibrational harmonic frequencies (cm-1):
38.8964 76.9371 110.5772
119.5059 156.2748 177.7062
187.2616 225.8999 232.1086
235.1569 253.9340 259.9693
283.8621 317.4863 332.5069
415.6692 429.1218 458.7620
466.7352 612.0385 734.8695
743.5979 804.6621 817.0763
849.7546 893.9516 948.9629
979.0277 986.6391 1024.7675
1027.3019 1034.7841 1040.1655
1104.7712 1108.8877 1135.2234
1143.2848 1152.7257 1203.7379
1234.5318 1290.7488 1301.0947
1302.8216 1311.4167 1365.7354
1373.4788 1391.4525 1395.0813
1407.3887 1409.1290 1418.4224
1437.7330 1481.4314 1486.5376
1491.4576 1493.0243 1501.0875
1504.1128 1507.4584 1510.8403
1512.3625 1515.8769 1653.9468
3037.4253 3052.6219 3054.3096
3060.3865 3061.4537 3062.3811
3065.4863 3069.6467 3106.7188
3118.3496 3131.9094 3132.1061
3136.6149 3141.5022 3144.3917
3145.6898 3153.7117 3160.5623
Zero-point correction (Hartree): 0.260297

dic2H5CH3CH_COO.cmmRR
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E (RM062X/Aug-CC-pVTZ) (Hartree): -504.06143931
Electronic state : 1-A
Cartesian coordinates (Angs):
C 0.133184 -0.056698 0.118772
O 0.251862 -0.970335 -0.723745
O -0.791608 -1.816198 -0.995691
C 1.365744 0.783972 0.326165
C 2.612792 0.233905 -0.363523
C 1.072918 2.229275 -0.101503

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H	1.537940	0.786988	1.409008
C	3.122413	-1.072134	0.235053
H	2.408140	0.107890	-1.427897
H	3.389361	0.996589	-0.281597
H	0.252796	2.665654	0.465587
H	0.820481	2.269076	-1.161849
H	1.958639	2.840861	0.062817
H	2.395667	-1.874544	0.124162
H	3.339252	-0.949969	1.297573
H	4.042037	-1.386562	-0.255964
C	-1.109394	0.203621	0.917493
C	-2.173028	1.015965	0.142281
C	-1.693779	-1.053287	1.573722
H	-0.767843	0.861716	1.721255
C	-2.706713	0.402680	-1.145220
H	-2.994347	1.170662	0.846527
H	-1.769440	2.005561	-0.076839
H	-0.910272	-1.701468	1.965711
H	-2.274132	-1.634268	0.867211
H	-2.326061	-0.739759	2.404842
H	-3.140701	-0.579415	-0.976938
H	-1.916353	0.273283	-1.882876
H	-3.472017	1.056176	-1.564684
Rotational constants (GHz): 1.5219700 0.7655700 0.6578500			
Vibrational harmonic frequencies (cm-1):			
38.5605	56.0112	110.1612	
133.6676	146.0301	172.9073	
196.6221	207.9047	227.9677	
252.7542	256.6482	284.4930	
294.5013	315.2389	339.4092	
350.8089	454.8382	459.8523	
509.2923	617.0160	713.9707	
759.7806	792.0252	808.7795	
845.5167	882.3412	957.2297	
984.4840	985.4575	1012.4265	
1033.9930	1038.6015	1045.1849	
1099.7625	1110.8336	1138.9781	
1147.7239	1151.4553	1196.9404	
1223.6913	1292.4540	1299.2480	
1304.0977	1320.1098	1371.9132	
1381.2813	1392.6091	1409.8041	
1410.3978	1418.6291	1431.3845	
1438.0118	1479.4594	1484.8690	
1489.1716	1492.5974	1499.0611	
1502.8498	1504.6097	1508.6147	
1511.0385	1513.7967	1644.8708	
3026.3120	3049.9962	3059.5688	
3064.1016	3066.0192	3068.8372	
3070.0851	3072.4657	3096.5867	
3105.3709	3131.2930	3132.4790	
3139.4456	3140.7720	3150.6881	
3152.2232	3163.0335	3198.6042	
Zero-point correction (Hartree): 0.260492			
dic2H5CH3CH_COO.cmmtrr			
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E(RM062X/Aug-CC-pVTZ) (Hartree): -504.06652158			
Electronic state : 1-A			
Cartesian coordinates (Angs):			
C	0.225500	-0.062076	-0.081024
O	0.515266	-0.917281	-0.942561
O	-0.434940	-1.817006	-1.370836
C	1.326772	0.886298	0.295330
C	2.722565	0.393706	-0.074822
C	1.012221	2.248629	-0.342373
H	1.264709	0.999097	1.383480
C	3.144574	-0.854026	0.691704
H	2.762802	0.208453	-1.149224
H	3.421162	1.206961	0.130929
H	0.018081	2.605467	-0.074068
H	1.069271	2.173502	-1.428563
H	1.740720	2.986044	-0.008966
H	2.493284	-1.697356	0.466358
H	3.113512	-0.675791	1.767917
H	4.161888	-1.142565	0.432470
C	-1.126671	0.055809	0.541571
C	-2.211391	0.386906	-0.499124
C	-1.432588	-1.203018	1.366619
H	-1.058420	0.904067	1.229125
C	-3.539197	0.740508	0.158696
H	-1.871085	1.231603	-1.103404
H	-2.317176	-0.461856	-1.170018
H	-0.615475	-1.426224	2.054072
H	-1.575971	-2.053677	0.706323
H	-2.328725	-1.038117	1.961594
H	-3.422600	1.548985	0.883320
H	-3.969122	-0.115791	0.676496
H	-4.260185	1.065081	-0.590126
Rotational constants (GHz): 1.5857000 0.6971000 0.6047600			
Vibrational harmonic frequencies (cm-1):			
22.3175	39.2517	73.7495	
120.2984	148.7783	169.7043	
183.6186	199.9901	215.4573	
230.8995	244.6142	263.4913	
283.0243	297.5421	341.9318	
362.4015	426.7763	456.3702	
495.0535	610.1511	730.2402	
772.5075	799.8135	816.7729	
844.5884	892.8554	946.3822	
972.5692	985.0491	995.3328	
1030.8914	1037.5919	1055.6636	
1100.7866	1118.3465	1127.7601	

1144.4533	1149.7605	1199.3604
1226.4379	1283.0553	1292.3325
1299.6165	1345.1158	1353.6571
1371.3512	1390.4669	1396.6349
1408.3979	1413.3015	1418.2954
1434.4731	1488.5383	1490.5118
1495.3391	1500.6818	1504.4589
1505.3551	1506.9048	1512.2420
1515.4987	1517.1996	1651.5601
3035.1309	3049.7640	3057.8105
3058.8848	3062.0588	3064.0922
3068.7316	3069.3995	3106.0876
3119.6701	3132.1722	3134.8158
3138.3261	3140.6112	3143.8253
3145.9738	3146.0879	3176.4388

Zero-point correction (Hartree): 0.259888

diC2H5CH3CH_COO.cmpRR
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E(RM062X/Aug-CC-pVT2) (Hartree): -504.06621556

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.026829  | 0.253544  | -0.394529 |
| O | 0.138322  | -0.506044 | -1.382382 |
| O | -0.973197 | -0.770452 | -2.143298 |
| C | 1.324057  | 0.577721  | 0.292514  |
| C | 2.340627  | -0.564541 | 0.255793  |
| C | 1.909708  | 1.830535  | -0.383276 |
| H | 1.091916  | 0.812516  | 1.333105  |
| C | 1.882567  | -1.823895 | 0.978181  |
| H | 2.578551  | -0.794968 | -0.783370 |
| H | 3.258439  | -0.188348 | 0.712075  |
| H | 1.200801  | 2.655533  | -0.425256 |
| H | 2.204681  | 1.586289  | -1.403723 |
| H | 2.791561  | 2.162730  | 0.162899  |
| H | 1.034751  | -2.282147 | 0.471957  |
| H | 1.584955  | -1.601447 | 2.004480  |
| H | 2.683800  | -2.560283 | 1.015249  |
| C | -1.297188 | 0.860286  | -0.054405 |
| C | -2.374995 | -0.213089 | 0.252322  |
| C | -1.219820 | 1.866648  | 1.091411  |
| H | -1.602652 | 1.356723  | -0.983122 |
| C | -1.830548 | -1.424438 | 0.997003  |
| H | -3.139665 | 0.283144  | 0.852621  |
| H | -2.828935 | -0.540106 | -0.676626 |
| H | -0.439423 | 2.613644  | 0.960683  |
| H | -1.050617 | 1.360991  | 2.043708  |
| H | -2.171568 | 2.389766  | 1.164439  |
| H | -1.219622 | -1.136777 | 1.856931  |
| H | -1.223439 | -2.031061 | 0.325046  |
| H | -2.641960 | -2.050860 | 1.364251  |

Rotational constants (GHz): 1.2439900 0.8622400 0.7774700

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| 51.9432   | 83.8032   | 101.9370  |
| 113.8002  | 171.5312  | 185.5850  |
| 206.5234  | 222.1566  | 243.9407  |
| 261.6551  | 277.8490  | 285.6820  |
| 296.1600  | 341.9732  | 376.4427  |
| 387.8316  | 437.1708  | 470.8623  |
| 527.6283  | 604.1160  | 684.9583  |
| 771.3712  | 785.8993  | 810.9675  |
| 845.7436  | 885.9848  | 953.8732  |
| 980.2631  | 986.9105  | 1023.5637 |
| 1032.0690 | 1034.5097 | 1042.0680 |
| 1083.2911 | 1096.2480 | 1134.1185 |
| 1142.2052 | 1178.7754 | 1188.1846 |
| 1253.1998 | 1266.6763 | 1291.9631 |
| 1302.6044 | 1303.6121 | 1347.0384 |
| 1373.9999 | 1377.5478 | 1406.2209 |
| 1410.3264 | 1417.6572 | 1419.9632 |
| 1426.0023 | 1484.8383 | 1487.7965 |
| 1493.9144 | 1498.3099 | 1502.6273 |
| 1504.2652 | 1507.1446 | 1509.3207 |
| 1515.7334 | 1521.6653 | 1627.5995 |
| 3036.6762 | 3047.9286 | 3062.9910 |
| 3066.1804 | 3067.2248 | 3069.5033 |
| 3072.2861 | 3083.2080 | 3109.8088 |
| 3117.0567 | 3132.9675 | 3134.5498 |
| 3140.0646 | 3143.4408 | 3146.9797 |
| 3152.4668 | 3156.4856 | 3172.7548 |

Zero-point correction (Hartree): 0.260787

diC2H5CH3CH\_COO.cmptRR

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E(RM062X/Aug-CC-pVT2) (Hartree): -504.06877178

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-0.237222	-0.174000	-0.452367
O	-0.486010	0.591753	-1.411209
O	0.550875	1.022409	-2.208935
C	-1.434683	-0.581394	0.358613
C	-2.378147	0.596645	0.615857
C	-2.160492	-1.728513	-0.358362
H	-1.059642	-0.945601	1.317135
C	-1.710550	1.740324	1.368398
H	-2.767985	0.951656	-0.338893
H	-3.228560	0.217791	1.185771
H	-1.503209	-2.575695	-0.548468
H	-2.549537	-1.376756	-1.313531
H	-2.994620	-2.072882	0.251654
H	-0.895918	2.171870	0.785498
H	-1.301023	1.394981	2.319495

H	-2.422011	2.536479	1.580847
C	1.163755	-0.585554	-0.177980
C	1.843507	0.618013	0.516720
C	1.288425	-1.873485	0.627774
H	1.629752	-0.687220	-1.160997
C	3.348510	0.430775	0.652251
H	1.636702	1.507463	-0.077872
H	1.390752	0.753472	1.503511
H	0.681547	-2.676850	0.211896
H	1.000153	-1.728119	1.669850
H	2.322939	-2.210317	0.617826
H	3.799413	0.262483	-0.326197
H	3.598613	-0.413242	1.294391
H	3.805101	1.320329	1.083807
Rotational constants (GHz): 1.3171200 0.7394700 0.7083500			
Vibrational harmonic frequencies (cm-1):			
45.8998	49.4484	78.6589	
111.2511	161.9408	187.8366	
193.2475	214.4971	223.5929	
232.7760	257.7433	270.6305	
292.8135	311.5041	335.3588	
374.1707	433.2401	455.8105	
551.8967	605.5977	701.6327	
764.5957	789.2064	814.4157	
850.7909	880.8867	944.8869	
974.2312	983.5846	1012.6684	
1023.5613	1032.0250	1045.8531	
1081.5492	1109.1534	1143.3920	
1144.8684	1183.2906	1188.3427	
1260.2630	1281.7807	1300.5324	
1308.4157	1319.3797	1350.9180	
1372.4702	1377.3515	1404.8489	
1409.8567	1416.7375	1420.0291	
1426.2726	1482.7371	1489.5991	
1499.0526	1499.3667	1501.4312	
1503.4826	1507.3392	1508.3346	
1510.2903	1519.0136	1626.3963	
3044.5346	3056.8017	3063.8474	
3064.9459	3067.2093	3069.7618	
3078.0599	3081.5256	3107.3296	
3114.8128	3128.6134	3134.4640	
3136.3953	3138.5051	3140.4278	
3144.6432	3144.7970	3152.0127	
Zero-point correction (Hartree): 0.260216			
dic2H5CH3CH_COO.cmtmRR			
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E(RM062X/Aug-CC-pVTZ) (Hartree): -504.06903731			
Electronic state : 1-A			
Cartesian coordinates (Angs):			
C	-0.026726	0.403735	-0.080081
O	0.414811	1.396115	-0.704728
O	-0.449472	2.147426	-1.463399
C	0.977158	-0.300277	0.790025
C	2.418019	-0.106979	0.318420
C	0.785383	0.189451	2.234339
H	0.742433	-1.365972	0.761651
C	2.689894	-0.728084	-1.046032
H	2.652417	0.957961	0.302847
H	3.068122	-0.562856	1.067464
H	-0.218852	-0.012584	2.603625
H	0.965547	1.262962	2.295151
H	1.495650	-0.318075	2.885768
H	2.082633	-0.262776	-1.821781
H	2.470541	-1.797328	-1.035454
H	3.734773	-0.607077	-1.327057
C	-1.476115	0.068455	-0.171793
C	-1.798135	-1.382713	0.170096
C	-2.267262	1.070488	0.689192
H	-1.734230	0.279197	-1.213971
C	-1.275338	-2.365052	-0.872250
H	-1.418293	-1.630844	1.164814
H	-2.883843	-1.470669	0.236399
H	-1.960234	2.089021	0.462879
H	-2.126206	0.868141	1.750725
H	-3.327921	0.970524	0.463535
H	-0.197521	-2.268245	-1.016002
H	-1.746016	-2.177849	-1.837499
H	-1.482976	-3.395991	-0.589576
Rotational constants (GHz): 1.1524600 0.8584400 0.7515200			
Vibrational harmonic frequencies (cm-1):			
45.1054	88.7938	118.7553	
140.3038	162.3321	183.6893	
194.5322	205.0511	212.6003	
234.1773	244.6896	256.4548	
280.6147	326.2728	346.8164	
411.0950	431.6096	465.5039	
521.9814	604.8309	687.2774	
745.8874	798.7159	811.1070	
866.2590	896.2289	950.2512	
976.6091	987.6915	1021.1642	
1027.1945	1036.1971	1042.1308	
1066.9501	1114.1794	1132.9318	
1145.1218	1188.1930	1194.7753	
1252.2233	1277.1145	1294.9713	
1306.8462	1313.6300	1365.1630	
1373.1941	1375.9790	1394.2156	
1406.4469	1415.2589	1421.1542	
1424.4376	1487.8016	1489.5319	
1499.4403	1501.1342	1503.5194	
1504.3136	1508.4225	1510.7452	
1512.3271	1514.2164	1619.6833	

3052.8079	3059.9162	3060.2699
3064.0041	3065.7381	3069.6399
3072.3495	3086.2679	3093.6051
3110.0293	3125.7125	3131.5991
3139.4689	3140.3283	3142.4078
3143.8858	3149.4373	3162.4209

Zero-point correction (Hartree): 0.260408

dic2H5CH3CH_COO.cmtprR

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E(RM062X/Aug-CC-pVTZ) (Hartree): -504.06600756

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.134391  | 0.449746  | 0.028777  |
| O | 0.761032  | 1.523232  | 0.190249  |
| O | 0.153846  | 2.713380  | -0.131403 |
| C | 0.890262  | -0.777512 | 0.458990  |
| C | 2.382873  | -0.686415 | 0.134351  |
| C | 0.656658  | -0.989087 | 1.962513  |
| H | 0.471561  | -1.624891 | -0.084750 |
| C | 2.656569  | -0.561185 | -1.358920 |
| H | 2.814805  | 0.159611  | 0.669684  |
| H | 2.857751  | -1.587270 | 0.527558  |
| H | -0.402745 | -1.054387 | 2.208033  |
| H | 1.085916  | -0.158486 | 2.522605  |
| H | 1.140073  | -1.911520 | 2.282415  |
| H | 2.240019  | 0.363452  | -1.759169 |
| H | 2.218263  | -1.397649 | -1.906331 |
| H | 3.726209  | -0.554892 | -1.561427 |
| C | -1.250414 | 0.490436  | -0.518990 |
| C | -1.723614 | -0.808533 | -1.181068 |
| C | -2.209550 | 1.008764  | 0.567428  |
| H | -1.190691 | 1.283523  | -1.271126 |
| C | -2.253245 | -1.887468 | -0.240586 |
| H | -2.523230 | -0.534766 | -1.871787 |
| H | -0.920743 | -1.211153 | -1.803343 |
| H | -1.871326 | 1.980287  | 0.918178  |
| H | -2.269653 | 0.318215  | 1.407856  |
| H | -3.207921 | 1.112230  | 0.142081  |
| H | -3.152806 | -1.551357 | 0.273191  |
| H | -1.527539 | -2.171125 | 0.521710  |
| H | -2.510552 | -2.785195 | -0.801115 |

Rotational constants (GHz): 1.1972900 0.8769700 0.6944800

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| 40.8880   | 80.1052   | 112.5942  |
| 146.0234  | 159.5975  | 191.3707  |
| 207.4931  | 211.3217  | 235.1337  |
| 243.9071  | 255.8423  | 268.2867  |
| 296.8021  | 321.3261  | 344.0599  |
| 347.6532  | 453.6052  | 464.2909  |
| 572.7882  | 613.8434  | 683.5126  |
| 744.6325  | 790.7708  | 808.9794  |
| 862.5339  | 892.3299  | 950.0041  |
| 969.1551  | 986.3080  | 999.2787  |
| 1025.5246 | 1033.3437 | 1041.7792 |
| 1079.2529 | 1120.0811 | 1141.1632 |
| 1148.7944 | 1166.0960 | 1191.0173 |
| 1257.2761 | 1292.3785 | 1303.2285 |
| 1314.0745 | 1316.8325 | 1368.8942 |
| 1373.9625 | 1378.0033 | 1395.4406 |
| 1404.8856 | 1415.5693 | 1419.6166 |
| 1426.0033 | 1487.5989 | 1490.8836 |
| 1495.0211 | 1499.1209 | 1502.7151 |
| 1506.1951 | 1510.0565 | 1510.5962 |
| 1513.1954 | 1521.7440 | 1616.6136 |
| 3050.1758 | 3058.6009 | 3059.9940 |
| 3064.6279 | 3068.6881 | 3069.7911 |
| 3072.8611 | 3091.3550 | 3096.0019 |
| 3110.8236 | 3130.5160 | 3134.9703 |
| 3138.1657 | 3140.8086 | 3142.3541 |
| 3143.3856 | 3144.4493 | 3169.3672 |

Zero-point correction (Hartree): 0.260641

dic2H5CH3CH\_COO.cmttrR

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E(RM062X/Aug-CC-pVTZ) (Hartree): -504.06836434

Electronic state : 1-A

Cartesian coordinates (Angs):

C	0.223796	0.347109	0.030122
O	0.820686	1.448216	0.004148
O	0.097459	2.593908	-0.226088
C	1.081158	-0.843386	0.349096
C	2.563795	-0.618266	0.056340
C	0.850618	-1.215877	1.822771
H	0.722662	-1.669152	-0.270245
C	2.863881	-0.407541	-1.422644
H	2.919846	0.232646	0.638494
H	3.101284	-1.496069	0.420012
H	-0.196982	-1.423826	2.034407
H	1.176284	-0.400792	2.469551
H	1.430914	-2.104408	2.067711
H	2.387762	0.496650	-1.799143
H	2.509017	-1.253058	-2.014423
H	3.935391	-0.311698	-1.590310
C	-1.249685	0.307059	-0.184606
C	-1.769436	-1.064469	-0.613067
C	-1.944567	0.849810	1.079518
H	-1.423167	1.043148	-0.976198
C	-3.257332	-1.039135	-0.941850
H	-1.215326	-1.400680	-1.492325
H	-1.584718	-1.798736	0.175775
H	-1.444446	1.751988	1.423589

H	-1.945337	0.099002	1.870715
H	-2.976830	1.105314	0.850088
H	-3.476089	-0.269360	-1.683163
H	-3.858141	-0.832635	-0.057455
H	-3.580638	-1.997146	-1.345645
Rotational constants (GHz):			1.3449800 0.7357000 0.6382200
Vibrational harmonic frequencies (cm-1):			
51.0399	97.2394	105.2571	
130.6717	153.0013	164.1995	
193.4259	200.0284	226.1112	
245.0943	256.1846	272.7525	
300.6326	319.3909	348.0011	
373.2022	430.0844	458.8174	
544.4828	604.2699	692.8949	
750.6815	799.5289	811.7262	
866.5233	905.9413	949.9564	
975.0302	982.6032	990.0726	
1025.3947	1037.0262	1049.6195	
1076.9993	1124.0768	1136.3691	
1150.8703	1187.5026	1193.2945	
1255.9905	1286.2213	1299.3859	
1308.7856	1319.0224	1334.1735	
1374.6402	1382.7597	1400.1995	
1407.0668	1414.3970	1417.3367	
1428.0459	1485.7687	1488.3258	
1493.8923	1500.2683	1502.8984	
1503.4678	1508.6280	1512.5875	
1513.1255	1523.8843	1621.4242	
3044.5877	3052.5138	3062.4274	
3065.2859	3066.0298	3067.8845	
3070.2663	3073.6978	3087.7094	
3108.4495	3132.9246	3134.3816	
3140.7907	3141.4143	3146.5533	
3146.9302	3151.2706	3164.0812	
Zero-point correction (Hartree): 0.260439			

dic2H5CH3CH_COO.cpmRR

E(RM062X/Aug-CC-pVTZ) (Hartree): -504.06677566

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-0.028593	-0.289155	0.233153
O	0.115566	-1.049770	-0.746438
O	-0.994827	-1.522274	-1.406683
C	1.234429	0.164832	0.907915
C	2.495312	-0.568788	0.438120
C	1.371093	1.690709	0.792462
H	1.075259	-0.068461	1.967703
C	3.030338	-0.129010	-0.921989
H	3.264932	-0.401941	1.194370
H	2.294909	-1.640198	0.424044
H	0.543285	2.211351	1.269919
H	1.408872	1.998666	-0.251404
H	2.295473	2.005381	1.276341
H	3.378657	0.903148	-0.898418
H	2.272741	-0.218633	-1.698528
H	3.876015	-0.752176	-1.208488
C	-1.368183	0.087404	0.781311
C	-2.335768	0.706799	-0.238988
C	-1.973020	-1.154769	1.456055
H	-1.167170	0.832437	1.554146
C	-1.662653	1.683502	-1.192468
H	-2.803008	-0.092270	-0.806604
H	-3.112778	1.214629	0.337173
H	-1.341351	-1.519337	2.266470
H	-2.104540	-1.942164	0.717318
H	-2.943696	-0.890244	1.874322
H	-0.938788	1.157942	-1.818426
H	-1.149278	2.482863	-0.654216
H	-2.393178	2.146218	-1.854184

Rotational constants (GHz):			1.4690100 0.7636900 0.7229200
Vibrational harmonic frequencies (cm-1):			
44.8214	83.1542	118.9992	
130.8833	176.4808	192.5067	
208.7806	225.2551	232.6161	
247.5939	257.9827	293.0620	
304.7800	321.0553	333.3462	
399.7998	426.2851	435.9817	
530.7859	625.7061	734.8377	
744.6056	797.6636	819.1710	
836.3984	890.9983	944.5900	
983.6849	996.7605	1003.3710	
1022.1603	1031.4486	1038.6222	
1098.6069	1117.9847	1127.6207	
1146.3086	1168.0476	1185.2193	
1228.1267	1289.6874	1301.7472	
1316.6387	1327.6354	1365.2352	
1374.9365	1380.7455	1394.0325	
1410.3974	1412.5744	1418.8080	
1434.5721	1482.7420	1486.5878	
1493.8431	1496.6541	1498.7819	
1505.0418	1509.8436	1514.0373	
1516.3442	1520.8525	1649.4936	
3024.7836	3051.8886	3060.3885	
3065.0115	3066.8260	3069.1660	
3073.3724	3075.1136	3108.4076	
3115.5890	3132.9773	3135.1215	
3139.2702	3144.5550	3151.2961	
3153.6037	3158.4040	3166.7062	

Rotational constants (GHz):			1.4690100 0.7636900 0.7229200
Vibrational harmonic frequencies (cm-1):			
44.8214	83.1542	118.9992	
130.8833	176.4808	192.5067	
208.7806	225.2551	232.6161	
247.5939	257.9827	293.0620	
304.7800	321.0553	333.3462	
399.7998	426.2851	435.9817	
530.7859	625.7061	734.8377	
744.6056	797.6636	819.1710	
836.3984	890.9983	944.5900	
983.6849	996.7605	1003.3710	
1022.1603	1031.4486	1038.6222	
1098.6069	1117.9847	1127.6207	
1146.3086	1168.0476	1185.2193	
1228.1267	1289.6874	1301.7472	
1316.6387	1327.6354	1365.2352	
1374.9365	1380.7455	1394.0325	
1410.3974	1412.5744	1418.8080	
1434.5721	1482.7420	1486.5878	
1493.8431	1496.6541	1498.7819	
1505.0418	1509.8436	1514.0373	
1516.3442	1520.8525	1649.4936	
3024.7836	3051.8886	3060.3885	
3065.0115	3066.8260	3069.1660	
3073.3724	3075.1136	3108.4076	
3115.5890	3132.9773	3135.1215	
3139.2702	3144.5550	3151.2961	
3153.6037	3158.4040	3166.7062	

Rotational constants (GHz):			1.4690100 0.7636900 0.7229200
Vibrational harmonic frequencies (cm-1):			
44.8214	83.1542	118.9992	
130.8833	176.4808	192.5067	
208.7806	225.2551	232.6161	
247.5939	257.9827	293.0620	
304.7800	321.0553	333.3462	
399.7998	426.2851	435.9817	
530.7859	625.7061	734.8377	
744.6056	797.6636	819.1710	
836.3984	890.9983	944.5900	
983.6849	996.7605	1003.3710	
1022.1603	1031.4486	1038.6222	
1098.6069	1117.9847	1127.6207	
1146.3086	1168.0476	1185.2193	
1228.1267	1289.6874	1301.7472	
1316.6387	1327.6354	1365.2352	
1374.9365	1380.7455	1394.0325	
1410.3974	1412.5744	1418.8080	
1434.5721	1482.7420	1486.5878	
1493.8431	1496.6541	1498.7819	
1505.0418	1509.8436	1514.0373	
1516.3442	1520.8525	1649.4936	
3024.7836	3051.8886	3060.3885	
3065.0115	3066.8260	3069.1660	
3073.3724	3075.1136	3108.4076	
3115.5890	3132.9773	3135.1215	
3139.2702	3144.5550	3151.2961	
3153.6037	3158.4040	3166.7062	

Rotational constants (GHz):			1.4690100 0.7636900 0.7229200
Vibrational harmonic frequencies (cm-1):			
44.8214	83.1542	118.9992	
130.8833	176.4808	192.5067	
208.7806	225.2551	232.6161	
247.5939	257.9827	293.0620	
304.7800	321.0553	333.3462	
399.7998	426.2851	435.9817	
530.7859	625.7061	734.8377	
744.6056	797.6636	819.1710	
836.3984	890.9983	944.5900	
983.6849	996.7605	1003.3710	
1022.1603	1031.4486	1038.6222	
1098.6069	1117.9847	1127.6207	
1146.3086	1168.0476	1185.2193	
1228.1267	1289.6874	1301.7472	
1316.6387	1327.6354	1365.2352	
1374.9365	1380.7455	1394.0325	
1410.3974	1412.5744	1418.8080	
1434.5721	1482.7420	1486.5878	
1493.8431	1496.6541	1498.7819	
1505.0418	1509.8436	1514.0373	
1516.3442	1520.8525	1649.4936	
3024.7836	3051.8886	3060.3885	
3065.0115	3066.8260	3069.1660	
3073.3724	3075.1136	3108.4076	
3115.5890	3132.9773	3135.1215	
3139.2702	3144.5550	3151.2961	
3153.6037	3158.4040	3166.7062	

Rotational constants (GHz):			1.4690100 0.7636900 0.7229200
Vibrational harmonic frequencies (cm-1):			
44.8214	83.1542	118.9992	
130.8833	176.4808	192.5067	
208.7806	225.2551	232.6161	
247.5939	257.9827	293.0620	
304.7800	321.0553	333.3462	
399.7998	426.2851	435.9817	
530.7859	625.7061	734.8377	
744.6056	797.6636	819.1710	
836.3984	890.9983	944.5900	
983.6849	996.7605	1003.3710	
1022.1603	1031.4486	1038.6222	
1098.6069	1117.9847	1127.6207	
1146.3086	1168.0476	1185.2193	
1228.1267	1289.6874	1301.7472	
1316.6387	1327.6354	1365.2352	
1374.9365	1380.7455	1394.0325	
1410.3974	1412.5744	1418.8080	
1434.5721	1482.7420	1486.5878	
1493.8431	1496.6541	1498.7819	
1505.0418	1509.8436	1514.0373	
1516.3442	1520.8525	1649.4936	
3024.7836	3051.8886	3060.3885	
3065.0115	3066.8260	3069.1660	
3073.3724	3075.1136	3108.4076	
3115.5890	3132.9773	3135.1215	
3139.2702	3144.5550	3151.2961	
3153.6037	3158.4040	3166.7062	

Rotational constants (GHz):			1.4690100 0.7636900 0.7229200
Vibrational harmonic frequencies (cm-1):			
44.8214	83.1542	118.9992	
130.8833	176.4808	192.5067	
208.7806	225.2551	232.6161	
247.5939	257.9827	293.0620	
304.7800	321.0553	333.3462	
399.7998	426.2851	435.9817	
530.7859	625.7061	734.8377	
744.6056	797.6636	819.1710	
836.3984	890.9983	944.5900	
983.6849	996.7605	1003.3710	
1022.1603	1031.4486	1038.6222	
1098.6069	1117.9847	1127.6207	
1146.3086	1168.0476	1185.2193	
1228.1267	1289.6874	1301.7472	
1316.6387	1327.6354	1365.2352	
1374.9365	1380.7455	1394.0325	
1410.3974	1412.5744	1418.8080	
1434.5721	1482.7420	1486.5878	
1493.8431	1496.6541	1498.7819	
1505.0418	1509.8436	1514.0373	
1516.3442	1520.8525	1649.4936	
3024.7836	3051.8886	3060.3885	
3065.0115	3066.8260	3069.1660	
3073.3724	3075.1136	3108.4076	
3115.5890	3132.9773	3135.1215	
3139.2702	3144.5550	3151.2961	
3153.6037	3158.4040	3166.7062	

Rotational constants (GHz):			1.4690100 0.7636900 0.7229200
Vibrational harmonic frequencies (cm-1):			
44.8214	83.1542	118.9992	
130.8833			

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E(RM062X/Aug-CC-pVTZ) (Hartree): -504.06095002
Electronic state : 1-A
Cartesian coordinates (Angs):
C      -0.032407      -0.149632      -0.466034
O      -0.117571      -1.335568      -0.083787
O       1.006195      -2.060820       0.215597
C      -1.348855       0.516337      -0.774876
C      -2.568345      -0.365741      -0.491221
C      -1.453222       1.882978      -0.084640
H      -1.309620       0.703486      -1.855312
C      -2.881106      -0.556507       0.990137
H      -3.424164       0.101356      -0.982575
H      -2.424107      -1.336459      -0.963892
H      -0.694743       2.579050      -0.437292
H      -1.352583       1.786758       0.995789
H      -2.431205       2.314444      -0.296503
H      -3.169514       0.382668       1.461521
H      -2.026610      -0.963473       1.529270
H      -3.710416      -1.251281       1.112272
C       1.261372       0.576700      -0.683454
C       1.786649       1.220847       0.620564
C       2.338349      -0.238585      -1.408460
H       0.988176       1.407040      -1.340017
C       2.003262       0.269477       1.790198
H       2.727559       1.709683       0.356867
H       1.102888       2.014360       0.925317
H       1.911285      -0.868470      -2.187601
H       2.871895      -0.888534      -0.725320
H       3.034187       0.461056      -1.873063
H       2.706444      -0.521356       1.543420
H       1.073031      -0.218821       2.081901
H       2.384318       0.824358       2.647459
Rotational constants (GHz):      1.4922400      0.7769000      0.7042600
Vibrational harmonic frequencies (cm-1):
43.3665      69.9409      125.0258
138.3033      167.4279      181.4994
200.0597      215.0454      241.0696
253.5339      268.6521      299.6256
319.0382      323.7649      334.3020
358.7525      409.3820      496.2229
536.3120      628.8110      711.9488
768.8195      788.2220      807.5755
836.1286      879.9313      949.8889
987.3335      995.1986      1007.5304
1014.7293      1027.3407      1041.3127
1101.3933      1105.7121      1132.5613
1142.8587      1173.8164      1187.9598
1218.4431      1288.9058      1295.4627
1318.1365      1326.3091      1367.4786
1377.9456      1380.8348      1412.9677
1415.8160      1419.9612      1429.7796
1435.3335      1478.3231      1483.6997
1489.3063      1492.6294      1499.3786
1502.4894      1504.8269      1508.2217
1510.1172      1520.8348      1640.1954
3018.2443      3053.1787      3062.1159
3068.3984      3069.1667      3070.6023
3071.2638      3072.8958      3099.5060
3115.5436      3131.2845      3135.1673
3139.1487      3142.9018      3146.6250
3151.0787      3164.3682      3196.9510
Zero-point correction (Hartree): 0.260842

diC2H5CH3CH_COO.cpmtrr
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E(RM062X/Aug-CC-pVTZ) (Hartree): -504.06462648
Electronic state : 1-A
Cartesian coordinates (Angs):
C       0.175174       0.240889      -0.277330
O       0.474284       1.316482       0.281469
O      -0.516250       2.157642       0.734402
C       1.326848      -0.615007      -0.721435
C       2.698072       0.054957      -0.588681
C       1.264409      -1.972348      -0.003447
H       1.136917      -0.801697      -1.785075
C       3.246654       0.130514       0.833450
H       3.394208      -0.512142      -1.209899
H       2.642246       1.057330      -1.013284
H       0.341244      -2.506344      -0.221687
H       1.336733      -1.844488       1.075707
H       2.100149      -2.590873      -0.329597
H       3.452346      -0.861444       1.234844
H       2.553878       0.636266       1.503651
H       4.183032       0.686087       0.842164
C      -1.235160      -0.194822      -0.508503
C      -1.923099      -0.510524       0.833360
C      -2.008073       0.816682      -1.366654
H      -1.166596      -1.127652      -1.074444
C      -3.330264      -1.059439       0.637332
H      -1.319225      -1.245039       1.371833
H      -1.938860       0.399983       1.429458
H      -1.412464       1.142300      -2.220049
H      -2.269441       1.691559      -0.780185
H      -2.908271       0.341761      -1.753033
H      -3.330350      -1.923077      -0.031044
H      -3.994303      -0.306838       0.214796
H      -3.752890      -1.374099       1.590312
Rotational constants (GHz):      1.6390500      0.6931100      0.5976700
Vibrational harmonic frequencies (cm-1):
44.5286      65.2715      82.0260
130.6748      142.0511      179.6448

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182.4179	216.9401	229.0318
255.4160	264.3849	269.5442
304.7669	315.1383	326.4890
364.9071	429.4828	444.1872
537.0588	627.5501	726.8673
772.1653	799.0463	820.9738
829.7523	888.0498	942.3616
974.6548	995.0451	996.7044
1003.1661	1029.4002	1057.9525
1108.5020	1113.0992	1119.3041
1150.2874	1168.4797	1183.5172
1221.0341	1289.2902	1290.5832
1327.2400	1342.7223	1357.1675
1373.3725	1381.4948	1400.6122
1411.3368	1413.0110	1422.1524
1432.4815	1486.3550	1489.3137
1495.6996	1499.8687	1503.3248
1505.8973	1511.3089	1512.7734
1515.1381	1521.0361	1648.7258
3026.4030	3056.8053	3057.8286
3059.7183	3067.3678	3070.6426
3073.0094	3073.8136	3109.7573
3118.6734	3134.6014	3137.5710
3138.2176	3143.6702	3145.1845
3149.5848	3152.7491	3185.4420

Zero-point correction (Hartree): 0.260494

diC2H5CH3CH_COO.cppmRR

E(RM062X/Aug-CC-pVTZ) (Hartree): -504.06001162

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-0.035656	-0.349951	0.087510
O	-0.165197	-1.597304	0.131623
O	-1.159433	-2.229494	-0.574418
C	1.097393	0.122442	0.976145
C	2.405904	-0.593024	0.582695
C	1.290178	1.631950	1.080257
H	0.824346	-0.241968	1.971262
C	2.821556	-0.361230	-0.865456
H	3.188081	-0.243125	1.258810
H	2.284519	-1.660928	0.756647
H	0.362328	2.154153	1.304801
H	1.709319	2.057305	0.171836
H	1.988078	1.832134	1.892472
H	2.961196	0.697103	-1.086488
H	2.074134	-0.759070	-1.554409
H	3.761869	-0.867149	-1.077931
C	-0.977904	0.451867	-0.748385
C	-2.133325	0.982927	0.126981
C	-0.329797	1.581789	-1.551277
H	-1.400108	-0.285551	-1.431507
C	-2.923747	-0.098762	0.850755
H	-1.737574	1.706202	0.844323
H	-2.790785	1.544134	-0.540548
H	0.627333	1.287509	-1.981426
H	-0.182097	2.480136	-0.955947
H	-0.995899	1.839046	-2.373898
H	-2.287957	-0.679119	1.520966
H	-3.356813	-0.802368	0.143654
H	-3.720542	0.347895	1.444392

Rotational constants (GHz): 1.3998800 0.8287400 0.6969000

Vibrational harmonic frequencies (cm-1):

35.4970	62.9071	91.9291
113.2050	171.8646	186.8572
209.9360	240.1050	260.1639
261.2256	263.7425	280.4126
286.0954	325.9347	333.5384
366.5244	432.6499	506.9699
515.0936	616.9826	671.3065
735.6513	790.2660	806.8754
844.1807	874.3654	940.0878
985.4794	989.1558	1012.6544
1025.8888	1034.5840	1054.2592
1074.2735	1104.6693	1129.8040
1148.1833	1178.4808	1196.3666
1270.8929	1285.2491	1302.3391
1320.0300	1333.1942	1364.4224
1372.7140	1377.5793	1386.3492
1416.2883	1417.6306	1424.0269
1428.7730	1481.4865	1490.1881
1492.7140	1494.3068	1501.4718
1502.3317	1506.3531	1510.8271
1516.0869	1526.2349	1595.9016
3044.6643	3052.3837	3059.9724
3067.2859	3072.9438	3074.3322
3081.6134	3085.0588	3099.4885
3116.2375	3130.3529	3133.9005
3138.3986	3140.9396	3146.7725
3156.4717	3157.8489	3167.5711

Zero-point correction (Hartree): 0.260626

diC2H5CH3CH_COO.cpppRR

E(RM062X/Aug-CC-pVTZ) (Hartree): -504.06459745

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-0.046686	-0.177968	-0.347508
O	0.391481	-1.335520	-0.539867
O	-0.440843	-2.291772	-1.074978
C	0.930823	0.795738	0.247047
C	1.995012	0.133913	1.139156

C	1.556570	1.655150	-0.862329
H	0.332942	1.455228	0.880362
C	3.166811	-0.520593	0.413192
H	2.382059	0.914421	1.797616
H	1.505521	-0.600872	1.780657
H	0.809894	2.247820	-1.384839
H	2.069609	1.027992	-1.589705
H	2.285544	2.335885	-0.422441
H	3.747833	0.213377	-0.144471
H	2.834228	-1.292567	-0.276672
H	3.836243	-0.982540	1.137494
C	-1.472692	0.123861	-0.657191
C	-2.328328	-0.495921	0.477009
C	-1.788395	1.597049	-0.889410
H	-1.695076	-0.460528	-1.551989
C	-2.088804	0.117328	1.851975
H	-3.372644	-0.365489	0.188713
H	-2.127408	-1.565759	0.494782
H	-1.347753	1.960379	-1.815942
H	-1.450928	2.240464	-0.077433
H	-2.868848	1.714669	-0.971156
H	-2.262029	1.194311	1.857666
H	-1.069519	-0.063944	2.198979
H	-2.760634	-0.325852	2.585491
Rotational constants (GHz):			
	1.3667100	0.7892200	0.7012600
Vibrational harmonic frequencies (cm-1):			
49.5954	79.0296		81.6249
127.2758	167.3116		186.1183
207.4414	225.0689		237.8603
250.6437	273.0587		275.3502
314.1410	318.0347		345.2241
365.4476	409.2346		502.8477
582.1662	618.3227		707.9493
744.3383	795.3712		800.6583
830.3928	868.1899		940.9109
985.6060	991.8984		1007.5501
1012.8603	1023.5452		1034.0425
1076.3155	1119.4870		1129.4526
1155.0415	1167.6792		1176.2819
1251.0371	1287.5354		1296.1441
1300.6298	1333.2092		1359.1051
1369.0098	1379.6893		1397.5584
1415.9262	1418.2929		1420.4614
1428.7212	1484.5732		1492.7702
1497.1414	1500.7380		1504.5605
1508.5597	1511.1871		1512.5574
1516.5522	1523.0535		1623.9280
3056.4661	3058.3406		3069.4899
3072.5368	3073.4734		3075.4836
3076.3028	3083.6137		3098.5175
3112.4187	3132.9156		3136.2781
3136.6719	3139.2433		3143.6093
3146.8067	3160.9161		3165.3442
Zero-point correction (Hartree): 0.260747			
diC2H5CH3CH_COO.cpptRR			
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E(RM062X/Aug-CC-pVTZ) (Hartree): -504.06473601			
Electronic state : 1-A			
Cartesian coordinates (Angs):			
C	0.099445	-0.090220	-0.183373
O	0.378163	-1.274218	-0.486065
O	-0.613664	-2.082427	-0.993301
C	1.216111	0.711217	0.421032
C	2.301528	-0.149979	1.087440
C	1.808612	1.680100	-0.614362
H	0.741295	1.311125	1.203426
C	3.317590	-0.786988	0.143802
H	2.830999	0.498703	1.788415
H	1.817473	-0.925443	1.682186
H	1.082428	2.416079	-0.947884
H	2.173169	1.136160	-1.484381
H	2.649835	2.209936	-0.167321
H	3.905639	-0.031693	-0.376858
H	2.836373	-1.420420	-0.597921
H	4.011684	-1.404259	0.712349
C	-1.302177	0.380345	-0.348449
C	-2.097592	-0.236891	0.832267
C	-1.482086	1.890073	-0.432427
H	-1.662715	-0.108711	-1.255700
C	-3.583844	-0.342429	0.521140
H	-1.712826	-1.236410	1.031740
H	-1.930115	0.379259	1.720080
H	-1.073433	2.297878	-1.355045
H	-1.021147	2.407353	0.410134
H	-2.544752	2.125756	-0.416966
H	-3.734716	-1.006547	-0.329718
H	-4.024339	0.625973	0.284270
H	-4.126366	-0.752946	1.371701
Rotational constants (GHz):			
	1.6539800	0.6992800	0.5787600
Vibrational harmonic frequencies (cm-1):			
33.4439	53.9530		90.5404
125.8909	167.2816		181.0147
212.3255	218.1651		232.4250
258.9718	261.7579		296.1240
301.3014	312.9107		345.8366
368.0744	415.9307		476.2325
576.9869	618.8127		710.9163
757.6401	779.3992		798.5693
844.5570	876.7472		941.8752
980.7799	994.2599		1004.3082
1022.5569	1028.8115		1036.0303

1080.9810	1119.9885	1129.9421
1157.9973	1167.9619	1185.8538
1258.0397	1286.0803	1294.1528
1319.2947	1329.9473	1350.8952
1376.2880	1384.2649	1398.3819
1409.5166	1417.7531	1421.5945
1428.0963	1478.1854	1486.6480
1494.2072	1499.8191	1503.2348
1504.6137	1508.7716	1511.7801
1519.1704	1521.2720	1619.1386
3047.7002	3049.2584	3064.4469
3065.2742	3069.8588	3073.5253
3076.1324	3081.4861	3103.4519
3114.2181	3136.0319	3137.1790
3140.0090	3140.8601	3144.0462
3149.2652	3158.9566	3171.7483

Zero-point correction (Hartree): 0.260649

diC2H5CH3CH_COO.cptmRR

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E(RM062X/Aug-CC-pVTZ) (Hartree): -504.06631190

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.028304 | 0.307419  | -0.173127 |
| O | 0.555889  | 1.325367  | -0.611569 |
| O | -0.144656 | 2.501387  | -0.730621 |
| C | 0.828817  | -0.914322 | -0.003012 |
| C | 2.179508  | -0.831231 | -0.727829 |
| C | 0.994245  | -1.217063 | 1.495965  |
| H | 0.263169  | -1.741142 | -0.439411 |
| C | 3.244359  | 0.019100  | -0.040746 |
| H | 2.551127  | -1.853577 | -0.822665 |
| H | 2.013101  | -0.462671 | -1.740396 |
| H | 0.045413  | -1.460756 | 1.968766  |
| H | 1.427183  | -0.365722 | 2.019579  |
| H | 1.663506  | -2.068912 | 1.616702  |
| H | 3.527090  | -0.400660 | 0.924316  |
| H | 2.905384  | 1.041212  | 0.114452  |
| H | 4.142503  | 0.054984  | -0.655482 |
| C | -1.472561 | 0.396071  | 0.187827  |
| C | -2.222242 | -0.931050 | 0.102282  |
| C | -1.588370 | 1.070747  | 1.566382  |
| H | -1.883979 | 1.101924  | -0.538884 |
| C | -2.399292 | -1.415584 | -1.332832 |
| H | -1.730169 | -1.695437 | 0.707401  |
| H | -3.204150 | -0.779595 | 0.554069  |
| H | -1.011361 | 1.993254  | 1.581559  |
| H | -1.243894 | 0.408123  | 2.359948  |
| H | -2.632853 | 1.314002  | 1.755933  |
| H | -1.441344 | -1.534751 | -1.841933 |
| H | -2.981742 | -0.695251 | -1.907219 |
| H | -2.915805 | -2.373573 | -1.368671 |

Rotational constants (GHz): 1.3119300 0.8029000 0.6806000

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| 56.6064   | 96.1303   | 131.6367  |
| 147.0955  | 164.6424  | 179.5997  |
| 194.1333  | 217.7388  | 222.5148  |
| 243.3552  | 246.3407  | 278.6762  |
| 302.6307  | 322.1765  | 359.5325  |
| 381.0183  | 432.8754  | 459.0247  |
| 560.5734  | 625.6125  | 685.5115  |
| 746.6790  | 793.5174  | 803.5980  |
| 856.0239  | 894.7219  | 943.9329  |
| 980.7330  | 994.9688  | 1004.9955 |
| 1019.0475 | 1029.4741 | 1042.2232 |
| 1074.6646 | 1109.0492 | 1134.9323 |
| 1162.1505 | 1169.6067 | 1196.2934 |
| 1253.2991 | 1279.3295 | 1297.8698 |
| 1313.9981 | 1330.2854 | 1366.7455 |
| 1374.9452 | 1382.1234 | 1390.2765 |
| 1404.2889 | 1419.5024 | 1421.3879 |
| 1426.4669 | 1486.9116 | 1491.1956 |
| 1495.4903 | 1500.8786 | 1504.6753 |
| 1506.0188 | 1509.5440 | 1512.0543 |
| 1514.2412 | 1521.6864 | 1620.2696 |
| 3058.7358 | 3061.0767 | 3063.5024 |
| 3068.0265 | 3069.8551 | 3073.0513 |
| 3075.5870 | 3075.6528 | 3097.2387 |
| 3107.7652 | 3127.4525 | 3138.0320 |
| 3140.9693 | 3141.0078 | 3143.4576 |
| 3156.2569 | 3157.3999 | 3160.0073 |

Zero-point correction (Hartree): 0.260856

diC2H5CH3CH\_COO.cptpRR

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E(RM062X/Aug-CC-pVTZ) (Hartree): -504.06230776

Electronic state : 1-A

Cartesian coordinates (Angs):

C	0.067569	0.432089	-0.223588
O	0.813351	1.438308	-0.170146
O	0.252985	2.692895	-0.126218
C	0.776107	-0.891061	-0.205370
C	2.202158	-0.847442	-0.780893
C	0.745178	-1.444741	1.229172
H	0.184634	-1.557110	-0.836233
C	3.288401	-0.310319	0.146632
H	2.457796	-1.870919	-1.063199
H	2.187527	-0.264390	-1.702609
H	-0.272063	-1.583375	1.588794
H	1.255689	-0.764921	1.909752
H	1.254105	-2.408520	1.258196
H	3.415358	-0.947044	1.021719

H	3.068450	0.699635	0.484636
H	4.241778	-0.288086	-0.379451
C	-1.409197	0.630962	-0.273045
C	-2.215448	-0.480649	-0.957384
C	-1.919075	0.995671	1.131948
H	-1.503950	1.545211	-0.866580
C	-2.523186	-1.736605	-0.147266
H	-3.165494	-0.024008	-1.241950
H	-1.728225	-0.754854	-1.896061
H	-1.390993	1.876300	1.490202
H	-1.780699	0.178410	1.838213
H	-2.984361	1.220772	1.077462
H	-3.010178	-1.490885	0.796005
H	-1.634020	-2.323146	0.077471
H	-3.201079	-2.380124	-0.706695
Rotational constants (GHz): 1.3608900 0.8353800 0.6235400			
Vibrational harmonic frequencies (cm-1):			
38.8633	99.8090	125.2083	
127.4129	166.9235	189.1324	
209.7229	220.6128	238.6892	
250.9907	266.9000	284.5216	
306.5368	319.4338	341.8930	
362.5541	403.1077	510.5234	
594.8250	626.0360	688.6259	
740.2849	780.9536	795.1361	
848.5319	889.8989	941.0978	
969.9614	988.3901	999.2113	
1011.9135	1025.9494	1045.1613	
1082.9694	1123.6783	1143.6307	
1150.3397	1166.4024	1181.5314	
1256.9745	1296.2980	1311.7606	
1321.1505	1333.0585	1371.0150	
1375.7537	1383.2120	1392.3798	
1403.1579	1417.9594	1420.6186	
1429.4844	1484.8938	1491.0756	
1492.3210	1495.8725	1507.9409	
1507.9667	1510.6587	1513.7001	
1520.0598	1526.7873	1617.5406	
3053.3323	3060.3537	3061.3991	
3068.9341	3070.7725	3075.7982	
3076.2415	3084.5781	3090.8887	
3102.6186	3135.5259	3136.8724	
3139.9676	3144.0359	3149.1911	
3160.8513	3162.2449	3164.5293	
Zero-point correction (Hartree): 0.261026			
diC2H5CH3CH_COO.cpttRR			
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E(RM062X/Aug-CC-pVTZ) (Hartree): -504.06602886			
Electronic state : 1-A			
Cartesian coordinates (Angs):			
C	0.147237	0.325412	-0.239167
O	0.773554	1.408334	-0.307274
O	0.080776	2.590246	-0.193213
C	0.980753	-0.920125	-0.315842
C	2.410440	-0.683048	-0.821568
C	0.959627	-1.629112	1.048949
H	0.472245	-1.572628	-1.030843
C	3.378462	-0.086761	0.196570
H	2.795032	-1.650610	-1.150495
H	2.369347	-0.045129	-1.704743
H	-0.042421	-1.947179	1.327538
H	1.337700	-0.972930	1.831792
H	1.597620	-2.511749	1.004838
H	3.546517	-0.765998	1.031932
H	3.015273	0.860232	0.590518
H	4.343701	0.095685	-0.273403
C	-1.332187	0.350362	-0.061948
C	-2.039930	-0.902817	-0.577785
C	-1.638265	0.671094	1.413040
H	-1.650500	1.222159	-0.641287
C	-3.557106	-0.773096	-0.507311
H	-1.746042	-1.076510	-1.615354
H	-1.726585	-1.782263	-0.010951
H	-1.028122	1.508841	1.744247
H	-1.451073	-0.196711	2.046545
H	-2.683100	0.954857	1.519525
H	-3.891975	0.130385	-1.018568
H	-3.906140	-0.723968	0.523054
H	-4.040296	-1.626591	-0.980083
Rotational constants (GHz): 1.5502400 0.7173200 0.5869100			
Vibrational harmonic frequencies (cm-1):			
59.4282	88.7789	116.8947	
137.4418	160.8432	171.1018	
192.1992	208.0511	235.4495	
243.5804	269.7034	301.2491	
303.3885	321.9789	330.6702	
369.8541	431.7209	459.2873	
565.7131	635.7260	692.1166	
748.5061	794.1751	804.8746	
854.8519	903.4041	943.7081	
976.2713	984.4343	994.6085	
1007.5844	1020.7562	1053.9610	
1078.9541	1115.5791	1150.4327	
1159.2710	1169.6464	1194.1948	
1259.0594	1290.7829	1295.6859	
1316.4781	1332.8162	1339.7277	
1375.9780	1382.8212	1395.3046	
1402.7696	1414.9735	1420.7384	
1428.2367	1485.7264	1489.8273	
1495.3513	1496.8263	1502.9529	
1507.0055	1511.0148	1513.1418	

1521.0571	1523.0512	1620.6903
3053.1420	3057.0645	3060.0356
3065.7101	3069.2027	3069.4611
3071.9098	3075.7442	3095.8498
3107.5770	3134.8968	3137.8764
3140.5622	3143.5487	3146.6738
3158.1026	3158.4029	3160.4833

Zero-point correction (Hartree): 0.260802

diC2H5CH3CH_COO.ctmmRR

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E(RM062X/Aug-CC-pVTZ) (Hartree): -504.06780858

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.077524 | -0.262955 | 0.004046  |
| O | -0.151336 | -0.861256 | -1.089240 |
| O | -1.371610 | -1.322259 | -1.525066 |
| C | 1.295370  | 0.191983  | 0.406664  |
| C | 2.406129  | -0.484960 | -0.395248 |
| C | 1.355866  | 1.724166  | 0.316848  |
| H | 1.397037  | -0.085595 | 1.463180  |
| C | 3.798726  | -0.155451 | 0.127679  |
| H | 2.249545  | -1.563908 | -0.368498 |
| H | 2.317729  | -0.190965 | -1.442369 |
| H | 0.551679  | 2.194689  | 0.879927  |
| H | 1.275339  | 2.040140  | -0.723970 |
| H | 2.299889  | 2.085613  | 0.718536  |
| H | 3.881670  | -0.380463 | 1.192481  |
| H | 4.048906  | 0.895064  | -0.013967 |
| H | 4.551374  | -0.743035 | -0.395282 |
| C | -1.249153 | -0.059719 | 0.909981  |
| C | -2.481687 | 0.586087  | 0.258526  |
| C | -1.592956 | -1.418320 | 1.543134  |
| H | -0.891227 | 0.607100  | 1.698539  |
| C | -2.140782 | 1.720373  | -0.696830 |
| H | -3.036865 | -0.180714 | -0.273369 |
| H | -3.106885 | 0.954105  | 1.075647  |
| H | -0.755315 | -1.820837 | 2.113204  |
| H | -1.870025 | -2.121849 | 0.760759  |
| H | -2.435542 | -1.288294 | 2.221510  |
| H | -1.573089 | 1.336550  | -1.546300 |
| H | -1.558239 | 2.502223  | -0.205805 |
| H | -3.046356 | 2.181082  | -1.088571 |

Rotational constants (GHz): 1.5961400 0.6823600 0.6350100

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| 49.0541   | 79.2752   | 93.1385   |
| 122.8496  | 155.9845  | 179.0599  |
| 200.4408  | 221.4901  | 231.8776  |
| 241.4666  | 251.9960  | 278.0490  |
| 306.4851  | 322.7395  | 353.9549  |
| 390.9537  | 425.6155  | 431.3025  |
| 461.2189  | 662.1237  | 734.7721  |
| 750.1818  | 787.6111  | 817.1794  |
| 850.9851  | 894.1496  | 949.7582  |
| 980.6382  | 984.3159  | 998.5807  |
| 1026.4750 | 1031.2387 | 1055.9630 |
| 1102.8553 | 1105.8328 | 1137.2746 |
| 1148.8753 | 1160.3767 | 1199.7732 |
| 1231.2510 | 1293.4346 | 1301.7371 |
| 1311.9617 | 1328.1455 | 1342.4066 |
| 1374.8042 | 1394.5616 | 1397.5912 |
| 1407.9751 | 1411.3401 | 1418.1966 |
| 1435.6633 | 1482.0084 | 1488.0437 |
| 1494.2327 | 1495.6271 | 1500.3372 |
| 1504.5937 | 1509.6371 | 1512.8824 |
| 1516.8202 | 1519.0610 | 1649.5108 |
| 3023.9619 | 3054.3830 | 3056.8816 |
| 3062.4106 | 3063.3191 | 3065.2077 |
| 3069.6778 | 3074.0954 | 3108.1976 |
| 3118.7899 | 3132.5825 | 3133.1543 |
| 3136.3769 | 3141.3601 | 3143.5217 |
| 3156.7449 | 3159.0202 | 3160.6472 |

Zero-point correction (Hartree): 0.260527

diC2H5CH3CH\_COO.ctmpRR

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E(RM062X/Aug-CC-pVTZ) (Hartree): -504.06100153

Electronic state : 1-A

Cartesian coordinates (Angs):

C	0.012158	-0.249363	-0.197527
O	0.087850	-1.308583	0.459782
O	1.294551	-1.926378	0.657899
C	-1.381236	0.300584	-0.357365
C	-2.450061	-0.605245	0.253554
C	-1.446396	1.735303	0.182688
H	-1.545194	0.351052	-1.441621
C	-3.869435	-0.137312	-0.044492
H	-2.312086	-1.616373	-0.128546
H	-2.291606	-0.664899	1.332072
H	-0.718142	2.384767	-0.298834
H	-1.261541	1.744776	1.257941
H	-2.432481	2.155846	-0.000304
H	-4.016706	0.012328	-1.115708
H	-4.108389	0.797237	0.460919
H	-4.591726	-0.880773	0.288318
C	1.181144	0.429003	-0.847830
C	1.978278	1.320820	0.132379
C	2.083910	-0.516996	-1.648483
H	0.718822	1.116416	-1.561673
C	2.596744	0.627972	1.339333
H	2.761904	1.791392	-0.466682
H	1.332275	2.128710	0.479441

H	1.501657	-1.252889	-2.202318
H	2.761792	-1.059838	-1.001076
H	2.650441	0.080057	-2.363812
H	3.271500	-0.171754	1.045524
H	1.835218	0.177660	1.974164
H	3.154421	1.357371	1.927205

Rotational constants (GHz): 1.6928500 0.6678100 0.5999800

Vibrational harmonic frequencies (cm-1):

38.9045	61.8998	92.4690
129.4776	154.3054	164.6752
196.9434	212.0748	231.4533
256.4707	266.8865	295.6322
311.8155	319.3632	342.6387
374.4759	396.0995	454.8314
504.9225	661.4136	714.3758
764.2563	787.0253	794.3297
847.3613	881.8708	956.5743
979.7958	986.4732	1006.3089
1012.8302	1040.9132	1050.1967
1095.2796	1110.6741	1141.4826
1149.7819	1166.1830	1194.8128
1225.1023	1293.9758	1302.9865
1319.3412	1322.4137	1344.7170
1381.1437	1397.1991	1409.8749
1412.1002	1418.3874	1429.5031
1437.3580	1478.8818	1484.5788
1487.1543	1493.8606	1499.5334
1501.3416	1504.4414	1509.6776
1511.4166	1522.4891	1640.9205
3015.2798	3049.8162	3058.8514
3061.1642	3068.3994	3070.4660
3072.2525	3075.3654	3095.8740
3112.6769	3132.0192	3132.2893
3138.8528	3141.8867	3145.7938
3158.8738	3162.3786	3203.7373

Zero-point correction (Hartree): 0.260558

dic2H5CH3CH_COO.ctmtrr

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E(RM062X/Aug-CC-pVTZ) (Hartree): -504.06563979

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.083837  | -0.339857 | 0.021466  |
| O | 0.195521  | -1.399689 | -0.628103 |
| O | -0.928786 | -2.137759 | -0.921482 |
| C | 1.352320  | 0.424960  | 0.256050  |
| C | 2.610821  | -0.400163 | -0.002819 |
| C | 1.298619  | 1.702878  | -0.597987 |
| H | 1.328975  | 0.724737  | 1.310542  |
| C | 3.888154  | 0.340775  | 0.372274  |
| H | 2.543209  | -1.329495 | 0.563977  |
| H | 2.637126  | -0.686882 | -1.055272 |
| H | 0.362790  | 2.243833  | -0.459648 |
| H | 1.393239  | 1.445943  | -1.653729 |
| H | 2.113586  | 2.371401  | -0.329516 |
| H | 3.849291  | 0.692609  | 1.404749  |
| H | 4.060090  | 1.203609  | -0.270010 |
| H | 4.752294  | -0.314434 | 0.276991  |
| C | -1.221485 | 0.171843  | 0.532868  |
| C | -2.241230 | 0.431891  | -0.592801 |
| C | -1.760447 | -0.775490 | 1.615241  |
| H | -0.994035 | 1.132054  | 1.003892  |
| C | -3.257566 | 1.489613  | -0.181479 |
| H | -1.718441 | 0.758396  | -1.494828 |
| H | -2.724112 | -0.507913 | -0.845583 |
| H | -1.069267 | -0.847887 | 2.455282  |
| H | -1.917007 | -1.763817 | 1.191279  |
| H | -2.705569 | -0.388959 | 1.993752  |
| H | -2.774143 | 2.448993  | 0.011839  |
| H | -3.792950 | 1.198160  | 0.722595  |
| H | -3.997084 | 1.640532  | -0.966515 |

Rotational constants (GHz): 1.6454800 0.6384000 0.5509800

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| 47.8859   | 56.4496   | 75.2813   |
| 89.9567   | 146.3532  | 175.3840  |
| 200.0760  | 210.6178  | 217.4488  |
| 231.6351  | 247.7654  | 268.6602  |
| 287.0007  | 300.6905  | 332.2413  |
| 373.1933  | 408.5523  | 441.4296  |
| 480.9757  | 666.8238  | 730.5896  |
| 775.0105  | 785.9018  | 815.1255  |
| 846.8182  | 898.0379  | 945.5825  |
| 978.4068  | 984.1391  | 995.3044  |
| 999.6947  | 1048.3879 | 1055.6905 |
| 1097.8798 | 1121.5706 | 1124.1829 |
| 1146.1227 | 1160.3332 | 1197.0045 |
| 1225.2560 | 1284.7442 | 1292.0403 |
| 1316.2521 | 1339.0248 | 1342.5969 |
| 1359.1260 | 1392.5136 | 1399.6204 |
| 1408.4664 | 1414.7487 | 1417.8049 |
| 1436.6454 | 1487.0937 | 1491.9015 |
| 1493.7176 | 1500.4700 | 1504.3520 |
| 1504.7986 | 1508.1454 | 1509.8717 |
| 1518.4727 | 1521.0645 | 1651.3231 |
| 3027.8936 | 3056.5826 | 3057.7060 |
| 3061.8668 | 3065.3356 | 3066.3084 |
| 3069.9368 | 3074.7529 | 3108.2421 |
| 3117.4022 | 3132.2628 | 3134.2230 |
| 3135.1171 | 3137.8029 | 3141.8945 |
| 3155.0456 | 3155.6654 | 3173.4967 |

Zero-point correction (Hartree): 0.260066

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diC2H5CH3CH_COO.ctpmRR
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E(RM062X/Aug-CC-pVTZ) (Hartree): -504.06664583
Electronic state : 1-A
Cartesian coordinates (Angs):
C -0.206185 0.155820 -0.451018
O -0.245369 -0.568158 -1.469141
O -1.452772 -0.844467 -2.071896
C 1.164207 0.363377 0.129544
C 1.948178 -0.954107 0.184892
C 1.894213 1.447859 -0.674541
H 1.023255 0.723627 1.151369
C 3.285359 -0.815901 0.900349
H 1.335625 -1.700374 0.695451
H 2.097535 -1.318773 -0.831907
H 1.302807 2.359486 -0.745722
H 2.092483 1.087328 -1.684052
H 2.840355 1.699201 -0.199514
H 3.155384 -0.388855 1.896354
H 3.974728 -0.178510 0.348478
H 3.760149 -1.789000 1.014697
C -1.445104 0.728332 0.146789
C -1.836051 -0.152580 1.350728
C -1.267735 2.188019 0.561535
H -2.216454 0.637181 -0.615832
C -2.145120 -1.596495 0.976348
H -1.035913 -0.113128 2.096786
H -2.709330 0.311635 1.812934
H -0.491025 2.310198 1.317523
H -2.202349 2.548945 0.988931
H -1.024389 2.821595 -0.290206
H -1.288293 -2.082235 0.507226
H -2.961037 -1.642135 0.257805
H -2.418974 -2.171134 1.860210
Rotational constants (GHz): 1.2914100 0.7330300 0.7051200
Vibrational harmonic frequencies (cm-1):
40.2098 57.2903 74.2247
104.2929 137.2283 156.8261
197.3796 209.2263 223.7795
230.3017 254.1191 266.0213
289.5822 300.7567 332.8764
367.8905 412.8637 452.8970
538.7802 626.9943 730.1059
734.7258 789.0781 809.0336
854.7275 881.4864 937.8443
978.6890 982.7461 995.5560
1021.0593 1045.8641 1059.2910
1077.2660 1111.5716 1125.4883
1151.1816 1177.8472 1188.0516
1256.7362 1280.6145 1297.6712
1324.8215 1346.5587 1351.9815
1362.9581 1378.4501 1405.2732
1413.4465 1415.9587 1420.3649
1428.0251 1482.4039 1489.4660
1496.6201 1496.7741 1498.8282
1500.2360 1505.0233 1509.2635
1511.1773 1517.5624 1635.2944
3039.8624 3061.7634 3062.7707
3064.9387 3067.4313 3069.7827
3074.4024 3086.5113 3109.6386
3119.8221 3131.8362 3133.2998
3138.8019 3141.2945 3142.7858
3146.1536 3152.6057 3155.4335
Zero-point correction (Hartree): 0.260052

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diC2H5CH3CH_COO.ctppRR
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E(RM062X/Aug-CC-pVTZ) (Hartree): -504.06663714
Electronic state : 1-A
Cartesian coordinates (Angs):
C      -0.211199     -0.513162     -0.206078
O      -0.138005     -1.660965      0.289940
O      -1.286206     -2.405598      0.430965
C       1.098513      0.210427     -0.328773
C       2.057126     -0.144402      0.812433
C       1.705157     -0.091789     -1.708007
H       0.873617      1.278515     -0.276362
C       3.316459      0.712284      0.809729
H       1.532328     -0.020856      1.761725
H       2.317558     -1.200948      0.742773
H       1.002481      0.110208     -2.513833
H       1.993769     -1.141948     -1.759026
H       2.588123      0.522042     -1.873512
H       3.068106      1.775042      0.821882
H       3.934575      0.521522     -0.066548
H       3.923393      0.502455      1.688928
C      -1.538535      0.036471     -0.598470
C      -2.261216      0.468893      0.701563
C      -1.489422      1.147932     -1.640487
H      -2.094327     -0.822109     -0.980302
C      -1.579623      1.612326      1.444861
H      -3.273971      0.760621      0.418668
H      -2.342960     -0.408907      1.340583
H      -1.133256      0.783287     -2.602352
H      -0.860833      1.985846     -1.342022
H      -2.498021      1.533507     -1.788599
H      -1.488191      2.506830      0.827733
H      -0.579868      1.330328      1.781904
H      -2.152391      1.883186      2.330499
Rotational constants (GHz):  1.2863400    0.7522500    0.6949700
Vibrational harmonic frequencies (cm-1):
49.6583      52.9034      76.8233

```

|           |           |           |
|-----------|-----------|-----------|
| 89.5409   | 149.4023  | 170.9262  |
| 202.1424  | 203.1228  | 231.4718  |
| 240.3561  | 268.5827  | 281.0785  |
| 300.8055  | 322.5562  | 352.8639  |
| 361.4601  | 404.4094  | 468.8366  |
| 553.6747  | 629.5455  | 725.0684  |
| 751.9216  | 787.5944  | 801.5571  |
| 840.9191  | 876.3645  | 945.0488  |
| 980.4654  | 985.6230  | 999.3456  |
| 1012.2393 | 1020.1414 | 1057.9327 |
| 1078.9412 | 1106.4225 | 1132.4377 |
| 1148.2509 | 1174.6187 | 1187.0227 |
| 1250.2960 | 1286.3865 | 1295.2666 |
| 1297.9155 | 1343.9246 | 1346.8803 |
| 1364.9892 | 1374.7808 | 1406.3679 |
| 1414.4563 | 1415.5039 | 1418.9140 |
| 1424.6821 | 1488.2129 | 1493.2323 |
| 1498.1658 | 1500.6471 | 1502.4894 |
| 1507.5985 | 1509.2944 | 1511.7824 |
| 1518.1261 | 1519.0229 | 1623.2332 |
| 3057.0582 | 3062.1742 | 3066.7629 |
| 3070.6430 | 3072.9619 | 3074.5900 |
| 3076.7733 | 3083.5267 | 3109.6865 |
| 3112.9629 | 3132.9790 | 3133.4089 |
| 3137.0234 | 3139.4893 | 3141.8116 |
| 3145.5842 | 3150.9258 | 3160.2714 |

Zero-point correction (Hartree): 0.260310

diC2H5CH3CH\_COO.ctptRR  
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E(RM062X/Aug-CC-pVTZ) (Hartree): -504.06675493

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-0.008245	-0.358796	0.309181
O	-0.105244	-1.607344	0.306812
O	1.035337	-2.364957	0.452862
C	-1.305604	0.379557	0.151777
C	-2.187052	-0.260531	-0.927888
C	-2.008903	0.439911	1.516343
H	-1.058113	1.397238	-0.157089
C	-3.448917	0.543842	-1.210942
H	-1.600118	-0.357180	-1.843392
H	-2.445319	-1.273476	-0.617634
H	-1.348097	0.817689	2.295256
H	-2.336370	-0.559429	1.803591
H	-2.876835	1.094209	1.466961
H	-3.207528	1.578801	-1.459631
H	-4.122612	0.552154	-0.355168
H	-3.993692	0.117642	-2.051765
C	1.328191	0.278454	0.437703
C	2.007823	0.148412	-0.946223
C	1.288689	1.717971	0.937660
H	1.885589	-0.363581	1.124069
C	3.474459	0.555643	-0.909219
H	1.922943	-0.890351	-1.263015
H	1.463575	0.771484	-1.662296
H	0.674523	1.825209	1.830905
H	0.909445	2.400482	0.175707
H	2.295017	2.041479	1.195457
H	4.013928	-0.037663	-0.170286
H	3.599782	1.609004	-0.660307
H	3.940494	0.387922	-1.879113

Rotational constants (GHz): 1.4973800 0.6468500 0.5892700

Vibrational harmonic frequencies (cm-1):

35.5519	51.5948	70.5043
85.6128	151.0085	168.5557
192.4268	206.1413	219.4580
232.4659	264.7857	280.2094
297.4484	310.7186	347.7724
353.6026	421.0876	437.5293
543.6808	635.5870	713.1649
774.9763	783.9791	799.3572
849.1487	880.3741	942.5557
973.9567	978.8476	992.8501
1018.7912	1030.1388	1059.9542
1080.8629	1115.2024	1131.6343
1153.3555	1182.7904	1187.2778
1255.2613	1281.4309	1295.7679
1315.9104	1346.1992	1346.9464
1360.1804	1378.4159	1405.4578
1409.6419	1414.6738	1418.0903
1422.5015	1484.3423	1489.7023
1497.9444	1499.7048	1501.0407
1504.2104	1506.3925	1509.6591
1516.4907	1517.7334	1625.5377
3041.8109	3061.2823	3063.7678
3065.2384	3067.9096	3069.9473
3074.8877	3080.0913	3109.5768
3115.5150	3132.3929	3134.6698
3136.6641	3139.4689	3141.5226
3143.0786	3150.7821	3155.2413

Zero-point correction (Hartree): 0.260035

diC2H5CH3CH_COO.cttmRR
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E(RM062X/Aug-CC-pVTZ) (Hartree): -504.06761698

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.208855 | 0.455153  | -0.161975 |
| O | -0.051181 | 1.596229  | -0.655425 |
| O | -1.158090 | 2.343033  | -0.975819 |
| C | 1.056408  | -0.254169 | 0.227283  |

|                                                           |           |           |           |
|-----------------------------------------------------------|-----------|-----------|-----------|
| C                                                         | 2.285925  | 0.310063  | -0.487633 |
| C                                                         | 1.193044  | -0.195788 | 1.757736  |
| H                                                         | 0.937942  | -1.302948 | -0.056048 |
| C                                                         | 3.540206  | -0.520738 | -0.247589 |
| H                                                         | 2.077034  | 0.356631  | -1.557240 |
| H                                                         | 2.447516  | 1.339276  | -0.164450 |
| H                                                         | 0.326533  | -0.623933 | 2.258016  |
| H                                                         | 1.303139  | 0.838833  | 2.084588  |
| H                                                         | 2.070167  | -0.755953 | 2.074786  |
| H                                                         | 3.375480  | -1.566538 | -0.512854 |
| H                                                         | 3.861010  | -0.484697 | 0.792622  |
| H                                                         | 4.364430  | -0.150230 | -0.854806 |
| C                                                         | -1.590450 | -0.059916 | 0.060289  |
| C                                                         | -1.682103 | -1.581122 | 0.138922  |
| C                                                         | -2.184667 | 0.639492  | 1.296688  |
| H                                                         | -2.152613 | 0.306874  | -0.803607 |
| C                                                         | -1.429229 | -2.259640 | -1.203026 |
| H                                                         | -1.001114 | -1.966736 | 0.901713  |
| H                                                         | -2.687011 | -1.830394 | 0.483912  |
| H                                                         | -2.041853 | 1.715536  | 1.226194  |
| H                                                         | -1.731431 | 0.265373  | 2.214343  |
| H                                                         | -3.253485 | 0.435011  | 1.339209  |
| H                                                         | -0.453859 | -1.994667 | -1.614816 |
| H                                                         | -2.179987 | -1.951241 | -1.930636 |
| H                                                         | -1.469416 | -3.344310 | -1.115140 |
| Rotational constants (GHz): 1.2423100 0.7785300 0.6451400 |           |           |           |
| Vibrational harmonic frequencies (cm-1):                  |           |           |           |
| 51.5347                                                   | 76.1987   | 95.7266   |           |
| 137.0018                                                  | 153.8399  | 167.5371  |           |
| 192.0228                                                  | 198.3829  | 220.1306  |           |
| 230.7662                                                  | 248.9704  | 274.8484  |           |
| 290.8231                                                  | 325.5402  | 360.3844  |           |
| 389.4311                                                  | 413.4186  | 445.0036  |           |
| 516.4132                                                  | 637.1352  | 701.8815  |           |
| 750.9442                                                  | 782.7167  | 804.4028  |           |
| 867.1739                                                  | 896.4782  | 949.0487  |           |
| 977.4265                                                  | 985.3137  | 994.3008  |           |
| 1022.7074                                                 | 1034.3636 | 1049.8630 |           |
| 1077.1557                                                 | 1112.2126 | 1131.8153 |           |
| 1155.3003                                                 | 1183.6260 | 1194.6545 |           |
| 1249.4466                                                 | 1277.0720 | 1299.0436 |           |
| 1302.6508                                                 | 1342.8812 | 1350.1722 |           |
| 1367.6533                                                 | 1376.5087 | 1396.3257 |           |
| 1407.4892                                                 | 1415.9910 | 1419.0926 |           |
| 1422.7927                                                 | 1485.8465 | 1491.1875 |           |
| 1497.1579                                                 | 1500.6091 | 1502.1711 |           |
| 1503.8990                                                 | 1509.6398 | 1510.8200 |           |
| 1513.3828                                                 | 1519.2789 | 1617.3943 |           |
| 3054.0860                                                 | 3060.1019 | 3062.3898 |           |
| 3065.3883                                                 | 3067.8187 | 3071.6440 |           |
| 3073.5819                                                 | 3078.0101 | 3094.2227 |           |
| 3109.8456                                                 | 3125.9989 | 3132.9952 |           |
| 3139.6959                                                 | 3140.3256 | 3140.9003 |           |
| 3147.9215                                                 | 3157.7004 | 3162.7296 |           |
| Zero-point correction (Hartree): 0.260304                 |           |           |           |
| diC2H5CH3CH_COO.cttpRR                                    |           |           |           |
| ~~~~~                                                     |           |           |           |
| E(RM062X/Aug-CC-pVTZ) (Hartree): -504.06450120            |           |           |           |
| Electronic state : 1-A                                    |           |           |           |
| Cartesian coordinates (Angs):                             |           |           |           |
| C                                                         | -0.138124 | 0.589701  | -0.150432 |
| O                                                         | 0.120539  | 1.813726  | -0.067224 |
| O                                                         | -0.896990 | 2.726919  | -0.200584 |
| C                                                         | 1.042182  | -0.313849 | 0.063525  |
| C                                                         | 2.349695  | 0.312531  | -0.432064 |
| C                                                         | 1.106820  | -0.673030 | 1.557805  |
| H                                                         | 0.857128  | -1.227054 | -0.505303 |
| C                                                         | 3.525795  | -0.652774 | -0.358368 |
| H                                                         | 2.210023  | 0.643467  | -1.462380 |
| H                                                         | 2.560389  | 1.208422  | 0.152390  |
| H                                                         | 0.151809  | -1.039727 | 1.930289  |
| H                                                         | 1.380456  | 0.211020  | 2.134562  |
| H                                                         | 1.852404  | -1.447423 | 1.728000  |
| H                                                         | 3.305679  | -1.582018 | -0.886923 |
| H                                                         | 3.779917  | -0.903672 | 0.670645  |
| H                                                         | 4.410698  | -0.212233 | -0.814703 |
| C                                                         | -1.541364 | 0.160144  | -0.413456 |
| C                                                         | -1.696417 | -1.226193 | -1.049921 |
| C                                                         | -2.382632 | 0.347792  | 0.861424  |
| H                                                         | -1.895608 | 0.920160  | -1.117004 |
| C                                                         | -1.621984 | -2.424738 | -0.108376 |
| H                                                         | -2.675447 | -1.234431 | -1.532835 |
| H                                                         | -0.968801 | -1.338541 | -1.856922 |
| H                                                         | -2.312824 | 1.380155  | 1.194421  |
| H                                                         | -2.054401 | -0.315215 | 1.660649  |
| H                                                         | -3.424340 | 0.117391  | 0.637260  |
| H                                                         | -2.410324 | -2.384339 | 0.642155  |
| H                                                         | -0.669163 | -2.488574 | 0.416011  |
| H                                                         | -1.749799 | -3.350048 | -0.668673 |
| Rotational constants (GHz): 1.2506500 0.8267100 0.6002000 |           |           |           |
| Vibrational harmonic frequencies (cm-1):                  |           |           |           |
| 47.5667                                                   | 77.2874   | 97.5197   |           |
| 122.4614                                                  | 166.5539  | 173.4492  |           |
| 198.7410                                                  | 222.1504  | 234.6688  |           |
| 249.8019                                                  | 260.4136  | 280.1934  |           |
| 305.1310                                                  | 316.6901  | 336.3488  |           |
| 372.1050                                                  | 400.8699  | 465.8072  |           |
| 573.2753                                                  | 637.3118  | 711.3432  |           |
| 742.9904                                                  | 783.1279  | 797.8806  |           |
| 863.0812                                                  | 890.5749  | 947.4898  |           |
| 969.7151                                                  | 983.7716  | 995.8907  |           |

|           |           |           |
|-----------|-----------|-----------|
| 999.5385  | 1029.6984 | 1057.5334 |
| 1084.4734 | 1121.0839 | 1142.7951 |
| 1149.4054 | 1167.3520 | 1187.4754 |
| 1251.6290 | 1296.7282 | 1299.4830 |
| 1314.7630 | 1346.7424 | 1352.6415 |
| 1370.6924 | 1377.8448 | 1396.2309 |
| 1405.4448 | 1415.5330 | 1418.9602 |
| 1423.9566 | 1487.4863 | 1492.1209 |
| 1495.4999 | 1498.6908 | 1502.0398 |
| 1509.5899 | 1511.7527 | 1513.3775 |
| 1519.7493 | 1522.2440 | 1614.8036 |
| 3047.8137 | 3061.1947 | 3061.3707 |
| 3067.4764 | 3069.8240 | 3073.7146 |
| 3075.0332 | 3084.8386 | 3092.6480 |
| 3111.7066 | 3133.1260 | 3135.4820 |
| 3139.1834 | 3140.6625 | 3144.1413 |
| 3147.3286 | 3154.1499 | 3165.6247 |

Zero-point correction (Hartree): 0.260638

diC2H5CH3CH\_COO.ctttRR

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E(RM062X/Aug-CC-pVT2) (Hartree): -504.06736976

Electronic state : 1-A

Cartesian coordinates (Angs):

C	0.045278	0.516110	-0.149306
O	0.390574	1.716314	-0.251436
O	-0.581128	2.681557	-0.357863
C	1.167266	-0.466052	0.015860
C	2.516530	0.103873	-0.425088
C	1.186090	-0.938506	1.479236
H	0.926798	-1.328357	-0.612577
C	3.626684	-0.939511	-0.420134
H	2.409467	0.520822	-1.427137
H	2.781474	0.938846	0.224976
H	0.219769	-1.327749	1.793880
H	1.450296	-0.107330	2.134138
H	1.921672	-1.729733	1.607381
H	3.349572	-1.811196	-1.015628
H	3.860194	-1.281472	0.587248
H	4.540508	-0.525574	-0.843050
C	-1.403737	0.168830	-0.154284
C	-1.687607	-1.281757	-0.542823
C	-2.010858	0.566607	1.205045
H	-1.834570	0.848541	-0.896272
C	-3.181054	-1.564129	-0.657198
H	-1.210423	-1.496421	-1.501600
H	-1.245180	-1.963500	0.187997
H	-1.664563	1.556506	1.493063
H	-1.745542	-0.159206	1.974664
H	-3.095425	0.600463	1.127007
H	-3.657285	-0.855953	-1.336676
H	-3.677167	-1.486306	0.309060
H	-3.356726	-2.568143	-1.039934

Rotational constants (GHz): 1.3933700 0.7024900 0.5587100

Vibrational harmonic frequencies (cm-1):

59.3574	82.1851	95.0189
117.3165	138.2628	167.7879
182.2794	210.0852	216.2953
250.0979	274.9205	287.8757
304.1406	320.2544	341.5427
374.8833	414.3661	437.6101
538.7075	642.2464	701.2440
756.5613	785.8701	806.0294
866.8645	907.0043	949.1863
975.2774	982.1441	988.8621
995.1601	1032.4065	1064.2410
1080.8301	1120.6997	1144.3778
1152.8534	1184.3967	1194.3234
1253.6496	1288.4579	1294.0897
1319.2483	1335.1464	1342.7474
1351.0891	1384.6022	1399.3842
1408.9739	1414.3904	1417.2851
1425.2967	1485.0674	1488.7426
1494.7404	1498.8898	1502.5891
1504.0697	1510.7890	1512.1250
1518.0364	1524.8812	1618.6208
3047.6356	3054.6548	3059.9520
3062.3061	3065.8169	3069.1552
3072.3655	3075.9845	3090.6595
3109.4014	3132.9074	3134.4317
3141.1453	3141.7541	3146.1506
3148.9321	3159.0307	3163.9349

Zero-point correction (Hartree): 0.260423

diC2H5CH3CH_COO.mmmmmRR

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E(RM062X/Aug-CC-pVT2) (Hartree): -504.06578129

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.019154 | -0.181933 | -0.303734 |
| O | 0.231128  | -0.711588 | -1.406911 |
| O | 1.390123  | -0.392303 | -2.073529 |
| C | -1.299320 | -0.638099 | 0.341406  |
| C | -2.444974 | 0.352511  | 0.049800  |
| C | -1.691609 | -2.046688 | -0.093072 |
| H | -1.111561 | -0.626048 | 1.419580  |
| C | -2.273328 | 1.747128  | 0.637253  |
| H | -2.575275 | 0.409432  | -1.033301 |
| H | -3.355725 | -0.096898 | 0.449554  |
| H | -0.879665 | -2.754385 | 0.067748  |
| H | -1.946731 | -2.066462 | -1.151342 |
| H | -2.558458 | -2.376106 | 0.477697  |



|                                                           |           |           |           |
|-----------------------------------------------------------|-----------|-----------|-----------|
| H                                                         | -1.434509 | 2.279734  | 0.192045  |
| H                                                         | -2.107538 | 1.699557  | 1.714787  |
| H                                                         | -3.168056 | 2.343486  | 0.465170  |
| C                                                         | 0.904224  | 0.787988  | 0.361267  |
| C                                                         | 2.166375  | 0.045101  | 0.842874  |
| C                                                         | 1.268873  | 2.002462  | -0.501087 |
| H                                                         | 0.367727  | 1.134127  | 1.247817  |
| C                                                         | 1.864415  | -1.112693 | 1.785892  |
| H                                                         | 2.703991  | -0.305982 | -0.035926 |
| H                                                         | 2.793547  | 0.784352  | 1.344706  |
| H                                                         | 1.644345  | 2.790417  | 0.152004  |
| H                                                         | 0.410050  | 2.392541  | -1.046739 |
| H                                                         | 2.026249  | 1.734355  | -1.229232 |
| H                                                         | 1.293788  | -1.895971 | 1.282247  |
| H                                                         | 1.290409  | -0.781989 | 2.653923  |
| H                                                         | 2.784394  | -1.567685 | 2.149185  |
| Rotational constants (GHz): 1.2089900 0.8235000 0.7650200 |           |           |           |
| Vibrational harmonic frequencies (cm-1):                  |           |           |           |
| 37.9801                                                   | 61.1551   | 98.4315   |           |
| 104.8910                                                  | 143.0911  | 181.3798  |           |
| 188.3519                                                  | 229.3542  | 241.8730  |           |
| 261.1398                                                  | 264.1804  | 272.7893  |           |
| 274.4257                                                  | 280.5496  | 334.4657  |           |
| 389.0374                                                  | 398.3789  | 448.1845  |           |
| 497.5400                                                  | 620.9143  | 723.8110  |           |
| 746.7912                                                  | 803.8729  | 826.3203  |           |
| 845.7935                                                  | 877.6799  | 958.7766  |           |
| 979.1451                                                  | 987.4998  | 1021.1347 |           |
| 1035.1623                                                 | 1043.6978 | 1056.9874 |           |
| 1099.7974                                                 | 1112.2398 | 1135.3957 |           |
| 1151.3951                                                 | 1163.4087 | 1183.1280 |           |
| 1221.9681                                                 | 1277.3284 | 1289.4283 |           |
| 1321.7995                                                 | 1326.6996 | 1357.2265 |           |
| 1364.2166                                                 | 1391.4603 | 1406.1371 |           |
| 1414.5164                                                 | 1417.2078 | 1418.8691 |           |
| 1441.8182                                                 | 1482.0782 | 1489.4826 |           |
| 1492.4238                                                 | 1497.9446 | 1500.6773 |           |
| 1503.1043                                                 | 1506.3077 | 1509.8582 |           |
| 1511.3324                                                 | 1515.3734 | 1646.0333 |           |
| 3047.6383                                                 | 3050.3101 | 3061.2240 |           |
| 3065.8523                                                 | 3069.0613 | 3070.9469 |           |
| 3073.3808                                                 | 3074.1195 | 3100.2536 |           |
| 3106.1287                                                 | 3132.6892 | 3134.2492 |           |
| 3135.6278                                                 | 3141.5463 | 3147.2335 |           |
| 3150.2783                                                 | 3151.7124 | 3186.7181 |           |
| Zero-point correction (Hartree): 0.260354                 |           |           |           |
| dic2H5CH3CH_COO.mmmppRR                                   |           |           |           |
| ~~~~~                                                     |           |           |           |
| E (RM062X/Aug-CC-pVTZ) (Hartree): -504.06291171           |           |           |           |
| Electronic state : 1-A                                    |           |           |           |
| Cartesian coordinates (Angs):                             |           |           |           |
| C                                                         | -0.115079 | -0.115340 | -0.158423 |
| O                                                         | 0.061010  | -0.500285 | -1.331853 |
| O                                                         | 1.180622  | -0.119826 | -2.033731 |
| C                                                         | -1.365452 | -0.651782 | 0.489545  |
| C                                                         | -2.583368 | 0.155640  | 0.008588  |
| C                                                         | -1.549464 | -2.142698 | 0.217093  |
| H                                                         | -1.250834 | -0.490005 | 1.564395  |
| C                                                         | -2.485443 | 1.650768  | 0.282088  |
| H                                                         | -2.701309 | -0.023094 | -1.062257 |
| H                                                         | -3.466384 | -0.256828 | 0.499844  |
| H                                                         | -0.682973 | -2.715115 | 0.547420  |
| H                                                         | -1.687678 | -2.321753 | -0.847730 |
| H                                                         | -2.427745 | -2.508569 | 0.747405  |
| H                                                         | -1.649805 | 2.101948  | -0.255612 |
| H                                                         | -2.345551 | 1.847849  | 1.346340  |
| H                                                         | -3.392726 | 2.162046  | -0.034919 |
| C                                                         | 0.805250  | 0.781856  | 0.605239  |
| C                                                         | 1.802032  | -0.104262 | 1.389811  |
| C                                                         | 1.479361  | 1.913802  | -0.168977 |
| H                                                         | 0.155388  | 1.237890  | 1.357359  |
| C                                                         | 2.703906  | -0.974788 | 0.523832  |
| H                                                         | 2.401382  | 0.571281  | 2.003976  |
| H                                                         | 1.239941  | -0.736537 | 2.082657  |
| H                                                         | 1.809497  | 2.664300  | 0.550984  |
| H                                                         | 0.789578  | 2.385178  | -0.867391 |
| H                                                         | 2.324833  | 1.560663  | -0.746629 |
| H                                                         | 3.302176  | -0.377175 | -0.159641 |
| H                                                         | 2.123180  | -1.664178 | -0.089216 |
| H                                                         | 3.375507  | -1.556194 | 1.154911  |
| Rotational constants (GHz): 1.3799500 0.7981200 0.7236200 |           |           |           |
| Vibrational harmonic frequencies (cm-1):                  |           |           |           |
| 34.4789                                                   | 70.0253   | 106.2622  |           |
| 111.6608                                                  | 160.8789  | 178.7102  |           |
| 196.4013                                                  | 229.1996  | 235.2115  |           |
| 241.5037                                                  | 254.4223  | 278.3459  |           |
| 287.1230                                                  | 306.6932  | 327.3511  |           |
| 360.9022                                                  | 399.3028  | 489.6736  |           |
| 509.2938                                                  | 628.2991  | 716.6654  |           |
| 764.1366                                                  | 790.4712  | 814.0276  |           |
| 846.0900                                                  | 873.4165  | 950.5087  |           |
| 980.6759                                                  | 989.8616  | 1009.4897 |           |
| 1030.7277                                                 | 1036.7710 | 1046.2585 |           |
| 1104.6127                                                 | 1124.7196 | 1132.0050 |           |
| 1143.1755                                                 | 1160.3456 | 1192.9228 |           |
| 1229.9662                                                 | 1277.1405 | 1288.1828 |           |
| 1312.7487                                                 | 1323.5341 | 1364.2830 |           |
| 1374.0613                                                 | 1392.5932 | 1413.3655 |           |
| 1417.1408                                                 | 1419.4287 | 1431.4155 |           |
| 1442.8931                                                 | 1478.7398 | 1485.1892 |           |
| 1488.7209                                                 | 1493.2526 | 1498.1813 |           |

|           |           |           |
|-----------|-----------|-----------|
| 1500.2539 | 1503.5270 | 1505.8064 |
| 1507.8939 | 1510.5452 | 1652.9655 |
| 3044.3175 | 3054.1843 | 3056.5491 |
| 3060.5635 | 3067.3644 | 3068.9629 |
| 3069.7810 | 3072.2602 | 3086.6050 |
| 3100.4719 | 3125.3000 | 3134.5835 |
| 3136.4838 | 3138.8918 | 3140.6911 |
| 3152.1849 | 3159.2931 | 3198.4564 |

Zero-point correction (Hartree): 0.260375

diC2H5CH3CH\_COO.mmmtrR  
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E(RM062X/Aug-CC-pVTZ) (Hartree): -504.06499331

Electronic state : 1-A

Cartesian coordinates (Angs):

C	0.263183	-0.407609	0.062529
O	0.291479	-1.452709	0.745416
O	-0.815648	-1.816784	1.476157
C	1.512785	-0.124531	-0.723972
C	2.447906	0.809055	0.070479
C	2.246075	-1.401274	-1.123154
H	1.188392	0.409393	-1.622653
C	1.874969	2.181159	0.399739
H	2.737934	0.291004	0.987407
H	3.356086	0.926556	-0.523360
H	1.589539	-2.086438	-1.657115
H	2.624860	-1.918130	-0.243030
H	3.088583	-1.152945	-1.766978
H	1.020472	2.115792	1.072643
H	1.551714	2.698872	-0.504884
H	2.627632	2.800160	0.885491
C	-0.939639	0.470743	-0.028076
C	-1.973601	-0.246321	-0.923742
C	-1.522429	0.897508	1.325945
H	-0.609000	1.363941	-0.563361
C	-3.193817	0.626003	-1.185724
H	-1.501076	-0.507289	-1.874337
H	-2.256628	-1.174709	-0.428569
H	-2.032224	1.853600	1.210175
H	-0.745115	1.014380	2.080167
H	-2.216990	0.150486	1.695835
H	-2.907720	1.581125	-1.630216
H	-3.735756	0.832424	-0.263841
H	-3.879937	0.129321	-1.870110

Rotational constants (GHz): 1.3217100 0.7511000 0.6608100

Vibrational harmonic frequencies (cm-1):

38.0864	75.9227	108.6865
116.2816	146.8114	182.3232
187.0031	228.2936	241.7953
256.6889	266.0354	283.2273
286.3306	296.7609	324.7490
375.4859	424.5193	441.2479
512.6313	624.8578	722.4800
775.4283	800.9454	824.1218
847.9944	881.8187	956.4639
978.0512	986.2965	1001.6005
1031.8303	1046.5743	1064.1315
1108.4734	1113.4496	1128.0178
1146.3510	1165.1440	1186.3924
1224.5255	1277.3818	1289.8599
1322.1750	1339.4729	1359.9790
1361.4973	1389.4458	1411.7594
1414.0169	1417.9169	1419.5440
1437.8844	1486.3454	1489.7815
1494.1178	1499.5947	1503.0167
1505.9268	1507.6029	1508.8016
1511.9145	1513.3886	1648.2859
3046.8782	3053.7648	3059.6528
3060.2782	3063.2927	3068.4709
3072.9743	3075.0652	3100.1718
3116.3668	3131.6151	3134.3790
3136.5315	3143.2777	3144.3626
3146.8162	3151.5051	3182.3250

Zero-point correction (Hartree): 0.260634

diC2H5CH3CH_COO.mmprrR
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E(RM062X/Aug-CC-pVTZ) (Hartree): -504.06091850

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.011645 | 0.715176  | -0.160168 |
| O | 0.058254  | 1.741313  | 0.557650  |
| O | 1.271447  | 2.346718  | 0.761993  |
| C | -1.419760 | 0.209365  | -0.357074 |
| C | -1.845970 | -0.778001 | 0.761675  |
| C | -2.401927 | 1.380611  | -0.442328 |
| H | -1.435281 | -0.330045 | -1.304259 |
| C | -1.701986 | -2.246835 | 0.386363  |
| H | -1.295377 | -0.553609 | 1.676961  |
| H | -2.893756 | -0.575229 | 0.987377  |
| H | -2.092911 | 2.110266  | -1.189227 |
| H | -2.474455 | 1.890113  | 0.516810  |
| H | -3.387830 | 1.003023  | -0.709650 |
| H | -0.670904 | -2.511812 | 0.162388  |
| H | -2.305606 | -2.475315 | -0.493089 |
| H | -2.038555 | -2.889060 | 1.199452  |
| C | 1.232928  | 0.178011  | -0.786877 |
| C | 2.221873  | -0.380123 | 0.263600  |
| C | 0.975388  | -0.797483 | -1.928816 |
| H | 1.716490  | 1.086107  | -1.167022 |
| C | 1.770011  | -1.650420 | 0.969183  |
| H | 3.156710  | -0.569818 | -0.267058 |

|                                                           |           |           |           |
|-----------------------------------------------------------|-----------|-----------|-----------|
| H                                                         | 2.414973  | 0.406634  | 0.987743  |
| H                                                         | 0.445398  | -1.690625 | -1.599520 |
| H                                                         | 1.930109  | -1.114384 | -2.347507 |
| H                                                         | 0.396138  | -0.339100 | -2.730029 |
| H                                                         | 1.605332  | -2.474667 | 0.274251  |
| H                                                         | 0.848973  | -1.486966 | 1.530968  |
| H                                                         | 2.529473  | -1.971573 | 1.680910  |
| Rotational constants (GHz): 1.1288300 0.9656000 0.6987900 |           |           |           |
| Vibrational harmonic frequencies (cm-1):                  |           |           |           |
| 42.6238                                                   | 51.2138   | 109.7113  |           |
| 134.9488                                                  | 176.2464  | 198.1421  |           |
| 216.6854                                                  | 235.5859  | 257.3782  |           |
| 273.1565                                                  | 283.3190  | 301.9280  |           |
| 305.3497                                                  | 323.3883  | 353.5313  |           |
| 383.0349                                                  | 403.4689  | 479.9708  |           |
| 521.3484                                                  | 628.4183  | 679.1949  |           |
| 743.5016                                                  | 785.3273  | 812.0379  |           |
| 841.0824                                                  | 872.6872  | 960.1358  |           |
| 984.5821                                                  | 990.8255  | 1015.8723 |           |
| 1022.9384                                                 | 1038.4262 | 1056.3372 |           |
| 1084.8561                                                 | 1126.3903 | 1134.1910 |           |
| 1143.7540                                                 | 1169.1579 | 1183.6750 |           |
| 1246.1407                                                 | 1276.3352 | 1292.5131 |           |
| 1296.5564                                                 | 1323.1244 | 1362.5522 |           |
| 1370.3106                                                 | 1376.3744 | 1408.6881 |           |
| 1412.9409                                                 | 1413.4389 | 1416.3770 |           |
| 1420.4549                                                 | 1489.8224 | 1494.4674 |           |
| 1498.6969                                                 | 1501.3824 | 1502.7740 |           |
| 1508.2634                                                 | 1509.7552 | 1511.2568 |           |
| 1517.1783                                                 | 1519.3888 | 1608.1170 |           |
| 3029.3938                                                 | 3059.8536 | 3066.3872 |           |
| 3068.9588                                                 | 3069.4961 | 3071.6946 |           |
| 3073.4013                                                 | 3097.5713 | 3104.6257 |           |
| 3122.3157                                                 | 3132.1051 | 3132.4875 |           |
| 3136.1332                                                 | 3143.6054 | 3145.9962 |           |
| 3154.1958                                                 | 3156.7629 | 3161.1724 |           |
| Zero-point correction (Hartree): 0.260913                 |           |           |           |
| dic2H5CH3CH_COO.mpmRR                                     |           |           |           |
| ~~~~~                                                     |           |           |           |
| E(RM062X/Aug-CC-pVTZ) (Hartree): -504.06910758            |           |           |           |
| Electronic state : 1-A                                    |           |           |           |
| Cartesian coordinates (Angs):                             |           |           |           |
| C                                                         | -0.014426 | -0.202563 | 0.067263  |
| O                                                         | -0.144260 | -0.599940 | 1.244228  |
| O                                                         | -1.215311 | -0.166238 | 1.989158  |
| C                                                         | 1.186646  | -0.718149 | -0.668272 |
| C                                                         | 2.149115  | 0.455869  | -0.952694 |
| C                                                         | 1.869775  | -1.880632 | 0.038413  |
| H                                                         | 0.805429  | -1.058576 | -1.637002 |
| C                                                         | 2.775456  | 1.049099  | 0.304102  |
| H                                                         | 2.928944  | 0.085872  | -1.620131 |
| H                                                         | 1.615274  | 1.233273  | -1.502427 |
| H                                                         | 1.189953  | -2.723960 | 0.146562  |
| H                                                         | 2.203957  | -1.599467 | 1.034555  |
| H                                                         | 2.734849  | -2.202167 | -0.540880 |
| H                                                         | 3.437399  | 0.336875  | 0.794098  |
| H                                                         | 2.014718  | 1.346224  | 1.028173  |
| H                                                         | 3.363863  | 1.931276  | 0.056556  |
| C                                                         | -0.961063 | 0.757659  | -0.579867 |
| C                                                         | -2.420787 | 0.270528  | -0.573003 |
| C                                                         | -0.825358 | 2.146582  | 0.060103  |
| H                                                         | -0.638097 | 0.818890  | -1.622432 |
| C                                                         | -2.555756 | -1.219839 | -0.852040 |
| H                                                         | -2.864209 | 0.504003  | 0.390430  |
| H                                                         | -2.942726 | 0.849242  | -1.338322 |
| H                                                         | 0.171351  | 2.562950  | -0.085556 |
| H                                                         | -1.037390 | 2.079531  | 1.124895  |
| H                                                         | -1.545902 | 2.819218  | -0.404727 |
| H                                                         | -2.140398 | -1.796850 | -0.024130 |
| H                                                         | -2.040630 | -1.504164 | -1.772997 |
| H                                                         | -3.601426 | -1.504068 | -0.957794 |
| Rotational constants (GHz): 1.4593500 0.7931700 0.7234200 |           |           |           |
| Vibrational harmonic frequencies (cm-1):                  |           |           |           |
| 57.4834                                                   | 64.8276   | 91.9876   |           |
| 120.4861                                                  | 169.0162  | 198.9847  |           |
| 207.4654                                                  | 215.3200  | 228.4296  |           |
| 249.3244                                                  | 263.0186  | 282.4083  |           |
| 295.5687                                                  | 303.2854  | 356.2881  |           |
| 382.8073                                                  | 430.3277  | 456.2569  |           |
| 515.3936                                                  | 619.9349  | 730.3860  |           |
| 749.3006                                                  | 798.3958  | 818.6063  |           |
| 833.4897                                                  | 883.7694  | 960.3590  |           |
| 981.0393                                                  | 991.2349  | 1005.3372 |           |
| 1027.2221                                                 | 1031.5959 | 1037.4543 |           |
| 1097.4949                                                 | 1123.4956 | 1128.2716 |           |
| 1144.0075                                                 | 1158.1507 | 1195.0360 |           |
| 1228.9063                                                 | 1279.0750 | 1297.7124 |           |
| 1302.5173                                                 | 1321.5666 | 1371.2093 |           |
| 1374.6753                                                 | 1382.3538 | 1393.1814 |           |
| 1410.2821                                                 | 1420.8912 | 1423.3441 |           |
| 1440.4209                                                 | 1483.8034 | 1486.4558 |           |
| 1493.9860                                                 | 1496.8972 | 1497.9260 |           |
| 1502.5104                                                 | 1506.0524 | 1514.1957 |           |
| 1517.7002                                                 | 1518.7845 | 1647.4789 |           |
| 3039.5135                                                 | 3046.7910 | 3056.6958 |           |
| 3064.2237                                                 | 3065.7958 | 3066.7917 |           |
| 3069.9486                                                 | 3076.1927 | 3101.5424 |           |
| 3111.2084                                                 | 3132.0306 | 3134.9229 |           |
| 3136.8546                                                 | 3143.6577 | 3146.3414 |           |
| 3158.6389                                                 | 3160.9505 | 3162.7688 |           |
| Zero-point correction (Hartree): 0.260600                 |           |           |           |

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dic2H5CH3CH_COO.mpmtrr
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E(RM062X/Aug-CC-pVTZ) (Hartree): -504.06671301
Electronic state : 1-A
Cartesian coordinates (Angs):
C 0.179910 -0.357524 -0.113732
O 0.310322 -1.361236 0.617864
O -0.700996 -1.724003 1.478130
C 1.356539 -0.021406 -0.980042
C 1.997341 1.283629 -0.454315
C 2.360762 -1.158561 -1.105417
H 0.938247 0.204617 -1.966525
C 2.654719 1.134638 0.912905
H 2.734965 1.606250 -1.190823
H 1.236973 2.065921 -0.413656
H 1.901957 -2.035897 -1.557733
H 2.747312 -1.455701 -0.133303
H 3.195864 -0.841153 -1.729381
H 3.514286 0.467600 0.872078
H 1.958356 0.732104 1.650509
H 3.003000 2.101034 1.273937
C -1.049609 0.490389 -0.136657
C -2.238754 -0.325839 -0.679879
C -1.319830 1.142716 1.224931
H -0.844607 1.285691 -0.858775
C -3.489552 0.527666 -0.844274
H -1.956956 -0.744704 -1.649258
H -2.420624 -1.159243 -0.005074
H -0.420565 1.624012 1.611812
H -1.647684 0.396554 1.942286
H -2.082116 1.911411 1.110629
H -3.289440 1.416181 -1.446645
H -3.877202 0.854225 0.119554
H -4.275517 -0.041233 -1.338706
Rotational constants (GHz): 1.5405400 0.6903300 0.6499300
Vibrational harmonic frequencies (cm-1):
50.3149 62.2174 69.4114
104.5602 133.8302 181.4293
192.7336 205.7663 221.0755
242.1175 268.6161 287.4712
294.7540 305.5365 321.4532
373.4157 424.9473 467.9226
519.1238 622.9181 731.8012
770.5611 799.1910 813.8625
833.2626 878.0111 953.6973
974.1087 988.3237 998.6436
1009.5945 1028.2496 1058.1414
1102.0546 1121.1906 1127.9255
1143.8507 1154.9436 1191.8810
1227.3723 1278.3160 1293.1966
1301.4554 1343.0550 1360.8545
1374.4891 1382.8841 1397.1948
1412.7575 1420.7116 1423.9887
1440.5053 1487.2908 1490.8791
1496.2562 1497.4509 1501.5675
1505.4083 1507.8737 1513.8735
1516.6960 1519.8037 1648.2519
3040.5511 3052.5236 3055.9028
3058.1821 3064.4674 3067.9017
3069.8894 3075.4904 3100.3406
3120.8591 3132.4602 3133.7120
3141.2730 3143.4961 3145.7755
3147.4121 3161.3611 3177.5651
Zero-point correction (Hartree): 0.260304

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dic2H5CH3CH_COO.mppmrr
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E(RM062X/Aug-CC-pVTZ) (Hartree): -504.06710595
Electronic state : 1-A
Cartesian coordinates (Angs):
C     -0.053037      0.551307      -0.374292
O      0.022163      1.639257      0.242826
O      1.245875      2.207258      0.490277
C     -1.450803      0.055514      -0.624577
C     -1.695182      -1.310456      0.049997
C     -2.511426      1.081096      -0.239095
H     -1.508254      -0.115396      -1.704037
C     -1.598891      -1.276838      1.569959
H     -2.690849      -1.640745      -0.251251
H     -0.995964      -2.045710      -0.347658
H     -2.388768      2.004685      -0.801045
H     -2.457616      1.333352      0.817633
H     -3.499588      0.673126      -0.449223
H     -2.358025      -0.628449      2.004685
H     -0.624071      -0.914843      1.899286
H     -1.739883      -2.274556      1.983104
C      1.185988      -0.125522      -0.865476
C      1.761418      -1.096934      0.188998
C      0.963993      -0.840032      -2.197842
H      1.906111      0.686134      -0.987085
C      2.204165      -0.448694      1.493865
H      1.032009      -1.885623      0.387275
H      2.615378      -1.587231      -0.283265
H      0.557324      -0.169343      -2.954289
H      0.294165      -1.694782      -2.099968
H      1.920269      -1.211658      -2.562959
H      1.391640      0.092244      1.977364
H      2.991777      0.280050      1.315986
H      2.572695      -1.210019      2.181397
Rotational constants (GHz):      1.2061800      0.8784100      0.8050600
Vibrational harmonic frequencies (cm-1):

```

|           |           |           |
|-----------|-----------|-----------|
| 61.6493   | 108.9410  | 130.0592  |
| 143.8075  | 160.9913  | 210.9839  |
| 220.2059  | 229.5410  | 248.8599  |
| 258.3658  | 280.8776  | 285.9015  |
| 293.9246  | 304.7212  | 343.5393  |
| 360.8317  | 433.8238  | 498.8893  |
| 557.8217  | 599.3833  | 674.0502  |
| 740.4970  | 786.8505  | 821.1451  |
| 841.3153  | 877.5918  | 958.5311  |
| 982.6979  | 989.0995  | 1002.1023 |
| 1027.2036 | 1030.4040 | 1056.2592 |
| 1077.5622 | 1100.8116 | 1139.2405 |
| 1155.5105 | 1178.8168 | 1181.4470 |
| 1263.0466 | 1277.0466 | 1296.7351 |
| 1303.8616 | 1320.2318 | 1366.8035 |
| 1371.0440 | 1375.9673 | 1412.5524 |
| 1418.2445 | 1421.4875 | 1422.6412 |
| 1429.7868 | 1481.3909 | 1490.3290 |
| 1493.8508 | 1497.9406 | 1499.8074 |
| 1502.7316 | 1506.3872 | 1509.5832 |
| 1512.6220 | 1517.0609 | 1615.6383 |
| 3052.8884 | 3058.0089 | 3065.3799 |
| 3070.3620 | 3072.2271 | 3075.9982 |
| 3077.7693 | 3079.8654 | 3096.1879 |
| 3114.2582 | 3136.5505 | 3137.8101 |
| 3140.5075 | 3142.1333 | 3145.2770 |
| 3149.6790 | 3155.1277 | 3160.6699 |

Zero-point correction (Hartree): 0.261059

diC2H5CH3CH\_COO.mpppRR

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E(RM062X/Aug-CC-pVTZ) (Hartree): -504.06645537

Electronic state : 1-A

Cartesian coordinates (Angs):

C	0.108232	0.670762	0.228860
O	0.374588	1.569782	-0.604397
O	-0.645302	2.316170	-1.137557
C	1.301070	-0.050032	0.791656
C	1.395156	-1.478518	0.214998
C	2.598205	0.729184	0.600375
H	1.107491	-0.153745	1.861860
C	1.727015	-1.515651	-1.272392
H	2.165498	-2.005957	0.780252
H	0.459789	-2.006071	0.400968
H	2.547247	1.699965	1.089991
H	2.807917	0.903365	-0.452222
H	3.425230	0.164664	1.030393
H	2.746173	-1.181999	-1.460741
H	1.059414	-0.872827	-1.849036
H	1.633276	-2.529491	-1.659313
C	-1.310204	0.449332	0.636738
C	-2.175059	-0.138865	-0.505015
C	-1.462306	-0.314243	1.947751
H	-1.679932	1.474364	0.756306
C	-1.950607	-1.611725	-0.822914
H	-3.212360	0.005939	-0.197614
H	-2.019481	0.472961	-1.390495
H	-1.006180	0.221332	2.779722
H	-1.024556	-1.310977	1.907607
H	-2.523029	-0.430176	2.169313
H	-2.055499	-2.246810	0.057870
H	-0.966998	-1.788327	-1.256677
H	-2.687297	-1.945283	-1.552897

Rotational constants (GHz): 1.2023600 0.9053600 0.7619500

Vibrational harmonic frequencies (cm-1):

53.3079	65.2643	114.2691
140.3738	184.0612	203.4539
225.0038	228.8245	241.5088
270.7033	291.8757	298.5588
303.8076	308.4583	344.9443
379.0397	452.1633	483.0020
551.4345	620.6378	669.5733
747.3122	788.5507	819.5123
832.5169	871.1832	957.4289
982.1532	990.2253	1004.3718
1015.7269	1025.3504	1029.6758
1085.7730	1113.0063	1131.2150
1151.4762	1174.4263	1185.4215
1254.8203	1276.5169	1287.6693
1302.4885	1306.0671	1360.4568
1372.7154	1379.2924	1414.7202
1416.6035	1418.8300	1421.4682
1423.7696	1487.1613	1494.2884
1495.3675	1501.1149	1503.4204
1505.5224	1509.6806	1517.3818
1518.4794	1520.7412	1610.6422
3036.4092	3063.8576	3065.3508
3069.8994	3070.3565	3072.0363
3075.7657	3079.1273	3115.3616
3123.5046	3131.7529	3136.8260
3138.5304	3142.4540	3145.4476
3146.9140	3150.5408	3163.1270

Zero-point correction (Hartree): 0.260992

diC2H5CH3CH_COO.mpptRR

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E(RM062X/Aug-CC-pVTZ) (Hartree): -504.06945277

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |          |           |
|---|-----------|----------|-----------|
| C | -0.242678 | 0.494442 | -0.413588 |
| O | -0.402999 | 1.619132 | 0.116817  |
| O | 0.708051  | 2.352417 | 0.461447  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -1.494502 | -0.279186 | -0.694492 |
| C | -1.604553 | -1.441692 | 0.320285  |
| C | -2.742117 | 0.596228  | -0.708801 |
| H | -1.364008 | -0.731111 | -1.680661 |
| C | -1.761482 | -0.988556 | 1.766685  |
| H | -2.461538 | -2.048459 | 0.022544  |
| H | -0.725839 | -2.081825 | 0.232515  |
| H | -2.674230 | 1.359913  | -1.481530 |
| H | -2.884653 | 1.104090  | 0.241952  |
| H | -3.616713 | -0.022571 | -0.907274 |
| H | -2.685803 | -0.432465 | 1.914764  |
| H | -0.934637 | -0.348210 | 2.076817  |
| H | -1.783499 | -1.850245 | 2.432080  |
| C | 1.138390  | 0.001610  | -0.663365 |
| C | 1.760771  | -0.429293 | 0.686734  |
| C | 1.227436  | -1.081657 | -1.731232 |
| H | 1.684011  | 0.896871  | -0.976240 |
| C | 3.282130  | -0.404097 | 0.640858  |
| H | 1.422469  | 0.258171  | 1.461057  |
| H | 1.400987  | -1.430858 | 0.936574  |
| H | 0.819788  | -0.742535 | -2.683388 |
| H | 0.702426  | -1.991197 | -1.438073 |
| H | 2.270578  | -1.343387 | -1.898185 |
| H | 3.628953  | 0.610065  | 0.442437  |
| H | 3.678910  | -1.060963 | -0.133346 |
| H | 3.702015  | -0.724460 | 1.593342  |

Rotational constants (GHz): 1.3740500 0.7811700 0.7025200  
 Vibrational harmonic frequencies (cm-1):  
 43.3135 68.6671 90.8722  
 113.0035 162.1612 192.1467  
 209.0885 216.5878 242.8963  
 244.1657 275.6497 282.0468  
 300.0027 319.7988 329.3727  
 364.4597 420.7386 480.3675  
 566.0641 628.8724 677.2186  
 769.3125 782.6859 805.0794  
 837.3439 877.9354 954.4027  
 981.4895 988.7647 1003.9006  
 1021.9680 1029.5623 1033.0215  
 1082.3105 1111.8255 1144.5952  
 1150.3496 1175.8255 1188.8127  
 1257.4093 1277.5852 1292.4662  
 1304.1123 1325.6327 1348.9774  
 1371.8540 1382.9491 1409.5932  
 1418.8821 1421.7786 1424.0213  
 1428.1400 1476.2366 1487.3427  
 1497.4292 1499.8959 1501.4275  
 1502.9818 1506.1603 1508.1589  
 1514.0230 1517.4085 1617.1982  
 3049.9546 3062.6563 3064.9323  
 3066.5085 3069.0735 3069.7628  
 3075.7188 3077.4259 3107.5399  
 3114.3848 3134.2370 3136.4167  
 3136.8791 3139.9561 3143.8235  
 3146.0282 3149.3598 3163.3217

Zero-point correction (Hartree): 0.260546

diC2H5CH3CH\_COO.mptmRR  
 ~~~~~  
 E(RM062X/Aug-CC-pVT2) (Hartree): -504.06464366
 Electronic state : 1-A
 Cartesian coordinates (Angs):
 C -0.089409 -0.329590 0.088465
 O 0.454826 -1.285272 0.689146
 O -0.333336 -2.221416 1.316450
 C 0.858732 0.588746 -0.633357
 C 1.979953 1.141427 0.271239
 C 1.405264 -0.124998 -1.877422
 H 0.269966 1.440763 -0.968485
 C 3.123014 0.184893 0.592496
 H 2.384436 2.018878 -0.238259
 H 1.534608 1.502496 1.200410
 H 0.603410 -0.379031 -2.569687
 H 1.918540 -1.043612 -1.599630
 H 2.110480 0.526514 -2.394029
 H 3.644761 -0.127581 -0.311555
 H 2.773586 -0.705529 1.109353
 H 3.849189 0.685167 1.231922
 C -1.578021 -0.247183 0.052235
 C -2.136669 1.148889 -0.196628
 C -2.064376 -1.264417 -0.996897
 H -1.898840 -0.615793 1.029886
 C -1.756648 2.150663 0.886822
 H -1.832401 1.510125 -1.182283
 H -3.223322 1.054896 -0.238611
 H -1.637343 -2.244984 -0.798010
 H -1.794072 -0.938990 -2.002430
 H -3.149725 -1.339160 -0.945765
 H -0.676178 2.292882 0.943873
 H -2.092138 1.801401 1.863639
 H -2.207924 3.124487 0.703177

Rotational constants (GHz):	1.2587900	0.8253700	0.6917900
Vibrational harmonic frequencies (cm-1):			
22.5695	73.8952		93.1892
142.3612	151.0197		176.6912
206.5190	213.7137		225.0601
235.2403	243.1426		267.8533
293.9497	313.4055		348.2115
368.8612	433.6616		462.1686
555.7729	628.3511		707.2167
741.9566	794.0403		799.0769
849.7414	894.3460		942.6155

972.8522	987.1146	1008.8900
1020.6390	1029.1260	1041.7535
1071.7628	1117.7866	1133.3683
1156.4729	1170.6113	1197.3035
1254.0989	1280.4425	1306.5144
1308.7959	1326.6398	1363.0209
1373.8077	1377.6738	1393.4954
1403.4626	1419.6407	1419.9942
1429.2187	1484.6081	1489.4625
1496.5154	1502.3567	1504.0843
1505.8952	1509.7701	1511.3616
1512.4004	1519.9350	1620.6590
3054.6000	3056.0447	3060.9943
3063.8125	3066.4263	3072.9683
3074.8416	3092.4170	3092.8781
3115.7957	3129.1927	3133.9636
3136.3964	3138.2783	3139.7490
3154.2396	3159.2413	3161.0781

Zero-point correction (Hartree): 0.260415

dic2H5CH3CH_COO.mptpRR

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E(RM062X/Aug-CC-pVTZ) (Hartree): -504.06367821

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.122886 | -0.560808 | 0.068574  |
| O | -0.672452 | -1.669540 | -0.138635 |
| O | 0.016121  | -2.654840 | -0.802718 |
| C | -0.973471 | 0.424326  | 0.819490  |
| C | -1.437357 | 1.572956  | -0.107906 |
| C | -2.165554 | -0.246611 | 1.498709  |
| H | -0.329872 | 0.850371  | 1.593072  |
| C | -1.971447 | 1.086108  | -1.450097 |
| H | -2.216141 | 2.117202  | 0.428596  |
| H | -0.624923 | 2.279385  | -0.268932 |
| H | -1.849653 | -1.074264 | 2.130545  |
| H | -2.868418 | -0.641482 | 0.767749  |
| H | -2.682981 | 0.486567  | 2.115446  |
| H | -2.754473 | 0.338951  | -1.323137 |
| H | -1.181303 | 0.629192  | -2.049322 |
| H | -2.386614 | 1.913621  | -2.022816 |
| C | 1.281484  | -0.365061 | -0.390648 |
| C | 1.745499  | 1.063182  | -0.699166 |
| C | 2.181131  | -1.080394 | 0.634977  |
| H | 1.333764  | -0.955753 | -1.308091 |
| C | 2.043820  | 1.980887  | 0.482961  |
| H | 2.669151  | 0.948568  | -1.270640 |
| H | 1.039479  | 1.539104  | -1.381245 |
| H | 1.906439  | -2.131360 | 0.689741  |
| H | 2.093072  | -0.629402 | 1.623705  |
| H | 3.220722  | -1.001506 | 0.316546  |
| H | 2.795531  | 1.544984  | 1.139940  |
| H | 1.163575  | 2.201615  | 1.084468  |
| H | 2.435971  | 2.931744  | 0.123832  |

Rotational constants (GHz): 1.1334200 0.9853700 0.7027500

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| 60.3772   | 71.5441   | 101.5162  |
| 145.7719  | 165.5052  | 198.5024  |
| 213.1885  | 231.0775  | 240.9559  |
| 246.7930  | 257.2555  | 283.7926  |
| 303.5644  | 310.9581  | 330.5962  |
| 376.2601  | 447.1686  | 497.8687  |
| 582.1719  | 625.5726  | 696.8133  |
| 750.0317  | 783.1397  | 793.5884  |
| 845.8234  | 889.0523  | 961.4564  |
| 963.7315  | 988.6494  | 1002.8068 |
| 1004.3521 | 1031.7516 | 1035.7080 |
| 1077.0928 | 1111.6315 | 1140.3854 |
| 1148.6778 | 1157.5347 | 1180.7315 |
| 1261.6686 | 1281.2445 | 1304.6399 |
| 1308.6496 | 1321.7475 | 1364.0896 |
| 1367.3992 | 1379.5635 | 1393.6820 |
| 1416.5624 | 1419.1205 | 1422.0586 |
| 1426.4249 | 1484.8513 | 1494.2224 |
| 1497.1385 | 1498.1181 | 1503.3034 |
| 1506.9701 | 1508.0403 | 1511.7096 |
| 1517.9258 | 1522.2945 | 1609.4154 |
| 3059.9827 | 3060.6446 | 3063.4649 |
| 3066.7098 | 3074.9376 | 3076.7372 |
| 3077.9469 | 3080.3066 | 3097.8444 |
| 3118.8405 | 3130.9318 | 3134.0612 |
| 3138.1541 | 3145.1706 | 3148.1941 |
| 3151.6436 | 3157.2454 | 3160.0888 |

Zero-point correction (Hartree): 0.260889

dic2H5CH3CH\_COO.mpttRR

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E(RM062X/Aug-CC-pVTZ) (Hartree): -504.06639825

Electronic state : 1-A

Cartesian coordinates (Angs):

C	0.253127	0.492284	0.043530
O	0.794384	1.489449	-0.488252
O	0.025290	2.345244	-1.240853
C	1.167410	-0.365125	0.870106
C	1.551458	-1.658851	0.109170
C	2.412516	0.396977	1.318063
H	0.592867	-0.655870	1.754375
C	1.942328	-1.415155	-1.343776
H	2.386507	-2.105456	0.651219
H	0.734479	-2.376202	0.155149
H	2.150800	1.327460	1.818454
H	3.048001	0.646732	0.470555

H	2.983632	-0.222414	2.007846
H	2.711520	-0.647858	-1.429694
H	1.086524	-1.082808	-1.934383
H	2.325419	-2.327851	-1.796913
C	-1.211825	0.283591	-0.120267
C	-1.671545	-1.164161	0.042885
C	-1.883478	1.251230	0.874552
H	-1.442869	0.644713	-1.125072
C	-3.181053	-1.312173	-0.113073
H	-1.178163	-1.779289	-0.711501
H	-1.368421	-1.552747	1.018970
H	-1.468778	2.250185	0.755892
H	-1.738073	0.907123	1.900648
H	-2.951971	1.303096	0.678018
H	-3.520350	-0.853925	-1.043109
H	-3.717971	-0.840856	0.708465
H	-3.464166	-2.363284	-0.133231
Rotational constants (GHz):			
Vibrational harmonic frequencies (cm-1):			
43.3634	70.9440	93.8442	
119.7066	161.6248	173.4978	
215.0248	219.9434	232.4012	
239.3942	250.6949	295.7565	
300.3979	326.8956	344.5852	
376.3897	436.5144	480.2306	
560.4469	611.7523	727.0064	
751.8062	787.5207	805.6052	
851.1464	900.2702	956.8739	
972.3011	987.0863	989.5287	
1007.7804	1036.0080	1044.4552	
1075.8574	1111.6446	1136.2155	
1149.5005	1176.0666	1193.6836	
1263.1920	1279.9001	1291.5660	
1309.9994	1311.4667	1338.8116	
1365.7303	1380.5577	1397.6691	
1413.8048	1418.2837	1421.6403	
1426.1017	1485.0754	1492.1408	
1495.8451	1497.5443	1502.4270	
1504.0967	1506.6341	1511.2057	
1518.0888	1523.7792	1619.3202	
3048.6064	3057.2624	3058.5434	
3060.8316	3066.5480	3076.3226	
3077.1073	3079.1818	3097.0481	
3118.8891	3134.6589	3135.7723	
3139.6269	3144.9947	3146.5594	
3150.3164	3155.3585	3161.7736	
Zero-point correction (Hartree): 0.260618			
diC2H5CH3CH_COO.mtmmRR			
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E(RM062X/Aug-CC-pVT2) (Hartree): -504.06828045			
Electronic state : 1-A			
Cartesian coordinates (Angs):			
C	0.127779	-0.194195	-0.199767
O	0.499724	-1.010780	-1.068172
O	1.759962	-0.898963	-1.606128
C	-1.259969	-0.398821	0.332323
C	-2.138473	0.789931	-0.107915
C	-1.852463	-1.744569	-0.061652
H	-1.164917	-0.346187	1.423700
C	-3.539113	0.745592	0.489508
H	-1.653396	1.723573	0.181437
H	-2.195723	0.788941	-1.199364
H	-1.172574	-2.558018	0.184118
H	-2.044063	-1.782610	-1.133931
H	-2.789831	-1.910384	0.464549
H	-3.495300	0.661326	1.576581
H	-4.111725	-0.098247	0.108843
H	-4.087468	1.653951	0.245236
C	0.980590	0.939308	0.273608
C	2.329188	0.477036	0.853942
C	1.172908	1.968274	-0.848924
H	0.413751	1.404314	1.084608
C	2.217254	-0.784271	1.698907
H	3.022803	0.308518	0.035404
H	2.706935	1.306021	1.456426
H	1.795723	2.781575	-0.476936
H	0.223233	2.389064	-1.178518
H	1.668353	1.495905	-1.693634
H	1.957887	-1.637572	1.069833
H	1.459242	-0.679263	2.479072
H	3.163377	-1.012668	2.186795
Rotational constants (GHz):			
Vibrational harmonic frequencies (cm-1):			
52.9522	58.8541	86.8492	
111.5887	167.4618	199.9335	
206.3394	220.7888	226.2768	
244.4769	263.9911	278.8127	
289.7626	316.3784	355.7751	
373.0709	428.5851	435.4193	
475.3642	643.2150	728.2960	
753.9148	792.1403	816.8213	
847.8575	885.9722	962.8117	
975.5256	985.0897	1003.2155	
1031.2432	1035.6039	1059.7839	
1098.5098	1122.8032	1124.4364	
1152.4434	1166.9574	1193.3701	
1230.5219	1275.7766	1298.4094	
1318.9122	1327.9623	1361.2288	
1372.9584	1378.6641	1393.2864	
1409.8016	1414.3094	1419.3279	
1437.8565	1483.3790	1486.7242	

1493.9500	1496.5002	1497.3530
1502.0553	1506.5014	1514.7850
1517.9887	1518.7088	1648.3097
3025.5734	3047.3010	3054.9155
3058.5317	3065.4836	3066.1618
3067.6475	3075.9379	3100.8582
3110.7471	3133.9836	3134.9043
3137.7776	3145.0968	3148.1621
3156.5416	3159.5443	3164.7877

Zero-point correction (Hartree): 0.260467

diC2H5CH3CH_COO.mtmpRR

E(RM062X/Aug-CC-pVTZ) (Hartree): -504.06266269

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-0.047474	0.170343	-0.163394
O	-0.342563	1.134581	-0.897851
O	-1.569640	1.192197	-1.514375
C	1.329369	0.221886	0.434725
C	2.252453	-0.662965	-0.428529
C	1.858644	1.643073	0.581394
H	1.250473	-0.245754	1.421962
C	3.635073	-0.851331	0.182163
H	1.784959	-1.638896	-0.575117
H	2.334704	-0.202034	-1.415479
H	1.142965	2.274162	1.105873
H	2.042744	2.087577	-0.395935
H	2.789775	1.642481	1.143985
H	3.561796	-1.251441	1.194597
H	4.183281	0.088071	0.229435
H	4.224514	-1.548006	-0.411760
C	-0.937127	-0.995857	0.131032
C	-1.821318	-0.666945	1.356793
C	-1.722451	-1.566192	-1.050549
H	-0.245350	-1.771668	0.471296
C	-2.782451	0.501270	1.180397
H	-2.375299	-1.579639	1.587991
H	-1.170543	-0.476646	2.214410
H	-2.035887	-2.578778	-0.792584
H	-1.107211	-1.614275	-1.948202
H	-2.588778	-0.960343	-1.286232
H	-3.465230	0.337395	0.350308
H	-2.249968	1.427857	0.969176
H	-3.367634	0.636010	2.089897

Rotational constants (GHz): 1.5950400 0.6654300 0.6303000

Vibrational harmonic frequencies (cm-1):

45.9532	57.4356	77.7038
106.6866	154.7329	177.3849
192.5293	212.3427	223.5458
254.7464	274.5517	275.2758
291.0928	315.9665	316.7922
361.6065	393.4195	473.6647
513.4355	650.5404	727.6785
760.1662	784.9915	801.1291
849.1362	874.0741	954.2919
976.6016	985.2136	1005.2659
1016.9466	1039.2806	1056.7738
1105.1748	1117.9317	1130.4666
1146.2772	1161.1628	1194.1841
1233.8739	1277.5919	1293.1748
1314.4721	1326.5613	1364.4041
1378.6490	1382.9760	1413.5651
1414.9448	1418.3982	1432.2978
1445.4711	1478.4663	1484.4496
1487.1643	1494.0166	1496.2772
1500.6175	1503.1664	1506.8985
1509.7436	1515.0822	1653.4271
3040.3406	3043.4155	3054.5755
3059.1613	3065.5347	3069.4150
3073.3513	3075.8993	3084.2338
3096.3543	3133.4976	3134.4710
3139.3310	3144.4522	3147.0423
3157.5553	3159.0966	3200.0107

Zero-point correction (Hartree): 0.260302

diC2H5CH3CH_COO.mtmtrR

E(RM062X/Aug-CC-pVTZ) (Hartree): -504.06615834

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-0.064261	0.445149	-0.044629
O	0.059296	1.659623	0.217094
O	1.255776	2.141050	0.697504
C	-1.417377	0.018354	-0.529652
C	-2.080893	-0.815313	0.586754
C	-2.285601	1.184649	-0.980823
H	-1.233385	-0.654580	-1.375535
C	-3.394931	-1.451021	0.151400
H	-1.391962	-1.596446	0.913380
H	-2.246215	-0.161310	1.446479
H	-1.759208	1.810601	-1.698716
H	-2.560317	1.810341	-0.131981
H	-3.195601	0.816566	-1.449519
H	-3.257279	-2.048387	-0.751245
H	-4.155424	-0.699704	-0.053987
H	-3.779884	-2.105792	0.931520
C	1.040817	-0.546677	0.113165
C	2.154961	-0.241002	-0.907579
C	1.543150	-0.634612	1.559818
H	0.607928	-1.514097	-0.156863
C	3.263012	-1.285374	-0.871146

H	1.713652	-0.215774	-1.907163
H	2.547808	0.751776	-0.697403
H	2.138506	-1.538345	1.678880
H	0.709326	-0.689901	2.260521
H	2.137636	0.239331	1.807035
H	2.863299	-2.294206	-0.992844
H	3.809282	-1.250639	0.070289
H	3.978003	-1.109734	-1.673491
Rotational constants (GHz): 1.4940300 0.6617700 0.5686700			
Vibrational harmonic frequencies (cm-1):			
53.5086	54.3570	78.6334	
91.5859	126.6659	174.1110	
193.2773	215.1864	215.8811	
253.4249	264.1657	279.2441	
296.0310	306.3516	331.7598	
362.1765	417.7515	429.7329	
501.0828	646.9969	733.4876	
771.4133	786.4492	817.4470	
849.6670	881.4045	957.0196	
973.4895	981.3666	994.8930	
1008.2105	1053.6921	1062.2139	
1102.7354	1118.3784	1134.4393	
1137.5637	1168.3136	1192.1764	
1229.4257	1275.4126	1291.1944	
1325.5173	1343.0171	1357.9789	
1368.7574	1380.2999	1401.7578	
1411.6337	1414.4302	1419.7235	
1437.8944	1487.2208	1490.1690	
1496.6172	1496.7197	1502.0816	
1505.0633	1507.5891	1513.3690	
1514.7091	1516.7890	1649.8427	
3028.9979	3052.2942	3055.6897	
3057.8837	3058.6172	3065.7490	
3072.3986	3076.5822	3097.1986	
3120.1707	3134.3977	3134.4618	
3139.8376	3144.6147	3145.2945	
3148.5714	3159.1399	3184.6890	
Zero-point correction (Hartree): 0.260235			
diC2H5CH3CH_COO.mtppRR			
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E(RM062X/Aug-CC-pVTZ) (Hartree): -504.06568783			
Electronic state : 1-A			
Cartesian coordinates (Angs):			
C	-0.211590	0.668688	0.224396
O	-0.445249	1.746099	-0.372377
O	-1.741866	2.166948	-0.522068
C	1.248121	0.345428	0.391257
C	1.651818	-0.806533	-0.549268
C	2.132912	1.573822	0.201370
H	1.361645	-0.020604	1.415938
C	3.089122	-1.265494	-0.336371
H	0.979909	-1.650797	-0.401168
H	1.512687	-0.472843	-1.580704
H	1.781635	2.408605	0.804377
H	2.133629	1.892783	-0.840477
H	3.154891	1.345452	0.495035
H	3.265421	-1.516077	0.711184
H	3.805172	-0.498008	-0.624263
H	3.298081	-2.152301	-0.932589
C	-1.347171	-0.130949	0.772907
C	-2.250449	-0.726209	-0.333240
C	-0.923776	-1.168348	1.807921
H	-1.967940	0.638336	1.248208
C	-1.601485	-1.780667	-1.219572
H	-3.108689	-1.161650	0.181842
H	-2.618198	0.097432	-0.939153
H	-0.437916	-0.707412	2.667226
H	-0.246400	-1.917450	1.399212
H	-1.809809	-1.689164	2.169221
H	-1.181568	-2.607465	-0.644390
H	-0.808053	-1.351397	-1.831607
H	-2.342591	-2.200242	-1.898726
Rotational constants (GHz): 1.2546600 0.8430100 0.6490800			
Vibrational harmonic frequencies (cm-1):			
53.5486	68.0510	98.1876	
121.8945	171.2631	208.0503	
221.8571	224.1127	250.5620	
268.4060	281.7097	297.2603	
307.0041	328.3629	353.7720	
384.5181	408.2869	471.2372	
528.9010	639.5659	669.4219	
759.8156	795.4475	807.1907	
845.5684	877.4665	961.5334	
979.1601	985.0068	998.4069	
1019.2888	1026.4378	1057.2521	
1084.4310	1119.2063	1126.4232	
1156.0790	1181.1890	1185.3139	
1252.6085	1275.5428	1292.2346	
1298.0390	1333.4026	1358.4707	
1365.6619	1379.1356	1405.5283	
1413.2367	1415.8851	1420.9207	
1421.8904	1483.4728	1495.8250	
1497.0084	1501.1418	1502.8317	
1508.2126	1510.1772	1514.4949	
1517.2157	1519.8588	1613.7628	
3029.2611	3054.1101	3059.5854	
3063.3693	3069.5766	3071.0021	
3072.6996	3078.3987	3119.3815	
3122.5495	3133.5750	3135.0356	
3137.8093	3143.0351	3148.5780	
3150.5916	3154.1112	3160.6902	

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Zero-point correction (Hartree): 0.260898

diC2H5CH3CH_COO.mttmRR
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E (RM062X/Aug-CC-pVTZ) (Hartree): -504.06522673
Electronic state : 1-A
Cartesian coordinates (Angs):
  C    0.297587    -0.551044    -0.116229
  O    0.422341    -1.541504    -0.870623
  O    1.670184    -1.879319    -1.342652
  C   -1.089607    -0.327530    0.419040
  C   -1.863436    0.645822    -0.491399
  C   -1.831083    -1.650173    0.608353
  H   -0.967265    0.153535    1.394111
  C   -3.265335    0.949013    0.023071
  H   -1.306592    1.577950    -0.579782
  H   -1.914783    0.209814    -1.491823
  H   -1.220761    -2.362975    1.160680
  H   -2.076771    -2.095429    -0.354936
  H   -2.752684    -1.487701    1.162741
  H   -3.233377    1.298183    1.056727
  H   -3.908090    0.071504    -0.016547
  H   -3.731367    1.727587    -0.578718
  C    1.499299    0.225919    0.301294
  C    1.251685    1.719425    0.506421
  C    2.010276    -0.481098    1.570598
  H    2.239490    0.070835    -0.483162
  C    1.250203    2.488274    -0.811507
  H    0.322751    1.888752    1.056177
  H    2.048424    2.104262    1.145248
  H    2.185630    -1.537070    1.369483
  H    1.296252    -0.380613    2.390142
  H    2.949893    -0.026368    1.880704
  H    0.560113    2.048490    -1.532642
  H    2.241514    2.463365    -1.263337
  H    0.969894    3.530826    -0.666712
Rotational constants (GHz):    1.1691200    0.8490000    0.6392600
Vibrational harmonic frequencies (cm-1):
  37.7579    58.5446    75.9046
 123.3477    142.2860    182.0388
 205.2803    213.8291    224.6336
 242.8456    246.1332    276.3592
 301.5987    316.0624    352.8181
 394.4599    411.0069    442.3495
 542.9776    620.2478    717.3348
 752.4308    788.5198    810.6039
 857.9584    892.3048    950.8237
 978.2465    982.0737    999.8234
1025.0655    1036.3969    1055.0376
1069.6934    1114.7333    1122.6606
1149.5281    1184.2049    1189.9427
1261.5976    1274.6900    1292.8526
1325.8693    1336.9010    1353.0448
1364.6102    1380.4466    1399.6986
1409.9291    1416.7485    1417.2428
1421.9065    1487.5596    1493.3132
1497.3426    1501.0408    1502.5937
1503.9116    1506.7587    1507.1622
1517.7800    1519.6319    1627.3346
3050.5360    3056.8531    3061.4952
3062.8504    3064.5111    3071.1601
3075.8708    3091.5716    3106.9445
3119.5598    3130.3672    3132.8623
3134.5793    3140.7099    3146.9738
3148.3033    3148.9012    3159.2504
Zero-point correction (Hartree): 0.260420

diC2H5CH3CH_COO.mttpRR
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E (RM062X/Aug-CC-pVTZ) (Hartree): -504.06318952
Electronic state : 1-A
Cartesian coordinates (Angs):
  C   -0.441898    0.584668    -0.108964
  O   -0.798117    1.765177    -0.334795
  O   -2.078890    2.017937    -0.765196
  C    0.961261    0.438393    0.403023
  C    1.883570    -0.011391    -0.747596
  C    1.465937    1.714884    1.071439
  H    0.929246    -0.361843    1.146980
  C    3.279495    -0.392079    -0.270192
  H    1.438686    -0.859464    -1.267191
  H    1.939946    0.804484    -1.471673
  H    0.760886    2.068518    1.821536
  H    1.600181    2.509251    0.338652
  H    2.419322    1.527635    1.560531
  H    3.228672    -1.160241    0.503899
  H    3.812567    0.463631    0.140245
  H    3.872142    -0.786303    -1.094141
  C   -1.436092    -0.513490    -0.273560
  C   -0.935884    -1.914273    -0.650306
  C   -2.275449    -0.504540    1.019412
  H   -2.093980    -0.159721    -1.068419
  C   -0.090104    -2.688814    0.358326
  H   -1.845355    -2.489783    -0.835964
  H   -0.420416    -1.870750    -1.610876
  H   -2.741845    0.470881    1.143360
  H   -1.666465    -0.726844    1.896112
  H   -3.056091    -1.261489    0.945521
  H   -0.518463    -2.646127    1.359718
  H    0.935970    -2.328817    0.412622
  H   -0.043966    -3.738077    0.069524
Rotational constants (GHz):    1.1799000    0.9142200    0.6143100

```

Vibrational harmonic frequencies (cm-1):

57.2360	67.5133	80.3925
148.1762	154.0598	183.7050
218.2697	230.0782	238.1734
252.8129	269.6022	280.6337
304.9833	312.5818	337.4163
358.2748	402.5255	470.7715
594.2233	633.4320	702.5613
751.8785	784.3788	787.0412
854.2868	890.0799	958.6564
961.1032	982.4338	998.9709
1004.6627	1033.8467	1057.5531
1079.5385	1115.3669	1140.7754
1151.8766	1159.8484	1187.0013
1262.6907	1287.9902	1305.4451
1328.3739	1331.1220	1359.4534
1367.8835	1380.8719	1394.4368
1412.1997	1417.2254	1419.1316
1425.0437	1487.1098	1494.8131
1495.7802	1497.0722	1504.7591
1505.4134	1508.8552	1515.9475
1516.8201	1522.3739	1616.3268
3059.9834	3060.5996	3062.7909
3064.2324	3073.7608	3076.8229
3079.0857	3089.9414	3096.1956
3118.7231	3131.0325	3131.8940
3137.3668	3146.7367	3148.3466
3150.1756	3155.0616	3160.2579

Zero-point correction (Hartree): 0.260843

diC2H5CH3CH_COO.mtttRR

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E(RM062X/Aug-CC-pVTZ) (Hartree): -504.06622983

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.011221 | 0.596928  | -0.085447 |
| O | 0.181010  | 1.736908  | -0.566419 |
| O | -0.885213 | 2.425303  | -1.098518 |
| C | 1.219334  | -0.077339 | 0.447903  |
| C | 1.991123  | -0.693743 | -0.736848 |
| C | 2.082914  | 0.891234  | 1.255960  |
| H | 0.886375  | -0.889723 | 1.096270  |
| C | 3.150810  | -1.575558 | -0.293686 |
| H | 1.305388  | -1.278989 | -1.352186 |
| H | 2.349979  | 0.124752  | -1.364202 |
| H | 1.497842  | 1.377855  | 2.035293  |
| H | 2.495020  | 1.665252  | 0.610290  |
| H | 2.903622  | 0.358509  | 1.731632  |
| H | 2.806028  | -2.363308 | 0.378032  |
| H | 3.916725  | -1.001131 | 0.224797  |
| H | 3.620770  | -2.050750 | -1.153319 |
| C | -1.383837 | 0.022190  | -0.067432 |
| C | -1.426186 | -1.499872 | 0.073298  |
| C | -2.143609 | 0.742176  | 1.064142  |
| H | -1.836393 | 0.336488  | -1.011859 |
| C | -2.809991 | -2.063315 | -0.230453 |
| H | -0.702305 | -1.957005 | -0.604185 |
| H | -1.133678 | -1.787002 | 1.086193  |
| H | -2.072046 | 1.819226  | 0.931522  |
| H | -1.733383 | 0.458825  | 2.035316  |
| H | -3.194572 | 0.461759  | 1.042440  |
| H | -3.127397 | -1.785811 | -1.235951 |
| H | -3.556282 | -1.692583 | 0.470596  |
| H | -2.808089 | -3.150255 | -0.165803 |

Rotational constants (GHz): 1.2236500 0.7729100 0.5721000

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| 41.0238   | 59.6792   | 65.5569   |
| 75.9906   | 145.5585  | 161.9107  |
| 201.8902  | 205.7642  | 218.1469  |
| 226.1745  | 264.2600  | 276.2151  |
| 300.2455  | 309.5592  | 341.4446  |
| 351.1989  | 424.4961  | 425.5416  |
| 554.0245  | 632.1272  | 736.4007  |
| 747.6086  | 784.3386  | 795.7050  |
| 859.7924  | 903.9778  | 950.2491  |
| 972.7449  | 980.8115  | 987.4515  |
| 1002.0171 | 1037.8495 | 1062.8670 |
| 1078.3216 | 1123.9205 | 1127.3669 |
| 1155.3979 | 1182.3470 | 1194.0213 |
| 1258.6797 | 1285.9652 | 1301.8848 |
| 1311.0952 | 1331.0368 | 1335.9968 |
| 1364.4816 | 1382.3677 | 1398.9469 |
| 1410.5311 | 1414.4753 | 1416.7214 |
| 1421.5638 | 1486.9494 | 1489.1853 |
| 1496.9427 | 1497.9800 | 1501.8651 |
| 1504.3176 | 1507.8115 | 1511.8524 |
| 1515.7258 | 1520.2749 | 1625.3444 |
| 3052.0268 | 3059.0152 | 3061.6795 |
| 3064.7849 | 3068.9826 | 3070.5263 |
| 3074.5689 | 3082.4641 | 3096.6203 |
| 3103.1408 | 3132.5370 | 3136.8453 |
| 3139.3141 | 3142.2566 | 3146.0865 |
| 3146.6295 | 3158.3859 | 3165.9476 |

Zero-point correction (Hartree): 0.260071

diC2H5CH3CH\_COO.pmmmRR

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E(RM062X/Aug-CC-pVTZ) (Hartree): -504.06872399

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-0.002058	-0.354840	0.408317
O	0.344974	-0.043719	1.569190

O	1.659766	0.258409	1.820405
C	-1.457783	-0.697559	0.263093
C	-2.190315	0.373852	-0.560272
C	-1.628776	-2.090008	-0.350051
H	-1.874874	-0.699790	1.271713
C	-2.366785	1.684504	0.194680
H	-1.655531	0.539183	-1.499309
H	-3.166802	-0.030981	-0.832704
H	-1.113715	-2.851567	0.233853
H	-1.252118	-2.125410	-1.372751
H	-2.688262	-2.340787	-0.376947
H	-1.410484	2.087270	0.525761
H	-2.986192	1.534925	1.079320
H	-2.847903	2.434743	-0.431126
C	0.961008	-0.458141	-0.731270
C	1.852886	0.773806	-0.960324
C	1.816148	-1.721638	-0.532112
H	0.344067	-0.592468	-1.622614
C	1.133846	2.099582	-0.767572
H	2.700996	0.721687	-0.283944
H	2.228976	0.691093	-1.982938
H	1.211206	-2.627171	-0.532174
H	2.357497	-1.645282	0.408800
H	2.533968	-1.790103	-1.349084
H	0.882335	2.232163	0.285538
H	0.219225	2.155213	-1.362884
H	1.770658	2.932421	-1.062201
Rotational constants (GHz): 1.2395700 0.9028200 0.7538500			
Vibrational harmonic frequencies (cm-1):			
62.1548	107.1401	128.7223	
137.6435	171.7942	200.6256	
213.9848	220.0602	237.2115	
245.4623	259.3586	282.7465	
297.6432	310.0657	346.3217	
406.8026	435.2042	436.5679	
493.4105	603.0113	733.9543	
738.7754	796.6485	819.4941	
854.1820	888.5537	960.0266	
979.9194	986.0000	1019.7968	
1032.7925	1034.4555	1051.7531	
1068.8976	1111.7784	1132.3705	
1146.1539	1182.4029	1188.6031	
1257.9288	1280.8243	1303.7614	
1318.2974	1324.3922	1372.0379	
1372.7808	1376.4061	1393.9929	
1407.0892	1414.3551	1420.9655	
1432.6080	1482.7101	1487.2394	
1495.4916	1497.9999	1501.4075	
1503.7770	1506.6094	1507.9792	
1517.7310	1517.9977	1640.9639	
3050.1154	3055.5446	3059.5358	
3066.2622	3070.0482	3070.8339	
3073.8649	3082.7257	3096.1004	
3117.3576	3136.5075	3137.6347	
3140.0645	3141.7280	3145.5081	
3150.1978	3154.8471	3161.7826	
Zero-point correction (Hartree): 0.261006			
dic2H5CH3CH_COO.pnmpRR			
~~			
E (RM062X/Aug-CC-pVT2) (Hartree): -504.06350400			
Electronic state : 1-A			
Cartesian coordinates (Angs):			
C	0.120666	0.484428	0.333914
O	-0.325104	0.619703	1.494677
O	-1.673686	0.640136	1.726176
C	1.621990	0.526280	0.253250
C	2.187316	-0.737334	-0.403813
C	2.071767	1.793958	-0.481419
H	1.979031	0.573161	1.283586
C	1.920438	-1.997035	0.409892
H	1.779085	-0.835953	-1.413124
H	3.262601	-0.593127	-0.524509
H	1.639553	2.688093	-0.033669
H	1.791384	1.764371	-1.534356
H	3.156714	1.875707	-0.428371
H	0.852303	-2.153804	0.567432
H	2.387336	-1.925233	1.392521
H	2.317694	-2.879766	-0.088784
C	-0.729517	0.363478	-0.893910
C	-1.221692	-1.082469	-1.136930
C	-1.859880	1.395989	-0.976542
H	-0.040344	0.573755	-1.715018
C	-2.067166	-1.707373	-0.035544
H	-1.793197	-1.047682	-2.067744
H	-0.356781	-1.718464	-1.335598
H	-1.528216	2.377521	-0.638459
H	-2.705022	1.109553	-0.362260
H	-2.167906	1.478587	-2.019386
H	-2.961132	-1.122682	0.165654
H	-1.520323	-1.769466	0.904626
H	-2.365989	-2.712821	-0.332749
Rotational constants (GHz): 1.2797400 0.8710300 0.7512000			
Vibrational harmonic frequencies (cm-1):			
56.6178	84.0521	135.4750	
139.1905	171.4125	183.3220	
196.0832	208.3014	231.9451	
236.8713	263.0253	268.8777	
303.4956	313.6559	341.6625	
358.9004	428.4846	487.6301	
516.0278	604.5209	715.3287	
764.7605	797.0468	807.3926	

855.0013	877.0269	964.1796
978.3646	987.2259	1010.7730
1027.3608	1042.7539	1045.1638
1073.7247	1112.7040	1127.0797
1149.1852	1182.9328	1191.2767
1256.7749	1282.8391	1300.7622
1317.6016	1323.8901	1371.1098
1376.9579	1383.1984	1412.2672
1412.6521	1421.4663	1431.3765
1441.2354	1481.5964	1486.3566
1488.7350	1495.8839	1499.6155
1502.2110	1504.2116	1505.9217
1509.4664	1512.7590	1638.7594
3054.1999	3057.5786	3064.0455
3064.8625	3067.7768	3071.3749
3074.5722	3082.0267	3092.0035
3096.5416	3130.8549	3131.2074
3137.8044	3139.8861	3141.0219
3142.5766	3161.4128	3201.1374

Zero-point correction (Hartree): 0.260867

diC2H5CH3CH_COO.pmmRR
 ~~~~~  
 E(RM062X/Aug-CC-pVT2) (Hartree): -504.06710505  
 Electronic state : 1-A  
 Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.293300 | -0.557936 | 0.265046  |
| O | -0.195882 | -1.023447 | 1.421913  |
| O | 1.037959  | -1.150274 | 2.011230  |
| C | -1.697404 | -0.463616 | -0.253906 |
| C | -2.088798 | 1.009913  | -0.440325 |
| C | -1.850578 | -1.259957 | -1.552015 |
| H | -2.340971 | -0.899397 | 0.512270  |
| C | -2.152132 | 1.775499  | 0.875115  |
| H | -1.384084 | 1.486820  | -1.127238 |
| H | -3.061675 | 1.033421  | -0.934763 |
| H | -1.549146 | -2.298598 | -1.421188 |
| H | -1.256770 | -0.827784 | -2.357531 |
| H | -2.894232 | -1.244927 | -1.863405 |
| H | -1.195069 | 1.755031  | 1.397866  |
| H | -2.895040 | 1.335361  | 1.540705  |
| H | -2.421836 | 2.817270  | 0.709546  |
| C | 0.883122  | -0.117363 | -0.542290 |
| C | 1.563631  | 1.102450  | 0.110290  |
| C | 1.840101  | -1.288191 | -0.809031 |
| H | 0.482051  | 0.212441  | -1.503709 |
| C | 2.747188  | 1.601195  | -0.708715 |
| H | 0.825308  | 1.902990  | 0.198210  |
| H | 1.874661  | 0.827944  | 1.116204  |
| H | 1.293897  | -2.164519 | -1.159544 |
| H | 2.373255  | -1.554624 | 0.098412  |
| H | 2.545905  | -1.004532 | -1.587619 |
| H | 2.463982  | 1.783952  | -1.747519 |
| H | 3.564820  | 0.882139  | -0.704027 |
| H | 3.127354  | 2.534808  | -0.296819 |

Rotational constants (GHz): 1.2275400 0.7803200 0.7285800  
 Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| 54.1730   | 64.6061   | 69.4048   |
| 118.1947  | 142.2588  | 179.8079  |
| 184.5965  | 198.5343  | 217.1026  |
| 240.9057  | 244.6275  | 258.3047  |
| 276.2582  | 315.0542  | 338.3758  |
| 399.9935  | 422.4306  | 435.8838  |
| 494.6487  | 604.3112  | 729.7924  |
| 771.9729  | 804.3404  | 817.7295  |
| 850.2234  | 882.5146  | 955.2720  |
| 975.5032  | 978.5133  | 997.8015  |
| 1021.7526 | 1045.7750 | 1059.9499 |
| 1077.8834 | 1108.2201 | 1122.2612 |
| 1147.6498 | 1182.9291 | 1185.8650 |
| 1249.7625 | 1281.4584 | 1296.6441 |
| 1321.4333 | 1350.5214 | 1360.3037 |
| 1371.3948 | 1375.8922 | 1396.6840 |
| 1410.4754 | 1414.0381 | 1424.3087 |
| 1428.9226 | 1487.6824 | 1491.1269 |
| 1495.3513 | 1501.5450 | 1503.1844 |
| 1504.1539 | 1505.5608 | 1508.3251 |
| 1514.8520 | 1516.0893 | 1641.1764 |
| 3053.1812 | 3057.3943 | 3061.6358 |
| 3063.7327 | 3065.4648 | 3069.8707 |
| 3072.5472 | 3082.7129 | 3095.7106 |
| 3120.3663 | 3131.0818 | 3135.5469 |
| 3138.9564 | 3140.5514 | 3142.6325 |
| 3143.4215 | 3146.8735 | 3179.6827 |

Zero-point correction (Hartree): 0.260230

diC2H5CH3CH\_COO.pmpmRR  
 ~~~~~  
 E(RM062X/Aug-CC-pVT2) (Hartree): -504.06560668
 Electronic state : 1-A
 Cartesian coordinates (Angs):

C	0.010635	-0.372878	0.176222
O	-0.189708	-1.541073	0.591708
O	-1.159188	-2.323062	0.022581
C	1.113897	0.328460	0.920394
C	2.410322	0.415318	0.094695
C	0.689186	1.700303	1.445713
H	1.322238	-0.320731	1.773425
C	2.828597	-0.919478	-0.507085
H	2.304793	1.169698	-0.684832
H	3.186776	0.778972	0.770605
H	-0.222289	1.638947	2.039671

H	0.524697	2.408697	0.635068
H	1.481301	2.098940	2.078860
H	2.104237	-1.272882	-1.242928
H	2.903469	-1.687318	0.263647
H	3.794804	-0.838147	-1.002079
C	-0.818027	0.166802	-0.942075
C	-2.032203	0.944770	-0.384271
C	-0.041503	1.028598	-1.935653
H	-1.201077	-0.723728	-1.441722
C	-2.869732	0.183416	0.634384
H	-1.683955	1.888274	0.041504
H	-2.646718	1.206806	-1.247806
H	0.814318	0.500822	-2.354330
H	0.307841	1.960563	-1.492296
H	-0.706886	1.287644	-2.758586
H	-2.282340	-0.090526	1.512718
H	-3.252044	-0.742187	0.211497
H	-3.705028	0.797370	0.969327
Rotational constants (GHz): 1.3468900 0.8429000 0.7375600			
Vibrational harmonic frequencies (cm-1):			
56.4986	73.5165	105.2361	
131.7851	183.9707	195.1502	
220.8674	231.0624	255.2674	
261.9921	276.7020	285.3548	
294.9868	306.3340	339.8035	
365.3343	435.5221	455.2654	
512.9104	635.8939	676.7732	
726.2446	805.9226	812.1251	
853.0815	876.4009	955.8721	
976.5593	983.0533	1012.8198	
1029.4758	1049.7426	1058.2007	
1073.4613	1110.3023	1136.2687	
1143.7135	1181.2678	1191.7931	
1277.9225	1285.5568	1320.7939	
1323.3954	1336.4341	1361.8953	
1371.9505	1376.9970	1392.5516	
1411.1407	1419.6617	1424.0451	
1427.5736	1484.1904	1487.6753	
1495.8740	1501.4661	1502.3098	
1502.8857	1505.0598	1509.9771	
1510.8949	1516.4036	1608.6084	
3059.9354	3060.2814	3065.1747	
3067.0726	3070.0330	3072.6854	
3073.6067	3086.8893	3102.7548	
3110.5623	3126.9050	3129.0468	
3137.3365	3138.9125	3143.0698	
3143.5643	3152.2806	3163.8521	
Zero-point correction (Hartree): 0.260932			
diC2H5CH3CH_COO.pmptrR			
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E(RM062X/Aug-CC-pVTZ) (Hartree): -504.06696490			
Electronic state : 1-A			
Cartesian coordinates (Angs):			
C	0.195818	0.509219	-0.204091
O	0.022474	1.736612	-0.416215
O	-1.126060	2.333485	0.034954
C	1.454400	-0.029544	-0.821792
C	2.456190	-0.566636	0.210247
C	1.122404	-1.067783	-1.898051
H	1.914853	0.833698	-1.306810
C	2.702487	0.406532	1.355348
H	2.121571	-1.530797	0.591669
H	3.388753	-0.756329	-0.324648
H	0.453595	-0.655272	-2.652546
H	0.652448	-1.952941	-1.471725
H	2.042203	-1.382156	-2.390545
H	1.796735	0.567533	1.943513
H	3.018725	1.379245	0.976810
H	3.474589	0.036439	2.027687
C	-0.865932	-0.232258	0.526491
C	-2.037767	-0.453672	-0.465398
C	-0.440770	-1.521484	1.217346
H	-1.226446	0.490593	1.264078
C	-3.370625	-0.584442	0.257424
H	-2.091894	0.396112	-1.145116
H	-1.826350	-1.349295	-1.055146
H	0.325205	-1.347168	1.971601
H	-0.072357	-2.269055	0.516142
H	-1.304650	-1.948393	1.724478
H	-3.590993	0.340663	0.789822
H	-3.367157	-1.403986	0.976295
H	-4.177373	-0.769255	-0.450620
Rotational constants (GHz): 1.4010000 0.7633500 0.6818000			
Vibrational harmonic frequencies (cm-1):			
48.0385	74.3312	81.1831	
129.8124	182.0537	200.7918	
218.2307	221.5433	221.9041	
256.6605	274.7582	275.5687	
304.2724	319.7573	343.5822	
394.5341	423.1289	443.7307	
511.2171	640.7886	683.9997	
770.4194	779.4854	805.0057	
855.7416	879.1592	960.8943	
977.2736	986.4564	1010.8845	
1027.7757	1035.5517	1048.5653	
1077.8078	1112.2709	1133.6306	
1145.2548	1186.3422	1197.0651	
1281.0689	1283.3668	1313.8639	
1325.5998	1328.3494	1360.1346	
1379.0540	1383.3499	1393.3604	
1407.8907	1412.1250	1421.4124	

1424.9338	1477.6720	1488.5142
1496.5765	1500.6160	1503.8027
1504.1508	1504.8839	1506.9887
1513.1445	1519.4241	1604.1347
3049.7778	3057.5879	3062.5944
3064.8896	3068.1350	3072.5481
3074.3566	3077.7407	3111.2562
3114.2242	3128.6898	3136.1717
3140.0025	3140.6514	3142.2792
3143.2206	3145.0487	3154.5474

Zero-point correction (Hartree): 0.260754

diC2H5CH3CH_COO.pmtmRR

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E(RM062X/Aug-CC-pVTZ) (Hartree): -504.05867538

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.407363 | -0.602893 | -0.013970 |
| O | -1.184732 | -1.594317 | -0.013005 |
| O | -2.537496 | -1.407372 | 0.063556  |
| C | 1.036130  | -1.074437 | -0.007287 |
| C | 2.103832  | -0.093671 | -0.484237 |
| C | 1.374275  | -1.651770 | 1.377539  |
| H | 1.037563  | -1.918624 | -0.702650 |
| C | 1.935587  | 0.339896  | -1.933607 |
| H | 2.156894  | 0.769087  | 0.179056  |
| H | 3.061076  | -0.607811 | -0.377420 |
| H | 0.644280  | -2.402957 | 1.670599  |
| H | 1.399221  | -0.878625 | 2.143223  |
| H | 2.357768  | -2.118802 | 1.339541  |
| H | 0.996411  | 0.867942  | -2.089650 |
| H | 1.938908  | -0.526315 | -2.596331 |
| H | 2.743609  | 1.001623  | -2.242274 |
| C | -1.043023 | 0.751689  | 0.020365  |
| C | -0.209876 | 1.958073  | 0.441943  |
| C | -1.736742 | 1.004831  | -1.335911 |
| H | -1.856532 | 0.605359  | 0.740921  |
| C | 0.289431  | 1.917766  | 1.879812  |
| H | 0.613025  | 2.127048  | -0.253062 |
| H | -0.868065 | 2.822073  | 0.327790  |
| H | -2.266648 | 0.118702  | -1.674014 |
| H | -1.016149 | 1.320844  | -2.088669 |
| H | -2.462773 | 1.806470  | -1.208899 |
| H | 1.015533  | 1.122682  | 2.038206  |
| H | -0.538818 | 1.750780  | 2.569219  |
| H | 0.769020  | 2.857121  | 2.152116  |

Rotational constants (GHz): 1.0805000 0.9100100 0.7804500

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| 56.0007   | 105.1270  | 130.9120  |
| 148.1315  | 153.6606  | 161.3296  |
| 195.1670  | 200.5887  | 212.8216  |
| 226.3615  | 252.1606  | 270.6703  |
| 296.6645  | 310.0985  | 354.8380  |
| 401.1263  | 427.5239  | 467.0691  |
| 497.1855  | 616.8667  | 663.2083  |
| 725.1738  | 786.6077  | 812.6045  |
| 870.2551  | 902.6299  | 970.5195  |
| 973.9223  | 985.4090  | 1015.6943 |
| 1021.2852 | 1038.4420 | 1046.9713 |
| 1087.7867 | 1099.5014 | 1130.7421 |
| 1135.8913 | 1196.0363 | 1208.8014 |
| 1268.3520 | 1279.1659 | 1295.5134 |
| 1304.7744 | 1332.8893 | 1371.1496 |
| 1374.3170 | 1385.4394 | 1395.3918 |
| 1402.6116 | 1410.0956 | 1416.2234 |
| 1422.0686 | 1480.6081 | 1490.1987 |
| 1495.9172 | 1500.3522 | 1503.3869 |
| 1504.5943 | 1509.2077 | 1512.9037 |
| 1514.0124 | 1522.6627 | 1572.9279 |
| 3028.4473 | 3054.4270 | 3067.5298 |
| 3069.1302 | 3070.0860 | 3072.5291 |
| 3077.0846 | 3078.2460 | 3107.2161 |
| 3119.0215 | 3136.1143 | 3137.7435 |
| 3142.2785 | 3144.2600 | 3154.5696 |
| 3158.0478 | 3165.4928 | 3173.5332 |

Zero-point correction (Hartree): 0.260568

diC2H5CH3CH\_COO.pmtprR

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E(RM062X/Aug-CC-pVTZ) (Hartree): -504.05832328

Electronic state : 1-A

Cartesian coordinates (Angs):

C	0.631107	0.537376	0.016033
O	1.659645	1.175232	-0.333577
O	2.884086	0.566967	-0.307781
C	-0.567702	1.452811	0.102720
C	-1.888153	0.877052	-0.401108
C	-0.686276	2.002517	1.533164
H	-0.304625	2.295438	-0.540864
C	-1.820571	0.418828	-1.851639
H	-2.221756	0.068746	0.248524
H	-2.635379	1.667184	-0.303670
H	0.255499	2.438900	1.861756
H	-0.977085	1.231389	2.244359
H	-1.450005	2.779475	1.552926
H	-1.059773	-0.349659	-1.993060
H	-1.565228	1.252448	-2.506696
H	-2.773761	0.008997	-2.182974
C	0.799306	-0.892694	0.418132
C	-0.332089	-1.539951	1.238338
C	1.220125	-1.746062	-0.793803
H	1.701357	-0.825438	1.039341

C	-1.327117	-2.401686	0.461920
H	0.146798	-2.178676	1.982245
H	-0.866437	-0.782789	1.809746
H	2.050517	-1.275409	-1.310546
H	0.391067	-1.896744	-1.482264
H	1.540758	-2.724863	-0.437449
H	-0.847369	-3.297986	0.072180
H	-1.770009	-1.877744	-0.383770
H	-2.136192	-2.720013	1.118541
Rotational constants (GHz): 1.0766200 0.9840000 0.7307000			
Vibrational harmonic frequencies (cm-1):			
80.4905	99.1269	131.4855	
162.5180	181.8545	193.0729	
213.0878	227.5057	233.7111	
252.8782	266.2844	291.0366	
304.5769	326.5242	338.7941	
356.1858	452.6987	485.9843	
523.5037	627.1712	655.4053	
732.0971	779.3375	812.6823	
867.9534	898.6007	967.2009	
976.6874	981.6641	1009.3003	
1023.6734	1034.6441	1046.6177	
1078.0332	1103.3450	1128.1931	
1158.5295	1168.1734	1203.5645	
1276.1495	1287.9079	1305.5869	
1315.2518	1336.7201	1368.4786	
1372.0878	1379.2184	1393.6773	
1398.5483	1413.0576	1416.2739	
1422.7154	1487.0159	1494.0767	
1495.6476	1500.7040	1501.8945	
1505.1680	1509.1360	1511.9755	
1520.0273	1527.5246	1584.6593	
3019.6771	3064.3703	3067.2178	
3070.7816	3073.5607	3075.0635	
3077.0999	3078.7816	3117.9839	
3121.7287	3135.7660	3139.7198	
3141.3591	3144.1672	3145.9861	
3151.7757	3157.0607	3183.7556	
Zero-point correction (Hartree): 0.261223			
dic2H5CH3CH_COO.pmttRR			
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E(RM062X/Aug-CC-pVT2) (Hartree): -504.06213425			
Electronic state : 1-A			
Cartesian coordinates (Angs):			
C	-0.310625	0.720571	0.112218
O	-0.452266	1.968805	0.032212
O	0.655546	2.766806	-0.050936
C	-1.628249	0.028953	0.365295
C	-1.852000	-1.287758	-0.377846
C	-1.836059	-0.130006	1.879180
H	-2.375335	0.742556	0.010298
C	-1.611797	-1.179526	-1.876794
H	-1.238740	-2.076479	0.056633
H	-2.888393	-1.577022	-0.192466
H	-1.732025	0.825576	2.390294
H	-1.127468	-0.834629	2.311468
H	-2.840206	-0.511445	2.062914
H	-0.571100	-0.939493	-2.095455
H	-2.227477	-0.390809	-2.311219
H	-1.851981	-2.112424	-2.384249
C	1.078434	0.176130	0.077936
C	1.252959	-1.276034	0.518569
C	1.709325	0.426281	-1.311160
H	1.605817	0.842574	0.772746
C	2.722297	-1.612361	0.752087
H	0.694602	-1.469127	1.434865
H	0.852550	-1.942713	-0.247505
H	1.325424	1.337027	-1.761398
H	1.522390	-0.424723	-1.966646
H	2.785580	0.543950	-1.207584
H	3.160224	-0.940419	1.491203
H	3.300531	-1.522108	-0.166484
H	2.833656	-2.632678	1.115480
Rotational constants (GHz): 1.0571400 0.9038300 0.7138900			
Vibrational harmonic frequencies (cm-1):			
51.9817	84.8345	105.4492	
119.0693	155.5536	182.0335	
196.8818	204.9056	212.7010	
235.1456	248.0969	273.1238	
300.8969	316.7036	349.4301	
400.1204	438.5214	454.4674	
500.1573	624.3181	680.4103	
748.6886	804.3031	807.4407	
872.6421	916.5948	969.6658	
976.1939	980.0925	992.5620	
1021.5908	1036.4457	1057.2878	
1081.9161	1096.8849	1129.5829	
1154.0484	1191.3867	1205.8818	
1268.5051	1285.6259	1309.2288	
1313.2428	1322.1894	1336.4397	
1371.8483	1386.1972	1392.2025	
1405.6157	1412.6190	1416.7006	
1420.9060	1480.8336	1490.2202	
1497.3448	1502.2103	1503.2451	
1503.9323	1506.4695	1508.9980	
1518.1341	1521.1347	1589.6905	
3016.5365	3064.5403	3066.1845	
3066.8555	3068.8278	3070.6112	
3073.1376	3075.0329	3109.3054	
3116.5634	3135.7486	3137.7131	
3141.9318	3143.9273	3145.2009	

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3150.1148      3154.5333      3173.8869
Zero-point correction (Hartree): 0.260513

diC2H5CH3CH_COO.ppmprR
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E(RM062X/Aug-CC-pVTZ) (Hartree): -504.05847566
Electronic state : 1-A
Cartesian coordinates (Angs):
  C   -0.050640   -0.628230   -0.205800
  O   -0.754728   -1.382034   -0.914887
  O   -2.115362   -1.402373   -0.777314
  C    1.421940   -0.767339   -0.484230
  C    2.106308    0.553082   -0.901837
  C    2.117074   -1.450809    0.697803
  H    1.478812   -1.439497   -1.340524
  C    2.568845    1.484093    0.215362
  H    2.984208    0.267540   -1.484557
  H    1.450617    1.088679   -1.591522
  H    1.696615   -2.440357    0.870865
  H    2.021323   -0.872884    1.616300
  H    3.180159   -1.562549    0.482859
  H    3.280659    0.988044    0.874268
  H    1.749180    1.856940    0.826544
  H    3.071480    2.349414   -0.214889
  C   -0.594891    0.282769    0.850515
  C   -1.047670    1.634790    0.251307
  C   -1.653221   -0.346831    1.763754
  H    0.269734    0.508314    1.476706
  C   -2.146444    1.569280   -0.801261
  H   -1.376265    2.243133    1.097713
  H   -0.178607    2.142530   -0.171791
  H   -1.688084    0.231812    2.687662
  H   -1.402080   -1.377247    2.013275
  H   -2.630548   -0.356271    1.296980
  H   -3.044917    1.092401   -0.418495
  H   -1.831625    0.991899   -1.669807
  H   -2.397746    2.578523   -1.127657
Rotational constants (GHz):   1.3834300   0.8259000   0.7023700
Vibrational harmonic frequencies (cm-1):
  53.7365      55.5532      124.3107
 146.6281      161.7683      188.5933
 194.0782      210.5998      236.6779
 257.7077      273.1974      286.9866
 303.6535      310.2100      331.5267
 351.0295      367.5899      508.1788
 552.1040      618.6733      717.8436
 762.2000      786.7157      799.2792
 837.8163      871.5788      954.9834
 980.3148      994.1996     1010.9654
1016.4338     1029.2898     1041.2720
1083.2352     1124.3666     1134.1024
1147.9622     1157.5466     1187.5734
1258.4691     1295.8600     1311.8697
1322.2516     1335.0800     1372.7979
1380.5320     1386.4005     1411.2075
1412.5446     1422.3467     1429.9734
1438.8286     1477.0002     1483.0442
1486.7460     1494.3746     1498.5785
1500.3416     1504.5782     1508.4874
1512.8024     1517.9041     1632.9550
3054.0653     3059.3911     3065.7008
3068.3083     3071.8270     3076.1464
3087.8633     3090.1976     3092.9598
3096.9900     3132.0772     3136.7823
3136.9858     3138.6374     3145.7750
3153.7454     3163.1502     3199.8570
Zero-point correction (Hartree): 0.260932

diC2H5CH3CH_COO.ppmtrR
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E(RM062X/Aug-CC-pVTZ) (Hartree): -504.06422315
Electronic state : 1-A
Cartesian coordinates (Angs):
  C    0.211588   -0.763898   -0.146782
  O   -0.106033   -1.706215   -0.906420
  O   -1.429950   -1.939176   -1.181051
  C    1.693697   -0.618355    0.054389
  C    2.268149    0.512600   -0.824589
  C    2.056192   -0.461566    1.531752
  H    2.130516   -1.548580   -0.310566
  C    1.760051    1.920632   -0.534339
  H    3.352022    0.485547   -0.694370
  H    2.073025    0.263855   -1.868994
  H    1.711914   -1.316400    2.112669
  H    1.630099    0.438543    1.971613
  H    3.139599   -0.399776    1.631146
  H    1.896696    2.195597    0.511870
  H    0.703721    2.028414   -0.778933
  H    2.308301    2.643936   -1.136050
  C   -0.803131    0.112396    0.508142
  C   -1.757854    0.797102   -0.491320
  C   -1.562038   -0.699956    1.571111
  H   -0.241374    0.896022    1.018373
  C   -2.236804    2.137968    0.051334
  H   -1.259116    0.939809   -1.452386
  H   -2.591686    0.129492   -0.687915
  H   -2.325946   -0.068939    2.023783
  H   -0.894036   -1.039556    2.362458
  H   -2.038512   -1.557909    1.103111
  H   -1.406121    2.834477    0.180738
  H   -2.723911    2.020597    1.020395
  H   -2.956421    2.596460   -0.625365

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Rotational constants (GHz): 1.1888200 0.8743400 0.7059800
 Vibrational harmonic frequencies (cm-1):
 50.1095 86.7262 90.6841
 132.8011 160.4090 184.5988
 206.9994 217.5178 225.4794
 244.9172 259.6485 270.9598
 292.5546 304.7327 338.8600
 362.2894 413.3525 442.4397
 538.1336 626.5244 738.0689
 776.9195 795.8809 810.1715
 832.0260 888.3621 951.6827
 977.8829 989.5852 1003.8392
 1015.1925 1027.5520 1050.0932
 1079.1725 1117.1821 1121.8429
 1147.3136 1172.5519 1184.7066
 1251.5701 1286.0975 1301.5883
 1319.6713 1335.6841 1354.8474
 1375.7390 1383.2649 1393.7716
 1413.1138 1417.5519 1420.4479
 1434.0599 1486.8196 1491.9206
 1495.0273 1500.2965 1502.8343
 1504.4237 1507.6239 1512.4237
 1515.1193 1521.6956 1636.4178
 3054.7578 3061.6195 3068.8726
 3069.4389 3070.8525 3072.1064
 3088.8793 3090.9797 3101.1781
 3114.0768 3134.6709 3135.7904
 3137.2394 3140.5352 3144.9409
 3149.7805 3155.0055 3164.5224
 Zero-point correction (Hartree): 0.260729

diC2H5CH3CH_COO.pppmRR
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 E(RM062X/Aug-CC-pVTZ) (Hartree): -504.06581691  
 Electronic state : 1-A  
 Cartesian coordinates (Angs):  
 C -0.061909 0.410800 -0.375044  
 O 0.241859 -0.107483 -1.473070  
 O -0.741758 -0.572902 -2.315785  
 C 1.104742 0.773816 0.499469  
 C 1.641991 -0.481039 1.230035  
 C 2.198524 1.497281 -0.286131  
 H 0.722873 1.445496 1.267893  
 C 2.328475 -1.506187 0.336601  
 H 2.345452 -0.123771 1.985149  
 H 0.823143 -0.956916 1.772162  
 H 1.830908 2.443330 -0.681692  
 H 2.544035 0.895395 -1.123175  
 H 3.045385 1.703130 0.368387  
 H 3.211551 -1.087963 -0.144695  
 H 1.665121 -1.872673 -0.445799  
 H 2.650179 -2.359539 0.932035  
 C -1.489985 0.601607 0.014453  
 C -1.915774 -0.495710 1.006182  
 C -1.738204 1.995358 0.593006  
 H -2.053522 0.468712 -0.907882  
 C -1.729354 -1.907616 0.466736  
 H -1.364842 -0.363286 1.942125  
 H -2.966563 -0.318339 1.243861  
 H -1.327497 2.779169 -0.043497  
 H -1.315759 2.103239 1.592172  
 H -2.812267 2.158149 0.671442  
 H -0.682237 -2.110394 0.233026  
 H -2.287280 -2.043741 -0.457525  
 H -2.060536 -2.646766 1.195011

Rotational constants (GHz): 1.2230800 0.8537200 0.7992800  
 Vibrational harmonic frequencies (cm-1):  
 35.0287 67.0273 108.2787  
 135.3805 156.5046 188.3511  
 189.3486 221.3140 233.8656  
 240.0267 255.5239 271.0527  
 291.5717 305.7273 335.5342  
 365.7512 413.7403 484.3902  
 562.1308 624.4089 704.3384  
 736.6674 792.4707 819.7766  
 837.9458 879.8193 939.6077  
 976.3440 985.7590 1005.5323  
 1024.6802 1031.9619 1047.8262  
 1076.0307 1110.0757 1132.7953  
 1149.1287 1176.7334 1183.4791  
 1261.1799 1282.5425 1300.6183  
 1307.2715 1320.1758 1358.4753  
 1373.5167 1376.5346 1411.1885  
 1414.1793 1422.3643 1426.9128  
 1428.5691 1482.0860 1492.7372  
 1497.1773 1499.0028 1501.8740  
 1502.5643 1505.5609 1509.8253  
 1511.5648 1518.6733 1626.7562  
 3045.2718 3062.0785 3063.2963  
 3065.8312 3070.2302 3073.4614  
 3086.2925 3100.8759 3101.8761  
 3113.5908 3129.2595 3136.4252  
 3138.4379 3140.2227 3141.2864  
 3146.6786 3153.3651 3162.5181  
 Zero-point correction (Hartree): 0.260527

diC2H5CH3CH\_COO.ppppRR  
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 E(RM062X/Aug-CC-pVTZ) (Hartree): -504.06089268
 Electronic state : 1-A
 Cartesian coordinates (Angs):
 C -0.007308 0.475252 0.199025

O	0.036175	1.679609	0.557562
O	0.920546	2.541893	-0.038325
C	-1.095379	-0.272327	0.940179
C	-2.473553	0.246023	0.475208
C	-1.019238	-1.795617	0.919139
H	-0.979086	0.049901	1.977945
C	-2.738692	0.077758	-1.015902
H	-3.234693	-0.282850	1.052044
H	-2.545952	1.300883	0.737985
H	-0.022488	-2.158965	1.162109
H	-1.310947	-2.213259	-0.040966
H	-1.707340	-2.181424	1.670624
H	-2.708196	-0.968268	-1.320657
H	-2.006476	0.628532	-1.610001
H	-3.723469	0.464898	-1.272147
C	0.948764	0.025992	-0.854572
C	2.372115	-0.042366	-0.247836
C	0.590571	-1.233570	-1.634777
H	0.969234	0.884571	-1.534410
C	2.530529	-1.048098	0.885978
H	3.048880	-0.295048	-1.066100
H	2.632850	0.956127	0.095846
H	-0.438069	-1.219858	-1.991326
H	0.742897	-2.144706	-1.061657
H	1.240857	-1.282328	-2.507870
H	2.290005	-2.065504	0.575477
H	1.892931	-0.791152	1.734770
H	3.558438	-1.051850	1.245789
Rotational constants (GHz):			
Vibrational harmonic frequencies (cm-1):			
60.0820	88.9175	91.6542	
128.3915	187.5390	205.6350	
242.5700	255.0265	271.8381	
274.5057	285.8840	298.3243	
312.8990	314.2345	338.9765	
367.2170	452.3257	483.1819	
522.9360	644.6163	681.0491	
739.8063	788.0779	807.0291	
835.6257	859.2065	949.7142	
990.4462	991.3828	1012.6560	
1021.5508	1029.0903	1032.9427	
1078.2491	1097.9758	1135.9803	
1146.7670	1182.1030	1197.1209	
1268.9755	1282.7320	1298.3817	
1307.7056	1331.4676	1360.5784	
1376.0126	1379.5601	1389.0660	
1413.0393	1416.9439	1419.2587	
1425.4139	1491.3468	1492.6923	
1493.4829	1497.1058	1506.9211	
1507.2657	1510.9428	1511.9708	
1520.9312	1525.8972	1587.5465	
3043.6448	3053.1661	3056.8826	
3060.7366	3071.6719	3073.0656	
3079.1930	3083.0189	3112.2412	
3113.2721	3130.6105	3133.1163	
3140.2403	3141.4311	3145.1831	
3147.9062	3165.4764	3169.7533	
Zero-point correction (Hartree): 0.261168			
diC2H5CH3CH_COO.ppptRR			
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E(RM062X/Aug-CC-pVTZ) (Hartree): -504.06173205			
Electronic state : 1-A			
Cartesian coordinates (Angs):			
C	-0.160469	0.512769	0.230749
O	-0.103207	1.767365	0.289075
O	0.962612	2.427587	-0.269643
C	-1.403201	-0.019334	0.906945
C	-2.650281	0.324625	0.066277
C	-1.354662	-1.489839	1.310452
H	-1.481119	0.571831	1.822138
C	-2.645333	-0.246146	-1.346070
H	-3.522589	-0.039595	0.612600
H	-2.734234	1.410043	0.016456
H	-0.419475	-1.743135	1.809050
H	-1.479634	-2.158453	0.462689
H	-2.167680	-1.683621	2.009180
H	-2.589885	-1.334714	-1.346718
H	-1.803196	0.139948	-1.923699
H	-3.556761	0.035362	-1.870966
C	0.965167	-0.205421	-0.428677
C	2.146590	-0.205123	0.571944
C	0.681394	-1.593318	-0.994233
H	1.255439	0.476110	-1.234082
C	3.455649	-0.608564	-0.092431
H	2.243047	0.798510	0.983659
H	1.913270	-0.892333	1.389837
H	-0.273776	-1.640973	-1.513585
H	0.697682	-2.362658	-0.223704
H	1.455358	-1.838566	-1.719256
H	3.677384	0.060018	-0.924910
H	3.422821	-1.629704	-0.471520
H	4.278990	-0.545577	0.617637
Rotational constants (GHz):			
Vibrational harmonic frequencies (cm-1):			
49.6042	69.4331	82.9170	
122.8933	182.3665	198.3610	
226.1794	238.9264	269.4498	
272.6305	281.6654	303.4392	
319.4086	321.1859	341.0362	
358.4771	430.4348	483.2952	
520.8487	634.6468	703.1703	

745.6021	786.7757	795.0202
845.1515	869.6091	949.0358
984.6492	991.7191	1013.2081
1023.2156	1030.1529	1045.1091
1081.2968	1105.0400	1141.5147
1150.0286	1182.2119	1198.4535
1278.8424	1287.0363	1308.6266
1325.6213	1333.7123	1357.4010
1376.5442	1381.5778	1389.8113
1410.4383	1418.0614	1420.5110
1425.0210	1481.4182	1489.0152
1494.5818	1498.1741	1501.7398
1506.5673	1507.7977	1513.1528
1522.1655	1527.3028	1590.0378
3044.7190	3058.1019	3059.2941
3064.3592	3064.5635	3072.3689
3075.8771	3081.7985	3110.4039
3117.0398	3130.6332	3136.7906
3138.3013	3139.2544	3140.2393
3147.3994	3160.1542	3165.8518

Zero-point correction (Hartree): 0.261079

diC2H5CH3CH_COO.pptmRR

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E(RM062X/Aug-CC-pVTZ) (Hartree): -504.05917149

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.423452  | -0.570346 | -0.392186 |
| O | 1.144029  | -1.507070 | -0.828594 |
| O | 2.457399  | -1.584267 | -0.457725 |
| C | -1.013585 | -0.729521 | -0.826852 |
| C | -1.942702 | -1.153204 | 0.336351  |
| C | -1.580823 | 0.428347  | -1.649868 |
| H | -0.968842 | -1.594041 | -1.490665 |
| C | -2.516571 | -0.052416 | 1.220371  |
| H | -2.776894 | -1.680841 | -0.130563 |
| H | -1.422810 | -1.892716 | 0.948742  |
| H | -0.983650 | 0.596650  | -2.544696 |
| H | -1.638486 | 1.361524  | -1.096733 |
| H | -2.591041 | 0.165091  | -1.966018 |
| H | -3.040307 | 0.701039  | 0.631994  |
| H | -1.755595 | 0.451344  | 1.811535  |
| H | -3.236974 | -0.481741 | 1.915716  |
| C | 1.054612  | 0.414927  | 0.534118  |
| C | 0.459876  | 1.820530  | 0.553871  |
| C | 1.115248  | -0.249904 | 1.924308  |
| H | 2.089160  | 0.467954  | 0.184802  |
| C | 0.838488  | 2.629351  | -0.682187 |
| H | -0.621013 | 1.793917  | 0.681701  |
| H | 0.851759  | 2.321769  | 1.441147  |
| H | 1.580892  | -1.230481 | 1.846153  |
| H | 0.124558  | -0.348976 | 2.366120  |
| H | 1.722190  | 0.368171  | 2.584374  |
| H | 0.549617  | 2.117916  | -1.600379 |
| H | 1.917348  | 2.779193  | -0.720608 |
| H | 0.360680  | 3.608339  | -0.679626 |

Rotational constants (GHz): 1.1125700 0.9029900 0.7655600

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| 70.9668   | 85.2990   | 134.8989  |
| 144.8927  | 158.8079  | 201.7602  |
| 209.0212  | 234.0295  | 239.9843  |
| 258.4502  | 260.4691  | 265.9312  |
| 321.6022  | 329.7621  | 345.3223  |
| 376.0044  | 429.1881  | 454.5642  |
| 551.4941  | 643.9891  | 670.1998  |
| 735.5690  | 782.3809  | 806.1441  |
| 843.3794  | 894.8537  | 958.8244  |
| 978.9303  | 994.0263  | 1020.3177 |
| 1023.2360 | 1035.0701 | 1041.1690 |
| 1066.2645 | 1118.8072 | 1129.2484 |
| 1151.3910 | 1173.7693 | 1200.9203 |
| 1283.1015 | 1289.8972 | 1316.0138 |
| 1326.7805 | 1345.4215 | 1369.3559 |
| 1380.3321 | 1383.0454 | 1395.1591 |
| 1400.9357 | 1415.6880 | 1417.3213 |
| 1421.3125 | 1485.0918 | 1490.3485 |
| 1497.3306 | 1499.5004 | 1501.8466 |
| 1505.7424 | 1512.2067 | 1516.5372 |
| 1517.5653 | 1524.9845 | 1591.2273 |
| 3058.0768 | 3062.7077 | 3067.8073 |
| 3071.5388 | 3072.9623 | 3073.8371 |
| 3075.9932 | 3082.7698 | 3095.8290 |
| 3123.6106 | 3134.3566 | 3135.4637 |
| 3141.1030 | 3142.4360 | 3144.7424 |
| 3157.7207 | 3164.9230 | 3175.0861 |

Zero-point correction (Hartree): 0.261326

diC2H5CH3CH\_COO.pptpRR

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E(RM062X/Aug-CC-pVTZ) (Hartree): -504.05463377

Electronic state : 1-A

Cartesian coordinates (Angs):

C	0.482333	0.646269	0.374949
O	1.201653	1.680473	0.302839
O	2.535070	1.575908	0.027400
C	-0.952268	1.039068	0.671533
C	-1.699069	1.441231	-0.619381
C	-1.763445	0.087748	1.545919
H	-0.838350	1.969152	1.231356
C	-2.113264	0.301405	-1.537959
H	-2.590216	1.987665	-0.303408
H	-1.075644	2.150990	-1.164415

H	-1.282772	-0.074944	2.509279
H	-1.937672	-0.878667	1.082548
H	-2.735485	0.544998	1.733358
H	-2.786392	-0.395199	-1.038049
H	-1.251008	-0.257692	-1.898361
H	-2.636426	0.693879	-2.408853
C	1.174285	-0.666729	0.182296
C	0.547877	-1.930247	0.786040
C	1.560802	-0.845847	-1.297565
H	2.123197	-0.470631	0.695295
C	-0.448691	-2.681527	-0.092106
H	1.381197	-2.604692	0.993600
H	0.108914	-1.704907	1.756482
H	2.077367	0.039394	-1.657757
H	0.690932	-1.046830	-1.919419
H	2.234382	-1.699272	-1.379935
H	0.048008	-3.124037	-0.954621
H	-1.240620	-2.038410	-0.471664
H	-0.914560	-3.490069	0.470299
Rotational constants (GHz): 1.0948000 0.9855900 0.7210900			
Vibrational harmonic frequencies (cm-1):			
53.3403	105.0807	126.1361	
149.7322	176.5234	216.8652	
233.0723	234.7265	251.5449	
277.2979	291.2374	304.5891	
319.7796	325.6168	340.6426	
356.5989	422.8034	535.8706	
544.2162	617.2785	656.6387	
738.6583	786.9489	799.0627	
839.7371	894.2086	959.8116	
969.7791	990.1493	1004.1489	
1026.0776	1030.9110	1036.2983	
1074.6859	1120.2419	1133.6679	
1162.9773	1165.2390	1195.8674	
1271.2504	1309.8020	1310.3832	
1314.2507	1341.1463	1372.5660	
1378.5238	1383.2748	1390.5412	
1395.8592	1412.9312	1418.9762	
1421.8159	1487.2251	1491.1204	
1493.5493	1500.0836	1503.5830	
1507.5062	1510.6756	1515.5740	
1523.5030	1529.8461	1571.6517	
3026.2873	3061.5703	3070.0900	
3070.7715	3074.5684	3075.0479	
3076.6391	3078.9116	3104.6608	
3120.6989	3136.5447	3137.0549	
3140.4808	3142.6649	3152.0386	
3156.9862	3173.5462	3184.6056	
Zero-point correction (Hartree): 0.261549			
dic2H5CH3CH_COO.ppttRR			
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E(RM062X/Aug-CC-pVT2) (Hartree): -504.05950741			
Electronic state : 1-A			
Cartesian coordinates (Angs):			
C	-0.116393	0.857299	0.272582
O	-0.033452	2.114364	0.249316
O	1.171726	2.710187	0.004069
C	-1.538172	0.403171	0.494595
C	-2.214199	-0.086414	-0.806834
C	-1.730367	-0.559895	1.666969
H	-2.050156	1.330681	0.755267
C	-1.923695	-1.513930	-1.252118
H	-3.289292	0.010117	-0.641096
H	-1.965926	0.611630	-1.608716
H	-1.275686	-0.166791	2.575647
H	-1.317986	-1.546047	1.478220
H	-2.799489	-0.674559	1.848768
H	-2.187512	-2.237819	-0.481511
H	-0.877842	-1.662211	-1.510603
H	-2.514098	-1.749404	-2.136743
C	1.133787	0.079407	0.034409
C	1.173539	-1.335130	0.610851
C	1.448625	0.145967	-1.474338
H	1.900325	0.689265	0.523417
C	2.538367	-1.986771	0.413371
H	0.954862	-1.290376	1.678759
H	0.406234	-1.963218	0.157036
H	1.331259	1.166114	-1.832784
H	0.803046	-0.523018	-2.042831
H	2.481540	-0.149346	-1.645175
H	3.333913	-1.342134	0.789953
H	2.739069	-2.186883	-0.638009
H	2.592606	-2.934642	0.946391
Rotational constants (GHz): 1.0683600 0.9326400 0.6799700			
Vibrational harmonic frequencies (cm-1):			
48.8934	62.8392	115.2520	
145.4664	148.9363	177.2536	
195.6516	228.4577	245.3935	
250.1844	265.1515	288.6000	
321.3893	326.5916	344.7461	
362.5572	430.5371	461.1190	
548.2792	640.1901	688.0781	
740.7431	785.5918	812.9149	
843.5644	904.2087	960.2573	
973.3812	981.9405	992.9615	
1025.4727	1030.1584	1048.0963	
1073.5900	1119.8522	1135.1744	
1161.3311	1178.2117	1199.4533	
1284.8043	1300.7092	1317.1396	
1325.4104	1337.4010	1349.5962	
1379.8045	1386.2601	1395.7740	

1399.6514	1415.5395	1417.8232
1420.8266	1482.9700	1487.2613
1493.7751	1499.6809	1503.8247
1504.6068	1512.2185	1517.9827
1523.5852	1527.2913	1591.0119
3044.5471	3058.6003	3064.8596
3071.7517	3073.6555	3075.4540
3079.4157	3083.0033	3096.9111
3113.0955	3134.5726	3136.2282
3136.9013	3142.8247	3151.1029
3162.0533	3166.2698	3181.0922

Zero-point correction (Hartree): 0.261100

dic2H5CH3CH_COO.ptmmRR

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E(RM062X/Aug-CC-pVTZ) (Hartree): -504.06804000

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.162765 | -0.348999 | -0.409662 |
| O | -0.673702 | -0.391506 | -1.550366 |
| O | -2.036528 | -0.301847 | -1.683713 |
| C | 1.333528  | -0.464330 | -0.397247 |
| C | 1.960592  | 0.852862  | 0.088097  |
| C | 1.769079  | -1.668937 | 0.442192  |
| H | 1.636812  | -0.625431 | -1.433406 |
| C | 3.482536  | 0.845037  | 0.009155  |
| H | 1.567568  | 1.668199  | -0.521779 |
| H | 1.645742  | 1.049180  | 1.115999  |
| H | 1.273960  | -2.579699 | 0.107789  |
| H | 1.540555  | -1.519189 | 1.498522  |
| H | 2.842428  | -1.819856 | 0.348254  |
| H | 3.818260  | 0.580560  | -0.994484 |
| H | 3.920158  | 0.135297  | 0.709578  |
| H | 3.881494  | 1.829806  | 0.246684  |
| C | -0.970907 | -0.247789 | 0.843757  |
| C | -1.955292 | 0.933829  | 0.878225  |
| C | -1.697511 | -1.583112 | 1.074982  |
| H | -0.246494 | -0.102938 | 1.648399  |
| C | -1.382745 | 2.221865  | 0.305787  |
| H | -2.850522 | 0.657825  | 0.329310  |
| H | -2.228771 | 1.074751  | 1.926608  |
| H | -0.997051 | -2.406716 | 1.208482  |
| H | -2.347618 | -1.792181 | 0.228307  |
| H | -2.303638 | -1.500830 | 1.976804  |
| H | -1.183532 | 2.103244  | -0.760819 |
| H | -0.457160 | 2.509563  | 0.808682  |
| H | -2.089442 | 3.042681  | 0.417986  |

Rotational constants (GHz): 1.4200600 0.7446400 0.6750600

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| 60.3571   | 86.8735   | 88.7025   |
| 118.1742  | 164.9222  | 197.6013  |
| 205.5169  | 217.4965  | 222.9997  |
| 252.0487  | 265.1768  | 283.4861  |
| 305.0317  | 307.6945  | 345.3452  |
| 366.4859  | 427.1998  | 433.4300  |
| 489.4986  | 656.4386  | 733.2684  |
| 741.6905  | 791.2176  | 816.1342  |
| 856.8994  | 887.0000  | 959.5003  |
| 974.6678  | 984.5034  | 1008.2183 |
| 1024.9360 | 1033.1578 | 1040.7794 |
| 1077.0364 | 1113.6490 | 1141.8113 |
| 1146.5620 | 1185.5741 | 1191.5177 |
| 1262.1779 | 1289.2616 | 1304.6842 |
| 1319.0205 | 1325.1201 | 1361.9755 |
| 1372.1469 | 1382.7782 | 1393.0057 |
| 1410.1576 | 1412.5876 | 1416.6540 |
| 1431.4374 | 1480.8701 | 1486.1216 |
| 1495.5687 | 1498.5999 | 1499.9703 |
| 1502.5131 | 1508.8691 | 1511.8536 |
| 1517.2685 | 1520.4315 | 1642.3219 |
| 3053.0915 | 3055.9030 | 3060.9898 |
| 3064.8387 | 3066.8157 | 3069.1555 |
| 3073.9157 | 3081.6521 | 3100.9886 |
| 3117.8389 | 3135.1957 | 3136.1895 |
| 3136.5551 | 3139.0038 | 3142.5112 |
| 3154.3421 | 3157.5463 | 3163.7814 |

Zero-point correction (Hartree): 0.260755

dic2H5CH3CH\_COO.ptmpRR

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E(RM062X/Aug-CC-pVTZ) (Hartree): -504.06170159

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-0.090184	-0.482065	-0.258859
O	-0.620308	-1.007240	-1.262320
O	-1.982281	-1.105467	-1.361088
C	1.412395	-0.492018	-0.296814
C	1.990841	0.913417	-0.085311
C	1.939378	-1.503946	0.729048
H	1.687891	-0.834896	-1.295798
C	3.504112	0.956678	-0.261278
H	1.523002	1.596549	-0.797293
H	1.728238	1.269403	0.914064
H	1.449843	-2.469920	0.610778
H	1.774357	-1.154319	1.748997
H	3.008708	-1.652279	0.592805
H	3.794368	0.546589	-1.229487
H	4.015895	0.387297	0.513216
H	3.866760	1.981903	-0.209636
C	-0.843903	0.056725	0.917657
C	-1.318351	1.509982	0.680966
C	-1.963197	-0.856271	1.430157

H	-0.091415	0.120318	1.707533
C	-2.228577	1.733464	-0.519167
H	-1.830385	1.809251	1.598806
H	-0.442558	2.155434	0.594186
H	-1.668239	-1.904803	1.402259
H	-2.861819	-0.756974	0.833274
H	-2.173343	-0.585525	2.465509
H	-3.130201	1.129545	-0.459885
H	-1.732374	1.463736	-1.450926
H	-2.513104	2.784556	-0.569535
Rotational constants (GHz): 1.4935800 0.7139200 0.6467800			
Vibrational harmonic frequencies (cm-1):			
51.3911	59.6740	101.9786	
130.4624	150.3835	173.0769	
187.4700	198.5899	221.4254	
259.5341	264.5667	290.4831	
301.3824	313.3717	345.4713	
355.0349	369.5272	490.5201	
511.0134	658.3196	718.6389	
762.4325	793.5926	800.6752	
856.7244	877.6072	962.1985	
975.0294	987.9413	1003.3257	
1012.6673	1037.7529	1046.0993	
1077.9351	1123.7531	1126.4969	
1152.0074	1182.4558	1194.1053	
1262.1924	1292.8116	1299.3936	
1320.9209	1324.7583	1357.7061	
1378.7589	1388.3920	1410.5104	
1411.7946	1416.0075	1430.3008	
1439.2871	1479.8403	1485.1174	
1487.5108	1494.9123	1499.9864	
1501.1267	1502.6393	1507.3331	
1510.0198	1518.1106	1638.6925	
3052.1165	3054.5124	3063.0435	
3066.2792	3067.6966	3070.7927	
3072.5912	3080.4299	3095.8876	
3096.4368	3132.9839	3135.0682	
3136.1213	3138.1296	3142.8005	
3152.3979	3162.5023	3198.6853	
Zero-point correction (Hartree): 0.260626			
diC2H5CH3CH_COO.ptmtRR			
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E(RM062X/Aug-CC-pVTZ) (Hartree): -504.06563134			
Electronic state : 1-A			
Cartesian coordinates (Angs):			
C	0.024351	-0.690413	-0.142459
O	-0.292571	-1.654192	-0.872679
O	-1.616633	-1.886680	-1.156069
C	1.498677	-0.521389	0.067938
C	1.960322	0.784994	-0.600845
C	1.837251	-0.574988	1.560309
H	1.983253	-1.357983	-0.438605
C	3.466740	0.995391	-0.509168
H	1.658847	0.760666	-1.649780
H	1.441341	1.631115	-0.142870
H	1.427172	-1.472056	2.022775
H	1.444857	0.295627	2.087697
H	2.916417	-0.592747	1.697790
H	4.004206	0.130831	-0.901033
H	3.789054	1.156058	0.518574
H	3.766719	1.866981	-1.088523
C	-0.975229	0.234136	0.466988
C	-1.820582	0.960447	-0.598839
C	-1.832572	-0.516704	1.496893
H	-0.394979	0.993271	0.996723
C	-2.369873	2.276637	-0.063520
H	-1.208062	1.154608	-1.482445
H	-2.617874	0.295860	-0.919511
H	-1.218880	-0.907031	2.308882
H	-2.353552	-1.337627	1.011708
H	-2.559888	0.169191	1.928588
H	-1.563658	2.961699	0.204918
H	-2.985423	2.121866	0.822893
H	-2.990322	2.767982	-0.811588
Rotational constants (GHz): 1.3150300 0.7171000 0.6179100			
Vibrational harmonic frequencies (cm-1):			
31.2364	55.9640	59.4789	
77.6117	154.0358	171.9220	
188.3664	200.5350	212.2942	
235.0765	253.3583	264.6615	
283.1960	304.8076	350.1640	
356.0328	401.3034	435.8248	
493.9178	652.6741	736.1975	
774.2063	785.5112	807.9968	
852.7048	888.2695	954.6930	
974.1019	981.7135	998.5732	
1009.4961	1032.4523	1055.0149	
1077.8952	1119.2996	1121.1503	
1149.8906	1183.1044	1189.7672	
1254.2861	1284.0641	1297.1885	
1323.0834	1342.6347	1356.3200	
1363.2979	1383.2117	1392.8023	
1411.7072	1412.6038	1415.7919	
1434.0095	1485.8028	1492.0382	
1493.4707	1499.0321	1501.5223	
1504.4175	1507.1948	1507.6111	
1518.4296	1520.0560	1645.7258	
3052.0655	3057.4989	3063.6617	
3064.8740	3066.8642	3069.0747	
3070.4816	3081.9785	3097.1392	
3118.0927	3134.3775	3135.3903	

3136.5012 3138.5744 3143.2505
 3153.5616 3155.7109 3169.4215
 Zero-point correction (Hartree): 0.260006

diC2H5CH3CH_COO.ptpmRR

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 E(RM062X/Aug-CC-pVTZ) (Hartree): -504.06381370

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.175098 | -0.506181 | -0.097959 |
| O | -0.527435 | -1.703526 | 0.038725  |
| O | -1.720263 | -2.140372 | -0.474463 |
| C | 1.158462  | -0.217904 | 0.536831  |
| C | 2.279681  | -0.116205 | -0.515563 |
| C | 1.109263  | 0.999217  | 1.462928  |
| H | 1.369988  | -1.102196 | 1.142206  |
| C | 3.664002  | -0.243659 | 0.109965  |
| H | 2.143129  | -0.909103 | -1.253527 |
| H | 2.203700  | 0.832134  | -1.047278 |
| H | 0.289044  | 0.921494  | 2.175953  |
| H | 0.991834  | 1.926165  | 0.902693  |
| H | 2.035927  | 1.066110  | 2.029736  |
| H | 3.757145  | -1.181467 | 0.658553  |
| H | 3.871259  | 0.573516  | 0.799751  |
| H | 4.434540  | -0.227180 | -0.659174 |
| C | -1.063964 | 0.448769  | -0.824757 |
| C | -1.966520 | 1.212815  | 0.170454  |
| C | -0.316882 | 1.423465  | -1.732370 |
| H | -1.709329 | -0.194938 | -1.422942 |
| C | -2.722331 | 0.329239  | 1.153881  |
| H | -1.363373 | 1.948406  | 0.706710  |
| H | -2.674023 | 1.780896  | -0.436644 |
| H | 0.306590  | 0.906149  | -2.459922 |
| H | 0.307901  | 2.117426  | -1.170751 |
| H | -1.050193 | 2.013714  | -2.281040 |
| H | -2.039598 | -0.242498 | 1.785545  |
| H | -3.344304 | -0.392604 | 0.630259  |
| H | -3.348331 | 0.937819  | 1.805315  |

Rotational constants (GHz):            1.4730800            0.7253000            0.6551300

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| 48.1206   | 67.0175   | 81.2002   |
| 123.6655  | 152.5575  | 195.7823  |
| 213.1190  | 229.7202  | 241.2619  |
| 246.0623  | 270.0554  | 289.7929  |
| 294.9044  | 308.8212  | 352.9930  |
| 359.0858  | 389.0877  | 451.8217  |
| 519.0600  | 652.3672  | 701.2303  |
| 733.6248  | 785.4021  | 811.4954  |
| 858.0275  | 877.8033  | 956.0425  |
| 975.1988  | 982.5002  | 1013.3901 |
| 1016.4148 | 1038.9776 | 1058.4222 |
| 1074.2225 | 1118.0030 | 1129.6892 |
| 1148.9429 | 1181.9414 | 1194.0389 |
| 1281.1747 | 1297.3239 | 1323.9987 |
| 1328.0621 | 1335.1498 | 1365.2692 |
| 1367.0507 | 1382.8151 | 1387.9933 |
| 1409.1853 | 1416.1603 | 1421.0552 |
| 1425.9636 | 1483.7499 | 1487.3350 |
| 1494.6044 | 1500.2964 | 1502.5745 |
| 1503.7970 | 1508.2000 | 1510.0219 |
| 1513.0256 | 1516.8060 | 1608.1094 |
| 3060.7013 | 3063.2545 | 3065.3694 |
| 3066.3364 | 3069.4262 | 3071.7582 |
| 3075.0921 | 3089.5226 | 3105.0065 |
| 3115.7392 | 3125.4200 | 3136.5606 |
| 3139.2155 | 3140.4694 | 3143.5644 |
| 3147.8705 | 3153.4130 | 3161.6875 |

Zero-point correction (Hartree): 0.260718

diC2H5CH3CH\_COO.ptppRR

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 E(RM062X/Aug-CC-pVTZ) (Hartree): -504.06211193

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-0.141440	-0.541922	0.056367
O	-0.326999	-1.723908	0.441906
O	-1.418668	-2.421571	-0.003805
C	1.180812	-0.000875	0.536951
C	2.270924	-0.388899	-0.484006
C	1.207952	1.489799	0.874710
H	1.391920	-0.566180	1.447755
C	3.669962	-0.024474	-0.003610
H	2.208815	-1.463392	-0.659641
H	2.069804	0.103251	-1.437775
H	0.298133	1.809627	1.378687
H	1.345535	2.101830	-0.015068
H	2.043104	1.689169	1.543683
H	3.869105	-0.462314	0.975679
H	3.800004	1.054030	0.076113
H	4.421317	-0.398291	-0.697266
C	-1.147249	0.078057	-0.854320
C	-2.485905	0.307354	-0.109940
C	-0.695999	1.328925	-1.600651
H	-1.351689	-0.728982	-1.567407
C	-2.386833	1.203002	1.118590
H	-3.170464	0.749139	-0.836448
H	-2.881851	-0.664472	0.171347
H	0.287526	1.216922	-2.053968
H	-0.677986	2.208254	-0.960500
H	-1.407528	1.522017	-2.402703
H	-1.980234	2.187947	0.885309
H	-1.760231	0.746733	1.887672

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H          -3.373290      1.352741      1.555175
Rotational constants (GHz): 1.4493100      0.7555900      0.6253000
Vibrational harmonic frequencies (cm-1):
63.8296      76.6102      93.3671
108.4601      158.4582      203.2314
212.3686      241.3410      249.0676
272.8004      289.0282      304.5139
323.0040      327.9465      352.9438
368.2333      388.8994      475.0007
518.2058      657.4433      688.5621
742.6835      787.6076      797.2618
848.4089      868.1434      957.7077
979.0544      987.6456      1014.3325
1022.1684      1027.8523      1046.9140
1078.5818      1101.6600      1137.5732
1151.0716      1179.8666      1196.2904
1270.1866      1283.2451      1299.5891
1320.8512      1331.9243      1360.1066
1360.1819      1380.8791      1387.5496
1412.1198      1414.6284      1419.8572
1423.6199      1487.3182      1492.3513
1495.2409      1499.0536      1502.4280
1507.2813      1508.6849      1514.8931
1519.3602      1524.7373      1596.9683
3036.3813      3053.6727      3060.6624
3064.6878      3071.9843      3072.7749
3079.3801      3083.0653      3108.6129
3115.0363      3132.6754      3134.7793
3141.8297      3144.1840      3150.0799
3155.1570      3158.6777      3162.6128
Zero-point correction (Hartree): 0.260936

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diC2H5CH3CH_COO.ptptRR
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E (RM062X/Aug-CC-pVTZ) (Hartree): -504.06506655
Electronic state : 1-A
Cartesian coordinates (Angs):
C      0.012889      -0.614276      -0.087278
O      -0.265754      -1.840095      -0.057745
O      -1.523619      -2.244732      -0.423710
C      1.392682      -0.305686      0.417020
C      2.299667      0.346027      -0.642097
C      1.305422      0.521463      1.705297
H      1.822092      -1.278819      0.664689
C      3.775680      0.148795      -0.315727
H      2.086949      -0.089371      -1.620541
H      2.078862      1.410789      -0.713622
H      0.698891      0.014868      2.455159
H      0.870587      1.502840      1.519922
H      2.301376      0.667785      2.120019
H      4.026399      -0.911597      -0.281705
H      4.034978      0.586504      0.647940
H      4.404308      0.618737      -1.070406
C      -1.047024      0.336720      -0.514937
C      -2.044684      0.476484      0.664296
C      -0.569915      1.685828      -1.035986
H      -1.581960      -0.204316      -1.300224
C      -3.438297      0.850732      0.180564
H      -2.103288      -0.473939      1.193880
H      -1.659263      1.229498      1.356357
H      0.068827      1.581011      -1.911306
H      -0.030148      2.256458      -0.281152
H      -1.436534      2.274849      -1.332163
H      -3.829178      0.058937      -0.458256
H      -3.437690      1.782319      -0.385708
H      -4.118744      0.975539      1.021846

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Rotational constants (GHz): 1.5995000      0.6736100      0.5807000
Vibrational harmonic frequencies (cm-1):
47.8331      70.4863      80.5702
103.9401      160.8021      196.3567
211.0236      215.5480      229.6140
257.4657      268.3466      288.7361
302.5876      306.5212      352.3329
364.7688      411.9609      434.1290
520.5942      662.2625      714.1330
763.4576      781.0131      796.2878
860.8659      882.1762      963.2609
978.9954      985.5177      1007.8620
1013.6601      1027.4848      1054.0018
1078.1345      1115.1412      1132.1375
1152.6478      1186.7653      1197.2634
1285.1814      1300.6295      1320.9690
1324.8443      1327.8947      1357.9614
1372.3532      1387.5995      1394.2658
1406.7058      1410.7941      1417.7655
1425.5983      1477.2244      1488.5935
1496.6890      1500.5764      1503.0864
1503.9093      1506.3036      1509.0663
1512.3831      1519.4978      1605.1470
3052.9533      3063.8351      3065.5740
3067.1092      3067.9459      3071.5347
3075.0644      3078.5344      3114.2743
3115.7414      3135.5502      3138.6102
3140.3286      3141.3683      3142.1725
3147.4870      3148.0764      3154.5938
Zero-point correction (Hartree): 0.260742

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diC2H5CH3CH_COO.pttmRR
~~~~~
E (RM062X/Aug-CC-pVTZ) (Hartree): -504.06355171
Electronic state : 1-A
Cartesian coordinates (Angs):

```

C	0.314075	-0.572744	-0.387733
O	0.679841	-1.614543	-0.989255
O	1.962765	-2.066946	-0.835809
C	-1.149293	-0.273677	-0.580554
C	-1.891184	-0.319295	0.766427
C	-1.418493	1.013285	-1.367557
H	-1.517788	-1.106760	-1.183302
C	-3.402916	-0.218086	0.601182
H	-1.643090	-1.257367	1.266624
H	-1.538924	0.484920	1.414691
H	-0.813976	1.051344	-2.272464
H	-1.219916	1.906842	-0.778200
H	-2.463604	1.035005	-1.670702
H	-3.768256	-0.969999	-0.099845
H	-3.702984	0.761501	0.232037
H	-3.903017	-0.378244	1.554904
C	1.299321	0.116872	0.496111
C	1.090182	1.613663	0.712903
C	1.342534	-0.673507	1.819877
H	2.260577	-0.053127	0.005260
C	1.540371	2.452117	-0.478429
H	0.054337	1.832466	0.973923
H	1.679697	1.896106	1.587246
H	1.449313	-1.738616	1.622722
H	0.445187	-0.493671	2.411566
H	2.204454	-0.343989	2.398143
H	1.050209	2.140047	-1.400021
H	2.614296	2.344702	-0.630126
H	1.325055	3.508992	-0.325300

Rotational constants (GHz): 1.1635400 0.8220600 0.6807700

Vibrational harmonic frequencies (cm-1):

68.8412	87.5331	112.8475
141.2132	151.7771	191.8812
207.6123	222.8109	235.4197
244.9823	266.8962	272.4693
312.2123	331.4272	355.9343
373.7548	407.1463	438.4403
519.6523	658.0243	693.1920
737.6996	791.7728	808.0110
861.7998	895.5584	962.8515
974.3993	986.4564	1010.5049
1023.0453	1041.5744	1044.8976
1071.0393	1105.4317	1132.6167
1152.1482	1189.4442	1198.4564
1275.5208	1297.4219	1302.5887
1331.8181	1337.3931	1367.6131
1370.0135	1385.6528	1389.8564
1401.8581	1411.7266	1416.2694
1418.6490	1484.5739	1492.9215
1497.4533	1500.7264	1502.1812
1503.7358	1508.6264	1511.5602
1517.4772	1522.7332	1601.3896
3062.3801	3065.2331	3067.6216
3069.0804	3070.4196	3071.8652
3074.9965	3078.3450	3102.5899
3113.6880	3135.4305	3139.0232
3141.8488	3142.9485	3144.4299
3150.0538	3156.9769	3157.8135

Zero-point correction (Hartree): 0.261024

dic2H5CH3CH_COO.pttpRR

~~~~~

E(RM062X/Aug-CC-pVTZ) (Hartree): -504.05971692

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.451878 | -0.711076 | 0.308223  |
| O | -0.915938 | -1.881753 | 0.307844  |
| O | -2.253866 | -2.085259 | 0.105147  |
| C | 1.044316  | -0.699341 | 0.458542  |
| C | 1.694963  | -0.380727 | -0.901059 |
| C | 1.556567  | 0.177837  | 1.603808  |
| H | 1.299393  | -1.734469 | 0.696123  |
| C | 3.215488  | -0.460306 | -0.851237 |
| H | 1.312383  | -1.093642 | -1.634058 |
| H | 1.388433  | 0.608884  | -1.240230 |
| H | 0.972247  | 0.020419  | 2.509655  |
| H | 1.535719  | 1.237160  | 1.357654  |
| H | 2.587262  | -0.091973 | 1.826685  |
| H | 3.541759  | -1.421388 | -0.450772 |
| H | 3.637630  | 0.325862  | -0.226319 |
| H | 3.637281  | -0.352060 | -1.849084 |
| C | -1.408008 | 0.414384  | 0.089509  |
| C | -1.073748 | 1.792139  | 0.679167  |
| C | -1.749748 | 0.461141  | -1.411642 |
| H | -2.310828 | 0.042731  | 0.582264  |
| C | -0.182076 | 2.718809  | -0.141349 |
| H | -2.036343 | 2.293171  | 0.801715  |
| H | -0.675563 | 1.677495  | 1.687442  |
| H | -2.117039 | -0.511028 | -1.732270 |
| H | -0.884396 | 0.741657  | -2.010990 |
| H | -2.532265 | 1.202518  | -1.575120 |
| H | -0.612803 | 2.911278  | -1.123278 |
| H | 0.820533  | 2.324295  | -0.292497 |
| H | -0.080223 | 3.678031  | 0.365383  |

Rotational constants (GHz): 1.1537100 0.8858100 0.6564000

Vibrational harmonic frequencies (cm-1):

|          |          |          |
|----------|----------|----------|
| 48.4985  | 86.6499  | 113.3071 |
| 135.2133 | 163.4971 | 207.4742 |
| 237.7652 | 239.0440 | 249.8613 |
| 262.4119 | 267.0679 | 283.2068 |
| 312.9793 | 317.5483 | 353.9850 |
| 363.3012 | 377.6707 | 491.1323 |

|           |           |           |
|-----------|-----------|-----------|
| 549.8546  | 654.1743  | 680.8152  |
| 740.3838  | 781.9017  | 795.2107  |
| 856.6049  | 893.7739  | 960.7335  |
| 966.2270  | 977.6530  | 1000.8464 |
| 1020.1121 | 1035.7924 | 1047.8525 |
| 1075.2704 | 1112.4060 | 1141.8981 |
| 1158.4630 | 1177.7049 | 1192.6581 |
| 1290.1424 | 1292.6326 | 1322.8682 |
| 1331.6253 | 1348.0012 | 1370.2373 |
| 1372.9844 | 1384.0341 | 1385.9757 |
| 1402.7827 | 1412.2129 | 1415.9329 |
| 1422.1966 | 1485.8171 | 1490.6018 |
| 1495.0296 | 1501.2105 | 1504.7829 |
| 1507.2972 | 1514.4103 | 1515.7104 |
| 1517.1431 | 1523.9913 | 1593.5215 |
| 3054.5602 | 3062.8316 | 3066.5637 |
| 3069.2015 | 3069.6578 | 3070.9609 |
| 3076.7262 | 3079.7246 | 3108.1778 |
| 3114.1496 | 3134.7881 | 3136.1752 |
| 3139.9519 | 3141.4353 | 3146.3316 |
| 3155.0744 | 3162.1765 | 3167.8445 |

Zero-point correction (Hartree): 0.261279

diC2H5CH3CH\_COO.ptttRR

E(RM062X/Aug-CC-pVTZ) (Hartree): -504.06436165

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.045812 | 0.792929  | -0.289905 |
| O | -0.140076 | 2.042999  | -0.382815 |
| O | -1.359948 | 2.639534  | -0.205311 |
| C | 1.366835  | 0.299259  | -0.429031 |
| C | 1.846031  | -0.324642 | 0.892782  |
| C | 1.574392  | -0.630801 | -1.631064 |
| H | 1.956727  | 1.202480  | -0.598800 |
| C | 3.327381  | -0.680105 | 0.858168  |
| H | 1.657525  | 0.383632  | 1.701945  |
| H | 1.258932  | -1.218373 | 1.112568  |
| H | 1.034075  | -0.273544 | -2.507006 |
| H | 1.253386  | -1.648299 | -1.416301 |
| H | 2.632308  | -0.659539 | -1.885320 |
| H | 3.928275  | 0.188806  | 0.585958  |
| H | 3.532272  | -1.470786 | 0.137528  |
| H | 3.662154  | -1.026974 | 1.834323  |
| C | -1.274340 | 0.009187  | 0.022889  |
| C | -1.263258 | -1.450398 | -0.429471 |
| C | -1.543612 | 0.175354  | 1.532635  |
| H | -2.071379 | 0.549920  | -0.495029 |
| C | -2.595961 | -2.139153 | -0.154689 |
| H | -1.057310 | -1.493383 | -1.499705 |
| H | -0.464226 | -2.002350 | 0.069632  |
| H | -1.440148 | 1.220369  | 1.817643  |
| H | -0.857051 | -0.439558 | 2.116150  |
| H | -2.561541 | -0.132828 | 1.760757  |
| H | -3.421831 | -1.566648 | -0.579267 |
| H | -2.778382 | -2.249074 | 0.913108  |
| H | -2.613531 | -3.133895 | -0.597056 |

Rotational constants (GHz): 1.1612400 0.8051000 0.6176700

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| 64.9476   | 93.3971   | 99.6238   |
| 114.6150  | 154.3124  | 159.0307  |
| 204.7802  | 214.4539  | 236.4140  |
| 261.1172  | 264.2576  | 280.9341  |
| 308.7280  | 321.1377  | 357.5339  |
| 362.3260  | 411.7329  | 437.5725  |
| 522.4306  | 654.7991  | 710.4859  |
| 751.5951  | 794.3456  | 811.7391  |
| 863.5903  | 904.7221  | 961.8722  |
| 972.2114  | 980.5071  | 988.0022  |
| 1012.6383 | 1034.4545 | 1060.6949 |
| 1073.4928 | 1103.4082 | 1144.5148 |
| 1157.0197 | 1188.6530 | 1197.6666 |
| 1278.4890 | 1297.8155 | 1316.2035 |
| 1328.0810 | 1333.8705 | 1346.0211 |
| 1364.3566 | 1383.5846 | 1391.9136 |
| 1399.5435 | 1413.5990 | 1415.5640 |
| 1418.6716 | 1482.4523 | 1490.3996 |
| 1494.6649 | 1501.9728 | 1502.5690 |
| 1506.2308 | 1507.6425 | 1513.2038 |
| 1519.8298 | 1523.6073 | 1605.5108 |
| 3055.8704 | 3061.7899 | 3064.5741 |
| 3065.3446 | 3067.7306 | 3071.3131 |
| 3073.4169 | 3076.7934 | 3101.3671 |
| 3109.5424 | 3134.4061 | 3135.6339 |
| 3141.6451 | 3142.1897 | 3146.9765 |
| 3147.5218 | 3157.3596 | 3159.2277 |

Zero-point correction (Hartree): 0.260814

Population analysis as 298K (%)

Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)

| Compound                           | Qtot      | Erel | Erel2 | n*Q*MB    | %    |
|------------------------------------|-----------|------|-------|-----------|------|
| TS.diC2H5CH3CH_COO.14Hshift.ctptRR | 3.772e+43 | 0.00 | 0.00  | 3.772e+43 | 15   |
| TS.diC2H5CH3CH_COO.14Hshift.mmmRR  | 8.549e+43 | 0.56 | 0.56  | 3.302e+43 | 13.1 |
| TS.diC2H5CH3CH_COO.14Hshift.cmpmRR | 4.204e+43 | 0.18 | 0.18  | 3.111e+43 | 12.3 |
| TS.diC2H5CH3CH_COO.14Hshift.mtptRR | 5.267e+43 | 0.45 | 0.45  | 2.463e+43 | 9.77 |
| TS.diC2H5CH3CH_COO.14Hshift.mpmRR  | 4.529e+43 | 0.40 | 0.40  | 2.317e+43 | 9.19 |
| TS.diC2H5CH3CH_COO.14Hshift.mtmRR  | 4.803e+43 | 0.78 | 0.78  | 1.277e+43 | 5.07 |
| TS.diC2H5CH3CH_COO.14Hshift.mmmRR  | 2.455e+43 | 0.57 | 0.57  | 9.303e+42 | 3.69 |
| TS.diC2H5CH3CH_COO.14Hshift.mtppRR | 7.490e+43 | 1.24 | 1.24  | 9.298e+42 | 3.69 |
| TS.diC2H5CH3CH_COO.14Hshift.mppRR  | 3.487e+43 | 0.80 | 0.80  | 9.056e+42 | 3.59 |

|                                    |           |      |      |           |          |
|------------------------------------|-----------|------|------|-----------|----------|
| TS.dic2H5CH3CH_COO.14Hshift.mtmpRR | 5.109e+43 | 1.08 | 1.08 | 8.223e+42 | 3.26     |
| TS.dic2H5CH3CH_COO.14Hshift.mmmRR  | 3.104e+43 | 0.87 | 0.87 | 7.115e+42 | 2.82     |
| TS.dic2H5CH3CH_COO.14Hshift.pmptRR | 1.349e+43 | 0.39 | 0.39 | 7.008e+42 | 2.78     |
| TS.dic2H5CH3CH_COO.14Hshift.cpptRR | 2.671e+43 | 0.81 | 0.81 | 6.828e+42 | 2.71     |
| TS.dic2H5CH3CH_COO.14Hshift.mpptRR | 3.455e+43 | 1.00 | 1.00 | 6.396e+42 | 2.54     |
| TS.dic2H5CH3CH_COO.14Hshift.ctpmRR | 3.215e+43 | 1.05 | 1.05 | 5.448e+42 | 2.16     |
| TS.dic2H5CH3CH_COO.14Hshift.mtmmRR | 3.820e+43 | 1.21 | 1.21 | 4.915e+42 | 1.95     |
| TS.dic2H5CH3CH_COO.14Hshift.ctmtRR | 6.901e+43 | 1.58 | 1.58 | 4.778e+42 | 1.9      |
| TS.dic2H5CH3CH_COO.14Hshift.mppmRR | 3.619e+43 | 1.46 | 1.46 | 3.060e+42 | 1.21     |
| TS.dic2H5CH3CH_COO.14Hshift.pmmRR  | 3.747e+43 | 1.72 | 1.72 | 2.042e+42 | 0.81     |
| TS.dic2H5CH3CH_COO.14Hshift.mppmRR | 3.033e+43 | 1.71 | 1.71 | 1.687e+42 | 0.669    |
| TS.dic2H5CH3CH_COO.14Hshift.ptptRR | 2.728e+43 | 1.75 | 1.75 | 1.424e+42 | 0.565    |
| TS.dic2H5CH3CH_COO.14Hshift.cppmRR | 1.887e+43 | 1.61 | 1.61 | 1.248e+42 | 0.495    |
| TS.dic2H5CH3CH_COO.14Hshift.pmpmRR | 1.099e+43 | 1.63 | 1.63 | 7.019e+41 | 0.278    |
| TS.dic2H5CH3CH_COO.14Hshift.ptpmRR | 2.192e+43 | 2.42 | 2.42 | 3.705e+41 | 0.147    |
| TS.dic2H5CH3CH_COO.14Hshift.ptmtRR | 5.755e+43 | 3.15 | 3.15 | 2.797e+41 | 0.111    |
| TS.dic2H5CH3CH_COO.14Hshift.pmpmRR | 1.757e+43 | 2.66 | 2.66 | 1.964e+41 | 0.0779   |
| TS.dic2H5CH3CH_COO.14Hshift.ptmpRR | 4.244e+43 | 3.68 | 3.68 | 8.499e+40 | 0.0337   |
| TS.dic2H5CH3CH_COO.14Hshift.ppptRR | 1.092e+43 | 2.89 | 2.89 | 8.308e+40 | 0.033    |
| TS.dic2H5CH3CH_COO.14Hshift.pmmRR  | 1.676e+43 | 3.47 | 3.47 | 4.748e+40 | 0.0188   |
| TS.dic2H5CH3CH_COO.14Hshift.ctmmRR | 5.740e+43 | 4.22 | 4.22 | 4.651e+40 | 0.0185   |
| TS.dic2H5CH3CH_COO.14Hshift.ptmmRR | 2.528e+43 | 4.62 | 4.62 | 1.033e+40 | 0.0041   |
| TS.dic2H5CH3CH_COO.14Hshift.cpmRR  | 3.747e+43 | 5.61 | 5.61 | 2.875e+39 | 0.00114  |
| TS.dic2H5CH3CH_COO.14Hshift.pppmRR | 1.257e+43 | 4.98 | 4.98 | 2.792e+39 | 0.00111  |
| TS.dic2H5CH3CH_COO.14Hshift.pppmRR | 1.734e+43 | 7.25 | 7.25 | 8.345e+37 | 3.31e-05 |
| Total                              |           |      |      | 2.521e+44 | 100      |

TS.dic2H5CH3CH\_COO.14Hshift.cmpmRR

E(RM062X/Aug-CC-pVTZ) (Hartree): -504.03734346

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.104528  | -0.093641 | -0.262935 |
| O | 0.370345  | -0.848817 | -1.284452 |
| O | -0.491273 | -1.947590 | -1.322953 |
| C | 1.170912  | 0.919377  | 0.029792  |
| C | 2.566330  | 0.288321  | 0.057495  |
| C | 1.080326  | 2.043280  | -1.010908 |
| H | 0.947188  | 1.334959  | 1.013374  |
| C | 2.688021  | -0.822534 | 1.091930  |
| H | 2.795313  | -0.098184 | -0.936550 |
| H | 3.288276  | 1.079937  | 0.266739  |
| H | 0.090194  | 2.497789  | -1.026036 |
| H | 1.295195  | 1.652784  | -2.005088 |
| H | 1.809698  | 2.817694  | -0.777159 |
| H | 1.978276  | -1.626622 | 0.887399  |
| H | 2.490531  | -0.443676 | 2.096093  |
| H | 3.687124  | -1.255013 | 1.089129  |
| C | -1.020329 | -0.463150 | 0.510232  |
| H | -0.831604 | -1.673944 | -0.049339 |
| C | -0.983314 | -0.100609 | 1.980467  |
| C | -2.413359 | -0.306080 | -0.136834 |
| C | -2.988581 | 1.095767  | 0.044183  |
| H | -2.349588 | -0.549213 | -1.193912 |
| H | -3.084783 | -1.038100 | 0.316922  |
| H | -1.144680 | 0.964656  | 2.161315  |
| H | -0.037946 | -0.382239 | 2.442152  |
| H | -1.775925 | -0.639601 | 2.501037  |
| H | -2.316659 | 1.847893  | -0.373164 |
| H | -3.153456 | 1.337316  | 1.093627  |
| H | -3.946941 | 1.180442  | -0.467833 |

Rotational constants (GHz): 1.3938100 0.7575300 0.7191300

Vibrational harmonic frequencies (cm-1):

|            |           |           |
|------------|-----------|-----------|
| i1599.3776 | 37.5073   | 74.4858   |
| 79.6536    | 125.7270  | 173.5967  |
| 181.9640   | 216.3025  | 218.5595  |
| 236.4783   | 239.1904  | 260.4473  |
| 277.8366   | 307.4201  | 314.4172  |
| 361.1565   | 423.8549  | 456.3500  |
| 500.8973   | 584.3275  | 649.1654  |
| 726.9071   | 761.4156  | 802.6304  |
| 808.5583   | 862.2902  | 919.8589  |
| 973.8560   | 1000.6509 | 1013.8112 |
| 1028.3806  | 1031.7651 | 1046.2538 |
| 1055.6223  | 1090.8471 | 1121.2098 |
| 1133.7289  | 1150.1775 | 1196.7710 |
| 1216.4084  | 1283.9656 | 1305.1454 |
| 1310.0196  | 1318.2027 | 1360.3221 |
| 1367.3974  | 1380.7057 | 1399.3886 |
| 1407.9612  | 1414.2603 | 1418.5526 |
| 1435.9437  | 1487.1719 | 1489.0610 |
| 1495.2734  | 1499.6400 | 1500.0962 |
| 1503.0210  | 1504.5785 | 1507.6994 |
| 1508.6846  | 1516.9405 | 1561.7779 |
| 1860.1987  | 3048.7922 | 3054.2207 |
| 3057.7337  | 3065.7029 | 3066.7943 |
| 3068.0008  | 3088.5866 | 3105.3064 |
| 3108.3373  | 3124.2442 | 3125.4324 |
| 3131.2549  | 3136.0006 | 3138.1396 |
| 3141.0712  | 3145.8094 | 3154.4021 |

Zero-point correction (Hartree): 0.255739

TS.dic2H5CH3CH\_COO.14Hshift.cpmRR

E(RM062X/Aug-CC-pVTZ) (Hartree): -504.02924560

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.026406  | -0.364988 | 0.103148  |
| O | 0.678410  | -1.481284 | -0.046966 |
| O | -0.122405 | -2.464250 | -0.626767 |
| C | 0.912098  | 0.804303  | 0.447906  |
| C | 2.320342  | 0.385715  | 0.908348  |

|                                                |           |           |           |
|------------------------------------------------|-----------|-----------|-----------|
| C                                              | 0.987698  | 1.823030  | -0.700416 |
| H                                              | 0.422935  | 1.294609  | 1.293611  |
| C                                              | 3.293709  | 0.002731  | -0.202986 |
| H                                              | 2.730469  | 1.236162  | 1.457099  |
| H                                              | 2.235326  | -0.434164 | 1.621418  |
| H                                              | 0.053539  | 2.358365  | -0.838532 |
| H                                              | 1.253033  | 1.337687  | -1.638913 |
| H                                              | 1.762129  | 2.553825  | -0.466695 |
| H                                              | 3.497054  | 0.846113  | -0.862370 |
| H                                              | 2.913744  | -0.819377 | -0.805243 |
| H                                              | 4.243962  | -0.308816 | 0.228579  |
| C                                              | -1.352842 | -0.433937 | -0.212786 |
| H                                              | -0.992749 | -1.528123 | -0.940581 |
| C                                              | -2.202529 | -1.293237 | 0.743905  |
| C                                              | -2.094737 | 0.793003  | -0.711818 |
| C                                              | -2.419781 | 1.858107  | 0.336694  |
| H                                              | -1.558166 | 1.243139  | -1.545853 |
| H                                              | -3.035193 | 0.430786  | -1.134273 |
| H                                              | -2.534193 | -0.690755 | 1.590770  |
| H                                              | -1.651327 | -2.148742 | 1.120994  |
| H                                              | -3.086192 | -1.660533 | 0.221700  |
| H                                              | -1.518214 | 2.283467  | 0.778250  |
| H                                              | -3.020548 | 1.446159  | 1.146525  |
| H                                              | -2.985840 | 2.676114  | -0.108594 |
| Rotational constants (GHz):                    |           |           |           |
|                                                |           | 1.3995000 | 0.6050900 |
| Vibrational harmonic frequencies (cm-1):       |           |           |           |
| i1609.6478                                     | 21.2115   | 96.3011   |           |
| 120.2625                                       | 145.4439  | 163.0046  |           |
| 177.9850                                       | 193.4005  | 209.0125  |           |
| 245.4095                                       | 259.3074  | 279.5349  |           |
| 302.8021                                       | 321.1071  | 338.3802  |           |
| 363.0680                                       | 396.0648  | 432.8735  |           |
| 554.4797                                       | 628.2807  | 663.1727  |           |
| 736.7587                                       | 749.4024  | 786.0699  |           |
| 801.0127                                       | 849.4829  | 941.8286  |           |
| 966.0522                                       | 988.5439  | 1007.6187 |           |
| 1019.0796                                      | 1034.9212 | 1039.4552 |           |
| 1055.5807                                      | 1094.1976 | 1117.0789 |           |
| 1126.9985                                      | 1160.5903 | 1185.4110 |           |
| 1214.4359                                      | 1293.5879 | 1297.6532 |           |
| 1316.5337                                      | 1327.2394 | 1355.5401 |           |
| 1365.5907                                      | 1379.8313 | 1394.5196 |           |
| 1402.1394                                      | 1410.4194 | 1420.2267 |           |
| 1432.7557                                      | 1482.6869 | 1489.7238 |           |
| 1493.9978                                      | 1496.6470 | 1501.8023 |           |
| 1504.9957                                      | 1510.2038 | 1513.2516 |           |
| 1515.8745                                      | 1527.0870 | 1551.1133 |           |
| 1874.7153                                      | 3055.2684 | 3059.8182 |           |
| 3061.2509                                      | 3066.8605 | 3069.7504 |           |
| 3072.8360                                      | 3075.0851 | 3109.2777 |           |
| 3109.4562                                      | 3119.0184 | 3131.0302 |           |
| 3136.8253                                      | 3139.5049 | 3140.4623 |           |
| 3155.6869                                      | 3176.4400 | 3179.9032 |           |
| Zero-point correction (Hartree): 0.256299      |           |           |           |
| TS.diC2H5CH3CH_COO.14Hshift.cppmRR             |           |           |           |
| ~~~~~                                          |           |           |           |
| E(RM062X/Aug-CC-pVTZ) (Hartree): -504.03533904 |           |           |           |
| Electronic state : 1-A                         |           |           |           |
| Cartesian coordinates (Angs):                  |           |           |           |
| C                                              | -0.078018 | 0.325543  | 0.282858  |
| O                                              | -0.499414 | 1.497348  | -0.082702 |
| O                                              | 0.531580  | 2.435951  | -0.016511 |
| C                                              | -1.150651 | -0.683333 | 0.568371  |
| C                                              | -2.578147 | -0.125357 | 0.529880  |
| C                                              | -0.965895 | -1.902411 | -0.344675 |
| H                                              | -0.944899 | -1.010350 | 1.592823  |
| C                                              | -3.127467 | 0.137322  | -0.869088 |
| H                                              | -3.220915 | -0.849188 | 1.034794  |
| H                                              | -2.614787 | 0.792089  | 1.117031  |
| H                                              | 0.005309  | -2.369500 | -0.192298 |
| H                                              | -1.042341 | -1.617467 | -1.393410 |
| H                                              | -1.741406 | -2.639111 | -0.135054 |
| H                                              | -3.233288 | -0.787656 | -1.435368 |
| H                                              | -2.482796 | 0.811452  | -1.430700 |
| H                                              | -4.113165 | 0.595620  | -0.805029 |
| C                                              | 1.305108  | 0.224001  | 0.568674  |
| H                                              | 1.226710  | 1.570052  | 0.714544  |
| C                                              | 1.719967  | -0.800584 | 1.604796  |
| C                                              | 2.293111  | 0.347283  | -0.610781 |
| C                                              | 2.499645  | -0.969046 | -1.355024 |
| H                                              | 1.944211  | 1.111184  | -1.300458 |
| H                                              | 3.248535  | 0.693571  | -0.210751 |
| H                                              | 1.626535  | -1.833092 | 1.260637  |
| H                                              | 1.145710  | -0.701855 | 2.525274  |
| H                                              | 2.769135  | -0.643178 | 1.857726  |
| H                                              | 1.565847  | -1.314487 | -1.800296 |
| H                                              | 2.872483  | -1.755313 | -0.698304 |
| H                                              | 3.225881  | -0.839670 | -2.157527 |
| Rotational constants (GHz):                    |           |           |           |
|                                                |           | 1.4473600 | 0.6587500 |
| Vibrational harmonic frequencies (cm-1):       |           |           |           |
| i1599.5473                                     | 50.4622   | 74.3369   |           |
| 120.8425                                       | 136.2845  | 175.1323  |           |
| 192.5974                                       | 212.8763  | 222.2397  |           |
| 233.5529                                       | 256.0749  | 284.5723  |           |
| 294.2540                                       | 310.1857  | 321.1455  |           |
| 358.3245                                       | 417.1679  | 450.3724  |           |
| 553.8723                                       | 578.3998  | 638.5212  |           |
| 730.3653                                       | 755.3404  | 790.4494  |           |
| 810.0278                                       | 849.4516  | 921.4912  |           |
| 969.5883                                       | 1001.5026 | 1014.6600 |           |
| 1016.9163                                      | 1031.0423 | 1042.0599 |           |

|           |           |           |
|-----------|-----------|-----------|
| 1049.3232 | 1087.6276 | 1112.4479 |
| 1135.0125 | 1165.3122 | 1181.2054 |
| 1218.4578 | 1285.2854 | 1297.4609 |
| 1318.9352 | 1325.6936 | 1355.8417 |
| 1359.8378 | 1377.6685 | 1401.6126 |
| 1407.5391 | 1416.7161 | 1420.0145 |
| 1438.1772 | 1485.0764 | 1490.8495 |
| 1492.6715 | 1494.9392 | 1500.2279 |
| 1503.1441 | 1506.8041 | 1510.4155 |
| 1514.0888 | 1519.7175 | 1552.9287 |
| 1865.7426 | 3048.1333 | 3051.4647 |
| 3060.3685 | 3064.6795 | 3068.3135 |
| 3069.0281 | 3073.4776 | 3108.0572 |
| 3110.5904 | 3124.7573 | 3129.7433 |
| 3130.5855 | 3137.2236 | 3141.5813 |
| 3150.5779 | 3151.1169 | 3152.4557 |

Zero-point correction (Hartree): 0.256014

TS.diC2H5CH3CH\_COO.14Hshift.cpptRR

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E(RM062X/Aug-CC-pVTZ) (Hartree): -504.03643313

Electronic state : 1-A

Cartesian coordinates (Angs):

C	0.148025	0.080154	-0.243707
O	0.323549	1.366081	-0.232089
O	-0.892770	2.027079	-0.422318
C	1.392834	-0.748561	-0.323070
C	2.674727	0.041649	-0.610286
C	1.489123	-1.606578	0.946686
H	1.217915	-1.427785	-1.162778
C	3.227236	0.828714	0.574310
H	3.427999	-0.674987	-0.943579
H	2.491385	0.716954	-1.446202
H	0.617455	-2.249872	1.054465
H	1.557766	-0.978803	1.834063
H	2.379211	-2.234051	0.902737
H	3.550278	0.165884	1.376637
H	2.486592	1.518077	0.976028
H	4.092778	1.412449	0.264691
C	-1.192750	-0.355041	-0.342147
H	-1.411400	0.883731	-0.848204
C	-1.447409	-1.705477	-0.974423
C	-2.095218	-0.071783	0.880964
C	-3.510111	0.341675	0.501597
H	-2.118850	-0.990124	1.476140
H	-1.647206	0.703099	1.499298
H	-1.195532	-2.535280	-0.307686
H	-0.897623	-1.837035	-1.905556
H	-2.506345	-1.799955	-1.213153
H	-4.132221	0.457679	1.388602
H	-3.984374	-0.398745	-0.142883
H	-3.492796	1.294966	-0.026915

Rotational constants (GHz): 1.7426600 0.7015400 0.5872600

Vibrational harmonic frequencies (cm-1):

i1599.6432	44.6380	78.7491
99.5164	133.5227	175.4400
184.1333	210.6718	216.6042
222.9743	265.2356	273.9267
296.7967	308.3863	313.3302
364.8588	376.5163	456.7098
564.8612	571.2640	634.6817
737.9984	773.9278	786.0128
807.4568	848.6981	923.5857
968.2820	1002.5430	1011.5486
1020.6945	1030.8723	1041.9038
1056.6646	1097.9075	1110.2279
1136.4061	1163.8803	1177.8221
1216.8813	1285.8881	1295.6692
1324.4716	1333.0837	1343.7783
1364.1134	1379.8947	1402.2816
1410.5317	1418.4829	1420.7465
1442.6765	1475.7988	1487.6210
1493.8393	1496.4954	1499.5278
1502.5949	1503.5874	1509.5808
1511.3469	1518.2253	1559.8443
1868.6068	3037.7020	3041.7534
3055.5485	3063.1673	3068.7239
3069.5028	3073.8175	3108.2394
3110.2874	3119.9780	3134.9427
3135.6720	3137.8954	3140.5222
3143.3408	3149.2313	3152.2507

Zero-point correction (Hartree): 0.255832

TS.diC2H5CH3CH_COO.14Hshift.ctmmRR

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E(RM062X/Aug-CC-pVTZ) (Hartree): -504.03094499

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.155309 | -0.488858 | -0.033935 |
| O | 0.056056  | -1.756695 | -0.233048 |
| O | -1.128176 | -2.420154 | -0.554149 |
| C | 1.109396  | 0.322544  | -0.011934 |
| C | 2.304471  | -0.503277 | 0.483754  |
| C | 1.360942  | 0.907761  | -1.408809 |
| H | 0.947397  | 1.142946  | 0.688713  |
| C | 3.540413  | 0.351019  | 0.736299  |
| H | 2.021907  | -1.012734 | 1.406037  |
| H | 2.528380  | -1.284629 | -0.243016 |
| H | 0.529156  | 1.520668  | -1.748322 |
| H | 1.511531  | 0.100491  | -2.126160 |
| H | 2.251309  | 1.533121  | -1.396715 |
| H | 3.317825  | 1.169632  | 1.422764  |

|                                                |           |           |                               |
|------------------------------------------------|-----------|-----------|-------------------------------|
| H                                              | 3.934178  | 0.781447  | -0.183329                     |
| H                                              | 4.333563  | -0.248565 | 1.180181                      |
| C                                              | -1.513993 | -0.092297 | -0.065660                     |
| H                                              | -1.693509 | -1.243560 | -0.761131                     |
| C                                              | -2.380007 | -0.606180 | 1.101125                      |
| C                                              | -1.905550 | 1.308750  | -0.506898                     |
| C                                              | -1.468725 | 2.468407  | 0.391652                      |
| H                                              | -1.568410 | 1.492777  | -1.527182                     |
| H                                              | -2.996512 | 1.307451  | -0.559367                     |
| H                                              | -2.383180 | 0.131311  | 1.906003                      |
| H                                              | -2.016258 | -1.550385 | 1.494407                      |
| H                                              | -3.408022 | -0.750070 | 0.769099                      |
| H                                              | -0.410600 | 2.697800  | 0.272642                      |
| H                                              | -1.648380 | 2.246427  | 1.444019                      |
| H                                              | -2.023248 | 3.373448  | 0.145365                      |
| Rotational constants (GHz):                    |           |           | 1.3023600 0.8016200 0.5968700 |
| Vibrational harmonic frequencies (cm-1):       |           |           |                               |
| i1610.2706                                     | 48.9959   | 66.7961   |                               |
| 82.4973                                        | 106.9279  | 151.0401  |                               |
| 168.0832                                       | 183.9681  | 201.5609  |                               |
| 232.7652                                       | 257.8053  | 259.2745  |                               |
| 295.9926                                       | 308.9287  | 326.7861  |                               |
| 344.4192                                       | 388.9117  | 416.5221  |                               |
| 491.8335                                       | 637.6794  | 699.6026  |                               |
| 745.8286                                       | 757.3392  | 780.9436  |                               |
| 787.0073                                       | 862.1159  | 945.0968  |                               |
| 968.4498                                       | 986.4715  | 997.2829  |                               |
| 1006.6682                                      | 1037.3388 | 1061.0388 |                               |
| 1063.1804                                      | 1093.7530 | 1105.4605 |                               |
| 1138.6936                                      | 1159.9584 | 1191.6094 |                               |
| 1212.4105                                      | 1287.5647 | 1301.9269 |                               |
| 1322.5321                                      | 1324.2759 | 1352.1764 |                               |
| 1361.4019                                      | 1384.6543 | 1395.5869 |                               |
| 1400.8539                                      | 1413.4440 | 1416.0172 |                               |
| 1433.7314                                      | 1487.3810 | 1488.5204 |                               |
| 1492.9761                                      | 1497.3515 | 1498.3004 |                               |
| 1503.2282                                      | 1506.4222 | 1510.7690 |                               |
| 1515.9858                                      | 1523.3040 | 1556.2128 |                               |
| 1876.2737                                      | 3056.5820 | 3063.3334 |                               |
| 3064.1540                                      | 3066.5618 | 3073.4918 |                               |
| 3074.0111                                      | 3087.2888 | 3100.7580 |                               |
| 3111.5676                                      | 3118.0027 | 3131.7647 |                               |
| 3133.8659                                      | 3140.3499 | 3141.5961 |                               |
| 3151.2491                                      | 3162.6019 | 3172.8760 |                               |
| Zero-point correction (Hartree): 0.255774      |           |           |                               |
| TS.dic2H5CH3CH_COO.14Hshift.ctmtRR             |           |           |                               |
| ~~~~~                                          |           |           |                               |
| E(RM062X/Aug-CC-pVTZ) (Hartree): -504.03506559 |           |           |                               |
| Electronic state : 1-A                         |           |           |                               |
| Cartesian coordinates (Angs):                  |           |           |                               |
| C                                              | -0.030827 | 0.416849  | -0.049113                     |
| O                                              | -0.235630 | 1.623599  | -0.478454                     |
| O                                              | 0.979064  | 2.273323  | -0.711644                     |
| C                                              | -1.245472 | -0.459629 | -0.102563                     |
| C                                              | -2.384016 | 0.185416  | 0.705125                      |
| C                                              | -1.639345 | -0.723438 | -1.560509                     |
| H                                              | -0.978111 | -1.404533 | 0.373753                      |
| C                                              | -3.610671 | -0.710780 | 0.811572                      |
| H                                              | -2.014881 | 0.419414  | 1.705667                      |
| H                                              | -2.648435 | 1.135627  | 0.238827                      |
| H                                              | -0.794881 | -1.106019 | -2.133000                     |
| H                                              | -1.976194 | 0.200954  | -2.029033                     |
| H                                              | -2.441322 | -1.457222 | -1.612281                     |
| H                                              | -3.346374 | -1.689579 | 1.215182                      |
| H                                              | -4.083141 | -0.862737 | -0.157748                     |
| H                                              | -4.353089 | -0.266209 | 1.472477                      |
| C                                              | 1.316889  | 0.059883  | 0.181973                      |
| H                                              | 1.586794  | 1.068328  | -0.668096                     |
| C                                              | 2.035066  | 0.759786  | 1.349264                      |
| C                                              | 1.657666  | -1.412822 | 0.050032                      |
| C                                              | 3.140319  | -1.633626 | -0.235619                     |
| H                                              | 1.388036  | -1.945662 | 0.969131                      |
| H                                              | 1.073198  | -1.861578 | -0.755253                     |
| H                                              | 1.967326  | 0.126557  | 2.237082                      |
| H                                              | 1.593196  | 1.726831  | 1.567539                      |
| H                                              | 3.088499  | 0.917420  | 1.123749                      |
| H                                              | 3.354487  | -2.691189 | -0.383307                     |
| H                                              | 3.758627  | -1.281504 | 0.589250                      |
| H                                              | 3.441138  | -1.094099 | -1.134122                     |
| Rotational constants (GHz):                    |           |           | 1.4597600 0.6729400 0.5739100 |
| Vibrational harmonic frequencies (cm-1):       |           |           |                               |
| i1609.2434                                     | 40.0848   | 77.9578   |                               |
| 84.2830                                        | 98.3399   | 141.8176  |                               |
| 173.3623                                       | 186.5301  | 211.0367  |                               |
| 223.1692                                       | 242.8305  | 277.5830  |                               |
| 286.6568                                       | 295.7300  | 329.0951  |                               |
| 350.6396                                       | 368.4109  | 432.8183  |                               |
| 541.5090                                       | 559.9094  | 688.2494  |                               |
| 748.4473                                       | 779.8796  | 787.6433  |                               |
| 809.0037                                       | 858.2566  | 954.6315  |                               |
| 968.7408                                       | 995.2538  | 999.2997  |                               |
| 1002.1113                                      | 1028.8178 | 1060.8553 |                               |
| 1070.9414                                      | 1105.6082 | 1121.1963 |                               |
| 1140.1380                                      | 1155.2445 | 1196.5663 |                               |
| 1221.5283                                      | 1294.2440 | 1299.9533 |                               |
| 1318.7262                                      | 1336.1770 | 1352.4699 |                               |
| 1371.0861                                      | 1382.9610 | 1396.0626 |                               |
| 1405.6503                                      | 1411.6465 | 1415.1790 |                               |
| 1441.5999                                      | 1484.3785 | 1489.4687 |                               |
| 1494.4032                                      | 1497.6989 | 1498.4691 |                               |
| 1503.5159                                      | 1507.9301 | 1508.3741 |                               |



|           |           |           |
|-----------|-----------|-----------|
| 1516.5574 | 1516.7446 | 1567.1143 |
| 1857.4797 | 3020.9999 | 3052.7010 |
| 3062.5733 | 3065.0811 | 3065.1320 |
| 3069.5088 | 3080.8405 | 3085.5819 |
| 3107.3405 | 3124.0282 | 3133.5257 |
| 3135.2571 | 3140.1119 | 3140.5828 |
| 3143.0212 | 3154.3839 | 3175.3082 |

Zero-point correction (Hartree): 0.255697

TS.diC2H5CH3CH\_COO.14Hshift.ctpmRR

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E(RM062X/Aug-CC-pVTZ) (Hartree): -504.03603718

Electronic state : 1-A

Cartesian coordinates (Angs):

C	0.034722	0.441402	0.086067
O	-0.102479	1.639142	-0.392681
O	1.042488	2.398918	-0.149868
C	-1.231459	-0.357448	0.171560
C	-2.485456	0.468168	-0.118902
C	-1.105460	-1.591278	-0.731892
H	-1.278102	-0.710701	1.207581
C	-3.773527	-0.313806	0.106767
H	-2.477383	1.353612	0.516869
H	-2.443325	0.831814	-1.147362
H	-0.193560	-2.146268	-0.517879
H	-1.084994	-1.289736	-1.780373
H	-1.950789	-2.259534	-0.582834
H	-3.796870	-0.749586	1.107351
H	-3.890491	-1.122346	-0.613538
H	-4.639504	0.338756	0.008454
C	1.298269	0.131428	0.643464
H	1.424105	1.478324	0.737217
C	1.314137	-0.898125	1.755634
C	2.508123	0.025720	-0.310035
C	2.609670	-1.329057	-1.005359
H	2.459927	0.817626	-1.052311
H	3.408992	0.199075	0.282367
H	1.083426	-1.909816	1.412676
H	0.612596	-0.647665	2.550487
H	2.310323	-0.929851	2.197990
H	1.757064	-1.492140	-1.665404
H	2.650310	-2.153201	-0.292598
H	3.514097	-1.374868	-1.612120

Rotational constants (GHz): 1.5276100 0.7140100 0.5946200

Vibrational harmonic frequencies (cm-1):

i1601.8326	49.7537	69.1108
93.6519	122.5175	149.4286
198.3431	203.8292	222.3896
237.1900	257.9615	286.4034
293.3221	304.4172	339.7855
355.4887	406.1642	450.8805
487.6848	591.2274	658.3845
729.0589	760.8704	785.1218
809.0119	860.9343	924.0200
969.8350	990.7662	1013.6757
1016.0187	1040.1153	1049.8561
1061.2004	1086.8250	1110.0992
1137.3020	1160.4709	1200.4910
1219.3372	1281.3334	1296.9285
1318.8872	1335.2194	1340.3510
1360.2677	1385.2109	1405.6331
1408.1109	1416.6421	1417.6087
1436.3210	1485.7747	1490.1853
1494.5509	1497.9539	1500.5572
1502.6715	1505.9043	1512.0050
1512.5884	1520.8017	1556.1107
1863.7079	3043.0448	3048.5561
3059.8388	3060.8053	3066.2663
3067.3905	3073.9409	3106.9277
3109.3558	3124.0821	3128.9888
3131.0543	3131.5627	3139.8152
3143.5843	3153.0202	3157.1815

Zero-point correction (Hartree): 0.255824

TS.diC2H5CH3CH_COO.14Hshift.ctptRR

~~~~~  
E(RM062X/Aug-CC-pVTZ) (Hartree): -504.03749756

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.052799 | 0.252900  | 0.070602  |
| O | -0.025362 | 1.538441  | -0.101081 |
| O | 1.249476  | 2.037607  | 0.178268  |
| C | -1.411558 | -0.372773 | 0.047084  |
| C | -2.550206 | 0.639461  | 0.168562  |
| C | -1.506915 | -1.234056 | -1.221907 |
| H | -1.441855 | -1.046568 | 0.909123  |
| C | -3.917962 | -0.023339 | 0.273202  |
| H | -2.373773 | 1.262154  | 1.046208  |
| H | -2.523822 | 1.310854  | -0.691613 |
| H | -0.645167 | -1.894501 | -1.314490 |
| H | -1.544832 | -0.594998 | -2.105095 |
| H | -2.404413 | -1.848466 | -1.201433 |
| H | -3.940797 | -0.747141 | 1.089920  |
| H | -4.186786 | -0.545179 | -0.644409 |
| H | -4.690745 | 0.719121  | 0.465379  |
| C | 1.181500  | -0.353696 | 0.390337  |
| H | 1.530479  | 0.894111  | 0.792344  |
| C | 1.133108  | -1.651548 | 1.166570  |
| C | 2.254543  | -0.350452 | -0.723553 |
| C | 3.661124  | -0.094698 | -0.201501 |
| H | 2.206927  | -1.329872 | -1.210206 |
| H | 2.006849  | 0.396677  | -1.474431 |

|                                                |           |           |                               |
|------------------------------------------------|-----------|-----------|-------------------------------|
| H                                              | 0.784524  | -2.488570 | 0.553547                      |
| H                                              | 0.494112  | -1.584664 | 2.046188                      |
| H                                              | 2.133577  | -1.905854 | 1.515105                      |
| H                                              | 4.395180  | -0.180394 | -1.002191                     |
| H                                              | 3.933693  | -0.806629 | 0.577963                      |
| H                                              | 3.728923  | 0.910748  | 0.214216                      |
| Rotational constants (GHz):                    |           |           | 1.9118000 0.5424400           |
| Vibrational harmonic frequencies (cm-1):       |           |           | 0.6271000                     |
| i1600.5853                                     | 50.5132   |           | 73.3701                       |
| 87.8947                                        | 111.0409  |           | 146.7422                      |
| 201.1594                                       | 206.5536  |           | 215.5030                      |
| 222.9312                                       | 258.4735  |           | 277.3504                      |
| 291.8344                                       | 302.1319  |           | 328.4005                      |
| 359.4334                                       | 381.4856  |           | 426.1927                      |
| 523.0271                                       | 577.4746  |           | 663.5414                      |
| 738.5825                                       | 773.9329  |           | 789.0910                      |
| 806.4003                                       | 861.3076  |           | 926.3612                      |
| 969.1081                                       | 989.8027  |           | 1006.8287                     |
| 1020.5672                                      | 1042.3290 |           | 1049.4328                     |
| 1066.2875                                      | 1093.7979 |           | 1118.5318                     |
| 1130.1337                                      | 1156.3485 |           | 1198.3926                     |
| 1218.4471                                      | 1283.6542 |           | 1294.1826                     |
| 1321.2921                                      | 1335.8183 |           | 1338.9568                     |
| 1353.1427                                      | 1387.5923 |           | 1405.8272                     |
| 1411.1678                                      | 1416.8485 |           | 1417.8941                     |
| 1441.2274                                      | 1476.5922 |           | 1487.2057                     |
| 1495.4787                                      | 1498.5523 |           | 1499.3730                     |
| 1502.1378                                      | 1504.7825 |           | 1507.6254                     |
| 1510.2886                                      | 1517.5757 |           | 1562.8926                     |
| 1867.7920                                      | 3036.7762 |           | 3037.8936                     |
| 3053.1990                                      | 3060.7357 |           | 3062.6083                     |
| 3066.0698                                      | 3073.2728 |           | 3107.2112                     |
| 3109.3487                                      | 3119.9630 |           | 3131.1025                     |
| 3134.9589                                      | 3135.4392 |           | 3136.1609                     |
| 3140.4637                                      | 3140.5961 |           | 3154.9798                     |
| Zero-point correction (Hartree): 0.255609      |           |           |                               |
| TS.dic2H5CH3CH_COO.14Hshift.mmmmmRR            |           |           |                               |
| ~~~~~                                          |           |           |                               |
| E(RM062X/Aug-CC-pVTZ) (Hartree): -504.03635031 |           |           |                               |
| Electronic state : 1-A                         |           |           |                               |
| Cartesian coordinates (Angs):                  |           |           |                               |
| C                                              | 0.180961  | -0.493153 | -0.146769                     |
| O                                              | 0.677999  | -1.668982 | 0.085674                      |
| O                                              | -0.335273 | -2.625134 | 0.169618                      |
| C                                              | 1.212433  | 0.517329  | -0.556745                     |
| C                                              | 2.146961  | 0.790048  | 0.633032                      |
| C                                              | 1.992263  | 0.055513  | -1.788827                     |
| H                                              | 0.679681  | 1.440451  | -0.787041                     |
| C                                              | 1.408395  | 1.276224  | 1.873523                      |
| H                                              | 2.698111  | -0.125193 | 0.856339                      |
| H                                              | 2.878991  | 1.533933  | 0.313975                      |
| H                                              | 1.326893  | -0.132498 | -2.631128                     |
| H                                              | 2.534088  | -0.863604 | -1.571875                     |
| H                                              | 2.709538  | 0.821713  | -2.081191                     |
| H                                              | 0.711865  | 0.520156  | 2.240330                      |
| H                                              | 0.836075  | 2.180045  | 1.658221                      |
| H                                              | 2.103811  | 1.504039  | 2.679603                      |
| C                                              | -1.230391 | -0.404035 | -0.169723                     |
| H                                              | -1.168808 | -1.731160 | -0.400098                     |
| C                                              | -1.979317 | -0.596183 | 1.158165                      |
| C                                              | -1.827708 | 0.666882  | -1.066824                     |
| C                                              | -2.086908 | 2.012448  | -0.389886                     |
| H                                              | -1.191280 | 0.810416  | -1.942366                     |
| H                                              | -2.774088 | 0.280108  | -1.452875                     |
| H                                              | -1.925377 | 0.313133  | 1.758643                      |
| H                                              | -1.567562 | -1.420156 | 1.732570                      |
| H                                              | -3.030236 | -0.805454 | 0.955109                      |
| H                                              | -1.183943 | 2.398064  | 0.087435                      |
| H                                              | -2.852144 | 1.926629  | 0.380187                      |
| H                                              | -2.427564 | 2.751870  | -1.113851                     |
| Rotational constants (GHz):                    |           |           | 1.1205400 0.9070200 0.7488400 |
| Vibrational harmonic frequencies (cm-1):       |           |           |                               |
| i1606.3501                                     | 41.8153   |           | 68.6657                       |
| 115.8832                                       | 139.1504  |           | 163.5123                      |
| 185.9649                                       | 199.5157  |           | 222.0153                      |
| 228.2778                                       | 239.2102  |           | 248.7696                      |
| 270.2704                                       | 314.3316  |           | 350.2472                      |
| 363.1242                                       | 379.7244  |           | 443.4764                      |
| 501.8014                                       | 613.3978  |           | 653.6079                      |
| 735.2635                                       | 761.7037  |           | 785.2536                      |
| 822.7629                                       | 860.2109  |           | 941.1200                      |
| 973.3902                                       | 993.3934  |           | 1003.5459                     |
| 1031.4181                                      | 1037.8971 |           | 1043.5369                     |
| 1050.0843                                      | 1097.9799 |           | 1126.2366                     |
| 1134.4222                                      | 1146.8946 |           | 1194.7135                     |
| 1223.7724                                      | 1279.9472 |           | 1293.4078                     |
| 1322.2932                                      | 1330.8455 |           | 1351.7319                     |
| 1368.2785                                      | 1377.6447 |           | 1393.1439                     |
| 1405.8946                                      | 1411.5061 |           | 1418.7212                     |
| 1440.0028                                      | 1488.0123 |           | 1490.7517                     |
| 1494.0349                                      | 1497.3256 |           | 1499.8267                     |
| 1505.7492                                      | 1506.2835 |           | 1508.7905                     |
| 1510.0069                                      | 1519.6909 |           | 1567.9552                     |
| 1859.6174                                      | 3054.2418 |           | 3055.9807                     |
| 3058.6149                                      | 3060.8880 |           | 3065.3029                     |
| 3066.9214                                      | 3086.1284 |           | 3093.3286                     |
| 3106.0047                                      | 3117.2488 |           | 3124.6633                     |
| 3127.4477                                      | 3137.9769 |           | 3139.3765                     |
| 3140.1320                                      | 3150.4791 |           | 3173.4817                     |
| Zero-point correction (Hartree): 0.255852      |           |           |                               |

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TS.dic2H5CH3CH_COO.14Hshift.mmmppRR
~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -504.03675267
Electronic state : 1-A
Cartesian coordinates (Angs):
C 0.048156 0.133969 0.398947
O 0.225990 0.713596 1.546319
O -0.956218 1.314519 1.983234
C 1.193333 -0.736582 -0.023700
C 2.326115 0.161252 -0.555470
C 1.689031 -1.640723 1.103630
H 0.835127 -1.343161 -0.856462
C 1.889746 1.081814 -1.687967
H 2.721816 0.747270 0.276409
H 3.129579 -0.496098 -0.892154
H 0.888443 -2.268989 1.492322
H 2.077712 -1.043887 1.927007
H 2.486908 -2.284970 0.735995
H 1.171127 1.824746 -1.340267
H 1.419092 0.514641 -2.493234
H 2.741089 1.615793 -2.106817
C -1.227574 0.306282 -0.188237
H -1.619306 0.596722 1.076796
C -1.568457 1.719312 -0.692135
C -1.727707 -0.785311 -1.116121
C -1.873037 -2.148738 -0.448776
H -2.703901 -0.468902 -1.488541
H -1.088610 -0.861751 -2.003454
H -2.642633 1.891906 -0.633272
H -1.267722 1.805457 -1.739222
H -1.067316 2.490595 -0.114577
H -0.919137 -2.519574 -0.071973
H -2.263595 -2.890026 -1.145221
H -2.554493 -2.082332 0.399214
Rotational constants (GHz): 1.1128700 0.8677400 0.8149300
Vibrational harmonic frequencies (cm-1):
i1607.4965 46.1092 81.3856
117.3973 145.8440 157.6468
180.2758 215.8668 223.5619
229.2412 232.1393 246.2534
265.4066 292.3800 323.4251
361.7506 431.5238 450.0289
505.3212 559.5670 649.7707
744.1377 760.2924 793.1650
824.6463 859.1191 939.4171
976.6109 1001.4179 1016.5438
1030.0515 1036.0127 1049.6479
1060.3759 1108.5752 1125.7314
1135.5633 1143.5942 1188.0466
1218.8862 1281.2476 1288.4836
1321.1699 1323.6387 1357.6591
1365.8961 1370.3388 1397.6971
1411.3205 1416.5023 1418.1580
1441.1551 1488.0056 1489.8984
1496.1276 1498.2929 1499.5125
1502.3614 1504.8514 1508.9518
1509.2718 1512.4742 1561.8379
1866.9523 3021.9259 3048.7873
3057.4651 3063.6779 3064.2571
3069.2053 3081.7546 3091.4800
3105.4931 3116.7267 3127.5411
3131.2577 3136.0367 3139.7758
3141.4486 3150.2198 3168.7830
Zero-point correction (Hartree): 0.255780

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TS.dic2H5CH3CH_COO.14Hshift.mmmmtRR
~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -504.03670979
Electronic state : 1-A
Cartesian coordinates (Angs):
C     -0.257954      0.409791     -0.109910
O     -0.602796      1.639836      0.113937
O      0.517634      2.416309      0.419754
C     -1.347245     -0.430665     -0.704456
C     -2.382901     -0.742734      0.390213
C     -1.994598      0.235508     -1.917652
H     -0.886677     -1.373003     -1.003479
C     -1.776624     -1.421574      1.612011
H     -2.873037      0.189034      0.679075
H     -3.147757     -1.380850     -0.055592
H     -1.257496      0.450308     -2.690742
H     -2.467922      1.173005     -1.630770
H     -2.754135     -0.422153     -2.338902
H     -1.077007     -0.760642      2.125834
H     -1.232831     -2.323925      1.326440
H     -2.548195     -1.705867      2.325516
C      1.107025      0.102759      0.089880
H      1.288593      1.431127     -0.069870
C      1.615386      0.138600      1.541798
C      1.675971     -1.041738     -0.728381
C      3.195468     -0.963251     -0.842526
H      1.400492     -2.002706     -0.277962
H      1.247559     -1.029202     -1.732390
H      2.650006      0.474390      1.588543
H      1.563560     -0.870682      1.958831
H      1.020922      0.807703      2.156821
H      3.577855     -1.753666     -1.486839
H      3.671974     -1.069195      0.131326
H      3.498217     -0.003011     -1.261238
Rotational constants (GHz):  1.2625600      0.7618900      0.7107800
Vibrational harmonic frequencies (cm-1):
i1608.3360      17.7423      83.5887

```

|           |           |           |
|-----------|-----------|-----------|
| 91.5029   | 131.0827  | 150.0796  |
| 172.3340  | 211.5333  | 219.3773  |
| 226.7183  | 241.0645  | 255.2000  |
| 275.5003  | 292.6148  | 340.8156  |
| 361.4533  | 375.4198  | 451.5612  |
| 540.2705  | 560.4221  | 649.9406  |
| 748.9236  | 761.4938  | 800.1641  |
| 825.1243  | 859.4148  | 955.0085  |
| 973.9906  | 997.1883  | 999.8824  |
| 1026.9628 | 1031.9083 | 1045.3017 |
| 1071.4242 | 1106.8208 | 1129.4581 |
| 1139.5771 | 1148.9111 | 1193.0428 |
| 1223.0460 | 1281.5808 | 1298.7430 |
| 1321.7117 | 1327.2823 | 1349.6495 |
| 1362.1439 | 1382.4138 | 1394.9966 |
| 1409.9526 | 1411.5933 | 1419.3764 |
| 1443.0389 | 1483.0403 | 1489.2202 |
| 1494.9463 | 1497.4576 | 1499.3874 |
| 1501.7881 | 1506.8033 | 1508.1638 |
| 1510.1312 | 1517.2871 | 1567.0005 |
| 1859.3989 | 3016.7383 | 3048.1199 |
| 3056.6716 | 3064.8632 | 3065.1326 |
| 3068.7820 | 3081.5643 | 3091.5764 |
| 3105.3760 | 3123.2175 | 3126.3063 |
| 3134.9821 | 3139.2738 | 3140.0077 |
| 3140.8765 | 3151.7148 | 3169.3755 |

Zero-point correction (Hartree): 0.255719

TS.dic2H5CH3CH\_COO.14Hshift.mppmRR

E(RM062X/Aug-CC-pVTZ) (Hartree): -504.03541519

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.093813  | -0.452680 | -0.283167 |
| O | 0.639621  | -1.630123 | -0.242294 |
| O | -0.331958 | -2.621690 | -0.110177 |
| C | 1.028693  | 0.655179  | -0.652715 |
| C | 1.451294  | 1.384568  | 0.644560  |
| C | 2.222065  | 0.197060  | -1.485022 |
| H | 0.435428  | 1.364618  | -1.233462 |
| C | 2.300981  | 0.542026  | 1.587756  |
| H | 1.998862  | 2.281763  | 0.349462  |
| H | 0.553288  | 1.718807  | 1.166628  |
| H | 1.893953  | -0.238148 | -2.427552 |
| H | 2.808584  | -0.554740 | -0.962421 |
| H | 2.865981  | 1.049226  | -1.701689 |
| H | 3.247458  | 0.257430  | 1.130432  |
| H | 1.783733  | -0.372556 | 1.880083  |
| H | 2.526855  | 1.102597  | 2.493569  |
| C | -1.310988 | -0.411910 | -0.107674 |
| H | -1.245350 | -1.726430 | -0.453690 |
| C | -1.850188 | -0.737465 | 1.293793  |
| C | -2.084386 | 0.679170  | -0.829125 |
| C | -2.177972 | 2.029789  | -0.119961 |
| H | -1.673321 | 0.821152  | -1.830423 |
| H | -3.096908 | 0.296371  | -0.980099 |
| H | -1.749935 | 0.126692  | 1.952634  |
| H | -1.324140 | -1.576282 | 1.739887  |
| H | -2.908974 | -0.990459 | 1.227643  |
| H | -1.195599 | 2.486337  | 0.005955  |
| H | -2.628797 | 1.931218  | 0.866827  |
| H | -2.792302 | 2.722477  | -0.694684 |

Rotational constants (GHz): 1.1939700 0.8962100 0.7059200

Vibrational harmonic frequencies (cm-1):

|            |           |           |
|------------|-----------|-----------|
| i1593.6309 | 46.8723   | 63.8961   |
| 103.9517   | 110.8290  | 158.8036  |
| 186.5933   | 194.5287  | 215.9326  |
| 238.0114   | 246.9990  | 279.7926  |
| 295.2782   | 299.9917  | 322.4176  |
| 359.9428   | 395.3579  | 439.4792  |
| 542.4066   | 612.0896  | 647.5568  |
| 738.6723   | 763.6716  | 783.6689  |
| 814.7649   | 840.7087  | 938.5290  |
| 976.3569   | 995.1020  | 1008.4807 |
| 1012.4674  | 1030.6636 | 1040.3926 |
| 1049.0555  | 1095.9397 | 1116.5621 |
| 1140.9910  | 1147.2238 | 1187.9912 |
| 1225.0139  | 1277.5181 | 1294.9538 |
| 1305.6623  | 1331.3308 | 1356.6918 |
| 1373.0760  | 1374.7502 | 1393.7532 |
| 1409.1039  | 1418.1388 | 1422.0863 |
| 1438.1446  | 1486.2658 | 1488.8009 |
| 1495.4530  | 1498.4840 | 1500.1796 |
| 1502.9962  | 1508.0548 | 1509.2715 |
| 1514.7510  | 1518.6969 | 1561.0894 |
| 1868.9060  | 3054.3202 | 3055.9584 |
| 3062.3120  | 3066.3116 | 3068.6302 |
| 3073.8676  | 3083.1311 | 3088.1940 |
| 3101.9847  | 3114.4995 | 3130.8576 |
| 3136.7306  | 3139.8780 | 3142.5959 |
| 3143.7976  | 3161.3847 | 3168.9655 |

Zero-point correction (Hartree): 0.255858

TS.dic2H5CH3CH\_COO.14Hshift.mppmRR

E(RM062X/Aug-CC-pVTZ) (Hartree): -504.03618913

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.017526  | -0.212192 | -0.344411 |
| O | 0.290258  | -1.171478 | -1.174313 |
| O | -0.789619 | -2.050270 | -1.280226 |
| C | 1.019414  | 0.897833  | -0.299545 |

|                                                           |           |           |           |
|-----------------------------------------------------------|-----------|-----------|-----------|
| C                                                         | 1.726772  | 0.839777  | 1.072503  |
| C                                                         | 1.990515  | 0.894300  | -1.474264 |
| H                                                         | 0.442831  | 1.824956  | -0.315612 |
| C                                                         | 2.514374  | -0.443492 | 1.306219  |
| H                                                         | 2.388945  | 1.704767  | 1.139466  |
| H                                                         | 0.976221  | 0.953890  | 1.857174  |
| H                                                         | 1.460721  | 1.008732  | -2.418397 |
| H                                                         | 2.553000  | -0.035396 | -1.525683 |
| H                                                         | 2.694563  | 1.719100  | -1.368582 |
| H                                                         | 3.313984  | -0.563167 | 0.576482  |
| H                                                         | 1.868939  | -1.321036 | 1.240610  |
| H                                                         | 2.967505  | -0.437576 | 2.296311  |
| C                                                         | -1.228973 | -0.301000 | 0.318891  |
| H                                                         | -1.550816 | -1.154699 | -0.705757 |
| C                                                         | -1.342266 | -1.406110 | 1.382482  |
| C                                                         | -1.888538 | 1.003979  | 0.730711  |
| C                                                         | -2.388237 | 1.829940  | -0.451514 |
| H                                                         | -2.737770 | 0.755444  | 1.369444  |
| H                                                         | -1.220371 | 1.606621  | 1.356407  |
| H                                                         | -0.975902 | -1.025529 | 2.339743  |
| H                                                         | -0.771328 | -2.290454 | 1.113877  |
| H                                                         | -2.384017 | -1.698111 | 1.512279  |
| H                                                         | -1.581057 | 2.077298  | -1.142539 |
| H                                                         | -2.841988 | 2.763787  | -0.120623 |
| H                                                         | -3.132104 | 1.267145  | -1.014717 |
| Rotational constants (GHz): 1.2055500 0.8433500 0.7662600 |           |           |           |
| Vibrational harmonic frequencies (cm-1):                  |           |           |           |
| i1597.4778                                                | 49.6423   | 61.6561   |           |
| 110.5101                                                  | 122.7014  | 150.3406  |           |
| 173.0935                                                  | 207.8190  | 215.8110  |           |
| 225.0078                                                  | 232.7570  | 273.8217  |           |
| 285.4270                                                  | 295.1874  | 320.4732  |           |
| 360.0330                                                  | 437.3539  | 451.7734  |           |
| 538.3620                                                  | 564.0804  | 631.0159  |           |
| 749.1580                                                  | 761.6540  | 793.9801  |           |
| 810.7865                                                  | 845.1605  | 938.7256  |           |
| 982.6119                                                  | 999.7648  | 1005.5494 |           |
| 1020.2901                                                 | 1029.4376 | 1038.0880 |           |
| 1058.4705                                                 | 1101.2899 | 1121.5528 |           |
| 1132.0141                                                 | 1149.4921 | 1184.7215 |           |
| 1222.9600                                                 | 1279.1554 | 1288.0638 |           |
| 1303.4311                                                 | 1318.0445 | 1354.9681 |           |
| 1367.3265                                                 | 1373.6637 | 1394.5905 |           |
| 1415.6489                                                 | 1418.4314 | 1422.1613 |           |
| 1441.0665                                                 | 1483.2341 | 1489.9261 |           |
| 1493.8176                                                 | 1498.4440 | 1500.3462 |           |
| 1501.0161                                                 | 1502.8139 | 1507.9106 |           |
| 1509.2662                                                 | 1517.2327 | 1556.4605 |           |
| 1873.0473                                                 | 3026.7698 | 3042.7233 |           |
| 3060.3909                                                 | 3061.6466 | 3065.3056 |           |
| 3075.3282                                                 | 3084.1431 | 3084.8947 |           |
| 3099.6356                                                 | 3111.8475 | 3126.6181 |           |
| 3132.5613                                                 | 3136.5283 | 3142.5731 |           |
| 3145.5576                                                 | 3158.2188 | 3166.2069 |           |
| Zero-point correction (Hartree): 0.255573                 |           |           |           |
| TS.diC2H5CH3CH_COO.14Hshift.mpmtrr                        |           |           |           |
| ~~~~~                                                     |           |           |           |
| E(RM062X/Aug-CC-pVTZ) (Hartree): -504.03684395            |           |           |           |
| Electronic state : 1-A                                    |           |           |           |
| Cartesian coordinates (Angs):                             |           |           |           |
| C                                                         | -0.212558 | 0.418593  | -0.254819 |
| O                                                         | -0.564775 | 1.664115  | -0.169797 |
| O                                                         | 0.538846  | 2.468643  | 0.121090  |
| C                                                         | -1.256126 | -0.506302 | -0.795549 |
| C                                                         | -1.640946 | -1.503576 | 0.317559  |
| C                                                         | -2.458789 | 0.213525  | -1.394772 |
| H                                                         | -0.758909 | -1.083873 | -1.579368 |
| C                                                         | -2.266896 | -0.843403 | 1.540014  |
| H                                                         | -2.331334 | -2.231540 | -0.111891 |
| H                                                         | -0.747843 | -2.053899 | 0.618511  |
| H                                                         | -2.160643 | 0.848138  | -2.227099 |
| H                                                         | -2.951035 | 0.847714  | -0.660533 |
| H                                                         | -3.179050 | -0.519556 | -1.756592 |
| H                                                         | -3.199858 | -0.339251 | 1.291936  |
| H                                                         | -1.593318 | -0.103406 | 1.976200  |
| H                                                         | -2.485052 | -1.585859 | 2.306018  |
| C                                                         | 1.139787  | 0.136557  | 0.049927  |
| H                                                         | 1.327416  | 1.462112  | -0.208689 |
| C                                                         | 1.536713  | 0.295738  | 1.528331  |
| C                                                         | 1.769715  | -1.068407 | -0.624149 |
| C                                                         | 3.294571  | -1.006891 | -0.595686 |
| H                                                         | 1.444997  | -1.997530 | -0.141236 |
| H                                                         | 1.444350  | -1.123996 | -1.664198 |
| H                                                         | 1.426705  | -0.668953 | 2.032045  |
| H                                                         | 0.915273  | 1.029926  | 2.032711  |
| H                                                         | 2.573339  | 0.614009  | 1.626180  |
| H                                                         | 3.726047  | -1.835003 | -1.156266 |
| H                                                         | 3.675998  | -1.062127 | 0.423116  |
| H                                                         | 3.647522  | -0.073973 | -1.036338 |
| Rotational constants (GHz): 1.3428300 0.7758000 0.6721500 |           |           |           |
| Vibrational harmonic frequencies (cm-1):                  |           |           |           |
| i1603.7521                                                | 49.2976   | 68.2037   |           |
| 76.2346                                                   | 114.6724  | 147.6242  |           |
| 172.3065                                                  | 213.3982  | 215.0001  |           |
| 225.7431                                                  | 267.9918  | 274.5544  |           |
| 288.3607                                                  | 302.6371  | 317.4329  |           |
| 349.9385                                                  | 386.5092  | 483.7189  |           |
| 546.6229                                                  | 571.1981  | 623.5205  |           |
| 751.4845                                                  | 761.4785  | 796.0018  |           |
| 811.8035                                                  | 847.0669  | 953.0932  |           |
| 981.5206                                                  | 990.3225  | 1004.9577 |           |

|           |           |           |
|-----------|-----------|-----------|
| 1011.0039 | 1024.3388 | 1031.6413 |
| 1068.3100 | 1104.2118 | 1113.7341 |
| 1144.7936 | 1149.2782 | 1189.5222 |
| 1223.2462 | 1280.0594 | 1297.2125 |
| 1305.4694 | 1322.0722 | 1342.9202 |
| 1371.3793 | 1374.3545 | 1392.6751 |
| 1410.7182 | 1418.6788 | 1421.7727 |
| 1442.8276 | 1480.9577 | 1486.4421 |
| 1490.5317 | 1496.8344 | 1498.2476 |
| 1500.5271 | 1505.5955 | 1508.4035 |
| 1516.0254 | 1516.0971 | 1559.1415 |
| 1867.4438 | 3018.1832 | 3042.6787 |
| 3061.3000 | 3064.3899 | 3065.3039 |
| 3071.3992 | 3075.9204 | 3086.3568 |
| 3103.1490 | 3119.6174 | 3131.5851 |
| 3134.9080 | 3141.0700 | 3142.1418 |
| 3147.3950 | 3157.6811 | 3167.8727 |

Zero-point correction (Hartree): 0.255588

TS.dic2H5CH3CH\_COO.14Hshift.mppmRR

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E(RM062X/Aug-CC-pVT2) (Hartree): -504.03512277

Electronic state : 1-A

Cartesian coordinates (Angs):

C	0.049234	0.270135	0.140121
O	0.311841	1.533959	-0.009139
O	-0.519906	2.100762	-0.978116
C	1.107327	-0.488283	0.882829
C	2.103346	-1.140970	-0.107295
C	1.834482	0.401559	1.891132
H	0.597246	-1.292399	1.418569
C	2.584782	-0.205670	-1.209943
H	2.950481	-1.490770	0.485673
H	1.648982	-2.025704	-0.550131
H	1.135592	0.892120	2.566869
H	2.410790	1.176495	1.389922
H	2.515398	-0.209474	2.481683
H	3.003012	0.715052	-0.804249
H	1.766866	0.074722	-1.875925
H	3.354396	-0.689702	-1.808993
C	-1.058064	-0.219697	-0.589238
H	-0.862328	0.881909	-1.362468
C	-1.030094	-1.683453	-0.979703
C	-2.446560	0.263172	-0.112964
C	-2.963252	-0.552361	1.069304
H	-2.397912	1.315851	0.152660
H	-3.140143	0.177211	-0.951788
H	-0.909482	-2.354571	-0.123871
H	-0.231936	-1.897428	-1.688396
H	-1.971849	-1.945647	-1.462219
H	-2.286499	-0.468731	1.921745
H	-3.061476	-1.609176	0.820874
H	-3.943821	-0.194111	1.382630

Rotational constants (GHz): 1.4341400 0.7752800 0.7248200

Vibrational harmonic frequencies (cm-1):

i1612.2927	41.1358	70.8907
86.0455	122.5190	173.3058
191.4104	220.0593	236.1917
245.9913	251.8821	267.1307
287.6873	318.8738	326.8050
363.4613	420.6942	447.3766
528.2055	603.0320	683.9363
737.7335	748.5663	782.6037
805.9685	850.0427	916.3947
979.2759	1003.7683	1008.2130
1011.8129	1037.7029	1045.9530
1050.8949	1090.8016	1114.6541
1133.9035	1141.9196	1190.4547
1211.6807	1278.3999	1299.5133
1307.8245	1312.4007	1355.9815
1364.1235	1373.3753	1406.5765
1410.7000	1415.6619	1424.2379
1436.1202	1485.9634	1491.2031
1493.5205	1498.4143	1501.0264
1501.7570	1504.9435	1510.5507
1513.7036	1520.6841	1551.6810
1867.8886	3038.8122	3054.4972
3062.0718	3064.7986	3067.6276
3073.7122	3075.3860	3107.4404
3116.6011	3119.4664	3128.6867
3132.5193	3138.1796	3144.1812
3145.6061	3152.1420	3156.8062

Zero-point correction (Hartree): 0.255961

TS.dic2H5CH3CH_COO.14Hshift.mpptRR

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E(RM062X/Aug-CC-pVT2) (Hartree): -504.03626163

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.172298  | -0.258689 | -0.287630 |
| O | 0.205091  | -1.440967 | 0.251142  |
| O | -0.926048 | -1.647727 | 1.045302  |
| C | 1.482104  | 0.191016  | -0.859780 |
| C | 2.256036  | 1.048197  | 0.172056  |
| C | 2.324856  | -0.991476 | -1.337856 |
| H | 1.248860  | 0.831476  | -1.713452 |
| C | 2.301039  | 0.445224  | 1.570834  |
| H | 3.268296  | 1.169678  | -0.218057 |
| H | 1.819940  | 2.044713  | 0.216744  |
| H | 1.772738  | -1.618608 | -2.035873 |
| H | 2.635748  | -1.617397 | -0.503982 |
| H | 3.215324  | -0.616122 | -1.839821 |

|                                                           |           |           |           |
|-----------------------------------------------------------|-----------|-----------|-----------|
| H                                                         | 2.690086  | -0.572462 | 1.559570  |
| H                                                         | 1.306058  | 0.408544  | 2.017683  |
| H                                                         | 2.938845  | 1.042004  | 2.220860  |
| C                                                         | -1.008997 | 0.480453  | -0.063633 |
| H                                                         | -1.158762 | -0.336588 | 1.003595  |
| C                                                         | -0.910836 | 1.989396  | -0.125727 |
| C                                                         | -2.289389 | -0.076540 | -0.733884 |
| C                                                         | -3.523438 | 0.043867  | 0.148074  |
| H                                                         | -2.431135 | 0.489861  | -1.659106 |
| H                                                         | -2.142121 | -1.118235 | -1.009612 |
| H                                                         | -0.515190 | 2.340984  | -1.084063 |
| H                                                         | -0.287853 | 2.397044  | 0.668270  |
| H                                                         | -1.903068 | 2.423992  | -0.010579 |
| H                                                         | -4.417817 | -0.272094 | -0.388186 |
| H                                                         | -3.678548 | 1.071174  | 0.479375  |
| H                                                         | -3.415786 | -0.587105 | 1.030361  |
| Rotational constants (GHz): 1.6502400 0.7257500 0.6570300 |           |           |           |
| Vibrational harmonic frequencies (cm-1):                  |           |           |           |
| i1610.7327                                                | 35.6068   |           | 72.2788   |
| 103.4123                                                  | 110.0865  |           | 162.5843  |
| 192.0287                                                  | 221.9381  |           | 233.1827  |
| 241.8865                                                  | 250.8981  |           | 272.4531  |
| 290.9873                                                  | 306.4507  |           | 330.8505  |
| 352.4961                                                  | 397.9466  |           | 462.4466  |
| 544.8118                                                  | 579.2695  |           | 684.4203  |
| 737.2829                                                  | 766.5916  |           | 788.1220  |
| 795.8531                                                  | 849.8254  |           | 918.9423  |
| 980.5336                                                  | 1003.7428 |           | 1007.4748 |
| 1019.1944                                                 | 1034.8179 |           | 1039.8686 |
| 1063.3744                                                 | 1102.0515 |           | 1114.1122 |
| 1129.2946                                                 | 1140.7461 |           | 1189.2608 |
| 1212.3037                                                 | 1281.2264 |           | 1296.8843 |
| 1307.2488                                                 | 1332.9470 |           | 1348.1306 |
| 1364.3191                                                 | 1375.2658 |           | 1409.3497 |
| 1412.5849                                                 | 1418.7754 |           | 1424.6670 |
| 1438.2202                                                 | 1478.1174 |           | 1486.8679 |
| 1492.6837                                                 | 1498.5954 |           | 1500.1518 |
| 1502.1359                                                 | 1505.2653 |           | 1507.7044 |
| 1513.5565                                                 | 1519.5666 |           | 1559.0448 |
| 1863.5182                                                 | 3036.2467 |           | 3043.6373 |
| 3062.1204                                                 | 3062.7220 |           | 3066.3730 |
| 3074.9765                                                 | 3076.9400 |           | 3111.9448 |
| 3119.5017                                                 | 3121.8651 |           | 3133.7360 |
| 3135.5956                                                 | 3140.2295 |           | 3142.6115 |
| 3145.4390                                                 | 3147.2915 |           | 3158.0599 |
| Zero-point correction (Hartree): 0.255965                 |           |           |           |
| TS.diC2H5CH3CH_COO.14Hshift.mtmmRR                        |           |           |           |
| ~~~~~                                                     |           |           |           |
| E(RM062X/Aug-CC-pVTZ) (Hartree): -504.03572325            |           |           |           |
| Electronic state : 1-A                                    |           |           |           |
| Cartesian coordinates (Angs):                             |           |           |           |
| C                                                         | -0.271210 | -0.627527 | -0.100221 |
| O                                                         | -0.465423 | -1.893226 | 0.107786  |
| O                                                         | -1.829573 | -2.180871 | 0.156461  |
| C                                                         | 1.146018  | -0.260232 | -0.407325 |
| C                                                         | 1.781860  | 0.250530  | 0.903134  |
| C                                                         | 1.942598  | -1.397555 | -1.039087 |
| H                                                         | 1.099765  | 0.583767  | -1.100020 |
| C                                                         | 3.135014  | 0.913280  | 0.683744  |
| H                                                         | 1.099963  | 0.959826  | 1.376324  |
| H                                                         | 1.878829  | -0.595265 | 1.587833  |
| H                                                         | 1.427550  | -1.798004 | -1.910616 |
| H                                                         | 2.081407  | -2.212366 | -0.329538 |
| H                                                         | 2.921665  | -1.043046 | -1.354789 |
| H                                                         | 3.050692  | 1.737184  | -0.027229 |
| H                                                         | 3.870113  | 0.208967  | 0.297448  |
| H                                                         | 3.522233  | 1.315738  | 1.618506  |
| C                                                         | -1.430307 | 0.184434  | -0.144389 |
| H                                                         | -2.064727 | -0.991834 | -0.391247 |
| C                                                         | -2.193521 | 0.396496  | 1.172453  |
| C                                                         | -1.389541 | 1.415860  | -1.033780 |
| C                                                         | -0.762622 | 2.666955  | -0.418028 |
| H                                                         | -0.883411 | 1.177475  | -1.971068 |
| H                                                         | -2.422712 | 1.643239  | -1.307638 |
| H                                                         | -1.699752 | 1.154681  | 1.782310  |
| H                                                         | -2.261501 | -0.521367 | 1.748211  |
| H                                                         | -3.204190 | 0.743934  | 0.955392  |
| H                                                         | 0.281681  | 2.501336  | -0.147703 |
| H                                                         | -1.292883 | 2.976080  | 0.481836  |
| H                                                         | -0.794486 | 3.498996  | -1.120993 |
| Rotational constants (GHz): 1.1886800 0.8882800 0.6226700 |           |           |           |
| Vibrational harmonic frequencies (cm-1):                  |           |           |           |
| i1594.6085                                                | 40.3305   |           | 80.4770   |
| 95.2255                                                   | 118.0371  |           | 160.1115  |
| 189.7796                                                  | 195.2643  |           | 215.1819  |
| 233.6273                                                  | 253.6258  |           | 279.1141  |
| 280.0231                                                  | 309.9114  |           | 320.7162  |
| 359.3415                                                  | 388.9729  |           | 422.4478  |
| 503.2070                                                  | 620.0856  |           | 662.0513  |
| 739.4188                                                  | 782.0060  |           | 783.6635  |
| 797.6549                                                  | 854.6785  |           | 939.3872  |
| 973.8795                                                  | 987.6240  |           | 1004.4342 |
| 1010.1548                                                 | 1037.4354 |           | 1043.9613 |
| 1061.0033                                                 | 1095.5183 |           | 1116.0397 |
| 1135.6826                                                 | 1152.1053 |           | 1196.4942 |
| 1225.5069                                                 | 1274.0125 |           | 1295.0795 |
| 1319.2536                                                 | 1332.7956 |           | 1353.7178 |
| 1362.3519                                                 | 1377.4412 |           | 1393.5236 |
| 1410.1956                                                 | 1413.1529 |           | 1417.4894 |
| 1439.2950                                                 | 1486.6338 |           | 1490.2194 |
| 1496.2778                                                 | 1497.1249 |           | 1499.9024 |

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1503.6866      1507.0735      1512.1902
1514.3424      1515.8132      1562.8537
1866.4087      3054.8670      3056.2879
3057.0897      3062.3784      3064.6277
3074.1956      3077.1645      3088.9214
3096.4894      3115.2480      3128.2164
3131.1481      3139.1646      3142.9758
3147.8937      3155.8404      3172.3954
Zero-point correction (Hartree): 0.255770

TS.dic2H5CH3CH_COO.14Hshift.mtmpRR
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E(RM062X/Aug-CC-pVTZ) (Hartree): -504.03564771
Electronic state : 1-A
Cartesian coordinates (Angs):
C -0.225434 -0.505115 -0.090486
O -0.447316 -1.758368 -0.340109
O -1.804644 -2.053107 -0.196252
C 1.157423 -0.030727 -0.407436
C 1.882199 0.170006 0.939654
C 1.910894 -0.951589 -1.359698
H 1.049007 0.956090 -0.863558
C 3.260015 0.799718 0.784342
H 1.260253 0.799159 1.580169
H 1.965190 -0.800000 1.436022
H 1.327525 -1.145704 -2.258009
H 2.121577 -1.909968 -0.885494
H 2.854230 -0.497750 -1.655864
H 3.197357 1.736951 0.228854
H 3.945505 0.139637 0.255298
H 3.695281 1.015579 1.758823
C -1.340538 0.249205 0.343653
H -2.065215 -0.765679 -0.220874
C -1.857566 -0.064536 1.757902
C -1.335738 1.733717 0.022924
C -1.482749 2.035632 -1.465789
H -2.171398 2.188052 0.557879
H -0.436849 2.218814 0.421837
H -1.319668 0.552462 2.482237
H -1.724022 -1.110350 2.018323
H -2.917924 0.174929 1.833443
H -0.688902 1.572668 -2.053796
H -1.458796 3.107879 -1.658524
H -2.428498 1.641159 -1.836281
Rotational constants (GHz): 1.2212400 0.7901000 0.6722700
Vibrational harmonic frequencies (cm-1):
i1603.5214 34.1078 77.7909
97.3623 127.7029 147.9894
169.7036 199.5698 213.6313
222.0872 235.8113 272.4896
291.5651 297.6031 321.5400
357.2612 406.9312 444.8845
503.0489 567.7053 654.2722
747.8233 777.3868 789.0496
807.8925 854.8142 939.8759
974.3311 1000.5420 1001.5787
1019.2506 1037.8188 1053.1873
1063.8842 1101.4872 1122.0974
1127.2794 1157.9953 1190.0081
1222.9635 1277.4352 1288.0182
1318.3281 1318.4946 1350.4280
1364.7092 1373.1485 1395.3521
1413.8686 1415.5126 1418.7065
1440.9360 1485.6370 1492.2480
1495.8826 1497.2403 1499.6475
1500.9705 1503.4253 1506.7189
1509.2458 1517.1164 1557.3565
1871.4145 3018.2248 3045.9199
3053.8692 3060.3935 3063.1688
3074.1131 3078.6270 3084.3874
3095.0910 3113.5631 3126.2741
3132.1780 3136.3492 3143.2022
3146.8244 3156.9830 3170.6762
Zero-point correction (Hartree): 0.255483

TS.dic2H5CH3CH_COO.14Hshift.mtmtRR
~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -504.03623743
Electronic state : 1-A
Cartesian coordinates (Angs):
C      -0.022812      0.612243      -0.094807
O      -0.027950      1.906603      -0.017447
O      1.274903      2.395162      0.102356
C      -1.331797      -0.011384      -0.459528
C      -1.843259      -0.767354      0.783504
C      -2.346281      0.983891      -1.009560
H      -1.105236      -0.761636      -1.222838
C      -3.089650      -1.596833      0.505165
H      -1.045497      -1.415173      1.152301
H      -2.045687      -0.037723      1.571601
H      -1.924546      1.561223      -1.829915
H      -2.658649      1.684378      -0.235077
H      -3.226474      0.460292      -1.376406
H      -2.920152      -2.283843      -0.325574
H      -3.942596      -0.968411      0.254025
H      -3.360719      -2.187369      1.378931
C      1.237616      -0.012435      0.049960
H      1.725412      1.213561      -0.288285
C      1.860973      0.051469      1.455994
C      1.427250      -1.351549      -0.638933
C      2.900698      -1.727350      -0.766521
H      0.904963      -2.144652      -0.089655

```



|                                                           |           |           |           |
|-----------------------------------------------------------|-----------|-----------|-----------|
| H                                                         | 0.989262  | -1.320237 | -1.637839 |
| H                                                         | 1.597993  | -0.858976 | 2.001708  |
| H                                                         | 1.503681  | 0.912111  | 2.013301  |
| H                                                         | 2.946781  | 0.114246  | 1.404666  |
| H                                                         | 3.017527  | -2.649601 | -1.333891 |
| H                                                         | 3.358975  | -1.878225 | 0.210070  |
| H                                                         | 3.452917  | -0.938283 | -1.278044 |
| Rotational constants (GHz): 1.2871400 0.7648800 0.5813700 |           |           |           |
| Vibrational harmonic frequencies (cm-1):                  |           |           |           |
| i1605.1156                                                | 44.2253   | 75.8891   |           |
| 87.5995                                                   | 104.3506  | 150.7751  |           |
| 169.0405                                                  | 214.1444  | 218.0549  |           |
| 233.8049                                                  | 257.6621  | 278.6070  |           |
| 294.7579                                                  | 305.4057  | 327.0082  |           |
| 355.5978                                                  | 374.3646  | 422.4492  |           |
| 548.2113                                                  | 561.2899  | 646.7544  |           |
| 750.5475                                                  | 775.7154  | 791.2160  |           |
| 811.7809                                                  | 855.5267  | 955.0091  |           |
| 973.2144                                                  | 989.7184  | 1001.5874 |           |
| 1011.6068                                                 | 1028.3975 | 1054.0109 |           |
| 1072.2589                                                 | 1102.9853 | 1118.8861 |           |
| 1139.7229                                                 | 1158.6455 | 1195.4297 |           |
| 1222.2479                                                 | 1273.7933 | 1299.6518 |           |
| 1315.7023                                                 | 1325.8489 | 1341.4257 |           |
| 1366.7301                                                 | 1375.3554 | 1394.3718 |           |
| 1411.4546                                                 | 1414.7413 | 1419.3444 |           |
| 1443.5468                                                 | 1482.6319 | 1488.1536 |           |
| 1492.5924                                                 | 1497.3553 | 1498.0213 |           |
| 1503.4256                                                 | 1505.2520 | 1507.1557 |           |
| 1515.8578                                                 | 1517.6364 | 1560.0483 |           |
| 1866.6397                                                 | 3011.9534 | 3044.5152 |           |
| 3051.3379                                                 | 3061.9400 | 3064.0111 |           |
| 3064.6985                                                 | 3075.3221 | 3085.2831 |           |
| 3094.7515                                                 | 3120.2287 | 3132.3214 |           |
| 3134.2224                                                 | 3140.6505 | 3142.5685 |           |
| 3147.1323                                                 | 3157.7509 | 3171.1006 |           |
| Zero-point correction (Hartree): 0.255599                 |           |           |           |

TS.dic2H5CH3CH\_COO.14Hshift.mtpmRR

E(RM062X/Aug-CC-pVTZ) (Hartree): -504.03550371

Electronic state : 1-A

Cartesian coordinates (Angs):

|                                                           |           |           |           |
|-----------------------------------------------------------|-----------|-----------|-----------|
| C                                                         | -0.090838 | 0.373627  | -0.010633 |
| O                                                         | -0.062162 | 1.670973  | 0.004054  |
| O                                                         | -1.136225 | 2.193348  | -0.721151 |
| C                                                         | 1.193782  | -0.264098 | 0.422462  |
| C                                                         | 2.281002  | -0.012991 | -0.637717 |
| C                                                         | 1.597116  | 0.257069  | 1.805143  |
| H                                                         | 1.010641  | -1.338450 | 0.486469  |
| C                                                         | 3.577827  | -0.755246 | -0.344514 |
| H                                                         | 1.899249  | -0.317906 | -1.614136 |
| H                                                         | 2.459692  | 1.062179  | -0.694712 |
| H                                                         | 0.784137  | 0.139836  | 2.521032  |
| H                                                         | 1.854589  | 1.314247  | 1.751983  |
| H                                                         | 2.456776  | -0.294710 | 2.179330  |
| H                                                         | 3.396334  | -1.824274 | -0.221179 |
| H                                                         | 4.055110  | -0.387840 | 0.562740  |
| H                                                         | 4.285542  | -0.628962 | -1.162400 |
| C                                                         | -1.207887 | -0.220996 | -0.640834 |
| H                                                         | -1.322020 | 0.975972  | -1.255916 |
| C                                                         | -0.978609 | -1.587483 | -1.252228 |
| C                                                         | -2.575951 | -0.075306 | 0.058925  |
| C                                                         | -2.786785 | -1.114626 | 1.157063  |
| H                                                         | -2.665044 | 0.925265  | 0.472997  |
| H                                                         | -3.356289 | -0.177475 | -0.698135 |
| H                                                         | -0.905923 | -2.380392 | -0.504050 |
| H                                                         | -0.074299 | -1.617424 | -1.858716 |
| H                                                         | -1.817803 | -1.834954 | -1.903390 |
| H                                                         | -1.994613 | -1.052268 | 1.905852  |
| H                                                         | -2.798046 | -2.130166 | 0.762707  |
| H                                                         | -3.738881 | -0.946939 | 1.660294  |
| Rotational constants (GHz): 1.4972500 0.6866100 0.6235900 |           |           |           |
| Vibrational harmonic frequencies (cm-1):                  |           |           |           |
| i1612.1086                                                | 43.0230   | 62.8555   |           |
| 73.9367                                                   | 85.8889   | 165.7514  |           |
| 182.3638                                                  | 192.4867  | 215.5362  |           |
| 216.7807                                                  | 244.6266  | 284.3680  |           |
| 292.1136                                                  | 304.2769  | 313.3728  |           |
| 354.8887                                                  | 393.6289  | 432.7761  |           |
| 505.3016                                                  | 596.8295  | 699.0869  |           |
| 731.6638                                                  | 751.5602  | 784.9531  |           |
| 802.0457                                                  | 864.4010  | 918.2788  |           |
| 971.4145                                                  | 996.8113  | 1001.6148 |           |
| 1013.9145                                                 | 1041.3885 | 1048.1981 |           |
| 1061.5856                                                 | 1090.6844 | 1116.5764 |           |
| 1134.4952                                                 | 1158.2235 | 1194.7151 |           |
| 1214.6236                                                 | 1285.2804 | 1300.3649 |           |
| 1316.2254                                                 | 1337.2951 | 1357.1666 |           |
| 1360.2306                                                 | 1378.7076 | 1404.9655 |           |
| 1408.2028                                                 | 1413.4593 | 1415.4099 |           |
| 1436.5449                                                 | 1486.4120 | 1489.8631 |           |
| 1494.6534                                                 | 1497.9986 | 1499.9819 |           |
| 1502.4164                                                 | 1504.4730 | 1509.6193 |           |
| 1516.5635                                                 | 1517.2250 | 1559.8715 |           |
| 1861.4532                                                 | 3049.0107 | 3055.0409 |           |
| 3062.2972                                                 | 3065.3558 | 3067.1983 |           |
| 3071.7732                                                 | 3079.2229 | 3104.4033 |           |
| 3107.5381                                                 | 3122.1121 | 3130.3778 |           |
| 3132.3205                                                 | 3134.0353 | 3141.0908 |           |
| 3143.7946                                                 | 3154.0053 | 3157.5685 |           |
| Zero-point correction (Hartree): 0.255584                 |           |           |           |

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TS.dic2H5CH3CH_COO.14Hshift.mtptRR
~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -504.03687427
Electronic state : 1-A
Cartesian coordinates (Angs):
 C 0.017824 0.303619 0.100115
 O -0.092372 1.502003 -0.386126
 O -1.317734 1.648484 -1.043330
 C 1.414667 -0.068653 0.492217
 C 2.265722 -0.266754 -0.775728
 C 2.004819 0.991258 1.426591
 H 1.354726 -1.020756 1.023206
 C 3.661013 -0.798186 -0.476491
 H 1.748550 -0.956913 -1.445161
 H 2.324219 0.689448 -1.298811
 H 1.351041 1.171406 2.278961
 H 2.139482 1.932816 0.895524
 H 2.969900 0.662440 1.806004
 H 3.610810 -1.720491 0.104751
 H 4.253991 -0.077944 0.085150
 H 4.195239 -1.014493 -1.400380
 C -1.117225 -0.524328 -0.033930
 H -1.431685 0.300935 -1.045022
 C -0.872682 -2.017138 -0.046907
 C -2.382017 -0.118940 0.758784
 C -3.670064 -0.332209 -0.023377
 H -2.391421 -0.724884 1.669351
 H -2.310361 0.923287 1.060320
 H -0.711193 -2.410753 0.960776
 H -0.016566 -2.293972 -0.660902
 H -1.742558 -2.529429 -0.456968
 H -4.540380 -0.109767 0.593243
 H -3.761603 -1.362105 -0.369439
 H -3.693682 0.325277 -0.892593
Rotational constants (GHz): 1.8344300 0.6280700 0.5587500
Vibrational harmonic frequencies (cm-1):
i1609.6952 45.7991 70.0616
 76.9185 99.8986 166.6374
 184.4289 202.9332 216.9125
 225.2361 258.6367 275.3097
 285.8607 293.6048 319.0989
 349.8522 377.8957 428.3168
 530.5240 576.2445 701.9097
 729.9019 768.6671 786.9955
 795.4851 864.5843 920.0450
 971.7411 996.8933 1001.6470
1020.1773 1041.7699 1050.4563
1065.2572 1100.6806 1121.0177
1126.3038 1156.2115 1193.2011
1215.0971 1286.3206 1297.8001
1330.5912 1338.6153 1352.7789
1361.0458 1378.3166 1408.0844
1411.9502 1413.4884 1418.1670
1440.1088 1477.9643 1489.5447
1496.6641 1497.8515 1501.2211
1501.9832 1505.2854 1508.6673
1511.4813 1517.3291 1566.1006
1859.9680 3042.3844 3046.9768
3061.8185 3061.9975 3065.3217
3071.8225 3077.9936 3103.9101
3112.1187 3122.5848 3132.0547
3135.2997 3137.8761 3141.6604
3142.6477 3144.1421 3156.5600
Zero-point correction (Hartree): 0.255703

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TS.dic2H5CH3CH_COO.14Hshift.pmmmmRR
~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -504.03244233
Electronic state : 1-A
Cartesian coordinates (Angs):
  C     -0.115844     -0.689250      0.219620
  O     -0.382202     -1.963213      0.156042
  O     -1.554742     -2.204737     -0.552320
  C      1.255624     -0.445005      0.780894
  C      2.183361      0.308357     -0.178322
  C      1.135572      0.248499      2.140977
  H      1.684417     -1.438377      0.934303
  C      2.332958     -0.391008     -1.522912
  H      1.834909      1.332828     -0.308284
  H      3.155797      0.377682      0.313023
  H      0.539669     -0.346239      2.832407
  H      0.667531      1.226485      2.045378
  H      2.127171      0.383024      2.572563
  H      1.373366     -0.482432     -2.034686
  H      2.726399     -1.399344     -1.390090
  H      3.012217      0.153518     -2.176940
  C     -1.107813      0.159438     -0.335880
  H     -1.506252     -0.967379     -0.991942
  C     -2.428701      0.228309      0.452600
  C     -0.749820      1.472442     -1.013123
  C     -0.618209      2.710395     -0.126254
  H      0.148222      1.355603     -1.618197
  H     -1.555902      1.659901     -1.727980
  H     -2.337198      0.928101      1.284575
  H     -2.715720     -0.742363      0.845234
  H     -3.225359      0.582508     -0.202831
  H      0.226315      2.636352      0.557723
  H     -1.516573      2.871197      0.468497
  H     -0.466226      3.599478     -0.738130
Rotational constants (GHz):      1.0953000      0.9700400      0.7487700
Vibrational harmonic frequencies (cm-1):

```

|            |           |           |
|------------|-----------|-----------|
| 11590.5258 | 53.8649   | 104.8458  |
| 117.1592   | 147.3088  | 164.6838  |
| 192.2287   | 195.8715  | 207.4701  |
| 222.0822   | 225.9190  | 261.3049  |
| 288.7154   | 310.6435  | 347.9066  |
| 358.4989   | 394.6181  | 438.9425  |
| 492.2226   | 615.8100  | 648.4804  |
| 727.8413   | 766.1698  | 777.8429  |
| 813.0387   | 871.0376  | 942.2436  |
| 974.0554   | 987.1768  | 1009.0373 |
| 1025.2625  | 1042.2845 | 1047.7178 |
| 1051.8791  | 1093.6968 | 1099.4772 |
| 1123.0144  | 1177.2951 | 1192.4973 |
| 1236.5046  | 1278.2329 | 1303.1689 |
| 1317.1152  | 1326.3047 | 1349.3072 |
| 1366.4186  | 1377.6414 | 1396.3403 |
| 1399.8094  | 1412.0353 | 1421.8138 |
| 1440.1458  | 1480.7676 | 1491.3093 |
| 1492.0516  | 1500.0149 | 1502.8304 |
| 1503.3653  | 1507.3347 | 1511.4206 |
| 1512.9990  | 1519.4448 | 1553.1260 |
| 1877.7731  | 3052.3267 | 3057.0006 |
| 3061.0579  | 3065.0930 | 3068.5371 |
| 3072.4234  | 3074.8293 | 3113.7377 |
| 3115.4621  | 3118.1190 | 3133.1030 |
| 3134.5167  | 3139.0975 | 3141.2449 |
| 3144.2061  | 3159.8770 | 3172.4954 |

Zero-point correction (Hartree): 0.256090

TS.dic2H5CH3CH\_COO.14Hshift.pmpRR

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E(RM062X/Aug-CC-pVTZ) (Hartree): -504.03356034

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-0.104112	0.704679	-0.096443
O	-0.261279	1.685657	0.744532
O	-1.433804	1.533047	1.482348
C	1.278056	0.679241	-0.678721
C	2.159731	-0.383706	-0.000545
C	1.249142	0.534665	-2.199318
H	1.707456	1.652161	-0.425938
C	2.257333	-0.201329	1.508290
H	1.787983	-1.379998	-0.242177
H	3.151914	-0.306808	-0.449940
H	0.638695	1.312326	-2.656879
H	0.852274	-0.431333	-2.506366
H	2.261221	0.621896	-2.593545
H	1.279236	-0.274398	1.985966
H	2.663408	0.780425	1.753776
H	2.904942	-0.957432	1.949713
C	-1.182186	-0.210114	-0.167232
H	-1.500361	0.275982	1.057879
C	-2.475126	0.350525	-0.793293
C	-0.917630	-1.665041	-0.527247
C	-0.632650	-2.538212	0.693039
H	-1.802250	-2.051850	-1.035484
H	-0.102250	-1.766881	-1.245189
H	-2.443709	0.193713	-1.873539
H	-2.601089	1.409682	-0.591010
H	-3.341776	-0.178750	-0.398102
H	0.255597	-2.198041	1.225412
H	-0.478477	-3.578826	0.406755
H	-1.467496	-2.495745	1.392446

Rotational constants (GHz): 1.1256000 0.9018800 0.8117000

Vibrational harmonic frequencies (cm-1):

i1607.9516	57.1903	92.7639
119.0211	148.4221	164.5625
177.4481	186.0122	210.8387
223.6362	241.6004	260.5684
282.0754	306.6581	342.1439
362.1129	415.9733	456.5513
486.2530	580.4091	641.1709
742.6693	760.8687	780.9289
807.2550	867.4310	942.1963
977.9646	998.4985	1003.0712
1024.3071	1037.1822	1054.6079
1061.2700	1096.2890	1106.0673
1131.9797	1169.6223	1185.8708
1235.0381	1275.9776	1296.0349
1308.2436	1323.4273	1348.5812
1364.2108	1366.2320	1394.6589
1410.1600	1415.5697	1422.7920
1447.2640	1483.6416	1491.8933
1495.3532	1496.3541	1500.7044
1503.3335	1504.5511	1505.9846
1511.4311	1514.9395	1556.9420
1866.8259	3052.7529	3061.7763
3062.7726	3063.3049	3067.8258
3069.2168	3073.8980	3099.1758
3111.8477	3117.4296	3130.6146
3132.6602	3138.7848	3139.6050
3140.8551	3151.8533	3174.8757

Zero-point correction (Hartree): 0.255913

TS.dic2H5CH3CH_COO.14Hshift.pmmRR

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E(RM062X/Aug-CC-pVTZ) (Hartree): -504.03495198

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |          |           |
|---|-----------|----------|-----------|
| C | -0.259077 | 0.661078 | 0.194275  |
| O | -0.384722 | 1.867675 | -0.275830 |
| O | 0.775316  | 2.272748 | -0.933771 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -1.563708 | 0.098845  | 0.674874  |
| C | -2.124638 | -0.987332 | -0.258542 |
| C | -1.433423 | -0.403511 | 2.112240  |
| H | -2.261993 | 0.938855  | 0.646679  |
| C | -2.105162 | -0.587615 | -1.727202 |
| H | -1.578901 | -1.918276 | -0.103854 |
| H | -3.149853 | -1.177404 | 0.064635  |
| H | -1.093676 | 0.386495  | 2.780855  |
| H | -0.726383 | -1.230344 | 2.172089  |
| H | -2.400284 | -0.759608 | 2.467193  |
| H | -1.083843 | -0.452686 | -2.088652 |
| H | -2.629373 | 0.356488  | -1.879356 |
| H | -2.583277 | -1.345643 | -2.345340 |
| C | 1.024317  | 0.084723  | 0.039828  |
| H | 1.178659  | 1.019387  | -0.939511 |
| C | 2.123344  | 0.724325  | 0.911538  |
| C | 1.146631  | -1.422384 | -0.089261 |
| C | 2.527626  | -1.837430 | -0.592114 |
| H | 0.957726  | -1.919615 | 0.868944  |
| H | 0.402822  | -1.795047 | -0.792331 |
| H | 2.228382  | 0.141738  | 1.830640  |
| H | 1.881198  | 1.750587  | 1.171007  |
| H | 3.083358  | 0.728674  | 0.398216  |
| H | 2.564069  | -2.910437 | -0.774702 |
| H | 3.305813  | -1.597084 | 0.130884  |
| H | 2.765350  | -1.323653 | -1.524399 |

Rotational constants (GHz): 1.1614200 0.8605200 0.7360200  
 Vibrational harmonic frequencies (cm-1):  
 i1599.6448 37.8850 70.2964  
 95.1347 148.1039 155.4993  
 186.0114 203.3366 214.6199  
 221.1525 250.2173 267.7427  
 285.9608 311.6235 339.0413  
 349.4518 408.8451 437.1356  
 494.1700 577.2591 652.7469  
 742.7725 762.5210 799.7085  
 813.7943 869.1640 957.2452  
 972.9757 990.7618 1003.1188  
 1022.2881 1029.8496 1054.0486  
 1070.7388 1097.3050 1114.2365  
 1128.1590 1177.3072 1191.6040  
 1232.6306 1278.2814 1295.7435  
 1316.9418 1323.7048 1333.7247  
 1364.4558 1368.8270 1398.2846  
 1410.0331 1410.5985 1421.3003  
 1445.2674 1481.4153 1489.6791  
 1494.1428 1497.1368 1501.2072  
 1503.0551 1504.4626 1508.0830  
 1516.2268 1518.3389 1557.9860  
 1870.8096 3023.2420 3047.5927  
 3058.8852 3064.6544 3066.2427  
 3067.7558 3071.6991 3103.7875  
 3113.9935 3123.8715 3128.2290  
 3134.2948 3138.8477 3141.3894  
 3143.5597 3143.8275 3169.2590  
 Zero-point correction (Hartree): 0.255809

TS.dic2H5CH3CH\_COO.14Hshift.pmpmRR  
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 E(RM062X/Aug-CC-pVT2) (Hartree): -504.03561047
 Electronic state : 1-A
 Cartesian coordinates (Angs):

C	0.154620	-0.674010	-0.225630
O	-0.027563	-1.430859	-1.268240
O	-1.339379	-1.899672	-1.323671
C	1.603725	-0.368302	0.014409
C	1.830961	1.146536	-0.039040
C	2.133374	-0.975150	1.318145
H	2.140325	-0.831179	-0.817386
C	1.516187	1.736652	-1.407395
H	1.219949	1.622823	0.732013
H	2.872558	1.341999	0.223424
H	1.830369	-2.015369	1.432136
H	1.789386	-0.415190	2.184793
H	3.221914	-0.937140	1.304985
H	0.487985	1.521982	-1.704937
H	2.170836	1.313174	-2.169766
H	1.645925	2.817918	-1.412000
C	-1.005774	-0.407771	0.539780
H	-1.495279	-1.516092	-0.067069
C	-0.868195	-0.164693	2.028400
C	-2.071735	0.490882	-0.134729
C	-1.906588	1.966266	0.219322
H	-2.030005	0.357658	-1.213131
H	-3.060333	0.151813	0.182468
H	-0.332440	0.755436	2.275547
H	-0.371507	-0.991747	2.530474
H	-1.866654	-0.076423	2.459019
H	-0.922200	2.336084	-0.071286
H	-2.028983	2.143119	1.287515
H	-2.655763	2.562931	-0.301082

 Rotational constants (GHz): 1.1292200 0.9008700 0.8066100
 Vibrational harmonic frequencies (cm-1):
 i1608.8528 59.7713 86.4058
 110.0716 167.4460 193.1123
 195.7239 219.6391 238.4385
 248.9161 253.2505 266.5725
 304.5679 312.5884 334.8881
 375.4551 396.7539 454.1885
 488.9772 616.1266 636.7385
 725.0160 749.2289 792.6500
 818.1630 867.0649 918.3243

980.5834	1001.4256	1013.7488
1028.1505	1043.1858	1047.7718
1058.6199	1083.1176	1101.9369
1130.3933	1173.1773	1190.7350
1227.5333	1279.9435	1306.4033
1312.7353	1321.6480	1340.7156
1365.6827	1376.5084	1405.9323
1408.0943	1417.2376	1420.0571
1442.9159	1485.0787	1488.6347
1492.5692	1498.1843	1501.0304
1502.5255	1504.1204	1509.3366
1516.9684	1522.4815	1554.3978
1876.9663	3048.1235	3055.9668
3059.1456	3062.4283	3065.1142
3068.1287	3072.8404	3095.1042
3107.0131	3123.3682	3126.1804
3130.9825	3139.4940	3141.6570
3145.3641	3147.4051	3161.6783

Zero-point correction (Hartree): 0.256318

TS.dic2H5CH3CH_COO.14Hshift.pmptrr

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E(RM062X/Aug-CC-pVTZ) (Hartree): -504.03738742

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.227002  | -0.564385 | -0.199341 |
| O | -0.169544 | -1.638958 | -0.815425 |
| O | -1.516150 | -1.893672 | -0.553248 |
| C | 1.725981  | -0.479335 | -0.141601 |
| C | 2.272952  | 0.946897  | -0.122949 |
| C | 2.249550  | -1.315869 | 1.034177  |
| H | 2.062526  | -0.964861 | -1.062311 |
| C | 1.714123  | 1.820371  | -1.238236 |
| H | 2.081250  | 1.403750  | 0.848423  |
| H | 3.358475  | 0.876698  | -0.216090 |
| H | 1.877665  | -2.337277 | 0.980151  |
| H | 1.947346  | -0.886013 | 1.988291  |
| H | 3.338548  | -1.339364 | 1.005960  |
| H | 0.638610  | 1.964392  | -1.125246 |
| H | 1.885459  | 1.362028  | -2.213466 |
| H | 2.183691  | 2.802723  | -1.242453 |
| C | -0.790244 | 0.158274  | 0.464290  |
| H | -1.438767 | -1.013458 | 0.469979  |
| C | -0.422217 | 1.030130  | 1.643051  |
| C | -1.872859 | 0.801161  | -0.437409 |
| C | -3.279070 | 0.678626  | 0.131800  |
| H | -1.606138 | 1.857275  | -0.543820 |
| H | -1.842386 | 0.355542  | -1.429081 |
| H | -0.062577 | 2.013143  | 1.325931  |
| H | 0.332168  | 0.578806  | 2.284267  |
| H | -1.307214 | 1.196227  | 2.257325  |
| H | -3.996677 | 1.210887  | -0.491755 |
| H | -3.340591 | 1.094262  | 1.137840  |
| H | -3.577149 | -0.368925 | 0.172754  |

Rotational constants (GHz): 1.4058500 0.8062900 0.6712300

Vibrational harmonic frequencies (cm-1):

|            |           |           |
|------------|-----------|-----------|
| i1601.8284 | 67.8020   | 92.9010   |
| 105.6335   | 128.3249  | 192.2317  |
| 207.4462   | 209.8414  | 219.9758  |
| 234.4137   | 248.9923  | 279.0932  |
| 282.8174   | 292.1019  | 337.1812  |
| 370.6325   | 421.4900  | 455.3455  |
| 473.2726   | 591.0318  | 635.7507  |
| 736.9799   | 764.8354  | 789.6767  |
| 806.9681   | 874.5302  | 918.0479  |
| 972.3837   | 1002.9049 | 1020.0598 |
| 1023.9661  | 1038.7331 | 1044.8374 |
| 1056.9217  | 1097.0758 | 1104.2552 |
| 1127.9955  | 1173.2458 | 1200.8003 |
| 1231.9158  | 1282.8600 | 1301.0520 |
| 1312.7576  | 1324.2013 | 1347.0004 |
| 1365.0878  | 1377.7747 | 1404.7659 |
| 1410.5926  | 1416.8535 | 1419.4285 |
| 1445.1577  | 1474.1180 | 1489.2399 |
| 1492.5187  | 1500.4492 | 1503.3242 |
| 1503.9793  | 1506.5113 | 1508.0320 |
| 1511.4717  | 1514.9554 | 1561.9617 |
| 1864.4454  | 3039.9926 | 3045.0321 |
| 3055.5872  | 3061.6746 | 3063.7789 |
| 3070.5679  | 3072.9969 | 3109.0820 |
| 3113.1836  | 3123.1144 | 3131.7037 |
| 3136.8445  | 3140.0999 | 3140.1579 |
| 3142.5277  | 3149.1797 | 3156.0494 |

Zero-point correction (Hartree): 0.256117

TS.dic2H5CH3CH\_COO.14Hshift.pmprr

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E(RM062X/Aug-CC-pVTZ) (Hartree): -504.02652048

Electronic state : 1-A

Cartesian coordinates (Angs):

C	0.441271	0.691938	-0.083852
O	1.123154	1.483745	-0.863090
O	2.333717	0.907106	-1.240064
C	-0.953799	1.214952	0.127547
C	-2.016517	0.609893	-0.830667
C	-1.350674	1.175690	1.602375
H	-0.863690	2.263047	-0.163362
C	-2.875053	-0.524458	-0.283307
H	-2.684873	1.426771	-1.106322
H	-1.524675	0.304438	-1.755558
H	-0.607537	1.687459	2.212831
H	-1.453066	0.158502	1.974481

H	-2.307092	1.680075	1.740829
H	-3.447243	-0.201123	0.585641
H	-2.294886	-1.397987	0.002820
H	-3.587446	-0.840194	-1.044783
C	1.115083	-0.495121	0.293578
H	1.893677	-0.246624	-0.795599
C	2.292880	-0.286756	1.265798
C	0.317097	-1.757557	0.555985
C	-0.046852	-2.496216	-0.729986
H	0.924788	-2.415280	1.179539
H	-0.583281	-1.554775	1.140411
H	3.032515	-1.076073	1.134644
H	1.921730	-0.334341	2.292034
H	2.784899	0.669037	1.111503
H	-0.599752	-1.851115	-1.413561
H	-0.656968	-3.377208	-0.527452
H	0.857320	-2.815615	-1.247694
Rotational constants (GHz):			
	1.2645000	0.8646800	0.7160200
Vibrational harmonic frequencies (cm-1):			
i1605.9730	49.8916		91.9020
113.6088	148.8412		170.2858
172.4258	198.1393		222.5781
250.8889	263.7476		284.7096
285.5164	298.9443		324.3338
358.7322	404.8237		447.1264
532.8058	592.2488		631.5639
739.3915	756.5791		775.1985
795.3053	857.4522		938.9840
971.8214	1002.7319		1010.1907
1025.9358	1039.5088		1042.2430
1059.3258	1102.7978		1104.9595
1142.2338	1161.1165		1177.3793
1240.9803	1292.4151		1299.5648
1309.8585	1329.2027		1350.4152
1366.6220	1376.8068		1395.7056
1410.5938	1416.7603		1419.6865
1442.4216	1485.3935		1490.1539
1493.0804	1494.3578		1497.7644
1500.7593	1504.9995		1507.4165
1514.5860	1522.2698		1554.8581
1874.8536	3050.5789		3059.3819
3063.0031	3064.2064		3071.5800
3078.2834	3079.3747		3092.4898
3102.6363	3116.3158		3129.8741
3133.2883	3135.4091		3137.9702
3157.1799	3170.9360		3172.6997
Zero-point correction (Hartree): 0.256187			
TS.dic2H5CH3CH_COO.14Hshift.pppmRR			
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E(RM062X/Aug-CC-pVT2) (Hartree): -504.03059173			
Electronic state : 1-A			
Cartesian coordinates (Angs):			
C	-0.135623	-0.790372	-0.129373
O	-0.732110	-1.761455	-0.763212
O	-2.083108	-1.827601	-0.441400
C	1.359124	-0.914433	-0.255115
C	1.957388	0.204038	-1.132273
C	2.069920	-1.056423	1.092248
H	1.502722	-1.850151	-0.798374
C	2.176285	1.546592	-0.446855
H	2.915942	-0.164899	-1.503526
H	1.320969	0.334248	-2.010349
H	1.647988	-1.875649	1.673325
H	2.012316	-0.149196	1.686490
H	3.122951	-1.274121	0.911208
H	2.905270	1.469343	0.358984
H	1.252027	1.943006	-0.032354
H	2.554726	2.274964	-1.163147
C	-0.994019	0.033632	0.642897
H	-1.837765	-1.019749	0.587027
C	-0.487128	0.679476	1.916873
C	-1.995387	0.917860	-0.138227
C	-1.405421	2.249729	-0.589979
H	-2.372217	0.372847	-0.999185
H	-2.849599	1.101280	0.517150
H	0.251211	1.467549	1.759855
H	-0.057901	-0.051487	2.598680
H	-1.336636	1.136786	2.426337
H	-0.607527	2.094791	-1.317454
H	-0.998832	2.822330	0.244584
H	-2.174728	2.859969	-1.063530
Rotational constants (GHz):			
	1.2068800	0.9245000	0.7248900
Vibrational harmonic frequencies (cm-1):			
i1588.9687	54.1903		84.3740
108.7952	133.4476		188.4869
206.3056	228.1745		238.9321
257.7717	270.2561		284.1191
304.4152	321.8188		341.3289
353.4397	416.1273		430.6409
547.1689	620.4099		635.3579
725.0126	748.4539		786.0872
810.2025	848.7020		915.9509
976.3783	1000.7231		1018.2749
1023.3586	1034.1823		1049.4524
1052.0497	1092.6033		1104.2775
1137.3103	1165.6910		1181.4686
1229.8271	1300.3068		1308.3507
1326.3808	1328.9264		1341.7040
1369.7434	1378.8784		1405.3635
1407.4681	1413.9377		1422.2299
1438.1354	1485.8720		1487.3476

1492.2373	1496.4667	1501.4981
1504.6311	1507.3767	1511.1404
1521.4638	1527.9132	1552.5828
1870.0130	3054.4896	3056.2523
3060.9396	3064.4748	3071.1594
3077.0592	3077.8147	3091.5806
3113.1176	3121.7171	3127.0197
3135.6903	3136.9514	3143.0203
3153.4326	3167.2455	3175.5166

Zero-point correction (Hartree): 0.256642

TS.dic2H5CH3CH_COO.14Hshift.ppptRR

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E(RM062X/Aug-CC-pVT2) (Hartree): -504.03383364

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.168507 | 0.699474  | 0.084318  |
| O | 0.308622  | 1.847445  | -0.306418 |
| O | 1.689683  | 1.896319  | -0.142033 |
| C | -1.670894 | 0.718031  | 0.122790  |
| C | -2.235323 | 0.000908  | -1.120417 |
| C | -2.278786 | 0.193228  | 1.423740  |
| H | -1.942767 | 1.771247  | 0.031693  |
| C | -1.937161 | -1.490952 | -1.202765 |
| H | -3.315606 | 0.161711  | -1.118981 |
| H | -1.847106 | 0.500024  | -2.010089 |
| H | -1.852471 | 0.693994  | 2.292045  |
| H | -2.139467 | -0.876959 | 1.545788  |
| H | -3.349855 | 0.394640  | 1.409292  |
| H | -2.351568 | -2.034748 | -0.354389 |
| H | -0.864180 | -1.678694 | -1.234701 |
| H | -2.374069 | -1.913059 | -2.106613 |
| C | 0.809674  | -0.245171 | 0.477321  |
| H | 1.597585  | 0.836329  | 0.656036  |
| C | 0.469101  | -1.325626 | 1.480088  |
| C | 1.734181  | -0.763574 | -0.655954 |
| C | 3.197791  | -0.858295 | -0.248669 |
| H | 1.363629  | -1.755772 | -0.931461 |
| H | 1.643133  | -0.127554 | -1.534193 |
| H | -0.185936 | -2.094583 | 1.061223  |
| H | 0.007203  | -0.931437 | 2.381968  |
| H | 1.390909  | -1.822460 | 1.782593  |
| H | 3.791469  | -1.309713 | -1.043099 |
| H | 3.324422  | -1.466714 | 0.647162  |
| H | 3.597788  | 0.135487  | -0.049381 |

Rotational constants (GHz): 1.4436800 0.7830000 0.6874200

Vibrational harmonic frequencies (cm-1):

|            |           |           |
|------------|-----------|-----------|
| i1598.1227 | 62.4870   | 94.1226   |
| 110.1647   | 121.3714  | 194.9673  |
| 209.7979   | 228.8907  | 252.1659  |
| 259.8801   | 267.7911  | 280.2701  |
| 296.7898   | 315.6346  | 328.8610  |
| 350.4890   | 393.8350  | 454.6440  |
| 531.0660   | 595.4878  | 650.8817  |
| 739.1884   | 769.3849  | 788.4779  |
| 807.7853   | 845.1302  | 917.7532  |
| 979.2504   | 1001.7095 | 1022.0192 |
| 1025.8178  | 1030.6277 | 1044.6035 |
| 1059.4551  | 1095.9168 | 1104.6212 |
| 1131.1447  | 1166.5124 | 1180.2358 |
| 1232.0710  | 1292.7274 | 1316.1690 |
| 1318.5282  | 1324.1779 | 1344.7357 |
| 1364.0712  | 1378.5104 | 1408.5358 |
| 1412.6613  | 1417.3059 | 1420.2178 |
| 1442.9840  | 1473.5202 | 1487.9113 |
| 1493.3658  | 1495.3655 | 1499.0303 |
| 1505.7759  | 1506.0281 | 1511.7963 |
| 1512.5772  | 1524.5248 | 1557.3989 |
| 1869.0757  | 3040.5571 | 3049.0258 |
| 3058.2692  | 3064.2681 | 3071.9798 |
| 3074.5078  | 3078.8471 | 3096.8586 |
| 3113.9079  | 3119.1661 | 3135.2635 |
| 3137.2584  | 3138.7688 | 3141.4966 |
| 3146.4598  | 3152.3879 | 3174.5186 |

Zero-point correction (Hartree): 0.256549

TS.dic2H5CH3CH\_COO.14Hshift.ptmmRR

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E(RM062X/Aug-CC-pVT2) (Hartree): -504.03054225

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-0.329182	-0.724112	-0.022838
O	-0.767999	-1.943785	-0.157626
O	-2.073666	-1.964947	-0.637512
C	1.138439	-0.707427	0.295667
C	1.982722	0.141255	-0.665362
C	1.308720	-0.289757	1.762144
H	1.468265	-1.744273	0.193213
C	3.472667	-0.147253	-0.519623
H	1.676174	-0.069207	-1.691457
H	1.796483	1.200389	-0.486424
H	0.715451	-0.926864	2.417191
H	0.991885	0.741522	1.912463
H	2.351027	-0.378298	2.062810
H	3.681240	-1.205360	-0.681380
H	3.841551	0.121581	0.469267
H	4.045789	0.422623	-1.249333
C	-1.285616	0.290054	-0.283978
H	-1.943536	-0.696446	-0.956273
C	-2.418920	0.412069	0.750974
C	-0.869823	1.626021	-0.875580
C	-0.474069	2.722861	0.112578

H	-0.079659	1.484069	-1.610658
H	-1.732921	1.982906	-1.444475
H	-2.078520	0.976454	1.620502
H	-2.769402	-0.560470	1.082598
H	-3.259370	0.947410	0.307099
H	0.381867	2.432928	0.721840
H	-1.294582	2.961520	0.788014
H	-0.208053	3.637106	-0.417795
Rotational constants (GHz): 1.2514600 0.8387200 0.6281200			
Vibrational harmonic frequencies (cm-1):			
i1594.0138	53.6436		86.8712
110.8150	130.8981		168.3961
175.6975	197.2061		203.4608
213.4098	240.5946		268.3411
297.3082	321.3786		324.9761
358.1970	384.5795		417.9797
488.9804	625.6655		697.8294
728.5270	758.9086		781.8719
803.6907	880.0459		942.4300
967.9745	985.5359		1000.7703
1021.9720	1038.9257		1046.8786
1048.7023	1087.6945		1095.2106
1142.4346	1175.8919		1194.2686
1239.1114	1291.3641		1304.1236
1306.2012	1327.7906		1355.9172
1364.6214	1375.2720		1395.6702
1401.8623	1412.3617		1417.0877
1436.1289	1484.1403		1490.2348
1493.5169	1496.3809		1501.2131
1503.2074	1507.2730		1512.3449
1515.2855	1519.4115		1553.4997
1876.2487	3052.8498		3055.9379
3063.6114	3065.8482		3067.8597
3070.8109	3074.7108		3113.4943
3114.8970	3121.1708		3132.5156
3138.3080	3140.1861		3141.9120
3147.6494	3156.7240		3171.8730
Zero-point correction (Hartree): 0.256017			
TS.dic2H5CH3CH_COO.14Hshift.ptmpRR			
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E(RM062X/Aug-CC-pVTZ) (Hartree): -504.03167900			
Electronic state : 1-A			
Cartesian coordinates (Angs):			
C	-0.284071	-0.685147	-0.051362
O	-0.638638	-1.665816	-0.829926
O	-1.938848	-1.489443	-1.299658
C	1.184452	-0.713208	0.256106
C	1.964486	0.327874	-0.566333
C	1.426856	-0.601436	1.762346
H	1.522412	-1.696875	-0.080822
C	3.470957	0.109976	-0.490117
H	1.639725	0.262836	-1.606561
H	1.719990	1.331860	-0.218355
H	0.820708	-1.324116	2.307601
H	1.184323	0.393469	2.133775
H	2.471367	-0.803294	1.992317
H	3.733621	-0.900988	-0.804113
H	3.848555	0.258730	0.520676
H	3.992029	0.809631	-1.141803
C	-1.298797	0.260244	0.232076
H	-1.887602	-0.235798	-0.889291
C	-2.438037	-0.253234	1.134343
C	-0.915529	1.708178	0.494512
C	-0.814270	2.530659	-0.788539
H	-1.680065	2.149075	1.136066
H	0.017106	1.788049	1.056754
H	-2.168739	-0.085997	2.179540
H	-2.633054	-1.310673	0.983056
H	-3.355959	0.296546	0.928011
H	-0.076759	2.107436	-1.470523
H	-0.532362	3.562742	-0.578619
H	-1.771684	2.536006	-1.309221
Rotational constants (GHz): 1.2813500 0.7835300 0.6676800			
Vibrational harmonic frequencies (cm-1):			
i1612.6622	50.3857		69.2583
107.2175	119.8247		151.8252
170.3689	182.9368		195.8142
213.1187	235.4081		262.0316
292.3761	300.1328		338.3111
363.9139	378.7640		451.5717
488.7590	581.5869		696.0555
741.6993	758.4494		782.2634
793.8960	875.3599		941.9299
974.2907	988.4083		1005.3734
1026.5917	1034.8057		1050.1267
1059.0322	1087.0065		1106.2821
1146.5135	1168.5301		1189.8290
1237.4620	1287.5662		1296.6243
1302.6482	1326.1224		1355.5106
1364.8191	1372.9706		1394.3916
1411.1090	1412.9549		1417.5486
1443.0089	1486.2072		1490.2473
1493.9167	1497.9306		1498.6816
1500.0316	1503.1390		1505.0007
1514.6242	1516.0661		1555.6096
1871.3441	3050.8185		3059.8483
3061.5169	3064.7360		3065.2535
3069.5048	3074.7422		3094.8133
3113.4348	3116.0271		3132.4617
3135.0676	3137.5015		3140.0387
3143.4719	3152.8969		3171.5964


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Zero-point correction (Hartree): 0.255654

TS.dic2H5CH3CH_COO.14Hshift.ptmtRR
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E(RM062X/Aug-CC-pVTZ) (Hartree): -504.03263368
Electronic state : 1-A
Cartesian coordinates (Angs):
  C   -0.004901   -0.730487    0.020209
  O   -0.128044   -1.951448   -0.411324
  O   -1.409675   -2.178463   -0.910977
  C    1.415636   -0.378278    0.344008
  C    2.023839    0.635030   -0.643984
  C    1.506387    0.101302    1.794579
  H    1.975296   -1.310953    0.238043
  C    3.546889    0.576514   -0.643607
  H    1.653448    0.431471   -1.650458
  H    1.693904    1.639511   -0.377984
  H    1.124554   -0.652226    2.482422
  H    0.929323    1.015294    1.934080
  H    2.541299    0.307890    2.062459
  H    3.896051   -0.408828   -0.952754
  H    3.955581    0.783266    0.345212
  H    3.961642    1.311485   -1.331808
  C   -1.189939    0.042264   -0.008401
  H   -1.609324   -0.880379   -0.922352
  C   -2.259872   -0.391377    1.013420
  C   -1.082439    1.546414   -0.179723
  C   -2.430392    2.175651   -0.524454
  H   -0.694365    2.022069    0.728748
  H   -0.383060    1.777285   -0.981500
  H   -2.154516    0.218582    1.914717
  H   -2.155341   -1.438138    1.282923
  H   -3.264702   -0.248043    0.619716
  H   -2.315486    3.236538   -0.742095
  H   -3.138998    2.080143    0.297045
  H   -2.864800    1.692117   -1.400283
Rotational constants (GHz):    1.2968600    0.7528500    0.6044000
Vibrational harmonic frequencies (cm-1):
  i1603.1162      37.0226      71.1012
    88.2409      124.2225      155.7042
   169.8272      197.0995      208.1391
   223.5189      247.8161      266.1182
   295.3703      313.8145      325.0219
   352.3920      363.7890      432.9406
   504.6319      577.9925      706.9190
   741.1512      761.2166      796.4610
   804.4185      879.6164      958.0682
   969.1324      991.6898      1001.3228
  1018.8145     1029.6721      1045.0892
  1071.3225     1086.4362      1112.9472
  1142.2896     1177.0430      1193.4567
  1233.1615     1292.1592      1296.4264
  1303.6408     1330.0926      1347.0518
  1362.3569     1377.1097      1397.6018
  1409.9807     1411.0898      1416.8009
  1443.8747     1483.0893      1489.3888
  1494.3335     1498.4754      1499.4332
  1501.3513     1506.3450      1509.2315
  1512.2421     1518.3939      1557.1578
  1872.9511     3017.7734      3046.4808
  3063.8301     3064.7267      3065.3559
  3070.0335     3071.7759      3107.7236
  3118.0193     3123.3019      3134.4238
  3137.4405     3139.8719      3141.6414
  3144.6617     3148.8974      3169.4306
Zero-point correction (Hartree): 0.255772

TS.dic2H5CH3CH_COO.14Hshift.ptpmRR
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E(RM062X/Aug-CC-pVTZ) (Hartree): -504.03413871
Electronic state : 1-A
Cartesian coordinates (Angs):
  C   -0.189069   -0.701466   -0.147605
  O   -0.620437   -1.711287   -0.845514
  O   -1.980602   -1.924570   -0.629124
  C    1.308762   -0.625427   -0.124786
  C    1.784989    0.744043   -0.625163
  C    1.878308   -0.979524    1.256229
  H    1.647807   -1.388702   -0.829605
  C    3.302756    0.839333   -0.715998
  H    1.348224    0.927121   -1.608985
  H    1.400688    1.522838    0.037456
  H    1.363603   -1.837089    1.688109
  H    1.795696   -0.140412    1.944911
  H    2.931815   -1.235065    1.159853
  H    3.706789    0.030421   -1.326855
  H    3.766636    0.781162    0.267875
  H    3.603547    1.782860   -1.168317
  C   -1.179213    0.007662    0.573823
  H   -1.905959   -1.128189    0.426615
  C   -0.789094    0.688507    1.870232
  C   -2.186109    0.826165   -0.267502
  C   -1.683712    2.232945   -0.578600
  H   -2.407982    0.297248   -1.190538
  H   -3.121037    0.888195    0.293628
  H   -0.067242    1.498899    1.742863
  H   -0.380758   -0.015683    2.591832
  H   -1.683374    1.127365    2.314751
  H   -0.762345    2.197307   -1.161236
  H   -1.486415    2.804225    0.328619
  H   -2.427097    2.780931   -1.157655
Rotational constants (GHz):    1.2992700    0.7868300    0.6596900

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Vibrational harmonic frequencies (cm-1):

i1600.3959	55.9153	77.1166
106.1079	109.4478	182.0909
192.0386	207.2546	223.4080
244.2013	279.0921	282.6243
292.1287	303.1303	338.4035
359.5911	381.0498	436.2383
495.0219	615.7471	678.6558
728.6789	761.0145	794.4071
803.0116	867.1946	921.5057
974.8294	989.4539	1014.0090
1019.5285	1032.6772	1047.2001
1066.0436	1083.8291	1098.0451
1145.1184	1173.1020	1191.0961
1228.4209	1284.5049	1303.7211
1314.6987	1321.6424	1350.8632
1361.1220	1376.5746	1405.5490
1407.8416	1415.1475	1417.9910
1439.7976	1485.0382	1489.9633
1492.2903	1499.0749	1501.4188
1502.3903	1507.5151	1512.0989
1515.6159	1520.5264	1554.7506
1872.4214	3048.4781	3058.3836
3060.4451	3063.6687	3064.5331
3065.9032	3073.3146	3098.8594
3107.8038	3124.4519	3128.9407
3132.5885	3141.7619	3141.9837
3147.4160	3150.7825	3155.1152

Zero-point correction (Hartree): 0.256101

TS.dic2H5CH3CH_COO.14Hshift.ptptRR

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E(RM062X/Aug-CC-pVTZ) (Hartree): -504.03510536

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.010684 | 0.603080  | 0.093111  |
| O | 0.413459  | 1.810656  | -0.140997 |
| O | 1.794719  | 1.891627  | 0.033084  |
| C | -1.505145 | 0.514737  | 0.145338  |
| C | -1.992284 | -0.454728 | -0.941621 |
| C | -2.026104 | 0.145396  | 1.539958  |
| H | -1.867858 | 1.517131  | -0.095076 |
| C | -3.511402 | -0.514283 | -1.037092 |
| H | -1.576086 | -0.141329 | -1.901110 |
| H | -1.591772 | -1.450119 | -0.736301 |
| H | -1.497542 | 0.693924  | 2.318707  |
| H | -1.920150 | -0.920869 | 1.732182  |
| H | -3.082411 | 0.397833  | 1.610774  |
| H | -3.930314 | 0.482416  | -1.184297 |
| H | -3.952443 | -0.934358 | -0.133955 |
| H | -3.821217 | -1.135004 | -1.876183 |
| C | 0.998875  | -0.349521 | 0.356453  |
| H | 1.756239  | 0.734784  | 0.666481  |
| C | 0.671932  | -1.556319 | 1.208936  |
| C | 1.906483  | -0.692582 | -0.852177 |
| C | 3.371880  | -0.859382 | -0.477241 |
| H | 1.518451  | -1.622263 | -1.280190 |
| H | 1.815683  | 0.077159  | -1.615707 |
| H | -0.035676 | -2.237722 | 0.727721  |
| H | 0.273344  | -1.281265 | 2.182842  |
| H | 1.586170  | -2.122450 | 1.385446  |
| H | 3.958266  | -1.182390 | -1.337043 |
| H | 3.501901  | -1.601071 | 0.311188  |
| H | 3.778680  | 0.088933  | -0.126165 |

Rotational constants (GHz): 1.6220400 0.6604900 0.6001900

Vibrational harmonic frequencies (cm-1):

|             |           |           |
|-------------|-----------|-----------|
| i11594.5353 | 54.9535   | 72.5731   |
| 88.0891     | 116.3279  | 175.8652  |
| 199.5346    | 205.6050  | 217.2530  |
| 253.2949    | 266.8404  | 279.4374  |
| 292.1377    | 319.1140  | 327.2992  |
| 356.0951    | 378.8278  | 437.1564  |
| 493.4383    | 592.7614  | 680.8693  |
| 743.4941    | 782.0418  | 788.6112  |
| 790.8098    | 864.3598  | 921.5875  |
| 975.4563    | 989.9383  | 1017.8015 |
| 1022.5453   | 1036.9805 | 1040.3994 |
| 1071.2835   | 1088.2512 | 1102.7270 |
| 1144.6235   | 1168.0934 | 1189.5572 |
| 1230.2318   | 1284.5036 | 1299.4111 |
| 1311.3632   | 1335.1513 | 1350.2060 |
| 1360.4208   | 1377.2033 | 1407.8340 |
| 1411.7680   | 1414.4215 | 1419.8861 |
| 1444.2508   | 1475.2715 | 1487.6026 |
| 1494.5936   | 1496.6706 | 1501.1609 |
| 1501.8021   | 1506.7289 | 1509.4258 |
| 1515.3183   | 1520.2476 | 1559.5624 |
| 1873.9715   | 3038.5979 | 3043.6648 |
| 3058.5509   | 3062.9789 | 3063.8391 |
| 3066.8222   | 3073.4504 | 3097.0980 |
| 3114.0689   | 3119.7082 | 3132.6139 |
| 3135.0470   | 3139.4684 | 3141.3293 |
| 3145.6918   | 3148.3939 | 3155.9502 |

Zero-point correction (Hartree): 0.256003

#####  
(S-CH(CH3)(C2H5))(R-CH(CH3)(C2H5))COO  
#####

Population analysis as 298K (%)  
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)

| Compound               | Qtot      | Erel | Erel2 | n*Q*MB    | %        |
|------------------------|-----------|------|-------|-----------|----------|
| dic2H5CH3CH_COO.cmmtRS | 4.241e+43 | 0.00 | 0.00  | 4.241e+43 | 11.9     |
| dic2H5CH3CH_COO.cmpRS  | 4.010e+43 | 0.18 | 0.18  | 2.984e+43 | 8.36     |
| dic2H5CH3CH_COO.cmttRS | 7.846e+43 | 0.58 | 0.58  | 2.954e+43 | 8.28     |
| dic2H5CH3CH_COO.ctmRS  | 5.196e+43 | 0.59 | 0.59  | 1.933e+43 | 5.42     |
| dic2H5CH3CH_COO.pmpRS  | 2.154e+43 | 0.10 | 0.10  | 1.835e+43 | 5.14     |
| dic2H5CH3CH_COO.mtmRS  | 1.553e+44 | 1.28 | 1.28  | 1.780e+43 | 4.99     |
| dic2H5CH3CH_COO.pmpRS  | 1.053e+44 | 1.15 | 1.15  | 1.513e+43 | 4.24     |
| dic2H5CH3CH_COO.mptRS  | 2.703e+43 | 0.40 | 0.40  | 1.384e+43 | 3.88     |
| dic2H5CH3CH_COO.mptRS  | 2.026e+43 | 0.23 | 0.23  | 1.370e+43 | 3.84     |
| dic2H5CH3CH_COO.cmpRS  | 5.446e+43 | 0.82 | 0.82  | 1.362e+43 | 3.82     |
| dic2H5CH3CH_COO.mmpRS  | 2.210e+44 | 1.68 | 1.68  | 1.294e+43 | 3.63     |
| dic2H5CH3CH_COO.ctpRS  | 5.043e+43 | 0.86 | 0.86  | 1.180e+43 | 3.31     |
| dic2H5CH3CH_COO.mttRS  | 4.516e+43 | 0.85 | 0.85  | 1.067e+43 | 2.99     |
| dic2H5CH3CH_COO.mtpRS  | 3.618e+43 | 0.74 | 0.74  | 1.039e+43 | 2.91     |
| dic2H5CH3CH_COO.mpmRS  | 9.301e+43 | 1.39 | 1.39  | 8.936e+42 | 2.5      |
| dic2H5CH3CH_COO.cmpRS  | 9.277e+43 | 1.39 | 1.39  | 8.903e+42 | 2.5      |
| dic2H5CH3CH_COO.mtpRS  | 3.277e+43 | 0.79 | 0.79  | 8.567e+42 | 2.4      |
| dic2H5CH3CH_COO.mtmRS  | 8.429e+43 | 1.40 | 1.40  | 7.885e+42 | 2.21     |
| dic2H5CH3CH_COO.mtmRS  | 8.551e+43 | 1.43 | 1.43  | 7.689e+42 | 2.16     |
| dic2H5CH3CH_COO.ptpRS  | 3.139e+43 | 0.92 | 0.92  | 6.598e+42 | 1.85     |
| dic2H5CH3CH_COO.mptRS  | 1.273e+44 | 1.78 | 1.78  | 6.253e+42 | 1.75     |
| dic2H5CH3CH_COO.cttRS  | 1.287e+44 | 1.82 | 1.82  | 5.985e+42 | 1.68     |
| dic2H5CH3CH_COO.mppRS  | 1.606e+43 | 0.61 | 0.61  | 5.730e+42 | 1.61     |
| dic2H5CH3CH_COO.ctpRS  | 1.166e+44 | 1.98 | 1.98  | 4.086e+42 | 1.15     |
| dic2H5CH3CH_COO.ptpRS  | 1.227e+44 | 2.03 | 2.03  | 3.992e+42 | 1.12     |
| dic2H5CH3CH_COO.mptRS  | 5.478e+43 | 1.58 | 1.58  | 3.802e+42 | 1.07     |
| dic2H5CH3CH_COO.mpmRS  | 4.830e+43 | 1.54 | 1.54  | 3.599e+42 | 1.01     |
| dic2H5CH3CH_COO.mmtRS  | 2.625e+43 | 1.28 | 1.28  | 3.001e+42 | 0.841    |
| dic2H5CH3CH_COO.cpmRS  | 3.681e+43 | 1.73 | 1.73  | 1.977e+42 | 0.554    |
| dic2H5CH3CH_COO.cpmRS  | 2.892e+43 | 1.63 | 1.63  | 1.852e+42 | 0.519    |
| dic2H5CH3CH_COO.mmmRS  | 3.976e+43 | 1.84 | 1.84  | 1.780e+42 | 0.499    |
| dic2H5CH3CH_COO.pmtRS  | 3.015e+43 | 1.98 | 1.98  | 1.063e+42 | 0.298    |
| dic2H5CH3CH_COO.ctmRS  | 4.533e+43 | 2.30 | 2.30  | 9.320e+41 | 0.261    |
| dic2H5CH3CH_COO.cmmRS  | 2.514e+43 | 2.09 | 2.09  | 7.374e+41 | 0.207    |
| dic2H5CH3CH_COO.mmpRS  | 3.411e+43 | 2.41 | 2.41  | 5.866e+41 | 0.164    |
| dic2H5CH3CH_COO.cpmRS  | 7.688e+43 | 2.95 | 2.95  | 5.267e+41 | 0.148    |
| dic2H5CH3CH_COO.pmtRS  | 2.264e+43 | 2.24 | 2.24  | 5.157e+41 | 0.145    |
| dic2H5CH3CH_COO.ptmRS  | 4.065e+43 | 2.71 | 2.71  | 4.194e+41 | 0.118    |
| dic2H5CH3CH_COO.ctmRS  | 3.014e+43 | 2.70 | 2.70  | 3.142e+41 | 0.0881   |
| dic2H5CH3CH_COO.cpmRS  | 2.365e+43 | 2.61 | 2.61  | 2.878e+41 | 0.0807   |
| dic2H5CH3CH_COO.cmpRS  | 4.904e+43 | 3.18 | 3.18  | 2.283e+41 | 0.064    |
| dic2H5CH3CH_COO.mmpRS  | 2.107e+43 | 2.74 | 2.74  | 2.049e+41 | 0.0574   |
| dic2H5CH3CH_COO.ppmRS  | 2.016e+43 | 2.93 | 2.93  | 1.432e+41 | 0.0401   |
| dic2H5CH3CH_COO.pmtRS  | 4.111e+43 | 3.37 | 3.37  | 1.380e+41 | 0.0387   |
| dic2H5CH3CH_COO.ppmRS  | 5.793e+43 | 3.60 | 3.60  | 1.325e+41 | 0.0371   |
| dic2H5CH3CH_COO.cmtRS  | 3.184e+43 | 3.27 | 3.27  | 1.280e+41 | 0.0359   |
| dic2H5CH3CH_COO.cptRS  | 4.088e+43 | 3.54 | 3.54  | 1.030e+41 | 0.0289   |
| dic2H5CH3CH_COO.pmpRS  | 4.121e+43 | 3.76 | 3.76  | 7.180e+40 | 0.0201   |
| dic2H5CH3CH_COO.ptmRS  | 2.684e+43 | 3.62 | 3.62  | 5.955e+40 | 0.0167   |
| dic2H5CH3CH_COO.ctpRS  | 6.966e+43 | 4.31 | 4.31  | 4.770e+40 | 0.0134   |
| dic2H5CH3CH_COO.cpmRS  | 1.874e+43 | 3.63 | 3.63  | 4.055e+40 | 0.0114   |
| dic2H5CH3CH_COO.pmmRS  | 1.016e+43 | 3.45 | 3.45  | 3.021e+40 | 0.00847  |
| dic2H5CH3CH_COO.ctmRS  | 3.936e+43 | 4.35 | 4.35  | 2.552e+40 | 0.00715  |
| dic2H5CH3CH_COO.ptpRS  | 5.422e+43 | 4.80 | 4.80  | 1.633e+40 | 0.00458  |
| dic2H5CH3CH_COO.mppRS  | 1.774e+43 | 4.20 | 4.20  | 1.485e+40 | 0.00416  |
| dic2H5CH3CH_COO.mmpRS  | 2.581e+43 | 4.60 | 4.60  | 1.096e+40 | 0.00307  |
| dic2H5CH3CH_COO.mtmRS  | 4.365e+43 | 5.12 | 5.12  | 7.625e+39 | 0.00214  |
| dic2H5CH3CH_COO.ptmRS  | 1.990e+43 | 4.74 | 4.74  | 6.615e+39 | 0.00185  |
| dic2H5CH3CH_COO.cpmRS  | 4.663e+43 | 5.61 | 5.61  | 3.574e+39 | 0.001    |
| dic2H5CH3CH_COO.cpmRS  | 2.779e+43 | 5.51 | 5.51  | 2.525e+39 | 0.000708 |
| dic2H5CH3CH_COO.pptRS  | 2.385e+43 | 5.60 | 5.60  | 1.863e+39 | 0.000522 |
| dic2H5CH3CH_COO.ppmRS  | 1.546e+43 | 5.54 | 5.54  | 1.337e+39 | 0.000375 |
| dic2H5CH3CH_COO.ppmRS  | 2.691e+43 | 5.91 | 5.91  | 1.239e+39 | 0.000347 |
| dic2H5CH3CH_COO.pmmRS  | 1.685e+43 | 6.23 | 6.23  | 4.515e+38 | 0.000127 |
| dic2H5CH3CH_COO.ppmRS  | 1.983e+43 | 7.03 | 7.03  | 1.389e+38 | 3.89e-05 |
| dic2H5CH3CH_COO.ppmRS  | 1.168e+43 | 8.32 | 8.32  | 9.255e+36 | 2.59e-06 |
| Total                  |           |      |       | 3.568e+44 | 100      |

dic2H5CH3CH\_COO.cmmRS

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E(RM062X/Aug-CC-pVTZ) (Hartree): -504.06635097

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-0.118669	0.283081	0.052213
O	-0.476941	1.287049	-0.606313
O	0.281838	2.429406	-0.564945
C	-1.067608	-0.884546	-0.013876
C	-2.494506	-0.469388	-0.377261
C	-0.536382	-1.945376	-0.987769
H	-1.081442	-1.325139	0.985996
C	-3.146469	0.439509	0.657562
H	-2.490943	0.013417	-1.355242
H	-3.078531	-1.385773	-0.480680
H	0.452990	-2.302880	-0.710624
H	-0.483211	-1.536473	-1.997309
H	-1.217667	-2.795081	-0.997270
H	-2.622529	1.390714	0.739537
H	-3.152002	-0.034566	1.640635
H	-4.179289	0.653621	0.387488
C	1.132335	0.338110	0.864945
C	2.401554	0.478185	-0.009372
C	1.247571	-0.794311	1.879997
H	1.042254	1.301086	1.382418
C	2.689050	-0.695488	-0.935738
H	2.308808	1.394191	-0.586064
H	3.233110	0.608771	0.685425
H	1.266116	-1.776019	1.406697
H	0.427896	-0.781203	2.597527
H	2.176972	-0.679336	2.436363
H	1.927119	-0.783395	-1.710623

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      H      2.745554      -1.644875      -0.400813
      H      3.644361      -0.547361      -1.437590
Rotational constants (GHz):      1.4106600      0.7978700      0.6830200
Vibrational harmonic frequencies (cm-1):
      49.3952      65.9443      108.6077
      129.3373      163.7447      193.1293
      215.6206      228.6033      255.5064
      267.0730      285.8968      292.8300
      303.3189      325.7247      369.7011
      380.7451      448.1306      475.6848
      522.5495      603.8012      672.2078
      749.6657      799.3430      809.9041
      843.2699      879.9964      950.6854
      979.6078      988.1019      1016.2198
      1026.5584      1034.0485      1040.8571
      1078.5857      1122.9507      1130.4409
      1141.3416      1181.5858      1191.1887
      1251.2433      1275.6114      1294.1051
      1302.7012      1307.6372      1362.1954
      1374.9317      1378.4654      1405.2295
      1413.7479      1416.1469      1420.7117
      1424.6639      1488.5052      1491.3011
      1497.3514      1500.3709      1504.3980
      1509.7155      1511.0884      1513.9072
      1517.7742      1519.3918      1617.4334
      3031.7780      3059.8294      3062.3069
      3066.3035      3068.2793      3070.4148
      3073.8632      3075.5193      3109.4247
      3122.3260      3132.7094      3134.8030
      3138.2758      3139.8972      3140.6107
      3147.1344      3160.1397      3161.8043
Zero-point correction (Hartree): 0.260887

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diC2H5CH3CH_COO.cmpRS

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E(RM062X/Aug-CC-pVTZ) (Hartree): -504.06780119

Electronic state : 1-A

Cartesian coordinates (Angs):

```

      C      -0.025811      -0.044889      -0.261071
      O      -0.059199      -0.720753      -1.312300
      O       0.873171      -0.506755      -2.303313
      C      -1.046939      -0.448335      0.769075
      C      -2.462833      -0.448609      0.181493
      C      -0.682715      -1.827221      1.334436
      H      -1.002066      0.285953      1.574468
      C      -2.888685      0.909450      -0.359996
      H      -2.508865      -1.199617      -0.608661
      H      -3.147508      -0.770683      0.968069
      H       0.312428      -1.833207      1.777990
      H      -0.709118      -2.573651      0.541173
      H      -1.402144      -2.109640      2.102248
      H      -2.254659      1.216514      -1.193493
      H      -2.826571      1.676304      0.414038
      H      -3.914918      0.881224      -0.722222
      C       1.001245      1.014128      -0.050775
      C       2.096687      0.450753      0.874612
      C       0.399465      2.298060      0.519837
      H       1.434913      1.200571      -1.031859
      C       2.819694      -0.756640      0.291929
      H       2.804577      1.260769      1.060974
      H       1.650930      0.204807      1.843847
      H       0.057517      2.169227      1.547118
      H      -0.436283      2.656166      -0.080067
      H       1.165554      3.072367      0.523490
      H       3.291544      -0.501364      -0.655025
      H       2.130252      -1.576751      0.085153
      H       3.581994      -1.119100      0.980418

```

Rotational constants (GHz): 1.3209100 0.7943200 0.7643500

Vibrational harmonic frequencies (cm-1):

```

      42.4238      58.7042      99.6801
      128.6945      162.6055      183.8473
      194.1940      213.7737      232.1287
      241.6392      259.1298      265.8597
      275.7049      289.7345      325.9781
      376.8701      429.5424      469.4936
      541.6361      604.1740      704.2775
      734.7811      807.4762      811.8043
      858.8269      880.5521      939.6587
      981.4761      982.0851      1017.3871
      1028.4896      1042.4225      1047.6809
      1076.1524      1105.3215      1135.9556
      1145.0836      1180.1439      1189.8868
      1257.8553      1281.3812      1299.8176
      1315.7588      1324.9834      1358.2635
      1373.5649      1377.8644      1402.6839
      1414.7760      1415.4164      1423.3557
      1429.2100      1484.0482      1489.1885
      1496.4811      1497.9608      1500.7664
      1502.6272      1504.7298      1508.0608
      1510.5823      1512.1264      1632.5834
      3041.5174      3055.5137      3065.1659
      3065.4460      3067.7323      3068.3929
      3086.5962      3090.2329      3106.0978
      3117.9366      3126.7855      3132.0190
      3139.6609      3139.9003      3141.2274
      3143.4156      3146.4196      3151.6023

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Zero-point correction (Hartree): 0.260315

diC2H5CH3CH\_COO.cmmtRS

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E(RM062X/Aug-CC-pVTZ) (Hartree): -504.06926330

Electronic state : 1-A

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Cartesian coordinates (Angs):
C      -0.202645      0.190548      0.041127
O      -0.410614      1.356186     -0.369678
O       0.610547      2.274827     -0.288931
C      -1.329964     -0.779677     -0.149801
C      -2.694511     -0.108532     -0.293417
C      -0.996352     -1.644789     -1.376376
H      -1.345167     -1.426778      0.730922
C      -3.140541      0.630011      0.962417
H      -2.669998      0.574442     -1.143573
H      -3.415851     -0.890541     -0.538080
H      -0.027835     -2.134222     -1.282566
H      -0.979865     -1.025572     -2.273609
H      -1.758307     -2.413129     -1.499656
H      -2.467744      1.453639      1.197242
H      -3.168227     -0.044443      1.819873
H      -4.139015      1.044580      0.833770
C       1.132034     -0.151265      0.597538
C       2.159110     -0.210172     -0.561957
C       1.147614     -1.414319      1.448105
H       1.398841      0.724406      1.197293
C       3.550909      0.185181     -0.090761
H       2.163508     -1.225420     -0.966285
H       1.849862      0.470296     -1.353928
H       0.864743     -2.295405      0.870568
H       0.478769     -1.335990      2.305047
H       2.153927     -1.581083      1.829317
H       3.887125     -0.434794      0.741352
H       3.543622      1.225065      0.235175
H       4.278223      0.084920     -0.895244

Rotational constants (GHz):      1.5921800      0.7112600      0.6160800
Vibrational harmonic frequencies (cm-1):
54.7731      57.9136      91.1675
121.7837      166.4603      184.2170
204.5485      215.0215      237.8586
259.6203      263.1052      276.0227
283.5358      331.3225      347.1749
370.1221      425.2352      457.7011
552.7973      608.1663      680.6659
772.5524      779.6125      811.9454
857.8644      886.6301      947.2410
980.4841      988.7268      1017.4221
1029.8047      1034.8987      1039.5259
1082.2457      1119.1870      1135.0400
1148.1936      1183.4597      1191.6919
1254.6232      1280.8321      1300.0924
1303.7714      1321.5191      1350.9905
1375.7059      1384.3088      1406.2498
1409.0101      1417.6157      1420.9677
1428.7244      1474.9656      1488.1098
1499.1927      1501.1773      1502.7476
1504.0925      1504.8552      1509.2230
1512.2684      1513.7100      1620.3271
3049.1218      3060.6533      3062.4532
3062.9152      3064.4127      3066.8328
3067.5990      3072.0878      3107.9401
3116.5435      3132.0234      3132.9743
3135.1756      3141.1913      3142.2266
3143.4682      3146.5156      3147.6842

Zero-point correction (Hartree): 0.260469

diC2H5CH3CH_COO.cmpmRS
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E(RM062X/Aug-CC-pVTZ) (Hartree): -504.06401796
Electronic state : 1-A
Cartesian coordinates (Angs):
C       0.101439      0.377071     -0.123422
O       0.113527      0.055930     -1.328217
O      -1.062555     -0.075442     -2.029782
C       1.456143      0.495483      0.519674
C       2.497712     -0.447094     -0.077445
C       1.895051      1.964234      0.425199
H       1.314368      0.245022      1.575762
C       2.141723     -1.917405      0.102973
H       2.621964     -0.216399     -1.136287
H       3.452051     -0.232199      0.407096
H       1.145899      2.640552      0.836980
H       2.064234      2.232987     -0.617439
H       2.823965      2.107739      0.975285
H       1.224385     -2.168817     -0.429174
H       1.999201     -2.156381      1.158456
H       2.932124     -2.560572     -0.280236
C      -1.122403      0.663294      0.686399
C      -1.619411     -0.656764      1.321192
C      -2.226767      1.467010      0.000465
H      -0.745747      1.265518      1.518678
C      -2.097401     -1.714948      0.335543
H      -0.816980     -1.070414      1.938548
H      -2.426459     -0.385583      2.005529
H      -2.803989      0.856743     -0.683023
H      -1.813123      2.294100     -0.575087
H      -2.877882      1.877040      0.773894
H      -1.304359     -2.008890     -0.350735
H      -2.920025     -1.351450     -0.275773
H      -2.433916     -2.598187      0.878051

Rotational constants (GHz):      1.3485500      0.8218300      0.7277600
Vibrational harmonic frequencies (cm-1):
46.2964      67.5238      109.0080
115.4631      158.6712      176.9665
188.1974      214.6900      215.6231
230.4888      258.1493      263.7906
299.3237      309.8405      326.2335

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347.3629	447.4521	466.7872
513.8668	615.7283	718.2793
759.0143	801.1990	807.8183
848.1567	878.6903	945.3057
983.7541	988.5820	1011.0304
1029.1365	1037.1468	1040.4009
1101.0226	1120.6882	1129.7264
1140.5978	1158.0513	1200.0745
1233.9356	1286.8750	1294.9939
1303.6186	1314.9111	1369.0453
1377.9301	1395.6475	1408.5821
1415.3080	1417.5849	1431.4897
1444.9899	1476.9648	1484.2695
1488.2063	1492.1621	1498.6332
1500.3397	1503.2547	1505.6295
1510.7206	1511.4092	1656.9600
3041.3694	3047.0433	3053.2680
3060.0132	3063.4118	3069.3639
3070.1218	3074.5600	3083.9346
3107.5675	3131.1084	3133.1855
3136.8280	3141.1872	3142.9124
3144.3441	3157.0750	3203.8327

Zero-point correction (Hartree): 0.260291

dic2H5CH3CH_COO.cmpPRS

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E(RM062X/Aug-CC-pVTZ) (Hartree): -504.06889729

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.007866 | 0.255889  | 0.135728  |
| O | -0.096601 | -0.252237 | 1.272368  |
| O | 1.048998  | -0.595332 | 1.952122  |
| C | -1.308087 | 0.593549  | -0.534596 |
| C | -2.525162 | -0.076841 | 0.096466  |
| C | -1.453269 | 2.122740  | -0.568180 |
| H | -1.204225 | 0.242057  | -1.567629 |
| C | -2.523474 | -1.595115 | -0.038170 |
| H | -2.586272 | 0.208716  | 1.147910  |
| H | -3.410656 | 0.333908  | -0.392393 |
| H | -0.601961 | 2.604156  | -1.047921 |
| H | -1.543502 | 2.512916  | 0.446013  |
| H | -2.352026 | 2.391164  | -1.121117 |
| H | -1.696829 | -2.042338 | 0.511135  |
| H | -2.436570 | -1.890927 | -1.085153 |
| H | -3.448212 | -2.017948 | 0.351236  |
| C | 1.299179  | 0.564573  | -0.521650 |
| C | 2.191063  | -0.677665 | -0.697383 |
| C | 2.030382  | 1.681277  | 0.236085  |
| H | 1.037179  | 0.929693  | -1.518401 |
| C | 1.411023  | -1.921846 | -1.099181 |
| H | 2.927937  | -0.425307 | -1.462895 |
| H | 2.718881  | -0.862483 | 0.233869  |
| H | 2.231785  | 1.359045  | 1.254618  |
| H | 1.448305  | 2.602212  | 0.259169  |
| H | 2.974184  | 1.887173  | -0.268451 |
| H | 0.784834  | -1.738864 | -1.976103 |
| H | 0.772458  | -2.247384 | -0.276190 |
| H | 2.082774  | -2.744592 | -1.338343 |

Rotational constants (GHz): 1.3183900 0.8505800 0.7211900

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| 53.4967   | 60.8652   | 104.8515  |
| 117.4513  | 173.5321  | 195.8088  |
| 200.9900  | 208.6872  | 221.0646  |
| 241.6266  | 250.2647  | 269.8206  |
| 278.5294  | 301.4578  | 345.4752  |
| 408.3496  | 428.5524  | 451.4362  |
| 477.6322  | 608.2654  | 729.7528  |
| 743.1554  | 807.1507  | 818.1868  |
| 849.8423  | 890.3466  | 951.9490  |
| 981.6990  | 986.7152  | 1025.1219 |
| 1028.8745 | 1036.1799 | 1045.3789 |
| 1092.7213 | 1123.2878 | 1132.7069 |
| 1141.8537 | 1155.6084 | 1200.4772 |
| 1228.6522 | 1289.7482 | 1298.1752 |
| 1299.2664 | 1321.1566 | 1367.8215 |
| 1372.8409 | 1393.1945 | 1393.8831 |
| 1409.2425 | 1410.1870 | 1419.2252 |
| 1435.8320 | 1483.3834 | 1486.9396 |
| 1492.0077 | 1495.1865 | 1500.5342 |
| 1503.5637 | 1506.6512 | 1510.0175 |
| 1516.9316 | 1519.3374 | 1651.8403 |
| 3032.8921 | 3047.2299 | 3055.7882 |
| 3062.4925 | 3065.0863 | 3067.1218 |
| 3067.5542 | 3069.4266 | 3104.7044 |
| 3111.5738 | 3132.3442 | 3135.8585 |
| 3137.5115 | 3140.3590 | 3145.7879 |
| 3149.9993 | 3155.4244 | 3168.3571 |

Zero-point correction (Hartree): 0.260382

dic2H5CH3CH\_COO.cmpTRS

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E(RM062X/Aug-CC-pVTZ) (Hartree): -504.06675852

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-0.220356	0.180316	0.205546
O	-0.464982	-0.332127	1.316699
O	0.570510	-0.679273	2.155657
C	-1.415607	0.542318	-0.626864
C	-2.687074	-0.208618	-0.243583
C	-1.600085	2.065471	-0.540045
H	-1.148406	0.289645	-1.658983
C	-2.594688	-1.709597	-0.490263

H	-2.915686	-0.011557	0.804788
H	-3.505979	0.213084	-0.829550
H	-0.688835	2.602190	-0.803534
H	-1.884166	2.347407	0.474032
H	-2.390449	2.379522	-1.220035
H	-1.815587	-2.163948	0.120605
H	-2.371377	-1.916541	-1.538289
H	-3.535009	-2.201754	-0.247586
C	1.160970	0.438961	-0.295779
C	1.834569	-0.914691	-0.600185
C	1.984646	1.335005	0.636788
H	1.032358	0.963494	-1.247086
C	3.210548	-0.737734	-1.228229
H	1.900250	-1.476168	0.330361
H	1.192694	-1.479477	-1.281725
H	2.328437	0.773313	1.499269
H	1.391698	2.176654	0.996071
H	2.835148	1.735910	0.087452
H	3.908344	-0.280760	-0.528045
H	3.162598	-0.106605	-2.117863
H	3.622202	-1.701789	-1.523052
Rotational constants (GHz): 1.4304100 0.6858300 0.6628100			
Vibrational harmonic frequencies (cm-1):			
38.3904	69.1743	85.3399	
113.6672	133.1166	175.0118	
182.5482	205.1732	216.4286	
236.9415	257.2057	265.1045	
278.1472	311.6177	336.4374	
369.4396	428.6392	455.1866	
498.7622	612.9301	727.0441	
773.6047	803.7227	821.7244	
846.5800	889.0940	946.6580	
977.5795	984.9971	998.5547	
1029.4317	1039.2726	1059.0220	
1101.9296	1115.8824	1127.0524	
1146.5373	1154.8629	1199.0879	
1229.8888	1284.9092	1297.2351	
1301.6034	1341.9206	1362.7490	
1370.1738	1394.1192	1404.0447	
1408.1942	1412.6659	1417.9345	
1437.8949	1488.6428	1489.1937	
1494.4800	1499.7890	1503.7759	
1504.1859	1506.8575	1511.6477	
1512.5615	1515.1916	1653.7080	
3036.1144	3050.8344	3052.2720	
3058.6589	3062.1116	3063.4013	
3068.3454	3072.5885	3106.8098	
3118.3167	3132.8505	3133.5325	
3136.4989	3136.9575	3143.8852	
3144.2585	3145.6617	3185.5456	
Zero-point correction (Hartree): 0.260176			
dic2H5CH3CH_COO.cmtmRS			
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E(RM062X/Aug-CC-pVTZ) (Hartree): -504.06425554			
Electronic state : 1-A			
Cartesian coordinates (Angs):			
C	-0.140689	0.355182	-0.389751
O	-0.966316	1.202892	-0.800572
O	-0.562440	2.501809	-1.006948
C	-0.709793	-1.011886	-0.138469
C	-2.194389	-0.974585	0.229142
C	-0.459130	-1.903192	-1.362657
H	-0.158079	-1.416183	0.712976
C	-2.470223	-0.218797	1.523058
H	-2.758590	-0.534201	-0.593496
H	-2.529800	-2.009022	0.325099
H	0.594564	-1.950777	-1.631882
H	-1.014616	-1.519138	-2.218285
H	-0.804548	-2.915121	-1.154342
H	-2.196573	0.832380	1.434075
H	-1.905098	-0.649506	2.351727
H	-3.526658	-0.264154	1.782366
C	1.259298	0.776547	-0.110478
C	2.378953	-0.252606	-0.319361
C	1.231929	1.369276	1.311203
H	1.430149	1.610699	-0.791432
C	2.471549	-1.445825	0.629775
H	2.359150	-0.601911	-1.353149
H	3.302638	0.322238	-0.224581
H	0.920676	0.630473	2.050785
H	0.544462	2.213098	1.338910
H	2.229933	1.718646	1.575738
H	1.732191	-2.214891	0.414138
H	2.353862	-1.142470	1.670156
H	3.451360	-1.912459	0.536587
Rotational constants (GHz): 1.1701100 0.9003700 0.7091400			
Vibrational harmonic frequencies (cm-1):			
58.6314	69.5539	115.9755	
120.0966	147.9814	180.1093	
201.3791	223.4613	237.4205	
246.4699	263.9162	278.9117	
289.2270	305.2877	334.6419	
340.3444	457.8445	459.7936	
585.3663	622.6535	692.5435	
738.2829	783.9852	809.0140	
856.7056	890.7518	947.3449	
963.1372	987.0820	1001.1770	
1025.8542	1031.7610	1047.0712	
1079.3151	1111.7900	1139.4014	
1153.1526	1155.8805	1190.5878	
1265.1653	1296.7381	1308.5312	

1314.4423	1332.8080	1362.5483
1372.9194	1383.6661	1398.7774
1405.5166	1415.1630	1419.2813
1429.8224	1486.7543	1491.5037
1495.5780	1498.7302	1503.4913
1505.6130	1508.7076	1512.2449
1516.6513	1522.4773	1622.1315
3058.7681	3058.9822	3062.3744
3067.8790	3069.4230	3072.6790
3081.8178	3095.3422	3097.0820
3109.1243	3129.9116	3130.8745
3136.6242	3141.9889	3142.9856
3147.6298	3150.7291	3152.1902

Zero-point correction (Hartree): 0.260667

diC2H5CH3CH_COO.cmttRS

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E (RM062X/Aug-CC-pVTZ) (Hartree): -504.06803649

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.206900 | 0.166907  | -0.415459 |
| O | -0.786040 | 1.053580  | -1.082969 |
| O | -0.067257 | 2.148601  | -1.505676 |
| C | -1.083951 | -0.982129 | -0.002533 |
| C | -2.441797 | -0.501677 | 0.517925  |
| C | -1.252364 | -1.939997 | -1.190227 |
| H | -0.566484 | -1.505668 | 0.803195  |
| C | -2.324345 | 0.420205  | 1.724618  |
| H | -2.970858 | 0.003645  | -0.290951 |
| H | -3.025963 | -1.386766 | 0.776511  |
| H | -0.295512 | -2.293346 | -1.571926 |
| H | -1.776927 | -1.433021 | -1.999614 |
| H | -1.838834 | -2.805010 | -0.883092 |
| H | -1.800277 | 1.341317  | 1.466311  |
| H | -1.777303 | -0.065266 | 2.535001  |
| H | -3.307102 | 0.695440  | 2.103565  |
| C | 1.233402  | 0.316825  | -0.075710 |
| C | 1.935099  | -0.999222 | 0.261265  |
| C | 1.308212  | 1.340888  | 1.073294  |
| H | 1.685979  | 0.782767  | -0.955060 |
| C | 3.452085  | -0.848449 | 0.282372  |
| H | 1.594338  | -1.363536 | 1.233410  |
| H | 1.665418  | -1.761507 | -0.472502 |
| H | 0.868065  | 0.924877  | 1.981573  |
| H | 0.783991  | 2.252017  | 0.792674  |
| H | 2.346775  | 1.591472  | 1.279024  |
| H | 3.774095  | -0.147690 | 1.051290  |
| H | 3.816894  | -0.483310 | -0.678011 |
| H | 3.933448  | -1.803971 | 0.484490  |

Rotational constants (GHz): 1.2725500 0.7571100 0.6762700

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| 46.3884   | 70.0104   | 77.1294   |
| 106.8367  | 152.5953  | 161.4313  |
| 196.7485  | 212.2920  | 224.9899  |
| 232.4210  | 244.4942  | 260.1052  |
| 284.8398  | 315.8877  | 333.0329  |
| 373.7910  | 424.9863  | 456.6995  |
| 551.3885  | 605.9362  | 719.6078  |
| 743.8175  | 793.1229  | 813.1221  |
| 864.3503  | 904.4221  | 945.3164  |
| 974.2090  | 982.6950  | 989.0621  |
| 1023.8455 | 1030.6699 | 1055.1735 |
| 1078.8302 | 1111.2407 | 1144.2477 |
| 1150.4789 | 1184.6045 | 1194.4571 |
| 1263.3813 | 1294.1782 | 1306.9551 |
| 1308.8983 | 1314.7870 | 1336.9383 |
| 1373.2341 | 1381.6339 | 1398.5312 |
| 1404.8079 | 1414.7009 | 1417.9600 |
| 1426.8949 | 1483.7652 | 1489.1269 |
| 1495.7905 | 1499.8889 | 1501.7177 |
| 1503.4526 | 1507.0023 | 1508.7303 |
| 1511.9030 | 1519.4592 | 1627.6399 |
| 3052.6448 | 3056.1486 | 3059.1162 |
| 3066.5478 | 3068.2063 | 3069.5739 |
| 3072.8763 | 3084.9960 | 3095.8132 |
| 3107.6724 | 3128.1587 | 3135.9444 |
| 3138.6153 | 3140.5009 | 3143.4732 |
| 3145.2013 | 3145.8486 | 3160.6413 |

Zero-point correction (Hartree): 0.260164

diC2H5CH3CH\_COO.cpmnRS

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E (RM062X/Aug-CC-pVTZ) (Hartree): -504.06405567

Electronic state : 1-A

Cartesian coordinates (Angs):

C	0.031664	0.353962	-0.376642
O	0.485003	1.468152	-0.023141
O	-0.363966	2.541258	0.079828
C	1.057160	-0.736167	-0.534953
C	2.502174	-0.218509	-0.594382
C	0.887634	-1.826757	0.532126
H	0.829366	-1.194201	-1.501681
C	3.124489	0.156257	0.747645
H	3.101422	-1.007840	-1.052945
H	2.542111	0.637587	-1.267949
H	-0.090882	-2.298339	0.489157
H	1.021165	-1.415753	1.531476
H	1.646125	-2.594049	0.376526
H	3.232499	-0.714120	1.394235
H	2.531677	0.903342	1.271524
H	4.119507	0.570214	0.591224
C	-1.420201	0.230140	-0.703271

C	-2.317126	0.357135	0.550190
C	-1.763963	-0.985023	-1.558301
H	-1.610250	1.148535	-1.271060
C	-2.214548	-0.787517	1.549001
H	-2.080065	1.302403	1.032148
H	-3.342398	0.429507	0.182750
H	-1.535648	-1.928896	-1.065860
H	-1.239364	-0.966893	-2.513042
H	-2.832944	-0.975717	-1.769140
H	-1.230563	-0.821468	2.016163
H	-2.407785	-1.758100	1.089679
H	-2.945958	-0.652612	2.344817
Rotational constants (GHz): 1.3965400 0.8021600 0.6775200			
Vibrational harmonic frequencies (cm-1):			
56.0273	64.8396		126.8178
135.4410	184.5771		191.9447
213.1576	228.1026		248.0810
260.8436	285.7784		293.6780
305.4885	341.5948		354.7598
380.0528	425.1588		489.7088
553.6775	627.6400		673.7172
747.4045	794.0266		804.8613
835.1066	875.4805		944.8900
981.2604	996.1549		1005.4302
1015.5627	1024.1120		1033.4281
1084.7131	1111.7329		1133.1008
1159.7592	1172.1457		1185.6085
1251.8277	1282.2673		1293.6011
1301.0829	1328.2934		1361.7624
1375.7032	1382.1363		1397.3113
1413.9492	1415.6338		1420.3902
1425.1229	1485.0386		1494.0612
1495.5304	1497.3259		1506.2229
1509.1787	1511.5822		1512.4038
1517.8819	1524.4279		1613.7218
3033.1390	3056.0203		3063.3263
3067.9260	3071.8351		3073.1640
3074.0514	3075.5918		3108.2272
3124.0454	3136.3952		3137.0635
3137.5398	3144.2307		3147.8749
3153.6791	3153.8110		3168.5187
Zero-point correction (Hartree): 0.261052			
dic2H5CH3CH_COO.cmpmpRS			
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E(RM062X/Aug-CC-pVT2) (Hartree): -504.06543877			
Electronic state : 1-A			
Cartesian coordinates (Angs):			
C	0.038933	-0.054470	-0.529552
O	-0.290611	-1.236296	-0.780969
O	0.669863	-2.190369	-1.008850
C	-1.103027	0.896281	-0.297299
C	-2.482168	0.250410	-0.478319
C	-0.972587	1.584057	1.070893
H	-0.989627	1.671018	-1.063329
C	-2.908321	-0.674918	0.657999
H	-3.205097	1.063694	-0.567587
H	-2.500954	-0.293636	-1.422088
H	-0.116459	2.252262	1.114349
H	-0.874897	0.852481	1.872474
H	-1.870267	2.173270	1.257807
H	-3.025688	-0.128853	1.593760
H	-2.186522	-1.474929	0.814761
H	-3.867691	-1.134715	0.426137
C	1.480851	0.335901	-0.523619
C	2.086841	0.248065	0.894072
C	1.710212	1.716325	-1.136761
H	1.963378	-0.430088	-1.132205
C	1.834981	-1.069764	1.615054
H	3.160433	0.409260	0.778999
H	1.715317	1.080820	1.494042
H	1.266348	2.513261	-0.540011
H	1.309192	1.779561	-2.148029
H	2.781641	1.904909	-1.191366
H	2.238153	-1.907004	1.051379
H	0.766479	-1.258738	1.739031
H	2.287959	-1.050581	2.605627
Rotational constants (GHz): 1.3175700 0.8426800 0.7302200			
Vibrational harmonic frequencies (cm-1):			
44.8650	75.8266		128.7189
137.3055	172.6377		185.8310
212.3504	232.3777		236.5519
248.2385	257.3310		287.2850
302.5747	319.6025		347.3264
371.9565	420.1203		481.9845
572.0693	609.0547		675.5752
736.1021	797.5928		810.9297
847.0020	880.4071		942.6313
979.6014	996.8935		1004.8579
1016.3839	1027.4168		1052.5129
1080.5241	1102.1153		1135.6917
1162.2857	1170.8414		1182.9061
1259.2039	1283.7606		1296.6137
1318.2187	1327.2531		1364.0883
1368.7313	1378.2496		1398.0713
1414.7793	1418.8098		1422.5077
1425.7780	1482.9761		1489.4640
1495.0393	1497.3240		1501.7051
1506.0441	1506.9383		1510.2880
1514.1112	1521.3057		1618.0164
3040.9563	3061.2465		3064.7490
3066.7244	3069.8445		3072.0119

3074.1879	3085.6061	3104.0885
3113.4898	3124.6610	3137.7120
3138.2868	3140.1705	3141.9357
3149.8424	3163.6814	3165.4277

Zero-point correction (Hartree): 0.260805

diC2H5CH3CH_COO.cpmtrS

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E(RM062X/Aug-CC-pVTZ) (Hartree): -504.06680879

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.142436  | 0.160813  | -0.404434 |
| O | 0.449014  | 1.374487  | -0.342185 |
| O | -0.556844 | 2.313338  | -0.361806 |
| C | 1.276951  | -0.814514 | -0.309468 |
| C | 2.660696  | -0.191034 | -0.537612 |
| C | 1.184451  | -1.551138 | 1.037649  |
| H | 1.101268  | -1.550524 | -1.098779 |
| C | 3.231089  | 0.596025  | 0.638973  |
| H | 3.342070  | -1.009354 | -0.778990 |
| H | 2.615380  | 0.449418  | -1.418842 |
| H | 0.257293  | -2.112207 | 1.132053  |
| H | 1.238512  | -0.846541 | 1.866427  |
| H | 2.017234  | -2.248754 | 1.125633  |
| H | 3.417386  | -0.049381 | 1.496954  |
| H | 2.563055  | 1.396927  | 0.949070  |
| H | 4.182288  | 1.045036  | 0.357133  |
| C | -1.292056 | -0.212589 | -0.523501 |
| C | -1.967392 | -0.025728 | 0.857233  |
| C | -1.535147 | -1.592226 | -1.122500 |
| H | -1.708276 | 0.563712  | -1.172088 |
| C | -3.455653 | 0.261404  | 0.718910  |
| H | -1.802978 | -0.927905 | 1.451420  |
| H | -1.494702 | 0.810331  | 1.371727  |
| H | -1.129281 | -2.390907 | -0.501779 |
| H | -1.103170 | -1.679818 | -2.119252 |
| H | -2.606567 | -1.761786 | -1.215172 |
| H | -3.973273 | -0.529847 | 0.175818  |
| H | -3.600296 | 1.198766  | 0.182029  |
| H | -3.925554 | 0.354157  | 1.697064  |

Rotational constants (GHz): 1.6252200 0.7157600 0.6030400

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| 43.2301   | 61.2472   | 105.4439  |
| 136.9368  | 175.7470  | 186.8368  |
| 208.5737  | 228.3879  | 242.0143  |
| 251.9189  | 261.3454  | 276.9948  |
| 309.5250  | 321.6512  | 332.7907  |
| 364.9832  | 418.2356  | 469.9980  |
| 571.8850  | 639.9000  | 677.6405  |
| 771.0487  | 777.1752  | 804.3490  |
| 848.0235  | 883.3378  | 940.2876  |
| 980.0258  | 994.3682  | 1005.8828 |
| 1015.3418 | 1028.3607 | 1038.5860 |
| 1084.8125 | 1114.0484 | 1146.2757 |
| 1158.1070 | 1168.6592 | 1188.9376 |
| 1256.2681 | 1284.6213 | 1295.4826 |
| 1320.8245 | 1334.2884 | 1349.2436 |
| 1377.9412 | 1385.5016 | 1400.8269 |
| 1409.5727 | 1418.4611 | 1422.3517 |
| 1429.3940 | 1476.5107 | 1488.3843 |
| 1495.5322 | 1500.3932 | 1503.6180 |
| 1504.6398 | 1507.9985 | 1511.3958 |
| 1512.8559 | 1522.0476 | 1620.0931 |
| 3052.8236 | 3056.9387 | 3062.6496 |
| 3065.7137 | 3068.6796 | 3070.6369 |
| 3072.8517 | 3075.5928 | 3106.9140 |
| 3114.3459 | 3135.2759 | 3136.4050 |
| 3137.7341 | 3141.0553 | 3144.3122 |
| 3146.1205 | 3157.9138 | 3159.5926 |

Zero-point correction (Hartree): 0.260774

diC2H5CH3CH\_COO.cppmRS

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E(RM062X/Aug-CC-pVTZ) (Hartree): -504.06048034

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-0.030417	0.101786	0.080907
O	-0.154082	-1.015601	0.621612
O	0.909332	-1.604860	1.262465
C	-1.262685	0.640169	-0.592194
C	-2.305456	-0.426301	-0.951509
C	-1.850769	1.771872	0.265878
H	-0.900378	1.089796	-1.522702
C	-3.180458	-0.911570	0.200943
H	-2.946482	0.001725	-1.724944
H	-1.793102	-1.275916	-1.404649
H	-1.141559	2.586217	0.403508
H	-2.138911	1.400364	1.248085
H	-2.738955	2.173387	-0.221629
H	-3.808717	-0.110093	0.588667
H	-2.584015	-1.308474	1.019665
H	-3.841806	-1.704120	-0.145984
C	1.232789	0.904784	0.052339
C	2.091677	0.478696	-1.162106
C	2.020985	0.968119	1.361593
H	0.895434	1.918681	-0.176951
C	2.575967	-0.965109	-1.162806
H	1.522263	0.671376	-2.075150
H	2.944593	1.161062	-1.183611
H	2.591511	0.062876	1.529431
H	1.358512	1.097209	2.216737
H	2.691543	1.827171	1.313455

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H      1.742532      -1.666230      -1.171389
H      3.165732      -1.191784      -0.278073
H      3.190000      -1.144235      -2.045356
Rotational constants (GHz):      1.5903300      0.7170000      0.6673900
Vibrational harmonic frequencies (cm-1):
  42.3188      60.3812      108.0950
 130.6919      165.0504      180.7734
 185.7875      212.2421      225.6603
 253.5098      270.3611      281.1324
 304.0766      315.0449      317.9911
 359.3347      401.6015      498.8473
 542.5036      630.7587      720.9949
 760.9842      797.8808      800.0289
 835.2609      875.2470      939.9611
 986.3863      994.1062      1006.0097
1013.1431      1031.5055      1041.6769
1101.4156      1121.1971      1131.1755
1147.1441      1163.2798      1185.2742
1229.5288      1287.1482      1296.9496
1314.7463      1331.8843      1371.3890
1378.0788      1383.9832      1410.5891
1413.8561      1420.9514      1431.8604
1443.5964      1478.9663      1485.2240
1487.0415      1493.1060      1498.2377
1500.4282      1504.2499      1508.9930
1512.9057      1521.1892      1653.4616
3039.5746      3046.0008      3062.0408
3064.9755      3069.0720      3070.9729
3073.5961      3074.2590      3084.1063
3103.1525      3131.9949      3136.8741
3139.7560      3142.8861      3149.9606
3156.2342      3160.6247      3199.6200
Zero-point correction (Hartree): 0.260629

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diC2H5CH3CH_COO.cpuppRS

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E(RM062X/Aug-CC-pVTZ) (Hartree): -504.06693482

Electronic state : 1-A

Cartesian coordinates (Angs):

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C      -0.022921      -0.002565      0.004525
O       0.083955      0.967427      0.783228
O      -0.984118      1.324304      1.572713
C       1.185816      -0.315804      -0.829955
C       2.314591      0.712608      -0.712763
C       1.662242      -1.747452      -0.540578
H       0.812727      -0.299519      -1.861189
C       3.125552      0.638063      0.577876
H       2.981360      0.555609      -1.562977
H       1.892849      1.711666      -0.824221
H       0.897066      -2.486050      -0.772648
H       1.938707      -1.860843      0.506799
H       2.539597      -1.964409      -1.149300
H       3.676044      -0.299647      0.649242
H       2.489779      0.731535      1.456570
H       3.854103      1.446698      0.607388
C      -1.266629      -0.826394      -0.105172
C      -2.524106      -0.002433      -0.432217
C      -1.450519      -1.662229      1.169089
H      -1.090035      -1.501460      -0.946181
C      -2.269579      1.098803      -1.451716
H      -3.264053      -0.709458      -0.814194
H      -2.910681      0.430409      0.485463
H      -1.541119      -1.000057      2.027214
H      -0.616564      -2.345997      1.326574
H      -2.362207      -2.251859      1.075481
H      -1.798618      0.706989      -2.356747
H      -1.623864      1.866636      -1.022601
H      -3.200465      1.580313      -1.746730

```

Rotational constants (GHz): 1.5139600 0.7451500 0.6979700

Vibrational harmonic frequencies (cm-1):

```

  47.5597      73.8613      112.2331
 126.5420      176.0970      194.1075
 198.4375      216.4691      234.8607
 246.4912      271.0612      280.4815
 299.2855      315.3058      358.5352
 363.7719      429.7863      442.8408
 531.1429      623.6587      726.5809
 748.1008      800.8258      817.1122
 836.1782      889.9320      945.5852
 984.1550      996.5240      1002.6279
1024.0187      1034.3315      1036.6289
1101.3601      1113.0969      1128.7726
1149.3676      1169.3163      1190.1050
1223.7601      1288.0599      1298.7468
1320.7437      1328.2322      1369.8421
1371.8279      1381.5069      1395.4463
1409.1279      1413.2264      1420.4196
1436.0449      1482.3336      1486.5399
1494.8990      1497.3475      1500.7145
1504.1801      1511.2985      1514.2427
1516.6295      1522.4696      1649.6415
3025.7080      3047.6622      3059.6507
3066.2302      3067.1889      3067.3668
3070.9403      3073.8226      3108.5448
3112.6397      3135.2666      3137.6842
3138.3296      3143.7809      3149.2104
3151.7867      3157.5379      3161.0449

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Zero-point correction (Hartree): 0.260734

diC2H5CH3CH\_COO.cpptRS

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E(RM062X/Aug-CC-pVTZ) (Hartree): -504.06450636

```

Electronic state : 1-A
Cartesian coordinates (Angs):
C      0.146174      0.091637     -0.082497
O      0.426875      1.303766      0.020057
O     -0.535993      2.206512      0.411598
C      1.267680     -0.813876     -0.501883
C      2.525609     -0.083880     -0.983366
C      1.562171     -1.810393      0.630904
H      0.859209     -1.387550     -1.342288
C      3.389065      0.521188      0.120053
H      3.120850     -0.806622     -1.545074
H      2.231345      0.695299     -1.686752
H      0.693916     -2.421624      0.870577
H      1.870621     -1.287786      1.535281
H      2.372112     -2.473342      0.327726
H      3.818520     -0.250296      0.758628
H      2.819506      1.207248      0.744198
H      4.215531      1.078291     -0.318351
C     -1.220680     -0.456910      0.168643
C     -2.208232      0.098422     -0.876473
C     -1.667045     -0.233141      1.618932
H     -1.143231     -1.533946     -0.001533
C     -3.587623     -0.534962     -0.748953
H     -2.261753      1.178459     -0.760251
H     -1.808126     -0.104434     -1.873234
H     -1.883397      0.817407      1.787931
H     -0.889468     -0.543118      2.318040
H     -2.552267     -0.833712      1.820635
H     -4.073402     -0.244863      0.181540
H     -3.529912     -1.625094     -0.774303
H     -4.229828     -0.215053     -1.568161
Rotational constants (GHz):      1.7387500      0.6566600      0.5885500
Vibrational harmonic frequencies (cm-1):
42.7676      66.0931      74.7898
124.6126     140.3838     175.5539
188.8353     207.4249     219.4522
238.2132     270.1371     275.3475
299.7763     315.3141     321.7447
369.0150     425.1520     446.4662
535.4938     627.7631     727.9145
772.3116     798.7956     816.3842
832.2606     887.1440     940.4641
975.1953     994.0643     995.4180
1007.7031    1027.4239    1058.7153
1105.8769    1112.4416    1132.2130
1139.8249    1169.2028    1186.7098
1222.5292    1285.7177    1293.5723
1328.8362    1343.8369    1359.9649
1373.2383    1381.4761    1397.5464
1410.8540    1412.7300    1420.3787
1434.7399    1487.8713    1490.2938
1496.3633    1499.7143    1503.1417
1507.2202    1510.7972    1514.1270
1516.1677    1521.8116    1649.8229
3026.9537    3054.7682    3057.9926
3060.7149    3066.9736    3070.3238
3071.8943    3074.3516    3108.6915
3120.8576    3134.9006    3138.1280
3141.6801    3143.4799    3147.8134
3149.3160    3153.7226    3179.0521
Zero-point correction (Hartree): 0.260415

diC2H5CH3CH_COO.cptmRS
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E(RM062X/Aug-CC-pVTZ) (Hartree): -504.06102408
Electronic state : 1-A
Cartesian coordinates (Angs):
C     -0.057683      0.428227     -0.101263
O     -0.787173      1.439458     -0.236839
O     -0.227734      2.642092     -0.594918
C     -0.774384     -0.814286      0.349980
C     -2.158783     -0.536419      0.958686
C     -0.854774     -1.852020     -0.780331
H     -0.144591     -1.226464      1.143388
C     -3.281717     -0.273815     -0.040688
H     -2.418286     -1.412132      1.557311
H     -2.078462      0.303652      1.648769
H     0.122467     -2.226400     -1.070892
H     -1.336114     -1.426960     -1.659972
H     -1.454287     -2.697660     -0.442896
H     -3.472736     -1.146757     -0.664327
H     -3.054769      0.569541     -0.689142
H     -4.204160     -0.047003      0.491927
C      1.414059      0.584711     -0.289063
C      2.236626     -0.637991     -0.712563
C      1.937018      1.236251      1.006408
H      1.496888      1.344921     -1.067924
C      2.491856     -1.724843      0.328219
H      1.810026     -1.071794     -1.617622
H      3.206280     -0.235424     -1.013673
H      1.773003      0.592436      1.870972
H      1.435372      2.188581      1.163295
H      3.008725      1.411585      0.911490
H      1.589828     -2.262787      0.614581
H      2.935596     -1.309423      1.232342
H      3.191168     -2.459215     -0.069875
Rotational constants (GHz):      1.3411700      0.8536900      0.6114400
Vibrational harmonic frequencies (cm-1):
40.7774      81.5491      118.1607
151.9651     163.3328     172.6672
209.4021     223.1889     239.6862
249.8063     268.8321     287.6070

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305.0445	314.7331	349.9964
359.6933	414.5991	510.9178
606.1755	616.6565	696.0033
734.5948	786.3758	800.4487
847.1662	889.6790	944.6476
962.4944	993.3460	1001.9362
1011.4137	1031.0285	1035.2373
1076.6793	1120.1161	1138.2239
1154.9600	1162.2603	1174.0047
1262.2742	1295.3849	1310.8733
1323.5707	1331.5801	1364.5870
1376.2421	1380.1872	1390.7972
1403.8956	1415.7197	1418.8460
1427.6752	1486.2697	1489.5092
1495.2747	1501.4291	1502.5818
1510.0554	1512.3523	1514.2591
1520.5067	1524.1481	1612.4095
3057.1238	3061.1067	3063.8758
3068.0748	3072.7920	3075.4200
3076.9126	3084.9059	3100.9999
3107.4896	3130.8466	3136.8495
3138.1770	3141.1881	3148.9573
3155.6678	3158.7525	3175.8984

Zero-point correction (Hartree): 0.261012

diC2H5CH3CH_COO.cpttRS

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E(RM062X/Aug-CC-pVTZ) (Hartree): -504.06388105

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.132461 | 0.308704  | -0.108395 |
| O | -0.762269 | 1.332836  | -0.459375 |
| O | -0.062550 | 2.445455  | -0.865762 |
| C | -0.971980 | -0.834186 | 0.388783  |
| C | -2.324215 | -0.391574 | 0.973720  |
| C | -1.143093 | -1.901425 | -0.703491 |
| H | -0.390461 | -1.279799 | 1.201080  |
| C | -3.421228 | -0.082728 | -0.041002 |
| H | -2.664653 | -1.200511 | 1.623622  |
| H | -2.161514 | 0.476847  | 1.613309  |
| H | -0.196994 | -2.357769 | -0.981055 |
| H | -1.593086 | -1.468606 | -1.595671 |
| H | -1.804220 | -2.686181 | -0.335477 |
| H | -3.690413 | -0.967339 | -0.617461 |
| H | -3.121285 | 0.701053  | -0.732713 |
| H | -4.318358 | 0.252339  | 0.477669  |
| C | 1.357553  | 0.338766  | -0.097708 |
| C | 2.034459  | -1.025078 | -0.229908 |
| C | 1.734494  | 1.080564  | 1.201121  |
| H | 1.641497  | 0.985018  | -0.930306 |
| C | 3.554263  | -0.925428 | -0.151399 |
| H | 1.677237  | -1.709029 | 0.544480  |
| H | 1.762805  | -1.463258 | -1.190968 |
| H | 1.526985  | 0.456971  | 2.073301  |
| H | 1.176690  | 2.012481  | 1.270239  |
| H | 2.795072  | 1.321529  | 1.195889  |
| H | 3.888080  | -0.641763 | 0.845294  |
| H | 3.930028  | -0.182225 | -0.856070 |
| H | 4.014394  | -1.881770 | -0.394388 |

Rotational constants (GHz): 1.5376800 0.7172400 0.5730800

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| 44.1301   | 80.1126   | 100.7289  |
| 129.4260  | 155.4374  | 170.1216  |
| 193.6270  | 222.7117  | 233.6222  |
| 238.8333  | 255.4375  | 288.9520  |
| 310.7341  | 318.7365  | 341.5427  |
| 360.6173  | 438.3015  | 464.5440  |
| 568.4160  | 628.7584  | 724.3789  |
| 733.4632  | 799.7808  | 804.0710  |
| 851.8620  | 901.9396  | 941.5051  |
| 972.4536  | 983.1705  | 997.2397  |
| 1005.9257 | 1033.9372 | 1044.0967 |
| 1075.2989 | 1124.2999 | 1133.4632 |
| 1159.2369 | 1169.1951 | 1193.3347 |
| 1264.0344 | 1293.9448 | 1301.5065 |
| 1309.5887 | 1329.5852 | 1339.8834 |
| 1375.6705 | 1382.3168 | 1398.8804 |
| 1399.5328 | 1414.1223 | 1418.9955 |
| 1428.7345 | 1487.3050 | 1488.0840 |
| 1493.1248 | 1499.9504 | 1502.9026 |
| 1507.6451 | 1510.6313 | 1513.1329 |
| 1520.9033 | 1524.7548 | 1624.1711 |
| 3049.0605 | 3055.8482 | 3057.3313 |
| 3064.9440 | 3066.7102 | 3073.2529 |
| 3076.1522 | 3083.6691 | 3102.4730 |
| 3102.6566 | 3135.1082 | 3136.9757 |
| 3138.9365 | 3143.1436 | 3146.5776 |
| 3160.6579 | 3160.8334 | 3171.7127 |

Zero-point correction (Hartree): 0.260734

diC2H5CH3CH\_COO.ctmmRS

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E(RM062X/Aug-CC-pVTZ) (Hartree): -504.06531859

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-0.074917	0.473208	-0.210276
O	0.042043	1.631713	0.253953
O	-1.023169	2.493463	0.192049
C	1.177907	-0.358852	-0.156551
C	2.432125	0.498429	0.034870
C	1.056930	-1.445255	0.921341
H	1.246833	-0.861477	-1.125950

C	3.721607	-0.300747	-0.106722
H	2.419873	1.305417	-0.698351
H	2.392342	0.977361	1.014189
H	0.164841	-2.053541	0.794651
H	1.021012	-0.987343	1.910834
H	1.920933	-2.104810	0.877591
H	3.743590	-0.847674	-1.051111
H	3.847682	-1.020218	0.701061
H	4.584111	0.363427	-0.088104
C	-1.367585	0.055228	-0.829924
C	-2.516369	-0.044350	0.201714
C	-1.254182	-1.189267	-1.704451
H	-1.626513	0.923854	-1.447268
C	-2.360306	-1.131242	1.256361
H	-2.619245	0.927078	0.677644
H	-3.425029	-0.223769	-0.375819
H	-0.931630	-2.067237	-1.145810
H	-0.559319	-1.041483	-2.530432
H	-2.231643	-1.411993	-2.130849
H	-1.521389	-0.922076	1.920372
H	-2.212248	-2.119316	0.817593
H	-3.256460	-1.180525	1.873571
Rotational constants (GHz):			
	1.4623100	0.7325300	0.6163900
Vibrational harmonic frequencies (cm-1):			
55.0437	65.7199		91.2203
124.8765	159.9735		182.9848
213.6572	239.1917		242.9894
273.4071	285.1378		304.1723
307.2240	336.5223		357.3258
393.2793	408.8507		461.7883
526.3422	639.1632		683.7109
753.6958	785.8469		804.1945
845.4831	881.1617		950.2323
978.0251	985.9247		1001.3202
1016.3095	1026.7743		1054.3185
1083.8032	1120.7091		1126.0062
1154.1549	1181.3154		1188.1458
1248.5781	1278.6843		1292.3492
1299.1328	1343.1035		1347.5740
1363.0917	1380.9959		1406.5930
1412.4815	1415.1977		1418.1974
1423.6095	1485.5799		1494.2557
1496.8674	1498.8335		1505.7109
1509.0892	1509.9925		1514.8577
1518.2488	1524.6740		1613.7908
3030.7219	3056.5132		3060.0420
3061.5983	3071.2753		3073.0320
3073.6262	3077.1976		3110.5383
3121.7425	3132.4701		3134.7879
3138.0519	3141.2283		3142.7705
3150.2949	3154.7581		3169.5633
Zero-point correction (Hartree): 0.260831			
diC2H5CH3CH_COO.ctmpRS			
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E(RM062X/Aug-CC-pVTZ) (Hartree): -504.06567847			
Electronic state : 1-A			
Cartesian coordinates (Angs):			
C	0.108936	-0.267144	-0.367279
O	0.112268	-1.519520	-0.341678
O	1.267882	-2.209281	-0.606251
C	-1.216578	0.372965	-0.062123
C	-2.362440	-0.640533	-0.032684
C	-1.110356	1.170342	1.246373
H	-1.405121	1.085792	-0.871774
C	-3.732542	0.016356	0.082121
H	-2.322018	-1.241268	-0.941335
H	-2.205668	-1.333496	0.795713
H	-0.345640	1.941459	1.192177
H	-0.870158	0.504304	2.076327
H	-2.057900	1.659651	1.460475
H	-3.875777	0.764882	-0.699233
H	-3.875018	0.504751	1.045003
H	-4.520093	-0.727881	-0.023687
C	1.353689	0.480578	-0.719523
C	2.218876	0.796197	0.522322
C	1.057073	1.759794	-1.499368
H	1.915531	-0.222832	-1.337031
C	2.502573	-0.379179	1.447538
H	3.158166	1.201471	0.140905
H	1.746662	1.605272	1.082950
H	0.520385	2.490801	-0.892974
H	0.472743	1.562262	-2.397675
H	1.997726	2.214912	-1.806521
H	3.039855	-1.167338	0.927780
H	1.579888	-0.822965	1.825395
H	3.089840	-0.045630	2.302674
Rotational constants (GHz):			
	1.4693800	0.7248800	0.6366300
Vibrational harmonic frequencies (cm-1):			
51.0415	64.6151		86.0308
125.8021	157.9036		162.1321
201.3095	220.8882		244.3722
258.4338	266.5811		284.4576
298.8663	341.4513		352.7029
370.4991	400.6927		456.6947
529.7956	626.7119		686.9359
744.1994	786.6545		811.6767
855.0332	883.0043		948.4130
976.7795	983.4285		1002.1766
1020.5777	1044.3403		1061.8635
1083.9399	1104.1567		1138.7271
1158.0107	1179.6940		1187.0376

1254.7484	1285.7219	1296.3265
1316.8584	1342.3979	1347.9163
1366.1274	1377.9543	1407.4341
1414.6933	1416.7574	1420.5734
1427.8502	1481.3600	1489.4261
1493.3524	1500.6235	1501.6204
1503.0156	1506.7134	1509.4640
1512.6819	1523.2711	1616.8474
3045.3010	3061.6179	3062.0603
3062.5882	3066.5474	3073.1336
3075.9772	3080.0681	3099.9760
3110.9630	3126.9661	3132.0792
3132.5045	3140.5719	3142.0528
3150.7267	3165.0662	3168.5802

Zero-point correction (Hartree): 0.260550

diC2H5CH3CH_COO.ctmtrS
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 E(RM062X/Aug-CC-pVTZ) (Hartree): -504.06831231  
 Electronic state : 1-A  
 Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.047540  | 0.345741  | -0.239690 |
| O | 0.085708  | 1.583927  | -0.048391 |
| O | -1.087539 | 2.297206  | -0.130504 |
| C | 1.345285  | -0.382596 | -0.065298 |
| C | 2.560144  | 0.540957  | -0.161900 |
| C | 1.287417  | -1.133386 | 1.276071  |
| H | 1.400221  | -1.125691 | -0.866106 |
| C | 3.879950  | -0.219377 | -0.130758 |
| H | 2.489231  | 1.117363  | -1.085139 |
| H | 2.523806  | 1.265106  | 0.653060  |
| H | 0.388987  | -1.742354 | 1.362757  |
| H | 1.294085  | -0.418156 | 2.099453  |
| H | 2.148829  | -1.790071 | 1.377593  |
| H | 3.906965  | -0.991680 | -0.901523 |
| H | 4.049117  | -0.699850 | 0.832062  |
| H | 4.714455  | 0.456772  | -0.308709 |
| C | -1.255526 | -0.294787 | -0.557218 |
| C | -2.129904 | -0.321908 | 0.722125  |
| C | -1.135985 | -1.666589 | -1.208161 |
| H | -1.735296 | 0.415187  | -1.237891 |
| C | -3.610407 | -0.227368 | 0.383622  |
| H | -1.917687 | -1.246040 | 1.265395  |
| H | -1.861430 | 0.517714  | 1.361693  |
| H | -0.633995 | -2.384298 | -0.558395 |
| H | -0.594688 | -1.622215 | -2.153046 |
| H | -2.131945 | -2.054295 | -1.417261 |
| H | -3.919264 | -1.018267 | -0.301200 |
| H | -3.815798 | 0.734524  | -0.085653 |
| H | -4.222022 | -0.306941 | 1.281305  |

Rotational constants (GHz): 1.7566700 0.6473100 0.5518900  
 Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| 56.4017   | 60.5385   | 88.0621   |
| 100.2807  | 152.6842  | 177.8895  |
| 206.8994  | 219.6872  | 245.3970  |
| 260.0207  | 263.6894  | 286.3814  |
| 297.3957  | 319.7197  | 338.0748  |
| 375.6203  | 418.6305  | 428.6298  |
| 548.3866  | 648.8356  | 689.4400  |
| 772.5171  | 778.8078  | 802.3355  |
| 858.7585  | 888.4017  | 945.5787  |
| 979.3092  | 988.0001  | 996.7055  |
| 1019.0144 | 1030.9918 | 1058.6896 |
| 1085.4229 | 1115.9098 | 1140.9988 |
| 1152.0397 | 1182.2290 | 1189.9294 |
| 1250.1418 | 1283.6708 | 1293.9589 |
| 1321.1138 | 1336.6695 | 1343.4313 |
| 1365.4586 | 1383.9837 | 1406.1255 |
| 1409.7021 | 1416.8831 | 1421.1402 |
| 1426.6565 | 1473.9328 | 1488.9396 |
| 1498.6167 | 1500.3710 | 1501.7097 |
| 1503.6695 | 1507.4598 | 1510.7013 |
| 1514.0361 | 1518.4334 | 1618.4395 |
| 3050.2512 | 3058.1850 | 3061.2362 |
| 3061.4769 | 3063.0443 | 3067.2021 |
| 3071.1654 | 3076.1113 | 3109.7153 |
| 3115.2018 | 3132.4551 | 3133.0558 |
| 3134.6387 | 3141.1509 | 3141.5096 |
| 3142.7026 | 3145.1800 | 3156.7643 |

Zero-point correction (Hartree): 0.260451

diC2H5CH3CH\_COO.ctpmRS  
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 E(RM062X/Aug-CC-pVTZ) (Hartree): -504.06228193
 Electronic state : 1-A
 Cartesian coordinates (Angs):

C	-0.062090	0.220396	-0.171916
O	-0.159912	-0.104646	-1.372246
O	-1.388578	-0.139070	-1.987191
C	1.336194	0.226884	0.378421
C	2.268713	-0.738791	-0.352210
C	1.849954	1.675411	0.350104
H	1.250767	-0.082401	1.425773
C	3.640016	-0.841876	0.303245
H	1.798639	-1.723326	-0.380400
H	2.370296	-0.418432	-1.389845
H	1.137689	2.364972	0.802650
H	2.019544	1.985638	-0.681396
H	2.786890	1.756728	0.897051
H	3.552115	-1.102006	1.359607
H	4.193248	0.093838	0.232758
H	4.238401	-1.612263	-0.180147

C	-1.204043	0.603490	0.715591
C	-1.779494	-0.668128	1.382173
C	-2.274628	1.503115	0.097088
H	-0.727808	1.166508	1.523467
C	-2.365154	-1.701311	0.428618
H	-0.993705	-1.132485	1.983938
H	-2.543241	-0.326737	2.084616
H	-2.952812	0.943216	-0.535148
H	-1.828989	2.283603	-0.518317
H	-2.828773	1.977560	0.908244
H	-1.614168	-2.071401	-0.268544
H	-3.169530	-1.283563	-0.171830
H	-2.757453	-2.544857	0.996327
Rotational constants (GHz): 1.5859100 0.6549800 0.6419600			
Vibrational harmonic frequencies (cm-1):			
40.7707	67.7080		87.9544
115.5992	152.4916		165.1117
184.4793	213.0457		221.5405
251.6948	267.6353		282.4305
301.5051	313.0369		325.3335
372.1927	393.4222		458.5456
513.8780	668.2645		722.0606
765.1819	785.7061		802.9665
850.8558	878.7624		944.6797
982.8955	986.4189		997.6208
1012.4166	1038.7804		1056.6886
1102.0453	1118.2186		1130.4451
1152.0490	1158.1260		1197.5549
1232.7562	1288.2769		1295.4140
1313.0100	1331.1994		1344.0511
1377.1465	1400.3247		1409.0474
1415.5228	1417.4838		1432.4892
1442.3168	1479.2140		1485.6847
1488.5867	1494.5283		1500.2474
1500.5991	1505.1076		1508.1889
1510.8601	1518.1193		1652.8439
3039.7092	3043.0056		3054.0542
3061.3522	3066.1867		3069.1735
3071.4107	3072.8007		3084.4270
3107.5110	3132.0200		3133.2769
3135.8199	3138.4307		3140.9709
3153.5336	3158.8446		3200.8810
Zero-point correction (Hartree): 0.260364			
dic2H5CH3CH_COO.ctppRS			
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E(RM062X/Aug-CC-pVTZ) (Hartree): -504.06785829			
Electronic state : 1-A			
Cartesian coordinates (Angs):			
C	0.117818	-0.099783	-0.189625
O	0.204734	0.410443	-1.325821
O	1.439705	0.538436	-1.916307
C	-1.266753	-0.187071	0.383164
C	-2.290836	0.628868	-0.402820
C	-1.659530	-1.666807	0.511282
H	-1.186084	0.224722	1.396813
C	-3.658747	0.664199	0.267334
H	-1.912006	1.644993	-0.518916
H	-2.375320	0.218752	-1.410629
H	-0.907962	-2.240284	1.051889
H	-1.783039	-2.107522	-0.478828
H	-2.599449	-1.759684	1.050629
H	-3.580277	1.003524	1.301775
H	-4.135984	-0.314885	0.270499
H	-4.323009	1.348971	-0.257047
C	1.299532	-0.620815	0.564403
C	2.383845	0.446297	0.797953
C	1.871483	-1.863441	-0.131520
H	0.907811	-0.913792	1.542147
C	1.812949	1.814265	1.144711
H	3.010229	0.077700	1.613219
H	2.997874	0.521881	-0.094675
H	2.196341	-1.600659	-1.135250
H	1.138131	-2.667394	-0.190229
H	2.727133	-2.223259	0.439510
H	1.117700	1.757956	1.985981
H	1.289276	2.233369	0.283699
H	2.604555	2.510310	1.417142
Rotational constants (GHz): 1.5256800 0.6871100 0.6467300			
Vibrational harmonic frequencies (cm-1):			
47.4190	70.1422		93.5411
109.8108	155.1177		194.4197
197.9560	210.1789		221.0962
242.4914	259.1222		278.4944
297.5932	322.3037		353.6350
376.4387	428.8423		436.5516
459.6839	659.3165		728.0099
754.2774	789.7743		818.4236
850.6170	892.0715		951.4359
978.7907	986.9367		1000.0193
1029.9644	1035.6070		1052.6717
1093.0021	1122.6740		1132.7362
1154.7626	1160.5139		1198.8296
1227.0668	1293.4245		1296.7925
1320.1848	1326.7051		1342.5912
1372.6003	1394.6162		1397.2185
1409.7194	1410.8854		1417.9861
1434.4799	1484.8755		1486.6499
1493.2261	1497.5822		1501.0693
1504.7751	1508.3432		1513.8013
1517.5533	1521.9989		1648.7243
3023.0395	3047.2525		3056.2914

3061.5746	3066.5535	3067.3721
3068.5233	3073.9838	3107.9915
3110.7288	3132.1232	3135.1876
3137.2545	3139.8166	3142.3187
3156.1912	3158.3952	3164.8897

Zero-point correction (Hartree): 0.260435

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E(RM062X/Aug-CC-pVTZ) (Hartree): -504.06571797

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.072995  | 0.260631  | 0.071255  |
| O | 0.153843  | 1.505182  | 0.017523  |
| O | -0.983849 | 2.272761  | 0.119767  |
| C | 1.371676  | -0.484009 | -0.026154 |
| C | 2.521562  | 0.376015  | -0.545895 |
| C | 1.672773  | -1.102759 | 1.348710  |
| H | 1.189883  | -1.304726 | -0.730605 |
| C | 3.798584  | -0.422938 | -0.774530 |
| H | 2.211116  | 0.849904  | -1.477824 |
| H | 2.706106  | 1.186747  | 0.160688  |
| H | 0.820483  | -1.657911 | 1.738740  |
| H | 1.925736  | -0.316437 | 2.060941  |
| H | 2.513616  | -1.789131 | 1.277644  |
| H | 3.614936  | -1.279122 | -1.426155 |
| H | 4.216760  | -0.795786 | 0.159622  |
| H | 4.557984  | 0.197401  | -1.247422 |
| C | -1.217967 | -0.474277 | 0.224197  |
| C | -2.071198 | -0.281967 | -1.045326 |
| C | -1.952656 | -0.102020 | 1.518076  |
| H | -0.948032 | -1.532812 | 0.278206  |
| C | -3.354588 | -1.100763 | -0.998754 |
| H | -2.289181 | 0.778692  | -1.152718 |
| H | -1.478853 | -0.585743 | -1.912204 |
| H | -2.393357 | 0.886214  | 1.431940  |
| H | -1.269746 | -0.098467 | 2.368351  |
| H | -2.727160 | -0.841072 | 1.716431  |
| H | -4.027122 | -0.739115 | -0.222330 |
| H | -3.147425 | -2.154717 | -0.802324 |
| H | -3.882778 | -1.034940 | -1.948774 |

Rotational constants (GHz): 1.6628000 0.6053200 0.5646800

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| 43.4109   | 70.5445   | 80.7660   |
| 91.8679   | 126.5529  | 158.0716  |
| 181.0190  | 209.0452  | 211.9532  |
| 242.8659  | 263.4871  | 273.2811  |
| 287.8312  | 309.6692  | 336.0469  |
| 370.5335  | 420.0485  | 425.6102  |
| 487.4698  | 663.6544  | 727.7622  |
| 774.3062  | 785.7605  | 818.0106  |
| 847.5717  | 890.3228  | 945.7741  |
| 975.7452  | 981.3941  | 993.4075  |
| 1002.4880 | 1044.7356 | 1063.5754 |
| 1096.4193 | 1119.6088 | 1132.5420 |
| 1145.8039 | 1162.7691 | 1195.9521 |
| 1227.2837 | 1289.5861 | 1293.0574 |
| 1321.2679 | 1341.2273 | 1350.1571 |
| 1363.9443 | 1394.4484 | 1399.5874 |
| 1408.8049 | 1412.6989 | 1417.8262 |
| 1435.1070 | 1485.9903 | 1488.7667 |
| 1495.7005 | 1499.8113 | 1503.3917 |
| 1505.4089 | 1508.2455 | 1513.2748 |
| 1515.8278 | 1517.9420 | 1649.9679 |
| 3025.9115 | 3053.1050 | 3055.9497 |
| 3058.5203 | 3061.0310 | 3067.8115 |
| 3071.5845 | 3074.6593 | 3108.1406 |
| 3120.9166 | 3131.7058 | 3133.9732 |
| 3138.5433 | 3141.3747 | 3141.6941 |
| 3146.5868 | 3155.5575 | 3180.6835 |

Zero-point correction (Hartree): 0.260086

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E(RM062X/Aug-CC-pVTZ) (Hartree): -504.06255456

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-0.177392	0.584211	0.206027
O	0.104083	1.793335	0.379819
O	-0.908081	2.717038	0.488003
C	1.008091	-0.323647	0.049868
C	2.252328	0.426534	-0.435569
C	1.265820	-1.066684	1.369495
H	0.728074	-1.054381	-0.713584
C	3.409526	-0.508447	-0.763528
H	1.986643	1.006943	-1.320194
H	2.555293	1.148273	0.323613
H	0.368753	-1.545620	1.754995
H	1.628177	-0.363856	2.120387
H	2.019800	-1.837853	1.224712
H	3.103047	-1.280570	-1.471626
H	3.796971	-1.003233	0.126109
H	4.232157	0.045892	-1.212223
C	-1.608329	0.186705	0.082224
C	-2.020534	-1.225014	0.519777
C	-2.000918	0.503317	-1.374297
H	-2.138731	0.907495	0.706043
C	-1.528711	-2.419236	-0.295244
H	-1.773367	-1.366471	1.573018
H	-3.111824	-1.218386	0.477327
H	-1.418057	-0.083503	-2.084823
H	-1.845854	1.562500	-1.570158

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H      -3.054853      0.267762      -1.521448
H      -0.482258      -2.654197      -0.109992
H      -1.656161      -2.254982      -1.365198
H      -2.105122      -3.305228      -0.032044
Rotational constants (GHz):      1.1994500      0.8469900      0.6100500
Vibrational harmonic frequencies (cm-1):
60.4405      76.2101      87.1418
120.1068      154.1753      161.9284
206.4748      214.7342      234.8418
248.3241      275.5859      279.0965
301.8786      318.1629      331.2746
364.2697      405.6731      462.4576
590.1558      631.7945      720.0517
736.5949      783.5781      796.1629
858.7951      892.2702      947.0126
962.8560      985.2860      993.0329
1006.0365      1034.5427      1055.9503
1081.3646      1106.2877      1144.8028
1153.4965      1159.7799      1188.5570
1258.7378      1297.0050      1304.4687
1325.8309      1344.8771      1349.6421
1364.7346      1382.4204      1398.2351
1406.5903      1415.7759      1417.8827
1426.6665      1488.3558      1490.3757
1496.6447      1499.0095      1505.4811
1505.9788      1510.3907      1516.1545
1518.9873      1523.4257      1616.0301
3061.1072      3061.3194      3063.6588
3065.8153      3073.8277      3074.8097
3077.3067      3089.0424      3097.0136
3110.4394      3131.2265      3132.7565
3137.5114      3140.9040      3148.2219
3149.7319      3154.9832      3164.0379
Zero-point correction (Hartree): 0.260688

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E(RM062X/Aug-CC-pVT2) (Hartree): -504.06600553
Electronic state : 1-A
Cartesian coordinates (Angs):
C      -0.008390      0.482998      -0.204103
O      -0.333440      1.653217      -0.508475
O      0.647993      2.612298      -0.612901
C      -1.150787      -0.488549      -0.122407
C      -2.338291      0.112577      0.640988
C      -1.534460      -0.924163      -1.544595
H      -0.791326      -1.362015      0.424533
C      -3.462880      -0.889737      0.864458
H      -1.980796      0.483526      1.603633
H      -2.706953      0.979882      0.092451
H      -0.669462      -1.273844      -2.106640
H      -1.970174      -0.081063      -2.080954
H      -2.261083      -1.733330      -1.510210
H      -3.093162      -1.792179      1.354490
H      -3.932798      -1.184587      -0.072786
H      -4.237579      -0.460501      1.497734
C      1.418416      0.156381      0.062473
C      1.758701      -1.326773      -0.087240
C      1.736177      0.700597      1.468849
H      1.985799      0.757405      -0.653115
C      3.263914      -1.565584      -0.130411
H      1.326683      -1.892926      0.741428
H      1.311776      -1.719610      -1.002754
H      1.190893      0.134519      2.226550
H      1.467105      1.752786      1.528106
H      2.800781      0.605434      1.672036
H      3.745461      -1.254069      0.795370
H      3.719598      -1.008378      -0.949303
H      3.484423      -2.621654      -0.277639
Rotational constants (GHz):      1.3354700      0.6994100      0.5749800
Vibrational harmonic frequencies (cm-1):
47.9945      63.2111      70.5546
83.2604      138.3414      158.5589
192.3250      209.6918      217.8535
228.3126      262.5421      279.4902
296.6894      310.1271      342.2782
351.9893      425.8178      429.7662
543.9588      638.5029      724.7630
758.1918      789.3357      799.7688
862.9631      905.5104      942.5054
973.2046      979.6644      987.4187
995.9491      1045.2889      1059.0498
1077.9529      1116.3365      1135.4371
1156.5742      1184.2949      1194.0291
1257.0587      1290.4230      1302.9018
1309.0588      1333.4796      1348.8765
1355.9783      1382.1598      1398.2443
1406.6108      1412.9523      1416.2780
1423.2383      1486.7496      1489.3960
1496.8774      1499.0053      1502.3746
1503.6784      1509.1529      1511.7907
1517.3691      1520.1588      1625.8364
3052.3043      3057.9200      3062.0278
3066.8566      3068.1808      3069.3050
3071.4295      3083.7615      3095.5273
3110.3003      3133.3419      3135.8110
3138.7286      3141.8390      3142.6481
3145.1912      3155.3454      3163.9967
Zero-point correction (Hartree): 0.260107

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E(RM062X/Aug-CC-pVTZ) (Hartree): -504.06643418
Electronic state : 1-A
Cartesian coordinates (Angs):
  C    0.067893    0.278838   -0.232724
  O    0.227363    1.338282   -0.884046
  O   -0.604019    1.610557   -1.942916
  C    1.074028    0.092579    0.873145
  C    2.480703   -0.085377    0.275839
  C    1.056590    1.284917    1.834258
  H    0.804551   -0.814409    1.414348
  C    2.611165   -1.270390   -0.670670
  H    2.740580    0.838333   -0.244278
  H    3.180975   -0.192251    1.106100
  H    0.072772    1.442054    2.273206
  H    1.342448    2.193832    1.307219
  H    1.767242    1.113174    2.641679
  H    1.930989   -1.177051   -1.519922
  H    2.390490   -2.208245   -0.159570
  H    3.622551   -1.337477   -1.068059
  C   -1.027811   -0.655031   -0.617888
  C   -2.385236   -0.046898   -0.188544
  C   -0.844755   -2.084320   -0.125505
  H   -1.019673   -0.621894   -1.711600
  C   -2.642013   -0.099987    1.312780
  H   -2.421797    0.977232   -0.555320
  H   -3.164418   -0.600633   -0.714975
  H    0.085073   -2.519999   -0.487071
  H   -1.667927   -2.693001   -0.499934
  H   -0.853702   -2.155996    0.961159
  H   -1.831530    0.368379    1.874427
  H   -2.749974   -1.122141    1.674588
  H   -3.558781    0.433396    1.559562
Rotational constants (GHz):    1.2747600    0.7929900    0.7587100
Vibrational harmonic frequencies (cm-1):
  46.8826    68.9247    98.4306
  110.2040    172.0841    179.2792
  207.2477    225.6801    230.9742
  231.9675    265.2144    282.9059
  304.7535    321.8327    356.8594
  366.1921    433.3432    471.1215
  549.6780    613.9783    687.6346
  749.8374    802.0689    810.6760
  846.5085    869.3834    951.0847
  981.1570    986.0858    1014.9464
  1019.8699    1029.4351    1045.5498
  1085.2369    1113.3644    1135.6045
  1148.2952    1174.5117    1185.0825
  1250.6693    1287.9078    1291.9404
  1294.3453    1319.2046    1364.7932
  1371.4047    1373.1244    1405.3180
  1414.4965    1416.7340    1418.4263
  1421.8363    1488.3503    1492.8248
  1498.1452    1499.4430    1502.4879
  1505.9683    1509.4684    1510.2759
  1513.5957    1522.6963    1614.0506
  3054.0216    3057.0720    3062.7555
  3065.7668    3071.9313    3072.8156
  3075.6120    3095.6351    3107.8750
  3119.6451    3126.1396    3133.9029
  3137.3798    3139.4967    3144.3748
  3146.7809    3151.8764    3152.8075
Zero-point correction (Hartree): 0.260571

dic2H5CH3CH_COO.mmpmRS
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E(RM062X/Aug-CC-pVTZ) (Hartree): -504.06252224
Electronic state : 1-A
Cartesian coordinates (Angs):
  C   -0.288383   -0.409228    0.043574
  O   -0.083540   -1.236571   -0.870041
  O    1.208513   -1.465732   -1.285327
  C   -1.727184   -0.237965    0.441954
  C   -2.360756    0.926165   -0.345477
  C   -2.537866   -1.516298    0.253139
  H   -1.716100    0.038220    1.500679
  C   -1.687673    2.279148   -0.156439
  H   -2.362332    0.651839   -1.402764
  H   -3.405296    0.988235   -0.035338
  H   -2.088398   -2.354419    0.783365
  H   -2.599070   -1.780404   -0.801165
  H   -3.548372   -1.367117    0.630835
  H   -0.671754    2.284598   -0.551103
  H   -1.641078    2.551721    0.899251
  H   -2.244958    3.056930   -0.675996
  C    0.820779    0.320426    0.724528
  C    1.739989    1.094520   -0.266161
  C    1.532622   -0.691327    1.641959
  H    0.329708    1.047987    1.371179
  C    3.195460    0.650905   -0.309608
  H    1.329409    1.011355   -1.272067
  H    1.694923    2.149820    0.010219
  H    0.821621   -1.135318    2.340063
  H    2.298566   -0.183628    2.224477
  H    1.990532   -1.479577    1.050717
  H    3.263719   -0.393947   -0.601809
  H    3.691384    0.786453    0.651447
  H    3.735777    1.247592   -1.043859
Rotational constants (GHz):    1.4769600    0.7805500    0.6530700
Vibrational harmonic frequencies (cm-1):
  47.2215    85.8373    107.4649
  120.0160    175.0606    191.6519
  218.3645    242.2656    242.9194

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256.4009	264.8543	280.9628
297.0389	302.1774	328.4418
375.8040	404.4469	472.7575
533.9444	624.8898	731.0850
739.3908	800.1872	813.4859
836.2799	878.1441	955.6896
979.1606	983.5474	1023.5116
1029.1759	1047.4127	1058.7632
1109.4988	1128.4313	1133.8242
1143.2823	1154.3189	1179.7015
1217.5770	1280.3769	1317.9262
1322.7159	1340.0654	1360.3784
1370.2875	1387.4739	1391.5143
1408.8295	1418.0992	1420.6072
1438.6369	1486.0865	1489.0742
1490.9824	1499.6903	1504.1460
1505.1220	1509.0875	1512.0676
1513.3053	1528.1631	1646.7900
3049.8448	3059.9947	3060.9134
3064.6875	3066.6867	3072.0683
3073.9247	3088.3119	3100.9050
3110.1762	3131.2589	3132.2201
3138.4763	3143.0776	3147.4033
3152.9229	3163.9572	3176.6524

Zero-point correction (Hartree): 0.261055

diC2H5CH3CH_COO.mmppRS
 ~~~~~  
 E(RM062X/Aug-CC-pVTZ) (Hartree): -504.06529595  
 Electronic state : 1-A  
 Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.004076 | -0.536011 | 0.083063  |
| O | 0.393211  | -1.372835 | -0.755770 |
| O | 1.736615  | -1.466746 | -1.033349 |
| C | -1.486473 | -0.533228 | 0.327605  |
| C | -2.159815 | 0.694215  | -0.333710 |
| C | -2.147832 | -1.822075 | -0.149797 |
| H | -1.610024 | -0.437183 | 1.412111  |
| C | -2.030051 | 2.017173  | 0.412016  |
| H | -1.784931 | 0.790029  | -1.355544 |
| H | -3.219737 | 0.449564  | -0.419437 |
| H | -1.654281 | -2.701736 | 0.258782  |
| H | -2.109645 | -1.893001 | -1.236078 |
| H | -3.191852 | -1.829936 | 0.158980  |
| H | -1.011649 | 2.398574  | 0.420199  |
| H | -2.357180 | 1.910503  | 1.447539  |
| H | -2.656354 | 2.774830  | -0.057432 |
| C | 0.927720  | 0.340975  | 0.854280  |
| C | 1.911730  | 1.160157  | -0.000056 |
| C | 1.667547  | -0.539322 | 1.876986  |
| H | 0.287276  | 1.028683  | 1.407132  |
| C | 1.336607  | 1.649167  | -1.323081 |
| H | 2.226056  | 2.007771  | 0.613903  |
| H | 2.786849  | 0.548286  | -0.199929 |
| H | 0.974816  | -1.023092 | 2.566059  |
| H | 2.341596  | 0.089610  | 2.457745  |
| H | 2.247098  | -1.296155 | 1.353163  |
| H | 0.430673  | 2.241649  | -1.185641 |
| H | 1.111534  | 0.797684  | -1.966323 |
| H | 2.059016  | 2.274254  | -1.846115 |

Rotational constants (GHz): 1.2407300 0.9002000 0.7263200  
 Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| 51.8001   | 79.6155   | 107.8622  |
| 159.0530  | 178.7924  | 193.1746  |
| 215.2934  | 227.8396  | 246.9891  |
| 251.8772  | 258.3576  | 273.7127  |
| 285.4857  | 299.1020  | 358.7057  |
| 377.1191  | 430.7488  | 437.8559  |
| 490.4486  | 623.1888  | 722.7869  |
| 743.8310  | 796.2805  | 817.2813  |
| 844.9681  | 885.6534  | 962.9010  |
| 980.9129  | 990.0708  | 1020.5457 |
| 1030.5205 | 1041.8551 | 1056.0203 |
| 1101.4976 | 1112.8520 | 1129.4044 |
| 1148.0875 | 1157.0577 | 1185.5184 |
| 1228.2974 | 1273.8155 | 1304.8975 |
| 1319.1414 | 1322.2182 | 1357.7154 |
| 1375.0851 | 1388.1459 | 1393.9866 |
| 1409.1571 | 1418.7949 | 1420.6623 |
| 1439.1947 | 1480.8570 | 1487.2048 |
| 1494.5989 | 1497.3689 | 1498.5669 |
| 1503.0260 | 1507.2282 | 1515.6960 |
| 1516.9895 | 1520.5715 | 1642.5618 |
| 3036.9996 | 3058.0441 | 3060.9261 |
| 3062.6849 | 3063.3258 | 3067.3494 |
| 3074.5320 | 3092.7250 | 3099.9818 |
| 3125.8044 | 3131.0140 | 3132.2356 |
| 3138.4518 | 3148.4432 | 3152.1033 |
| 3153.0320 | 3158.9223 | 3162.9377 |

Zero-point correction (Hartree): 0.260874

diC2H5CH3CH\_COO.mmptRS  
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 E(RM062X/Aug-CC-pVTZ) (Hartree): -504.06550994
 Electronic state : 1-A
 Cartesian coordinates (Angs):

C	-0.367958	-0.504509	0.027270
O	-0.503175	-1.417291	-0.814251
O	0.614322	-2.049672	-1.308077
C	-1.647507	0.115749	0.513479
C	-1.972399	1.381705	-0.305337
C	-2.818373	-0.860874	0.471927

H	-1.460244	0.422953	1.547055
C	-0.929329	2.489889	-0.241784
H	-2.134262	1.076760	-1.341691
H	-2.927990	1.758836	0.063181
H	-2.594821	-1.773698	1.021622
H	-3.052221	-1.137012	-0.554854
H	-3.698463	-0.395221	0.913076
H	0.012402	2.189269	-0.700702
H	-0.723627	2.779099	0.790251
H	-1.282955	3.373825	-0.770184
C	0.963410	-0.085010	0.553229
C	1.994246	0.283350	-0.531441
C	1.481376	-1.192049	1.488324
H	0.772962	0.805861	1.155883
C	2.930104	1.377021	-0.031446
H	2.544658	-0.612003	-0.806458
H	1.488582	0.607436	-1.442577
H	0.811257	-1.346248	2.334450
H	2.456072	-0.901191	1.878538
H	1.581424	-2.119694	0.929384
H	3.425889	1.078517	0.893769
H	2.386234	2.302381	0.168207
H	3.704508	1.594197	-0.765656
Rotational constants (GHz): 1.2556600 0.8643300 0.6456400			
Vibrational harmonic frequencies (cm-1):			
47.3570	78.7025	101.6472	
140.0576	168.2314	180.3960	
218.1139	222.8728	240.5955	
245.0282	248.8422	263.0984	
286.8989	302.5807	322.3966	
375.0287	417.1387	445.7985	
503.7714	624.7885	728.5432	
778.5839	797.9735	818.1640	
842.6488	891.7870	954.7797	
977.4308	982.2078	1005.1512	
1029.6439	1048.0208	1049.7198	
1111.3340	1116.2335	1120.3356	
1144.8950	1162.2376	1188.7456	
1223.8280	1278.5683	1288.0030	
1322.0412	1333.1272	1346.7961	
1361.4308	1387.6609	1396.7886	
1411.0356	1418.2080	1420.1068	
1440.3019	1487.9315	1491.1212	
1494.4360	1499.7420	1500.9819	
1503.2558	1508.1396	1510.1111	
1512.8620	1520.0734	1647.9983	
3046.9911	3053.0702	3059.9297	
3063.5710	3064.7039	3072.6808	
3073.6646	3079.0042	3099.7942	
3111.5706	3132.1668	3132.6707	
3135.4047	3143.9618	3146.9685	
3151.3127	3151.4813	3162.9129	
Zero-point correction (Hartree): 0.260550			
diC2H5CH3CH_COO.mmtprS			
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E(RM062X/Aug-CC-pVTZ) (Hartree): -504.06725583			
Electronic state : 1-A			
Cartesian coordinates (Angs):			
C	-0.035034	-0.159985	0.433296
O	-0.507046	-0.826852	1.384218
O	0.225086	-1.864594	1.906249
C	-0.948940	0.940150	-0.042933
C	-2.265418	0.365017	-0.587635
C	-1.235747	1.922615	1.098819
H	-0.440181	1.462406	-0.853192
C	-2.079200	-0.636620	-1.718227
H	-2.803899	-0.101069	0.239199
H	-2.870404	1.207681	-0.927202
H	-0.323248	2.335440	1.525677
H	-1.779553	1.414775	1.893980
H	-1.846824	2.745245	0.729386
H	-1.594527	-1.545523	-1.361226
H	-1.465944	-0.217640	-2.518737
H	-3.038395	-0.922131	-2.146905
C	1.307307	-0.519625	-0.110163
C	1.993220	0.571247	-0.925825
C	1.181363	-1.824214	-0.920234
H	1.896648	-0.759150	0.780788
C	2.327022	1.828043	-0.132643
H	2.915970	0.137420	-1.315505
H	1.389779	0.817868	-1.803440
H	2.179692	-2.213622	-1.114039
H	0.699099	-1.632987	-1.878854
H	0.621708	-2.570973	-0.361966
H	2.923382	1.579595	0.745815
H	1.429347	2.340626	0.212152
H	2.895596	2.533848	-0.736399
Rotational constants (GHz): 1.0856400 0.8881100 0.7852100			
Vibrational harmonic frequencies (cm-1):			
53.1260	87.9334	103.0830	
135.4276	171.5141	192.5006	
199.4413	220.6843	226.7483	
237.6704	258.1238	266.8951	
286.7594	304.8300	344.7451	
404.1251	438.5074	456.7979	
518.0349	610.0777	692.9298	
738.6682	792.9503	814.8666	
864.0101	896.5313	950.9105	
975.3854	986.2110	1018.4472	
1028.7852	1038.5621	1044.1850	
1082.0236	1113.4152	1131.2883	

1147.8469	1179.9276	1193.8561
1247.0911	1280.7225	1291.2299
1307.5122	1317.0735	1363.6351
1373.6063	1374.5540	1394.7527
1404.8170	1414.0549	1417.2740
1423.8401	1484.7233	1489.9858
1498.0258	1500.5014	1503.0365
1503.5415	1510.3545	1512.4654
1513.5870	1515.4533	1614.1484
3047.1226	3056.2433	3058.5994
3065.6948	3068.4950	3069.2722
3071.3825	3091.1045	3097.4248
3110.5476	3128.9703	3135.8624
3139.1743	3141.3046	3143.2809
3147.3957	3151.9054	3162.0613

Zero-point correction (Hartree): 0.260508

diC2H5CH3CH_COO.mpmnRS

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E(RM062X/Aug-CC-pVT2) (Hartree): -504.06697775

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.016558  | 0.316710  | -0.083820 |
| O | 0.214508  | 1.546504  | -0.222047 |
| O | -0.584112 | 2.262580  | -1.082375 |
| C | 0.957131  | -0.376537 | 0.858005  |
| C | 2.059851  | -1.124048 | 0.067520  |
| C | 1.559217  | 0.587568  | 1.877046  |
| H | 0.365085  | -1.126819 | 1.387962  |
| C | 2.712901  | -0.281204 | -1.021939 |
| H | 2.808118  | -1.440176 | 0.796285  |
| H | 1.649930  | -2.033314 | -0.368730 |
| H | 0.782915  | 1.132790  | 2.412014  |
| H | 2.203525  | 1.321030  | 1.396827  |
| H | 2.150254  | 0.025687  | 2.598636  |
| H | 3.075798  | 0.669679  | -0.632744 |
| H | 2.009745  | -0.055031 | -1.825235 |
| H | 3.558530  | -0.810088 | -1.458278 |
| C | -1.107081 | -0.330523 | -0.814690 |
| C | -2.419745 | 0.058771  | -0.089855 |
| C | -0.963774 | -1.835960 | -1.003276 |
| H | -1.137971 | 0.174919  | -1.782435 |
| C | -2.525863 | -0.463913 | 1.338332  |
| H | -2.495925 | 1.144634  | -0.106142 |
| H | -3.240300 | -0.334842 | -0.691967 |
| H | -0.798270 | -2.367967 | -0.066587 |
| H | -0.146032 | -2.077172 | -1.680547 |
| H | -1.882418 | -2.224052 | -1.442903 |
| H | -1.756090 | -0.030648 | 1.980194  |
| H | -2.435342 | -1.549850 | 1.386650  |
| H | -3.489891 | -0.196635 | 1.768445  |

Rotational constants (GHz): 1.3181700 0.8227500 0.7564000

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| 41.2820   | 70.2448   | 74.3442   |
| 96.2257   | 169.5954  | 194.3997  |
| 217.1519  | 238.8200  | 242.3141  |
| 248.2789  | 260.5405  | 295.4933  |
| 309.4166  | 326.5327  | 348.8992  |
| 370.4518  | 433.3922  | 501.9683  |
| 561.3248  | 617.0149  | 720.9636  |
| 745.1365  | 782.2091  | 807.6001  |
| 833.3927  | 864.9300  | 955.9240  |
| 981.2595  | 993.0803  | 1007.6392 |
| 1013.1654 | 1022.2646 | 1036.4390 |
| 1074.7389 | 1110.5524 | 1131.7829 |
| 1141.3512 | 1175.2324 | 1177.5886 |
| 1251.8703 | 1280.3565 | 1287.8578 |
| 1294.4794 | 1308.3428 | 1358.4935 |
| 1367.5625 | 1373.3467 | 1414.6881 |
| 1417.9564 | 1420.2063 | 1420.5349 |
| 1425.9330 | 1487.9374 | 1496.1708 |
| 1498.1931 | 1500.3976 | 1501.9861 |
| 1506.1030 | 1507.6737 | 1510.7962 |
| 1513.8864 | 1522.2388 | 1618.7995 |
| 3056.0552 | 3062.5538 | 3066.4123 |
| 3069.7334 | 3072.2491 | 3075.3067 |
| 3077.6473 | 3078.6420 | 3112.3997 |
| 3118.2637 | 3133.3624 | 3134.2020 |
| 3136.3401 | 3139.8410 | 3143.2178 |
| 3145.7220 | 3146.2915 | 3157.9629 |

Zero-point correction (Hartree): 0.260634

diC2H5CH3CH\_COO.mpmprS

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E(RM062X/Aug-CC-pVT2) (Hartree): -504.06656870

Electronic state : 1-A

Cartesian coordinates (Angs):

C	0.034236	-0.114627	-0.147199
O	-0.049819	-1.207235	-0.750939
O	0.873032	-1.533677	-1.718373
C	-1.019654	0.124456	0.896082
C	-2.256485	0.821042	0.282292
C	-1.392184	-1.163094	1.629407
H	-0.583375	0.822233	1.614548
C	-2.955270	0.024095	-0.812382
H	-2.949451	1.008463	1.105016
H	-1.965629	1.797327	-0.105039
H	-0.520917	-1.596273	2.119444
H	-1.792064	-1.907910	0.945927
H	-2.143512	-0.946228	2.388080
H	-3.299482	-0.943157	-0.449130
H	-2.296844	-0.157014	-1.661473

H	-3.825418	0.570285	-1.173504
C	1.145805	0.837822	-0.429063
C	2.234074	0.620767	0.644191
C	0.688696	2.294447	-0.452758
H	1.551798	0.546421	-1.396270
C	2.813093	-0.787769	0.668163
H	3.023100	1.347394	0.441250
H	1.821762	0.880843	1.624162
H	0.267525	2.608090	0.503620
H	-0.050114	2.473530	-1.232597
H	1.549842	2.929495	-0.656878
H	3.249004	-1.043064	-0.295316
H	2.045065	-1.535123	0.872142
H	3.579146	-0.870838	1.438117
Rotational constants (GHz): 1.3953800 0.7931400 0.7216200			
Vibrational harmonic frequencies (cm-1):			
10.9471	66.0229	72.6415	
105.5078	149.0718	191.9631	
211.2152	220.2705	236.1180	
253.8242	266.8746	284.5005	
291.1850	314.1867	336.4499	
350.4187	446.6220	475.9311	
559.4001	614.6494	705.8934	
740.1697	787.5459	808.3288	
843.2216	873.7641	945.4359	
978.4569	989.6395	1006.0980	
1025.3812	1032.3918	1048.2827	
1076.6840	1108.8217	1130.7875	
1149.3561	1176.6671	1178.9294	
1262.2834	1282.6408	1294.4695	
1308.8759	1323.9966	1356.7447	
1372.9617	1376.4219	1413.7707	
1415.4007	1424.3230	1426.6371	
1428.7221	1482.8055	1486.9226	
1494.9233	1498.9856	1502.3894	
1505.4165	1506.5665	1507.5687	
1512.7508	1516.5616	1629.1674	
3041.0938	3062.0033	3065.8859	
3068.1830	3071.3402	3073.3378	
3075.6242	3086.8462	3113.0104	
3116.8563	3131.9182	3136.5917	
3139.9816	3141.3567	3142.0168	
3145.1295	3155.2067	3164.1484	
Zero-point correction (Hartree): 0.260453			
dic2H5CH3CH_COO.mpmtrS			
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E(RM062X/Aug-CC-pVTZ) (Hartree): -504.06715652			
Electronic state : 1-A			
Cartesian coordinates (Angs):			
C	-0.156960	0.315196	-0.044107
O	-0.245655	1.487048	0.393161
O	0.784039	1.989863	1.154082
C	-1.313760	-0.146540	-0.880185
C	-2.215728	-1.116570	-0.076538
C	-2.121678	1.023081	-1.436586
H	-0.880754	-0.707270	-1.713836
C	-2.520832	-0.631331	1.335892
H	-3.141838	-1.227189	-0.642788
H	-1.758911	-2.103371	-0.035414
H	-1.486027	1.727865	-1.969318
H	-2.623599	1.569728	-0.640525
H	-2.875847	0.643621	-2.124231
H	-2.917204	0.383859	1.335386
H	-1.622810	-0.628215	1.956592
H	-3.253948	-1.278371	1.814400
C	1.069630	-0.470923	0.248719
C	2.174565	0.080259	-0.688720
C	0.909941	-1.980282	0.130935
H	1.351891	-0.184633	1.264853
C	3.570447	-0.215270	-0.158482
H	2.036699	-0.359076	-1.680584
H	2.054548	1.159760	-0.772799
H	0.541078	-2.277358	-0.852024
H	0.235516	-2.376037	0.888778
H	1.877399	-2.457737	0.275351
H	3.744980	-1.283655	-0.032201
H	3.708916	0.272484	0.806300
H	4.329083	0.164592	-0.841448
Rotational constants (GHz): 1.5194600 0.7392400 0.6425900			
Vibrational harmonic frequencies (cm-1):			
28.6204	46.8826	76.9248	
108.7061	169.2896	197.1192	
207.8584	238.9121	242.8625	
254.6032	264.7188	297.8070	
299.9928	318.8097	342.9334	
386.4795	419.8690	482.7663	
565.6307	604.9712	731.4112	
755.1965	780.2193	792.0596	
845.2506	874.2671	956.4651	
981.5732	987.6337	1005.6146	
1021.7803	1032.3485	1037.2274	
1080.6783	1109.3698	1134.3335	
1145.2395	1176.1680	1186.1856	
1258.0709	1278.9916	1286.5290	
1304.0338	1319.2728	1349.2760	
1367.3542	1382.8399	1409.0675	
1417.5177	1420.1336	1421.5033	
1426.6934	1478.0286	1490.7319	
1498.4706	1498.6136	1502.5360	
1504.8103	1506.3685	1508.4600	
1512.8560	1521.0710	1616.4876	

3048.6740	3053.2030	3061.3068
3064.1409	3067.0295	3074.6011
3076.8278	3079.4865	3115.2340
3118.8747	3134.2079	3135.8081
3139.1257	3140.4895	3145.2409
3149.2310	3150.5031	3155.6822

Zero-point correction (Hartree): 0.260573

dic2H5CH3CH_COO.mppmRS

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E(RM062X/Aug-CC-pVTZ) (Hartree): -504.06303351

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.088046 | -0.577277 | 0.199650  |
| O | 0.093290  | -1.279608 | -0.817276 |
| O | 1.352125  | -1.462061 | -1.326828 |
| C | -1.517899 | -0.483317 | 0.660660  |
| C | -1.978230 | 0.987295  | 0.701429  |
| C | -2.462894 | -1.364807 | -0.145509 |
| H | -1.502356 | -0.836804 | 1.698030  |
| C | -2.028620 | 1.648817  | -0.670890 |
| H | -2.968448 | 1.005529  | 1.159398  |
| H | -1.324210 | 1.554574  | 1.365115  |
| H | -2.182055 | -2.413328 | -0.071873 |
| H | -2.451927 | -1.097878 | -1.200209 |
| H | -3.478283 | -1.247789 | 0.232045  |
| H | -2.786527 | 1.192164  | -1.305458 |
| H | -1.070831 | 1.567904  | -1.188547 |
| H | -2.268217 | 2.707073  | -0.578001 |
| C | 1.008267  | 0.091848  | 0.974906  |
| C | 1.434181  | 1.447904  | 0.366043  |
| C | 2.205050  | -0.818624 | 1.275018  |
| H | 0.538521  | 0.334594  | 1.931917  |
| C | 1.978711  | 1.414819  | -1.055782 |
| H | 0.588844  | 2.137019  | 0.410872  |
| H | 2.191699  | 1.851435  | 1.042489  |
| H | 2.867078  | -0.898072 | 0.421354  |
| H | 1.885386  | -1.827331 | 1.534792  |
| H | 2.743564  | -0.399933 | 2.125824  |
| H | 1.239902  | 1.034835  | -1.760111 |
| H | 2.847262  | 0.766750  | -1.139911 |
| H | 2.264161  | 2.422660  | -1.358039 |

Rotational constants (GHz): 1.3796600 0.8575400 0.7280900

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| 52.5244   | 88.1876   | 130.2941  |
| 141.6365  | 166.1533  | 178.5249  |
| 215.3266  | 222.9159  | 229.8296  |
| 265.0232  | 270.0194  | 295.1532  |
| 299.0073  | 319.7354  | 324.1228  |
| 364.8953  | 435.6232  | 502.3586  |
| 516.6684  | 623.9721  | 719.5588  |
| 764.0773  | 783.4505  | 811.1606  |
| 834.3259  | 875.4120  | 964.2422  |
| 980.7449  | 992.2521  | 1001.2524 |
| 1017.5510 | 1028.5885 | 1040.0256 |
| 1100.2418 | 1109.4629 | 1137.3865 |
| 1144.7416 | 1158.5057 | 1192.1613 |
| 1224.9398 | 1282.8643 | 1299.4332 |
| 1302.6510 | 1319.0537 | 1371.1367 |
| 1378.0757 | 1385.0429 | 1411.6873 |
| 1420.7827 | 1421.9241 | 1430.8476 |
| 1441.4098 | 1479.3284 | 1484.3578 |
| 1488.1822 | 1494.7641 | 1497.5565 |
| 1498.9182 | 1506.2697 | 1508.9413 |
| 1510.7943 | 1518.0590 | 1640.9838 |
| 3030.3960 | 3051.3683 | 3059.8490 |
| 3065.3486 | 3070.4570 | 3072.2803 |
| 3073.2539 | 3077.4987 | 3092.6794 |
| 3104.9202 | 3132.9707 | 3133.1883 |
| 3138.5789 | 3143.9748 | 3150.1207 |
| 3159.2421 | 3160.4278 | 3201.4659 |

Zero-point correction (Hartree): 0.260926

dic2H5CH3CH\_COO.mpppRS

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E(RM062X/Aug-CC-pVTZ) (Hartree): -504.06872400

Electronic state : 1-A

Cartesian coordinates (Angs):

C	0.022934	-0.507663	0.006523
O	0.117152	-0.779388	-1.208748
O	1.344001	-0.693261	-1.824835
C	-1.341873	-0.660733	0.611944
C	-1.929180	0.730010	0.938468
C	-2.282435	-1.506815	-0.235961
H	-1.168769	-1.163353	1.569814
C	-2.346079	1.523960	-0.293674
H	-2.790735	0.575798	1.590222
H	-1.201194	1.299822	1.518715
H	-1.890437	-2.513857	-0.366719
H	-2.418816	-1.076149	-1.225281
H	-3.255227	-1.571445	0.251002
H	-3.205641	1.071404	-0.785547
H	-1.536647	1.583596	-1.021784
H	-2.620430	2.540516	-0.015747
C	1.194846	-0.141681	0.860244
C	2.082255	0.995090	0.332199
C	2.007755	-1.424933	1.102112
H	0.765500	0.177984	1.813091
C	1.298693	2.131816	-0.306891
H	2.655669	1.361684	1.187089
H	2.780744	0.586935	-0.392506
H	2.372721	-1.805623	0.150331

H	1.412146	-2.193139	1.595875
H	2.857707	-1.189095	1.741640
H	0.522572	2.515757	0.359555
H	0.834275	1.783679	-1.230511
H	1.955843	2.962368	-0.560364
Rotational constants (GHz):			1.3509700 0.8562000 0.7421200
Vibrational harmonic frequencies (cm-1):			
57.5306	93.2346	128.6759	
134.9853	170.6181	200.7733	
203.6380	215.7220	233.2836	
253.2037	265.9334	278.8703	
308.8084	314.2715	336.0193	
420.8594	429.2380	435.8616	
518.3221	618.6866	735.9924	
744.6498	801.4030	818.9257	
835.8776	886.5960	956.2220	
983.6414	987.5580	1008.5049	
1027.0496	1032.2061	1032.8924	
1100.0758	1116.5608	1133.2964	
1143.5588	1159.5100	1193.6727	
1234.6243	1283.6868	1298.9576	
1303.4690	1316.4157	1370.0949	
1374.3048	1385.2316	1394.0172	
1407.3823	1420.7052	1422.2013	
1440.3297	1482.7146	1487.6416	
1494.7798	1495.2059	1497.8837	
1503.9527	1504.8503	1514.9366	
1516.1039	1521.0268	1649.3261	
3037.2116	3051.5422	3056.6559	
3062.6509	3064.5758	3069.3954	
3071.8937	3076.1122	3100.8451	
3117.8997	3132.8705	3136.8361	
3141.5812	3143.7814	3146.8507	
3155.6569	3158.4100	3161.4019	
Zero-point correction (Hartree): 0.260902			

diC2H5CH3CH_COO.mpptRS

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E(RM062X/Aug-CC-pVTZ) (Hartree): -504.06680960

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.251803 | -0.537695 | 0.171993  |
| O | -0.391527 | -1.348184 | -0.768002 |
| O | 0.709331  | -1.794245 | -1.462314 |
| C | -1.517495 | -0.083081 | 0.836558  |
| C | -1.734170 | 1.414961  | 0.525290  |
| C | -2.726750 | -0.936224 | 0.479419  |
| H | -1.325611 | -0.158987 | 1.911994  |
| C | -2.035994 | 1.696523  | -0.942176 |
| H | -2.558295 | 1.763280  | 1.149851  |
| H | -0.851929 | 1.978123  | 0.835626  |
| H | -2.581223 | -1.969190 | 0.790037  |
| H | -2.907609 | -0.939673 | -0.593003 |
| H | -3.611190 | -0.542948 | 0.979967  |
| H | -2.993240 | 1.272396  | -1.241002 |
| H | -1.269615 | 1.276914  | -1.596193 |
| H | -2.078838 | 2.769515  | -1.122549 |
| C | 1.075805  | -0.013279 | 0.613296  |
| C | 1.704021  | 0.868159  | -0.483226 |
| C | 1.994939  | -1.149211 | 1.084418  |
| H | 0.866852  | 0.628217  | 1.474121  |
| C | 3.022352  | 1.485180  | -0.034222 |
| H | 1.842199  | 0.258788  | -1.374140 |
| H | 1.000512  | 1.665184  | -0.736287 |
| H | 2.360008  | -1.717038 | 0.234399  |
| H | 1.464701  | -1.829990 | 1.751060  |
| H | 2.830595  | -0.726665 | 1.639391  |
| H | 3.791418  | 0.725801  | 0.098532  |
| H | 2.909557  | 2.020432  | 0.910986  |
| H | 3.383856  | 2.193270  | -0.778368 |

|                             |  |  |                               |
|-----------------------------|--|--|-------------------------------|
| Rotational constants (GHz): |  |  | 1.3948700 0.7861100 0.6514000 |
|-----------------------------|--|--|-------------------------------|

Vibrational harmonic frequencies (cm-1):

|           |           |           |  |
|-----------|-----------|-----------|--|
| 57.8231   | 65.2554   | 73.8985   |  |
| 111.3263  | 146.8881  | 187.3128  |  |
| 191.0606  | 210.1804  | 221.2036  |  |
| 254.7030  | 275.2658  | 284.3461  |  |
| 298.5966  | 301.1778  | 327.4789  |  |
| 369.8861  | 427.6447  | 465.6240  |  |
| 522.8369  | 620.7985  | 731.4930  |  |
| 772.5619  | 800.4489  | 819.2942  |  |
| 827.9719  | 881.1113  | 954.7857  |  |
| 976.5366  | 985.5824  | 998.7808  |  |
| 1009.7462 | 1028.0055 | 1058.3767 |  |
| 1104.1311 | 1118.5894 | 1123.9657 |  |
| 1146.1163 | 1156.0003 | 1190.4927 |  |
| 1225.6210 | 1279.7451 | 1293.2653 |  |
| 1302.5752 | 1345.6533 | 1360.7860 |  |
| 1373.9513 | 1383.3257 | 1399.2741 |  |
| 1412.6293 | 1419.8407 | 1422.8544 |  |
| 1439.7123 | 1487.8571 | 1489.9779 |  |
| 1495.9925 | 1497.2670 | 1501.4290 |  |
| 1504.6896 | 1508.5919 | 1515.3784 |  |
| 1516.2625 | 1518.1994 | 1646.5455 |  |
| 3041.1420 | 3053.2531 | 3057.0629 |  |
| 3063.9483 | 3065.0525 | 3069.0956 |  |
| 3073.6560 | 3076.2009 | 3100.9868 |  |
| 3120.8610 | 3133.4919 | 3135.3498 |  |
| 3142.2363 | 3144.2724 | 3147.2515 |  |
| 3148.9022 | 3160.9132 | 3188.2124 |  |

Zero-point correction (Hartree): 0.260533

diC2H5CH3CH\_COO.mptpRS

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E(RM062X/Aug-CC-pVTZ) (Hartree): -504.06913526
Electronic state : 1-A
Cartesian coordinates (Angs):
C 0.015229 0.237693 -0.433311
O -0.442884 1.157321 -1.151263
O 0.241508 2.345340 -1.230825
C -0.845721 -0.986981 -0.329724
C -1.520445 -1.017536 1.061887
C -1.858443 -1.091320 -1.464669
H -0.177181 -1.848737 -0.372879
C -2.442784 0.164784 1.332453
H -2.081814 -1.951626 1.123764
H -0.751292 -1.068385 1.833705
H -1.358532 -1.133130 -2.430973
H -2.531292 -0.237446 -1.480932
H -2.449334 -1.998073 -1.339548
H -3.275231 0.191975 0.631019
H -1.911529 1.114100 1.253097
H -2.858495 0.097963 2.336738
C 1.293906 0.453265 0.303053
C 2.034311 -0.834413 0.653886
C 1.009518 1.334955 1.532558
H 1.896771 1.058351 -0.380109
C 2.605200 -1.540148 -0.571377
H 2.850230 -0.567982 1.327903
H 1.387154 -1.507872 1.220781
H 0.448309 0.786741 2.289596
H 0.457645 2.225019 1.237280
H 1.956568 1.645661 1.971387
H 3.328075 -0.898723 -1.075528
H 1.828418 -1.784022 -1.298223
H 3.107929 -2.466889 -0.298909
Rotational constants (GHz): 1.1660800 0.8627600 0.7773500
Vibrational harmonic frequencies (cm-1):
59.2418 94.5472 105.5298
138.5169 160.9724 184.0382
218.7790 225.0581 229.9759
239.3515 250.9484 281.9425
292.7996 307.4024 361.2500
387.9704 429.4061 477.0387
547.4636 622.9799 683.3367
751.7048 793.7337 800.0842
845.4996 893.0597 957.9766
975.7397 993.6579 1005.7076
1027.0476 1030.7942 1036.4322
1070.7222 1108.5674 1132.0235
1150.8934 1178.8386 1194.8393
1254.0525 1274.6572 1287.2067
1304.3217 1312.9013 1363.2762
1372.0779 1377.6432 1395.6388
1418.2385 1421.4770 1424.2069
1425.6857 1484.0488 1494.7918
1498.6992 1500.0743 1502.9788
1504.0085 1506.6893 1511.6276
1516.6383 1517.6071 1616.3864
3055.8302 3060.2520 3065.4207
3066.2898 3069.6762 3071.7427
3076.7507 3085.8648 3094.6964
3105.2372 3126.1758 3136.9848
3139.7391 3140.2425 3144.5435
3146.2801 3158.3803 3163.4891
Zero-point correction (Hartree): 0.260710

diC2H5CH3CH_COO.mpttRS
~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -504.06877373
Electronic state : 1-A
Cartesian coordinates (Angs):
C     -0.221676      0.465012     -0.381262
O     -0.781015      1.583882     -0.303882
O     -0.047487      2.667745      0.114424
C     -1.109512     -0.676920     -0.775290
C     -1.368135     -1.568093      0.462360
C     -2.404575     -0.218041     -1.435811
H     -0.541926     -1.280459     -1.487291
C     -2.107655     -0.860792      1.591507
H     -1.942369     -2.431426      0.121524
H     -0.418509     -1.955272      0.833345
H     -2.201117      0.348493     -2.342743
H     -2.986586      0.419881     -0.775160
H     -3.005379     -1.088661     -1.696940
H     -3.103389     -0.545963      1.283400
H     -1.568818      0.025594      1.929158
H     -2.220938     -1.527476      2.445042
C      1.222333      0.343176     -0.034083
C      1.908896     -0.865616     -0.670013
C      1.360662      0.391721      1.499366
H      1.665295      1.268718     -0.414382
C      3.410691     -0.876356     -0.409600
H      1.470267     -1.793627     -0.295489
H      1.735293     -0.848553     -1.748284
H      1.035032     -0.547276      1.949570
H      0.774683      1.217054      1.898408
H      2.401284      0.558227      1.769270
H      3.632246     -1.023643      0.646342
H      3.863514      0.066483     -0.719253
H      3.893255     -1.679667     -0.963884
Rotational constants (GHz):      1.2928300      0.7906100      0.6772300
Vibrational harmonic frequencies (cm-1):
62.9522      87.8097      95.7622
128.6424      156.9364      161.0911

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|           |           |           |
|-----------|-----------|-----------|
| 212.1115  | 223.4947  | 224.5971  |
| 238.5563  | 282.0883  | 296.9957  |
| 298.5129  | 309.6508  | 332.8730  |
| 366.5667  | 430.5043  | 476.5033  |
| 560.5806  | 624.8380  | 691.2473  |
| 753.3634  | 789.3108  | 804.5989  |
| 844.0813  | 901.1810  | 957.8743  |
| 972.9767  | 985.8586  | 991.6992  |
| 1004.9321 | 1029.6902 | 1046.5257 |
| 1078.4022 | 1114.5369 | 1145.1923 |
| 1151.5242 | 1177.1492 | 1193.7654 |
| 1259.5145 | 1281.8246 | 1287.8790 |
| 1308.7348 | 1317.7626 | 1337.2838 |
| 1372.3189 | 1381.7282 | 1399.3010 |
| 1414.6011 | 1419.2449 | 1424.2537 |
| 1426.6041 | 1481.0966 | 1490.9561 |
| 1494.8873 | 1498.7073 | 1501.8578 |
| 1502.5695 | 1506.4394 | 1512.9841 |
| 1517.7648 | 1523.8116 | 1619.1463 |
| 3050.0203 | 3056.2785 | 3066.1600 |
| 3066.4542 | 3068.6103 | 3070.7041 |
| 3076.3086 | 3077.9682 | 3091.6644 |
| 3109.1924 | 3135.2861 | 3136.7161 |
| 3141.1787 | 3145.1898 | 3146.7777 |
| 3147.2592 | 3159.2863 | 3163.6608 |

Zero-point correction (Hartree): 0.260611

dic2H5CH3CH\_COO.mtmmRS

E(RM062X/Aug-CC-pVTZ) (Hartree): -504.06690212

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.199050 | 0.448129  | -0.238145 |
| O | -0.354692 | 1.689093  | -0.307857 |
| O | -1.488512 | 2.191468  | -0.903371 |
| C | 1.078821  | 0.005972  | 0.412705  |
| C | 2.154087  | -0.168361 | -0.679487 |
| C | 1.525083  | 0.971792  | 1.507813  |
| H | 0.885052  | -0.974217 | 0.854945  |
| C | 3.442532  | -0.783029 | -0.148172 |
| H | 1.760289  | -0.793600 | -1.481110 |
| H | 2.352273  | 0.813604  | -1.114725 |
| H | 0.718792  | 1.161663  | 2.215152  |
| H | 1.825514  | 1.926968  | 1.079601  |
| H | 2.366675  | 0.554547  | 2.056342  |
| H | 3.243525  | -1.734481 | 0.347720  |
| H | 3.936161  | -0.126530 | 0.566339  |
| H | 4.141246  | -0.969642 | -0.962158 |
| C | -1.259198 | -0.457705 | -0.761564 |
| C | -2.411580 | -0.460040 | 0.274098  |
| C | -0.788272 | -1.863461 | -1.116827 |
| H | -1.650418 | 0.050036  | -1.645304 |
| C | -2.035292 | -1.056645 | 1.625583  |
| H | -2.752843 | 0.567509  | 0.389616  |
| H | -3.232305 | -1.027731 | -0.167365 |
| H | -0.281032 | -2.365357 | -0.293744 |
| H | -0.118787 | -1.859696 | -1.975076 |
| H | -1.656663 | -2.467100 | -1.380435 |
| H | -1.248086 | -0.477786 | 2.113079  |
| H | -1.691007 | -2.087763 | 1.537660  |
| H | -2.895536 | -1.054832 | 2.293255  |

Rotational constants (GHz): 1.3340300 0.7608000 0.6645500

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| 42.1813   | 64.7911   | 71.1076   |
| 82.7893   | 147.3557  | 192.2575  |
| 207.4240  | 222.0290  | 232.2586  |
| 243.0038  | 273.7866  | 283.1107  |
| 299.1430  | 319.9231  | 351.5153  |
| 359.1687  | 402.3692  | 472.9769  |
| 561.4701  | 627.0749  | 731.3248  |
| 740.7775  | 784.2868  | 799.9729  |
| 844.1280  | 869.4815  | 953.2086  |
| 980.8981  | 985.1545  | 1001.7984 |
| 1012.0202 | 1020.7895 | 1055.8018 |
| 1080.2775 | 1113.8386 | 1126.9895 |
| 1148.4280 | 1172.0281 | 1185.2833 |
| 1251.8245 | 1285.2404 | 1289.8119 |
| 1298.2918 | 1332.0517 | 1358.5131 |
| 1363.3306 | 1374.3029 | 1409.7186 |
| 1415.4210 | 1417.3348 | 1420.3893 |
| 1422.1174 | 1486.4140 | 1494.2467 |
| 1497.7495 | 1500.7282 | 1503.5879 |
| 1504.8452 | 1507.6955 | 1511.9843 |
| 1516.0360 | 1518.2301 | 1623.2057 |
| 3056.2487 | 3061.9094 | 3065.1917 |
| 3071.8479 | 3073.2129 | 3075.6506 |
| 3078.4343 | 3081.9243 | 3109.8839 |
| 3113.0278 | 3132.5131 | 3133.7477 |
| 3137.0283 | 3140.0374 | 3144.1267 |
| 3146.9218 | 3147.9125 | 3159.1281 |

Zero-point correction (Hartree): 0.260381

dic2H5CH3CH\_COO.mtmpRS

E(RM062X/Aug-CC-pVTZ) (Hartree): -504.06683735

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.187390  | -0.193710 | -0.324814 |
| O | 0.402830  | -1.272222 | -0.918798 |
| O | 1.564333  | -1.442310 | -1.639450 |
| C | -1.103310 | -0.138371 | 0.441874  |
| C | -2.248606 | 0.208855  | -0.528697 |

|                                                           |           |           |           |
|-----------------------------------------------------------|-----------|-----------|-----------|
| C                                                         | -1.357529 | -1.441366 | 1.199269  |
| H                                                         | -1.009117 | 0.678837  | 1.161022  |
| C                                                         | -3.578262 | 0.432658  | 0.179673  |
| H                                                         | -1.982968 | 1.105240  | -1.091018 |
| H                                                         | -2.334899 | -0.603615 | -1.253203 |
| H                                                         | -0.497678 | -1.708841 | 1.812565  |
| H                                                         | -1.543534 | -2.258445 | 0.503664  |
| H                                                         | -2.219947 | -1.335568 | 1.853940  |
| H                                                         | -3.483088 | 1.194624  | 0.955149  |
| H                                                         | -3.943372 | -0.480391 | 0.646909  |
| H                                                         | -4.336293 | 0.767374  | -0.526665 |
| C                                                         | 1.172713  | 0.923860  | -0.357560 |
| C                                                         | 1.977680  | 0.876034  | 0.957692  |
| C                                                         | 0.507934  | 2.285968  | -0.548223 |
| H                                                         | 1.846270  | 0.706659  | -1.184577 |
| C                                                         | 2.756234  | -0.418478 | 1.153978  |
| H                                                         | 2.661435  | 1.726833  | 0.940546  |
| H                                                         | 1.297399  | 1.045118  | 1.798415  |
| H                                                         | -0.195042 | 2.517598  | 0.253250  |
| H                                                         | -0.019036 | 2.347448  | -1.499161 |
| H                                                         | 1.277429  | 3.056919  | -0.543287 |
| H                                                         | 3.454516  | -0.576632 | 0.334606  |
| H                                                         | 2.095475  | -1.286315 | 1.172886  |
| H                                                         | 3.309674  | -0.393281 | 2.091783  |
| Rotational constants (GHz): 1.4297000 0.7264800 0.6543200 |           |           |           |
| Vibrational harmonic frequencies (cm-1):                  |           |           |           |
| 47.4877                                                   | 57.6145   | 74.6512   |           |
| 111.5110                                                  | 128.5001  | 184.5668  |           |
| 204.4793                                                  | 215.6230  | 231.3572  |           |
| 240.1840                                                  | 257.3508  | 270.5206  |           |
| 287.3326                                                  | 305.1215  | 335.8403  |           |
| 363.1624                                                  | 410.4455  | 458.5031  |           |
| 544.5798                                                  | 624.2225  | 714.3943  |           |
| 749.9533                                                  | 785.1649  | 804.0345  |           |
| 857.6732                                                  | 876.4198  | 943.5216  |           |
| 977.3791                                                  | 983.1893  | 998.6015  |           |
| 1023.9779                                                 | 1045.1211 | 1058.6074 |           |
| 1078.0732                                                 | 1114.7016 | 1124.4465 |           |
| 1149.0312                                                 | 1177.4037 | 1186.3806 |           |
| 1258.5416                                                 | 1280.3414 | 1297.3129 |           |
| 1326.3927                                                 | 1340.2955 | 1356.7145 |           |
| 1367.1931                                                 | 1378.9026 | 1410.0000 |           |
| 1414.5200                                                 | 1415.9313 | 1418.9340 |           |
| 1428.7529                                                 | 1484.0945 | 1487.7635 |           |
| 1497.1744                                                 | 1498.5762 | 1499.4384 |           |
| 1502.4098                                                 | 1504.5329 | 1506.4420 |           |
| 1511.6481                                                 | 1516.6668 | 1634.9799 |           |
| 3041.5643                                                 | 3060.8854 | 3062.5476 |           |
| 3067.0021                                                 | 3068.2028 | 3073.4064 |           |
| 3075.6959                                                 | 3087.8055 | 3106.7754 |           |
| 3119.7805                                                 | 3132.4192 | 3132.5614 |           |
| 3137.9891                                                 | 3142.3862 | 3143.8901 |           |
| 3146.0066                                                 | 3153.3733 | 3158.3060 |           |
| Zero-point correction (Hartree): 0.260279                 |           |           |           |
| diC2H5CH3CH_COO.mtmtrs                                    |           |           |           |
| ~~~~~                                                     |           |           |           |
| E(RM062X/Aug-CC-pVTZ) (Hartree): -504.06701004            |           |           |           |
| Electronic state : 1-A                                    |           |           |           |
| Cartesian coordinates (Angs):                             |           |           |           |
| C                                                         | -0.000189 | 0.408690  | -0.141512 |
| O                                                         | -0.032764 | 1.628749  | -0.422431 |
| O                                                         | -1.169924 | 2.150540  | -0.997566 |
| C                                                         | 1.288013  | -0.068250 | 0.461832  |
| C                                                         | 2.292924  | -0.331460 | -0.678289 |
| C                                                         | 1.829756  | 0.924823  | 1.489471  |
| H                                                         | 1.077831  | -1.019385 | 0.955040  |
| C                                                         | 3.569509  | -1.008809 | -0.198169 |
| H                                                         | 1.820485  | -0.949585 | -1.443675 |
| H                                                         | 2.521825  | 0.626423  | -1.149889 |
| H                                                         | 1.074335  | 1.162704  | 2.237232  |
| H                                                         | 2.127847  | 1.852860  | 1.003917  |
| H                                                         | 2.692928  | 0.504842  | 2.001475  |
| H                                                         | 3.343259  | -1.939830 | 0.323963  |
| H                                                         | 4.132417  | -0.369528 | 0.479952  |
| H                                                         | 4.217036  | -1.246431 | -1.040710 |
| C                                                         | -1.192443 | -0.440932 | -0.398639 |
| C                                                         | -2.210949 | -0.112064 | 0.719179  |
| C                                                         | -0.892302 | -1.932474 | -0.492133 |
| H                                                         | -1.616341 | -0.062885 | -1.332298 |
| C                                                         | -3.579226 | -0.723996 | 0.451462  |
| H                                                         | -1.814696 | -0.479753 | 1.670383  |
| H                                                         | -2.300750 | 0.971537  | 0.781791  |
| H                                                         | -0.649157 | -2.357094 | 0.482996  |
| H                                                         | -0.069805 | -2.144862 | -1.173883 |
| H                                                         | -1.768397 | -2.456800 | -0.868099 |
| H                                                         | -3.546357 | -1.813097 | 0.444340  |
| H                                                         | -3.962856 | -0.386157 | -0.511740 |
| H                                                         | -4.288650 | -0.420449 | 1.219977  |
| Rotational constants (GHz): 1.5688800 0.6633700 0.5622400 |           |           |           |
| Vibrational harmonic frequencies (cm-1):                  |           |           |           |
| 41.3982                                                   | 43.5867   | 63.5373   |           |
| 85.3086                                                   | 152.6141  | 193.5883  |           |
| 194.6258                                                  | 212.9717  | 227.7679  |           |
| 241.8353                                                  | 268.3605  | 277.4322  |           |
| 298.7428                                                  | 316.3111  | 347.9784  |           |
| 354.6330                                                  | 417.9873  | 438.7757  |           |
| 554.9912                                                  | 628.6684  | 728.2244  |           |
| 758.4326                                                  | 783.4816  | 795.6474  |           |
| 857.1829                                                  | 872.0017  | 949.4792  |           |
| 977.1492                                                  | 981.5653  | 997.8479  |           |
| 1019.5827                                                 | 1031.3863 | 1059.1404 |           |

|           |           |           |
|-----------|-----------|-----------|
| 1082.7429 | 1123.5846 | 1125.6668 |
| 1151.7604 | 1182.1021 | 1187.0143 |
| 1258.5466 | 1282.1451 | 1292.5244 |
| 1320.0309 | 1334.2605 | 1350.3654 |
| 1366.9326 | 1378.2579 | 1409.2141 |
| 1411.5757 | 1416.4824 | 1419.6219 |
| 1420.8168 | 1484.7645 | 1488.8441 |
| 1497.9596 | 1500.9994 | 1502.0543 |
| 1505.1707 | 1506.6707 | 1508.8394 |
| 1515.6869 | 1518.7674 | 1625.5613 |
| 3043.8475 | 3061.7656 | 3063.8374 |
| 3064.9287 | 3067.5963 | 3074.3089 |
| 3075.5716 | 3081.9762 | 3103.5159 |
| 3117.7994 | 3133.0731 | 3135.5296 |
| 3136.6098 | 3140.3127 | 3143.1489 |
| 3146.5892 | 3151.4958 | 3157.9325 |

Zero-point correction (Hartree): 0.260260

diC2H5CH3CH\_COO.mtpmRS

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E(RM062X/Aug-CC-pVTZ) (Hartree): -504.06142182

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-0.071190	0.480482	0.212516
O	-0.465560	1.466797	-0.444671
O	-1.801664	1.676329	-0.661926
C	1.422097	0.392889	0.386144
C	1.937214	-0.943919	-0.181649
C	2.153543	1.595867	-0.194346
H	1.585447	0.363260	1.470970
C	3.438302	-1.129941	0.002591
H	1.416155	-1.766732	0.308286
H	1.681648	-0.994426	-1.243499
H	1.730881	2.528615	0.171576
H	2.082031	1.602026	-1.282299
H	3.204522	1.563439	0.083360
H	3.722933	-0.982877	1.045929
H	4.009189	-0.429465	-0.603944
H	3.735472	-2.136518	-0.287124
C	-0.979200	-0.531734	0.845751
C	-1.449491	-1.622663	-0.144459
C	-2.141241	0.084450	1.634345
H	-0.335823	-1.044564	1.565981
C	-2.227493	-1.149189	-1.364967
H	-0.582386	-2.195443	-0.476635
H	-2.063410	-2.309881	0.443097
H	-1.823533	0.963197	2.194845
H	-2.502478	-0.661579	2.342910
H	-2.946544	0.391669	0.978166
H	-1.627868	-0.486079	-1.986824
H	-3.119656	-0.594471	-1.086647
H	-2.524022	-2.012632	-1.960926

Rotational constants (GHz): 1.5002100 0.7305500 0.6200300

Vibrational harmonic frequencies (cm-1):

46.5157	53.3469	105.3287
139.0742	150.7866	181.5209
212.4310	221.3152	229.3180
265.1380	267.4808	291.3028
316.4956	320.6596	335.4151
366.7144	400.6315	472.4393
505.3972	645.2475	721.2462
764.1463	789.9407	801.9762
846.0892	879.8383	969.1541
976.2276	985.1023	999.6273
1020.8651	1041.8404	1059.2674
1102.1518	1109.6750	1140.3266
1144.8070	1173.1188	1192.4089
1226.9270	1279.2619	1301.4870
1314.0177	1334.9484	1361.7989
1378.7997	1382.3389	1412.6537
1415.2104	1421.7319	1430.6101
1438.5405	1479.3710	1485.6849
1487.5366	1495.9832	1497.1816
1500.9219	1502.4147	1508.4729
1509.3254	1520.2808	1641.0152
3017.3994	3049.8765	3056.5512
3059.3688	3065.0783	3070.5010
3072.2634	3076.9795	3096.3944
3109.4430	3132.6189	3133.6777
3138.5820	3146.0172	3151.0554
3162.7322	3163.8721	3201.5184

Zero-point correction (Hartree): 0.260793

diC2H5CH3CH_COO.mtppRS

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E(RM062X/Aug-CC-pVTZ) (Hartree): -504.06824556

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.145026  | -0.470655 | 0.043506  |
| O | 0.499148  | -1.194462 | -0.910298 |
| O | 1.832041  | -1.273141 | -1.240121 |
| C | -1.327162 | -0.455291 | 0.333959  |
| C | -1.896294 | 0.919834  | -0.069601 |
| C | -2.071574 | -1.609225 | -0.324935 |
| H | -1.413487 | -0.537143 | 1.424301  |
| C | -3.367340 | 1.081301  | 0.291906  |
| H | -1.317010 | 1.706064  | 0.416373  |
| H | -1.755747 | 1.046888  | -1.145900 |
| H | -1.593238 | -2.561591 | -0.105048 |
| H | -2.088821 | -1.487234 | -1.407782 |
| H | -3.096965 | -1.649047 | 0.035700  |
| H | -3.533209 | 0.871931  | 1.349991  |

|                                                           |           |           |           |
|-----------------------------------------------------------|-----------|-----------|-----------|
| H                                                         | -3.999457 | 0.410792  | -0.287543 |
| H                                                         | -3.698932 | 2.099615  | 0.095557  |
| C                                                         | 1.107020  | 0.287561  | 0.900494  |
| C                                                         | 2.094583  | 1.189811  | 0.144767  |
| C                                                         | 1.841157  | -0.729175 | 1.790747  |
| H                                                         | 0.486784  | 0.920628  | 1.540114  |
| C                                                         | 1.464157  | 1.944170  | -1.016746 |
| H                                                         | 2.496705  | 1.892138  | 0.878958  |
| H                                                         | 2.913412  | 0.578611  | -0.222773 |
| H                                                         | 1.148455  | -1.286472 | 2.421741  |
| H                                                         | 2.536499  | -0.194757 | 2.437224  |
| H                                                         | 2.397942  | -1.422538 | 1.163813  |
| H                                                         | 0.617881  | 2.553037  | -0.692908 |
| H                                                         | 1.123444  | 1.240885  | -1.778660 |
| H                                                         | 2.188786  | 2.609035  | -1.484395 |
| Rotational constants (GHz): 1.4223200 0.7475100 0.6576000 |           |           |           |
| Vibrational harmonic frequencies (cm-1):                  |           |           |           |
| 52.8048                                                   | 72.1844   | 91.2036   |           |
| 114.7463                                                  | 169.8319  | 197.2760  |           |
| 211.3809                                                  | 220.9600  | 227.4014  |           |
| 247.0471                                                  | 256.9444  | 286.2357  |           |
| 306.5166                                                  | 312.9518  | 348.7191  |           |
| 395.0004                                                  | 423.6102  | 432.7962  |           |
| 474.5918                                                  | 646.2605  | 739.3946  |           |
| 745.9800                                                  | 791.1038  | 815.6245  |           |
| 849.5997                                                  | 888.3266  | 960.4717  |           |
| 977.2939                                                  | 984.1607  | 1001.4276 |           |
| 1029.1842                                                 | 1032.4652 | 1058.7719 |           |
| 1105.0757                                                 | 1109.7420 | 1130.6245 |           |
| 1148.8778                                                 | 1163.9941 | 1197.0595 |           |
| 1234.3747                                                 | 1276.4916 | 1302.6145 |           |
| 1316.1807                                                 | 1328.4356 | 1362.8722 |           |
| 1370.4664                                                 | 1382.8473 | 1393.9728 |           |
| 1408.8549                                                 | 1414.5395 | 1420.4085 |           |
| 1438.7852                                                 | 1481.3750 | 1486.8641 |           |
| 1494.4505                                                 | 1497.4298 | 1498.6841 |           |
| 1502.7732                                                 | 1507.5835 | 1513.8190 |           |
| 1515.7014                                                 | 1517.7304 | 1649.4094 |           |
| 3025.7267                                                 | 3053.4936 | 3056.2093 |           |
| 3060.5572                                                 | 3063.5055 | 3065.0778 |           |
| 3066.4146                                                 | 3077.5596 | 3103.2510 |           |
| 3118.7370                                                 | 3133.6380 | 3133.9705 |           |
| 3134.9171                                                 | 3145.5106 | 3149.5648 |           |
| 3159.1855                                                 | 3160.6623 | 3160.7568 |           |
| Zero-point correction (Hartree): 0.260629                 |           |           |           |
| diC2H5CH3CH_COO.mtptRS                                    |           |           |           |
| ~~~~~                                                     |           |           |           |
| E(RM062X/Aug-CC-pVTZ) (Hartree): -504.06607536            |           |           |           |
| Electronic state : 1-A                                    |           |           |           |
| Cartesian coordinates (Angs):                             |           |           |           |
| C                                                         | 0.075359  | 0.575217  | 0.101814  |
| O                                                         | -0.051195 | 1.633252  | -0.549063 |
| O                                                         | -1.301868 | 2.067563  | -0.923477 |
| C                                                         | 1.484923  | 0.180276  | 0.430772  |
| C                                                         | 1.829818  | -1.092140 | -0.370734 |
| C                                                         | 2.486714  | 1.303563  | 0.201989  |
| H                                                         | 1.476998  | -0.095548 | 1.492030  |
| C                                                         | 3.192047  | -1.670144 | -0.008877 |
| H                                                         | 1.060848  | -1.847434 | -0.199222 |
| H                                                         | 1.797320  | -0.845092 | -1.434824 |
| H                                                         | 2.172629  | 2.217411  | 0.702231  |
| H                                                         | 2.582972  | 1.522540  | -0.861269 |
| H                                                         | 3.463429  | 1.019994  | 0.587676  |
| H                                                         | 3.266585  | -1.845933 | 1.065466  |
| H                                                         | 4.001320  | -1.002158 | -0.298282 |
| H                                                         | 3.350736  | -2.620403 | -0.516116 |
| C                                                         | -1.079252 | -0.273428 | 0.523949  |
| C                                                         | -1.808106 | -0.866614 | -0.696199 |
| C                                                         | -2.007054 | 0.501114  | 1.471048  |
| H                                                         | -0.642887 | -1.104165 | 1.086060  |
| C                                                         | -2.879867 | -1.868933 | -0.287408 |
| H                                                         | -2.234765 | -0.048001 | -1.271156 |
| H                                                         | -1.073971 | -1.362554 | -1.335874 |
| H                                                         | -1.438316 | 0.984684  | 2.265970  |
| H                                                         | -2.703602 | -0.192183 | 1.938806  |
| H                                                         | -2.551641 | 1.263652  | 0.922314  |
| H                                                         | -3.696508 | -1.383970 | 0.245371  |
| H                                                         | -2.470656 | -2.648017 | 0.359239  |
| H                                                         | -3.303475 | -2.352813 | -1.166212 |
| Rotational constants (GHz): 1.3878600 0.7265600 0.5643900 |           |           |           |
| Vibrational harmonic frequencies (cm-1):                  |           |           |           |
| 47.7404                                                   | 53.5941   | 64.2189   |           |
| 98.0100                                                   | 140.2091  | 181.9231  |           |
| 185.2241                                                  | 216.4255  | 220.1381  |           |
| 235.7725                                                  | 264.9803  | 270.9097  |           |
| 298.4187                                                  | 309.0371  | 328.7710  |           |
| 361.2148                                                  | 416.4606  | 429.0450  |           |
| 500.3427                                                  | 642.9912  | 733.2696  |           |
| 771.5220                                                  | 789.2836  | 816.5470  |           |
| 841.4333                                                  | 885.5643  | 957.3468  |           |
| 974.5113                                                  | 978.8351  | 990.6656  |           |
| 1010.2056                                                 | 1051.4404 | 1062.5053 |           |
| 1103.2922                                                 | 1119.7852 | 1124.2638 |           |
| 1144.1252                                                 | 1164.8621 | 1192.9396 |           |
| 1226.9237                                                 | 1277.3743 | 1289.3161 |           |
| 1327.3306                                                 | 1343.7843 | 1356.5699 |           |
| 1364.3501                                                 | 1382.1171 | 1396.6067 |           |
| 1411.1058                                                 | 1414.0853 | 1420.0870 |           |
| 1435.4734                                                 | 1486.8606 | 1490.1643 |           |
| 1496.1870                                                 | 1496.9333 | 1502.0803 |           |
| 1505.7550                                                 | 1506.3955 | 1514.8763 |           |

|           |           |           |
|-----------|-----------|-----------|
| 1516.0630 | 1516.7245 | 1647.5012 |
| 3027.4228 | 3050.6600 | 3057.3295 |
| 3058.4759 | 3062.2647 | 3066.1428 |
| 3070.2004 | 3077.2932 | 3098.8182 |
| 3120.6645 | 3134.3018 | 3134.5624 |
| 3142.0483 | 3145.5858 | 3149.3147 |
| 3149.4596 | 3160.0512 | 3174.7532 |

Zero-point correction (Hartree): 0.260125

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E(RM062X/Aug-CC-pVTZ) (Hartree): -504.06809519

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-0.287348	-0.538900	-0.188795
O	-0.427550	-1.769850	-0.378500
O	-1.636242	-2.355428	-0.093086
C	1.091162	-0.006467	-0.453128
C	1.779982	0.248861	0.904539
C	1.906431	-0.930403	-1.351507
H	0.975127	0.962643	-0.944346
C	3.166567	0.862434	0.756912
H	1.156480	0.911934	1.504978
H	1.841664	-0.699791	1.443408
H	1.354045	-1.186046	-2.253832
H	2.148426	-1.858652	-0.834947
H	2.833868	-0.443583	-1.644581
H	3.128675	1.765722	0.145548
H	3.865169	0.169499	0.291581
H	3.569429	1.133682	1.731419
C	-1.436656	0.254437	0.333787
C	-1.355865	1.746305	0.022578
C	-1.597662	-0.034600	1.837621
C	-2.307458	-0.186415	-0.160794
C	-1.554096	2.054599	-1.457568
H	-2.136621	2.243333	0.600857
H	-0.410354	2.161511	0.380589
H	-0.811526	0.449384	2.416495
H	-1.583474	-1.106911	2.019438
H	-2.556039	0.359544	2.172561
H	-2.543685	1.732894	-1.782150
H	-0.825471	1.534824	-2.082019
H	-1.463003	3.121060	-1.658139

Rotational constants (GHz): 1.1451500 0.8271400 0.6786300

Vibrational harmonic frequencies (cm-1):

54.1968	75.9842	108.7792
133.2437	154.6778	181.3655
208.5949	220.7284	228.4156
232.0712	244.0628	280.3460
296.4130	316.4562	361.0064
389.6349	419.2715	443.1854
528.1658	636.5195	681.7958
756.7001	791.0644	807.3186
858.3286	894.8190	960.4256
977.6328	983.4906	1001.5003
1027.5498	1037.9048	1057.8502
1074.9526	1111.6025	1131.2287
1156.7394	1178.8724	1195.2662
1253.4983	1278.7021	1285.6363
1308.9346	1338.2953	1358.4621
1370.5698	1378.0952	1395.5646
1409.7408	1417.2088	1419.5314
1423.7413	1483.5248	1495.4212
1497.1067	1500.6344	1503.1689
1504.1744	1507.2914	1510.0059
1512.7123	1518.9183	1617.3326
3052.9452	3058.5368	3061.0358
3064.2982	3065.3719	3071.1134
3075.6575	3079.3657	3093.6098
3109.6401	3126.7433	3133.2675
3140.8878	3141.4368	3146.4262
3148.7215	3158.9637	3161.2041

Zero-point correction (Hartree): 0.260567

dic2H5CH3CH_COO.mtttrS

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E(RM062X/Aug-CC-pVTZ) (Hartree): -504.06785236

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.025702 | 0.694953  | -0.214526 |
| O | -0.201957 | 1.928153  | -0.078221 |
| O | 0.873595  | 2.723740  | 0.233854  |
| C | -1.262960 | -0.103217 | -0.498294 |
| C | -1.648741 | -0.867625 | 0.786135  |
| C | -2.406278 | 0.758964  | -1.021610 |
| H | -0.994245 | -0.846988 | -1.253559 |
| C | -2.828685 | -1.809209 | 0.582000  |
| H | -0.789896 | -1.439020 | 1.139395  |
| H | -1.879234 | -0.134724 | 1.563230  |
| H | -2.082725 | 1.372216  | -1.860377 |
| H | -2.774509 | 1.426621  | -0.243329 |
| H | -3.227248 | 0.128462  | -1.355551 |
| H | -2.638949 | -2.495340 | -0.245182 |
| H | -3.745164 | -1.263775 | 0.364295  |
| H | -3.002573 | -2.403594 | 1.477564  |
| C | 1.342090  | 0.128547  | -0.046123 |
| C | 1.533706  | -1.228929 | -0.722101 |
| C | 1.694402  | 0.118204  | 1.454028  |
| H | 1.993437  | 0.875454  | -0.511199 |
| C | 2.975317  | -1.715646 | -0.633937 |
| H | 0.872067  | -1.973292 | -0.271335 |
| H | 1.248025  | -1.149936 | -1.773371 |

|                                                           |           |           |           |
|-----------------------------------------------------------|-----------|-----------|-----------|
| H                                                         | 1.201363  | -0.711584 | 1.961746  |
| H                                                         | 1.403070  | 1.060212  | 1.912823  |
| H                                                         | 2.769213  | 0.003990  | 1.578002  |
| H                                                         | 3.261836  | -1.929471 | 0.394654  |
| H                                                         | 3.661779  | -0.962830 | -1.023778 |
| H                                                         | 3.111758  | -2.627791 | -1.212529 |
| Rotational constants (GHz): 1.1859900 0.8089700 0.5862600 |           |           |           |
| Vibrational harmonic frequencies (cm-1):                  |           |           |           |
| 53.3687                                                   | 76.4366   | 97.9671   |           |
| 118.2161                                                  | 156.3711  | 157.2857  |           |
| 202.3563                                                  | 213.3604  | 223.5525  |           |
| 242.4945                                                  | 268.5317  | 296.2216  |           |
| 301.5167                                                  | 312.2510  | 340.1637  |           |
| 368.8889                                                  | 416.1101  | 434.5387  |           |
| 549.8466                                                  | 638.1275  | 684.3498  |           |
| 763.3958                                                  | 786.8056  | 810.5933  |           |
| 857.2198                                                  | 903.7637  | 959.4928  |           |
| 976.1390                                                  | 979.9821  | 986.8365  |           |
| 1002.0929                                                 | 1046.3111 | 1061.4730 |           |
| 1078.5323                                                 | 1120.1024 | 1143.0500 |           |
| 1151.6598                                                 | 1180.2571 | 1193.5732 |           |
| 1257.1175                                                 | 1279.6791 | 1298.8102 |           |
| 1316.7390                                                 | 1330.8924 | 1338.7586 |           |
| 1363.9009                                                 | 1381.3294 | 1401.5839 |           |
| 1408.5174                                                 | 1414.6667 | 1418.0053 |           |
| 1424.4204                                                 | 1483.2356 | 1489.3588 |           |
| 1495.9790                                                 | 1497.5562 | 1501.6254 |           |
| 1503.1511                                                 | 1506.1923 | 1511.6465 |           |
| 1516.5947                                                 | 1521.7315 | 1619.1770 |           |
| 3046.3798                                                 | 3053.5384 | 3056.8512 |           |
| 3064.1128                                                 | 3065.8711 | 3068.4057 |           |
| 3071.4344                                                 | 3077.3287 | 3089.2316 |           |
| 3109.1744                                                 | 3133.5029 | 3134.5503 |           |
| 3141.2950                                                 | 3146.0743 | 3147.8207 |           |
| 3149.5425                                                 | 3159.1722 | 3163.1059 |           |
| Zero-point correction (Hartree): 0.260420                 |           |           |           |

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E(RM062X/Aug-CC-pVTZ) (Hartree): -504.06013663

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.041719 | -0.269844 | -0.630258 |
| O | -0.421865 | 0.359642  | -1.650244 |
| O | -1.754867 | 0.404453  | -1.942701 |
| C | 1.459176  | -0.248005 | -0.473376 |
| C | 1.914017  | 0.618074  | 0.714479  |
| C | 2.095316  | -1.643286 | -0.421412 |
| H | 1.810791  | 0.240910  | -1.383840 |
| C | 1.824113  | 2.111052  | 0.428524  |
| H | 1.337894  | 0.359179  | 1.604437  |
| H | 2.949296  | 0.349822  | 0.935058  |
| H | 1.613366  | -2.342586 | -1.104208 |
| H | 2.069840  | -2.060149 | 0.582397  |
| H | 3.140537  | -1.553807 | -0.714777 |
| H | 0.823567  | 2.398097  | 0.109713  |
| H | 2.515311  | 2.386601  | -0.368354 |
| H | 2.076739  | 2.696171  | 1.311748  |
| C | -1.075006 | -0.967311 | 0.198565  |
| C | -2.114015 | 0.013437  | 0.819332  |
| C | -0.522264 | -1.924901 | 1.250908  |
| H | -1.630617 | -1.537944 | -0.556009 |
| C | -1.584738 | 1.401264  | 1.146388  |
| H | -2.946848 | 0.113894  | 0.131348  |
| H | -2.481205 | -0.463403 | 1.729351  |
| H | 0.089980  | -1.414249 | 1.994947  |
| H | 0.061695  | -2.730932 | 0.815532  |
| H | -1.361725 | -2.378048 | 1.775369  |
| H | -1.352254 | 1.938099  | 0.226602  |
| H | -0.692429 | 1.365560  | 1.774827  |
| H | -2.339369 | 1.977144  | 1.680512  |

Rotational constants (GHz): 1.1883200 0.8786600 0.8151200

Vibrational harmonic frequencies (cm-1):

|                                           |           |           |  |
|-------------------------------------------|-----------|-----------|--|
| 60.9037                                   | 69.1201   | 107.8537  |  |
| 141.4553                                  | 164.5013  | 202.2845  |  |
| 213.5034                                  | 226.4891  | 246.2308  |  |
| 261.2224                                  | 287.6224  | 304.1927  |  |
| 316.9482                                  | 348.8820  | 362.1242  |  |
| 423.6093                                  | 432.3587  | 461.0946  |  |
| 511.0656                                  | 630.6669  | 657.2597  |  |
| 761.6008                                  | 773.1753  | 801.6033  |  |
| 850.8927                                  | 874.3809  | 970.6800  |  |
| 988.7207                                  | 998.8202  | 1030.4568 |  |
| 1037.5664                                 | 1040.5625 | 1059.5962 |  |
| 1070.6738                                 | 1097.6263 | 1139.4422 |  |
| 1152.7079                                 | 1178.2380 | 1187.0117 |  |
| 1267.8063                                 | 1280.8478 | 1299.4826 |  |
| 1313.5045                                 | 1333.4914 | 1353.6715 |  |
| 1374.3513                                 | 1380.2706 | 1387.5470 |  |
| 1409.7990                                 | 1416.2114 | 1419.2560 |  |
| 1422.4865                                 | 1482.3374 | 1486.3864 |  |
| 1496.6198                                 | 1499.4733 | 1502.3243 |  |
| 1506.2795                                 | 1507.2432 | 1509.8221 |  |
| 1518.3478                                 | 1533.5889 | 1598.9674 |  |
| 3027.0300                                 | 3056.6389 | 3064.1772 |  |
| 3070.0744                                 | 3070.6908 | 3073.3460 |  |
| 3075.0819                                 | 3077.6832 | 3103.8078 |  |
| 3123.7536                                 | 3136.6442 | 3138.0375 |  |
| 3138.3339                                 | 3140.2627 | 3155.2269 |  |
| 3157.0837                                 | 3165.8772 | 3170.5433 |  |
| Zero-point correction (Hartree): 0.261277 |           |           |  |



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diC2H5CH3CH_COO.pmmprS
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E(RM062X/Aug-CC-pVTZ) (Hartree): -504.06452601
Electronic state : 1-A
Cartesian coordinates (Angs):
C -0.027182 0.499962 -0.459250
O 0.473808 0.649644 -1.601785
O 1.783752 1.019797 -1.741644
C -1.489092 0.136212 -0.512339
C -1.829950 -1.133126 0.276681
C -2.385348 1.312656 -0.097545
H -1.680144 -0.064439 -1.568677
C -1.210383 -2.392099 -0.315112
H -1.534046 -1.012950 1.320246
H -2.917830 -1.227117 0.279904
H -2.054468 2.248161 -0.547402
H -2.415854 1.436303 0.982428
H -3.400278 1.114043 -0.439867
H -0.122988 -2.326941 -0.351131
H -1.562787 -2.549899 -1.334785
H -1.472720 -3.271322 0.271522
C 0.819351 0.723317 0.752830
C 1.482303 -0.597073 1.206172
C 0.080606 1.378515 1.918128
H 1.615901 1.381708 0.402400
C 2.404464 -1.239655 0.178542
H 2.050831 -0.356854 2.106976
H 0.705481 -1.299598 1.517338
H -0.693143 0.734596 2.335593
H -0.373222 2.325807 1.632835
H 0.800969 1.580189 2.710002
H 3.236554 -0.580518 -0.058215
H 1.893434 -1.437277 -0.763522
H 2.795217 -2.181681 0.563139
Rotational constants (GHz): 1.1685200 0.8750800 0.8151400
Vibrational harmonic frequencies (cm-1):
66.2057 110.1463 136.9105
148.2691 171.4123 197.3941
223.5760 232.4396 243.7166
265.0138 269.1696 284.9511
296.6208 325.6238 333.9458
370.4598 426.2257 469.3514
505.8966 634.7288 676.7587
726.6181 791.9134 824.7693
854.5420 879.1445 961.5743
981.4083 984.3349 1019.4895
1035.3414 1045.5998 1057.0683
1066.2720 1106.7780 1132.7603
1148.8053 1178.3528 1192.2775
1276.4181 1286.3468 1313.7971
1320.1392 1336.5323 1364.4037
1375.1663 1380.5255 1387.6407
1414.8201 1417.8903 1421.6442
1430.9776 1483.5452 1488.4041
1496.4417 1498.2838 1500.2565
1504.2746 1507.0003 1510.7381
1513.8089 1520.6236 1604.1103
3057.5367 3065.1075 3068.8238
3070.6483 3071.0868 3074.0201
3074.0908 3082.0602 3096.8721
3105.1058 3136.3648 3137.7637
3139.5684 3141.0307 3145.1931
3149.7540 3154.9420 3163.6074
Zero-point correction (Hartree): 0.261222

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diC2H5CH3CH_COO.pmmtrS
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E(RM062X/Aug-CC-pVTZ) (Hartree): -504.06641909
Electronic state : 1-A
Cartesian coordinates (Angs):
C       0.252600      0.204269     -0.682158
O       0.078689      1.284192     -1.303291
O      -1.195463      1.667707     -1.630028
C       1.690794     -0.053549     -0.332082
C       1.896747      0.008123      1.190086
C       2.245676     -1.352810     -0.926002
H       2.237026      0.781693     -0.775141
C       1.624526      1.388008      1.773953
H       1.267159     -0.740572      1.675460
H       2.929768     -0.284261      1.389240
H       1.949708     -1.481039     -1.966711
H       1.924217     -2.225873     -0.363377
H       3.333732     -1.315326     -0.888273
H       0.596248      1.702664      1.595322
H       2.278622      2.133687      1.321355
H       1.794773      1.397095      2.849400
C      -0.947789     -0.601397     -0.326896
C      -1.661979      0.109799      0.850730
C      -0.708222     -2.080092     -0.051128
H      -1.605544     -0.479613     -1.192520
C      -3.140225     -0.247211      0.915327
H      -1.156622     -0.163337      1.781292
H      -1.571973      1.186880      0.715597
H      -0.054471     -2.242170      0.805426
H      -0.282450     -2.590674     -0.912885
H      -1.661789     -2.555894      0.170993
H      -3.300165     -1.318529      1.035610
H      -3.636763      0.075058      0.000027
H      -3.620052      0.254175      1.754760
Rotational constants (GHz):  1.2344600      0.7887800      0.7522800
Vibrational harmonic frequencies (cm-1):
52.1025      68.2495      111.5871

```

|           |           |           |
|-----------|-----------|-----------|
| 122.0342  | 160.4589  | 193.4449  |
| 198.2050  | 232.2252  | 243.9357  |
| 254.4405  | 255.7033  | 281.0573  |
| 307.4951  | 324.9322  | 355.0338  |
| 390.6799  | 414.7548  | 445.6617  |
| 510.7985  | 638.6244  | 683.8116  |
| 758.9182  | 787.0609  | 808.5772  |
| 853.5698  | 878.5604  | 959.9087  |
| 982.0282  | 987.4434  | 1015.8516 |
| 1025.1352 | 1036.7678 | 1056.1269 |
| 1076.6287 | 1102.9292 | 1140.1192 |
| 1149.7470 | 1182.6452 | 1192.5381 |
| 1277.3135 | 1284.5483 | 1310.6537 |
| 1327.6029 | 1332.4333 | 1360.6701 |
| 1372.5328 | 1382.6016 | 1393.5899 |
| 1409.5977 | 1415.9669 | 1421.7700 |
| 1423.9290 | 1476.9158 | 1485.1071 |
| 1496.7554 | 1499.9170 | 1503.1069 |
| 1503.6700 | 1505.8921 | 1508.0956 |
| 1512.4910 | 1522.5030 | 1601.5793 |
| 3047.0985 | 3060.4828 | 3061.9055 |
| 3065.2408 | 3067.7984 | 3073.0179 |
| 3074.3097 | 3077.4065 | 3100.9758 |
| 3115.4386 | 3136.5565 | 3137.2200 |
| 3139.4303 | 3140.1018 | 3143.1837 |
| 3146.9662 | 3150.1228 | 3163.7769 |

Zero-point correction (Hartree): 0.260782

diC2H5CH3CH\_COO.pmpmRS

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E(RM062X/Aug-CC-pVTZ) (Hartree): -504.06337132

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-0.132189	-0.053336	-0.328949
O	0.093267	-0.852310	-1.264482
O	1.183049	-1.680187	-1.226355
C	-1.390866	0.748104	-0.508849
C	-2.479698	0.233601	0.448279
C	-1.151235	2.245526	-0.318488
H	-1.724296	0.562826	-1.531341
C	-2.804561	-1.241503	0.254227
H	-2.172932	0.422913	1.479994
H	-3.371057	0.840175	0.277265
H	-0.385549	2.619787	-0.996977
H	-0.847281	2.472402	0.704065
H	-2.076127	2.785821	-0.516764
H	-1.945726	-1.875043	0.478439
H	-3.094283	-1.441880	-0.777701
H	-3.623779	-1.547839	0.902472
C	0.711812	0.076988	0.900749
C	1.901533	1.039368	0.672144
C	1.141380	-1.250096	1.535531
H	0.059168	0.582657	1.617167
C	2.864819	0.658387	-0.444157
H	1.512356	2.041919	0.486689
H	2.434039	1.087899	1.625102
H	1.994452	-1.678079	1.022931
H	0.341276	-1.988736	1.505096
H	1.392534	-1.059245	2.579582
H	2.361733	0.623426	-1.410008
H	3.300652	-0.324212	-0.283517
H	3.668321	1.392948	-0.498731

Rotational constants (GHz): 1.4191000 0.8169400 0.7055800

Vibrational harmonic frequencies (cm-1):

50.1323	61.6529	91.3220
133.9092	160.9086	172.2339
208.1634	213.6642	241.5203
256.7907	263.6245	269.3305
292.4428	314.8169	338.8373
353.0631	423.3861	493.8572
510.6506	602.8539	717.8137
762.2451	784.9623	813.6302
852.3770	872.9892	959.1869
976.1731	989.4981	1009.8528
1024.9917	1039.7104	1050.9544
1077.3033	1113.7726	1126.4245
1148.4241	1181.1973	1188.3313
1255.8034	1281.7216	1295.8504
1316.7198	1322.9785	1365.3454
1377.1056	1379.9532	1412.0684
1414.2477	1423.9125	1431.3293
1439.2919	1479.7553	1483.8311
1488.5014	1491.6870	1501.0891
1502.7073	1503.4473	1505.5728
1507.3412	1508.3210	1638.9711
3052.8658	3057.4670	3061.9307
3064.6175	3065.8976	3071.2413
3072.9050	3082.5377	3096.8426
3097.5450	3131.5519	3134.8695
3135.9182	3137.1836	3141.7738
3142.5480	3162.2209	3197.3714

Zero-point correction (Hartree): 0.260572

diC2H5CH3CH_COO.pmppRS

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E(RM062X/Aug-CC-pVTZ) (Hartree): -504.06940461

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |          |
|---|-----------|-----------|----------|
| C | 0.045068  | 0.011305  | 0.367506 |
| O | -0.225598 | -0.510491 | 1.471767 |
| O | -1.297777 | -1.360373 | 1.572463 |
| C | 1.253429  | 0.901939  | 0.382308 |

|                                                           |           |           |           |
|-----------------------------------------------------------|-----------|-----------|-----------|
| C                                                         | 2.358979  | 0.301087  | -0.498799 |
| C                                                         | 0.896637  | 2.325907  | -0.048712 |
| H                                                         | 1.606980  | 0.921430  | 1.414812  |
| C                                                         | 2.899106  | -1.014530 | 0.047150  |
| H                                                         | 1.979336  | 0.169389  | -1.515702 |
| H                                                         | 3.163399  | 1.035754  | -0.566104 |
| H                                                         | 0.107541  | 2.744290  | 0.574356  |
| H                                                         | 0.568231  | 2.358864  | -1.087823 |
| H                                                         | 1.778070  | 2.959484  | 0.042503  |
| H                                                         | 2.109810  | -1.759379 | 0.155692  |
| H                                                         | 3.343951  | -0.867070 | 1.031519  |
| H                                                         | 3.662693  | -1.428071 | -0.609782 |
| C                                                         | -0.728224 | -0.274634 | -0.880222 |
| C                                                         | -2.239772 | -0.012517 | -0.758652 |
| C                                                         | -0.452026 | -1.717229 | -1.335391 |
| H                                                         | -0.330523 | 0.407118  | -1.635152 |
| C                                                         | -2.578373 | 1.261551  | 0.000573  |
| H                                                         | -2.624123 | 0.042812  | -1.779778 |
| H                                                         | -2.701924 | -0.863966 | -0.268163 |
| H                                                         | -0.708962 | -2.408939 | -0.535652 |
| H                                                         | 0.589531  | -1.858871 | -1.621470 |
| H                                                         | -1.074871 | -1.933446 | -2.203106 |
| H                                                         | -2.095896 | 2.134171  | -0.444589 |
| H                                                         | -2.262602 | 1.176382  | 1.042043  |
| H                                                         | -3.652574 | 1.439681  | -0.002013 |
| Rotational constants (GHz): 1.3679700 0.8398800 0.7309900 |           |           |           |
| Vibrational harmonic frequencies (cm-1):                  |           |           |           |
| 57.5722                                                   | 83.7350   | 107.7525  |           |
| 136.7302                                                  | 168.6075  | 197.6699  |           |
| 212.7372                                                  | 220.5854  | 228.6529  |           |
| 246.2585                                                  | 255.9107  | 270.8606  |           |
| 293.8215                                                  | 317.6253  | 338.3663  |           |
| 404.4461                                                  | 429.1414  | 448.5498  |           |
| 493.1103                                                  | 601.3854  | 731.0702  |           |
| 743.7470                                                  | 799.5420  | 819.8154  |           |
| 855.1127                                                  | 885.0122  | 961.5510  |           |
| 978.9803                                                  | 988.3831  | 1018.0309 |           |
| 1031.3558                                                 | 1037.3008 | 1046.3127 |           |
| 1076.5740                                                 | 1104.5656 | 1132.4795 |           |
| 1146.2125                                                 | 1184.6006 | 1186.7385 |           |
| 1254.9773                                                 | 1281.0665 | 1303.8742 |           |
| 1317.6317                                                 | 1324.8998 | 1370.4400 |           |
| 1372.5096                                                 | 1376.7223 | 1393.1944 |           |
| 1411.2076                                                 | 1413.3951 | 1423.3247 |           |
| 1430.7796                                                 | 1482.3918 | 1487.4225 |           |
| 1495.0663                                                 | 1496.3211 | 1501.1476 |           |
| 1503.1883                                                 | 1507.7582 | 1509.1999 |           |
| 1513.6490                                                 | 1518.5393 | 1641.0067 |           |
| 3051.9327                                                 | 3056.7773 | 3061.8641 |           |
| 3064.7672                                                 | 3066.0673 | 3068.2402 |           |
| 3074.8541                                                 | 3082.1670 | 3096.6911 |           |
| 3115.7595                                                 | 3131.0301 | 3135.4457 |           |
| 3137.7797                                                 | 3139.3426 | 3141.7964 |           |
| 3146.3282                                                 | 3158.7078 | 3161.2145 |           |
| Zero-point correction (Hartree): 0.260762                 |           |           |           |
| diC2H5CH3CH_COO.pmptrS                                    |           |           |           |
| ~~~~~                                                     |           |           |           |
| E(RM062X/Aug-CC-pVTZ) (Hartree): -504.06708190            |           |           |           |
| Electronic state : 1-A                                    |           |           |           |
| Cartesian coordinates (Angs):                             |           |           |           |
| C                                                         | -0.265486 | -0.163452 | -0.479628 |
| O                                                         | -0.255190 | -1.110849 | -1.296055 |
| O                                                         | 0.814925  | -1.970489 | -1.339625 |
| C                                                         | -1.495606 | 0.693211  | -0.532373 |
| C                                                         | -2.297054 | 0.538537  | 0.768988  |
| C                                                         | -1.129056 | 2.154420  | -0.802058 |
| H                                                         | -2.101032 | 0.316356  | -1.358565 |
| C                                                         | -2.837970 | -0.871533 | 0.967423  |
| H                                                         | -1.670767 | 0.829833  | 1.616437  |
| H                                                         | -3.120524 | 1.254289  | 0.735631  |
| H                                                         | -0.560456 | 2.259072  | -1.725281 |
| H                                                         | -0.541196 | 2.575362  | 0.014095  |
| H                                                         | -2.040196 | 2.744131  | -0.894326 |
| H                                                         | -2.034809 | -1.608524 | 1.002804  |
| H                                                         | -3.497670 | -1.150105 | 0.145295  |
| H                                                         | -3.403186 | -0.946993 | 1.894867  |
| C                                                         | 0.850052  | 0.109579  | 0.474664  |
| C                                                         | 2.110360  | 0.535117  | -0.305587 |
| C                                                         | 1.087805  | -1.063804 | 1.434311  |
| H                                                         | 0.531432  | 0.967859  | 1.071408  |
| C                                                         | 3.249725  | 0.937825  | 0.621517  |
| H                                                         | 2.406410  | -0.287290 | -0.953400 |
| H                                                         | 1.850640  | 1.381095  | -0.946649 |
| H                                                         | 1.512228  | -1.909586 | 0.902189  |
| H                                                         | 0.155069  | -1.378977 | 1.902863  |
| H                                                         | 1.761653  | -0.744643 | 2.227474  |
| H                                                         | 3.629601  | 0.083727  | 1.179942  |
| H                                                         | 2.929911  | 1.695892  | 1.339601  |
| H                                                         | 4.078390  | 1.349808  | 0.047519  |
| Rotational constants (GHz): 1.3525500 0.7547800 0.6764100 |           |           |           |
| Vibrational harmonic frequencies (cm-1):                  |           |           |           |
| 48.0689                                                   | 58.5873   | 67.6251   |           |
| 109.2723                                                  | 132.9740  | 173.0005  |           |
| 188.1874                                                  | 206.0423  | 221.4042  |           |
| 240.2674                                                  | 250.1064  | 254.2567  |           |
| 275.7990                                                  | 315.7601  | 338.8995  |           |
| 402.6824                                                  | 419.2200  | 434.8144  |           |
| 494.7516                                                  | 602.9569  | 731.7752  |           |
| 769.2477                                                  | 797.7799  | 814.1161  |           |
| 853.2694                                                  | 880.1362  | 955.6989  |           |
| 973.8941                                                  | 981.7150  | 996.2817  |           |

|           |           |           |
|-----------|-----------|-----------|
| 1023.0817 | 1043.4912 | 1060.6198 |
| 1076.9599 | 1108.8632 | 1124.5370 |
| 1145.7104 | 1183.0973 | 1186.2761 |
| 1249.9077 | 1279.3803 | 1296.2773 |
| 1322.1631 | 1346.9730 | 1359.8549 |
| 1371.2289 | 1376.2227 | 1396.4393 |
| 1411.2977 | 1414.0201 | 1423.6058 |
| 1431.1897 | 1486.9865 | 1489.9245 |
| 1496.0991 | 1501.6690 | 1503.6480 |
| 1504.4924 | 1504.9493 | 1507.3159 |
| 1514.2568 | 1517.5593 | 1642.1489 |
| 3053.3840 | 3056.9664 | 3058.9472 |
| 3062.1645 | 3064.6607 | 3068.3208 |
| 3074.2907 | 3082.8637 | 3096.0045 |
| 3119.3254 | 3130.7503 | 3136.1693 |
| 3137.7386 | 3138.8009 | 3142.0654 |
| 3142.8272 | 3145.8336 | 3178.9697 |

Zero-point correction (Hartree): 0.260119

diC2H5CH3CH\_COO.pmttRS

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E(RM062X/Aug-CC-pVT2) (Hartree): -504.06597733

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-0.294182	0.685572	0.009625
O	-0.549643	1.851452	-0.385329
O	0.438656	2.591831	-0.977056
C	-1.457823	0.030216	0.700048
C	-1.996461	-1.198835	-0.046891
C	-1.122627	-0.287683	2.160242
H	-2.243898	0.788067	0.686185
C	-2.239541	-0.932053	-1.526289
H	-1.322111	-2.044271	0.085795
H	-2.933487	-1.476192	0.439867
H	-0.794101	0.602886	2.694684
H	-0.342093	-1.042951	2.239469
H	-2.012750	-0.674570	2.655611
H	-1.308529	-0.705392	-2.049636
H	-2.902091	-0.076520	-1.662420
H	-2.693504	-1.794033	-2.012201
C	1.088477	0.160994	-0.175615
C	1.224721	-1.359657	-0.247718
C	1.959403	0.797424	0.927272
H	1.412905	0.604301	-1.121484
C	2.660560	-1.784966	-0.537813
H	0.894830	-1.823645	0.683597
H	0.578526	-1.741941	-1.039379
H	1.770367	0.319899	1.889756
H	1.754500	1.863931	0.995234
H	3.012069	0.675316	0.682139
H	3.323627	-1.553677	0.294263
H	3.042976	-1.275869	-1.423612
H	2.715499	-2.857672	-0.715958

Rotational constants (GHz): 1.0892100 0.8885700 0.7163200

Vibrational harmonic frequencies (cm-1):

67.6056	91.7017	96.2540
137.3290	168.5275	185.6286
207.1808	217.9836	221.3468
234.4180	251.7168	272.3666
301.9479	326.0300	345.4811
394.9199	428.6557	444.2863
506.4344	630.3042	706.3337
741.2238	802.0307	816.8943
862.2605	905.2879	964.1796
971.6263	977.8622	989.0681
1014.4882	1044.8601	1051.5196
1072.5710	1113.7520	1133.2552
1153.2319	1190.2360	1199.4143
1281.0410	1286.5618	1315.5043
1321.5525	1335.2457	1341.5461
1377.1956	1377.9179	1391.2331
1399.3531	1413.4636	1417.7122
1422.6192	1483.5967	1491.3109
1497.0161	1500.5114	1502.2448
1503.1314	1505.2531	1509.7583
1518.6526	1522.6145	1605.1780
3054.6207	3057.1672	3064.4043
3066.5859	3069.3840	3071.2520
3072.4436	3074.8289	3105.6458
3111.8272	3129.5664	3135.5030
3140.0708	3141.3616	3142.6169
3148.3128	3149.6780	3161.2347

Zero-point correction (Hartree): 0.260752

diC2H5CH3CH_COO.ppmRS

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E(RM062X/Aug-CC-pVT2) (Hartree): -504.05712545

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.317075 | -0.804367 | -0.026521 |
| O | -0.993850 | -1.658229 | -0.662063 |
| O | -2.355442 | -1.654070 | -0.574869 |
| C | 1.165057  | -1.042017 | -0.217641 |
| C | 1.871440  | -0.041793 | -1.161132 |
| C | 1.921641  | -1.256458 | 1.095450  |
| H | 1.179230  | -1.994192 | -0.749365 |
| C | 2.402926  | 1.249225  | -0.551351 |
| H | 2.716893  | -0.585269 | -1.588149 |
| H | 1.207500  | 0.179131  | -1.998773 |
| H | 1.421520  | -1.996735 | 1.719294  |
| H | 2.033743  | -0.342636 | 1.670701  |
| H | 2.919947  | -1.629866 | 0.864716  |

|                                                 |           |           |                     |
|-------------------------------------------------|-----------|-----------|---------------------|
| H                                               | 3.122212  | 1.048114  | 0.241828            |
| H                                               | 1.613220  | 1.875363  | -0.144997           |
| H                                               | 2.915660  | 1.830882  | -1.316820           |
| C                                               | -1.066554 | 0.179425  | 0.810811            |
| C                                               | -1.841720 | 1.184301  | -0.077832           |
| C                                               | -0.285245 | 0.864107  | 1.925187            |
| H                                               | -1.850394 | -0.449973 | 1.247944            |
| C                                               | -0.992175 | 2.256085  | -0.744867           |
| H                                               | -2.397589 | 0.616718  | -0.820401           |
| H                                               | -2.578530 | 1.658338  | 0.573235            |
| H                                               | 0.578835  | 1.417803  | 1.565211            |
| H                                               | 0.055059  | 0.152027  | 2.674522            |
| H                                               | -0.947607 | 1.574925  | 2.419997            |
| H                                               | -0.266595 | 1.821767  | -1.433389           |
| H                                               | -0.451731 | 2.864940  | -0.018968           |
| H                                               | -1.626820 | 2.926002  | -1.323753           |
| Rotational constants (GHz):                     |           | 1.1957300 | 0.9106900 0.7315100 |
| Vibrational harmonic frequencies (cm-1):        |           |           |                     |
| 54.5806                                         | 84.7005   | 126.4083  |                     |
| 146.8369                                        | 189.9936  | 201.5933  |                     |
| 225.3783                                        | 236.8753  | 261.3679  |                     |
| 276.2040                                        | 296.2707  | 304.8030  |                     |
| 318.8506                                        | 340.2572  | 355.1357  |                     |
| 369.0581                                        | 411.2504  | 515.5110  |                     |
| 551.1301                                        | 618.6613  | 662.1227  |                     |
| 739.9866                                        | 782.3115  | 811.0028  |                     |
| 833.1638                                        | 866.7587  | 957.0807  |                     |
| 987.5643                                        | 992.5337  | 1016.3928 |                     |
| 1018.7909                                       | 1031.6619 | 1036.6404 |                     |
| 1081.2410                                       | 1115.6206 | 1133.6548 |                     |
| 1159.7291                                       | 1170.4443 | 1189.0262 |                     |
| 1272.4477                                       | 1294.5730 | 1306.1155 |                     |
| 1327.1210                                       | 1346.2277 | 1369.3519 |                     |
| 1379.3336                                       | 1383.1388 | 1390.8936 |                     |
| 1412.7625                                       | 1413.4278 | 1416.1910 |                     |
| 1424.1392                                       | 1487.5720 | 1491.7898 |                     |
| 1494.2650                                       | 1497.7501 | 1505.1510 |                     |
| 1511.1670                                       | 1512.8072 | 1517.7419 |                     |
| 1522.8335                                       | 1528.8783 | 1582.2010 |                     |
| 3031.9573                                       | 3059.5179 | 3062.7788 |                     |
| 3070.8616                                       | 3073.1514 | 3076.1074 |                     |
| 3079.1080                                       | 3083.8510 | 3097.2661 |                     |
| 3122.5560                                       | 3133.3568 | 3134.0656 |                     |
| 3135.9472                                       | 3138.7930 | 3148.2904 |                     |
| 3161.3277                                       | 3177.3799 | 3179.4516 |                     |
| Zero-point correction (Hartree): 0.261589       |           |           |                     |
| dic2H5CH3CH_COO.ppmprS                          |           |           |                     |
| ~~~~~                                           |           |           |                     |
| E (RM062X/Aug-CC-pVTZ) (Hartree): -504.05875224 |           |           |                     |
| Electronic state : 1-A                          |           |           |                     |
| Cartesian coordinates (Angs):                   |           |           |                     |
| C                                               | 0.278092  | -0.720204 | 0.028405            |
| O                                               | 1.060438  | -1.538879 | 0.576720            |
| O                                               | 2.397101  | -1.530952 | 0.288696            |
| C                                               | -1.138622 | -0.891315 | 0.519891            |
| C                                               | -1.687621 | 0.339843  | 1.280593            |
| C                                               | -2.092829 | -1.409011 | -0.560702           |
| H                                               | -1.041295 | -1.685694 | 1.260636            |
| C                                               | -2.450875 | 1.380035  | 0.468881            |
| H                                               | -2.364667 | -0.051397 | 2.042136            |
| H                                               | -0.869212 | 0.814709  | 1.825706            |
| H                                               | -1.695017 | -2.309859 | -1.026539           |
| H                                               | -2.284187 | -0.675280 | -1.338452           |
| H                                               | -3.046905 | -1.661665 | -0.096821           |
| H                                               | -3.325766 | 0.944140  | -0.012348           |
| H                                               | -1.841376 | 1.844171  | -0.303129           |
| H                                               | -2.801230 | 2.173815  | 1.127608            |
| C                                               | 0.829793  | 0.261139  | -0.953712           |
| C                                               | 1.152370  | 1.598293  | -0.251604           |
| C                                               | -0.040412 | 0.476760  | -2.190313           |
| H                                               | 1.779995  | -0.182227 | -1.253403           |
| C                                               | 2.103140  | 1.476851  | 0.932239            |
| H                                               | 1.590255  | 2.246092  | -1.013784           |
| H                                               | 0.223199  | 2.078781  | 0.060558            |
| H                                               | -0.970286 | 0.994958  | -1.964996           |
| H                                               | -0.280722 | -0.463399 | -2.684974           |
| H                                               | 0.516028  | 1.091827  | -2.896820           |
| H                                               | 3.054018  | 1.047784  | 0.625774            |
| H                                               | 1.699896  | 0.821770  | 1.706391            |
| H                                               | 2.278739  | 2.455774  | 1.377057            |
| Rotational constants (GHz):                     |           | 1.2769200 | 0.8549500 0.7495400 |
| Vibrational harmonic frequencies (cm-1):        |           |           |                     |
| 58.3516                                         | 69.7923   | 118.6813  |                     |
| 146.0004                                        | 167.0130  | 200.9813  |                     |
| 207.0207                                        | 222.1332  | 253.4985  |                     |
| 257.5245                                        | 268.0166  | 294.6655  |                     |
| 310.8300                                        | 314.0058  | 330.2794  |                     |
| 351.8193                                        | 411.8160  | 474.0978  |                     |
| 553.3931                                        | 641.9123  | 668.0520  |                     |
| 726.6984                                        | 778.2672  | 815.5250  |                     |
| 838.7660                                        | 876.7422  | 953.6105  |                     |
| 980.6223                                        | 984.5973  | 1014.4219 |                     |
| 1027.1580                                       | 1038.8152 | 1052.3208 |                     |
| 1074.8247                                       | 1121.2232 | 1131.2338 |                     |
| 1154.5499                                       | 1172.5082 | 1183.4028 |                     |
| 1275.7104                                       | 1304.1246 | 1325.6837 |                     |
| 1333.4276                                       | 1352.3298 | 1368.7174 |                     |
| 1378.0329                                       | 1383.1342 | 1390.6572 |                     |
| 1410.5241                                       | 1413.8365 | 1422.5788 |                     |
| 1428.1955                                       | 1480.3639 | 1490.2465 |                     |
| 1492.2976                                       | 1496.0127 | 1499.8444 |                     |

|           |           |           |
|-----------|-----------|-----------|
| 1504.2850 | 1507.6078 | 1511.9580 |
| 1516.1526 | 1522.0050 | 1598.1931 |
| 3060.6625 | 3064.0352 | 3066.6051 |
| 3071.1976 | 3073.1741 | 3077.8596 |
| 3085.9990 | 3089.5260 | 3097.1171 |
| 3107.0804 | 3128.1474 | 3135.5611 |
| 3137.0654 | 3139.5952 | 3150.0925 |
| 3160.7384 | 3166.6236 | 3173.3438 |

Zero-point correction (Hartree): 0.261159

diC2H5CH3CH\_COO.ppmtrS

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E(RM062X/Aug-CC-pVTZ) (Hartree): -504.06132548

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-0.124451	0.738978	0.226547
O	0.327925	1.860453	-0.128596
O	1.681733	2.049016	-0.166879
C	-1.632112	0.706783	0.169238
C	-2.135512	0.112085	-1.162123
C	-2.315715	0.089096	1.389226
H	-1.906236	1.762631	0.142612
C	-1.886330	-1.375536	-1.369280
H	-3.208819	0.309418	-1.205365
H	-1.681902	0.676785	-1.978357
H	-1.918672	0.498271	2.317621
H	-2.219914	-0.991799	1.426327
H	-3.378083	0.328770	1.345777
H	-2.347728	-1.978141	-0.587210
H	-0.821453	-1.601846	-1.391626
H	-2.308775	-1.696395	-2.320409
C	0.873362	-0.298205	0.608799
C	1.676087	-0.746799	-0.645723
C	0.373141	-1.496915	1.402683
H	1.583899	0.277098	1.213856
C	3.156636	-0.886444	-0.326106
H	1.271205	-1.702957	-0.983571
H	1.555131	-0.024666	-1.451770
H	-0.356734	-2.082236	0.845281
H	-0.062271	-1.212357	2.358590
H	1.224645	-2.146078	1.607513
H	3.318857	-1.568371	0.510639
H	3.560762	0.090226	-0.063213
H	3.708180	-1.272360	-1.182449

Rotational constants (GHz): 1.3715200 0.7955000 0.6896700

Vibrational harmonic frequencies (cm-1):

59.3672	90.4964	93.0868
123.1878	184.1721	221.0029
227.5032	238.5335	253.2856
270.4911	289.6902	301.0829
309.4117	333.5157	353.3012
374.6516	413.4944	492.2651
540.5859	640.1385	669.4385
765.5918	784.5391	804.5604
837.9791	880.7043	957.2517
992.3945	995.3461	1020.6936
1026.9904	1036.3394	1039.1370
1078.8141	1121.7487	1128.7258
1154.1030	1179.5730	1196.6596
1272.6096	1293.0490	1315.0978
1320.8731	1326.6133	1363.2850
1379.4593	1384.3306	1394.5403
1404.7724	1417.0253	1418.4159
1423.5152	1480.9535	1487.8595
1494.4898	1497.3847	1498.6128
1506.6878	1509.3863	1513.8368
1517.3662	1526.3204	1585.9088
3028.0429	3058.7714	3059.3582
3065.1502	3072.3604	3073.9105
3076.8866	3083.1183	3099.1965
3116.3232	3132.7594	3135.8493
3137.2579	3138.0224	3147.1580
3152.9794	3156.5696	3177.7714

Zero-point correction (Hartree): 0.261360

diC2H5CH3CH_COO.pppmRS

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E(RM062X/Aug-CC-pVTZ) (Hartree): -504.06035778

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.054074  | 0.138604  | -0.468038 |
| O | -0.404642 | 0.863104  | -1.379267 |
| O | -1.583393 | 1.538319  | -1.210031 |
| C | 1.375144  | -0.489404 | -0.830000 |
| C | 2.538427  | 0.422000  | -0.380358 |
| C | 1.523046  | -1.922697 | -0.323263 |
| H | 1.401669  | -0.505984 | -1.920132 |
| C | 2.651292  | 0.670854  | 1.119444  |
| H | 3.457962  | -0.042209 | -0.742583 |
| H | 2.440831  | 1.375654  | -0.900938 |
| H | 0.760892  | -2.572691 | -0.750667 |
| H | 1.457198  | -1.992754 | 0.761512  |
| H | 2.498237  | -2.306946 | -0.621313 |
| H | 2.714217  | -0.260733 | 1.682769  |
| H | 1.803687  | 1.241527  | 1.499054  |
| H | 3.551558  | 1.244224  | 1.334860  |
| C | -0.599998 | -0.053223 | 0.865326  |
| C | -1.645994 | -1.192271 | 0.815120  |
| C | -1.147078 | 1.225024  | 1.510220  |
| H | 0.202414  | -0.422081 | 1.506067  |
| C | -2.777941 | -1.012235 | -0.187600 |
| H | -1.130613 | -2.133724 | 0.616187  |

|                                                |           |           |                                     |
|------------------------------------------------|-----------|-----------|-------------------------------------|
| H                                              | -2.050617 | -1.271669 | 1.827022                            |
| H                                              | -0.504940 | 2.083265  | 1.315300                            |
| H                                              | -1.195199 | 1.066239  | 2.588390                            |
| H                                              | -2.131202 | 1.472566  | 1.130643                            |
| H                                              | -2.399646 | -0.946735 | -1.207396                           |
| H                                              | -3.337913 | -0.099117 | -0.003577                           |
| H                                              | -3.460088 | -1.860121 | -0.125914                           |
| Rotational constants (GHz):                    |           |           | 1.4453800    0.7780400    0.7352200 |
| Vibrational harmonic frequencies (cm-1):       |           |           |                                     |
| 54.0362                                        | 69.3715   | 103.5290  |                                     |
| 128.6797                                       | 169.7318  | 184.6038  |                                     |
| 202.2718                                       | 230.3558  | 250.4058  |                                     |
| 258.3277                                       | 271.7990  | 291.0055  |                                     |
| 297.8658                                       | 319.5048  | 342.7759  |                                     |
| 347.5852                                       | 383.0312  | 504.0392  |                                     |
| 543.9656                                       | 627.5222  | 718.6117  |                                     |
| 761.0806                                       | 782.5317  | 811.3223  |                                     |
| 832.8496                                       | 871.1152  | 951.1351  |                                     |
| 982.5460                                       | 994.8081  | 1013.2079 |                                     |
| 1021.1006                                      | 1030.2204 | 1041.7092 |                                     |
| 1077.2955                                      | 1123.9040 | 1126.5002 |                                     |
| 1146.8755                                      | 1175.3755 | 1185.3710 |                                     |
| 1255.1819                                      | 1294.4148 | 1301.0087 |                                     |
| 1314.5768                                      | 1319.3340 | 1377.9858 |                                     |
| 1378.6504                                      | 1384.8041 | 1415.2775 |                                     |
| 1419.7013                                      | 1420.8694 | 1429.7045 |                                     |
| 1437.3935                                      | 1478.9042 | 1484.3145 |                                     |
| 1489.7118                                      | 1492.5222 | 1500.4594 |                                     |
| 1503.0273                                      | 1506.2080 | 1506.8017 |                                     |
| 1509.5996                                      | 1517.2991 | 1631.3108 |                                     |
| 3056.2972                                      | 3061.7896 | 3066.3490 |                                     |
| 3067.7734                                      | 3070.9859 | 3072.3121 |                                     |
| 3087.5461                                      | 3091.1536 | 3094.2998 |                                     |
| 3103.4900                                      | 3132.4187 | 3134.5974 |                                     |
| 3136.5123                                      | 3139.2455 | 3140.2103 |                                     |
| 3148.5266                                      | 3163.0258 | 3196.6839 |                                     |
| Zero-point correction (Hartree): 0.260987      |           |           |                                     |
| diC2H5CH3CH_COO.ppppRS                         |           |           |                                     |
| ~~~~~                                          |           |           |                                     |
| E(RM062X/Aug-CC-pVTZ) (Hartree): -504.06523527 |           |           |                                     |
| Electronic state : 1-A                         |           |           |                                     |
| Cartesian coordinates (Angs):                  |           |           |                                     |
| C                                              | 0.085599  | 0.020211  | -0.562948                           |
| O                                              | 0.739058  | -0.073123 | -1.626717                           |
| O                                              | 1.985795  | -0.643073 | -1.609116                           |
| C                                              | -1.263235 | 0.657595  | -0.741419                           |
| C                                              | -2.424014 | -0.339115 | -0.521894                           |
| C                                              | -1.397281 | 1.920352  | 0.111648                            |
| H                                              | -1.298877 | 0.949627  | -1.791372                           |
| C                                              | -2.797539 | -0.668531 | 0.919915                            |
| H                                              | -3.295263 | 0.104449  | -1.008140                           |
| H                                              | -2.205088 | -1.257504 | -1.070460                           |
| H                                              | -0.657357 | 2.664197  | -0.179883                           |
| H                                              | -1.268832 | 1.713740  | 1.173339                            |
| H                                              | -2.390192 | 2.348766  | -0.028169                           |
| H                                              | -3.031925 | 0.231748  | 1.487390                            |
| H                                              | -2.011046 | -1.205765 | 1.446138                            |
| H                                              | -3.684543 | -1.300625 | 0.931726                            |
| C                                              | 0.592502  | -0.502729 | 0.742362                            |
| C                                              | 1.969339  | 0.048690  | 1.154964                            |
| C                                              | 0.600897  | -2.039210 | 0.695498                            |
| H                                              | -0.129900 | -0.175048 | 1.491074                            |
| C                                              | 2.131543  | 1.536806  | 0.882117                            |
| H                                              | 2.072877  | -0.153269 | 2.223601                            |
| H                                              | 2.740772  | -0.504903 | 0.628506                            |
| H                                              | -0.390791 | -2.446908 | 0.498973                            |
| H                                              | 0.941862  | -2.419093 | 1.658364                            |
| H                                              | 1.283549  | -2.371755 | -0.082929                           |
| H                                              | 1.342861  | 2.121518  | 1.360328                            |
| H                                              | 2.109302  | 1.727605  | -0.192493                           |
| H                                              | 3.086912  | 1.898377  | 1.259215                            |
| Rotational constants (GHz):                    |           |           | 1.3828500    0.7871300    0.7585400 |
| Vibrational harmonic frequencies (cm-1):       |           |           |                                     |
| 61.7222                                        | 75.7789   | 103.4037  |                                     |
| 130.3856                                       | 172.9813  | 201.0026  |                                     |
| 218.0720                                       | 230.8734  | 248.4085  |                                     |
| 250.7566                                       | 275.1638  | 277.3860  |                                     |
| 304.3354                                       | 311.5624  | 338.4489  |                                     |
| 368.2223                                       | 427.6573  | 438.4489  |                                     |
| 547.0141                                       | 620.5521  | 733.4679  |                                     |
| 743.8898                                       | 787.2278  | 818.0133  |                                     |
| 837.4945                                       | 882.3531  | 956.5399  |                                     |
| 983.2069                                       | 987.1406  | 1017.7469 |                                     |
| 1020.4341                                      | 1032.5938 | 1040.4038 |                                     |
| 1079.9562                                      | 1114.5864 | 1140.7967 |                                     |
| 1144.1399                                      | 1164.4157 | 1188.7379 |                                     |
| 1258.1676                                      | 1301.1465 | 1310.1977 |                                     |
| 1325.3100                                      | 1326.6564 | 1371.8929 |                                     |
| 1376.2127                                      | 1386.3131 | 1394.1434 |                                     |
| 1410.3097                                      | 1414.6762 | 1421.2375 |                                     |
| 1433.2958                                      | 1482.4403 | 1487.0396 |                                     |
| 1495.0282                                      | 1496.0012 | 1497.9093 |                                     |
| 1506.3663                                      | 1510.9403 | 1513.3539 |                                     |
| 1517.2916                                      | 1523.4079 | 1635.2720 |                                     |
| 3051.8102                                      | 3057.9374 | 3063.2691 |                                     |
| 3065.8774                                      | 3066.7900 | 3075.8264 |                                     |
| 3090.2551                                      | 3091.3240 | 3096.0174 |                                     |
| 3115.5845                                      | 3132.7514 | 3134.8243 |                                     |
| 3136.1654                                      | 3138.9476 | 3147.7610 |                                     |
| 3153.7743                                      | 3160.1015 | 3165.1885 |                                     |
| Zero-point correction (Hartree): 0.261110      |           |           |                                     |

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dic2H5CH3CH_COO.ppttRS
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E(RM062X/Aug-CC-pVTZ) (Hartree): -504.06371614
Electronic state : 1-A
Cartesian coordinates (Angs):
C -0.211524 0.649979 0.258170
O 0.067655 1.865233 0.364854
O 1.292976 2.322774 -0.048862
C -1.587866 0.298887 0.748659
C -2.573212 0.104272 -0.423546
C -1.562297 -0.894983 1.704469
H -1.931836 1.174324 1.300483
C -2.314153 -1.083807 -1.343500
H -3.564075 0.000860 0.023710
H -2.592032 1.024368 -1.010148
H -0.958856 -0.677841 2.584910
H -1.164185 -1.793941 1.236553
H -2.577606 -1.113465 2.035052
H -2.249866 -2.019762 -0.788092
H -1.395745 -0.964441 -1.916599
H -3.131209 -1.183502 -2.056545
C 0.751199 -0.351336 -0.287834
C 1.902664 -0.553354 0.719321
C 1.245681 0.004588 -1.698525
H 0.204394 -1.293503 -0.346355
C 2.870858 -1.633892 0.256441
H 2.413544 0.399633 0.845858
H 1.479786 -0.834844 1.686489
H 0.457671 0.466598 -2.293813
H 1.562963 -0.905440 -2.206379
H 2.069958 0.708146 -1.647108
H 3.385043 -1.338904 -0.657232
H 2.351169 -2.574409 0.062443
H 3.627724 -1.820067 1.016901
Rotational constants (GHz): 1.2939700 0.7821900 0.6913300
Vibrational harmonic frequencies (cm-1):
46.4456 67.8354 98.6759
102.0115 141.9205 171.4552
190.4796 217.2082 240.1120
260.6985 272.6846 274.3920
286.0247 305.7019 333.1349
363.6779 414.6310 444.5879
540.1840 633.6887 731.4899
770.0297 790.9607 819.0966
835.8740 879.6837 951.9860
977.8882 986.8809 1000.0233
1015.2552 1027.6507 1058.1111
1083.1183 1113.8783 1126.0212
1152.1922 1168.8228 1182.4690
1251.3926 1293.1880 1304.3811
1319.5937 1345.3955 1363.7211
1374.8165 1383.9902 1405.7050
1411.6216 1418.2355 1420.0721
1431.0896 1484.1293 1487.5841
1493.4574 1500.9389 1503.0180
1505.6274 1506.6644 1512.5619
1513.0203 1518.2639 1635.7056
3057.6303 3059.8046 3061.9359
3069.0488 3070.4944 3071.7036
3088.0251 3091.7127 3098.8738
3118.9135 3131.7775 3135.4682
3138.0681 3139.7930 3143.7512
3145.7936 3148.9881 3183.7834
Zero-point correction (Hartree): 0.260660

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dic2H5CH3CH_COO.ppttRS
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E(RM062X/Aug-CC-pVTZ) (Hartree): -504.06082019
Electronic state : 1-A
Cartesian coordinates (Angs):
C       0.217312     -0.709280      0.151986
O       0.435437     -1.883419     -0.239438
O      -0.568740     -2.600574     -0.839374
C       1.443597     -0.102883      0.796613
C       2.521442      0.174145     -0.272007
C       1.189138      1.099654      1.700289
H       1.837355     -0.907026      1.422340
C       2.097828      1.137582     -1.373171
H       3.400833      0.562962      0.245225
H       2.807299     -0.778769     -0.716829
H       0.359158      0.925178      2.384277
H       0.981387      2.006877      1.139019
H       2.081881      1.276371      2.299127
H       1.829064      2.117239     -0.978170
H       1.244164      0.747365     -1.930800
H       2.911379      1.282502     -2.082127
C      -1.153449     -0.153243     -0.034355
C      -1.296656      1.368362     -0.110507
C      -2.037205     -0.773965      1.066470
H      -1.477405     -0.600950     -0.979184
C      -2.587431      1.761617     -0.822568
H      -1.291645      1.798751      0.891466
H      -0.453768      1.802595     -0.648489
H      -3.079074     -0.513970      0.889542
H      -1.752117     -0.391069      2.047443
H      -1.947053     -1.857756      1.051396
H      -3.463613      1.363747     -0.311772
H      -2.595784      1.381297     -1.844189
H      -2.693095      2.844670     -0.864272
Rotational constants (GHz):      1.1427100      0.8844300      0.6824800
Vibrational harmonic frequencies (cm-1):

```



|           |           |           |
|-----------|-----------|-----------|
| 62.2939   | 77.6238   | 94.0854   |
| 131.9705  | 171.2865  | 183.4126  |
| 205.0706  | 231.4038  | 244.6029  |
| 269.6031  | 275.7696  | 286.9609  |
| 299.3526  | 313.6255  | 340.6854  |
| 368.0141  | 426.3201  | 480.6408  |
| 521.0538  | 628.6271  | 718.1618  |
| 736.4372  | 794.6789  | 802.5334  |
| 846.4412  | 907.5951  | 950.9125  |
| 974.4139  | 988.9909  | 993.0674  |
| 1018.8157 | 1030.4296 | 1047.4114 |
| 1078.0414 | 1100.9861 | 1144.4766 |
| 1153.9382 | 1186.8689 | 1202.4208 |
| 1285.2825 | 1292.7972 | 1310.3581 |
| 1316.0771 | 1334.3508 | 1339.7658 |
| 1376.6502 | 1383.2107 | 1393.3743 |
| 1399.7746 | 1416.6077 | 1417.7211 |
| 1423.6687 | 1485.2489 | 1489.4952 |
| 1495.3398 | 1499.7313 | 1504.6962 |
| 1506.6368 | 1509.4425 | 1513.7908 |
| 1516.8882 | 1523.4943 | 1592.5951 |
| 3048.3898 | 3058.3310 | 3063.9202 |
| 3065.5750 | 3068.9257 | 3071.7572 |
| 3075.7599 | 3081.6149 | 3110.4587 |
| 3118.3957 | 3130.5914 | 3137.5428 |
| 3139.4354 | 3140.0643 | 3140.8887 |
| 3145.0956 | 3164.2555 | 3167.3611 |

Zero-point correction (Hartree): 0.260951

dic2H5CH3CH\_COO.ptmmRS

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E(RM062X/Aug-CC-pVTZ) (Hartree): -504.06237985

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-0.284011	-0.751211	-0.030029
O	-0.728132	-1.700100	-0.727125
O	-2.073318	-1.942569	-0.761359
C	1.220391	-0.675972	-0.058380
C	1.734767	0.614193	-0.712705
C	1.837013	-0.919301	1.327436
H	1.517860	-1.506199	-0.702258
C	3.255455	0.640939	-0.812241
H	1.306744	0.689817	-1.713289
H	1.385179	1.484141	-0.153903
H	1.292878	-1.687744	1.875797
H	1.854643	-0.011325	1.927115
H	2.863018	-1.262364	1.208850
H	3.626945	-0.251265	-1.318774
H	3.721505	0.688029	0.171065
H	3.586795	1.510116	-1.377860
C	-1.257862	0.080432	0.736437
C	-2.110252	0.958572	-0.214125
C	-0.679817	0.879921	1.898859
H	-1.960097	-0.670001	1.116092
C	-1.386837	2.150261	-0.826573
H	-2.520179	0.315875	-0.989837
H	-2.952665	1.313642	0.382239
H	0.117528	1.556546	1.596430
H	-0.296060	0.231962	2.684006
H	-1.476931	1.486706	2.328898
H	-0.604921	1.834384	-1.515681
H	-0.933703	2.792451	-0.070085
H	-2.090030	2.759580	-1.393010

Rotational constants (GHz): 1.2623800 0.7940200 0.6835500

Vibrational harmonic frequencies (cm-1):

60.5035	77.7703	103.0414
126.6189	158.4244	201.2013
214.5061	235.2833	255.2339
277.8385	284.2702	305.0932
318.9823	325.1962	359.9072
374.4744	386.5242	481.8082
533.6937	658.5516	672.0461
747.1039	799.2792	806.7788
846.8337	878.0311	961.7942
977.9415	989.4818	1009.1762
1017.2606	1022.1237	1052.3654
1075.8633	1101.3715	1146.9412
1150.2321	1178.5075	1191.8364
1273.5720	1290.1652	1294.1510
1325.4554	1329.8486	1360.8874
1365.1247	1381.5736	1386.3401
1411.9795	1415.1944	1417.5629
1422.4331	1483.9512	1493.2511
1496.3661	1502.3453	1504.7049
1510.1481	1510.9350	1515.6279
1517.1080	1526.6402	1595.7749
3037.1498	3063.0819	3066.6610
3067.5724	3072.7609	3073.3139
3073.9491	3076.9542	3109.4564
3124.5910	3134.6022	3139.0452
3139.5466	3142.0919	3146.9219
3150.9506	3156.1017	3159.2524

Zero-point correction (Hartree): 0.261144

dic2H5CH3CH_COO.ptmpRS

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E(RM062X/Aug-CC-pVTZ) (Hartree): -504.06390729

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.274789 | -0.627557 | -0.159690 |
| O | -0.831933 | -1.327279 | -1.041067 |
| O | -2.188521 | -1.514386 | -1.023644 |

|                                                |           |           |                     |
|------------------------------------------------|-----------|-----------|---------------------|
| C                                              | 1.215243  | -0.534033 | -0.349447           |
| C                                              | 1.704192  | 0.920453  | -0.384004           |
| C                                              | 1.977071  | -1.388242 | 0.675319            |
| H                                              | 1.392205  | -0.969235 | -1.335517           |
| C                                              | 3.167800  | 1.024652  | -0.796135           |
| H                                              | 1.086985  | 1.485526  | -1.085708           |
| H                                              | 1.568010  | 1.379281  | 0.596860            |
| H                                              | 1.496247  | -2.355856 | 0.814768            |
| H                                              | 2.047007  | -0.891755 | 1.641445            |
| H                                              | 2.987904  | -1.570357 | 0.315364            |
| H                                              | 3.338335  | 0.525932  | -1.751269           |
| H                                              | 3.825474  | 0.569838  | -0.056544           |
| H                                              | 3.463570  | 2.066777  | -0.904579           |
| C                                              | -1.098331 | 0.002883  | 0.914584            |
| C                                              | -1.499846 | 1.441659  | 0.516633            |
| C                                              | -0.435216 | -0.007301 | 2.290204            |
| H                                              | -2.009239 | -0.596332 | 0.935313            |
| C                                              | -2.157860 | 1.570194  | -0.850606           |
| H                                              | -2.185459 | 1.789638  | 1.291787            |
| H                                              | -0.619818 | 2.085535  | 0.575169            |
| H                                              | 0.452248  | 0.624128  | 2.326034            |
| H                                              | -0.158039 | -1.012844 | 2.602604            |
| H                                              | -1.145209 | 0.384604  | 3.017754            |
| H                                              | -3.058965 | 0.964911  | -0.908072           |
| H                                              | -1.496786 | 1.226369  | -1.648295           |
| H                                              | -2.410419 | 2.610918  | -1.050571           |
| Rotational constants (GHz):                    |           |           | 1.3113300           |
| Vibrational harmonic frequencies (cm-1):       |           |           | 0.7555000 0.7139100 |
| 62.2486                                        | 67.6371   | 112.1489  |                     |
| 130.5931                                       | 152.5656  | 189.6116  |                     |
| 198.2015                                       | 238.5200  | 240.8497  |                     |
| 253.2231                                       | 272.0669  | 290.7518  |                     |
| 295.3503                                       | 309.9342  | 354.5781  |                     |
| 363.9049                                       | 385.6053  | 459.3169  |                     |
| 519.2616                                       | 654.1706  | 701.0401  |                     |
| 726.1248                                       | 795.9633  | 814.8191  |                     |
| 855.8883                                       | 882.4790  | 959.8072  |                     |
| 977.1929                                       | 983.0461  | 1003.6901 |                     |
| 1017.6579                                      | 1046.7854 | 1058.4164 |                     |
| 1074.2048                                      | 1115.9600 | 1128.4464 |                     |
| 1153.0527                                      | 1181.3097 | 1194.4337 |                     |
| 1279.2086                                      | 1293.7090 | 1324.1893 |                     |
| 1330.0139                                      | 1337.6544 | 1359.5398 |                     |
| 1366.0232                                      | 1380.9997 | 1392.0385 |                     |
| 1411.4590                                      | 1416.7143 | 1418.3897 |                     |
| 1427.0104                                      | 1482.3295 | 1488.9790 |                     |
| 1496.2619                                      | 1497.4420 | 1500.5834 |                     |
| 1503.2214                                      | 1507.5571 | 1512.9794 |                     |
| 1513.0577                                      | 1519.6871 | 1608.4240 |                     |
| 3059.1397                                      | 3062.4923 | 3065.0557 |                     |
| 3065.9603                                      | 3069.6600 | 3071.1880 |                     |
| 3075.8192                                      | 3088.3466 | 3103.6064 |                     |
| 3105.2709                                      | 3127.0858 | 3134.8257 |                     |
| 3138.8103                                      | 3141.6111 | 3146.9222 |                     |
| 3148.1379                                      | 3157.3917 | 3163.6356 |                     |
| Zero-point correction (Hartree):               |           |           | 0.260880            |
| diC2H5CH3CH_COO.ptmtrS                         |           |           |                     |
| ~~~~~                                          |           |           |                     |
| E(RM062X/Aug-CC-pVT2) (Hartree): -504.06533974 |           |           |                     |
| Electronic state : 1-A                         |           |           |                     |
| Cartesian coordinates (Angs):                  |           |           |                     |
| C                                              | 0.027319  | 0.725143  | 0.217487            |
| O                                              | 0.376237  | 1.880085  | -0.137158           |
| O                                              | 1.712396  | 2.180720  | -0.199027           |
| C                                              | -1.456536 | 0.507325  | 0.152729            |
| C                                              | -1.784331 | -0.515097 | -0.949137           |
| C                                              | -2.079324 | 0.142053  | 1.505658            |
| H                                              | -1.865639 | 1.470756  | -0.158833           |
| C                                              | -3.284179 | -0.658793 | -1.175809           |
| H                                              | -1.301116 | -0.196621 | -1.874931           |
| H                                              | -1.356842 | -1.485467 | -0.689336           |
| H                                              | -1.654037 | 0.738751  | 2.311923            |
| H                                              | -1.941791 | -0.910856 | 1.744024            |
| H                                              | -3.148827 | 0.341953  | 1.476145            |
| H                                              | -3.738860 | 0.310275  | -1.386253           |
| H                                              | -3.781609 | -1.082397 | -0.304187           |
| H                                              | -3.483851 | -1.314013 | -2.022042           |
| C                                              | 1.092281  | -0.258599 | 0.547066            |
| C                                              | 1.721296  | -0.726133 | -0.791693           |
| C                                              | 0.679761  | -1.427990 | 1.431154            |
| H                                              | 1.857335  | 0.342489  | 1.046253            |
| C                                              | 3.167872  | -1.162464 | -0.609632           |
| H                                              | 1.116424  | -1.544482 | -1.190384           |
| H                                              | 1.692913  | 0.096756  | -1.505136           |
| H                                              | -0.085308 | -2.049353 | 0.966906            |
| H                                              | 0.313765  | -1.096401 | 2.401330            |
| H                                              | 1.549572  | -2.058999 | 1.607562            |
| H                                              | 3.263224  | -1.964294 | 0.122934            |
| H                                              | 3.765920  | -0.315498 | -0.273831           |
| H                                              | 3.584703  | -1.521703 | -1.549610           |
| Rotational constants (GHz):                    |           |           | 1.4084400           |
| Vibrational harmonic frequencies (cm-1):       |           |           | 0.7051900 0.6259600 |
| 51.6497                                        | 73.4292   | 85.7199   |                     |
| 102.0352                                       | 160.1107  | 189.4748  |                     |
| 203.9773                                       | 241.6951  | 248.5154  |                     |
| 259.5674                                       | 275.5915  | 295.1397  |                     |
| 306.0581                                       | 314.3678  | 361.4159  |                     |
| 364.9685                                       | 408.2131  | 433.1499  |                     |
| 529.3313                                       | 663.8570  | 689.2082  |                     |
| 777.4030                                       | 780.3422  | 796.2103  |                     |
| 852.9839                                       | 882.8395  | 957.6748  |                     |

|           |           |           |
|-----------|-----------|-----------|
| 979.2812  | 988.8784  | 1011.6181 |
| 1019.8438 | 1028.8819 | 1059.9590 |
| 1076.5284 | 1107.7306 | 1137.3874 |
| 1153.7703 | 1185.4193 | 1194.7078 |
| 1281.3750 | 1290.4283 | 1324.7792 |
| 1325.9961 | 1331.2434 | 1362.3673 |
| 1369.0825 | 1385.3828 | 1393.8183 |
| 1409.7293 | 1413.6438 | 1417.7344 |
| 1422.3701 | 1477.0283 | 1489.2122 |
| 1496.4427 | 1498.8202 | 1502.4333 |
| 1503.8532 | 1505.8636 | 1512.9129 |
| 1517.1382 | 1521.1350 | 1604.4901 |
| 3052.4225 | 3062.0713 | 3063.4899 |
| 3065.1902 | 3066.2372 | 3072.6285 |
| 3074.3113 | 3076.7656 | 3104.0510 |
| 3115.1871 | 3134.1626 | 3135.8299 |
| 3140.5821 | 3140.6872 | 3143.7701 |
| 3145.8151 | 3147.8048 | 3157.9510 |

Zero-point correction (Hartree): 0.260862

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E(RM062X/Aug-CC-pVTZ) (Hartree): -504.06179483

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-0.036285	-0.292913	0.294193
O	-0.447186	-1.126905	1.130468
O	-1.700010	-1.667915	1.019099
C	1.374233	0.162798	0.541448
C	2.303711	-0.511263	-0.484930
C	1.488713	1.687389	0.526343
H	1.644543	-0.205812	1.532624
C	3.777412	-0.219622	-0.228915
H	2.133675	-1.588806	-0.446710
H	2.033128	-0.183002	-1.491442
H	0.781403	2.142257	1.218818
H	1.304191	2.090480	-0.470768
H	2.489836	1.987510	0.828861
H	4.051918	-0.477085	0.794915
H	4.014562	0.831123	-0.388599
H	4.404067	-0.804150	-0.900510
C	-0.817250	0.176325	-0.894247
C	-1.766650	1.343182	-0.534258
C	-1.517641	-0.939033	-1.677913
H	-0.061249	0.609152	-1.553873
C	-2.798060	1.059596	0.549570
H	-1.166012	2.207238	-0.244562
H	-2.268822	1.617323	-1.465266
H	-2.447331	-1.233235	-1.205855
H	-0.893349	-1.829172	-1.750101
H	-1.712583	-0.572641	-2.686496
H	-2.321381	0.804816	1.495633
H	-3.438637	0.221608	0.287641
H	-3.419486	1.942195	0.701420

Rotational constants (GHz): 1.6237200 0.6792700 0.6283500

Vibrational harmonic frequencies (cm-1):

55.3090	61.8621	70.5513
124.2007	150.0145	169.3392
208.6408	214.4659	238.5267
258.8197	269.6878	291.5021
306.3155	315.8912	343.8169
354.1739	370.7366	489.1864
511.2142	656.8428	714.7167
762.3055	784.3926	800.4598
855.2030	874.6685	957.4101
975.0956	989.2469	1008.9922
1017.7782	1039.9332	1041.7690
1077.3256	1122.4447	1128.8138
1153.1954	1182.0773	1191.4522
1263.3218	1290.5353	1299.1139
1317.4848	1324.6784	1365.4940
1379.3381	1381.0298	1411.5415
1413.5483	1417.4398	1429.3254
1438.3196	1479.5784	1483.9544
1487.5969	1492.8588	1500.2001
1501.2495	1505.6408	1507.2339
1509.1844	1519.1740	1639.2844
3052.7090	3056.8224	3062.6805
3066.0241	3066.1760	3070.8765
3072.4234	3081.3219	3094.8298
3099.4501	3132.4149	3134.9481
3135.1787	3137.0607	3142.5590
3152.9705	3162.8469	3196.1257

Zero-point correction (Hartree): 0.260652

diC2H5CH3CH_COO.ptppRS

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E(RM062X/Aug-CC-pVTZ) (Hartree): -504.06805438

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.115090  | -0.146184 | -0.433740 |
| O | 0.606580  | -0.433642 | -1.547176 |
| O | 1.892664  | -0.907908 | -1.615905 |
| C | -1.301158 | 0.347011  | -0.491964 |
| C | -2.223931 | -0.603398 | 0.288332  |
| C | -1.384450 | 1.792260  | 0.008208  |
| H | -1.590606 | 0.321774  | -1.544199 |
| C | -3.694896 | -0.222014 | 0.173935  |
| H | -2.081203 | -1.616544 | -0.092550 |
| H | -1.927993 | -0.616620 | 1.340361  |
| H | -0.675296 | 2.428924  | -0.518749 |
| H | -1.175040 | 1.854292  | 1.077155  |

|                                                |           |           |           |
|------------------------------------------------|-----------|-----------|-----------|
| H                                              | -2.383377 | 2.188030  | -0.163602 |
| H                                              | -3.993013 | -0.133551 | -0.871649 |
| H                                              | -3.904960 | 0.726229  | 0.666276  |
| H                                              | -4.323316 | -0.980190 | 0.638257  |
| C                                              | 0.847880  | -0.333976 | 0.855569  |
| C                                              | 2.221445  | 0.355207  | 0.917827  |
| C                                              | 0.967924  | -1.839520 | 1.144208  |
| H                                              | 0.213055  | 0.117334  | 1.621519  |
| C                                              | 2.229885  | 1.750595  | 0.311934  |
| H                                              | 2.494252  | 0.400777  | 1.974798  |
| H                                              | 2.948253  | -0.268910 | 0.406905  |
| H                                              | 1.517562  | -2.320063 | 0.337820  |
| H                                              | -0.008911 | -2.310396 | 1.249038  |
| H                                              | 1.514252  | -1.974630 | 2.077352  |
| H                                              | 1.481078  | 2.394933  | 0.777318  |
| H                                              | 2.032918  | 1.697146  | -0.760473 |
| H                                              | 3.201666  | 2.223971  | 0.443210  |
| Rotational constants (GHz):                    |           |           |           |
| Vibrational harmonic frequencies (cm-1):       |           |           |           |
| 57.9347                                        | 83.1896   | 93.9086   |           |
| 117.2022                                       | 159.6312  | 189.2590  |           |
| 208.5332                                       | 216.7009  | 226.6340  |           |
| 249.8469                                       | 258.0290  | 279.8980  |           |
| 305.6838                                       | 315.2793  | 344.3110  |           |
| 368.1454                                       | 426.8328  | 436.2371  |           |
| 487.9277                                       | 656.2269  | 733.9031  |           |
| 744.7568                                       | 791.2826  | 817.8450  |           |
| 857.8447                                       | 885.7946  | 960.3278  |           |
| 973.5025                                       | 985.4102  | 1005.5711 |           |
| 1021.8517                                      | 1031.5863 | 1047.4453 |           |
| 1077.7859                                      | 1111.4252 | 1141.5704 |           |
| 1147.6091                                      | 1185.1180 | 1191.4593 |           |
| 1261.7952                                      | 1293.6416 | 1303.3407 |           |
| 1318.5403                                      | 1324.1026 | 1360.7651 |           |
| 1372.2222                                      | 1383.9554 | 1391.6426 |           |
| 1409.6858                                      | 1411.7378 | 1415.8850 |           |
| 1432.0269                                      | 1483.5823 | 1488.9782 |           |
| 1494.8868                                      | 1496.9221 | 1497.8882 |           |
| 1503.3192                                      | 1507.9467 | 1514.2549 |           |
| 1517.0846                                      | 1519.1028 | 1642.9436 |           |
| 3052.2885                                      | 3055.7122 | 3061.2772 |           |
| 3065.0052                                      | 3066.5443 | 3067.8116 |           |
| 3073.0763                                      | 3081.4802 | 3099.0985 |           |
| 3116.5638                                      | 3135.2899 | 3136.2752 |           |
| 3138.2137                                      | 3139.1072 | 3143.7829 |           |
| 3153.7821                                      | 3160.1040 | 3162.9224 |           |
| Zero-point correction (Hartree): 0.260732      |           |           |           |
| diC2H5CH3CH_COO.ptptRS                         |           |           |           |
| ~~~~~                                          |           |           |           |
| E(RM062X/Aug-CC-pVT2) (Hartree): -504.06575424 |           |           |           |
| Electronic state : 1-A                         |           |           |           |
| Cartesian coordinates (Angs):                  |           |           |           |
| C                                              | 0.076272  | 0.565746  | -0.257160 |
| O                                              | -0.193918 | 1.728430  | -0.629589 |
| O                                              | -1.453573 | 2.239159  | -0.431294 |
| C                                              | 1.488763  | 0.139258  | -0.522961 |
| C                                              | 2.220319  | -0.077134 | 0.812640  |
| C                                              | 1.510931  | -1.102818 | -1.418610 |
| H                                              | 1.968810  | 0.966388  | -1.049001 |
| C                                              | 3.695035  | -0.414628 | 0.629914  |
| H                                              | 2.126394  | 0.832379  | 1.409154  |
| H                                              | 1.726280  | -0.874820 | 1.372980  |
| H                                              | 0.926955  | -0.942768 | -2.324176 |
| H                                              | 1.109993  | -1.974099 | -0.898673 |
| H                                              | 2.532347  | -1.329979 | -1.716834 |
| H                                              | 4.192518  | 0.337637  | 0.016341  |
| H                                              | 3.830207  | -1.383692 | 0.151891  |
| H                                              | 4.201301  | -0.449259 | 1.593144  |
| C                                              | -0.913910 | -0.334191 | 0.404633  |
| C                                              | -2.044983 | -0.696372 | -0.578070 |
| C                                              | -1.415562 | 0.259590  | 1.728471  |
| H                                              | -0.374667 | -1.256493 | 0.634410  |
| C                                              | -3.027573 | -1.691284 | 0.025713  |
| H                                              | -2.550085 | 0.220983  | -0.872925 |
| H                                              | -1.597855 | -1.129290 | -1.476192 |
| H                                              | -2.081061 | 1.096120  | 1.538976  |
| H                                              | -0.582351 | 0.611778  | 2.337619  |
| H                                              | -1.935779 | -0.512155 | 2.293115  |
| H                                              | -3.589254 | -1.246737 | 0.845887  |
| H                                              | -2.514211 | -2.575962 | 0.408372  |
| H                                              | -3.745373 | -2.019747 | -0.724443 |
| Rotational constants (GHz):                    |           |           |           |
| Vibrational harmonic frequencies (cm-1):       |           |           |           |
| 54.1827                                        | 67.7696   | 68.5884   |           |
| 79.6098                                        | 123.1150  | 168.8419  |           |
| 187.1617                                       | 197.7309  | 219.6788  |           |
| 244.0355                                       | 260.5129  | 264.5268  |           |
| 298.3247                                       | 306.6240  | 349.0940  |           |
| 354.6711                                       | 409.9963  | 431.3289  |           |
| 494.9450                                       | 656.4193  | 731.3993  |           |
| 771.0282                                       | 787.0414  | 814.9157  |           |
| 855.3523                                       | 881.5538  | 955.4512  |           |
| 971.2271                                       | 980.5365  | 995.5724  |           |
| 1007.5016                                      | 1035.7553 | 1060.5893 |           |
| 1078.6681                                      | 1115.2127 | 1128.8154 |           |
| 1150.9409                                      | 1182.2862 | 1190.5063 |           |
| 1254.6554                                      | 1293.2472 | 1297.1532 |           |
| 1323.1062                                      | 1349.9938 | 1361.1752 |           |
| 1365.8731                                      | 1383.4720 | 1397.5553 |           |
| 1410.8905                                      | 1412.0688 | 1415.6936 |           |
| 1428.9865                                      | 1487.5485 | 1488.9349 |           |

|           |           |           |
|-----------|-----------|-----------|
| 1496.1534 | 1498.9556 | 1501.7545 |
| 1505.3922 | 1507.2766 | 1514.1288 |
| 1515.9663 | 1517.7804 | 1643.2708 |
| 3054.0699 | 3056.7831 | 3060.1770 |
| 3062.6764 | 3066.6134 | 3068.2603 |
| 3071.0938 | 3081.7642 | 3098.1281 |
| 3120.0754 | 3133.8592 | 3135.4551 |
| 3136.4026 | 3141.0290 | 3143.2701 |
| 3146.9324 | 3153.1374 | 3179.4603 |

Zero-point correction (Hartree): 0.260193

dic2H5CH3CH\_COO.ptttRS

E(RM062X/Aug-CC-pVT2) (Hartree): -504.06409417

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.028385 | -0.775674 | -0.135742 |
| O | -0.105595 | -1.990996 | -0.447080 |
| O | -1.320136 | -2.518395 | -0.797494 |
| C | 1.351446  | -0.366073 | 0.296585  |
| C | 1.998628  | 0.681440  | -0.627516 |
| C | 1.343266  | 0.074140  | 1.765215  |
| H | 1.944378  | -1.279977 | 0.219325  |
| C | 3.518831  | 0.669215  | -0.512692 |
| H | 1.715675  | 0.477402  | -1.662060 |
| H | 1.620415  | 1.674081  | -0.384053 |
| H | 0.921278  | -0.700532 | 2.404415  |
| H | 0.765716  | 0.986964  | 1.905358  |
| H | 2.361666  | 0.266594  | 2.098410  |
| H | 3.920227  | -0.305628 | -0.790230 |
| H | 3.846429  | 0.891089  | 0.502581  |
| H | 3.961407  | 1.414722  | -1.171406 |
| C | -1.273756 | 0.042738  | -0.150994 |
| C | -1.077307 | 1.544667  | -0.352079 |
| C | -2.055293 | -0.303913 | 1.132815  |
| H | -1.849873 | -0.367979 | -0.984695 |
| C | -2.408832 | 2.280988  | -0.455977 |
| H | -0.494034 | 1.971278  | 0.466298  |
| H | -0.508147 | 1.712539  | -1.267306 |
| H | -1.600845 | 0.174618  | 2.001399  |
| H | -2.080505 | -1.382613 | 1.274031  |
| H | -3.081889 | 0.044598  | 1.044446  |
| H | -2.953355 | 2.260721  | 0.486714  |
| H | -3.042467 | 1.827745  | -1.219567 |
| H | -2.251815 | 3.324333  | -0.724752 |

Rotational constants (GHz): 1.1926100 0.7911600 0.6001200

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| 64.5561   | 74.2958   | 94.6467   |
| 124.9204  | 144.7309  | 170.5192  |
| 202.6404  | 213.6415  | 225.9371  |
| 233.5479  | 251.5821  | 275.7814  |
| 306.2866  | 316.9588  | 347.5819  |
| 360.2571  | 419.4606  | 438.9420  |
| 513.8825  | 655.4633  | 734.8060  |
| 740.3608  | 791.0820  | 807.4320  |
| 867.7885  | 907.3765  | 963.3947  |
| 971.5658  | 981.7292  | 988.9686  |
| 1008.4171 | 1019.6335 | 1062.5559 |
| 1071.0614 | 1113.9223 | 1139.0239 |
| 1157.5381 | 1190.1955 | 1199.7270 |
| 1285.7632 | 1304.1085 | 1317.3565 |
| 1328.0445 | 1334.5365 | 1342.0123 |
| 1364.4980 | 1387.2344 | 1393.3180 |
| 1398.8950 | 1411.2365 | 1415.8517 |
| 1419.2429 | 1483.9621 | 1491.7495 |
| 1496.7890 | 1499.7918 | 1500.4222 |
| 1502.3627 | 1509.2145 | 1511.9508 |
| 1513.9450 | 1522.5372 | 1606.0150 |
| 3058.0821 | 3064.4261 | 3065.6373 |
| 3066.5294 | 3069.1867 | 3070.8843 |
| 3073.7776 | 3076.1307 | 3106.2615 |
| 3115.7100 | 3135.6947 | 3138.9087 |
| 3141.1821 | 3142.0655 | 3146.1013 |
| 3147.6589 | 3152.3912 | 3159.7405 |

Zero-point correction (Hartree): 0.260676

Population analysis as 298K (%)

Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)

| Compound                           | Qtot      | Erel | Erel2 | n*Q*MB    | %     |
|------------------------------------|-----------|------|-------|-----------|-------|
| TS.dic2H5CH3CH_COO.14Hshift.mpmtrS | 3.819e+43 | 0.00 | 0.00  | 3.819e+43 | 25.5  |
| TS.dic2H5CH3CH_COO.14Hshift.mmmtrS | 5.074e+43 | 0.24 | 0.24  | 3.363e+43 | 22.5  |
| TS.dic2H5CH3CH_COO.14Hshift.mtmtrS | 3.830e+43 | 0.35 | 0.35  | 2.132e+43 | 14.2  |
| TS.dic2H5CH3CH_COO.14Hshift.cmptRS | 6.474e+43 | 0.95 | 0.95  | 1.302e+43 | 8.7   |
| TS.dic2H5CH3CH_COO.14Hshift.ctmtRS | 5.967e+43 | 1.19 | 1.19  | 8.026e+42 | 5.36  |
| TS.dic2H5CH3CH_COO.14Hshift.cmpmRS | 3.175e+43 | 1.03 | 1.03  | 5.543e+42 | 3.7   |
| TS.dic2H5CH3CH_COO.14Hshift.cmpmRS | 3.042e+43 | 1.14 | 1.14  | 4.416e+42 | 2.95  |
| TS.dic2H5CH3CH_COO.14Hshift.mpmprS | 1.527e+43 | 0.84 | 0.84  | 3.681e+42 | 2.46  |
| TS.dic2H5CH3CH_COO.14Hshift.pmmtrS | 1.829e+43 | 1.06 | 1.06  | 3.052e+42 | 2.04  |
| TS.dic2H5CH3CH_COO.14Hshift.ctmpRS | 7.774e+43 | 1.94 | 1.94  | 2.961e+42 | 1.98  |
| TS.dic2H5CH3CH_COO.14Hshift.cmpmRS | 2.142e+43 | 1.19 | 1.19  | 2.880e+42 | 1.92  |
| TS.dic2H5CH3CH_COO.14Hshift.mtmprS | 2.982e+43 | 1.42 | 1.42  | 2.715e+42 | 1.81  |
| TS.dic2H5CH3CH_COO.14Hshift.ctptRS | 4.650e+43 | 1.80 | 1.80  | 2.234e+42 | 1.49  |
| TS.dic2H5CH3CH_COO.14Hshift.mtmprS | 6.757e+43 | 2.16 | 2.16  | 1.747e+42 | 1.17  |
| TS.dic2H5CH3CH_COO.14Hshift.ctpmRS | 5.859e+43 | 2.08 | 2.08  | 1.747e+42 | 1.17  |
| TS.dic2H5CH3CH_COO.14Hshift.pmmprS | 1.470e+43 | 1.63 | 1.63  | 9.319e+41 | 0.623 |
| TS.dic2H5CH3CH_COO.14Hshift.ctppRS | 4.160e+43 | 2.30 | 2.30  | 8.551e+41 | 0.571 |
| TS.dic2H5CH3CH_COO.14Hshift.mpmtrS | 9.033e+43 | 2.89 | 2.89  | 6.812e+41 | 0.455 |
| TS.dic2H5CH3CH_COO.14Hshift.ptmtRS | 3.839e+43 | 2.42 | 2.42  | 6.468e+41 | 0.432 |
| TS.dic2H5CH3CH_COO.14Hshift.cpptRS | 3.472e+43 | 2.58 | 2.58  | 4.473e+41 | 0.299 |
| TS.dic2H5CH3CH_COO.14Hshift.pmptrS | 3.417e+43 | 2.83 | 2.83  | 2.860e+41 | 0.191 |

```

TS.dic2H5CH3CH_COO.14Hshift.ptmpRS 2.969e+43 3.05 3.05 1.728e+41 0.115
TS.dic2H5CH3CH_COO.14Hshift.cppmRS 2.236e+43 3.06 3.06 1.272e+41 0.085
TS.dic2H5CH3CH_COO.14Hshift.mmmpRS 2.318e+43 3.48 3.48 6.455e+40 0.0431
TS.dic2H5CH3CH_COO.14Hshift.ptptRS 3.564e+43 3.81 3.81 5.745e+40 0.0384
TS.dic2H5CH3CH_COO.14Hshift.pmpmRS 1.737e+43 3.45 3.45 5.114e+40 0.0342
TS.dic2H5CH3CH_COO.14Hshift.cpppRS 2.390e+43 3.66 3.66 4.934e+40 0.033
TS.dic2H5CH3CH_COO.14Hshift.mppmRS 1.463e+43 3.44 3.44 4.397e+40 0.0294
TS.dic2H5CH3CH_COO.14Hshift.mpppRS 1.603e+43 3.93 3.93 2.112e+40 0.0141
TS.dic2H5CH3CH_COO.14Hshift.pmpmRS 1.441e+43 4.13 4.13 1.344e+40 0.00898
TS.dic2H5CH3CH_COO.14Hshift.ptpmRS 2.526e+43 4.53 4.53 1.196e+40 0.00799
TS.dic2H5CH3CH_COO.14Hshift.mtpmRS 2.925e+43 4.78 4.78 9.149e+39 0.00611
TS.dic2H5CH3CH_COO.14Hshift.ppptRS 1.547e+43 4.97 4.97 3.530e+39 0.00236
TS.dic2H5CH3CH_COO.14Hshift.ptppRS 1.873e+43 5.17 5.17 3.017e+39 0.00202
TS.dic2H5CH3CH_COO.14Hshift.pppmRS 1.202e+43 6.18 6.18 3.548e+38 0.000237
Total 1.496e+44 100

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TS.dic2H5CH3CH\_COO.14Hshift.cmpmRS

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E(RM062X/Aug-CC-pVTZ) (Hartree): -504.03694282

Electronic state : 1-A

Cartesian coordinates (Angs):

C	0.173658	0.411549	-0.155145
O	0.436516	0.780609	-1.371363
O	-0.674855	1.403981	-1.946039
C	1.393201	0.070209	0.648730
C	2.255864	-0.960422	-0.090460
C	2.191801	1.341712	0.956986
H	1.043100	-0.373119	1.583022
C	1.513595	-2.255441	-0.393685
H	2.622481	-0.511490	-1.014815
H	3.128798	-1.164534	0.532087
H	1.589918	2.076726	1.489814
H	2.541720	1.794182	0.029889
H	3.056057	1.094553	1.572645
H	0.671036	-2.077701	-1.064198
H	1.126911	-2.707087	0.521444
H	2.169510	-2.979923	-0.873551
C	-1.154071	0.610154	0.284543
H	-1.202781	1.514445	-0.713424
C	-1.339442	0.828827	1.771284
C	-2.251556	-0.263713	-0.362228
C	-2.442858	-1.593675	0.362155
H	-3.188768	0.296739	-0.352725
H	-2.001697	-0.439759	-1.405195
H	-0.644737	1.570101	2.163783
H	-1.215813	-0.087832	2.352808
H	-2.349604	1.195129	1.958501
H	-2.802506	-1.455013	1.381139
H	-1.504522	-2.149324	0.408600
H	-3.173543	-2.208011	-0.163687

Rotational constants (GHz): 1.2320900 0.8220000 0.7558300

Vibrational harmonic frequencies (cm-1):

11619.7569	48.8003	76.1710
90.8525	128.0349	178.2599
185.6173	196.0794	206.8501
228.2607	234.1497	256.6592
275.4787	311.0721	333.5089
343.4468	416.1929	454.0054
498.4496	588.3668	655.5714
726.7012	751.4353	794.6660
824.1090	856.8512	921.1692
970.6191	998.1563	1013.1152
1028.0568	1036.0684	1048.8154
1050.3774	1090.2523	1119.7695
1132.7401	1150.1855	1198.8269
1214.2850	1282.2539	1303.3223
1316.0800	1318.4176	1358.8408
1370.8959	1375.4224	1400.5967
1406.1224	1414.6606	1417.1950
1438.9223	1486.2021	1489.5536
1494.4265	1497.1736	1499.9296
1501.5958	1503.0698	1507.6677
1509.6149	1516.7663	1561.4697
1862.4740	3049.6896	3055.4088
3057.8244	3065.7125	3066.7896
3068.2368	3077.7150	3104.4489
3108.6426	3124.7726	3126.4980
3130.1662	3134.7127	3137.8203
3142.2333	3147.1548	3151.5058

Zero-point correction (Hartree): 0.255642

TS.dic2H5CH3CH_COO.14Hshift.cmpmRS

~~~~~  
E(RM062X/Aug-CC-pVTZ) (Hartree): -504.03677164

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.052312  | 0.437258  | -0.005881 |
| O | -0.245001 | 1.340989  | 0.876362  |
| O | 0.846852  | 1.590430  | 1.711059  |
| C | -1.106695 | -0.050597 | -0.819918 |
| C | -2.450415 | 0.052696  | -0.101117 |
| C | -1.092170 | 0.741809  | -2.137097 |
| H | -0.904959 | -1.097255 | -1.055235 |
| C | -2.536452 | -0.846142 | 1.125715  |
| H | -2.625381 | 1.092046  | 0.180005  |
| H | -3.231211 | -0.216180 | -0.815112 |
| H | -0.130129 | 0.656018  | -2.642357 |
| H | -1.286743 | 1.796934  | -1.943941 |
| H | -1.867176 | 0.364129  | -2.802539 |
| H | -1.754445 | -0.603735 | 1.846074  |
| H | -2.427774 | -1.895453 | 0.846585  |
| H | -3.496471 | -0.733710 | 1.626897  |

|                                                           |           |           |           |
|-----------------------------------------------------------|-----------|-----------|-----------|
| C                                                         | 1.393278  | -0.011228 | -0.004925 |
| H                                                         | 1.408394  | 0.478588  | 1.267592  |
| C                                                         | 2.442760  | 1.004133  | -0.490081 |
| C                                                         | 1.656372  | -1.422200 | -0.499952 |
| C                                                         | 1.069972  | -2.504195 | 0.401483  |
| H                                                         | 1.298843  | -1.547620 | -1.528726 |
| H                                                         | 2.738508  | -1.554103 | -0.551643 |
| H                                                         | 2.162013  | 2.025981  | -0.253420 |
| H                                                         | 2.557522  | 0.908569  | -1.572675 |
| H                                                         | 3.408405  | 0.798235  | -0.029282 |
| H                                                         | 1.269582  | -3.500767 | 0.008508  |
| H                                                         | -0.009956 | -2.396806 | 0.511070  |
| H                                                         | 1.502401  | -2.435430 | 1.399469  |
| Rotational constants (GHz): 1.1891200 0.8496100 0.7646700 |           |           |           |
| Vibrational harmonic frequencies (cm-1):                  |           |           |           |
| i1609.6669                                                | 51.5508   |           | 92.4537   |
| 128.1315                                                  | 137.4528  |           | 156.1556  |
| 176.4038                                                  | 195.4483  |           | 205.1261  |
| 223.2582                                                  | 234.9754  |           | 248.8372  |
| 284.2949                                                  | 298.0804  |           | 334.1045  |
| 353.4636                                                  | 436.6169  |           | 464.0980  |
| 498.0278                                                  | 558.0054  |           | 633.1740  |
| 746.7789                                                  | 772.2614  |           | 794.3727  |
| 812.3744                                                  | 867.4159  |           | 941.4797  |
| 975.3512                                                  | 1000.8964 |           | 1013.9048 |
| 1031.5039                                                 | 1032.3619 |           | 1046.5464 |
| 1059.5517                                                 | 1102.0745 |           | 1123.5755 |
| 1134.2911                                                 | 1136.9714 |           | 1194.9553 |
| 1222.8466                                                 | 1284.6321 |           | 1292.5016 |
| 1302.8294                                                 | 1317.7591 |           | 1355.9819 |
| 1369.1804                                                 | 1379.3815 |           | 1397.3784 |
| 1402.9723                                                 | 1414.8231 |           | 1418.9866 |
| 1442.4468                                                 | 1488.1042 |           | 1490.7907 |
| 1494.9492                                                 | 1498.9483 |           | 1501.2387 |
| 1501.9669                                                 | 1506.5792 |           | 1507.0932 |
| 1507.4669                                                 | 1511.7609 |           | 1560.8912 |
| 1868.9130                                                 | 3021.8466 |           | 3048.3535 |
| 3059.3267                                                 | 3062.3330 |           | 3063.3346 |
| 3068.5793                                                 | 3085.4889 |           | 3087.9643 |
| 3107.1592                                                 | 3115.5164 |           | 3129.2347 |
| 3132.2473                                                 | 3135.8917 |           | 3137.2292 |
| 3140.2243                                                 | 3143.8068 |           | 3171.5626 |
| Zero-point correction (Hartree): 0.255717                 |           |           |           |
| TS.dic2H5CH3CH_COO.14Hshift.cmpPR                         |           |           |           |
| ~~~~~                                                     |           |           |           |
| E(RM062X/Aug-CC-pVTZ) (Hartree): -504.03701264            |           |           |           |
| Electronic state : 1-A                                    |           |           |           |
| Cartesian coordinates (Angs):                             |           |           |           |
| C                                                         | -0.096196 | 0.388154  | -0.205232 |
| O                                                         | -0.642831 | 1.557769  | -0.335514 |
| O                                                         | 0.181023  | 2.550351  | 0.196678  |
| C                                                         | -1.031073 | -0.750333 | -0.485131 |
| C                                                         | -2.442299 | -0.502402 | 0.049587  |
| C                                                         | -1.024448 | -1.007279 | -1.998996 |
| H                                                         | -0.613778 | -1.626843 | 0.012939  |
| C                                                         | -2.463076 | -0.296943 | 1.558627  |
| H                                                         | -2.868333 | 0.365801  | -0.454672 |
| H                                                         | -3.057938 | -1.361958 | -0.222384 |
| H                                                         | -0.015301 | -1.188435 | -2.369144 |
| H                                                         | -1.435074 | -0.147339 | -2.527786 |
| H                                                         | -1.637349 | -1.878518 | -2.226408 |
| H                                                         | -1.872941 | 0.575897  | 1.841966  |
| H                                                         | -2.051825 | -1.166237 | 2.074881  |
| H                                                         | -3.477829 | -0.142657 | 1.921581  |
| C                                                         | 1.213427  | 0.366917  | 0.330569  |
| H                                                         | 0.878357  | 1.580919  | 0.817452  |
| C                                                         | 2.345342  | 0.946459  | -0.533035 |
| C                                                         | 1.616567  | -0.866979 | 1.118682  |
| C                                                         | 2.184068  | -2.013999 | 0.282607  |
| H                                                         | 2.369678  | -0.555473 | 1.846547  |
| H                                                         | 0.768470  | -1.221540 | 1.707364  |
| H                                                         | 2.044169  | 1.867496  | -1.021788 |
| H                                                         | 2.647044  | 0.227156  | -1.295439 |
| H                                                         | 3.210948  | 1.154686  | 0.096712  |
| H                                                         | 3.121229  | -1.730444 | -0.194158 |
| H                                                         | 1.490338  | -2.311510 | -0.506425 |
| H                                                         | 2.380728  | -2.887543 | 0.903376  |
| Rotational constants (GHz): 1.2096200 0.8685500 0.7087300 |           |           |           |
| Vibrational harmonic frequencies (cm-1):                  |           |           |           |
| i1601.1846                                                | 37.1069   |           | 82.3862   |
| 112.5214                                                  | 141.8767  |           | 162.2045  |
| 183.4785                                                  | 195.2490  |           | 208.9405  |
| 237.1838                                                  | 242.0687  |           | 258.4222  |
| 277.2477                                                  | 311.7449  |           | 338.7708  |
| 365.8817                                                  | 388.1080  |           | 454.7800  |
| 499.3062                                                  | 611.8520  |           | 643.6330  |
| 736.7533                                                  | 776.1916  |           | 790.4060  |
| 811.8840                                                  | 866.3598  |           | 941.2769  |
| 974.4505                                                  | 989.2289  |           | 1004.8243 |
| 1029.9448                                                 | 1036.2753 |           | 1044.2223 |
| 1048.4176                                                 | 1097.9739 |           | 1120.7688 |
| 1135.9753                                                 | 1144.3761 |           | 1199.1941 |
| 1225.2052                                                 | 1282.6277 |           | 1296.1463 |
| 1305.0124                                                 | 1329.1283 |           | 1353.6536 |
| 1368.9028                                                 | 1381.5439 |           | 1394.0048 |
| 1401.6959                                                 | 1412.6776 |           | 1417.9027 |
| 1438.3570                                                 | 1489.2316 |           | 1491.8387 |
| 1494.4744                                                 | 1498.3218 |           | 1502.2403 |
| 1504.1354                                                 | 1508.1250 |           | 1509.4010 |
| 1510.1153                                                 | 1518.7062 |           | 1566.4788 |
| 1859.0791                                                 | 3056.0835 |           | 3056.4352 |

|           |           |           |
|-----------|-----------|-----------|
| 3059.6653 | 3061.5971 | 3062.5875 |
| 3067.8902 | 3087.6071 | 3092.6678 |
| 3106.7177 | 3118.2073 | 3126.0096 |
| 3127.2222 | 3137.1848 | 3140.1137 |
| 3141.2449 | 3143.9376 | 3175.4561 |

Zero-point correction (Hartree): 0.255886

TS.dic2H5CH3CH\_COO.14Hshift.cmptRS

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E(RM062X/Aug-CC-pVTZ) (Hartree): -504.03702618

Electronic state : 1-A

Cartesian coordinates (Angs):

C	0.226815	0.451661	0.045736
O	0.625739	1.319663	-0.831952
O	-0.431736	1.704366	-1.659836
C	1.343290	-0.220185	0.786240
C	2.458024	-0.692864	-0.150062
C	1.866273	0.754145	1.851182
H	0.909515	-1.084162	1.291422
C	1.960152	-1.679017	-1.198281
H	2.903683	0.177057	-0.634353
H	3.237350	-1.152125	0.461003
H	1.068680	1.087200	2.514899
H	2.306484	1.629876	1.375281
H	2.631490	0.263842	2.451464
H	1.191003	-1.225777	-1.826554
H	1.532736	-2.565910	-0.727324
H	2.769717	-2.004351	-1.849427
C	-1.157437	0.166136	0.049615
H	-1.117751	0.636083	-1.213777
C	-2.093294	1.296045	0.514594
C	-1.575465	-1.212027	0.527642
C	-2.964063	-1.593656	0.023061
H	-0.858947	-1.957419	0.178337
H	-1.569726	-1.253102	1.623086
H	-1.643229	2.272937	0.367885
H	-2.311335	1.158485	1.576608
H	-3.035224	1.276945	-0.031091
H	-3.729038	-0.931323	0.426549
H	-3.217489	-2.611297	0.316755
H	-3.005708	-1.530609	-1.064817

Rotational constants (GHz): 1.2806100 0.7723200 0.6899400

Vibrational harmonic frequencies (cm-1):

11599.9383	28.1652	77.3749
89.6271	135.7276	142.8881
168.2457	196.3863	206.5416
234.4432	240.4902	263.3349
285.0765	286.9142	321.5298
359.1804	391.4348	451.0150
538.7191	558.3980	643.0389
747.1881	775.1927	801.3318
809.4958	864.8483	955.2568
974.3823	993.4227	999.4922
1027.1398	1028.8194	1043.1772
1068.8000	1103.2286	1124.0713
1138.0225	1149.6604	1197.6990
1223.4567	1287.0523	1298.3099
1312.5371	1323.4655	1351.9124
1368.9305	1383.8928	1394.8642
1403.8603	1410.3252	1417.7244
1441.3867	1483.7522	1489.0736
1493.6664	1497.4615	1499.7574
1503.2204	1506.5394	1507.5021
1508.1042	1516.0079	1568.6840
1858.9719	3019.1688	3051.0568
3054.0649	3063.5363	3064.7294
3067.4091	3085.4731	3091.6479
3105.4361	3123.3263	3125.2000
3134.7618	3137.8577	3138.5240
3140.4321	3145.2410	3173.9990

Zero-point correction (Hartree): 0.255592

TS.dic2H5CH3CH_COO.14Hshift.cppmRS

~~~~~  
E(RM062X/Aug-CC-pVTZ) (Hartree): -504.03382713

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.011078 | 0.273911  | -0.044217 |
| O | 0.463833  | 1.375190  | -0.539320 |
| O | -0.563971 | 2.288917  | -0.782967 |
| C | 0.956706  | -0.865932 | 0.048888  |
| C | 2.259387  | -0.674252 | -0.736961 |
| C | 1.189904  | -1.167648 | 1.537420  |
| H | 0.428414  | -1.722780 | -0.375506 |
| C | 3.276056  | 0.263653  | -0.092766 |
| H | 2.712845  | -1.660384 | -0.855368 |
| H | 2.014993  | -0.318747 | -1.738451 |
| H | 0.256255  | -1.422914 | 2.036816  |
| H | 1.620796  | -0.305943 | 2.045420  |
| H | 1.879300  | -2.005498 | 1.640922  |
| H | 3.641619  | -0.135594 | 0.853023  |
| H | 2.851777  | 1.248800  | 0.092204  |
| H | 4.136508  | 0.388563  | -0.748424 |
| C | -1.401997 | 0.262248  | 0.216751  |
| H | -1.430016 | 1.314134  | -0.659942 |
| C | -1.872500 | 1.130759  | 1.395444  |
| C | -2.116662 | -1.075402 | 0.127416  |
| C | -2.237949 | -1.603476 | -1.299703 |
| H | -1.639805 | -1.825919 | 0.767662  |
| H | -3.118892 | -0.939788 | 0.537251  |
| H | -1.264669 | 2.023247  | 1.512091  |
| H | -1.821683 | 0.545124  | 2.316849  |



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H      -2.907455      1.438219      1.247975
H      -2.742298      -2.569133      -1.324707
H      -1.261808      -1.724087      -1.771622
H      -2.805985      -0.903316      -1.911539
Rotational constants (GHz):      1.3542900      0.7933600      0.6718400
Vibrational harmonic frequencies (cm-1):
i1592.1093      47.8044      110.1320
119.4051      131.0738      149.3532
167.8914      196.0608      203.1606
226.0999      242.9038      271.3908
295.2407      300.9247      314.0370
362.3452      418.7927      446.4083
554.4809      563.3124      637.2330
749.8446      765.2319      788.7918
803.1978      855.4694      939.7753
969.1009      999.6976      1008.7291
1023.2694      1031.4906      1037.7532
1059.6892      1101.8784      1116.0241
1131.6202      1163.7587      1176.7899
1219.9255      1287.8439      1289.6257
1318.7744      1324.5238      1349.7175
1367.7697      1378.3441      1394.3390
1402.7773      1414.9456      1418.7026
1443.5214      1485.1248      1489.3312
1495.8459      1496.5833      1499.5988
1500.4227      1504.8196      1508.8665
1511.2994      1519.3556      1556.1718
1872.8929      3028.5488      3046.5555
3061.1144      3063.5827      3066.7641
3072.5735      3079.8247      3085.8915
3105.7087      3113.5030      3127.9680
3136.7431      3137.1725      3141.7549
3144.9490      3151.1632      3169.3394
Zero-point correction (Hartree): 0.255757

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TS.dic2H5CH3CH_COO.14Hshift.cpppRS
~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -504.03311503
Electronic state : 1-A
Cartesian coordinates (Angs):
C 0.047481 0.359914 -0.079899
O 0.707028 1.476830 -0.032755
O -0.147057 2.565915 -0.209630
C 0.896356 -0.871718 -0.154810
C 2.271106 -0.673001 -0.812030
C 0.990707 -1.467756 1.259349
H 0.326655 -1.573128 -0.767780
C 3.347841 -0.050553 0.071721
H 2.612865 -1.656261 -1.142124
H 2.141507 -0.069357 -1.711328
H 0.002412 -1.687775 1.660094
H 1.484166 -0.773391 1.937791
H 1.569441 -2.391137 1.232167
H 3.592198 -0.696339 0.914777
H 3.039350 0.917880 0.459638
H 4.261375 0.093676 -0.503453
C -1.359057 0.474564 -0.206653
H -1.070847 1.722261 -0.656838
C -2.132126 1.017767 1.005121
C -2.096437 -0.614308 -0.967810
C -2.488897 -1.854054 -0.164834
H -3.005657 -0.156799 -1.365842
H -1.513889 -0.914038 -1.840914
H -1.610981 1.847118 1.473388
H -2.277018 0.232528 1.748669
H -3.115010 1.364625 0.684235
H -3.124791 -1.595622 0.680963
H -1.612671 -2.374651 0.223471
H -3.040717 -2.556673 -0.788766
Rotational constants (GHz): 1.3980400 0.8177700 0.6154000
Vibrational harmonic frequencies (cm-1):
i1598.6028 44.8376 100.1883
109.9715 123.9120 161.7910
191.4078 196.5421 202.4826
233.4549 253.1617 274.3412
282.5352 316.0007 328.5363
365.2244 389.1678 419.9568
557.0069 611.8049 656.3592
737.4639 766.7298 784.0424
798.8733 852.0760 939.2154
965.2083 987.7210 1011.4826
1016.3633 1034.6475 1039.8495
1049.1830 1096.5324 1117.7723
1136.9668 1157.0532 1182.2744
1223.9336 1288.5708 1292.9981
1328.2897 1329.6410 1352.3891
1369.2180 1381.4925 1394.1080
1399.6419 1410.1265 1420.1148
1441.4357 1483.7441 1490.0673
1493.1095 1495.3622 1500.8824
1506.2087 1508.2974 1512.5757
1515.0809 1522.1784 1560.1767
1865.3893 3054.6523 3057.5471
3061.2864 3065.5882 3067.3374
3073.5455 3082.9432 3089.4147
3102.4081 3115.6826 3130.0392
3136.1752 3139.2232 3142.9007
3148.1511 3155.5762 3172.3849
Zero-point correction (Hartree): 0.256002

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TS.dic2H5CH3CH_COO.14Hshift.cpptRS
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E(RM062X/Aug-CC-pVTZ) (Hartree): -504.03465023
Electronic state : 1-A
Cartesian coordinates (Angs):
  C    0.149059    0.247227   -0.108111
  O    0.647110    1.437257   -0.245445
  O   -0.368190    2.394756   -0.297371
  C    1.109381   -0.884656   -0.309318
  C    2.486093   -0.472243   -0.842901
  C    1.189405   -1.695630    0.991986
  H    0.632949   -1.521319   -1.060523
  C    3.406556    0.182166    0.183019
  H    2.966392   -1.374268   -1.227208
  H    2.348339    0.197093   -1.692193
  H    0.213098   -2.087053    1.272434
  H    1.555282   -1.078684    1.811675
  H    1.874510   -2.533541    0.863700
  H    3.674864   -0.513134    0.978032
  H    2.943010    1.057458    0.634918
  H    4.330637    0.503877   -0.294851
  C   -1.255553    0.183151    0.052458
  H   -1.235754    1.420426   -0.513580
  C   -1.804585    0.726168    1.383847
  C   -1.962954   -1.068318   -0.432879
  C   -3.455539   -0.831117   -0.647836
  H   -1.525654   -1.402174   -1.375148
  H   -1.836911   -1.889020    0.282595
  H   -1.141049    1.468316    1.817408
  H   -1.915400   -0.104373    2.086304
  H   -2.780338    1.190181    1.249270
  H   -3.959934   -0.599424    0.289396
  H   -3.931206   -1.714916   -1.070722
  H   -3.615368    0.003969   -1.330572
Rotational constants (GHz):    1.6039000    0.7113800    0.5864400
Vibrational harmonic frequencies (cm-1):
  i1599.1598    39.8575    76.2665
    110.2634    128.3693    152.7699
    173.5819    192.8101    217.1153
    236.1212    257.8054    282.2775
    296.2058    309.3843    314.2377
    354.5457    380.4334    468.5929
    543.6140    587.3741    628.3493
    751.4152    762.8114    795.7705
    804.9885    855.8324    956.2123
    969.2806    992.5214    1005.7261
   1013.0982   1030.7015   1031.4369
   1069.0369   1105.3902   1110.8349
   1144.7064   1164.9136   1178.5888
   1222.6737   1286.2085   1301.7628
   1314.2763   1326.2814   1343.3066
   1369.4030   1378.6567   1394.8638
   1404.4467   1411.7311   1420.2624
   1444.6650   1481.1767   1485.6996
   1491.3948   1496.5576   1497.8084
   1503.1024   1507.2800   1511.0039
   1516.1363   1519.1510   1557.7722
   1867.7533   3020.7204   3045.9296
   3055.7104   3064.8889   3068.7516
   3068.8932   3073.0875   3087.2437
   3108.3193   3121.0158   3134.8253
   3137.2788   3140.6575   3142.2818
   3149.3695   3150.9993   3170.4074
Zero-point correction (Hartree): 0.255809

TS.diC2H5CH3CH_COO.14Hshift.ctmpRS
~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -504.03540395
Electronic state : 1-A
Cartesian coordinates (Angs):
 C -0.086830 0.438405 -0.008492
 O -0.015569 1.466849 -0.796679
 O -1.247156 2.123404 -0.858323
 C 1.248845 -0.112368 0.389023
 C 2.040320 -0.503255 -0.870016
 C 1.998638 0.900402 1.261820
 H 1.059225 -1.016187 0.970974
 C 3.353092 -1.203666 -0.545932
 H 1.419189 -1.157965 -1.485134
 H 2.225678 0.396112 -1.459209
 H 1.386775 1.222342 2.103967
 H 2.257196 1.780599 0.673717
 H 2.911713 0.460642 1.658246
 H 3.186014 -2.069384 0.097010
 H 4.049459 -0.537225 -0.039075
 H 3.836473 -1.552266 -1.457214
 C -1.362439 0.145883 0.526256
 H -1.627784 1.436188 0.230505
 C -1.375370 -0.538291 1.877444
 C -2.439542 -0.376341 -0.447647
 C -2.330471 -1.879302 -0.691838
 H -3.419660 -0.143181 -0.026276
 H -2.363978 0.159209 -1.390063
 H -0.697626 -0.059233 2.583130
 H -1.106987 -1.595818 1.821022
 H -2.379884 -0.482667 2.298593
 H -2.495468 -2.454796 0.218399
 H -1.343054 -2.137372 -1.079787
 H -3.072940 -2.199830 -1.422506
Rotational constants (GHz): 1.3801200 0.7089100 0.6393300
Vibrational harmonic frequencies (cm-1):
 i1611.6502 37.5860 64.7378
 77.0340 96.4172 156.6163
 185.9145 200.7729 207.1840

```

|           |           |           |
|-----------|-----------|-----------|
| 217.6774  | 236.7349  | 276.8524  |
| 284.2076  | 303.9305  | 319.8693  |
| 355.3895  | 395.6470  | 435.6122  |
| 499.6247  | 595.1583  | 690.0496  |
| 727.8308  | 768.5104  | 788.8170  |
| 810.6072  | 852.8934  | 923.4234  |
| 967.1735  | 995.3623  | 1002.0445 |
| 1013.7720 | 1039.2089 | 1046.6382 |
| 1064.5943 | 1091.7318 | 1114.4029 |
| 1140.3296 | 1152.9531 | 1196.9878 |
| 1214.6202 | 1286.1754 | 1301.0258 |
| 1317.1273 | 1337.4114 | 1359.1521 |
| 1360.7170 | 1382.2245 | 1402.6029 |
| 1405.7633 | 1415.0586 | 1415.6497 |
| 1435.7856 | 1487.5527 | 1489.4778 |
| 1494.6979 | 1496.1650 | 1499.6931 |
| 1503.1867 | 1504.8860 | 1508.4801 |
| 1515.4236 | 1516.7467 | 1560.0020 |
| 1861.2677 | 3049.2658 | 3054.9489 |
| 3060.8178 | 3063.3468 | 3066.7161 |
| 3069.5860 | 3079.9975 | 3105.3815 |
| 3108.3544 | 3121.5975 | 3129.5991 |
| 3131.9659 | 3132.5183 | 3139.8387 |
| 3142.1453 | 3153.1440 | 3154.4799 |

Zero-point correction (Hartree): 0.255540

TS.diC2H5CH3CH\_COO.14Hshift.ctmtRS

E(RM062X/Aug-CC-pVTZ) (Hartree): -504.03672176

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.039982 | 0.193684  | -0.113718 |
| O | 0.013469  | 1.472202  | -0.330789 |
| O | 1.320312  | 1.857270  | -0.643943 |
| C | -1.428516 | -0.368988 | -0.123929 |
| C | -2.310042 | 0.390868  | 0.880084  |
| C | -1.994403 | -0.325665 | -1.548668 |
| H | -1.353157 | -1.409114 | 0.198937  |
| C | -3.700460 | -0.214853 | 1.018335  |
| H | -1.813537 | 0.391077  | 1.852429  |
| H | -2.380786 | 1.432926  | 0.564943  |
| H | -1.315241 | -0.799666 | -2.256609 |
| H | -2.141362 | 0.708520  | -1.859344 |
| H | -2.948399 | -0.847054 | -1.596513 |
| H | -3.642193 | -1.275294 | 1.269176  |
| H | -4.274884 | -0.117702 | 0.098250  |
| H | -4.258952 | 0.285088  | 1.808116  |
| C | 1.195316  | -0.488628 | -0.132117 |
| H | 1.606405  | 0.555242  | -0.869061 |
| C | 1.153187  | -1.958558 | -0.487271 |
| C | 2.202056  | -0.157616 | 0.994056  |
| C | 3.642707  | -0.095247 | 0.507243  |
| H | 1.936364  | 0.788289  | 1.459935  |
| H | 2.095907  | -0.938758 | 1.752357  |
| H | 0.482635  | -2.165474 | -1.320573 |
| H | 0.842140  | -2.573535 | 0.362077  |
| H | 2.146721  | -2.295205 | -0.781919 |
| H | 3.935506  | -1.018141 | 0.005926  |
| H | 4.327559  | 0.062890  | 1.339778  |
| H | 3.765854  | 0.730154  | -0.194143 |

Rotational constants (GHz): 1.8058100 0.6107800 0.5659900

Vibrational harmonic frequencies (cm-1):

|            |           |           |
|------------|-----------|-----------|
| i1602.5775 | 38.4498   | 73.4827   |
| 90.0204    | 92.5805   | 163.2720  |
| 185.3935   | 198.7275  | 210.6928  |
| 225.3671   | 248.3398  | 272.4466  |
| 283.1374   | 294.8370  | 325.0419  |
| 349.6067   | 377.4497  | 432.9151  |
| 525.3885   | 575.1692  | 690.9521  |
| 733.1568   | 783.5319  | 788.8807  |
| 804.7397   | 853.1701  | 925.6684  |
| 967.4513   | 995.3839  | 1000.7918 |
| 1019.8801  | 1039.6081 | 1049.7839 |
| 1067.4248  | 1101.9354 | 1116.7380 |
| 1135.2974  | 1150.5149 | 1196.3001 |
| 1215.1329  | 1288.5132 | 1301.4072 |
| 1333.7963  | 1337.7827 | 1350.2977 |
| 1360.5113  | 1385.1855 | 1403.2028 |
| 1411.0442  | 1416.0974 | 1417.7847 |
| 1438.9426  | 1477.3278 | 1489.4596 |
| 1496.2813  | 1496.5623 | 1500.6954 |
| 1500.8377  | 1504.8347 | 1508.1725 |
| 1510.4690  | 1517.5424 | 1567.1073 |
| 1859.8697  | 3041.6298 | 3046.6755 |
| 3061.8333  | 3062.6672 | 3065.6195 |
| 3069.1059  | 3077.9765 | 3106.5934 |
| 3111.5936  | 3122.7262 | 3133.3757 |
| 3135.5611  | 3136.8783 | 3140.0594 |
| 3142.4015  | 3143.2364 | 3154.5948 |

Zero-point correction (Hartree): 0.255667

TS.diC2H5CH3CH\_COO.14Hshift.ctpmRS

E(RM062X/Aug-CC-pVTZ) (Hartree): -504.03511093

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.197249  | -0.438740 | -0.040969 |
| O | 0.120723  | -1.574422 | -0.662695 |
| O | 1.383705  | -1.979536 | -1.099339 |
| C | -1.118702 | 0.191442  | 0.293419  |
| C | -2.274998 | -0.321532 | -0.564631 |
| C | -1.346614 | -0.015436 | 1.799931  |

|                                                           |           |           |           |
|-----------------------------------------------------------|-----------|-----------|-----------|
| H                                                         | -0.999194 | 1.263839  | 0.123282  |
| C                                                         | -3.576197 | 0.427274  | -0.306071 |
| H                                                         | -1.997561 | -0.226576 | -1.615616 |
| H                                                         | -2.412432 | -1.388272 | -0.380621 |
| H                                                         | -0.484493 | 0.321544  | 2.375487  |
| H                                                         | -1.510957 | -1.072238 | 2.013557  |
| H                                                         | -2.217015 | 0.545418  | 2.133820  |
| H                                                         | -3.439666 | 1.503355  | -0.427992 |
| H                                                         | -3.952686 | 0.249282  | 0.700517  |
| H                                                         | -4.348226 | 0.108887  | -1.004639 |
| C                                                         | 1.498936  | 0.086145  | 0.135781  |
| H                                                         | 1.823849  | -0.758475 | -0.890299 |
| C                                                         | 2.396800  | -0.660458 | 1.136974  |
| C                                                         | 1.626817  | 1.596574  | 0.227588  |
| C                                                         | 1.309286  | 2.315276  | -1.080661 |
| H                                                         | 1.007048  | 1.993783  | 1.040198  |
| H                                                         | 2.656068  | 1.822271  | 0.511601  |
| H                                                         | 2.189256  | -1.726236 | 1.154972  |
| H                                                         | 2.236230  | -0.251088 | 2.137638  |
| H                                                         | 3.446410  | -0.519840 | 0.880244  |
| H                                                         | 1.395175  | 3.396108  | -0.971975 |
| H                                                         | 0.299834  | 2.093825  | -1.430551 |
| H                                                         | 1.997471  | 1.992804  | -1.861518 |
| Rotational constants (GHz): 1.3207200 0.7527000 0.6445800 |           |           |           |
| Vibrational harmonic frequencies (cm-1):                  |           |           |           |
| i1599.8785                                                | 30.1952   | 78.3394   |           |
| 111.4846                                                  | 127.2013  | 142.7722  |           |
| 161.0269                                                  | 194.9928  | 205.3397  |           |
| 214.4298                                                  | 234.8355  | 266.6683  |           |
| 280.3680                                                  | 307.1297  | 327.2328  |           |
| 360.6223                                                  | 405.1818  | 446.2765  |           |
| 492.3837                                                  | 566.7986  | 674.1821  |           |
| 751.7487                                                  | 765.6650  | 790.9656  |           |
| 803.5920                                                  | 867.9613  | 941.5002  |           |
| 971.5806                                                  | 988.7696  | 1002.2928 |           |
| 1022.3724                                                 | 1036.7975 | 1052.7034 |           |
| 1064.2522                                                 | 1097.7880 | 1120.5403 |           |
| 1132.7059                                                 | 1156.3190 | 1193.4984 |           |
| 1222.5834                                                 | 1285.6278 | 1297.0478 |           |
| 1315.9747                                                 | 1319.8265 | 1341.4775 |           |
| 1366.2971                                                 | 1383.5149 | 1396.9416 |           |
| 1406.0118                                                 | 1415.6604 | 1417.3442 |           |
| 1441.9246                                                 | 1486.4041 | 1491.1076 |           |
| 1496.4157                                                 | 1497.8367 | 1500.0558 |           |
| 1500.6660                                                 | 1503.7336 | 1507.9801 |           |
| 1510.1445                                                 | 1516.7641 | 1559.1938 |           |
| 1870.9838                                                 | 3019.7426 | 3046.0684 |           |
| 3060.7291                                                 | 3061.2043 | 3064.1982 |           |
| 3069.7355                                                 | 3081.7456 | 3084.4807 |           |
| 3106.1095                                                 | 3113.5812 | 3126.7809 |           |
| 3130.9285                                                 | 3134.5834 | 3137.2025 |           |
| 3140.5859                                                 | 3154.2176 | 3169.9434 |           |
| Zero-point correction (Hartree): 0.255478                 |           |           |           |
| TS.diC2H5CH3CH_COO.14Hshift.ctppRS                        |           |           |           |
| ~~~~~                                                     |           |           |           |
| E(RM062X/Aug-CC-pVTZ) (Hartree): -504.03499014            |           |           |           |
| Electronic state : 1-A                                    |           |           |           |
| Cartesian coordinates (Angs):                             |           |           |           |
| C                                                         | 0.130838  | -0.526187 | -0.007603 |
| O                                                         | -0.080957 | -1.805516 | 0.036222  |
| O                                                         | 1.071846  | -2.508860 | -0.313246 |
| C                                                         | -1.106907 | 0.307916  | 0.111457  |
| C                                                         | -2.356267 | -0.382420 | -0.440740 |
| C                                                         | -1.255605 | 0.701684  | 1.590932  |
| H                                                         | -0.920430 | 1.218890  | -0.462348 |
| C                                                         | -3.574436 | 0.532106  | -0.453155 |
| H                                                         | -2.144640 | -0.728777 | -1.453597 |
| H                                                         | -2.562501 | -1.275067 | 0.151268  |
| H                                                         | -0.328050 | 1.115709  | 1.985159  |
| H                                                         | -1.518678 | -0.174609 | 2.184391  |
| H                                                         | -2.037645 | 1.449124  | 1.708350  |
| H                                                         | -3.364970 | 1.456692  | -0.994137 |
| H                                                         | -3.890429 | 0.797981  | 0.554908  |
| H                                                         | -4.416546 | 0.044482  | -0.941572 |
| C                                                         | 1.455981  | -0.122487 | -0.301006 |
| H                                                         | 1.569935  | -1.376753 | -0.807651 |
| C                                                         | 2.526557  | -0.385495 | 0.769905  |
| C                                                         | 1.639168  | 1.192862  | -1.038791 |
| C                                                         | 1.672783  | 2.445482  | -0.163333 |
| H                                                         | 2.582763  | 1.123295  | -1.585581 |
| H                                                         | 0.865833  | 1.299308  | -1.801693 |
| H                                                         | 2.406732  | -1.364175 | 1.224013  |
| H                                                         | 2.475759  | 0.371702  | 1.553772  |
| H                                                         | 3.516244  | -0.334169 | 0.314693  |
| H                                                         | 2.504291  | 2.416360  | 0.539524  |
| H                                                         | 0.753501  | 2.553786  | 0.414651  |
| H                                                         | 1.789049  | 3.340460  | -0.773949 |
| Rotational constants (GHz): 1.3128000 0.7946600 0.5956000 |           |           |           |
| Vibrational harmonic frequencies (cm-1):                  |           |           |           |
| i1599.2568                                                | 46.7521   | 76.4671   |           |
| 101.1530                                                  | 110.0738  | 151.8993  |           |
| 181.5717                                                  | 186.6496  | 211.5973  |           |
| 220.5597                                                  | 247.1076  | 271.5224  |           |
| 282.7221                                                  | 316.3555  | 324.1724  |           |
| 360.5816                                                  | 390.2574  | 420.9129  |           |
| 492.3785                                                  | 622.3274  | 679.9767  |           |
| 745.0493                                                  | 762.8820  | 787.0803  |           |
| 798.3021                                                  | 867.4866  | 940.6866  |           |
| 968.6828                                                  | 982.8948  | 1003.1249 |           |
| 1009.0277                                                 | 1037.2517 | 1045.8836 |           |
| 1061.0170                                                 | 1096.5372 | 1113.1947 |           |

|           |           |           |
|-----------|-----------|-----------|
| 1142.0726 | 1149.3281 | 1198.3857 |
| 1224.8643 | 1284.8979 | 1295.0496 |
| 1321.3300 | 1334.4053 | 1342.5660 |
| 1362.6262 | 1387.5982 | 1393.7528 |
| 1404.8014 | 1412.0234 | 1415.7255 |
| 1438.1508 | 1486.6977 | 1491.0374 |
| 1494.8179 | 1497.6812 | 1500.1593 |
| 1505.3786 | 1509.0071 | 1509.7639 |
| 1515.7849 | 1516.4470 | 1562.6087 |
| 1864.6368 | 3055.1783 | 3057.4400 |
| 3060.5149 | 3063.6538 | 3065.2978 |
| 3070.8582 | 3077.1260 | 3089.1813 |
| 3107.7971 | 3115.6541 | 3128.1949 |
| 3131.3354 | 3137.2871 | 3140.0626 |
| 3140.3290 | 3152.6128 | 3174.3586 |

Zero-point correction (Hartree): 0.255708

TS.dic2H5CH3CH\_COO.14Hshift.ctptRS

E(RM062X/Aug-CC-pVTZ) (Hartree): -504.03567823

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.041604  | 0.446186  | -0.001305 |
| O | 0.281349  | 1.707947  | -0.179936 |
| O | -0.903235 | 2.399254  | -0.443307 |
| C | 1.249818  | -0.435249 | 0.047090  |
| C | 2.521755  | 0.246411  | -0.456590 |
| C | 1.381778  | -0.966182 | 1.483220  |
| H | 1.023242  | -1.287249 | -0.601099 |
| C | 3.712038  | -0.702415 | -0.519826 |
| H | 2.328591  | 0.662473  | -1.445915 |
| H | 2.752335  | 1.094423  | 0.190751  |
| H | 0.439978  | -1.386617 | 1.834548  |
| H | 1.668924  | -0.157354 | 2.156434  |
| H | 2.140371  | -1.744157 | 1.535097  |
| H | 3.475624  | -1.588528 | -1.111757 |
| H | 4.019189  | -1.033931 | 0.471316  |
| H | 4.568625  | -0.213526 | -0.980943 |
| C | -1.320734 | 0.067042  | -0.011794 |
| H | -1.495289 | 1.239826  | -0.682051 |
| C | -2.159737 | 0.547638  | 1.186010  |
| C | -1.639548 | -1.351499 | -0.447230 |
| C | -3.112399 | -1.523573 | -0.807387 |
| H | -1.036270 | -1.616979 | -1.316787 |
| H | -1.382095 | -2.064862 | 0.345278  |
| H | -1.748268 | 1.450908  | 1.626095  |
| H | -2.178320 | -0.240196 | 1.944200  |
| H | -3.186385 | 0.757964  | 0.890560  |
| H | -3.754156 | -1.376875 | 0.060441  |
| H | -3.302107 | -2.523430 | -1.195174 |
| H | -3.406349 | -0.799656 | -1.568181 |

Rotational constants (GHz): 1.4952200 0.6771300 0.5610300

Vibrational harmonic frequencies (cm-1):

|            |           |           |
|------------|-----------|-----------|
| i1610.5855 | 47.0638   | 82.7552   |
| 84.1331    | 118.8390  | 131.6695  |
| 174.4961   | 190.8444  | 212.3346  |
| 235.4489   | 249.8043  | 284.5774  |
| 292.7576   | 305.4177  | 331.4288  |
| 354.0549   | 378.5704  | 421.4003  |
| 538.5942   | 562.5673  | 662.9161  |
| 754.4828   | 765.5967  | 792.8606  |
| 806.5389   | 867.7492  | 959.1883  |
| 969.2375   | 986.9847  | 998.8918  |
| 1009.2021  | 1030.1621 | 1054.7214 |
| 1070.4237  | 1099.0351 | 1122.2457 |
| 1141.4545  | 1156.1203 | 1199.7594 |
| 1222.6534  | 1287.4375 | 1300.8326 |
| 1307.3113  | 1326.7888 | 1339.0826 |
| 1362.5704  | 1387.1778 | 1395.5322 |
| 1406.8589  | 1412.5060 | 1416.9256 |
| 1444.1900  | 1482.3276 | 1487.7459 |
| 1491.7399  | 1498.4264 | 1499.4276 |
| 1503.8799  | 1505.5844 | 1508.9704 |
| 1517.2526  | 1517.9554 | 1560.6674 |
| 1867.1456  | 3012.9118 | 3044.2195 |
| 3055.6603  | 3060.7617 | 3064.4652 |
| 3066.1357  | 3072.8065 | 3085.5696 |
| 3106.8480  | 3120.5390 | 3130.8734 |
| 3134.1639  | 3135.9297 | 3140.6890 |
| 3140.8010  | 3154.2784 | 3171.2468 |

Zero-point correction (Hartree): 0.255595

TS.dic2H5CH3CH\_COO.14Hshift.mmmprRS

E(RM062X/Aug-CC-pVTZ) (Hartree): -504.03354644

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.210145  | 0.631383  | 0.066839  |
| O | 0.274213  | 1.762064  | -0.568432 |
| O | -0.927069 | 2.459944  | -0.467692 |
| C | 1.553713  | 0.002133  | 0.304991  |
| C | 1.790358  | -1.168265 | -0.675908 |
| C | 2.690012  | 1.019442  | 0.224600  |
| H | 1.514762  | -0.417019 | 1.313756  |
| C | 1.142852  | -2.478450 | -0.251385 |
| H | 1.449847  | -0.873299 | -1.671371 |
| H | 2.869552  | -1.310287 | -0.752724 |
| H | 2.506397  | 1.878302  | 0.867267  |
| H | 2.809111  | 1.385062  | -0.794526 |
| H | 3.621566  | 0.545236  | 0.529805  |
| H | 0.063457  | -2.382600 | -0.161115 |
| H | 1.532748  | -2.801294 | 0.715100  |

|                                                           |           |           |           |
|-----------------------------------------------------------|-----------|-----------|-----------|
| H                                                         | 1.347479  | -3.265991 | -0.975706 |
| C                                                         | -1.053005 | 0.304917  | 0.622502  |
| H                                                         | -1.267354 | 1.627167  | 0.548742  |
| C                                                         | -1.063375 | -0.538966 | 1.881514  |
| C                                                         | -2.245415 | 0.027313  | -0.320586 |
| C                                                         | -2.297642 | -1.397662 | -0.861779 |
| H                                                         | -3.155955 | 0.231502  | 0.246899  |
| H                                                         | -2.225921 | 0.729981  | -1.148329 |
| H                                                         | -0.351473 | -0.174617 | 2.621035  |
| H                                                         | -0.847178 | -1.593430 | 1.700508  |
| H                                                         | -2.055097 | -0.486172 | 2.332186  |
| H                                                         | -2.286425 | -2.143006 | -0.065678 |
| H                                                         | -1.455384 | -1.592564 | -1.526383 |
| H                                                         | -3.213138 | -1.544108 | -1.435201 |
| Rotational constants (GHz): 1.1679500 0.9642300 0.6741200 |           |           |           |
| Vibrational harmonic frequencies (cm-1):                  |           |           |           |
| i1596.2661                                                | 48.5999   | 69.0437   |           |
| 91.6087                                                   | 133.1715  | 169.3198  |           |
| 196.4377                                                  | 223.8996  | 238.3012  |           |
| 260.4449                                                  | 268.4839  | 280.2155  |           |
| 288.9251                                                  | 303.4277  | 329.9423  |           |
| 367.7034                                                  | 411.1140  | 448.2567  |           |
| 508.5541                                                  | 579.3931  | 642.5725  |           |
| 722.8645                                                  | 743.4343  | 783.9457  |           |
| 826.3382                                                  | 849.5496  | 919.1992  |           |
| 980.0282                                                  | 1010.1145 | 1019.4707 |           |
| 1028.3264                                                 | 1044.1034 | 1050.0056 |           |
| 1058.6439                                                 | 1092.0933 | 1121.9806 |           |
| 1133.3654                                                 | 1149.5505 | 1185.2881 |           |
| 1218.5070                                                 | 1271.0436 | 1305.7243 |           |
| 1316.4270                                                 | 1330.4179 | 1359.1884 |           |
| 1364.5361                                                 | 1371.9545 | 1404.6304 |           |
| 1411.5505                                                 | 1414.7258 | 1419.2606 |           |
| 1431.9153                                                 | 1486.8136 | 1490.1834 |           |
| 1496.6547                                                 | 1498.3787 | 1500.3112 |           |
| 1503.4898                                                 | 1505.0754 | 1509.2229 |           |
| 1511.8258                                                 | 1521.6990 | 1556.5990 |           |
| 1855.0026                                                 | 3055.5386 | 3057.3147 |           |
| 3059.1228                                                 | 3064.6714 | 3067.9804 |           |
| 3070.9323                                                 | 3073.3476 | 3098.8646 |           |
| 3115.1630                                                 | 3123.8908 | 3127.3616 |           |
| 3131.3757                                                 | 3132.1717 | 3146.5513 |           |
| 3151.6833                                                 | 3156.9358 | 3171.6906 |           |
| Zero-point correction (Hartree): 0.256151                 |           |           |           |
| TS.dic2H5CH3CH_COO.14Hshift.mmmtrS                        |           |           |           |
| ~~~~~                                                     |           |           |           |
| E(RM062X/Aug-CC-pVTZ) (Hartree): -504.03835596            |           |           |           |
| Electronic state : 1-A                                    |           |           |           |
| Cartesian coordinates (Angs):                             |           |           |           |
| C                                                         | 0.284718  | 0.431259  | 0.076206  |
| O                                                         | 0.220436  | 1.447111  | -0.728901 |
| O                                                         | -1.096443 | 1.900246  | -0.837720 |
| C                                                         | 1.677636  | 0.042339  | 0.466890  |
| C                                                         | 2.279862  | -0.836896 | -0.645184 |
| C                                                         | 2.564408  | 1.250567  | 0.760072  |
| H                                                         | 1.586427  | -0.574703 | 1.362098  |
| C                                                         | 1.458238  | -2.083005 | -0.949415 |
| H                                                         | 2.389967  | -0.227144 | -1.544408 |
| H                                                         | 3.285447  | -1.118166 | -0.327810 |
| H                                                         | 2.132031  | 1.880124  | 1.536660  |
| H                                                         | 2.692656  | 1.858364  | -0.133941 |
| H                                                         | 3.545593  | 0.914789  | 1.093529  |
| H                                                         | 0.482671  | -1.825233 | -1.362958 |
| H                                                         | 1.292023  | -2.670722 | -0.044860 |
| H                                                         | 1.967196  | -2.718210 | -1.672550 |
| C                                                         | -0.951310 | -0.041527 | 0.569397  |
| H                                                         | -1.389095 | 1.195127  | 0.270802  |
| C                                                         | -0.937604 | -0.760144 | 1.900894  |
| C                                                         | -1.916517 | -0.680837 | -0.456224 |
| C                                                         | -3.372546 | -0.301083 | -0.228415 |
| H                                                         | -1.623594 | -0.399242 | -1.465675 |
| H                                                         | -1.793158 | -1.764937 | -0.369205 |
| H                                                         | -0.568188 | -1.785663 | 1.807631  |
| H                                                         | -1.951578 | -0.817699 | 2.295750  |
| H                                                         | -0.332094 | -0.243263 | 2.644366  |
| H                                                         | -3.694044 | -0.542276 | 0.785060  |
| H                                                         | -4.025332 | -0.832648 | -0.920108 |
| H                                                         | -3.510188 | 0.768603  | -0.386744 |
| Rotational constants (GHz): 1.4383700 0.7714000 0.6722500 |           |           |           |
| Vibrational harmonic frequencies (cm-1):                  |           |           |           |
| i1608.8483                                                | 24.3559   | 74.4937   |           |
| 107.6701                                                  | 118.2901  | 172.6849  |           |
| 198.1799                                                  | 214.4931  | 222.8901  |           |
| 230.0863                                                  | 244.6933  | 260.0472  |           |
| 280.1336                                                  | 298.1572  | 316.3032  |           |
| 372.8156                                                  | 378.9399  | 449.5062  |           |
| 533.3931                                                  | 568.4386  | 646.8780  |           |
| 736.6794                                                  | 766.6810  | 793.9646  |           |
| 826.4480                                                  | 852.1267  | 922.8577  |           |
| 974.1271                                                  | 1000.2109 | 1020.8695 |           |
| 1027.1349                                                 | 1039.4599 | 1043.7397 |           |
| 1065.7977                                                 | 1102.8011 | 1126.6402 |           |
| 1137.8072                                                 | 1137.9540 | 1191.7978 |           |
| 1216.1432                                                 | 1277.9840 | 1300.3279 |           |
| 1321.2899                                                 | 1336.4978 | 1347.8107 |           |
| 1360.4831                                                 | 1377.7060 | 1410.7689 |           |
| 1412.1686                                                 | 1417.1769 | 1418.6755 |           |
| 1441.1172                                                 | 1478.1019 | 1490.2082 |           |
| 1497.0650                                                 | 1499.4846 | 1499.9179 |           |
| 1500.9677                                                 | 1505.2632 | 1506.8972 |           |
| 1508.5553                                                 | 1512.0158 | 1567.4995 |           |

|           |           |           |
|-----------|-----------|-----------|
| 1862.5293 | 3040.0274 | 3041.2562 |
| 3059.0584 | 3062.8209 | 3063.4982 |
| 3070.7418 | 3088.2312 | 3104.1256 |
| 3111.3243 | 3119.4897 | 3129.2082 |
| 3135.1119 | 3135.9668 | 3139.7274 |
| 3140.2579 | 3142.7226 | 3151.7759 |

Zero-point correction (Hartree): 0.255796

TS.dic2H5CH3CH\_COO.14Hshift.mpmprS

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E(RM062X/Aug-CC-pVTZ) (Hartree): -504.03770824

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.172602 | -0.612701 | 0.152210  |
| O | -0.388229 | -1.578108 | -0.687559 |
| O | 0.792100  | -2.276799 | -0.946726 |
| C | -1.403420 | 0.013400  | 0.731814  |
| C | -1.468566 | 1.489224  | 0.291581  |
| C | -2.681481 | -0.756424 | 0.417896  |
| H | -1.243595 | 0.011191  | 1.813965  |
| C | -1.630976 | 1.665967  | -1.213407 |
| H | -2.302548 | 1.958935  | 0.815798  |
| H | -0.561360 | 1.995520  | 0.625478  |
| H | -2.638207 | -1.767797 | 0.817201  |
| H | -2.845885 | -0.835559 | -0.654704 |
| H | -3.534170 | -0.242980 | 0.861205  |
| H | -2.588933 | 1.281580  | -1.560803 |
| H | -0.845441 | 1.140283  | -1.760651 |
| H | -1.577929 | 2.719340  | -1.484954 |
| C | 1.173536  | -0.412886 | 0.539851  |
| H | 1.332467  | -1.691839 | 0.120823  |
| C | 1.409233  | 0.156323  | 1.924098  |
| C | 2.155840  | 0.118526  | -0.527536 |
| C | 2.192205  | 1.642465  | -0.601902 |
| H | 3.152943  | -0.255348 | -0.284822 |
| H | 1.894432  | -0.294328 | -1.498522 |
| H | 0.880075  | -0.409940 | 2.689615  |
| H | 1.114899  | 1.204577  | 2.017675  |
| H | 2.473631  | 0.101402  | 2.155626  |
| H | 2.488767  | 2.090306  | 0.346481  |
| H | 1.216762  | 2.046213  | -0.876801 |
| H | 2.910509  | 1.964349  | -1.355958 |

Rotational constants (GHz): 1.2399600 0.9040500 0.7353500

Vibrational harmonic frequencies (cm-1):

|            |           |           |
|------------|-----------|-----------|
| 11595.6090 | 60.9321   | 72.7055   |
| 95.8189    | 158.2849  | 180.4038  |
| 195.7687   | 223.7193  | 228.5663  |
| 233.8411   | 265.5142  | 289.1913  |
| 298.4467   | 303.2377  | 309.6937  |
| 357.7062   | 420.5368  | 475.0029  |
| 538.1323   | 575.0717  | 635.1066  |
| 728.2030   | 758.4649  | 784.6518  |
| 819.9366   | 846.0514  | 918.7882  |
| 981.6665   | 1003.9430 | 1007.8670 |
| 1016.3071  | 1028.9493 | 1044.7067 |
| 1050.3976  | 1087.2417 | 1113.8575 |
| 1139.8879  | 1149.5642 | 1190.5167 |
| 1219.1673  | 1280.8991 | 1299.9122 |
| 1302.4666  | 1323.2311 | 1359.8172 |
| 1364.5083  | 1371.9042 | 1406.7566 |
| 1415.8884  | 1419.7157 | 1422.6716 |
| 1436.9966  | 1484.6765 | 1489.1746 |
| 1496.1223  | 1497.3126 | 1501.3986 |
| 1501.9994  | 1502.6757 | 1509.9326 |
| 1517.0719  | 1518.6353 | 1555.7363 |
| 1868.7727  | 3047.2906 | 3057.7249 |
| 3060.1424  | 3061.0922 | 3064.2118 |
| 3071.3447  | 3076.6794 | 3103.0317 |
| 3107.3566  | 3125.0253 | 3127.2848 |
| 3130.2860  | 3130.4666 | 3141.7227 |
| 3148.2089  | 3149.2505 | 3158.7626 |

Zero-point correction (Hartree): 0.256103

TS.dic2H5CH3CH\_COO.14Hshift.mpmtrS

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E(RM062X/Aug-CC-pVTZ) (Hartree): -504.03859706

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.225086  | 0.400373  | 0.296201  |
| O | 0.199951  | 1.587332  | -0.227849 |
| O | -1.115693 | 2.045719  | -0.332345 |
| C | 1.577374  | -0.102467 | 0.689301  |
| C | 1.916670  | -1.321077 | -0.194525 |
| C | 2.658673  | 0.971709  | 0.666352  |
| H | 1.464330  | -0.474165 | 1.711448  |
| C | 2.028241  | -0.988401 | -1.677380 |
| H | 2.854996  | -1.744613 | 0.167662  |
| H | 1.148952  | -2.083256 | -0.049992 |
| H | 2.424597  | 1.777375  | 1.359564  |
| H | 2.762793  | 1.412050  | -0.323016 |
| H | 3.614437  | 0.533408  | 0.951941  |
| H | 2.836237  | -0.284695 | -1.872360 |
| H | 1.103154  | -0.546869 | -2.052512 |
| H | 2.225683  | -1.888487 | -2.257408 |
| C | -1.033956 | -0.189891 | 0.544190  |
| H | -1.484862 | 1.089777  | 0.508725  |
| C | -1.117310 | -1.212426 | 1.656212  |
| C | -1.862707 | -0.572707 | -0.703881 |
| C | -3.353948 | -0.318638 | -0.535959 |
| H | -1.500266 | -0.023819 | -1.570664 |
| H | -1.680606 | -1.635910 | -0.891814 |
| H | -0.631849 | -0.869953 | 2.569232  |

|                                           |           |           |           |                     |
|-------------------------------------------|-----------|-----------|-----------|---------------------|
| H                                         | -0.677296 | -2.173579 | 1.374265  |                     |
| H                                         | -2.162294 | -1.399878 | 1.901153  |                     |
| H                                         | -3.751005 | -0.830446 | 0.340875  |                     |
| H                                         | -3.908746 | -0.669594 | -1.405600 |                     |
| H                                         | -3.541056 | 0.749394  | -0.423013 |                     |
| Rotational constants (GHz):               |           |           | 1.4965000 | 0.7506200 0.6756900 |
| Vibrational harmonic frequencies (cm-1):  |           |           |           |                     |
| i1608.5517                                | 46.6443   |           | 65.5520   |                     |
| 83.8307                                   | 108.2733  |           | 170.9382  |                     |
| 184.4794                                  | 215.1983  |           | 219.5338  |                     |
| 226.3994                                  | 273.9770  |           | 281.0068  |                     |
| 289.1621                                  | 299.7242  |           | 312.6191  |                     |
| 360.4355                                  | 387.7082  |           | 470.6657  |                     |
| 553.4984                                  | 571.3355  |           | 624.3748  |                     |
| 740.2759                                  | 769.9262  |           | 787.6579  |                     |
| 813.7361                                  | 843.7527  |           | 919.4478  |                     |
| 980.4054                                  | 1004.0010 |           | 1005.5120 |                     |
| 1019.6715                                 | 1027.8502 |           | 1041.2238 |                     |
| 1058.4653                                 | 1095.9528 |           | 1112.6294 |                     |
| 1136.1552                                 | 1148.8372 |           | 1188.0892 |                     |
| 1217.9333                                 | 1279.8310 |           | 1295.1088 |                     |
| 1302.4931                                 | 1332.9513 |           | 1345.7732 |                     |
| 1366.9200                                 | 1371.6359 |           | 1409.9301 |                     |
| 1417.2397                                 | 1418.3226 |           | 1422.4131 |                     |
| 1440.3170                                 | 1475.6964 |           | 1484.7029 |                     |
| 1494.3739                                 | 1497.8880 |           | 1499.8479 |                     |
| 1500.6009                                 | 1501.8763 |           | 1506.8434 |                     |
| 1510.3542                                 | 1518.2309 |           | 1560.5359 |                     |
| 1868.5455                                 | 3034.0822 |           | 3040.1282 |                     |
| 3061.4455                                 | 3063.1741 |           | 3065.1215 |                     |
| 3070.8978                                 | 3076.7819 |           | 3102.3487 |                     |
| 3110.3884                                 | 3119.3227 |           | 3132.5015 |                     |
| 3135.1704                                 | 3135.8406 |           | 3140.3189 |                     |
| 3143.3364                                 | 3148.2020 |           | 3158.5411 |                     |
| Zero-point correction (Hartree): 0.255649 |           |           |           |                     |

TS.diC2H5CH3CH\_COO.14Hshift.mppmRS

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E(RM062X/Aug-CC-pVTZ) (Hartree): -504.03372676

Electronic state : 1-A

Cartesian coordinates (Angs):

|                                           |           |           |           |                     |
|-------------------------------------------|-----------|-----------|-----------|---------------------|
| C                                         | 0.067476  | -0.588653 | -0.224366 |                     |
| O                                         | 0.412614  | -1.453842 | 0.681276  |                     |
| O                                         | -0.651251 | -1.719432 | 1.545744  |                     |
| C                                         | 1.232094  | 0.028208  | -0.939797 |                     |
| C                                         | 1.682396  | 1.320594  | -0.216847 |                     |
| C                                         | 2.388955  | -0.961045 | -1.085738 |                     |
| H                                         | 0.882438  | 0.310659  | -1.934618 |                     |
| C                                         | 1.917596  | 1.155199  | 1.279777  |                     |
| H                                         | 2.600788  | 1.651220  | -0.706277 |                     |
| H                                         | 0.942319  | 2.103029  | -0.383111 |                     |
| H                                         | 2.069723  | -1.872266 | -1.589091 |                     |
| H                                         | 2.795923  | -1.242026 | -0.117196 |                     |
| H                                         | 3.180826  | -0.500624 | -1.674914 |                     |
| H                                         | 2.642251  | 0.369887  | 1.491488  |                     |
| H                                         | 0.995690  | 0.896319  | 1.802641  |                     |
| H                                         | 2.295729  | 2.083618  | 1.705330  |                     |
| C                                         | -1.295721 | -0.211733 | -0.226839 |                     |
| H                                         | -1.274258 | -0.632967 | 1.054909  |                     |
| C                                         | -2.304938 | -1.300985 | -0.636941 |                     |
| C                                         | -1.651738 | 1.173707  | -0.743573 |                     |
| C                                         | -1.791869 | 2.199584  | 0.379739  |                     |
| H                                         | -0.917275 | 1.525961  | -1.472815 |                     |
| H                                         | -2.596296 | 1.111283  | -1.285964 |                     |
| H                                         | -1.988950 | -2.289891 | -0.320718 |                     |
| H                                         | -2.420834 | -1.290374 | -1.722349 |                     |
| H                                         | -3.277145 | -1.091877 | -0.191231 |                     |
| H                                         | -2.049478 | 3.184626  | -0.009895 |                     |
| H                                         | -0.865766 | 2.287687  | 0.948740  |                     |
| H                                         | -2.572096 | 1.892673  | 1.076414  |                     |
| Rotational constants (GHz):               |           |           | 1.2299100 | 0.9219200 0.7286300 |
| Vibrational harmonic frequencies (cm-1):  |           |           |           |                     |
| i1615.3356                                | 66.8486   |           | 80.0379   |                     |
| 109.4648                                  | 140.5132  |           | 169.1169  |                     |
| 185.2956                                  | 206.5526  |           | 225.6708  |                     |
| 240.7267                                  | 245.9492  |           | 253.1627  |                     |
| 297.7886                                  | 323.1310  |           | 336.9425  |                     |
| 368.1774                                  | 416.5702  |           | 477.2921  |                     |
| 542.4194                                  | 555.3891  |           | 685.4446  |                     |
| 750.7777                                  | 754.4973  |           | 782.8513  |                     |
| 797.1061                                  | 849.8045  |           | 940.6545  |                     |
| 982.5526                                  | 996.4689  |           | 1008.4920 |                     |
| 1015.6468                                 | 1034.4484 |           | 1042.4769 |                     |
| 1060.0950                                 | 1104.9944 |           | 1116.7560 |                     |
| 1134.4636                                 | 1141.7310 |           | 1189.1900 |                     |
| 1214.4472                                 | 1282.1604 |           | 1294.8473 |                     |
| 1311.5460                                 | 1318.5699 |           | 1361.5572 |                     |
| 1367.4088                                 | 1375.3416 |           | 1397.0458 |                     |
| 1410.1222                                 | 1412.4815 |           | 1426.0837 |                     |
| 1439.4491                                 | 1484.6958 |           | 1494.1610 |                     |
| 1496.2997                                 | 1497.9478 |           | 1502.0343 |                     |
| 1503.4894                                 | 1504.9281 |           | 1509.2999 |                     |
| 1513.1884                                 | 1517.7275 |           | 1559.7935 |                     |
| 1857.9849                                 | 3053.3608 |           | 3056.5814 |                     |
| 3059.5960                                 | 3064.0248 |           | 3068.0182 |                     |
| 3075.5246                                 | 3077.4325 |           | 3090.2596 |                     |
| 3112.6444                                 | 3118.9909 |           | 3130.6848 |                     |
| 3131.6042                                 | 3134.4504 |           | 3143.1411 |                     |
| 3145.3439                                 | 3162.0089 |           | 3178.9322 |                     |
| Zero-point correction (Hartree): 0.256259 |           |           |           |                     |

TS.diC2H5CH3CH\_COO.14Hshift.mpppRS

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E(RM062X/Aug-CC-pVTZ) (Hartree): -504.03298331
Electronic state : 1-A
Cartesian coordinates (Angs):
C      0.060776      -0.497812      -0.265436
O      0.521609      -1.690439      -0.024426
O     -0.352183      -2.414521       0.785276
C      1.101475       0.430635      -0.826814
C      1.614963       1.398845       0.265700
C      2.261655      -0.332228      -1.467451
H      0.609494       1.024743      -1.598071
C      1.957131       0.711802       1.582328
H      2.501028       1.888249      -0.142471
H      0.881609       2.185247       0.437870
H      1.909680      -1.046303      -2.209672
H      2.834899      -0.882745      -0.724568
H      2.924104       0.379223      -1.958217
H      2.664401      -0.104328       1.436961
H      1.066381       0.290696       2.052238
H      2.401045       1.420375       2.279662
C     -1.243474      -0.244685       0.224273
H     -0.983459      -1.284946       1.058097
C     -2.382034      -1.016584      -0.467514
C     -1.643407       1.162997       0.630980
C     -1.869411       2.163640      -0.503423
H     -2.576304       1.062957       1.190938
H     -0.921699       1.568223       1.340594
H     -2.062001      -1.999125      -0.799994
H     -2.741805      -0.455381      -1.331228
H     -3.214707      -1.145496       0.224048
H     -2.579416       1.780139      -1.235448
H     -0.944220       2.399112      -1.028765
H     -2.270477       3.099380      -0.114628
Rotational constants (GHz):      1.1951000      0.9610100      0.7125100
Vibrational harmonic frequencies (cm-1):
11606.8146      60.1217      91.4395
100.5436      139.0953      161.0462
182.1240      203.5542      237.0873
247.8066      248.5699      259.9174
291.3834      329.7943      337.7026
345.7719      399.6470      452.6752
523.9887      633.0168      678.5460
736.4099      756.2772      781.4877
797.9155      850.8125      940.2275
971.5073      998.6496      1008.9975
1010.3272      1035.2942      1037.4144
1058.0557      1094.0679      1113.6433
1134.4991      1144.2731      1191.8292
1214.2586      1278.7023      1299.2768
1307.8095      1322.6670      1356.9359
1369.1882      1371.0042      1395.5027
1408.8623      1414.4824      1424.9622
1433.0513      1480.0902      1494.7297
1496.7029      1500.6161      1501.3149
1505.7304      1505.9214      1508.9137
1513.7553      1523.3177      1555.3266
1870.0719      3059.7838      3061.4423
3062.7316      3068.5777      3073.8263
3077.0726      3085.5846      3102.8217
3117.8692      3119.4038      3132.9712
3133.5205      3140.7399      3143.2476
3148.4794      3158.0285      3175.0706
Zero-point correction (Hartree): 0.256294

TS.dic2H5CH3CH_COO.14Hshift.mpptRS
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E(RM062X/Aug-CC-pVTZ) (Hartree): -504.03423679
Electronic state : 1-A
Cartesian coordinates (Angs):
C 0.154341 -0.395244 -0.247471
O 0.631038 -1.433089 0.369754
O -0.345163 -2.010590 1.187444
C 1.200402 0.504769 -0.832779
C 1.840477 1.406536 0.248260
C 2.252919 -0.308859 -1.590255
H 0.687651 1.159600 -1.539061
C 2.566687 0.673041 1.369073
H 2.537084 2.066192 -0.274089
H 1.071813 2.048894 0.678919
H 1.801627 -0.866096 -2.409934
H 2.749149 -1.020391 -0.934725
H 3.002526 0.365181 -2.003747
H 3.357308 0.029591 0.985308
H 1.886275 0.053362 1.950832
H 3.026041 1.394473 2.043630
C -1.229926 -0.165185 -0.084192
H -1.077638 -0.881061 1.045001
C -2.175092 -1.216045 -0.698170
C -1.721222 1.258520 -0.262815
C -3.063690 1.492177 0.424560
H -0.994372 1.964626 0.138461
H -1.823065 1.485843 -1.330261
H -1.685247 -2.177584 -0.813027
H -2.502960 -0.861572 -1.678207
H -3.056927 -1.363590 -0.077035
H -3.845267 0.871333 -0.011713
H -3.373370 2.531938 0.329109
H -2.997010 1.250430 1.485696
Rotational constants (GHz): 1.4007400 0.7559000 0.6521400
Vibrational harmonic frequencies (cm-1):
11616.5391 24.3468 69.1074
84.6885 99.1768 141.0573

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|           |           |           |
|-----------|-----------|-----------|
| 167.6109  | 212.7153  | 218.1151  |
| 226.9586  | 266.9185  | 277.3438  |
| 293.5583  | 313.2340  | 319.2510  |
| 347.8562  | 374.2041  | 472.5626  |
| 542.9970  | 574.0079  | 682.1085  |
| 748.8069  | 754.1863  | 792.1626  |
| 799.4073  | 849.0752  | 952.4198  |
| 973.1985  | 989.9330  | 1007.1302 |
| 1016.2201 | 1029.1104 | 1035.5053 |
| 1071.4716 | 1108.5038 | 1120.5536 |
| 1137.9874 | 1146.2594 | 1188.9598 |
| 1221.3804 | 1292.8799 | 1296.8314 |
| 1314.7554 | 1318.6613 | 1350.8637 |
| 1376.9169 | 1381.7765 | 1397.4795 |
| 1409.4870 | 1412.1195 | 1425.8949 |
| 1443.8654 | 1481.5225 | 1487.0498 |
| 1493.7976 | 1498.7081 | 1499.8853 |
| 1503.5041 | 1507.4771 | 1509.7852 |
| 1517.0104 | 1519.5676 | 1567.5968 |
| 1856.5693 | 3022.6872 | 3053.8126 |
| 3060.8750 | 3065.5236 | 3071.7419 |
| 3074.2767 | 3083.1294 | 3098.7402 |
| 3110.6262 | 3125.6550 | 3135.7535 |
| 3138.6715 | 3141.6019 | 3141.8880 |
| 3148.8905 | 3162.8461 | 3176.8985 |

Zero-point correction (Hartree): 0.255901

TS.dic2H5CH3CH\_COO.14Hshift.mtmpRS

E(RM062X/Aug-CC-pVTZ) (Hartree): -504.03656776

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.132316 | 0.650369  | 0.110938  |
| O | -0.365077 | 1.794921  | -0.453305 |
| O | -1.715619 | 2.129000  | -0.346761 |
| C | 1.315990  | 0.338546  | 0.335849  |
| C | 1.687099  | -0.908536 | -0.487829 |
| C | 2.234623  | 1.524170  | 0.063751  |
| H | 1.391594  | 0.060630  | 1.392685  |
| C | 3.106276  | -1.396151 | -0.226950 |
| H | 0.979139  | -1.705566 | -0.256470 |
| H | 1.560144  | -0.674343 | -1.548229 |
| H | 1.905476  | 2.409099  | 0.604049  |
| H | 2.246152  | 1.767527  | -0.998877 |
| H | 3.250508  | 1.290820  | 0.374723  |
| H | 3.270405  | -1.556832 | 0.840038  |
| H | 3.849248  | -0.681840 | -0.577679 |
| H | 3.287570  | -2.339498 | -0.739656 |
| C | -1.261175 | -0.042245 | 0.610506  |
| H | -1.840268 | 1.182931  | 0.587361  |
| C | -1.026937 | -0.951659 | 1.800235  |
| C | -2.279520 | -0.605689 | -0.404296 |
| C | -1.866853 | -1.954630 | -0.986693 |
| H | -3.235245 | -0.710498 | 0.113639  |
| H | -2.431281 | 0.110873  | -1.206727 |
| H | -0.522056 | -0.432830 | 2.614243  |
| H | -0.441316 | -1.841758 | 1.556564  |
| H | -1.989085 | -1.296495 | 2.180338  |
| H | -1.695427 | -2.700732 | -0.210264 |
| H | -0.953994 | -1.860908 | -1.575743 |
| H | -2.649119 | -2.337000 | -1.642540 |

Rotational constants (GHz): 1.2840600 0.8301000 0.6235200

Vibrational harmonic frequencies (cm-1):

|            |           |           |
|------------|-----------|-----------|
| i1600.9115 | 47.8240   | 70.3691   |
| 91.4886    | 114.2303  | 184.6989  |
| 196.5983   | 215.8203  | 221.7750  |
| 231.6228   | 267.2071  | 281.8202  |
| 295.0389   | 309.4080  | 323.1016  |
| 354.4331   | 406.8586  | 446.5956  |
| 502.3226   | 586.4364  | 646.5937  |
| 728.6813   | 768.8945  | 790.0283  |
| 815.9989   | 851.9961  | 921.6959  |
| 971.7466   | 999.1157  | 1007.2773 |
| 1016.9003  | 1042.2811 | 1048.7769 |
| 1061.0411  | 1088.9366 | 1112.4011 |
| 1134.4999  | 1163.3396 | 1196.5844 |
| 1219.6926  | 1273.6581 | 1298.6028 |
| 1320.8634  | 1329.8580 | 1352.7303 |
| 1361.3817  | 1373.4539 | 1407.0960 |
| 1413.1736  | 1415.7029 | 1419.2786 |
| 1434.7289  | 1484.2695 | 1491.2562 |
| 1497.0875  | 1497.2766 | 1501.7860 |
| 1503.7991  | 1504.1380 | 1511.0812 |
| 1512.8802  | 1517.4932 | 1554.6396 |
| 1863.2478  | 3042.4857 | 3047.1690 |
| 3057.6852  | 3060.3543 | 3063.4965 |
| 3066.1809  | 3075.8511 | 3102.3694 |
| 3106.6924  | 3124.5595 | 3129.9176 |
| 3131.0144  | 3132.0343 | 3143.2042 |
| 3148.3937  | 3153.8993 | 3160.0266 |

Zero-point correction (Hartree): 0.255881

TS.dic2H5CH3CH\_COO.14Hshift.mtmRS

E(RM062X/Aug-CC-pVTZ) (Hartree): -504.03804828

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.034543  | 0.490687  | 0.163801  |
| O | -0.233199 | 1.702517  | -0.213761 |
| O | -1.609631 | 1.935627  | -0.154284 |
| C | 1.483022  | 0.187658  | 0.375214  |
| C | 1.917710  | -0.784500 | -0.739924 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 2.358236  | 1.432729  | 0.453109  |
| H | 1.539275  | -0.358664 | 1.321711  |
| C | 3.329237  | -1.321854 | -0.545676 |
| H | 1.209897  | -1.615108 | -0.777104 |
| H | 1.841813  | -0.264454 | -1.698147 |
| H | 1.974907  | 2.136108  | 1.189637  |
| H | 2.389870  | 1.942498  | -0.509791 |
| H | 3.373918  | 1.162544  | 0.733957  |
| H | 3.435292  | -1.786257 | 0.436117  |
| H | 4.074394  | -0.532146 | -0.627005 |
| H | 3.561232  | -2.073186 | -1.298912 |
| C | -1.080014 | -0.329046 | 0.445815  |
| H | -1.730946 | 0.850989  | 0.602124  |
| C | -0.871835 | -1.465505 | 1.422816  |
| C | -1.966686 | -0.717610 | -0.760361 |
| C | -3.453812 | -0.718938 | -0.436467 |
| H | -1.778807 | -0.041208 | -1.591416 |
| H | -1.650083 | -1.716941 | -1.075707 |
| H | -0.384878 | -1.138449 | 2.340670  |
| H | -0.279624 | -2.279280 | 0.992462  |
| H | -1.836551 | -1.886795 | 1.703755  |
| H | -3.676682 | -1.362436 | 0.414981  |
| H | -4.036871 | -1.075662 | -1.285044 |
| H | -3.785913 | 0.291573  | -0.197892 |

Rotational constants (GHz): 1.6018300 0.6932000 0.5672600

Vibrational harmonic frequencies (cm-1):

|            |           |           |
|------------|-----------|-----------|
| i1596.0941 | 49.6825   | 72.1106   |
| 78.6501    | 105.7422  | 171.3558  |
| 203.7111   | 216.0624  | 219.3588  |
| 224.2059   | 273.3026  | 274.2538  |
| 292.4117   | 300.3580  | 320.7438  |
| 358.0126   | 377.8086  | 426.7988  |
| 530.0619   | 578.9034  | 645.7301  |
| 743.2055   | 777.0416  | 787.4311  |
| 810.5480   | 849.7257  | 923.1989  |
| 972.9530   | 999.5341  | 1005.6771 |
| 1020.7750  | 1040.1131 | 1050.5357 |
| 1067.4295  | 1096.9223 | 1116.7653 |
| 1129.4866  | 1157.6110 | 1194.5809 |
| 1218.5246  | 1273.5856 | 1293.5470 |
| 1323.6972  | 1334.9321 | 1346.5198 |
| 1359.1519  | 1374.7345 | 1410.8153 |
| 1413.2020  | 1416.8853 | 1419.1623 |
| 1441.2928  | 1476.1980 | 1487.5752 |
| 1496.0394  | 1497.2519 | 1499.5018 |
| 1501.7182  | 1503.7241 | 1508.2117 |
| 1510.1527  | 1516.6311 | 1562.6404 |
| 1868.2875  | 3034.8550 | 3038.1961 |
| 3051.1984  | 3061.1519 | 3062.1482 |
| 3064.1147  | 3075.6835 | 3094.7607 |
| 3108.5988  | 3119.9247 | 3132.5023 |
| 3134.9302  | 3135.9788 | 3140.2830 |
| 3142.6885  | 3147.5003 | 3157.3423 |

Zero-point correction (Hartree): 0.255653

TS.diC2H5CH3CH\_COO.14Hshift.mtppRS

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E(RM062X/Aug-CC-pVTZ) (Hartree): -504.03145032

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.320668  | -0.564558 | 0.083238  |
| O | 0.521079  | -1.820155 | -0.191118 |
| O | 1.742026  | -2.005746 | -0.839915 |
| C | -1.098076 | -0.267959 | 0.477272  |
| C | -1.872977 | 0.237112  | -0.755485 |
| C | -1.774362 | -1.482418 | 1.113988  |
| H | -1.060857 | 0.538724  | 1.210798  |
| C | -3.294374 | 0.671598  | -0.420358 |
| H | -1.339236 | 1.075986  | -1.200458 |
| H | -1.884603 | -0.561922 | -1.500332 |
| H | -1.163930 | -1.899274 | 1.913014  |
| H | -1.943487 | -2.265347 | 0.376120  |
| H | -2.732792 | -1.190550 | 1.537489  |
| H | -3.294044 | 1.411490  | 0.382344  |
| H | -3.910309 | -0.168400 | -0.104110 |
| H | -3.770901 | 1.121924  | -1.289749 |
| C | 1.405127  | 0.295955  | -0.213669 |
| H | 1.795127  | -0.703076 | -1.046524 |
| C | 2.651221  | 0.106634  | 0.674687  |
| C | 1.173638  | 1.754076  | -0.577295 |
| C | 0.552845  | 2.648037  | 0.499232  |
| H | 2.157557  | 2.154638  | -0.830503 |
| H | 0.588009  | 1.829161  | -1.493841 |
| H | 2.736380  | -0.908601 | 1.049639  |
| H | 2.599046  | 0.791474  | 1.523513  |
| H | 3.553759  | 0.336292  | 0.108735  |
| H | 1.005285  | 2.468200  | 1.475197  |
| H | -0.520684 | 2.485725  | 0.591971  |
| H | 0.698567  | 3.699907  | 0.255295  |

Rotational constants (GHz): 1.2570300 0.8728500 0.6077800

Vibrational harmonic frequencies (cm-1):

|            |           |           |
|------------|-----------|-----------|
| i1608.8312 | 50.1197   | 70.6594   |
| 104.3794   | 125.2398  | 159.2611  |
| 170.9229   | 211.9189  | 231.5044  |
| 232.9897   | 260.3390  | 276.2655  |
| 295.8932   | 319.0408  | 322.0164  |
| 347.9881   | 385.0813  | 419.4536  |
| 502.5099   | 641.4496  | 697.7517  |
| 735.3519   | 751.8721  | 784.6659  |
| 788.1066   | 866.4479  | 943.8291  |
| 970.1619   | 984.2308  | 1005.1100 |
| 1011.2151  | 1037.3607 | 1054.5203 |

|           |           |           |
|-----------|-----------|-----------|
| 1067.4217 | 1093.2398 | 1113.9790 |
| 1132.8316 | 1164.6221 | 1185.2154 |
| 1212.6233 | 1284.7329 | 1300.3267 |
| 1321.0169 | 1323.9739 | 1359.1874 |
| 1360.0974 | 1373.2559 | 1396.6860 |
| 1409.3784 | 1413.9516 | 1416.6045 |
| 1434.2270 | 1485.9291 | 1491.2446 |
| 1494.3378 | 1497.8960 | 1500.6818 |
| 1504.9979 | 1506.0742 | 1508.8382 |
| 1519.3760 | 1520.4179 | 1555.1300 |
| 1876.7175 | 3054.6704 | 3060.0894 |
| 3063.3129 | 3065.2431 | 3067.2734 |
| 3077.5821 | 3089.3885 | 3098.5496 |
| 3116.8392 | 3117.9671 | 3131.1613 |
| 3131.6462 | 3137.5239 | 3145.6576 |
| 3149.7403 | 3159.4272 | 3174.2379 |

Zero-point correction (Hartree): 0.256118

TS.dic2H5CH3CH\_COO.14Hshift.mtptRS

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E(RM062X/Aug-CC-pVTZ) (Hartree): -504.03519074

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.006329  | -0.560789 | 0.082225  |
| O | -0.137364 | -1.669061 | -0.576356 |
| O | 1.053249  | -2.013184 | -1.221932 |
| C | -1.288409 | 0.067298  | 0.499955  |
| C | -2.027802 | 0.601405  | -0.740302 |
| C | -2.130930 | -0.940460 | 1.287975  |
| H | -1.040978 | 0.909384  | 1.148998  |
| C | -3.280684 | 1.392314  | -0.388909 |
| H | -1.346588 | 1.233500  | -1.313483 |
| H | -2.277247 | -0.247067 | -1.379890 |
| H | -1.564611 | -1.362423 | 2.117253  |
| H | -2.448437 | -1.757376 | 0.641067  |
| H | -3.013959 | -0.453809 | 1.696536  |
| H | -3.048748 | 2.203319  | 0.303552  |
| H | -4.038718 | 0.761549  | 0.072966  |
| H | -3.719770 | 1.832272  | -1.283001 |
| C | 1.308490  | -0.011995 | 0.097793  |
| H | 1.484878  | -0.749661 | -1.014346 |
| C | 2.385514  | -0.795021 | 0.869889  |
| C | 1.408003  | 1.491921  | 0.272612  |
| C | 2.725770  | 2.044460  | -0.263055 |
| H | 0.583291  | 1.985884  | -0.244035 |
| H | 1.315969  | 1.753602  | 1.333010  |
| H | 2.143883  | -1.851271 | 0.932325  |
| H | 2.464349  | -0.385276 | 1.879641  |
| H | 3.357817  | -0.702989 | 0.388692  |
| H | 3.575513  | 1.645681  | 0.289732  |
| H | 2.754918  | 3.129940  | -0.179253 |
| H | 2.853667  | 1.777908  | -1.312549 |

Rotational constants (GHz): 1.3492900 0.7341800 0.5787800

Vibrational harmonic frequencies (cm-1):

|            |           |           |
|------------|-----------|-----------|
| i1612.0760 | 44.2997   | 68.8306   |
| 85.8397    | 93.2602   | 144.5450  |
| 167.7206   | 199.8200  | 213.6281  |
| 222.3406   | 247.0993  | 281.5621  |
| 286.5603   | 298.8467  | 324.7603  |
| 352.0235   | 368.9351  | 427.2248  |
| 546.1444   | 560.3469  | 697.8307  |
| 753.3312   | 756.9192  | 788.4264  |
| 800.5332   | 866.5381  | 952.2383  |
| 973.3951   | 985.5160  | 999.1584  |
| 1014.8272  | 1028.3065 | 1056.0143 |
| 1071.9202  | 1103.9465 | 1125.0669 |
| 1133.0599  | 1159.8515 | 1195.1006 |
| 1221.0509  | 1287.0548 | 1301.9747 |
| 1320.2871  | 1331.2035 | 1356.3041 |
| 1363.4036  | 1381.0690 | 1395.6214 |
| 1408.3991  | 1411.2429 | 1414.1032 |
| 1441.9714  | 1484.5866 | 1489.9493 |
| 1495.0245  | 1497.7174 | 1498.9394 |
| 1505.0780  | 1506.9403 | 1510.0973 |
| 1516.1317  | 1516.5585 | 1567.5511 |
| 1857.8305  | 3021.7366 | 3053.4977 |
| 3061.3312  | 3064.0612 | 3065.7396 |
| 3072.0502  | 3078.6032 | 3087.6330 |
| 3103.3632  | 3124.8992 | 3131.7362 |
| 3135.8189  | 3140.9639 | 3141.3159 |
| 3144.0691  | 3156.8883 | 3176.3676 |

Zero-point correction (Hartree): 0.255692

TS.dic2H5CH3CH\_COO.14Hshift.pmmprS

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E(RM062X/Aug-CC-pVTZ) (Hartree): -504.03641387

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.121925 | -0.345934 | -0.410262 |
| O | -0.178355 | -1.487388 | -1.032570 |
| O | 0.672121  | -2.421634 | -0.444291 |
| C | -1.238563 | 0.572848  | -0.808562 |
| C | -2.297474 | 0.701930  | 0.300422  |
| C | -0.706479 | 1.936845  | -1.244003 |
| H | -1.721068 | 0.085783  | -1.659354 |
| C | -2.750412 | -0.639895 | 0.859084  |
| H | -1.915177 | 1.341094  | 1.096406  |
| H | -3.146047 | 1.230945  | -0.137401 |
| H | -0.028821 | 1.846106  | -2.091986 |
| H | -0.171299 | 2.427911  | -0.431529 |
| H | -1.537060 | 2.577964  | -1.538711 |
| H | -1.930657 | -1.161812 | 1.356434  |

|                                                           |           |           |           |
|-----------------------------------------------------------|-----------|-----------|-----------|
| H                                                         | -3.110856 | -1.290566 | 0.061592  |
| H                                                         | -3.554239 | -0.510447 | 1.581896  |
| C                                                         | 0.838575  | -0.264666 | 0.626650  |
| H                                                         | 0.777726  | -1.619919 | 0.603974  |
| C                                                         | 0.564170  | 0.643690  | 1.807994  |
| C                                                         | 2.320066  | -0.263463 | 0.185046  |
| C                                                         | 2.827054  | 1.135417  | -0.153475 |
| H                                                         | 2.914835  | -0.681261 | 1.000147  |
| H                                                         | 2.448442  | -0.923428 | -0.668850 |
| H                                                         | -0.356448 | 0.374562  | 2.322617  |
| H                                                         | 0.508719  | 1.703435  | 1.548908  |
| H                                                         | 1.378900  | 0.534973  | 2.525148  |
| H                                                         | 2.748022  | 1.813012  | 0.696828  |
| H                                                         | 2.259168  | 1.565019  | -0.979851 |
| H                                                         | 3.875654  | 1.098164  | -0.448746 |
| Rotational constants (GHz): 1.3129000 0.8626100 0.7227900 |           |           |           |
| Vibrational harmonic frequencies (cm-1):                  |           |           |           |
| i1612.3496                                                | 63.5815   |           | 77.3661   |
| 103.1208                                                  | 145.8735  |           | 176.5958  |
| 197.6319                                                  | 226.0873  |           | 233.1481  |
| 234.8333                                                  | 257.7182  |           | 264.0675  |
| 294.6350                                                  | 300.8473  |           | 335.3328  |
| 364.4748                                                  | 422.1349  |           | 428.3944  |
| 499.0782                                                  | 615.9003  |           | 634.4423  |
| 729.0698                                                  | 752.7573  |           | 793.8222  |
| 809.5612                                                  | 867.4913  |           | 917.5198  |
| 975.0291                                                  | 1000.5816 |           | 1013.0965 |
| 1022.2847                                                 | 1041.6060 |           | 1044.9239 |
| 1062.3416                                                 | 1090.1301 |           | 1106.3043 |
| 1127.2374                                                 | 1173.0791 |           | 1187.6064 |
| 1227.9606                                                 | 1278.2835 |           | 1306.1692 |
| 1314.6360                                                 | 1324.7584 |           | 1339.0198 |
| 1363.4994                                                 | 1367.7128 |           | 1403.9816 |
| 1408.3108                                                 | 1418.9760 |           | 1423.2178 |
| 1441.5960                                                 | 1485.6585 |           | 1489.3771 |
| 1490.4820                                                 | 1498.9155 |           | 1501.4239 |
| 1504.2834                                                 | 1506.0541 |           | 1507.3419 |
| 1511.9398                                                 | 1518.1552 |           | 1554.2027 |
| 1869.3809                                                 | 3053.4314 |           | 3059.3158 |
| 3059.4103                                                 | 3064.6230 |           | 3066.6920 |
| 3068.0354                                                 | 3071.5105 |           | 3108.5743 |
| 3110.0778                                                 | 3123.5210 |           | 3127.7243 |
| 3129.7010                                                 | 3138.4017 |           | 3139.5785 |
| 3141.5646                                                 | 3144.2618 |           | 3149.7300 |
| Zero-point correction (Hartree): 0.256069                 |           |           |           |
| TS.dic2H5CH3CH_COO.14Hshift.pmmtrS                        |           |           |           |
| ~~~~~                                                     |           |           |           |
| E(RM062X/Aug-CC-pVTZ) (Hartree): -504.03720837            |           |           |           |
| Electronic state : 1-A                                    |           |           |           |
| Cartesian coordinates (Angs):                             |           |           |           |
| C                                                         | 0.197462  | 0.290788  | -0.440405 |
| O                                                         | -0.049503 | 1.491541  | -0.876921 |
| O                                                         | -1.251255 | 1.970156  | -0.356588 |
| C                                                         | 1.590664  | -0.161853 | -0.757176 |
| C                                                         | 2.474809  | -0.259166 | 0.496466  |
| C                                                         | 1.558511  | -1.479523 | -1.531653 |
| H                                                         | 2.011616  | 0.620937  | -1.392679 |
| C                                                         | 2.414709  | 0.985142  | 1.371519  |
| H                                                         | 2.199977  | -1.145754 | 1.067929  |
| H                                                         | 3.496213  | -0.423218 | 0.147955  |
| H                                                         | 0.981908  | -1.385954 | -2.451011 |
| H                                                         | 1.117048  | -2.274128 | -0.930775 |
| H                                                         | 2.573376  | -1.778275 | -1.793194 |
| H                                                         | 1.413538  | 1.135705  | 1.779836  |
| H                                                         | 2.667481  | 1.876562  | 0.796322  |
| H                                                         | 3.110311  | 0.910861  | 2.205758  |
| C                                                         | -0.823535 | -0.284783 | 0.349182  |
| H                                                         | -1.217202 | 1.000015  | 0.539479  |
| C                                                         | -0.459323 | -1.322153 | 1.388855  |
| C                                                         | -2.131494 | -0.621482 | -0.410562 |
| C                                                         | -3.389391 | -0.311464 | 0.387876  |
| H                                                         | -2.162108 | -0.080546 | -1.354008 |
| H                                                         | -2.089363 | -1.688822 | -0.649024 |
| H                                                         | 0.276396  | -0.955327 | 2.102027  |
| H                                                         | -0.081730 | -2.251012 | 0.952636  |
| H                                                         | -1.352430 | -1.580242 | 1.957393  |
| H                                                         | -3.382698 | -0.810452 | 1.357175  |
| H                                                         | -4.279694 | -0.639352 | -0.148075 |
| H                                                         | -3.471043 | 0.762396  | 0.555719  |
| Rotational constants (GHz): 1.4932300 0.7471900 0.6895600 |           |           |           |
| Vibrational harmonic frequencies (cm-1):                  |           |           |           |
| i1601.3482                                                | 58.0125   |           | 77.6582   |
| 107.4955                                                  | 144.5961  |           | 170.0899  |
| 198.1365                                                  | 207.0901  |           | 220.1926  |
| 229.7644                                                  | 244.6651  |           | 276.5671  |
| 290.3600                                                  | 300.9794  |           | 339.3977  |
| 357.5200                                                  | 423.1869  |           | 431.1880  |
| 481.8666                                                  | 592.8716  |           | 644.2654  |
| 739.8082                                                  | 772.6736  |           | 786.3064  |
| 808.4083                                                  | 868.8844  |           | 918.7080  |
| 975.1307                                                  | 1001.4227 |           | 1019.5423 |
| 1023.5243                                                 | 1035.1534 |           | 1047.7501 |
| 1065.3129                                                 | 1100.1175 |           | 1102.9204 |
| 1126.6988                                                 | 1169.5975 |           | 1189.2307 |
| 1230.0505                                                 | 1278.9504 |           | 1304.5328 |
| 1318.1205                                                 | 1325.1229 |           | 1341.9412 |
| 1361.2917                                                 | 1370.5536 |           | 1405.8817 |
| 1411.1953                                                 | 1419.0019 |           | 1423.1998 |
| 1445.1675                                                 | 1476.1368 |           | 1487.2097 |
| 1492.9085                                                 | 1498.9653 |           | 1502.6719 |
| 1502.9073                                                 | 1504.2940 |           | 1507.5271 |

|           |           |           |
|-----------|-----------|-----------|
| 1510.1679 | 1518.0132 | 1558.9571 |
| 1871.3375 | 3040.2979 | 3046.6905 |
| 3059.7663 | 3063.9764 | 3066.8979 |
| 3068.4538 | 3072.8352 | 3109.3082 |
| 3114.2444 | 3120.6970 | 3128.8564 |
| 3135.6086 | 3139.4622 | 3140.1443 |
| 3141.4657 | 3143.4263 | 3143.9273 |

Zero-point correction (Hartree): 0.255950

TS.dic2H5CH3CH\_COO.14Hshift.pmpmRS

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E(RM062X/Aug-CC-pVTZ) (Hartree): -504.03338385

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.103307 | -0.343399 | -0.483436 |
| O | -0.048035 | -1.242922 | -1.421916 |
| O | 1.157038  | -1.941553 | -1.378126 |
| C | -1.271144 | 0.585061  | -0.653959 |
| C | -2.112252 | 0.632723  | 0.625866  |
| C | -0.856718 | 1.981214  | -1.130512 |
| H | -1.876184 | 0.134606  | -1.445164 |
| C | -2.646479 | -0.736695 | 1.025991  |
| H | -1.517443 | 1.054339  | 1.438245  |
| H | -2.940318 | 1.323458  | 0.455073  |
| H | -0.220508 | 1.925829  | -2.012876 |
| H | -0.328043 | 2.532073  | -0.355491 |
| H | -1.752698 | 2.543408  | -1.391980 |
| H | -1.831543 | -1.433258 | 1.230135  |
| H | -3.253865 | -1.164585 | 0.227540  |
| H | -3.262123 | -0.673530 | 1.921760  |
| C | 0.986212  | -0.346080 | 0.421067  |
| H | 1.634837  | -1.014976 | -0.571596 |
| C | 1.045852  | -1.563392 | 1.364705  |
| C | 1.415980  | 0.955390  | 1.079699  |
| C | 2.368167  | 1.771695  | 0.208383  |
| H | 0.559787  | 1.568667  | 1.369663  |
| H | 1.922451  | 0.706041  | 2.013454  |
| H | 0.637832  | -2.458287 | 0.903541  |
| H | 0.478424  | -1.339371 | 2.271451  |
| H | 2.077115  | -1.767138 | 1.651675  |
| H | 2.652077  | 2.704933  | 0.695348  |
| H | 1.915897  | 2.013246  | -0.753146 |
| H | 3.274400  | 1.201242  | 0.005877  |

Rotational constants (GHz): 1.1158500 0.9150500 0.7652300

Vibrational harmonic frequencies (cm-1):

|            |           |           |
|------------|-----------|-----------|
| i1612.7370 | 52.3286   | 104.4967  |
| 123.7604   | 125.6991  | 157.3883  |
| 180.4298   | 215.3029  | 225.3419  |
| 234.2310   | 242.5139  | 256.1359  |
| 271.4757   | 297.2502  | 352.2842  |
| 364.3028   | 429.1853  | 451.6015  |
| 479.6404   | 582.2306  | 641.0506  |
| 743.4599   | 757.7800  | 783.3510  |
| 809.6565   | 869.7069  | 942.5403  |
| 978.6561   | 1002.1801 | 1004.9076 |
| 1028.9373  | 1037.9254 | 1048.1627 |
| 1060.9042  | 1095.6243 | 1105.1459 |
| 1130.7067  | 1168.2152 | 1191.7413 |
| 1236.9112  | 1279.1006 | 1296.0339 |
| 1309.8680  | 1320.9944 | 1351.7852 |
| 1365.9280  | 1377.8325 | 1394.3694 |
| 1407.4565  | 1412.2284 | 1419.4654 |
| 1445.5444  | 1485.1565 | 1486.8846 |
| 1491.6690  | 1497.7226 | 1500.1471 |
| 1501.6755  | 1504.6800 | 1508.1859 |
| 1511.4325  | 1515.9722 | 1554.5266 |
| 1871.7167  | 3045.7874 | 3057.9899 |
| 3060.0792  | 3062.9202 | 3063.6015 |
| 3068.5994  | 3072.6810 | 3091.7235 |
| 3102.8782  | 3114.1525 | 3128.2163 |
| 3133.0796  | 3137.9845 | 3140.4744 |
| 3141.6721  | 3159.8008 | 3167.5610 |

Zero-point correction (Hartree): 0.255936

TS.dic2H5CH3CH\_COO.14Hshift.pmpmRS

~~~~~  
E(RM062X/Aug-CC-pVTZ) (Hartree): -504.03253167

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.191391 | -0.514848 | -0.452175 |
| O | -0.549544 | -1.732711 | -0.747072 |
| O | 0.534675  | -2.603762 | -0.716266 |
| C | -1.315467 | 0.454373  | -0.677245 |
| C | -1.847282 | 0.933865  | 0.683969  |
| C | -0.966520 | 1.634417  | -1.584688 |
| H | -2.104841 | -0.126214 | -1.160763 |
| C | -2.299394 | -0.204794 | 1.588665  |
| H | -1.073506 | 1.521134  | 1.181525  |
| H | -2.679989 | 1.612239  | 0.487267  |
| H | -0.514445 | 1.306590  | -2.519716 |
| H | -0.290136 | 2.332334  | -1.095694 |
| H | -1.884144 | 2.171621  | -1.821942 |
| H | -1.463972 | -0.852126 | 1.859350  |
| H | -3.045952 | -0.824800 | 1.091097  |
| H | -2.735504 | 0.179188  | 2.509396  |
| C | 1.166740  | -0.363988 | -0.071907 |
| H | 1.332492  | -1.560809 | -0.703884 |
| C | 1.543239  | -0.970091 | 1.292004  |
| C | 1.932598  | 0.907206  | -0.396275 |
| C | 1.879348  | 2.027589  | 0.641688  |
| H | 2.977704  | 0.605898  | -0.510503 |
| H | 1.634370  | 1.287334  | -1.371932 |

|                                                           |           |           |           |
|-----------------------------------------------------------|-----------|-----------|-----------|
| H                                                         | 1.068361  | -1.933873 | 1.450518  |
| H                                                         | 1.249714  | -0.297798 | 2.100283  |
| H                                                         | 2.624255  | -1.107703 | 1.341843  |
| H                                                         | 2.281129  | 1.698500  | 1.599232  |
| H                                                         | 0.861068  | 2.376161  | 0.813572  |
| H                                                         | 2.471125  | 2.881724  | 0.312834  |
| Rotational constants (GHz): 1.0561800 0.9982900 0.7528700 |           |           |           |
| Vibrational harmonic frequencies (cm-1):                  |           |           |           |
| i1597.3691                                                | 58.1388   |           | 90.0160   |
| 113.1535                                                  | 138.6524  |           | 172.6644  |
| 195.1677                                                  | 208.0899  |           | 236.8766  |
| 244.1740                                                  | 250.2612  |           | 260.6305  |
| 294.5360                                                  | 315.2304  |           | 337.5284  |
| 378.7124                                                  | 392.4521  |           | 431.5911  |
| 493.2655                                                  | 615.8993  |           | 646.9083  |
| 729.3111                                                  | 752.3082  |           | 782.9679  |
| 814.4336                                                  | 863.9906  |           | 940.7317  |
| 974.6676                                                  | 987.2032  |           | 1008.4445 |
| 1032.4665                                                 | 1039.9521 |           | 1044.1662 |
| 1060.4787                                                 | 1093.2445 |           | 1096.4566 |
| 1129.2063                                                 | 1174.6866 |           | 1192.1230 |
| 1236.5426                                                 | 1281.2009 |           | 1299.7652 |
| 1315.5437                                                 | 1325.0262 |           | 1347.6907 |
| 1363.6306                                                 | 1370.1771 |           | 1393.8666 |
| 1404.3495                                                 | 1414.3280 |           | 1421.5678 |
| 1441.1700                                                 | 1482.2776 |           | 1486.7010 |
| 1491.5387                                                 | 1499.8341 |           | 1502.5119 |
| 1503.7796                                                 | 1506.0307 |           | 1507.7703 |
| 1515.1446                                                 | 1520.9244 |           | 1554.2099 |
| 1877.6238                                                 | 3051.1003 |           | 3052.9647 |
| 3060.8129                                                 | 3062.5369 |           | 3066.8566 |
| 3070.3085                                                 | 3073.4395 |           | 3103.7471 |
| 3111.8302                                                 | 3117.6752 |           | 3129.3952 |
| 3135.8144                                                 | 3140.4983 |           | 3141.2875 |
| 3144.1596                                                 | 3159.7554 |           | 3168.7384 |
| Zero-point correction (Hartree): 0.256168                 |           |           |           |

TS.dic2H5CH3CH\_COO.14Hshift.pmptrS

~~~~~  
E(RM062X/Aug-CC-pVTZ) (Hartree): -504.03435302

Electronic state : 1-A

Cartesian coordinates (Angs):

|                                                           |           |           |           |
|-----------------------------------------------------------|-----------|-----------|-----------|
| C                                                         | 0.287738  | 0.464860  | -0.436145 |
| O                                                         | 0.422606  | 1.664977  | -0.919666 |
| O                                                         | -0.800427 | 2.333093  | -0.951659 |
| C                                                         | 1.527985  | -0.362621 | -0.603271 |
| C                                                         | 2.008319  | -0.868367 | 0.761794  |
| C                                                         | 1.357942  | -1.513536 | -1.601258 |
| H                                                         | 2.277825  | 0.323350  | -1.005141 |
| C                                                         | 2.310174  | 0.259786  | 1.739181  |
| H                                                         | 1.250982  | -1.535699 | 1.179028  |
| H                                                         | 2.901575  | -1.474356 | 0.597324  |
| H                                                         | 0.860908  | -1.187561 | -2.514114 |
| H                                                         | 0.789862  | -2.333097 | -1.166741 |
| H                                                         | 2.343249  | -1.894459 | -1.867097 |
| H                                                         | 1.415890  | 0.848942  | 1.948873  |
| H                                                         | 3.062802  | 0.935978  | 1.332030  |
| H                                                         | 2.681682  | -0.128569 | 2.686079  |
| C                                                         | -1.006700 | 0.150104  | 0.042584  |
| H                                                         | -1.405966 | 1.184580  | -0.752744 |
| C                                                         | -1.412715 | 0.900081  | 1.326643  |
| C                                                         | -1.477644 | -1.292575 | 0.002159  |
| C                                                         | -2.980227 | -1.407302 | 0.248821  |
| H                                                         | -1.259667 | -1.722268 | -0.974167 |
| H                                                         | -0.951196 | -1.903348 | 0.744938  |
| H                                                         | -0.889180 | 1.847238  | 1.419860  |
| H                                                         | -1.173145 | 0.275589  | 2.192273  |
| H                                                         | -2.481101 | 1.108552  | 1.341527  |
| H                                                         | -3.244824 | -1.108747 | 1.262184  |
| H                                                         | -3.315500 | -2.433735 | 0.107253  |
| H                                                         | -3.530859 | -0.769523 | -0.443811 |
| Rotational constants (GHz): 1.1661900 0.8391200 0.7235300 |           |           |           |
| Vibrational harmonic frequencies (cm-1):                  |           |           |           |
| i1602.0176                                                | 34.6633   |           | 81.0380   |
| 107.2550                                                  | 127.0407  |           | 151.4825  |
| 181.1563                                                  | 212.8786  |           | 225.1398  |
| 242.6856                                                  | 250.6962  |           | 275.3281  |
| 283.0471                                                  | 313.6703  |           | 332.3794  |
| 358.2323                                                  | 412.7597  |           | 441.2854  |
| 489.4778                                                  | 577.2596  |           | 652.7132  |
| 743.4951                                                  | 760.1721  |           | 802.1589  |
| 814.6049                                                  | 869.5991  |           | 958.7960  |
| 978.3902                                                  | 990.9495  |           | 1002.5261 |
| 1026.2890                                                 | 1033.1120 |           | 1050.8568 |
| 1071.9706                                                 | 1090.2181 |           | 1108.2438 |
| 1133.2555                                                 | 1176.2140 |           | 1193.2929 |
| 1231.2625                                                 | 1279.3223 |           | 1299.4731 |
| 1314.2872                                                 | 1322.2155 |           | 1335.5805 |
| 1369.2191                                                 | 1374.6758 |           | 1397.1097 |
| 1408.0342                                                 | 1411.1436 |           | 1420.2299 |
| 1445.7749                                                 | 1481.5945 |           | 1487.9173 |
| 1489.7712                                                 | 1499.6115 |           | 1501.1471 |
| 1504.3974                                                 | 1506.7021 |           | 1508.2502 |
| 1515.8228                                                 | 1519.8958 |           | 1556.9090 |
| 1871.4192                                                 | 3018.6910 |           | 3040.7394 |
| 3059.2343                                                 | 3061.6359 |           | 3064.5463 |
| 3067.6052                                                 | 3071.7655 |           | 3098.5122 |
| 3111.9081                                                 | 3121.4851 |           | 3128.8846 |
| 3134.2414                                                 | 3139.7662 |           | 3141.7055 |
| 3143.3176                                                 | 3158.4078 |           | 3167.1270 |
| Zero-point correction (Hartree): 0.255919                 |           |           |           |

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TS.dic2H5CH3CH_COO.14Hshift.pppmRS
~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -504.02952971
Electronic state : 1-A
Cartesian coordinates (Angs):
C      0.171153      -0.620977      -0.367783
O      0.759576      -1.649191      -0.912838
O      2.126733      -1.649417      -0.655597
C     -1.261837      -0.524577      -0.816105
C     -2.210042      -0.889205       0.343635
C     -1.637708       0.793758     -1.494331
H     -1.367579     -1.312011     -1.564885
C     -2.289423       0.122279       1.479171
H     -3.201979     -1.024774     -0.093011
H     -1.911469     -1.861702       0.740208
H     -1.036096       0.958094     -2.386537
H     -1.522244       1.654203     -0.841616
H     -2.683303       0.739000     -1.798965
H     -2.615344       1.100414       1.125399
H     -1.326342       0.243632       1.972680
H     -3.006251     -0.210743       2.228506
C      1.016799       0.184045       0.437476
H      2.025123     -0.397062     -0.265954
C      1.487847     -0.486714       1.745511
C      0.771515       1.676335       0.586772
C      1.223822       2.485449     -0.626033
H     -0.270166       1.900212       0.826227
H      1.342798       2.008995       1.455447
H      0.810079     -0.208480       2.555586
H      2.486520     -0.139549       2.009384
H      1.515945     -1.569245       1.665136
H      1.028922       3.549028     -0.487261
H      0.715107       2.164808     -1.533985
H      2.293053       2.351675     -0.788765
Rotational constants (GHz):  1.1448500      0.9034500      0.7731000
Vibrational harmonic frequencies (cm-1):
i1601.9403      59.6712      102.5389
132.9746      138.1063      156.8262
185.3514      207.7281      231.3282
249.9321      256.0277      270.8341
297.7233      306.7028      327.4485
358.6203      403.0156      460.9288
528.4322      592.7767      655.2924
740.6597      758.8977      788.2355
803.2044      848.2994      941.9059
981.4282      1002.4302      1007.3270
1022.1409      1034.4198      1041.8051
1063.1588      1095.7124      1107.7878
1137.9794      1162.4158      1177.0293
1239.0974      1295.5270      1298.0063
1309.2700      1325.9703      1353.8289
1368.4826      1379.1922      1397.6579
1409.6883      1411.9146      1418.3246
1444.0823      1485.7158      1486.3296
1493.0357      1497.7100      1498.3984
1502.4850      1507.1528      1510.0846
1514.8362      1521.9720      1553.3425
1875.9887      3052.4229      3056.0140
3065.5390      3066.3742      3072.1676
3074.8847      3077.4584      3092.4469
3094.4561      3115.7726      3133.7029
3135.5577      3138.3693      3146.5455
3151.8874      3171.3490      3177.5399
Zero-point correction (Hartree): 0.256425

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TS.dic2H5CH3CH_COO.14Hshift.ppptRS
~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -504.03162148
Electronic state : 1-A
Cartesian coordinates (Angs):
C 0.208957 0.738228 -0.263905
O 0.088459 2.033223 -0.339217
O -1.239900 2.426066 -0.205754
C 1.603935 0.302255 -0.615754
C 2.390482 0.001360 0.677194
C 1.688130 -0.844770 -1.622317
H 2.067449 1.178869 -1.072045
C 1.893806 -1.197545 1.475293
H 3.432012 -0.154147 0.387598
H 2.371777 0.893056 1.306360
H 1.126153 -0.622220 -2.528317
H 1.321653 -1.782674 -1.215126
H 2.733637 -0.982414 -1.898326
H 1.947599 -2.119584 0.897381
H 0.861891 -1.059362 1.796401
H 2.502972 -1.334538 2.367590
C -0.993095 0.050072 0.036261
H -1.598469 1.167874 -0.426230
C -1.545864 0.295641 1.457252
C -1.206532 -1.370064 -0.453314
C -2.680276 -1.766123 -0.392995
H -0.868783 -1.465347 -1.483613
H -0.623013 -2.080936 0.143378
H -1.314374 -0.572846 2.079187
H -2.626821 0.425150 1.448782
H -1.110641 1.180730 1.912200
H -3.047765 -1.790195 0.632074
H -2.830796 -2.755413 -0.822840
H -3.290202 -1.054635 -0.950982
Rotational constants (GHz): 1.1772600 0.8845800 0.7007100
Vibrational harmonic frequencies (cm-1):
i1602.1918 49.2333 88.5410

```



|           |           |           |
|-----------|-----------|-----------|
| 112.0450  | 137.4671  | 168.9134  |
| 189.7452  | 228.9951  | 238.4002  |
| 253.5086  | 269.2364  | 297.3252  |
| 301.2004  | 318.7112  | 327.1386  |
| 348.6375  | 372.7358  | 474.4397  |
| 523.6113  | 590.9571  | 660.9945  |
| 744.6796  | 762.0635  | 803.8264  |
| 815.3930  | 847.3966  | 958.7665  |
| 978.3568  | 994.7283  | 1002.3757 |
| 1023.3683 | 1031.8763 | 1036.7848 |
| 1072.3617 | 1091.8838 | 1115.6029 |
| 1132.2173 | 1169.5863 | 1187.9340 |
| 1233.9100 | 1296.8381 | 1298.5814 |
| 1318.3123 | 1321.6035 | 1339.1586 |
| 1370.8735 | 1378.3881 | 1401.1306 |
| 1411.7433 | 1413.2647 | 1419.6294 |
| 1444.3387 | 1481.6480 | 1487.5908 |
| 1491.4856 | 1496.4422 | 1502.8739 |
| 1503.3435 | 1509.4885 | 1510.7606 |
| 1515.1008 | 1524.5517 | 1556.6895 |
| 1871.5919 | 3022.7596 | 3050.0656 |
| 3059.0776 | 3064.5574 | 3073.0061 |
| 3075.5192 | 3078.7233 | 3098.2544 |
| 3117.3645 | 3123.7883 | 3134.0119 |
| 3137.9794 | 3139.4867 | 3144.2171 |
| 3149.7619 | 3165.5327 | 3174.0605 |

Zero-point correction (Hartree): 0.256587

TS.dic2H5CH3CH\_COO.14Hshift.ptmpRS

~~~~~  
E(RM062X/Aug-CC-pVTZ) (Hartree): -504.03398529

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.078626  | -0.575447 | -0.193596 |
| O | 0.269745  | -1.794587 | -0.606149 |
| O | 1.398557  | -2.353588 | -0.009205 |
| C | -1.275255 | -0.053387 | -0.572167 |
| C | -2.211079 | 0.050307  | 0.648222  |
| C | -1.152177 | 1.272051  | -1.324532 |
| H | -1.698512 | -0.806792 | -1.241076 |
| C | -3.678737 | 0.057784  | 0.237698  |
| H | -2.027107 | -0.791450 | 1.318723  |
| H | -1.978003 | 0.958538  | 1.204351  |
| H | -0.554713 | 1.156139  | -2.228009 |
| H | -0.681781 | 2.032015  | -0.700611 |
| H | -2.136464 | 1.633367  | -1.618095 |
| H | -3.938949 | -0.863272 | -0.284216 |
| H | -3.907028 | 0.894436  | -0.422044 |
| H | -4.322956 | 0.142397  | 1.111609  |
| C | 1.081387  | -0.056624 | 0.660127  |
| H | 1.388631  | -1.362275 | 0.867119  |
| C | 0.689284  | 0.971656  | 1.701784  |
| C | 2.456149  | 0.223202  | 0.010290  |
| C | 2.532725  | 1.609337  | -0.622982 |
| H | 3.219395  | 0.132913  | 0.786180  |
| H | 2.672056  | -0.538853 | -0.733832 |
| H | -0.072195 | 0.592399  | 2.379657  |
| H | 0.327487  | 1.912499  | 1.280102  |
| H | 1.568396  | 1.210708  | 2.301711  |
| H | 2.354868  | 2.399849  | 0.106313  |
| H | 1.795080  | 1.714085  | -1.419610 |
| H | 3.519841  | 1.775420  | -1.054494 |

Rotational constants (GHz): 1.4399700 0.7413200 0.6276500

Vibrational harmonic frequencies (cm-1):

|            |           |           |
|------------|-----------|-----------|
| i1606.5574 | 56.9009   | 75.1204   |
| 80.6419    | 121.8453  | 166.8148  |
| 192.9300   | 220.4539  | 225.5587  |
| 236.1514   | 242.7666  | 263.5389  |
| 291.4623   | 300.1291  | 331.6882  |
| 355.8417   | 385.5511  | 429.2125  |
| 493.7388   | 615.4000  | 692.2254  |
| 729.4521   | 745.1087  | 788.4489  |
| 801.5525   | 877.9630  | 918.6636  |
| 975.3813   | 992.3708  | 1014.0611 |
| 1024.6317  | 1029.9812 | 1048.9978 |
| 1058.6428  | 1086.9265 | 1097.0083 |
| 1141.8722  | 1171.2498 | 1190.9295 |
| 1228.7450  | 1290.5966 | 1302.4359 |
| 1315.1592  | 1321.9707 | 1350.6921 |
| 1361.9575  | 1374.5847 | 1404.9118 |
| 1408.3896  | 1415.5847 | 1421.0461 |
| 1439.2963  | 1485.2960 | 1488.9800 |
| 1490.9361  | 1497.6683 | 1500.6321 |
| 1502.4914  | 1505.8497 | 1509.7915 |
| 1513.5827  | 1515.6978 | 1553.2708 |
| 1872.1129  | 3051.4761 | 3060.0424 |
| 3063.1936  | 3064.9179 | 3065.3600 |
| 3069.0922  | 3071.8521 | 3108.6099 |
| 3110.7515  | 3124.1911 | 3129.5964 |
| 3136.7760  | 3139.2558 | 3141.9358 |
| 3144.9533  | 3148.9391 | 3150.6604 |

Zero-point correction (Hartree): 0.255894

TS.dic2H5CH3CH\_COO.14Hshift.ptmtRS

~~~~~  
E(RM062X/Aug-CC-pVTZ) (Hartree): -504.03489245

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |          |           |
|---|-----------|----------|-----------|
| C | -0.025645 | 0.512771 | 0.110582  |
| O | 0.302837  | 1.771119 | 0.068720  |
| O | 1.576488  | 1.931597 | -0.476378 |
| C | -1.468194 | 0.303186 | 0.455978  |

|                                                           |           |           |           |
|-----------------------------------------------------------|-----------|-----------|-----------|
| C                                                         | -2.279321 | -0.264955 | -0.723228 |
| C                                                         | -1.573663 | -0.568866 | 1.709469  |
| H                                                         | -1.863869 | 1.297719  | 0.676310  |
| C                                                         | -3.772728 | -0.010262 | -0.556941 |
| H                                                         | -1.935215 | 0.190754  | -1.653680 |
| H                                                         | -2.094531 | -1.336189 | -0.804927 |
| H                                                         | -1.036542 | -0.121215 | 2.544776  |
| H                                                         | -1.156573 | -1.559170 | 1.527010  |
| H                                                         | -2.615125 | -0.687344 | 2.003937  |
| H                                                         | -3.980346 | 1.059053  | -0.512740 |
| H                                                         | -4.158398 | -0.465753 | 0.354736  |
| H                                                         | -4.330616 | -0.426584 | -1.394355 |
| C                                                         | 0.986509  | -0.387938 | -0.289948 |
| H                                                         | 1.511579  | 0.692101  | -0.924538 |
| C                                                         | 0.593327  | -1.729630 | -0.868705 |
| C                                                         | 2.203440  | -0.474031 | 0.665609  |
| C                                                         | 3.535249  | -0.583472 | -0.062452 |
| H                                                         | 2.222412  | 0.393450  | 1.321965  |
| H                                                         | 2.044522  | -1.354847 | 1.295683  |
| H                                                         | -0.063710 | -1.633721 | -1.730111 |
| H                                                         | 0.108837  | -2.383703 | -0.138008 |
| H                                                         | 1.491604  | -2.245180 | -1.207553 |
| H                                                         | 3.544814  | -1.424169 | -0.756527 |
| H                                                         | 4.352920  | -0.726471 | 0.643519  |
| H                                                         | 3.729800  | 0.328732  | -0.626420 |
| Rotational constants (GHz): 1.7707500 0.6453500 0.5767900 |           |           |           |
| Vibrational harmonic frequencies (cm-1):                  |           |           |           |
| i1598.6008                                                | 49.9261   | 65.5667   |           |
| 91.6413                                                   | 108.3683  | 173.5357  |           |
| 194.9140                                                  | 210.3734  | 217.4338  |           |
| 228.7062                                                  | 241.6712  | 272.6007  |           |
| 289.4160                                                  | 305.8238  | 320.3017  |           |
| 354.5841                                                  | 376.6480  | 444.7294  |           |
| 484.7655                                                  | 593.2549  | 698.4466  |           |
| 737.6621                                                  | 765.0702  | 786.4884  |           |
| 796.0954                                                  | 878.3846  | 919.7572  |           |
| 975.0200                                                  | 992.1781  | 1015.4426 |           |
| 1024.0184                                                 | 1033.4665 | 1042.4966 |           |
| 1066.1689                                                 | 1091.9858 | 1101.9281 |           |
| 1140.5172                                                 | 1167.0039 | 1191.0656 |           |
| 1230.5370                                                 | 1291.5203 | 1300.1425 |           |
| 1308.7497                                                 | 1334.6366 | 1348.4019 |           |
| 1360.3304                                                 | 1375.8015 | 1405.6845 |           |
| 1411.2238                                                 | 1414.9850 | 1420.8156 |           |
| 1444.7630                                                 | 1475.7020 | 1487.1012 |           |
| 1494.2827                                                 | 1498.9448 | 1499.8416 |           |
| 1501.0933                                                 | 1504.3931 | 1508.7685 |           |
| 1512.9855                                                 | 1515.9235 | 1559.7297 |           |
| 1872.4112                                                 | 3038.3292 | 3045.1769 |           |
| 3063.0088                                                 | 3064.0567 | 3065.6770 |           |
| 3069.6831                                                 | 3071.9228 | 3111.6235 |           |
| 3114.2721                                                 | 3120.0873 | 3135.0871 |           |
| 3137.7366                                                 | 3139.5928 | 3139.9909 |           |
| 3141.5437                                                 | 3148.4777 | 3149.6552 |           |
| Zero-point correction (Hartree): 0.255798                 |           |           |           |
| TS.diC2H5CH3CH_COO.14Hshift.ptpmRS                        |           |           |           |
| ~~~~~                                                     |           |           |           |
| E(RM062X/Aug-CC-pVTZ) (Hartree): -504.03169865            |           |           |           |
| Electronic state : 1-A                                    |           |           |           |
| Cartesian coordinates (Angs):                             |           |           |           |
| C                                                         | 0.215290  | -0.622529 | -0.256340 |
| O                                                         | 0.645299  | -1.653940 | -0.922924 |
| O                                                         | 2.034523  | -1.747011 | -0.862353 |
| C                                                         | -1.241805 | -0.358189 | -0.498604 |
| C                                                         | -1.993012 | -0.283327 | 0.837829  |
| C                                                         | -1.474540 | 0.863730  | -1.395492 |
| H                                                         | -1.602275 | -1.234094 | -1.044497 |
| C                                                         | -3.502076 | -0.172104 | 0.659590  |
| H                                                         | -1.759225 | -1.179813 | 1.415671  |
| H                                                         | -1.624543 | 0.564402  | 1.418100  |
| H                                                         | -0.839855 | 0.822837  | -2.279694 |
| H                                                         | -1.275108 | 1.794956  | -0.867764 |
| H                                                         | -2.510465 | 0.877104  | -1.729377 |
| H                                                         | -3.879621 | -0.977857 | 0.027995  |
| H                                                         | -3.782981 | 0.774725  | 0.200196  |
| H                                                         | -4.008990 | -0.235351 | 1.621055  |
| C                                                         | 1.206850  | 0.094877  | 0.455079  |
| H                                                         | 2.072167  | -0.512919 | -0.404537 |
| C                                                         | 1.796074  | -0.645605 | 1.672262  |
| C                                                         | 1.031602  | 1.588698  | 0.678361  |
| C                                                         | 1.525080  | 2.425576  | -0.499867 |
| H                                                         | -0.004287 | 1.848383  | 0.908441  |
| H                                                         | 1.602621  | 1.863261  | 1.566693  |
| H                                                         | 1.825584  | -1.720552 | 1.521361  |
| H                                                         | 1.187556  | -0.425977 | 2.552386  |
| H                                                         | 2.810997  | -0.299568 | 1.866051  |
| H                                                         | 1.381544  | 3.491034  | -0.318504 |
| H                                                         | 1.000899  | 2.163394  | -1.418459 |
| H                                                         | 2.586616  | 2.246882  | -0.669804 |
| Rotational constants (GHz): 1.2566900 0.7807900 0.6657700 |           |           |           |
| Vibrational harmonic frequencies (cm-1):                  |           |           |           |
| i1607.5330                                                | 57.2153   | 75.4005   |           |
| 106.6843                                                  | 130.7036  | 150.4609  |           |
| 181.3305                                                  | 209.9450  | 217.1496  |           |
| 229.5114                                                  | 257.7980  | 269.6099  |           |
| 292.8203                                                  | 300.7949  | 341.7891  |           |
| 362.1656                                                  | 379.9539  | 449.7360  |           |
| 490.4858                                                  | 580.8108  | 687.4099  |           |
| 744.5667                                                  | 769.6735  | 783.4786  |           |
| 791.5953                                                  | 867.6345  | 943.5910  |           |
| 974.3641                                                  | 991.7968  | 1004.9024 |           |

|           |           |           |
|-----------|-----------|-----------|
| 1014.8763 | 1035.3052 | 1058.5692 |
| 1060.7717 | 1088.6260 | 1106.5206 |
| 1148.3732 | 1167.0960 | 1190.6514 |
| 1237.7149 | 1283.1233 | 1295.4915 |
| 1305.6719 | 1326.1211 | 1356.6883 |
| 1366.1686 | 1378.6465 | 1396.1264 |
| 1408.1494 | 1411.5995 | 1416.0039 |
| 1443.5380 | 1486.0063 | 1489.0945 |
| 1494.5765 | 1497.9507 | 1500.0353 |
| 1501.3929 | 1503.9629 | 1510.4455 |
| 1515.7252 | 1519.0934 | 1555.9143 |
| 1872.0971 | 3050.3136 | 3057.4659 |
| 3062.4973 | 3063.0201 | 3063.2757 |
| 3067.1454 | 3075.7263 | 3091.6112 |
| 3104.3523 | 3116.3069 | 3132.4214 |
| 3133.5092 | 3138.6950 | 3142.0647 |
| 3148.2369 | 3156.2763 | 3171.5544 |

Zero-point correction (Hartree): 0.255975

TS.dic2H5CH3CH\_COO.14Hshift.ptppRS

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E(RM062X/Aug-CC-pVTZ) (Hartree): -504.03099779

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.303023 | -0.713266 | 0.215798  |
| O | -0.685162 | -1.958386 | 0.255859  |
| O | -2.072204 | -2.065218 | 0.235540  |
| C | 1.176045  | -0.590105 | 0.439556  |
| C | 1.836251  | -0.240387 | -0.906990 |
| C | 1.566956  | 0.377266  | 1.558140  |
| H | 1.512200  | -1.589559 | 0.726420  |
| C | 3.357374  | -0.212965 | -0.829211 |
| H | 1.520771  | -0.978834 | -1.646654 |
| H | 1.460666  | 0.725369  | -1.250224 |
| H | 0.985328  | 0.195763  | 2.460645  |
| H | 1.434196  | 1.415914  | 1.259843  |
| H | 2.616746  | 0.230650  | 1.805056  |
| H | 3.742515  | -1.147472 | -0.418213 |
| H | 3.712957  | 0.603032  | -0.201470 |
| H | 3.789117  | -0.079764 | -1.819822 |
| C | -1.348497 | 0.231389  | 0.056101  |
| H | -2.143684 | -0.780075 | 0.505237  |
| C | -2.036178 | 0.230901  | -1.321373 |
| C | -1.251829 | 1.615325  | 0.675295  |
| C | -0.596724 | 2.703812  | -0.174677 |
| H | -2.280369 | 1.924664  | 0.881070  |
| H | -0.767342 | 1.560781  | 1.648516  |
| H | -2.185127 | -0.776318 | -1.698101 |
| H | -1.438532 | 0.789777  | -2.043171 |
| H | -3.010168 | 0.715470  | -1.240370 |
| H | -1.142641 | 2.861770  | -1.103917 |
| H | 0.431959  | 2.454197  | -0.435050 |
| H | -0.581920 | 3.651651  | 0.363177  |

Rotational constants (GHz): 1.2093900 0.8509500 0.6418300

Vibrational harmonic frequencies (cm-1):

|            |           |           |
|------------|-----------|-----------|
| i1591.8332 | 53.1391   | 90.9531   |
| 97.7020    | 137.6124  | 169.1854  |
| 193.3235   | 206.6563  | 226.8216  |
| 245.1946   | 269.9050  | 276.9123  |
| 305.1785   | 320.3611  | 337.1773  |
| 356.3132   | 385.7010  | 420.3127  |
| 492.8820   | 626.3626  | 678.7364  |
| 729.5155   | 773.7404  | 784.3553  |
| 791.4446   | 860.7425  | 942.4101  |
| 973.2477   | 985.4195  | 996.6847  |
| 1026.8841  | 1040.3575 | 1047.6777 |
| 1054.5239  | 1086.2930 | 1095.0627 |
| 1143.0349  | 1175.6040 | 1191.4644 |
| 1238.1110  | 1283.7951 | 1301.1986 |
| 1311.3189  | 1329.3587 | 1361.1068 |
| 1363.7834  | 1373.1750 | 1395.1875 |
| 1405.0831  | 1413.3839 | 1414.9047 |
| 1437.6549  | 1485.3239 | 1488.2557 |
| 1494.2738  | 1499.8301 | 1501.2641 |
| 1504.0420  | 1507.5705 | 1514.5526 |
| 1517.5171  | 1521.4627 | 1555.0240 |
| 1878.2014  | 3052.1956 | 3055.9879 |
| 3060.7915  | 3064.0205 | 3066.5743 |
| 3069.4567  | 3077.4181 | 3102.5265 |
| 3113.9426  | 3120.8985 | 3132.0870 |
| 3135.1233  | 3141.0778 | 3143.3553 |
| 3149.2330  | 3156.7955 | 3173.3625 |

Zero-point correction (Hartree): 0.256292

TS.dic2H5CH3CH\_COO.14Hshift.ptptRS

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E(RM062X/Aug-CC-pVTZ) (Hartree): -504.03285258

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.009708  | -0.734459 | -0.171743 |
| O | 0.222119  | -2.004397 | -0.356763 |
| O | 1.586769  | -2.289454 | -0.348781 |
| C | -1.423840 | -0.355049 | -0.389418 |
| C | -1.980430 | 0.263622  | 0.901483  |
| C | -1.629066 | 0.552174  | -1.609221 |
| H | -1.948088 | -1.294987 | -0.579130 |
| C | -3.471990 | 0.560252  | 0.814618  |
| H | -1.790325 | -0.422760 | 1.729076  |
| H | -1.428983 | 1.180710  | 1.121280  |
| H | -1.031512 | 0.220168  | -2.457287 |
| H | -1.369898 | 1.584927  | -1.382049 |
| H | -2.675694 | 0.525332  | -1.906571 |

```

H -4.030322 -0.335234 0.537206
H -3.683905 1.331206 0.074773
H -3.852400 0.908452 1.773481
C 1.164389 0.037565 0.097845
H 1.832279 -1.006907 -0.475157
C 1.801283 -0.230881 1.476337
C 1.182933 1.499772 -0.309006
C 2.589352 2.090301 -0.240322
H 0.819231 1.602592 -1.330105
H 0.518621 2.096468 0.327522
H 1.568712 -1.228249 1.837514
H 1.417942 0.502664 2.190833
H 2.885071 -0.135243 1.437234
H 2.959601 2.126254 0.783228
H 2.599784 3.106032 -0.633060
H 3.284745 1.489603 -0.827869
Rotational constants (GHz): 1.2783000 0.7583300 0.6102100
Vibrational harmonic frequencies (cm-1):
i1599.9028 47.2631 79.7064
 93.6617 104.2244 154.9014
 174.4645 208.4429 232.5701
 250.1704 268.5116 281.4340
 294.4480 310.4042 330.7250
 356.5823 369.0520 423.4773
 511.3936 576.6114 692.0827
 746.5848 772.8143 789.1919
 808.3749 867.7509 959.0262
 974.8906 988.6581 994.7556
 1016.2534 1030.2854 1056.9315
 1070.9616 1084.1950 1112.1900
 1145.2399 1176.8295 1191.6384
 1232.8157 1279.7804 1303.0897
 1305.9668 1328.0898 1354.3609
 1360.0023 1377.5916 1397.4640
 1410.0063 1410.4325 1414.2866
 1443.5492 1482.8911 1488.3182
 1491.3903 1498.9706 1502.1266
 1504.3831 1507.5388 1511.0382
 1516.7529 1518.8720 1557.4169
 1873.9059 3016.6474 3044.9168
 3057.4309 3063.3806 3064.9544
 3065.7343 3073.4201 3097.2093
 3112.8617 3122.3348 3132.2114
 3134.3488 3140.8156 3144.1889
 3147.2640 3153.8717 3169.9175
Zero-point correction (Hartree): 0.255973

```

```

#####
E-CHOCHOO
#####

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```

Population analysis as 298K (%)
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)
Compound Qtot Erel Erel2 n*Q*MB %

H_CHO_COO.t 1.486e+38 0.00 0.00 1.486e+38 99.8
H_CHO_COO.c 1.905e+38 3.86 3.86 2.829e+35 0.19
Total 1.489e+38 100

```

```

H_CHO_COO.c
~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -302.89202852
Electronic state : 1-A
Cartesian coordinates (Angs):
C      -0.095776      0.658006      0.000098
O      -0.845770     -0.342880     -0.000028
O      -2.150467     -0.166806     -0.000019
H      -0.557389      1.640147      0.000209
C       1.371520      0.420458      0.000097
O       1.862066     -0.671809     -0.000138
H       1.976298      1.341037      0.000095
Rotational constants (GHz):   23.7871600   3.0118600   2.6733600
Vibrational harmonic frequencies (cm-1):
  166.8838      216.4583      261.4737
  471.6325      763.6994      884.1501
  960.1769      1037.4131      1121.9229
 1354.5257      1430.1928      1565.1562
 1844.7366      3009.3603      3193.8759
Zero-point correction (Hartree): 0.041649

```

```

H_CHO_COO.t
~~~~~
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -302.49420257
E(CCSD/Aug-CC-pVTZ) (Hartree): -302.43826246
T1 diagnostic: 0.036963
E(MP2/Aug-CC-pVTZ) (Hartree): -302.43241404
E(MP3/Aug-CC-pVTZ) (Hartree): -302.42276069
E(RHF/Aug-CC-pVTZ) (Hartree): -301.39512167
E(RM062X/Aug-CC-pVTZ) (Hartree): -302.89828013
Electronic state : 1-A
Cartesian coordinates (Angs):
C 0.044533 -0.339764 0.000038
O 1.062592 0.388299 -0.000077
O 2.260576 -0.165842 -0.000053
H 0.158469 -1.418253 0.000159
C -1.252963 0.362896 -0.000003
O -2.287345 -0.245291 0.000101
H -1.194467 1.462131 -0.000141
Rotational constants (GHz): 46.1893000 2.4796200 2.3532800
Vibrational harmonic frequencies (cm-1):

```

```

154.3962 234.2742 324.9081
505.9116 576.6011 913.2032
1036.4570 1063.3841 1130.6633
1332.0408 1399.8437 1580.3558
1840.0956 3027.6316 3208.6052
Zero-point correction (Hartree): 0.041755

Population analysis as 298K (%)
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)
Compound Qtot Erel Erel2 n*Q*MB %

TS.H_CHO_COO.isomrot.t 1.403e+38 0.00 0.00 2.807e+38 93
TS.H_CHO_COO.isomrot.c 1.296e+38 1.49 1.49 2.106e+37 6.98
Total 3.017e+38 100

TS.H_CHO_COO.isomrot.c
~~~~~
E(UM062X/Aug-CC-pVTZ) (Hartree): -302.86439196
Electronic state : 1-A
Cartesian coordinates (Angs):
C      -0.030454      0.886700      -0.009089
O      -1.033160      0.113308      0.534750
O      -1.661332     -0.555563     -0.406698
H      -0.306724      1.895472     -0.280606
C       1.277297      0.322105     -0.173698
O       1.543991     -0.827342      0.117950
H       2.029667      1.008469     -0.590684
Rotational constants (GHz): 12.7960300      3.8479200      3.2706200
Vibrational harmonic frequencies (cm-1):
i248.9028          220.4509          246.7664
379.6130          598.2557          777.8357
937.6051          968.4360         1150.8493
1219.0300         1382.4810         1420.9724
1659.3519         3013.7605         3224.6192
Zero-point correction (Hartree): 0.039185

TS.H_CHO_COO.isomrot.t
~~~~~
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -302.45235580
E(CCSD/Aug-CC-pVTZ) (Hartree): -302.40852147
T1 diagnostic: 0.034212
E(MP2/Aug-CC-pVTZ) (Hartree): -302.36826823
E(MP3/Aug-CC-pVTZ) (Hartree): -302.38736639
E(PMP2/Aug-CC-pVTZ) (Hartree): -302.43952811
E(PMP3/Aug-CC-pVTZ) (Hartree): -302.45707051
E(PUHF/Aug-CC-pVTZ) (Hartree): -301.49565206
E(UHF/Aug-CC-pVTZ) (Hartree): -301.42327879
E(UM062X/Aug-CC-pVTZ) (Hartree): -302.86663685
Electronic state : 1-A
Cartesian coordinates (Angs):
C 0.008812 0.577461 -0.060156
O -1.237162 0.274846 0.459095
O -1.936863 -0.443616 -0.391901
H 0.086724 1.482646 -0.644844
C 1.100477 -0.304673 0.210053
O 2.223420 -0.071196 -0.199611
H 0.862377 -1.199651 0.804802
Rotational constants (GHz): 23.7047200 2.7124700 2.6227600
Vibrational harmonic frequencies (cm-1):
i296.3877 158.1457 309.3028
411.4750 557.2108 636.4835
971.3606 1088.1531 1152.6725
1212.3817 1302.1344 1437.6583
1654.9386 3020.6531 3233.2082
Zero-point correction (Hartree): 0.039061

Population analysis as 298K (%)
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)
Compound Qtot Erel Erel2 n*Q*MB %

TS.H_CHO_COO.introt 1.169e+38 0.00 0.00 4.677e+38 100
Total 4.677e+38 100

TS.H_CHO_COO.introt
~~~~~
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -302.47812389
E(CCSD/Aug-CC-pVTZ) (Hartree): -302.42475827
T1 diagnostic: 0.035974
E(MP2/Aug-CC-pVTZ) (Hartree): -302.41401683
E(MP3/Aug-CC-pVTZ) (Hartree): -302.40826857
E(RHF/Aug-CC-pVTZ) (Hartree): -301.38674879
E(RM062X/Aug-CC-pVTZ) (Hartree): -302.88319811
Electronic state : 1-A
Cartesian coordinates (Angs):
C       0.087894      0.465146      0.250003
O       0.942700     -0.229564     -0.317914
O       2.219829     -0.150949      0.094550
H       0.403774      1.120117      1.058758
C      -1.337666      0.338992     -0.235034
O      -2.068176     -0.496012      0.204425
H      -1.659971      1.067254     -0.997052
Rotational constants (GHz): 29.0356900      2.6333700      2.5598400
Vibrational harmonic frequencies (cm-1):
i213.1088          176.2697          277.5468
459.1456          627.2805          853.3671
944.1003         1021.9348          1083.4356
1338.0329         1413.8879          1631.8117
1868.5675         3004.1133          3162.5775
Zero-point correction (Hartree): 0.040693

```

Population analysis as 298K (%)  
 Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)  
 Compound Qtot Erel Erel2 n\*Q\*MB %  
 -----  
 TS.H\_CHO\_COO.13Hshift.t 3.169e+38 0.00 0.00 3.169e+38 100  
 Total 3.169e+38 100

TS.H\_CHO\_COO.13Hshift.t  
 ~~~~~  
 E(CCSO(T)/Aug-CC-pVTZ) (Hartree): -302.43318829
 E(CCSO(Aug-CC-pVTZ) (Hartree): -302.37902378
 Tl diagnostic: 0.028190
 E(MP2/Aug-CC-pVTZ) (Hartree): -302.37215360
 E(MP3/Aug-CC-pVTZ) (Hartree): -302.36541700
 E(RHF/Aug-CC-pVTZ) (Hartree): -301.33367470
 E(RM062X/Aug-CC-pVTZ) (Hartree): -302.83811159
 Electronic state : 1-A
 Cartesian coordinates (Angs):
 C -0.091824 -0.277523 0.000081
 O -1.021131 0.557442 -0.000068
 O -2.168521 -0.287000 -0.000012
 H -1.123686 -1.142195 0.000150
 C 1.290197 0.337198 0.000063
 O 2.265172 -0.352370 -0.000070
 H 1.329289 1.439569 0.000179
 Rotational constants (GHz): 36.3325400 2.5634500 2.3945100
 Vibrational harmonic frequencies (cm-1):
 i1785.0197 70.1603 243.6900
 255.0637 507.8738 730.1938
 914.6252 953.8467 1161.1839
 1194.8732 1382.4759 1603.3017
 1860.1366 2144.5723 2999.8851
 Zero-point correction (Hartree): 0.036501

Population analysis as 298K (%)
 Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)
 Compound Qtot Erel Erel2 n*Q*MB %

 TS.H_CHO_COO.ringclose.t 1.726e+38 0.00 0.00 3.453e+38 99.3
 TS.H_CHO_COO.ringclose.c 1.874e+38 2.97 2.97 2.500e+36 0.719
 Total 3.478e+38 100

TS.H_CHO_COO.ringclose.c
 ~~~~~  
 E(RM062X/Aug-CC-pVTZ) (Hartree): -302.85426943  
 Electronic state : 1-A  
 Cartesian coordinates (Angs):  
 C 0.199343 0.571648 0.199085  
 O 0.849937 -0.482774 0.441885  
 O 1.928319 -0.065684 -0.412617  
 H 0.683913 1.539343 0.284872  
 C -1.283370 0.463860 -0.060483  
 O -1.822728 -0.598117 -0.152043  
 H -1.823971 1.420210 -0.134283  
 Rotational constants (GHz): 18.6198100 3.2590500 2.9983500  
 Vibrational harmonic frequencies (cm-1):  
 i733.7604 115.0126 254.0846  
 346.9420 745.2716 769.5341  
 858.7096 963.7541 1037.5680  
 1352.8994 1408.6788 1562.0788  
 1853.8820 3021.1016 3180.7961  
 Zero-point correction (Hartree): 0.039800

TS.H\_CHO\_COO.ringclose.t  
 ~~~~~  
 E(CCSO(T)/Aug-CC-pVTZ) (Hartree): -302.45999884
 E(CCSO(Aug-CC-pVTZ) (Hartree): -302.40360870
 Tl diagnostic: 0.046136
 E(MP2/Aug-CC-pVTZ) (Hartree): -302.38936147
 E(MP3/Aug-CC-pVTZ) (Hartree): -302.38353921
 E(RHF/Aug-CC-pVTZ) (Hartree): -301.36430115
 E(RM062X/Aug-CC-pVTZ) (Hartree): -302.85899785
 Electronic state : 1-A
 Cartesian coordinates (Angs):
 C -0.139172 -0.144612 0.315507
 O -1.135131 0.622280 0.198194
 O -1.954273 -0.458637 -0.308450
 H -0.219041 -1.104475 0.816434
 C 1.201953 0.350248 -0.146678
 O 2.166737 -0.350960 -0.048140
 H 1.223698 1.369189 -0.562244
 Rotational constants (GHz): 24.0979900 2.8026500 2.6252400
 Vibrational harmonic frequencies (cm-1):
 i725.3631 123.5257 298.7677
 354.9311 526.8414 806.0387
 892.9188 1024.5454 1098.3809
 1312.5823 1381.1581 1571.5126
 1852.2796 3034.4996 3191.9825
 Zero-point correction (Hartree): 0.039800

 Z-CHOCHO
 #####

Population analysis as 298K (%)
 Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)
 Compound Qtot Erel Erel2 n*Q*MB %

 CHO_H_COO.t 2.200e+38 0.00 0.00 2.200e+38 100

```

CHO_H_COO.c 1.943e+38 6.28 6.28 4.832e+33 0.0022
Total_ 2.200e+38 100

CHO_H_COO.c
~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -302.88595444
Electronic state : 1-A
Cartesian coordinates (Angs):
  C 0.109372 0.974951 -0.000033
  O 1.218606 0.378081 -0.000160
  O 1.298307 -0.927722 -0.000142
  H 0.211950 2.052422 -0.000071
  C -1.229913 0.344613 0.000144
  O -1.447686 -0.833043 0.000197
  H -2.042516 1.091663 0.000246
Rotational constants (GHz): 11.1701700 4.7323300 3.3240700
Vibrational harmonic frequencies (cm-1):
  132.8860 231.3107 375.1177
  444.1417 812.1815 890.5977
  919.9533 1021.7844 1051.7260
  1390.7161 1443.9654 1550.4085
  1834.4236 2981.1899 3220.8837
Zero-point correction (Hartree): 0.041693

CHO_H_COO.t
~~~~~
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -302.49156112
E(CCSD/Aug-CC-pVTZ) (Hartree): -302.43650734
Tl diagnostic: 0.037540
E(MP2/Aug-CC-pVTZ) (Hartree): -302.42812268
E(MP3/Aug-CC-pVTZ) (Hartree): -302.42090639
E(RHF/Aug-CC-pVTZ) (Hartree): -301.39489842
E(RM062X/Aug-CC-pVTZ) (Hartree): -302.89595468
Electronic state : 1-A
Cartesian coordinates (Angs):
  C -0.012225 0.709963 -0.000048
  O -1.249521 0.531266 -0.000007
  O -1.747895 -0.703604 0.000061
  H 0.306928 1.744821 -0.000004
  C 0.986250 -0.392930 -0.000080
  O 2.153209 -0.106363 0.000084
  H 0.602585 -1.417406 -0.000329
Rotational constants (GHz): 19.7367500 3.1562200 2.7210800
Vibrational harmonic frequencies (cm-1):
  108.3900 263.0243 364.9635
  456.9939 678.0528 840.6365
  937.6769 1042.9620 1128.1886
  1337.9784 1390.2812 1592.9360
  1827.8246 3106.7271 3222.2482
Zero-point correction (Hartree): 0.041688

Population analysis as 298K (%)
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)
Compound Qtot Erel Erel2 n*Q*MB %
-----
TS_H_CHO_COO.isomrot.t 1.403e+38 0.00 0.00 2.807e+38 93
TS_H_CHO_COO.isomrot.c 1.296e+38 1.49 1.49 2.106e+37 6.98
Total_ 3.017e+38 100

TS_H_CHO_COO.isomrot.c
~~~~~
E(UM062X/Aug-CC-pVTZ) (Hartree): -302.86439196
Electronic state : 1-A
Cartesian coordinates (Angs):
  C -0.030454 0.886700 -0.009089
  O -1.033160 0.113308 0.534750
  O -1.661332 -0.555563 -0.406698
  H -0.306724 1.895472 -0.280606
  C 1.277297 0.322105 -0.173698
  O 1.543991 -0.827342 0.117950
  H 2.029667 1.008469 -0.590684
Rotational constants (GHz): 12.7960300 3.8479200 3.2706200
Vibrational harmonic frequencies (cm-1):
  1248.9028 220.4509 246.7664
  379.6130 598.2557 777.8357
  937.6051 968.4360 1150.8493
  1219.0300 1382.4810 1420.9724
  1659.3519 3013.7605 3224.6192
Zero-point correction (Hartree): 0.039185

TS_H_CHO_COO.isomrot.t
~~~~~
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -302.45235580
E(CCSD/Aug-CC-pVTZ) (Hartree): -302.40852147
Tl diagnostic: 0.034212
E(MP2/Aug-CC-pVTZ) (Hartree): -302.36826823
E(MP3/Aug-CC-pVTZ) (Hartree): -302.38736639
E(PMP2/Aug-CC-pVTZ) (Hartree): -302.43952811
E(PMP3/Aug-CC-pVTZ) (Hartree): -302.45707051
E(PUHF/Aug-CC-pVTZ) (Hartree): -301.49565206
E(UHF/Aug-CC-pVTZ) (Hartree): -301.42327879
E(UM062X/Aug-CC-pVTZ) (Hartree): -302.86663685
Electronic state : 1-A
Cartesian coordinates (Angs):
  C 0.008812 0.577461 -0.060156
  O -1.237162 0.274846 0.459095
  O -1.936863 -0.443616 -0.391901
  H 0.086724 1.482646 -0.644844
  C 1.100477 -0.304673 0.210053
  O 2.223420 -0.071196 -0.199611
  H 0.862377 -1.199651 0.804802

```

Rotational constants (GHz): 23.7047200 2.7124700 2.6227600
 Vibrational harmonic frequencies (cm-1):
 i296.3877 158.1457 309.3028
 411.4750 557.2108 636.4835
 971.3606 1088.1531 1152.6725
 1212.3817 1302.1344 1437.6583
 1654.9386 3020.6531 3233.2082
 Zero-point correction (Hartree): 0.039061

Population analysis as 298K (%)
 Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)
 Compound Qtot Erel Erel2 n*Q*MB %

 TS.CHO_H_COO.introt 1.026e+38 0.00 0.00 4.104e+38 100
 Total 4.104e+38 100

TS.CHO_H_COO.introt
 ~~~~~  
 E(CCSDF(T)/Aug-CC-pVTZ) (Hartree): -302.47874763  
 E(CCSDF(T)/Aug-CC-pVTZ) (Hartree): -302.42397105  
 T1 diagnostic: 0.036824  
 E(MP2/Aug-CC-pVTZ) (Hartree): -302.41561964  
 E(MP3/Aug-CC-pVTZ) (Hartree): -302.40772571  
 E(RHF/Aug-CC-pVTZ) (Hartree): -301.38094518  
 E(RM062X/Aug-CC-pVTZ) (Hartree): -302.88270647  
 Electronic state : 1-A  
 Cartesian coordinates (Angs):  
 C -0.135015 0.938602 -0.085345  
 O -1.231768 0.350280 -0.150857  
 O -1.326002 -0.935788 0.179221  
 H -0.179898 1.995317 -0.323410  
 C 1.158291 0.270852 0.300078  
 O 1.600612 -0.665644 -0.290373  
 H 1.697504 0.757179 1.131084  
 Rotational constants (GHz): 11.5568500 4.3052700 3.3329500  
 Vibrational harmonic frequencies (cm-1):  
 i162.6919 208.2469 318.8020  
 526.0417 720.0161 832.5004  
 914.3371 956.0828 1060.0774  
 1371.8623 1425.3552 1610.5597  
 1865.8950 2982.6005 3200.4282  
 Zero-point correction (Hartree): 0.040991

Population analysis as 298K (%)  
 Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)  
 Compound Qtot Erel Erel2 n\*Q\*MB %  
 -----  
 TS.CHO\_H\_COO.14Hshift 8.602e+37 0.00 0.00 1.720e+38 100  
 Total 1.720e+38 100

TS.CHO\_H\_COO.14Hshift  
 ~~~~~  
 E(CCSDF(T)/Aug-CC-pVTZ) (Hartree): -302.45453351
 E(CCSDF(T)/Aug-CC-pVTZ) (Hartree): -302.39456128
 T1 diagnostic: 0.034232
 E(MP2/Aug-CC-pVTZ) (Hartree): -302.40023220
 E(MP3/Aug-CC-pVTZ) (Hartree): -302.38177960
 E(RHF/Aug-CC-pVTZ) (Hartree): -301.33024238
 E(RM062X/Aug-CC-pVTZ) (Hartree): -302.85781976
 Electronic state : 1-A
 Cartesian coordinates (Angs):
 C 0.169916 0.923950 -0.097046
 O 1.341310 0.386589 0.023609
 O 1.178483 -0.965293 -0.083584
 C -0.875951 -0.035501 0.179054
 H 0.128824 1.983986 0.127172
 H 0.021167 -0.899464 0.629596
 O -2.009015 -0.223198 -0.096127
 Rotational constants (GHz): 14.7378900 4.0016900 3.1937600
 Vibrational harmonic frequencies (cm-1):
 i1767.1398 221.3751 417.6567
 550.9705 649.5216 750.9387
 824.8513 946.7787 1027.8993
 1288.0473 1308.0959 1477.4443
 1824.4490 1941.6158 3202.0856
 Zero-point correction (Hartree): 0.037434

Population analysis as 298K (%)
 Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)
 Compound Qtot Erel Erel2 n*Q*MB %

 TS.CHO_H_COO.ringclose.t 1.376e+38 0.00 0.00 2.752e+38 100
 TS.CHO_H_COO.ringclose.c 1.670e+38 7.12 7.12 2.005e+33 0.000729
 Total 2.752e+38 100

TS.CHO_H_COO.ringclose.c
 ~~~~~  
 E(RM062X/Aug-CC-pVTZ) (Hartree): -302.85483164  
 Electronic state : 1-A  
 Cartesian coordinates (Angs):  
 C 0.273028 -0.766837 0.302713  
 O 1.194640 -0.410139 -0.463724  
 O 1.172534 0.942624 0.122866  
 H 0.354229 -1.750128 0.780785  
 C -0.986660 0.066139 0.441094  
 O -1.727684 0.148572 -0.493051  
 H -1.188358 0.505862 1.427648  
 Rotational constants (GHz): 12.2497500 4.2019200 3.7597200  
 Vibrational harmonic frequencies (cm-1):



```
i736.8024      133.7950      270.8419
301.0876      710.7922      793.5750
872.9453      995.5813      1058.6783
1344.5102     1403.4261      1641.1834
1844.0270     3038.8872      3075.9842
Zero-point correction (Hartree): 0.039834
```

TS.CHO\_H\_COO.ringclose.t

```
~~~~~
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -302.46702362
E(CCSD/Aug-CC-pVTZ) (Hartree): -302.41031557
Tl diagnostic: 0.042387
E(MP2/Aug-CC-pVTZ) (Hartree): -302.39910477
E(MP3/Aug-CC-pVTZ) (Hartree): -302.39120388
E(RHF/Aug-CC-pVTZ) (Hartree): -301.36891671
E(RM062X/Aug-CC-pVTZ) (Hartree): -302.86663126
Electronic state : 1-A
Cartesian coordinates (Angs):
C 0.185044 0.714717 -0.096488
O 1.388189 0.477835 0.212180
O 1.265229 -0.884365 -0.263095
H -0.057294 1.652106 -0.604906
C -0.923595 -0.191974 0.319393
O -2.008484 -0.079563 -0.180440
H -0.670872 -0.899824 1.118318
Rotational constants (GHz): 15.9436900 3.6841900 3.1858500
Vibrational harmonic frequencies (cm-1):
i720.0726 134.2828 335.1165
423.0220 581.3749 834.7136
934.1892 1036.5748 1112.4488
1318.0739 1369.1802 1595.5555
1829.6379 3065.0731 3114.8991
Zero-point correction (Hartree): 0.040287
```

```
#####
E- (C(O)CH3)CHOO
#####
```

Population analysis as 298K (%)  
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)  
Compound Qtot Erel Erel2 n\*Q\*MB %  
-----  
H\_CH3CO\_COO.t 2.441e+39 0.00 0.00 2.441e+39 99.8  
H\_CH3CO\_COO.c 3.018e+39 3.89 3.89 4.216e+36 0.172  
Total 2.445e+39 100

H\_CH3CO\_COO.c

```
~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -342.21355142
Point group : CS
Electronic state : 1-A'
Cartesian coordinates (Angs):
C      0.000000      0.601123      0.000000
O      1.246510      0.649028      0.000000
O      1.844387      1.829104      0.000000
H     -0.539387      1.543428      0.000000
C     -0.647093      -0.751243      0.000000
O      0.016859      -1.751497      0.000000
C     -2.148214      -0.723780      0.000000
H     -2.530669      -1.739119      0.000000
H     -2.510074      -0.186997      0.878838
H     -2.510074      -0.186997      -0.878838
Rotational constants (GHz): 9.9951000  2.0783000  1.7389800
Vibrational harmonic frequencies (cm-1):
96.4407 ( A") 126.0649 ( A") 192.2804 ( A')
221.4909 ( A") 377.5917 ( A') 476.2543 ( A')
564.7006 ( A") 626.4242 ( A') 913.5727 ( A")
918.9613 ( A') 962.2729 ( A') 1050.1721 ( A")
1072.9804 ( A') 1217.0096 ( A') 1374.9527 ( A')
1401.1434 ( A') 1465.9460 ( A') 1474.5586 ( A")
1578.6269 ( A') 1850.5425 ( A') 3063.7878 ( A')
3124.7781 ( A") 3183.7774 ( A') 3191.8675 ( A')
Zero-point correction (Hartree): 0.069544
```

H\_CH3CO\_COO.t

```
~~~~~
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -341.74966793
E(CCSD/Aug-CC-pVTZ) (Hartree): -341.68629673
Tl diagnostic: 0.034179
E(MP2/Aug-CC-pVTZ) (Hartree): -341.66955499
E(MP3/Aug-CC-pVTZ) (Hartree): -341.67034321
E(RHF/Aug-CC-pVTZ) (Hartree): -340.45864039
E(RM062X/Aug-CC-pVTZ) (Hartree): -342.21996090
Point group : CS
Electronic state : 1-A'
Cartesian coordinates (Angs):
C 0.000000 0.712319 0.000000
O -1.218372 0.441669 0.000000
O -2.108048 1.428697 0.000000
H 0.313297 1.751148 0.000000
C 0.968295 -0.419895 0.000000
O 2.140451 -0.139930 0.000000
C 0.421869 -1.815387 0.000000
H 1.248965 -2.517714 0.000000
H -0.207749 -1.969573 0.876494
H -0.207749 -1.969573 -0.876494
Rotational constants (GHz): 9.0306000 2.1853900 1.7787600
Vibrational harmonic frequencies (cm-1):
105.6979 (A") 149.6053 (A") 188.4142 (A')
230.8511 (A") 405.5606 (A') 503.1091 (A')
563.1668 (A") 577.1179 (A') 847.4959 (A')
```

```

938.0443 (A") 1022.6987 (A') 1043.0178 (A')
1055.7710 (A") 1253.2283 (A') 1355.2840 (A')
1406.6908 (A') 1464.9451 (A') 1472.1347 (A")
1588.0431 (A') 1833.9864 (A') 3076.3318 (A')
3140.4888 (A") 3192.7802 (A') 3202.0574 (A')
Zero-point correction (Hartree): 0.069750

Population analysis as 298K (%)
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)
Compound Qtot Erel Erel2 n*Q*MB %

TS.H_CH3CO_COO.isomrot.t 1.732e+39 0.00 0.00 3.464e+39 89.8
TS.H_CH3CO_COO.isomrot.c 6.979e+39 2.11 2.11 3.934e+38 10.2
Total 3.857e+39 100

TS.H_CH3CO_COO.isomrot.c
~~~~~
E(UM062X/Aug-CC-pVTZ) (Hartree): -342.18299200
Electronic state : 1-A
Cartesian coordinates (Angs):
C -0.279453 -0.725778 -0.242067
O -1.517667 -0.182326 -0.509984
O -2.156814 0.087417 0.606302
H -0.246848 -1.803943 -0.173873
C 0.851721 0.162428 -0.060503
O 0.706126 1.367314 -0.123917
C 2.176778 -0.499922 0.220164
H 2.151843 -0.972761 1.202934
H 2.959182 0.252305 0.202372
H 2.388386 -1.275206 -0.516206
Rotational constants (GHz): 8.5306500 2.3186900 2.0180100
Vibrational harmonic frequencies (cm-1):
i255.7929 26.3988 113.8955
215.3744 323.2128 413.0108
484.5632 614.0773 666.5941
877.5992 973.8040 1028.8473
1123.7496 1197.0469 1226.9138
1382.4734 1416.3282 1473.1608
1479.2468 1711.7802 3070.4409
3135.0821 3185.1270 3220.7763
Zero-point correction (Hartree): 0.066886

TS.H_CH3CO_COO.isomrot.t
~~~~~
E(CCS(D)/T)/Aug-CC-pVTZ) (Hartree): -341.70677893
E(CCS(D)/Aug-CC-pVTZ) (Hartree): -341.65461854
T1 diagnostic: 0.030035
E(MP2/Aug-CC-pVTZ) (Hartree): -341.60780463
E(MP3/Aug-CC-pVTZ) (Hartree): -341.63461076
E(PMP2/Aug-CC-pVTZ) (Hartree): -341.66972915
E(PMP3/Aug-CC-pVTZ) (Hartree): -341.69525987
E(PUHF/Aug-CC-pVTZ) (Hartree): -340.54345633
E(UHF/Aug-CC-pVTZ) (Hartree): -340.48059195
E(UM062X/Aug-CC-pVTZ) (Hartree): -342.18656709
Electronic state : 1-A
Cartesian coordinates (Angs):
C 0.271858 -0.838703 0.203110
O 1.423503 -0.139180 0.523984
O 2.088509 0.199171 -0.558656
H 0.364510 -1.911396 0.119398
C -0.968825 -0.128019 0.000320
C -0.949517 1.373369 0.089216
O -1.971761 -0.778897 -0.240612
H -1.960364 1.746017 -0.040773
H -0.548893 1.693146 1.051343
H -0.298352 1.783603 -0.683568
Rotational constants (GHz): 7.5525000 2.4725600 2.0517400
Vibrational harmonic frequencies (cm-1):
i254.1488 115.6231 127.5561
215.2448 358.2426 446.5197
501.5471 556.2918 658.3464
825.0407 1003.0880 1029.7688
1103.4517 1208.6612 1263.2010
1355.3489 1404.2539 1469.5542
1476.9332 1695.3167 3073.0818
3136.1820 3190.5926 3236.7247
Zero-point correction (Hartree): 0.067093

Population analysis as 298K (%)
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)
Compound Qtot Erel Erel2 n*Q*MB %

TS.H_CH3CO_COO.introt 1.290e+39 0.00 0.00 5.160e+39 100
Total 5.160e+39 100

TS.H_CH3CO_COO.introt
~~~~~
E(CCS(D)/T)/Aug-CC-pVTZ) (Hartree): -341.73568641
E(CCS(D)/Aug-CC-pVTZ) (Hartree): -341.67450649
T1 diagnostic: 0.032650
E(MP2/Aug-CC-pVTZ) (Hartree): -341.65435429
E(MP3/Aug-CC-pVTZ) (Hartree): -341.65802999
E(RHF/Aug-CC-pVTZ) (Hartree): -340.45165102
E(RM062X/Aug-CC-pVTZ) (Hartree): -342.20690378
Electronic state : 1-A
Cartesian coordinates (Angs):
C -0.429743 -0.003937 0.501021
O -1.293945 0.017345 -0.385529
O -2.587150 -0.144691 -0.033803
H -0.750818 -0.156356 1.529499

```

```

C      1.013905      0.194609      0.076858
O      1.422243      1.309734     -0.080369
C      1.819241     -1.055731     -0.096651
H      2.849525     -0.802762     -0.328235
H      1.768735     -1.659870      0.810942
H      1.382955     -1.649762     -0.901969
Rotational constants (GHz):      8.8810100      2.0718900      1.7946700
Vibrational harmonic frequencies (cm-1):
i144.5976      144.2852      156.4814
205.7037      371.6873      455.9439
540.0043      618.7917      850.6337
907.8715      950.6856      1013.5381
1075.6020      1211.2379      1357.1327
1395.5092      1462.4022      1470.8126
1638.6488      1865.5295      3062.5628
3125.8605      3158.9251      3183.5698
Zero-point correction (Hartree): 0.068854

```

```

Population analysis as 298K (%)
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)
Compound      Qtot      Erel      Erel2      n*Q*MB      %
-----
TS.H_CH3CO_COO.13Hshift.g 6.182e+39 0.00      0.00      1.236e+40 100
Total      1.236e+40 100

```

```

TS.H_CH3CO_COO.13Hshift.g
~~~~~
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -341.68977424
E(CCSD/Aug-CC-pVTZ) (Hartree): -341.62801123
T1 diagnostic: 0.024722
E(MP2/Aug-CC-pVTZ) (Hartree): -341.61161883
E(MP3/Aug-CC-pVTZ) (Hartree): -341.61406090
E(RHF/Aug-CC-pVTZ) (Hartree): -340.39854542
E(UM062X/Aug-CC-pVTZ) (Hartree): -342.16082669
Electronic state : 1-A
Cartesian coordinates (Angs):
C -0.463416 -0.299053 0.329249
O -1.212784 0.330092 -0.440643
O -2.509205 -0.009050 0.086686
H -1.613353 -0.668754 0.887222
C 1.024596 -0.222304 0.056757
O 1.600062 -1.255164 -0.144749
C 1.645915 1.139513 0.084864
H 2.718305 1.054656 -0.062583
H 1.198029 1.753512 -0.698273
H 1.429868 1.624625 1.038060
Rotational constants (GHz): 8.6686500 2.1593700 1.8201600
Vibrational harmonic frequencies (cm-1):
i1778.0518 51.0080 126.1808
145.7229 221.5516 390.6497
483.2129 583.0146 636.6480
868.8606 940.2043 1023.4293
1068.0312 1151.3702 1254.8699
1392.6557 1460.4965 1469.6752
1621.4883 1856.2513 2141.1861
3065.9738 3130.3949 3186.0951
Zero-point correction (Hartree): 0.064401

```

```

Population analysis as 298K (%)
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)
Compound Qtot Erel Erel2 n*Q*MB %

TS.H_CH3CO_COO.ringclose.t 2.095e+39 0.00 0.00 4.191e+39 99.7
TS.H_CH3CO_COO.ringclose.c 2.904e+39 3.62 3.62 1.290e+37 0.307
Total 4.204e+39 100

```

```

TS.H_CH3CO_COO.ringclose.c
~~~~~
E(UM062X/Aug-CC-pVTZ) (Hartree): -342.17675713
Electronic state : 1-A
Cartesian coordinates (Angs):
C      -0.465211     -0.370277      0.268844
O      -1.426620      0.436929      0.374105
O      -2.284656     -0.414214     -0.415913
H      -0.624567     -1.424439      0.479258
C      0.927283      0.174186     -0.009353
O      1.070790      1.354346     -0.161302
C      2.022233     -0.847288     -0.043454
H      2.972885     -0.363987     -0.242813
H      2.063673     -1.380067      0.908459
H      1.806073     -1.587720     -0.816247
Rotational constants (GHz):      8.4211500      2.2851800      1.9072800
Vibrational harmonic frequencies (cm-1):
i713.9412      66.9465      137.9455
226.8492      247.7965      383.9464
607.4496      635.1045      750.6880
816.6620      952.1320      986.7735
1050.4566      1206.1978      1365.6896
1397.4485      1464.3576      1471.1664
1575.1288      1860.1579      3062.3412
3122.4652      3166.2927      3192.7212
Zero-point correction (Hartree): 0.067768

```

```

TS.H_CH3CO_COO.ringclose.t
~~~~~
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -341.71706429
E(CCSD/Aug-CC-pVTZ) (Hartree): -341.65315672
T1 diagnostic: 0.040917
E(MP2/Aug-CC-pVTZ) (Hartree): -341.62941217
E(MP3/Aug-CC-pVTZ) (Hartree): -341.63334274

```

```

E(RHF/Aug-CC-pVTZ) (Hartree): -340.42900768
E(UM062X/Aug-CC-pVTZ) (Hartree): -342.18268678
Electronic state : 1-A
Cartesian coordinates (Angs):
 C 0.487000 -0.488348 -0.248727
 O 1.287481 0.467667 -0.436127
 O 2.277099 -0.127982 0.446266
 H 0.811499 -1.520223 -0.343674
 C -0.978867 -0.200885 -0.002797
 O -1.710953 -1.151704 0.072293
 C -1.383454 1.231743 0.121615
 H -2.462156 1.300697 0.214825
 H -0.894591 1.667822 0.994287
 H -1.031842 1.792808 -0.745443
Rotational constants (GHz): 7.7730000 2.3901800 1.9541700
Vibrational harmonic frequencies (cm-1):
 i694.0943 88.9112 160.0396
 207.4003 254.2034 462.7103
 540.3800 611.2036 764.4826
 812.1296 928.1802 1020.8990
 1053.5139 1261.9515 1321.4439
 1403.0107 1460.0882 1467.0730
 1567.0297 1849.4354 3069.8959
 3130.7113 3189.0081 3194.9565
Zero-point correction (Hartree): 0.067932

#####
Z- (C (O) CH3) CHOO
#####

Population analysis as 298K (%)
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)
Compound Qtot Erel Erel2 n*Q*MB %

CH3CO_H_COO.t 3.034e+39 0.00 0.00 3.034e+39 100
CH3CO_H_COO.c 4.046e+39 7.17 7.17 2.226e+34 0.000734
Total 3.034e+39 100

CH3CO_H_COO.c
~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -342.20578859
Electronic state : 1-A
Cartesian coordinates (Angs):
  C   -0.258954    -0.858146    -0.000280
  O   -1.504418    -0.683013    -0.000102
  O   -2.048363    0.510142    0.000403
  H    0.006370    -1.908134    -0.000631
  C    0.797353    0.197080    -0.000104
  O    0.548765    1.371580    -0.000325
  C    2.197056    -0.364460    0.000306
  H    2.909070    0.454306    0.000069
  H    2.351845    -0.990957    0.880317
  H    2.352103    -0.991734    -0.879099
Rotational constants (GHz):    8.4509400    2.5893400    2.0066000
Vibrational harmonic frequencies (cm-1):
  46.7309            121.7345            225.2496
  309.9827           345.7488            471.3981
  605.0892           705.1197            835.2891
  884.8954           1000.6503            1035.5231
  1044.0914          1196.2697            1391.4108
  1420.4835          1468.6464            1476.8323
  1555.4779          1838.3138            3064.5611
  3126.8225          3189.7488            3211.5187
Zero-point correction (Hartree): 0.069647

CH3CO_H_COO.t
~~~~~
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -341.74660729
E(CCSD/Aug-CC-pVTZ) (Hartree): -341.68352136
T1 diagnostic: 0.033474
E(MP2/Aug-CC-pVTZ) (Hartree): -341.66597029
E(MP3/Aug-CC-pVTZ) (Hartree): -341.66801688
E(RHF/Aug-CC-pVTZ) (Hartree): -340.45537554
E(RM062X/Aug-CC-pVTZ) (Hartree): -342.21760539
Point group : CS
Electronic state : 1-A'
Cartesian coordinates (Angs):
 C -0.986741 -0.202047 0.000000
 O -0.760976 -1.429306 0.000000
 O 0.484941 -1.909472 0.000000
 H -2.039256 0.056608 0.000000
 C 0.000000 0.933670 0.000000
 O -0.517171 2.024804 0.000000
 C 1.472093 0.700291 0.000000
 H 1.974270 1.663237 0.000000
 H 1.749258 0.100237 0.866479
 H 1.749258 0.100237 -0.866479
Rotational constants (GHz): 7.1680300 2.8416700 2.0600500
Vibrational harmonic frequencies (cm-1):
 36.0538 (A'') 233.9273 (A'') 262.2465 (A')
 334.9488 (A'') 342.8914 (A') 505.9710 (A')
 597.1190 (A'') 673.7883 (A') 833.1323 (A')
 883.4859 (A'') 939.1266 (A') 1050.6830 (A')
 1055.6221 (A'') 1272.8722 (A') 1383.3584 (A')
 1408.1442 (A') 1443.2450 (A') 1454.4565 (A'')
 1598.1522 (A') 1816.0708 (A') 3076.1589 (A')
 3139.0484 (A'') 3188.4843 (A') 3212.6834 (A')
Zero-point correction (Hartree): 0.070035

Population analysis as 298K (%)

```

Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)

| Compound                 | Qtot      | Erel | Erel2 | n*Q*MB    | %    |
|--------------------------|-----------|------|-------|-----------|------|
| TS.H.CH3CO_COO.isomrot.t | 1.732e+39 | 0.00 | 0.00  | 3.464e+39 | 89.8 |
| TS.H.CH3CO_COO.isomrot.c | 6.979e+39 | 2.11 | 2.11  | 3.934e+38 | 10.2 |
| Total                    |           |      |       | 3.857e+39 | 100  |

TS.H.CH3CO\_COO.isomrot.c

~~~~~  
E(UM062X/Aug-CC-pVTZ) (Hartree): -342.18299200

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.279453 | -0.725778 | -0.242067 |
| O | -1.517667 | -0.182326 | -0.509984 |
| O | -2.156814 | 0.087417  | 0.606302  |
| H | -0.246848 | -1.803943 | -0.173873 |
| C | 0.851721  | 0.162428  | -0.060503 |
| O | 0.706126  | 1.367314  | -0.123917 |
| C | 2.176778  | -0.499922 | 0.220164  |
| H | 2.151843  | -0.972761 | 1.202934  |
| H | 2.959182  | 0.252305  | 0.202372  |
| H | 2.388386  | -1.275206 | -0.516206 |

Rotational constants (GHz): 8.5306500 2.3186900 2.0180100

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i255.7929 | 26.3988   | 113.8955  |
| 215.3744  | 323.2128  | 413.0108  |
| 484.5632  | 614.0773  | 666.5941  |
| 877.5992  | 973.8040  | 1028.8473 |
| 1123.7496 | 1197.0469 | 1226.9138 |
| 1382.4734 | 1416.3282 | 1473.1608 |
| 1479.2468 | 1711.7802 | 3070.4409 |
| 3135.0821 | 3185.1270 | 3220.7763 |

Zero-point correction (Hartree): 0.066886

TS.H.CH3CO\_COO.isomrot.t

~~~~~  
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -341.70677893

E(CCSD/Aug-CC-pVTZ) (Hartree): -341.65461854

T1 diagnostic: 0.030035

E(MP2/Aug-CC-pVTZ) (Hartree): -341.60780463

E(MP3/Aug-CC-pVTZ) (Hartree): -341.63461076

E(PMP2/Aug-CC-pVTZ) (Hartree): -341.66972915

E(PMP3/Aug-CC-pVTZ) (Hartree): -341.69525987

E(PUHF/Aug-CC-pVTZ) (Hartree): -340.54345633

E(UHF/Aug-CC-pVTZ) (Hartree): -340.48059195

E(UM062X/Aug-CC-pVTZ) (Hartree): -342.18656709

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.271858  | -0.838703 | 0.203110  |
| O | 1.423503  | -0.139180 | 0.523984  |
| O | 2.088509  | 0.199171  | -0.558656 |
| H | 0.364510  | -1.911396 | 0.119398  |
| C | -0.968825 | -0.128019 | 0.000320  |
| C | -0.949517 | 1.373369  | 0.089216  |
| O | -1.971761 | -0.778897 | -0.240612 |
| H | -1.960364 | 1.746017  | -0.040773 |
| H | -0.548893 | 1.693146  | 1.051343  |
| H | -0.298352 | 1.783603  | -0.683568 |

Rotational constants (GHz): 7.5525000 2.4725600 2.0517400

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i254.1488 | 115.6231  | 127.5561  |
| 215.2448  | 358.2426  | 446.5197  |
| 501.5471  | 556.2918  | 658.3464  |
| 825.0407  | 1003.0880 | 1029.7688 |
| 1103.4517 | 1208.6612 | 1263.2010 |
| 1355.3489 | 1404.2539 | 1469.5542 |
| 1476.9332 | 1695.3167 | 3073.0818 |
| 3136.1820 | 3190.5926 | 3236.7247 |

Zero-point correction (Hartree): 0.067093

Population analysis as 298K (%)

Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)

| Compound              | Qtot      | Erel | Erel2 | n*Q*MB    | %   |
|-----------------------|-----------|------|-------|-----------|-----|
| TS.CH3CO_H_COO.introt | 8.454e+38 | 0.00 | 0.00  | 3.381e+39 | 100 |
| Total                 |           |      |       | 3.381e+39 | 100 |

TS.CH3CO\_H\_COO.introt

~~~~~  
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -341.73563980

E(CCSD/Aug-CC-pVTZ) (Hartree): -341.67198196

T1 diagnostic: 0.034023

E(MP2/Aug-CC-pVTZ) (Hartree): -341.65604342

E(MP3/Aug-CC-pVTZ) (Hartree): -341.65586673

E(RHF/Aug-CC-pVTZ) (Hartree): -340.44076316

E(RM062X/Aug-CC-pVTZ) (Hartree): -342.20495648

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.315208  | -0.800299 | -0.365189 |
| O | 1.524589  | -0.606822 | -0.113162 |
| O | 1.940269  | 0.505233  | 0.473462  |
| H | 0.120587  | -1.774217 | -0.799898 |
| C | -0.801221 | 0.182444  | -0.121209 |
| O | -0.664391 | 1.348696  | -0.355379 |
| C | -2.076502 | -0.445128 | 0.367534  |
| H | -2.848684 | 0.314436  | 0.440066  |
| H | -2.392928 | -1.238676 | -0.311447 |
| H | -1.907626 | -0.900499 | 1.345103  |

Rotational constants (GHz): 7.5644100 2.6017800 2.1300300

Vibrational harmonic frequencies (cm-1):

|          |          |          |
|----------|----------|----------|
| i60.7538 | 129.0176 | 204.4003 |
|----------|----------|----------|

|           |           |           |
|-----------|-----------|-----------|
| 268.0903  | 404.3484  | 469.3439  |
| 590.9713  | 696.2721  | 820.8794  |
| 862.5761  | 979.2913  | 995.1340  |
| 1062.3026 | 1197.4728 | 1392.3289 |
| 1406.3785 | 1464.3341 | 1474.9384 |
| 1588.7352 | 1857.5394 | 3063.2684 |
| 3126.3522 | 3184.5772 | 3198.1905 |

Zero-point correction (Hartree): 0.069340

Population analysis as 298K (%)  
 Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)

| Compound                | Qtot      | Erel | Erel2 | n*Q*MB    | %   |
|-------------------------|-----------|------|-------|-----------|-----|
| TS.CH3CO_H_COO.15Hshift | 6.032e+38 | 0.00 | 0.00  | 1.206e+39 | 100 |
| Total                   |           |      |       | 1.206e+39 | 100 |

TS.CH3CO\_H\_COO.15Hshift  
 ~~~~~  
 E (CCSD(T)/Aug-CC-pVTZ) (Hartree): -341.70361222  
 E (CCSD/Aug-CC-pVTZ) (Hartree): -341.63825206  
 T1 diagnostic: 0.027362  
 E (MP2/Aug-CC-pVTZ) (Hartree): -341.62859477  
 E (MP3/Aug-CC-pVTZ) (Hartree): -341.62529376  
 E (RHF/Aug-CC-pVTZ) (Hartree): -340.40106638  
 E (UM062X/Aug-CC-pVTZ) (Hartree): -342.17798772  
 Electronic state : 1-A  
 Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.197164  | -0.908765 | 0.464783  |
| O | 1.355903  | -0.679650 | 0.053715  |
| O | 1.652672  | 0.597572  | -0.439763 |
| H | 0.050796  | -1.924124 | 0.820437  |
| C | -0.957146 | 0.009593  | 0.136331  |
| O | -1.779470 | -0.648648 | -0.491887 |
| C | -0.707230 | 1.380227  | 0.295807  |
| H | 0.574177  | 1.155581  | -0.322926 |
| H | -1.455955 | 2.068498  | -0.070442 |
| H | -0.198585 | 1.659533  | 1.214877  |

Rotational constants (GHz): 6.5049900 3.2205800 2.4253700  
 Vibrational harmonic frequencies (cm-1):

|            |           |           |
|------------|-----------|-----------|
| i1285.1360 | 112.9118  | 233.0368  |
| 447.6702   | 504.7904  | 533.9467  |
| 572.6097   | 708.1977  | 745.7430  |
| 850.1026   | 877.6622  | 928.7996  |
| 963.8121   | 1051.4783 | 1230.5449 |
| 1301.6236  | 1369.3726 | 1461.1819 |
| 1586.1148  | 1731.5956 | 1775.3648 |
| 3129.2859  | 3201.2876 | 3243.3692 |

Zero-point correction (Hartree): 0.065066

Population analysis as 298K (%)  
 Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)

| Compound                   | Qtot      | Erel | Erel2 | n*Q*MB    | %      |
|----------------------------|-----------|------|-------|-----------|--------|
| TS.CH3CO_H_COO.ringclose.t | 1.312e+39 | 0.00 | 0.00  | 2.625e+39 | 99.9   |
| TS.CH3CO_H_COO.ringclose.c | 3.488e+39 | 4.91 | 4.91  | 1.739e+36 | 0.0662 |
| Total                      |           |      |       | 2.627e+39 | 100    |

TS.CH3CO\_H\_COO.ringclose.c  
 ~~~~~  
 E (UM062X/Aug-CC-pVTZ) (Hartree): -342.17803879  
 Electronic state : 1-A  
 Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.597410 | 0.249241  | 0.764062  |
| O | -1.684723 | 0.300239  | 0.145315  |
| O | -1.279304 | -0.845119 | -0.688350 |
| H | -0.629258 | 0.361119  | 1.855254  |
| C | 0.745513  | 0.260160  | 0.048945  |
| O | 1.025581  | 1.286378  | -0.506488 |
| C | 1.627844  | -0.938271 | 0.175751  |
| H | 2.647603  | -0.672914 | -0.087234 |
| H | 1.586151  | -1.338946 | 1.190027  |
| H | 1.247397  | -1.708023 | -0.494409 |

Rotational constants (GHz): 6.2625300 3.0183600 2.5380600  
 Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i740.2104 | 58.6093   | 106.7543  |
| 223.0565  | 243.5819  | 418.8298  |
| 511.9345  | 650.4876  | 800.2080  |
| 820.2698  | 938.9263  | 1036.1138 |
| 1054.5178 | 1221.7121 | 1357.9563 |
| 1391.2861 | 1464.8761 | 1473.0518 |
| 1636.7726 | 1850.1355 | 3064.9734 |
| 3071.4380 | 3142.5495 | 3183.9835 |

Zero-point correction (Hartree): 0.067712

TS.CH3CO\_H\_COO.ringclose.t  
 ~~~~~  
 E (CCSD(T)/Aug-CC-pVTZ) (Hartree): -341.72041402  
 E (CCSD/Aug-CC-pVTZ) (Hartree): -341.65622428  
 T1 diagnostic: 0.038282  
 E (MP2/Aug-CC-pVTZ) (Hartree): -341.63472554  
 E (MP3/Aug-CC-pVTZ) (Hartree): -341.63711520  
 E (RHF/Aug-CC-pVTZ) (Hartree): -340.43002234  
 E (UM062X/Aug-CC-pVTZ) (Hartree): -342.18665769  
 Electronic state : 1-A  
 Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.521719  | -0.813714 | -0.342589 |
| O | 1.608922  | -0.183769 | -0.448665 |
| O | 1.369901  | 0.512981  | 0.803379  |
| H | 0.516044  | -1.886990 | -0.555725 |
| C | -0.804452 | -0.175755 | -0.029828 |

```

O -1.659865 -0.925065 0.369266
C -1.019627 1.281547 -0.316613
H -1.970886 1.382152 -0.835448
H -1.076607 1.813024 0.630917
H -0.206053 1.706172 -0.897410
Rotational constants (GHz): 6.4596100 3.0580400 2.4963800
Vibrational harmonic frequencies (cm-1):
i713.3587 95.2465 175.3577
259.7899 279.1418 483.8316
557.4596 611.2127 800.9584
828.3756 964.6043 1045.8093
1057.5896 1260.6562 1330.6809
1398.3201 1467.8083 1481.5053
1598.7826 1824.1960 3088.0783
3107.5511 3165.9930 3185.3549
Zero-point correction (Hartree): 0.068501

```

```

#####
E- (CH3) (CHO) COO
#####

```

```

Population analysis as 298K (%)
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)
Compound Qtot Erel Erel2 n*Q*MB %

CH3_CHO_COO.t 1.204e+39 0.00 0.00 1.204e+39 100
CH3_CHO_COO.c 1.637e+39 4.85 4.85 4.505e+35 0.0374
Total 1.205e+39 100

```

```

CH3_CHO_COO.c
~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -342.21938077
Electronic state : 1-A
Cartesian coordinates (Angs):
C      -0.032568      0.299778      0.000027
O      -0.511596      -0.861389      -0.000086
O      -1.839101      -0.977203      -0.000026
C      -0.917823      1.470181      0.000216
C      1.462904      0.369636      -0.000049
O      2.172313      -0.592777      -0.000148
H      1.861875      1.397891      0.000139
H      -0.351266      2.396676      0.000289
H      -1.579255      1.409310      0.868535
H      -1.579360      1.409511      -0.868038
Rotational constants (GHz):      6.8166700      2.8111600      2.0144600
Vibrational harmonic frequencies (cm-1):
104.2784      218.6029      229.3823
278.0111      324.6737      481.2375
495.0968      702.0410      843.7400
950.4930      1009.1735      1065.5409
1105.2485      1276.1808      1393.4049
1423.1714      1440.4274      1480.0766
1588.9220      1855.4162      2999.1006
3050.3207      3097.4219      3179.5534
Zero-point correction (Hartree): 0.069693

```

```

CH3_CHO_COO.t
~~~~~
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -341.75638503
E(CCSD/Aug-CC-pVTZ) (Hartree): -341.69284431
T1 diagnostic: 0.033592
E(MP2/Aug-CC-pVTZ) (Hartree): -341.67769460
E(MP3/Aug-CC-pVTZ) (Hartree): -341.67723498
E(RHF/Aug-CC-pVTZ) (Hartree): -340.46345221
E(RM062X/Aug-CC-pVTZ) (Hartree): -342.22744060
Electronic state : 1-A
Cartesian coordinates (Angs):
C -0.011614 0.026868 0.000001
O -0.972790 -0.786797 -0.000120
O -2.210212 -0.292192 -0.000090
C -0.228269 1.474256 0.000172
C 1.312938 -0.648044 -0.000053
O 2.338193 -0.025581 0.000065
H 1.272270 -1.748069 -0.000200
H 0.721758 1.997742 0.000259
H -0.836959 1.734095 0.869859
H -0.836918 1.734309 -0.869478
Rotational constants (GHz): 8.8891900 2.4389600 1.9362100
Vibrational harmonic frequencies (cm-1):
135.6817 213.6106 242.8612
306.5538 322.1857 489.0708
507.0809 691.4027 842.0585
969.3813 1007.6951 1065.4937
1077.7639 1311.1880 1391.8017
1394.3233 1450.1574 1480.3221
1604.8869 1842.8348 3028.5352
3055.8651 3104.0921 3198.6004
Zero-point correction (Hartree): 0.070016

```

```

Population analysis as 298K (%)
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)
Compound Qtot Erel Erel2 n*Q*MB %

TS.CH3_CHO_COO.isomrot.t 1.209e+39 0.00 0.00 2.417e+39 98.9
TS.CH3_CHO_COO.isomrot.c 1.125e+39 2.60 2.60 2.805e+37 1.15
Total 2.445e+39 100

```

```

TS.CH3_CHO_COO.isomrot.c
~~~~~

```

E(UM062X/Aug-CC-pVTZ) (Hartree): -342.18647441  
 Electronic state : 1-A  
 Cartesian coordinates (Angs):  
 C -0.202418 0.426296 0.122035  
 O -0.568340 -0.836816 0.571615  
 O -0.824756 -1.626679 -0.444619  
 C -1.303519 1.384213 -0.068814  
 C 1.191253 0.652724 -0.118915  
 O 2.047730 -0.200593 0.022690  
 H 1.437836 1.674901 -0.448729  
 H -1.864278 1.512360 0.859851  
 H -1.999643 0.997329 -0.818216  
 H -0.922886 2.348725 -0.396227  
 Rotational constants (GHz): 4.7848800 3.5449800 2.2256700  
 Vibrational harmonic frequencies (cm-1):  
 i147.5638 154.4822 191.6700  
 239.4501 271.1921 366.7374  
 561.5429 618.1401 845.6945  
 925.1530 983.4841 1020.0313  
 1222.4891 1251.0429 1326.1354  
 1407.1213 1436.5896 1459.7970  
 1486.2098 1649.2321 2997.9965  
 3042.9802 3097.6360 3161.5736  
 Zero-point correction (Hartree): 0.067699

TS.CH3\_CHO\_COO.isomrot.t  
 ~~~~~  
 E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -341.71009146
 E(CCSD/Aug-CC-pVTZ) (Hartree): -341.65782404
 T1 diagnostic: 0.031205
 E(MP2/Aug-CC-pVTZ) (Hartree): -341.60933845
 E(MP3/Aug-CC-pVTZ) (Hartree): -341.63687604
 E(PMP2/Aug-CC-pVTZ) (Hartree): -341.67718877
 E(PMP3/Aug-CC-pVTZ) (Hartree): -341.70325477
 E(PUHF/Aug-CC-pVTZ) (Hartree): -340.55144866
 E(UHF/Aug-CC-pVTZ) (Hartree): -340.48252772
 E(UM062X/Aug-CC-pVTZ) (Hartree): -342.19057060
 Electronic state : 1-A
 Cartesian coordinates (Angs):
 C 0.001794 0.194894 0.189179
 O -1.246473 -0.312662 0.550102
 O -1.958381 -0.595155 -0.516630
 C 0.086842 1.640283 -0.057664
 C 1.064067 -0.756549 0.090973
 O 2.205400 -0.427117 -0.190383
 H 0.786194 -1.803048 0.286037
 H -0.238188 2.197556 0.823597
 H -0.579332 1.909720 -0.881541
 H 1.110741 1.903483 -0.307737
 Rotational constants (GHz): 6.5696300 2.6348000 2.0630500
 Vibrational harmonic frequencies (cm-1):
 i183.4742 150.1293 176.1830
 250.5881 277.6890 387.7975
 490.8970 638.0047 824.0553
 947.1438 981.6426 1013.4506
 1214.3555 1228.1302 1352.6083
 1403.2416 1418.8259 1465.9316
 1480.7541 1646.4755 3023.0018
 3047.1478 3102.7594 3177.0808
 Zero-point correction (Hartree): 0.067657

Population analysis as 298K (%)
 Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)
 Compound Qtot Erel Erel2 n*Q*MB %

 TS.CH3_CHO_COO.introt 8.604e+38 0.00 0.00 3.442e+39 100
 Total 3.442e+39 100

TS.CH3_CHO_COO.introt
 ~~~~~  
 E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -341.73996902  
 E(CCSD/Aug-CC-pVTZ) (Hartree): -341.67896022  
 T1 diagnostic: 0.031522  
 E(MP2/Aug-CC-pVTZ) (Hartree): -341.65956575  
 E(MP3/Aug-CC-pVTZ) (Hartree): -341.66280899  
 E(RHF/Aug-CC-pVTZ) (Hartree): -340.45513481  
 E(RM062X/Aug-CC-pVTZ) (Hartree): -342.21184014  
 Electronic state : 1-A  
 Cartesian coordinates (Angs):  
 C -0.014476 0.163846 0.142163  
 O -0.741695 -0.848937 0.109350  
 O -2.062973 -0.651635 -0.140098  
 C -0.567717 1.507980 -0.069217  
 C 1.448381 -0.106009 0.414816  
 O 2.212840 -0.351717 -0.468827  
 H 1.767079 -0.033021 1.468693  
 H -1.386389 1.656461 0.639620  
 H -1.036902 1.523144 -1.056785  
 H 0.193697 2.276821 0.018507  
 Rotational constants (GHz): 7.4325600 2.5192100 2.0334500  
 Vibrational harmonic frequencies (cm-1):  
 i153.2593 164.7995 215.7509  
 260.6351 312.9689 412.6959  
 522.9256 683.6775 818.8702  
 930.8347 986.0470 1038.0789  
 1077.2258 1280.4040 1383.6504  
 1408.6613 1438.4836 1475.6379  
 1630.9840 1868.7685 2992.0497  
 3051.7087 3102.0835 3182.2144  
 Zero-point correction (Hartree): 0.068890



Population analysis as 298K (%)  
 Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)  
 Compound Qtot Erel Erel2 n\*Q\*MB %  
 -----  
 TS.CH3\_CHO\_COO.14Hshift.t 6.784e+38 0.00 0.00 1.357e+39 98.5  
 TS.CH3\_CHO\_COO.14Hshift.c 8.241e+38 2.60 2.60 2.048e+37 1.49  
 Total 1.377e+39 100

TS.CH3\_CHO\_COO.14Hshift.c

~~~~~

E(RM062X/Aug-CC-pVTZ) (Hartree): -342.19113100

Electronic state : 1-A

Cartesian coordinates (Angs):

C	0.003698	0.290871	0.060092
O	0.508553	-0.888293	-0.005907
O	1.879742	-0.799488	-0.049961
C	0.910246	1.364176	0.045964
C	-1.481802	0.376188	-0.109210
H	1.590038	1.421364	0.895404
H	0.519396	2.320004	-0.275609
H	1.775649	0.539453	-0.478820
O	-2.218261	-0.542478	0.092460
H	-1.838216	1.373837	-0.414781

Rotational constants (GHz): 7.9545000 2.7066600 2.0468000

Vibrational harmonic frequencies (cm-1):

i1652.8814	111.3572	219.2448
270.2048	472.3814	534.6289
553.7064	744.3871	783.9037
868.2862	947.5729	999.6333
1046.6979	1084.7519	1324.1005
1376.8482	1412.7163	1511.7872
1562.4035	1860.5266	1871.7383
3001.0739	3111.0305	3225.6909

Zero-point correction (Hartree): 0.065827

TS.CH3_CHO_COO.14Hshift.t

~~~~~

E(CCS(D)T)/Aug-CC-pVTZ) (Hartree): -341.72182029

E(CCS(D)/Aug-CC-pVTZ) (Hartree): -341.65739876

T1 diagnostic: 0.026978

E(MP2/Aug-CC-pVTZ) (Hartree): -341.64981726

E(MP3/Aug-CC-pVTZ) (Hartree): -341.64510785

E(RHF/Aug-CC-pVTZ) (Hartree): -340.41708894

E(RM062X/Aug-CC-pVTZ) (Hartree): -342.19540999

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.016583 | 0.019919  | 0.125984  |
| O | 0.924216  | -0.861842 | 0.056112  |
| O | 2.134347  | -0.229276 | -0.104694 |
| C | 0.361335  | 1.360360  | 0.017181  |
| C | -1.385347 | -0.574878 | 0.027314  |
| H | 1.024902  | 1.731819  | 0.797019  |
| H | -0.415597 | 2.045978  | -0.288527 |
| H | 1.466301  | 0.913568  | -0.550217 |
| O | -2.360320 | 0.110084  | -0.080244 |
| H | -1.417976 | -1.675489 | 0.049460  |

Rotational constants (GHz): 9.8457500 2.4372500 1.9775300

Vibrational harmonic frequencies (cm-1):

|            |           |           |
|------------|-----------|-----------|
| i1666.1593 | 127.0143  | 231.2769  |
| 283.8072   | 467.8853  | 553.5485  |
| 571.4638   | 704.9714  | 770.2351  |
| 893.5815   | 961.2370  | 1001.9607 |
| 1047.4964  | 1061.5969 | 1330.2148 |
| 1357.1539  | 1410.7261 | 1502.0967 |
| 1586.1193  | 1852.1340 | 1860.1228 |
| 3022.3609  | 3115.4394 | 3242.8841 |

Zero-point correction (Hartree): 0.065965

Population analysis as 298K (%)  
 Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)

| Compound                   | Qtot      | Erel | Erel2 | n*Q*MB    | %     |
|----------------------------|-----------|------|-------|-----------|-------|
| -----                      |           |      |       |           |       |
| TS.CH3_CHO_COO.ringclose.t | 1.180e+39 | 0.00 | 0.00  | 2.361e+39 | 99.8  |
| TS.CH3_CHO_COO.ringclose.c | 1.434e+39 | 3.84 | 3.84  | 4.415e+36 | 0.187 |
| Total                      |           |      |       | 2.365e+39 | 100   |

TS.CH3\_CHO\_COO.ringclose.c

~~~~~

E(RM062X/Aug-CC-pVTZ) (Hartree): -342.17444804

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-0.145037	0.227550	0.121089
O	-0.458008	-0.928313	0.530521
O	-1.534776	-1.025656	-0.447281
C	-1.035293	1.410701	0.050958
C	1.346126	0.454392	-0.119008
O	2.128862	-0.444463	-0.090915
H	1.641627	1.499307	-0.313135
H	-2.013764	1.167957	0.449244
H	-0.560691	2.234110	0.593566
H	-1.150569	1.730217	-0.986516

Rotational constants (GHz): 6.1882000 3.0306100 2.2094200

Vibrational harmonic frequencies (cm-1):

i663.5827	82.0890	234.5889
254.5745	354.4500	385.4803
413.7927	623.5676	767.8449
878.1571	939.2471	979.3390
1053.3631	1213.5914	1397.5830
1404.2978	1441.2542	1462.7281
1598.2947	1869.3006	2994.9577

3044.3422 3106.0699 3201.2349
Zero-point correction (Hartree): 0.067662

TS.CH3_CHO_COO.ringclose.t

~~~~~  
E (CCSD(T)/Aug-CC-pVTZ) (Hartree): -341.71344917  
E (CCSD/Aug-CC-pVTZ) (Hartree): -341.65034485  
T1 diagnostic: 0.040271  
E (MP2/Aug-CC-pVTZ) (Hartree): -341.62635145  
E (MP3/Aug-CC-pVTZ) (Hartree): -341.63143149  
E (RHF/Aug-CC-pVTZ) (Hartree): -340.42803896  
E (RM062X/Aug-CC-pVTZ) (Hartree): -342.18077017  
Electronic state : 1-A

Cartesian coordinates (Angs):  
C -0.124179 0.004275 0.183785  
O -1.064051 -0.796786 0.478405  
O -1.921652 -0.237832 -0.567746  
C -0.181476 1.480896 0.164570  
C 1.228698 -0.672273 0.020356  
O 2.206074 -0.044544 -0.262124  
H 1.222764 -1.762762 0.171968  
H -1.157998 1.818402 0.491570  
H 0.632477 1.861631 0.785396  
H 0.001535 1.838640 -0.849468  
Rotational constants (GHz): 7.4068300 2.6695900 2.1688700  
Vibrational harmonic frequencies (cm-1):  
i674.3522 98.9349 238.3329  
263.3832 342.0435 391.5613  
453.2512 566.3667 795.7035  
811.2487 949.2087 1012.3727  
1057.2364 1263.4143 1374.0545  
1402.1696 1433.4928 1458.7883  
1596.3998 1860.0536 3029.8576  
3064.5194 3122.9061 3206.9977  
Zero-point correction (Hartree): 0.067872

#####  
Z- (CHO) (CH3) COO  
#####

Population analysis as 298K (%)  
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)  
Compound Qtot Erel Erel2 n\*Q\*MB %  
-----  
CHO\_CH3\_COO.t 3.549e+39 0.00 0.00 3.549e+39 100  
CHO\_CH3\_COO.c 2.795e+39 8.47 8.47 1.724e+33 4.86e-05  
Total 3.549e+39 100

CHO\_CH3\_COO.c

~~~~~  
E (RM062X/Aug-CC-pVTZ) (Hartree): -342.20480930
Electronic state : 1-A
Cartesian coordinates (Angs):
C 0.538720 -0.026854 -0.000063
O 0.155805 1.172634 0.000196
O -1.125973 1.503219 0.000134
C 2.008968 -0.247621 0.000070
C -0.377786 -1.205393 -0.000537
O -1.572703 -1.178340 0.000014
H 0.183416 -2.158412 0.000119
H 2.303984 -0.823463 0.879262
H 2.304219 -0.822971 -0.879364
H 2.531944 0.703946 0.000405
Rotational constants (GHz): 4.7557200 3.8204600 2.1465900
Vibrational harmonic frequencies (cm-1):
82.9639 131.4436 251.2871
277.9558 338.6106 397.1418
449.8791 649.8671 873.9613
963.5775 998.8438 1064.9416
1085.0586 1289.7969 1417.8069
1440.5344 1471.0639 1474.7765
1573.7140 1848.1234 2959.0349
3061.1445 3115.7403 3181.8811
Zero-point correction (Hartree): 0.069254

CHO_CH3_COO.t

~~~~~  
E (CCSD(T)/Aug-CC-pVTZ) (Hartree): -341.74686002  
E (CCSD/Aug-CC-pVTZ) (Hartree): -341.68490187  
T1 diagnostic: 0.034240  
E (MP2/Aug-CC-pVTZ) (Hartree): -341.66573811  
E (MP3/Aug-CC-pVTZ) (Hartree): -341.66913910  
E (RHF/Aug-CC-pVTZ) (Hartree): -340.46035318  
E (RM062X/Aug-CC-pVTZ) (Hartree): -342.21848314  
Electronic state : 1-A  
Cartesian coordinates (Angs):  
C -0.022790 0.359407 0.000033  
O -1.273197 0.431175 0.000153  
O -2.021213 -0.690488 0.000124  
C 0.750334 1.620717 0.000078  
C 0.675449 -0.969465 -0.000150  
O 1.876652 -0.987242 -0.000255  
H 0.044056 -1.861623 -0.000206  
H 1.400904 1.648300 0.874803  
H 1.400755 1.648455 -0.874753  
H 0.078389 2.473360 0.000211  
Rotational constants (GHz): 5.8257100 3.0527900 2.0279100  
Vibrational harmonic frequencies (cm-1):  
64.0033 134.7041 257.5687  
271.5464 311.0098 403.5970  
531.7946 633.0643 794.5198

```

971.6546          979.8679          1031.5199
1078.6819         1339.8042         1369.2756
1424.8490         1460.4460         1461.6561
1617.8565         1829.9014         3072.9052
3119.0174         3131.2016         3187.4213
Zero-point correction (Hartree): 0.069434

Population analysis as 298K (%)
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)
Compound      Qtot      Erel  Erel2  n*Q*MB      %
-----
TS.CH3_CHO_COO.isomrot.t 1.209e+39 0.00  0.00  2.417e+39 98.9
TS.CH3_CHO_COO.isomrot.c 1.125e+39 2.60  2.60  2.805e+37 1.15
Total                                2.445e+39 100

TS.CH3_CHO_COO.isomrot.c
~~~~~
E(UM062X/Aug-CC-pVTZ) (Hartree): -342.18647441
Electronic state : 1-A
Cartesian coordinates (Angs):
C -0.202418 0.426296 0.122035
O -0.568340 -0.836816 0.571615
O -0.824756 -1.626679 -0.444619
C -1.303519 1.384213 -0.068814
C 1.191253 0.652724 -0.118915
O 2.047730 -0.200593 0.022690
H 1.437836 1.674901 -0.448729
H -1.864278 1.512360 0.859851
H -1.999643 0.997329 -0.818216
H -0.922886 2.348725 -0.396227
Rotational constants (GHz): 4.7848800 3.5449800 2.2256700
Vibrational harmonic frequencies (cm-1):
i147.5638 154.4822 191.6700
239.4501 271.1921 366.7374
561.5429 618.1401 845.6945
925.1530 983.4841 1020.0313
1222.4891 1251.0429 1326.1354
1407.1213 1436.5896 1459.7970
1486.2098 1649.2321 2997.9965
3042.9802 3097.6360 3161.5736
Zero-point correction (Hartree): 0.067699

TS.CH3_CHO_COO.isomrot.t
~~~~~
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -341.71009146
E(CCSD/Aug-CC-pVTZ) (Hartree): -341.65782404
T1 diagnostic: 0.031205
E(MP2/Aug-CC-pVTZ) (Hartree): -341.60933845
E(MP3/Aug-CC-pVTZ) (Hartree): -341.63687604
E(PMP2/Aug-CC-pVTZ) (Hartree): -341.67718877
E(PMP3/Aug-CC-pVTZ) (Hartree): -341.70325477
E(PUHF/Aug-CC-pVTZ) (Hartree): -340.55144866
E(UHF/Aug-CC-pVTZ) (Hartree): -340.48252772
E(UM062X/Aug-CC-pVTZ) (Hartree): -342.19057060
Electronic state : 1-A
Cartesian coordinates (Angs):
C       0.001794      0.194894      0.189179
O      -1.246473     -0.312662      0.550102
O      -1.958381     -0.595155     -0.516630
C       0.086842      1.640283     -0.057664
C       1.064067     -0.756549      0.090973
O       2.205400     -0.427117     -0.190383
H       0.786194     -1.803048      0.286037
H      -0.238188      2.197556      0.823597
H      -0.579332      1.909720     -0.881541
H       1.110741      1.903483     -0.307737
Rotational constants (GHz):   6.5696300   2.6348000   2.0630500
Vibrational harmonic frequencies (cm-1):
i183.4742          150.1293          176.1830
250.5881           277.6890          387.7975
490.8970           638.0047          824.0553
947.1438           981.6426         1013.4506
1214.3555          1228.1302         1352.6083
1403.2416          1418.8259         1465.9316
1480.7541          1646.4755         3023.0018
3047.1478          3102.7594         3177.0808
Zero-point correction (Hartree): 0.067657

Population analysis as 298K (%)
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)
Compound      Qtot      Erel  Erel2  n*Q*MB      %
-----
TS.CHO_CH3_COO.introt.a 1.041e+39 0.00  0.00  4.165e+39 100
Total                                4.165e+39 100

TS.CHO_CH3_COO.introt.a
~~~~~
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -341.73328847
E(CCSD/Aug-CC-pVTZ) (Hartree): -341.67071849
T1 diagnostic: 0.034372
E(MP2/Aug-CC-pVTZ) (Hartree): -341.65276488
E(MP3/Aug-CC-pVTZ) (Hartree): -341.65430015
E(RHF/Aug-CC-pVTZ) (Hartree): -340.44303833
E(RM062X/Aug-CC-pVTZ) (Hartree): -342.20373691
Electronic state : 1-A
Cartesian coordinates (Angs):
C -0.526257 0.006435 0.034798
O -0.171861 -1.189229 -0.058148
O 1.109420 -1.548529 0.094706
C -1.975920 0.302869 -0.089366

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C 0.438247 1.137835 0.278439
O 1.481076 1.269975 -0.283770
H 0.052144 1.893140 0.987998
H -2.535729 -0.617705 -0.226063
H -2.327179 0.815662 0.808312
H -2.154737 0.968334 -0.935779
Rotational constants (GHz): 4.4492400 3.9086600 2.1712800
Vibrational harmonic frequencies (cm-1):
i110.7265 130.2039 223.7126
267.7949 327.5882 341.8941
514.5515 642.5333 854.1936
945.0517 984.1060 1054.3566
1062.1543 1284.2968 1413.1997
1429.9392 1468.3259 1471.1626
1612.5102 1867.7122 2958.6929
3059.7594 3115.7874 3178.7658
Zero-point correction (Hartree): 0.068820

Population analysis as 298K (%)
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)
Compound Qtot Erel Erel2 n*Q*MB %

TS.CHO_CH3_COO.14Hshift 1.588e+39 0.00 0.00 3.177e+39 100
Total 3.177e+39 100

TS.CHO_CH3_COO.14Hshift
~~~~~
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -341.70912739
E(CCSD/Aug-CC-pVTZ) (Hartree): -341.64208081
T1 diagnostic: 0.032819
E(MP2/Aug-CC-pVTZ) (Hartree): -341.63549166
E(MP3/Aug-CC-pVTZ) (Hartree): -341.62838024
E(RHF/Aug-CC-pVTZ) (Hartree): -340.39547809
E(RM062X/Aug-CC-pVTZ) (Hartree): -342.17896225
Electronic state : 1-A
Cartesian coordinates (Angs):
C      -0.426519     -0.270083     -0.122296
O      -0.982427     0.896543     -0.009463
O      0.016313      1.843677     -0.056919
C      0.990031     -0.188989     0.189776
C     -1.298581     -1.458426     0.028233
H      0.827525      1.059160     0.639391
O      1.979382     -0.772820     -0.104066
H     -2.214797     -1.212727     0.561790
H     -1.550122     -1.837095     -0.964211
H     -0.758330     -2.243551     0.552339
Rotational constants (GHz):      4.5261100      3.9105300      2.1480800
Vibrational harmonic frequencies (cm-1):
i1750.3334      83.1641      191.9676
261.2466      303.9876      406.2001
593.1323      641.0544      699.9771
796.4741      973.1140      1022.1120
1054.4909      1235.2465      1357.7414
1414.5090      1433.2542      1473.7325
1506.1459      1844.9871      1916.5558
3066.4062      3136.0258      3169.7932
Zero-point correction (Hartree): 0.065113

Population analysis as 298K (%)
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)
Compound      Qtot      Erel      Erel2      n*Q*MB      %
-----
TS.CHO_CH3_COO.ringclose.t 1.295e+39 0.00 0.00 2.590e+39 100
TS.CHO_CH3_COO.ringclose.c 1.930e+39 7.67 7.67 9.105e+33 0.000352
Total 2.590e+39 100

TS.CHO_CH3_COO.ringclose.c
~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -342.18333803
Electronic state : 1-A
Cartesian coordinates (Angs):
C -0.433268 -0.156312 -0.056840
O -0.636327 0.943098 -0.634625
O 0.081706 1.658174 0.440522
C -1.527341 -1.131744 0.108440
C 0.976729 -0.476047 0.406324
O 1.826681 -0.697328 -0.406067
H 1.129186 -0.569807 1.491788
H -1.894730 -1.010570 1.134148
H -2.343381 -0.914193 -0.575451
H -1.164267 -2.152361 0.003326
Rotational constants (GHz): 4.6970800 3.8012900 2.4739600
Vibrational harmonic frequencies (cm-1):
i490.9332 103.2116 125.6573
256.3981 304.8313 332.3573
418.2237 616.3165 835.4516
859.9651 953.0680 1004.2729
1040.2953 1244.4432 1381.6889
1401.9675 1440.4517 1471.2764
1633.2713 1841.6855 3021.0472
3045.9110 3127.4191 3184.8489
Zero-point correction (Hartree): 0.067534

TS.CHO_CH3_COO.ringclose.t
~~~~~
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -341.72903024
E(CCSD/Aug-CC-pVTZ) (Hartree): -341.66512809
T1 diagnostic: 0.036126
E(MP2/Aug-CC-pVTZ) (Hartree): -341.64547557
E(MP3/Aug-CC-pVTZ) (Hartree): -341.64689940

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E(RHF/Aug-CC-pVTZ) (Hartree): -340.43889879
E(RM062X/Aug-CC-pVTZ) (Hartree): -342.19612294
Electronic state : 1-A
Cartesian coordinates (Angs):
  C    0.189444    0.366995   -0.184200
  O    1.412758    0.075245   -0.379975
  O    1.316124   -1.076232    0.497896
  C   -0.209606    1.741443    0.147639
  C   -0.823145   -0.729998   -0.316060
  O   -1.920289   -0.608967    0.157345
  H   -0.493061   -1.586909   -0.915083
  H   -0.247401    1.783329    1.242902
  H    0.539548    2.450746   -0.194929
  H   -1.207995    1.961828   -0.219290
Rotational constants (GHz):    5.2974300    3.5922400    2.3589300
Vibrational harmonic frequencies (cm-1):
  i471.7492         111.1344         145.5716
  265.3612         380.9708         421.9026
  479.5167         606.9210         780.8173
  863.0952         967.1245        1015.5715
 1035.3622        1299.9419        1369.9243
 1383.1587        1436.5353        1464.6151
 1595.1124        1824.4756        3044.0655
 3068.4757        3133.4188        3195.4685
Zero-point correction (Hartree): 0.068091

#####
E- (CH3) (C (O) CH3) COO
#####

Population analysis as 298K (%)
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)
Compound      Qtot      Erel      Erel2      n*Q*MB      %
-----
CH3_CH3CO_COO.t 1.606e+40 0.00    0.00    1.606e+40 100
CH3_CH3CO_COO.c 1.973e+40 5.62    5.62    1.496e+36 0.00932
Total                      1.606e+40 100

CH3_CH3CO_COO.c
~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -381.53936829
Electronic state : 1-A
Cartesian coordinates (Angs):
 C -0.308141 0.164173 0.000018
 O -1.165484 -0.752921 -0.000099
 O -2.453050 -0.395662 -0.000058
 C -0.757065 1.564446 0.000193
 C 1.121907 -0.333542 -0.000041
 O 1.347353 -1.512261 -0.000190
 C 2.199062 0.714868 0.000105
 H -1.407385 1.715555 0.866263
 H -1.407382 1.715772 -0.865841
 H 0.069408 2.265304 0.000283
 H 3.165927 0.222444 0.000051
 H 2.107161 1.354116 -0.879239
 H 2.107143 1.353889 0.879612
Rotational constants (GHz): 4.9311500 1.9888500 1.4420800
Vibrational harmonic frequencies (cm-1):
 36.3904 182.4051 212.5573
 229.2029 266.3396 344.0151
 391.4829 464.0837 486.4331
 590.7438 619.1803 772.9088
 956.0280 988.7468 1010.1951
1061.0760 1080.2090 1174.4437
1312.8547 1392.7321 1396.5889
1442.2985 1468.5093 1480.6986
1481.1918 1582.1296 1849.0692
3051.7016 3067.2640 3093.3713
3130.0396 3190.3306 3203.6845
Zero-point correction (Hartree): 0.097981

CH3_CH3CO_COO.t
~~~~~
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -381.01115982
E(CCSD/Aug-CC-pVTZ) (Hartree): -380.94004743
T1 diagnostic: 0.031188
E(MP2/Aug-CC-pVTZ) (Hartree): -380.91440550
E(MP3/Aug-CC-pVTZ) (Hartree): -380.92418198
E(RHF/Aug-CC-pVTZ) (Hartree): -379.52543228
E(RM062X/Aug-CC-pVTZ) (Hartree): -381.54828627
Electronic state : 1-A
Cartesian coordinates (Angs):
  C    0.324355    0.248748   -0.000060
  O    0.952192   -0.839734    0.000066
  O    2.292275   -0.793316    0.000078
  C    1.031985    1.531118   -0.000190
  C   -1.173209    0.104285   -0.000070
  O   -1.838046    1.108569   -0.000081
  C   -1.742420   -1.283372    0.000208
  H    1.695475    1.557958   -0.868323
  H    1.695441    1.558152    0.867963
  H    0.327070    2.354361   -0.000295
  H   -2.825388   -1.217331    0.000275
  H   -1.394179   -1.831132   -0.875254
  H   -1.394054   -1.830834    0.875807
Rotational constants (GHz):    4.5959100    2.0877300    1.4610300
Vibrational harmonic frequencies (cm-1):
  74.6140         129.4376         186.7147
 214.9067         237.8304         314.7637
 405.3276         470.2393         494.3536
 601.4795         620.1731         772.9774

```

|           |           |           |
|-----------|-----------|-----------|
| 967.4324  | 997.8774  | 999.5282  |
| 1067.9005 | 1070.6704 | 1147.3839 |
| 1333.7823 | 1390.7812 | 1403.7941 |
| 1450.6490 | 1463.0782 | 1472.7326 |
| 1479.4008 | 1606.6851 | 1836.3965 |
| 3056.1510 | 3079.6031 | 3102.3447 |
| 3143.5809 | 3194.0170 | 3206.5774 |

Zero-point correction (Hartree): 0.097946

Population analysis as 298K (%)  
 Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)

| Compound                | Qtot      | Erel | Erel2 | n*Q*MB    | %   |
|-------------------------|-----------|------|-------|-----------|-----|
| TS.CH3_CH3CO_COO.introt | 6.668e+39 | 0.00 | 0.00  | 2.667e+40 | 100 |
| Total                   |           |      |       | 2.667e+40 | 100 |

TS.CH3\_CH3CO\_COO.introt  
 ~~~~~  
 E (CCSD(T)/Aug-CC-pVTZ) (Hartree): -380.99769648
 E (CCSD/Aug-CC-pVTZ) (Hartree): -380.92868476
 T1 diagnostic: 0.029093
 E (MP2/Aug-CC-pVTZ) (Hartree): -380.90017596
 E (MP3/Aug-CC-pVTZ) (Hartree): -380.91252239
 E (RHF/Aug-CC-pVTZ) (Hartree): -379.51900856
 E (RM062X/Aug-CC-pVTZ) (Hartree): -381.53537231
 Electronic state : 1-A
 Cartesian coordinates (Angs):

C	-0.323575	0.138103	-0.103565
O	-1.047899	-0.802597	0.276916
O	-2.389082	-0.567021	0.331731
C	-0.899200	1.440408	-0.467280
C	1.162955	-0.167374	-0.156483
O	1.610707	-0.741314	-1.108718
C	1.963804	0.315490	1.014914
H	-1.496817	1.798685	0.375012
H	-1.615218	1.275244	-1.276460
H	-0.132439	2.152969	-0.756499
H	3.020521	0.136551	0.840620
H	1.778171	1.377926	1.182113
H	1.632076	-0.213680	1.910279

Rotational constants (GHz): 4.6913900 1.7439100 1.6501800
 Vibrational harmonic frequencies (cm-1):

165.7462	137.5138	144.7133
193.2704	217.8088	300.8909
360.0966	409.0938	552.7934
594.2626	626.4004	765.3848
933.9349	952.8756	1017.7401
1045.8684	1074.1490	1150.7306
1319.0457	1384.0620	1392.7710
1437.6534	1460.4282	1469.4405
1479.5340	1633.4746	1864.2911
3052.2734	3063.0780	3103.2709
3126.3664	3179.6508	3183.4391

Zero-point correction (Hartree): 0.097110

Population analysis as 298K (%)
 Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)

Compound	Qtot	Erel	Erel2	n*Q*MB	%
TS.CH3_CH3CO_COO.14Hshift.t	8.240e+39	0.00	0.00	1.648e+40	99.6
TS.CH3_CH3CO_COO.14Hshift.c	8.401e+39	3.31	3.31	6.291e+37	0.38
Total				1.654e+40	100

TS.CH3_CH3CO_COO.14Hshift.c
 ~~~~~  
 E (RM062X/Aug-CC-pVTZ) (Hartree): -381.51193629  
 Electronic state : 1-A  
 Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.293467  | 0.128727  | 0.129720  |
| O | 1.131168  | -0.818781 | -0.098079 |
| O | 2.405336  | -0.306940 | -0.187643 |
| C | 0.837890  | 1.423423  | 0.217912  |
| C | -1.158194 | -0.286179 | 0.039015  |
| H | 1.527541  | 1.579755  | 1.047152  |
| H | 0.167535  | 2.251695  | 0.040724  |
| H | 1.874197  | 0.963985  | -0.433387 |
| O | -1.457327 | -1.435493 | 0.207157  |
| C | -2.147564 | 0.808788  | -0.239684 |
| H | -3.129177 | 0.367782  | -0.380089 |
| H | -2.172198 | 1.505920  | 0.598862  |
| H | -1.854918 | 1.372026  | -1.126510 |

Rotational constants (GHz): 5.2271300 1.9605900 1.4751600  
 Vibrational harmonic frequencies (cm-1):

|            |           |           |
|------------|-----------|-----------|
| i1626.9788 | 55.5997   | 182.9429  |
| 205.1806   | 223.7144  | 375.4170  |
| 474.9291   | 499.5696  | 540.1326  |
| 607.0526   | 672.8959  | 749.7642  |
| 874.4115   | 933.8398  | 967.7892  |
| 1018.5569  | 1054.3731 | 1062.9687 |
| 1198.2340  | 1339.6588 | 1381.6821 |
| 1403.6193  | 1470.0302 | 1476.1190 |
| 1511.9289  | 1544.6473 | 1854.3226 |
| 1876.8375  | 3070.7241 | 3109.6158 |
| 3135.3035  | 3189.1916 | 3237.2709 |

Zero-point correction (Hartree): 0.094085

TS.CH3\_CH3CO\_COO.14Hshift.t  
 ~~~~~  
 E (CCSD(T)/Aug-CC-pVTZ) (Hartree): -380.97769527
 E (CCSD/Aug-CC-pVTZ) (Hartree): -380.90528159

T1 diagnostic: 0.025088
 E(MP2/Aug-CC-pVTZ) (Hartree): -380.88808947
 E(MP3/Aug-CC-pVTZ) (Hartree): -380.89277429
 E(RHF/Aug-CC-pVTZ) (Hartree): -379.47885503
 E(RM062X/Aug-CC-pVTZ) (Hartree): -381.51715831
 Electronic state : 1-A
 Cartesian coordinates (Angs):
 C 0.305684 0.239408 0.121754
 O 0.925846 -0.888749 0.026238
 O 2.279297 -0.663138 -0.115664
 C 1.089757 1.394980 0.059768
 C -1.198175 0.144855 0.006215
 H 1.827268 1.510355 0.852993
 H 0.571072 2.299946 -0.219925
 H 2.004272 0.644718 -0.521008
 O -1.820872 1.165445 -0.113491
 C -1.806075 -1.224380 0.039993
 H -2.885664 -1.135941 -0.022598
 H -1.421885 -1.818398 -0.789417
 H -1.516376 -1.738318 0.956908
 Rotational constants (GHz): 4.9856200 2.0490500 1.4800800
 Vibrational harmonic frequencies (cm-1):
 i1655.6513 66.1366 151.8496
 206.1956 213.9988 386.5822
 469.9725 513.4557 550.5052
 604.1148 664.7821 747.1894
 858.7941 938.0984 987.4293
 1010.5650 1049.3493 1061.7347
 1187.5078 1332.7859 1379.4039
 1405.9550 1465.2620 1472.0427
 1499.6696 1576.4285 1851.5810
 1856.2582 3075.7136 3115.0357
 3139.1117 3193.5678 3245.2267
 Zero-point correction (Hartree): 0.094034

 Population analysis as 298K (%)
 Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)
 Compound Qtot Erel Erel2 n*Q*MB %

 TS.CH3_CH3CO_COO.ringclose.t 1.312e+40 0.00 0.00 2.624e+40 100
 Total 2.624e+40 100

 TS.CH3_CH3CO_COO.ringclose.t
 ~~~~~  
 E(CCS(D)/Aug-CC-pVTZ) (Hartree): -380.97018808  
 E(CCS(D)/Aug-CC-pVTZ) (Hartree): -380.89932551  
 T1 diagnostic: 0.036521  
 E(MP2/Aug-CC-pVTZ) (Hartree): -380.86592776  
 E(MP3/Aug-CC-pVTZ) (Hartree): -380.88067833  
 E(RHF/Aug-CC-pVTZ) (Hartree): -379.49160870  
 E(RM062X/Aug-CC-pVTZ) (Hartree): -381.50393373  
 Electronic state : 1-A  
 Cartesian coordinates (Angs):  
 C -0.419929 0.176095 0.174153  
 O -0.938005 -0.933918 0.503189  
 O -1.965876 -0.831066 -0.540706  
 C -1.107551 1.483242 0.131333  
 C 1.103118 0.151134 -0.027450  
 O 1.667198 1.198123 -0.196655  
 C 1.753928 -1.193675 -0.013111  
 H -2.131015 1.373212 0.469592  
 H -0.528245 2.187581 0.731822  
 H -1.103416 1.866372 -0.889711  
 H 2.825763 -1.081192 -0.137344  
 H 1.521057 -1.706177 0.921229  
 H 1.331924 -1.805677 -0.811759  
 Rotational constants (GHz): 4.1849000 2.2772400 1.5960100  
 Vibrational harmonic frequencies (cm-1):  
 i640.8420 49.5491 174.7674  
 214.5935 235.2341 270.9654  
 365.7066 384.8915 494.3649  
 537.0266 616.4886 698.8948  
 806.0169 938.0208 972.8373  
 1012.7101 1058.8638 1152.5439  
 1300.0016 1395.0383 1407.1811  
 1429.1849 1454.4857 1459.3560  
 1465.8934 1587.4693 1854.5475  
 3067.6732 3070.4448 3124.8730  
 3131.0034 3194.5651 3208.9710  
 Zero-point correction (Hartree): 0.095989  
  
 Population analysis as 298K (%)  
 Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)  
 Compound Qtot Erel Erel2 n\*Q\*MB %  
 -----  
 TS.CH3\_CH3CO\_COO.isomrot.t 1.400e+40 0.00 0.00 2.800e+40 99.8  
 TS.CH3\_CH3CO\_COO.isomrot.c 1.294e+40 3.62 3.62 5.734e+37 0.204  
 Total 2.806e+40 100  
  
 TS.CH3\_CH3CO\_COO.isomrot.c  
 ~~~~~  
 E(UM062X/Aug-CC-pVTZ) (Hartree): -381.50354708
 Electronic state : 1-A
 Cartesian coordinates (Angs):
 C 0.270686 0.384315 -0.201006
 O 1.431825 -0.322808 -0.498154
 O 2.036337 -0.697790 0.603773
 C 0.459871 1.838070 -0.041781
 C -0.936061 -0.404272 -0.058341
 O -0.895557 -1.616782 -0.172061

C -2.220186 0.335299 0.234976
H 0.920040 2.259710 -0.938598
H 1.145463 2.025280 0.790053
H -0.480227 2.346045 0.150517
H -3.027392 -0.388585 0.285539
H -2.149710 0.867778 1.184093
H -2.434868 1.068335 -0.543153
Rotational constants (GHz): 3.9508800 2.2789000 1.5787400
Vibrational harmonic frequencies (cm-1):
1143.6042 92.3988 127.5312
164.1664 198.8751 251.1489
360.8717 399.4838 500.6388
563.0747 608.8458 715.7917
958.8714 978.5649 983.1410
1035.6750 1137.3881 1221.8318
1258.3045 1363.5189 1402.8251
1407.6085 1461.2233 1476.2765
1486.4473 1487.3165 1687.0759
3041.8544 3069.3941 3093.0930
3133.2203 3179.2760 3184.4826
Zero-point correction (Hartree): 0.095752

TS.CH3_CH3COO.isomrot.t

~~~~~  
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -380.96345684  
E(CCSD/Aug-CC-pVTZ) (Hartree): -380.90281046  
T1 diagnostic: 0.027899  
E(MP2/Aug-CC-pVTZ) (Hartree): -380.84770320  
E(MP3/Aug-CC-pVTZ) (Hartree): -380.88290843  
E(PMP2/Aug-CC-pVTZ) (Hartree): -380.90680712  
E(PMP3/Aug-CC-pVTZ) (Hartree): -380.94081782  
E(PUHF/Aug-CC-pVTZ) (Hartree): -379.59856316  
E(UHF/Aug-CC-pVTZ) (Hartree): -379.53856013  
E(UM062X/Aug-CC-pVTZ) (Hartree): -381.50918000  
Electronic state : 1-A

Cartesian coordinates (Angs):  
C -0.330391 0.421936 0.182392  
O -1.213718 -0.608556 0.513395  
O -1.763079 -1.120337 -0.563297  
C -0.915599 1.763420 0.042678  
C 1.058131 0.065850 -0.005416  
O 1.864986 0.947097 -0.261768  
C 1.441789 -1.385562 0.119379  
H -1.423703 2.057363 0.963869  
H -1.662482 1.756803 -0.755855  
H -0.130608 2.476100 -0.191727  
H 2.516870 -1.472158 -0.000203  
H 1.136698 -1.782287 1.087586  
H 0.934123 -1.975311 -0.644508  
Rotational constants (GHz): 3.6834000 2.4195200 1.5901700  
Vibrational harmonic frequencies (cm-1):  
1165.2160 102.0234 132.5100  
142.0050 186.4474 237.0881  
334.1584 450.0094 471.5945  
548.4034 611.2828 718.8838  
942.9389 976.3850 988.0311  
1038.8700 1139.7900 1217.4996  
1242.7825 1368.9100 1396.0884  
1418.1685 1467.3837 1468.5036  
1476.9015 1481.4768 1686.2396  
3044.9702 3074.2678 3098.4456  
3137.2880 3182.0501 3189.4151  
Zero-point correction (Hartree): 0.095617

#####  
Z- (C(O)CH3) (CH3)COO  
#####

Population analysis as 298K (%)  
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)  
Compound Qtot Erel Erel2 n\*Q\*MB %  
-----  
CH3CO\_CH3\_COO.t 5.751e+40 0.00 0.00 5.751e+40 100  
Total 5.751e+40 100

CH3CO\_CH3\_COO.t

~~~~~  
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -381.00077515
E(CCSD/Aug-CC-pVTZ) (Hartree): -380.93096022
T1 diagnostic: 0.030625

E(MP2/Aug-CC-pVTZ) (Hartree): -380.90246168
E(MP3/Aug-CC-pVTZ) (Hartree): -380.91517074
E(RHF/Aug-CC-pVTZ) (Hartree): -379.51995609
E(RM062X/Aug-CC-pVTZ) (Hartree): -381.53887035
Electronic state : 1-A
Cartesian coordinates (Angs):
C -0.671638 0.139237 0.052180
O -1.079978 -1.038023 -0.026298
O -0.215203 -2.049317 -0.279473
C -1.690853 1.199979 0.235114
C 0.792653 0.535588 -0.052806
O 0.989762 1.658617 -0.444297
C 1.875207 -0.393054 0.389478
H 2.742683 0.202554 0.662600
H 1.536961 -1.030046 1.204664
H 2.114487 -1.064277 -0.434397
H -2.679076 0.760014 0.325285
H -1.454553 1.794572 1.117675
H -1.649361 1.876469 -0.619073
Rotational constants (GHz): 3.2654000 2.8291700 1.6203600
Vibrational harmonic frequencies (cm-1):

14.1644	143.2783	224.8779
259.4587	270.7007	299.8185
320.1427	411.5256	529.4461
625.9219	646.0774	686.7977
945.5459	998.4779	1008.0874
1040.1704	1068.9431	1162.4865
1349.0696	1397.0974	1414.8104
1447.7166	1460.5429	1463.4590
1467.1579	1629.8651	1825.9151
3074.6781	3078.5762	3133.8928
3149.7844	3180.3462	3189.5635

Zero-point correction (Hartree): 0.097775

Population analysis as 298K (%)

Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)

Compound	Qtot	Erel	Erel2	n*Q*MB	%
TS.CH3CO_CH3_COO.introt	4.459e+39	0.00	0.00	8.917e+39	100
Total				8.917e+39	100

TS.CH3CO_CH3_COO.introt

~~~~~

E (CCSD(T)/Aug-CC-pVTZ) (Hartree): -380.98821286

E (CCSD/Aug-CC-pVTZ) (Hartree): -380.91537568

T1 diagnostic: 0.032040

E (MP2/Aug-CC-pVTZ) (Hartree): -380.89248935

E (MP3/Aug-CC-pVTZ) (Hartree): -380.89943335

E (RHF/Aug-CC-pVTZ) (Hartree): -379.49455905

E (RM062X/Aug-CC-pVTZ) (Hartree): -381.52330406

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.249822  | 0.545401  | -0.000011 |
| O | 1.502138  | 0.399585  | -0.000000 |
| O | 2.102638  | -0.778985 | -0.000005 |
| C | -0.198735 | 1.967221  | 0.000008  |
| C | -0.730546 | -0.599776 | -0.000012 |
| O | -0.383865 | -1.748562 | 0.000016  |
| C | -2.185247 | -0.192872 | -0.000008 |
| H | -2.791103 | -1.093118 | -0.000273 |
| H | -2.419654 | 0.408164  | 0.879327  |
| H | -2.419557 | 0.408640  | -0.879041 |
| H | 0.668392  | 2.621277  | 0.000212  |
| H | -0.808414 | 2.179505  | -0.879039 |
| H | -0.808720 | 2.179379  | 0.878870  |

Rotational constants (GHz): 3.6988000 2.5531000 1.5391500

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| 133.4094  | 107.1109  | 221.7503  |
| 256.1735  | 292.4242  | 325.9906  |
| 334.5961  | 401.7045  | 467.4201  |
| 624.2326  | 636.4577  | 698.3348  |
| 973.8668  | 1004.7948 | 1007.9706 |
| 1063.4559 | 1084.3905 | 1171.3843 |
| 1321.8447 | 1393.8129 | 1420.9273 |
| 1457.3581 | 1470.6748 | 1477.9495 |
| 1488.5511 | 1555.5734 | 1835.8383 |
| 3066.6373 | 3072.7967 | 3124.2915 |
| 3135.8920 | 3176.4916 | 3188.8524 |

Zero-point correction (Hartree): 0.097641

Population analysis as 298K (%)

Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)

| Compound                  | Qtot      | Erel | Erel2 | n*Q*MB    | %   |
|---------------------------|-----------|------|-------|-----------|-----|
| TS.CH3CO_CH3_COO.15Hshift | 6.483e+39 | 0.00 | 0.00  | 1.297e+40 | 100 |
| Total                     |           |      |       | 1.297e+40 | 100 |

TS.CH3CO\_CH3\_COO.15Hshift

~~~~~

E (CCSD(T)/Aug-CC-pVTZ) (Hartree): -380.96360657

E (CCSD/Aug-CC-pVTZ) (Hartree): -380.89147306

T1 diagnostic: 0.023884

E (MP2/Aug-CC-pVTZ) (Hartree): -380.87191663

E (MP3/Aug-CC-pVTZ) (Hartree): -380.87928222

E (RHF/Aug-CC-pVTZ) (Hartree): -379.47067035

E (UM062X/Aug-CC-pVTZ) (Hartree): -381.50484993

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-0.634879	-0.218879	0.124183
O	-0.253854	-1.380733	-0.164854
O	1.115260	-1.628223	-0.376595
C	-2.079778	-0.028193	0.333289
C	0.344265	0.951498	0.046684
O	-0.053500	1.805893	-0.735312
C	1.588156	0.695716	0.649880
H	1.595277	-0.559759	-0.045004
H	2.350731	1.455052	0.546657
H	1.552274	0.176702	1.604774
H	-2.638847	-0.936615	0.131880
H	-2.236429	0.296120	1.364339
H	-2.392836	0.792146	-0.312774

Rotational constants (GHz): 3.1635300 2.9748700 1.7784200

Vibrational harmonic frequencies (cm-1):

i1223.3602	88.8560	128.9544
234.4632	274.5162	292.7813
451.9080	498.2140	572.1872
616.1720	669.1956	703.7695
753.0461	876.9681	937.1796
1001.9395	1036.0757	1060.7244
1204.0178	1267.1089	1348.7819
1403.9846	1451.4440	1454.2696

```

1463.7654          1600.4545          1740.6383
1769.7975          3067.6485          3125.8463
3134.0411          3190.4503          3237.5433
Zero-point correction (Hartree): 0.092623

Population analysis as 298K (%)
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)
Compound          Qtot          Erel    Erel2  n*Q*MB    %
-----
TS.CH3CO_CH3_COO.ringclose.t 1.142e+40 0.00    0.00    2.284e+40 100
TS.CH3CO_CH3_COO.ringclose.c 2.600e+40 5.49    5.49    4.859e+36 0.0213
Total                    2.285e+40 100

TS.CH3CO_CH3_COO.ringclose.c
~~~~~
E(UM062X/Aug-CC-pVTZ) (Hartree): -381.50585968
Electronic state : 1-A
Cartesian coordinates (Angs):
  C    -0.634021    0.245357   -0.121814
  O    -1.410011   -0.727646   -0.314399
  O    -0.657954   -1.557324    0.644755
  C    -1.197210    1.592214    0.110114
  C     0.870930    0.050001   -0.262828
  O     1.270845   -0.175591   -1.372393
  C     1.730788    0.274292    0.941172
  H     2.772821    0.325560    0.639688
  H     1.441162    1.197410    1.447291
  H     1.568766   -0.547742    1.636257
  H    -2.181885    1.669099   -0.345924
  H    -1.321115    1.693696    1.193975
  H    -0.525718    2.375287   -0.234854
Rotational constants (GHz):    3.4009700    2.4304900    2.0725600
Vibrational harmonic frequencies (cm-1):
  i498.3817          55.1124          105.6594
    149.1766          207.6156          229.8082
    297.7994          391.3304          459.8989
    548.2749          610.5527          707.0507
    849.9160          945.1508          996.9006
   1031.3651         1052.8249         1141.3978
   1296.9267         1376.7618         1390.3522
   1444.4697         1464.0768         1471.4127
   1477.8407         1626.2073         1846.1470
   3048.4752         3069.7091         3128.0765
   3143.1620         3179.5530         3186.1515
Zero-point correction (Hartree): 0.095522

TS.CH3CO_CH3_COO.ringclose.t
~~~~~
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -380.98178385
E(CCSD/Aug-CC-pVTZ) (Hartree): -380.91032590
T1 diagnostic: 0.032885
E(MP2/Aug-CC-pVTZ) (Hartree): -380.88061954
E(MP3/Aug-CC-pVTZ) (Hartree): -380.89213819
E(RHF/Aug-CC-pVTZ) (Hartree): -379.49880095
E(UM062X/Aug-CC-pVTZ) (Hartree): -381.51521468
Electronic state : 1-A
Cartesian coordinates (Angs):
  C     0.679758    0.033904    0.196148
  O     0.938669   -1.200723    0.339277
  O     0.133527   -1.551030   -0.822269
  C     1.769150    1.021996    0.233953
  C    -0.747480    0.488229   -0.022828
  O    -0.901386    1.541017   -0.589814
  C    -1.869100   -0.313880    0.575170
  H    -2.500737   -0.671021   -0.234873
  H    -1.508298   -1.167522    1.139752
  H    -2.456277    0.352945    1.205254
  H     2.640679    0.610338    0.735696
  H     2.027817    1.213801   -0.814277
  H     1.436356    1.965858    0.656226
Rotational constants (GHz):    3.4118200    2.8384000    1.8657700
Vibrational harmonic frequencies (cm-1):
  i471.4872          90.0003          119.0825
    155.3217         251.9704          258.3303
    335.2971         401.2756          520.0510
    567.0477         593.3486          704.9936
    858.0796         927.0139          1015.2988
   1033.5144         1047.9701          1132.5374
   1324.4467         1381.2747          1395.9779
   1432.4979         1461.3594          1469.6736
   1482.3568         1594.0690          1821.3682
   3046.3914         3085.9264          3135.2344
   3161.2042         3192.4973          3196.7249
Zero-point correction (Hartree): 0.096121

Population analysis as 298K (%)
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)
Compound          Qtot          Erel    Erel2  n*Q*MB    %
-----
TS.CH3_CH3CO_COO.isomrot.t 1.400e+40 0.00    0.00    2.800e+40 99.8
TS.CH3_CH3CO_COO.isomrot.c 1.294e+40 3.62    3.62    5.734e+37 0.204
Total                    2.806e+40 100

TS.CH3_CH3CO_COO.isomrot.c
~~~~~
E(UM062X/Aug-CC-pVTZ) (Hartree): -381.50354708
Electronic state : 1-A
Cartesian coordinates (Angs):
  C     0.270686    0.384315   -0.201006
  O     1.431825   -0.322808   -0.498154

```

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O      2.036337      -0.697790      0.603773
C      0.459871      1.838070      -0.041781
C     -0.936061     -0.404272     -0.058341
O     -0.895557     -1.616782     -0.172061
C     -2.220186      0.335299      0.234976
H      0.920040      2.259710     -0.938598
H      1.145463      2.025280      0.790053
H     -0.480227      2.346045      0.150517
H     -3.027392     -0.388585      0.285539
H     -2.149710      0.867778      1.184093
H     -2.434868      1.068335     -0.543153
Rotational constants (GHz):   3.9508800   2.2789000   1.5787400
Vibrational harmonic frequencies (cm-1):
i143.6042      92.3988      127.5312
164.1664      198.8751      251.1489
360.8717      399.4838      500.6388
563.0747      608.8458      715.7917
958.8714      978.5649      983.1410
1035.6750     1137.3881      1221.8318
1258.3045     1363.5189      1402.8251
1407.6085     1461.2233      1476.2765
1486.4473     1487.3165      1687.0759
3041.8544     3069.3941      3093.0930
3133.2203     3179.2760      3184.4826
Zero-point correction (Hartree): 0.095752

```

```

TS.CH3_CH3CO_COO.isomrot.t
~~~~~
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -380.96345684
E(CCSD/Aug-CC-pVTZ) (Hartree): -380.90281046
T1 diagnostic: 0.027899
E(MP2/Aug-CC-pVTZ) (Hartree): -380.84770320
E(MP3/Aug-CC-pVTZ) (Hartree): -380.88290843
E(PMP2/Aug-CC-pVTZ) (Hartree): -380.90680712
E(PMP3/Aug-CC-pVTZ) (Hartree): -380.94081782
E(PUHF/Aug-CC-pVTZ) (Hartree): -379.59856316
E(UHF/Aug-CC-pVTZ) (Hartree): -379.53856013
E(UM062X/Aug-CC-pVTZ) (Hartree): -381.50918000
Electronic state : 1-A
Cartesian coordinates (Angs):
C      -0.330391      0.421936      0.182392
O     -1.213718     -0.608556      0.513395
O     -1.763079     -1.120337     -0.563297
C     -0.915599      1.763420      0.042678
C      1.058131      0.065850     -0.005416
O      1.864986      0.947097     -0.261768
C      1.441789     -1.385562      0.119379
H     -1.423703      2.057363      0.963869
H     -1.662482      1.756803     -0.755855
H     -0.130608      2.476100     -0.191727
H      2.516870     -1.472158     -0.000203
H      1.136698     -1.782287      1.087586
H      0.934123     -1.975311     -0.644508
Rotational constants (GHz):   3.6834000   2.4195200   1.5901700
Vibrational harmonic frequencies (cm-1):
i165.2160      102.0234      132.5100
142.0050      186.4474      237.0881
334.1584      450.0094      471.5945
548.4034      611.2828      718.8838
942.9389      976.3850      988.0311
1038.8700     1139.7900      1217.4996
1242.7825     1368.9100      1396.0884
1418.1685     1467.3837      1468.5036
1476.9015     1481.4768      1686.2396
3044.9702     3074.2678      3098.4456
3137.2880     3182.0501      3189.4151
Zero-point correction (Hartree): 0.095617

```

```

#####
CH2OO (geometry + vib at ROHF-UCCSD(T)/aug-cc-pVTZ level of theory)
#####

```

```

Population analysis as 298K (%)
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)
Compound      Qtot      Erel      Erel2  n*Q*MB      %
-----
CH2O2.gradopt.Cs 3.093e+36 0.00 0.00 3.093e+36 100
Total          3.093e+36 100

```

```

CH2O2.gradopt.Cs
~~~~~
E(CCSD(T)/AUG-CC-PVQZ) (Hartree): -189.38009575
E(CCSD-T/AUG-CC-PVQZ) (Hartree): -189.37837091
E(CCSD/AUG-CC-PVQZ) (Hartree): -189.34204642
T1 diagnostic: 0.044439
D1 diagnostic: 0.178499
E(CCSD[T]/AUG-CC-PVQZ) (Hartree): -189.38576300
E(RHF/AUG-CC-PVQZ) (Hartree): -188.64228299
E(CCSD(T)/AUG-CC-PV5Z) (Hartree): -189.39551396
E(CCSD-T/AUG-CC-PV5Z) (Hartree): -189.39384553
E(CCSD/AUG-CC-PV5Z) (Hartree): -189.35664756
T1 diagnostic: 0.044016
D1 diagnostic: 0.176728
E(CCSD[T]/AUG-CC-PV5Z) (Hartree): -189.40108274
E(RHF/AUG-CC-PV5Z) (Hartree): -188.64515513
E(CCSD(T)/AUG-CC-PV6Z) (Hartree): -189.40089000
E(CCSD-T/AUG-CC-PV6Z) (Hartree): -189.39924692
E(CCSD/AUG-CC-PV6Z) (Hartree): -189.36173501
T1 diagnostic: 0.043826
D1 diagnostic: 0.175934

```

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E(CCSD[T]/AUG-CC-PV6Z) (Hartree): -189.40641476
E(RHF/AUG-CC-PV6Z) (Hartree): -188.64547670
E(CCSD(T)/AUG-CC-PVTZ) (Hartree): -189.33199213
E(CCSD-T/AUG-CC-PVTZ) (Hartree): -189.33011144
E(CCSD/AUG-CC-PVTZ) (Hartree): -189.29610902
  T1 diagnostic: 0.045571
  D1 diagnostic: 0.183198
E(CCSD[T]/AUG-CC-PVTZ) (Hartree): -189.33790817
E(RHF/AUG-CC-PVTZ) (Hartree): -188.63038395
Point group : Cs
Cartesian coordinates (Angs):
  C      1.070475      -0.195549      0.000000
  O      -0.014012      0.474814      0.000000
  O      -1.177108      -0.210703      0.000000
  H       1.013525      -1.277556      0.000000
  H       1.972175       0.400140      0.000000
Rotational constants (GHz):  77.0292797  12.3586560  10.6499648
Vibrational harmonic frequencies (cm-1):
  531.9100 ( A)      638.0400 ( A)      864.3500 ( A)
  934.4800 ( A)     1232.6900 ( A)     1306.6000 ( A)
 1483.9700 ( A)     3137.5900 ( A)     3294.9800 ( A)
Zero-point correction (Hartree): 0.030584

CH2O2.gradopt.Cs
-----
E(CCSD(T)/AUG-CC-PVTZ) (Hartree): -189.33199213
E(CCSD-T/AUG-CC-PVTZ) (Hartree): -189.33011144
E(CCSD/AUG-CC-PVTZ) (Hartree): -189.29610902
  T1 diagnostic: 0.045571
  D1 diagnostic: 0.183198
E(CCSD[T]/AUG-CC-PVTZ) (Hartree): -189.33790817
E(RHF/AUG-CC-PVTZ) (Hartree): -188.63038395
Cartesian coordinates (Angs):
  C      1.070475      -0.195549      0.000000
  O      -0.014012      0.474814      0.000000
  O      -1.177108      -0.210703      0.000000
  H       1.013525      -1.277556      0.000000
  H       1.972175       0.400140      0.000000
Rotational constants (GHz):  77.0292797  12.3586560  10.6499648

Population analysis as 298K (%)
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)
Compound      Qtot      Erel      Erel2  n*Q*MB      %
-----
TS.CH2O2.13Hshift.gradopt 3.042e+36 0.00  0.00  3.042e+36 100
Total                               3.042e+36 100

TS.CH2O2.13Hshift.gradopt
-----
E(CCSD(T)/AUG-CC-PVTZ) (Hartree): -189.27840028
E(CCSD-T/AUG-CC-PVTZ) (Hartree): -189.27733031
E(CCSD/AUG-CC-PVTZ) (Hartree): -189.24349049
  T1 diagnostic: 0.029735
  D1 diagnostic: 0.100448
E(CCSD[T]/AUG-CC-PVTZ) (Hartree): -189.28192927
E(RHF/AUG-CC-PVTZ) (Hartree): -188.57402559
Point group : C1
Cartesian coordinates (Angs):
  C      -0.973426      0.368173      0.000043
  O      -0.149489     -0.587579     -0.000012
  O       1.116414      0.173010     -0.000033
  H       0.148698      1.104453      0.000027
  H      -2.019378      0.034113      0.000068
Rotational constants (GHz):  57.0717088  14.1168912  11.3174736
Vibrational harmonic frequencies (cm-1):
 11823.0500      667.7400 ( A)      719.1000 ( A)
   873.2100 ( A)     1156.2800 ( A)     1262.9800 ( A)
  1499.6300 ( A)     2121.2800 ( A)     3048.0200 ( A)
Zero-point correction (Hartree): 0.025853

TS.CH2O2.13Hshift.gradopt
-----
E(CCSD(T)/AUG-CC-PVTZ) (Hartree): -189.27840028
E(CCSD-T/AUG-CC-PVTZ) (Hartree): -189.27733031
E(CCSD/AUG-CC-PVTZ) (Hartree): -189.24349049
  T1 diagnostic: 0.029735
  D1 diagnostic: 0.100448
E(CCSD[T]/AUG-CC-PVTZ) (Hartree): -189.28192927
E(RHF/AUG-CC-PVTZ) (Hartree): -188.57402559
Cartesian coordinates (Angs):
  C      -0.973426      0.368173      0.000043
  O      -0.149489     -0.587579     -0.000012
  O       1.116414      0.173010     -0.000033
  H       0.148698      1.104453      0.000027
  H      -2.019378      0.034113      0.000068
Rotational constants (GHz):  57.0717088  14.1168912  11.3174736

Population analysis as 298K (%)
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)
Compound      Qtot      Erel      Erel2  n*Q*MB      %
-----
TS.CH2O2.ringclose.gradopt 3.228e+36 0.00  0.00  6.457e+36 100
Total                               6.457e+36 100

TS.CH2O2.ringclose.gradopt
-----
E(CCSD(T)/AUG-CC-PVQZ) (Hartree): -189.34808636
E(CCSD-T/AUG-CC-PVQZ) (Hartree): -189.34573721
E(CCSD/AUG-CC-PVQZ) (Hartree): -189.30912922
  T1 diagnostic: 0.053021

```

D1 diagnostic: 0.213387
 E(CCSD[T]/AUG-CC-PVQZ) (Hartree): -189.35507641
 E(RHF/AUG-CC-PVQZ) (Hartree): -188.61302509
 E(CCSD(T)/AUG-CC-PV5Z) (Hartree): -189.36342695
 E(CCSD-T/AUG-CC-PV5Z) (Hartree): -189.36115929
 E(CCSD/AUG-CC-PV5Z) (Hartree): -189.32367210
 T1 diagnostic: 0.052483
 D1 diagnostic: 0.211135
 E(CCSD[T]/AUG-CC-PV5Z) (Hartree): -189.37029612
 E(RHF/AUG-CC-PV5Z) (Hartree): -188.61588858
 E(CCSD(T)/AUG-CC-PV6Z) (Hartree): -189.36876585
 E(CCSD-T/AUG-CC-PV6Z) (Hartree): -189.36653370
 E(CCSD/AUG-CC-PV6Z) (Hartree): -189.32872865
 T1 diagnostic: 0.052255
 D1 diagnostic: 0.210184
 E(CCSD[T]/AUG-CC-PV6Z) (Hartree): -189.37558355
 E(RHF/AUG-CC-PV6Z) (Hartree): -188.61620415
 E(CCSD(T)/AUG-CC-PVTZ) (Hartree): -189.30065712
 E(CCSD-T/AUG-CC-PVTZ) (Hartree): -189.29809371
 E(CCSD/AUG-CC-PVTZ) (Hartree): -189.26382444
 T1 diagnostic: 0.054369
 D1 diagnostic: 0.218991
 E(CCSD[T]/AUG-CC-PVTZ) (Hartree): -189.30794453
 E(RHF/AUG-CC-PVTZ) (Hartree): -188.60154670
 Point group : C1
 Cartesian coordinates (Angs):
 C -0.911324 -0.293899 0.000908
 O -0.052099 0.662355 -0.087476
 O 1.071139 -0.269750 0.080862
 H -1.785633 -0.133429 0.630473
 H -0.768872 -1.190395 -0.589080
 Rotational constants (GHz): 43.5992121 15.2511466 11.7816676
 Vibrational harmonic frequencies (cm-1):
 i745.0800 664.0600 (A) 792.7400 (A)
 953.8900 (A) 1190.5200 (A) 1326.7800 (A)
 1520.6500 (A) 3089.4700 (A) 3245.2600 (A)
 Zero-point correction (Hartree): 0.029123

 TS.CH2O2.ringclose.gradopt

 E(CCSD(T)/AUG-CC-PVTZ) (Hartree): -189.30065712
 E(CCSD-T/AUG-CC-PVTZ) (Hartree): -189.29809371
 E(CCSD/AUG-CC-PVTZ) (Hartree): -189.26382444
 T1 diagnostic: 0.054369
 D1 diagnostic: 0.218991
 E(CCSD[T]/AUG-CC-PVTZ) (Hartree): -189.30794453
 E(RHF/AUG-CC-PVTZ) (Hartree): -188.60154670
 Cartesian coordinates (Angs):
 C -0.911324 -0.293899 0.000908
 O -0.052099 0.662355 -0.087476
 O 1.071139 -0.269750 0.080862
 H -1.785633 -0.133429 0.630473
 H -0.768872 -1.190395 -0.589080
 Rotational constants (GHz): 43.5992121 15.2511466 11.7816676

 Population analysis as 298K (%)
 Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)
 Compound Qtot Erel Erel2 n*Q*MB %

 TS.CH2O2.ringclose.gradopt 3.228e+36 0.00 0.00 6.457e+36 100
 Total 6.457e+36 100

 TS.CH2O2.ringclose.gradopt
 ~~~~~  
 E(CCSD(T)/AUG-CC-PVQZ) (Hartree): -189.34808636  
 E(CCSD-T/AUG-CC-PVQZ) (Hartree): -189.34573721  
 E(CCSD/AUG-CC-PVQZ) (Hartree): -189.30912922  
 T1 diagnostic: 0.053021  
 D1 diagnostic: 0.213387  
 E(CCSD[T]/AUG-CC-PVQZ) (Hartree): -189.35507641  
 E(RHF/AUG-CC-PVQZ) (Hartree): -188.61302509  
 E(CCSD(T)/AUG-CC-PV5Z) (Hartree): -189.36342695  
 E(CCSD-T/AUG-CC-PV5Z) (Hartree): -189.36115929  
 E(CCSD/AUG-CC-PV5Z) (Hartree): -189.32367210  
 T1 diagnostic: 0.052483  
 D1 diagnostic: 0.211135  
 E(CCSD[T]/AUG-CC-PV5Z) (Hartree): -189.37029612  
 E(RHF/AUG-CC-PV5Z) (Hartree): -188.61588858  
 E(CCSD(T)/AUG-CC-PV6Z) (Hartree): -189.36876585  
 E(CCSD-T/AUG-CC-PV6Z) (Hartree): -189.36653370  
 E(CCSD/AUG-CC-PV6Z) (Hartree): -189.32872865  
 T1 diagnostic: 0.052255  
 D1 diagnostic: 0.210184  
 E(CCSD[T]/AUG-CC-PV6Z) (Hartree): -189.37558355  
 E(RHF/AUG-CC-PV6Z) (Hartree): -188.61620415  
 E(CCSD(T)/AUG-CC-PVTZ) (Hartree): -189.30065712  
 E(CCSD-T/AUG-CC-PVTZ) (Hartree): -189.29809371  
 E(CCSD/AUG-CC-PVTZ) (Hartree): -189.26382444  
 T1 diagnostic: 0.054369  
 D1 diagnostic: 0.218991  
 E(CCSD[T]/AUG-CC-PVTZ) (Hartree): -189.30794453  
 E(RHF/AUG-CC-PVTZ) (Hartree): -188.60154670  
 Point group : C1  
 Cartesian coordinates (Angs):  
 C -0.911324 -0.293899 0.000908  
 O -0.052099 0.662355 -0.087476  
 O 1.071139 -0.269750 0.080862  
 H -1.785633 -0.133429 0.630473  
 H -0.768872 -1.190395 -0.589080  
 Rotational constants (GHz): 43.5992121 15.2511466 11.7816676  
 Vibrational harmonic frequencies (cm-1):

```

i745.0800          664.0600 ( A)          792.7400 ( A)
953.8900 ( A)      1190.5200 ( A)          1326.7800 ( A)
1520.6500 ( A)     3089.4700 ( A)          3245.2600 ( A)
Zero-point correction (Hartree): 0.029123

TS.CH2O2.ringclose.gradopt
-----
E(CCSD(T)/AUG-CC-PVTZ) (Hartree): -189.30065712
E(CCSD-T/AUG-CC-PVTZ) (Hartree): -189.29809371
E(CCSD/AUG-CC-PVTZ) (Hartree): -189.26382444
T1 diagnostic: 0.054369
D1 diagnostic: 0.218991
E(CCSD[T]/AUG-CC-PVTZ) (Hartree): -189.30794453
E(RHF/AUG-CC-PVTZ) (Hartree): -188.60154670
Cartesian coordinates (Angs):
C      -0.911324      -0.293899      0.000908
O      -0.052099      0.662355     -0.087476
O       1.071139     -0.269750      0.080862
H      -1.785633     -0.133429      0.630473
H      -0.768872     -1.190395     -0.589080
Rotational constants (GHz):  43.5992121  15.2511466  11.7816676

#####
CH2OO (geometry + vib at ROHF-UCCSD(T)/aug-cc-pVQZ level of theory)
#####

Population analysis as 298K (%)
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)
Compound      Qtot      Erel      Erel2  n*Q*MB      %
-----
CH2O2.gradoptQ.Cs 3.048e+36 0.00  0.00  3.048e+36 100
Total              3.048e+36 100

CH2O2.gradoptQ.Cs
~~~~~
E(CCSD(T)/AUG-CC-PV5Z) (Hartree): -189.39559627
E(CCSD-T/AUG-CC-PV5Z) (Hartree): -189.39398139
E(CCSD/AUG-CC-PV5Z) (Hartree): -189.35696488
T1 diagnostic: 0.043321
D1 diagnostic: 0.173959
E(CCSD[T]/AUG-CC-PV5Z) (Hartree): -189.40104327
E(RHF/AUG-CC-PV5Z) (Hartree): -188.64580111
E(CCSD(T)/AUG-CC-PV6Z) (Hartree): -189.40098143
E(CCSD-T/AUG-CC-PV6Z) (Hartree): -189.39939077
E(CCSD/AUG-CC-PV6Z) (Hartree): -189.36206085
T1 diagnostic: 0.043137
D1 diagnostic: 0.173187
E(CCSD[T]/AUG-CC-PV6Z) (Hartree): -189.40638597
E(RHF/AUG-CC-PV6Z) (Hartree): -188.64612363
E(CCSD(T)/AUG-CC-PVQZ) (Hartree): -189.38015319
E(CCSD-T/AUG-CC-PVQZ) (Hartree): -189.37848348
E(CCSD/AUG-CC-PVQZ) (Hartree): -189.34233830
T1 diagnostic: 0.043742
D1 diagnostic: 0.175723
E(CCSD[T]/AUG-CC-PVQZ) (Hartree): -189.38569727
E(RHF/AUG-CC-PVQZ) (Hartree): -188.64292465
Point group : Cs
Cartesian coordinates (Angs):
C 1.068448 -0.195230 0.000000
O -0.012958 0.471270 0.000000
O -1.171117 -0.209097 0.000000
H 1.011881 -1.276190 0.000000
H 1.968800 0.400393 0.000000
Rotational constants (GHz): 77.8348806 12.4486379 10.7321720
Vibrational harmonic frequencies (cm-1):
533.6400 (A) 636.7100 (A) 873.1200 (A)
944.4300 (A) 1237.2500 (A) 1315.1400 (A)
1487.6800 (A) 3139.3100 (A) 3301.8300 (A)
Zero-point correction (Hartree): 0.030685

CH2O2.gradoptQ.Cs

E(CCSD(T)/AUG-CC-PVQZ) (Hartree): -189.38015319
E(CCSD-T/AUG-CC-PVQZ) (Hartree): -189.37848348
E(CCSD/AUG-CC-PVQZ) (Hartree): -189.34233830
T1 diagnostic: 0.043742
D1 diagnostic: 0.175723
E(CCSD[T]/AUG-CC-PVQZ) (Hartree): -189.38569727
E(RHF/AUG-CC-PVQZ) (Hartree): -188.64292465
Cartesian coordinates (Angs):
C 1.068448 -0.195230 0.000000
O -0.012958 0.471270 0.000000
O -1.171117 -0.209097 0.000000
H 1.011881 -1.276190 0.000000
H 1.968800 0.400393 0.000000
Rotational constants (GHz): 77.8348806 12.4486379 10.7321720

Population analysis as 298K (%)
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)
Compound Qtot Erel Erel2 n*Q*MB %

TS.CH2O2.ringclose.gradoptQ 3.181e+36 0.00 0.00 6.363e+36 100
Total 6.363e+36 100

TS.CH2O2.ringclose.gradoptQ
~~~~~
E(CCSD(T)/AUG-CC-PV5Z) (Hartree): -189.36349175
E(CCSD-T/AUG-CC-PV5Z) (Hartree): -189.36127781
E(CCSD/AUG-CC-PV5Z) (Hartree): -189.32396398
T1 diagnostic: 0.051880

```

D1 diagnostic: 0.208742  
 E(CCSD[T]/AUG-CC-PV5Z) (Hartree): -189.37024420  
 E(RHF/AUG-CC-PV5Z) (Hartree): -188.61643224  
 E(CCSD(T)/AUG-CC-PV6Z) (Hartree): -189.36883878  
 E(CCSD-T/AUG-CC-PV6Z) (Hartree): -189.36665945  
 E(CCSD/AUG-CC-PV6Z) (Hartree): -189.32902849  
 T1 diagnostic: 0.051655  
 D1 diagnostic: 0.207803  
 E(CCSD[T]/AUG-CC-PV6Z) (Hartree): -189.37554073  
 E(RHF/AUG-CC-PV6Z) (Hartree): -188.61674853  
 E(CCSD(T)/AUG-CC-PVQZ) (Hartree): -189.34812651  
 E(CCSD-T/AUG-CC-PVQZ) (Hartree): -189.34583637  
 E(CCSD/AUG-CC-PVQZ) (Hartree): -189.30940238  
 T1 diagnostic: 0.052372  
 D1 diagnostic: 0.210798  
 E(CCSD[T]/AUG-CC-PVQZ) (Hartree): -189.35499194  
 E(RHF/AUG-CC-PVQZ) (Hartree): -188.61356523  
 Point group : C1  
 Cartesian coordinates (Angs):  
 C -0.909213 -0.293302 0.001241  
 O -0.053170 0.659439 -0.086811  
 O 1.065772 -0.269606 0.080069  
 H -1.783325 -0.132758 0.629531  
 H -0.766852 -1.188891 -0.588342  
 Rotational constants (GHz): 43.8880752 15.3640488 11.8680640  
 Vibrational harmonic frequencies (cm-1):  
 i749.1300 674.6300 ( A) 799.3900 ( A)  
 967.5600 ( A) 1201.3600 ( A) 1337.1900 ( A)  
 1528.5800 ( A) 3093.7300 ( A) 3251.4600 ( A)  
 Zero-point correction (Hartree): 0.029283  
  
 TS.CH2O2.ringclose.gradoptQ  
 -----  
 E(CCSD(T)/AUG-CC-PVQZ) (Hartree): -189.34812651  
 E(CCSD-T/AUG-CC-PVQZ) (Hartree): -189.34583637  
 E(CCSD/AUG-CC-PVQZ) (Hartree): -189.30940238  
 T1 diagnostic: 0.052372  
 D1 diagnostic: 0.210798  
 E(CCSD[T]/AUG-CC-PVQZ) (Hartree): -189.35499194  
 E(RHF/AUG-CC-PVQZ) (Hartree): -188.61356523  
 Cartesian coordinates (Angs):  
 C -0.909213 -0.293302 0.001241  
 O -0.053170 0.659439 -0.086811  
 O 1.065772 -0.269606 0.080069  
 H -1.783325 -0.132758 0.629531  
 H -0.766852 -1.188891 -0.588342  
 Rotational constants (GHz): 43.8880752 15.3640488 11.8680640  
  
 Population analysis as 298K (%)  
 Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)  

| Compound                    | Qtot      | Erel | Erel2 | n*Q*MB    | %   |
|-----------------------------|-----------|------|-------|-----------|-----|
| TS.CH2O2.ringclose.gradoptQ | 3.181e+36 | 0.00 | 0.00  | 6.363e+36 | 100 |
| Total                       |           |      |       | 6.363e+36 | 100 |

  
 TS.CH2O2.ringclose.gradoptQ  
 ~~~~~  
 E(CCSD(T)/AUG-CC-PV5Z) (Hartree): -189.36349175
 E(CCSD-T/AUG-CC-PV5Z) (Hartree): -189.36127781
 E(CCSD/AUG-CC-PV5Z) (Hartree): -189.32396398
 T1 diagnostic: 0.051880
 D1 diagnostic: 0.208742
 E(CCSD[T]/AUG-CC-PV5Z) (Hartree): -189.37024420
 E(RHF/AUG-CC-PV5Z) (Hartree): -188.61643224
 E(CCSD(T)/AUG-CC-PV6Z) (Hartree): -189.36883878
 E(CCSD-T/AUG-CC-PV6Z) (Hartree): -189.36665945
 E(CCSD/AUG-CC-PV6Z) (Hartree): -189.32902849
 T1 diagnostic: 0.051655
 D1 diagnostic: 0.207803
 E(CCSD[T]/AUG-CC-PV6Z) (Hartree): -189.37554073
 E(RHF/AUG-CC-PV6Z) (Hartree): -188.61674853
 E(CCSD(T)/AUG-CC-PVQZ) (Hartree): -189.34812651
 E(CCSD-T/AUG-CC-PVQZ) (Hartree): -189.34583637
 E(CCSD/AUG-CC-PVQZ) (Hartree): -189.30940238
 T1 diagnostic: 0.052372
 D1 diagnostic: 0.210798
 E(CCSD[T]/AUG-CC-PVQZ) (Hartree): -189.35499194
 E(RHF/AUG-CC-PVQZ) (Hartree): -188.61356523
 Point group : C1
 Cartesian coordinates (Angs):
 C -0.909213 -0.293302 0.001241
 O -0.053170 0.659439 -0.086811
 O 1.065772 -0.269606 0.080069
 H -1.783325 -0.132758 0.629531
 H -0.766852 -1.188891 -0.588342
 Rotational constants (GHz): 43.8880752 15.3640488 11.8680640
 Vibrational harmonic frequencies (cm-1):
 i749.1300 674.6300 (A) 799.3900 (A)
 967.5600 (A) 1201.3600 (A) 1337.1900 (A)
 1528.5800 (A) 3093.7300 (A) 3251.4600 (A)
 Zero-point correction (Hartree): 0.029283

 TS.CH2O2.ringclose.gradoptQ

 E(CCSD(T)/AUG-CC-PVQZ) (Hartree): -189.34812651
 E(CCSD-T/AUG-CC-PVQZ) (Hartree): -189.34583637
 E(CCSD/AUG-CC-PVQZ) (Hartree): -189.30940238
 T1 diagnostic: 0.052372
 D1 diagnostic: 0.210798
 E(CCSD[T]/AUG-CC-PVQZ) (Hartree): -189.35499194
 E(RHF/AUG-CC-PVQZ) (Hartree): -188.61356523

```

Cartesian coordinates (Angs):
  C   -0.909213   -0.293302    0.001241
  O   -0.053170    0.659439   -0.086811
  O    1.065772   -0.269606    0.080069
  H   -1.783325   -0.132758    0.629531
  H   -0.766852   -1.188891   -0.588342
Rotational constants (GHz):  43.8880752  15.3640488  11.8680640

#####
Z-CH3CHOO (geometry + vib at ROHF-UCCSD(T)/aug-cc-pVTZ level of theory)
#####

Population analysis as 298K (%)
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)
Compound      Qtot      Erel  Erel2  n*Q*MB      %
-----
CH3CHO2s.Cs.freq 1.016e+38 0.00  0.00  1.016e+38 100
Total              1.016e+38 100

CH3CHO2s.Cs.freq
~~~~~
E(CCSD(T)/AUG-CC-PVTZ) (Hartree): -228.59171671
E(CCSD-T/AUG-CC-PVTZ) (Hartree): -228.59000203
E(CCSD/AUG-CC-PVTZ) (Hartree): -228.54882230
  T1 diagnostic:  0.037662
  D1 diagnostic:  0.172936
E(CCSD[T]/AUG-CC-PVTZ) (Hartree): -228.59749783
E(RHF/AUG-CC-PVTZ) (Hartree): -227.69932479
Point group : Cs
Cartesian coordinates (Angs):
  C   0.480462    0.710905    0.000000
  O   -0.790234    0.593453    0.000000
  O   -1.277109   -0.684921    0.000000
  C   1.349635   -0.478579    0.000000
  H   0.807186    1.744095    0.000000
  H   1.102414   -1.094296   -0.871627
  H   1.102414   -1.094296    0.871627
  H   2.400422   -0.195890    0.000000
Rotational constants (GHz):  17.4531507  7.0986646  5.2054191
Vibrational harmonic frequencies (cm-1):
  66.4000 ( A)    294.8200 ( A)    424.2500 ( A)
  654.2500 ( A)    694.3500 ( A)    899.1400 ( A)
  959.1200 ( A)    1013.1400 ( A)    1099.1600 ( A)
  1291.3000 ( A)    1374.2800 ( A)    1423.2700 ( A)
  1444.6900 ( A)    1506.0500 ( A)    3018.5200 ( A)
  3071.3300 ( A)    3153.2000 ( A)    3199.9000 ( A)
Zero-point correction (Hartree): 0.058292

CH3CHO2s.Cs.freq
-----
E(CCSD(T)/AUG-CC-PVTZ) (Hartree): -228.59171671
E(CCSD-T/AUG-CC-PVTZ) (Hartree): -228.59000203
E(CCSD/AUG-CC-PVTZ) (Hartree): -228.54882230
  T1 diagnostic:  0.037662
  D1 diagnostic:  0.172936
E(CCSD[T]/AUG-CC-PVTZ) (Hartree): -228.59749783
E(RHF/AUG-CC-PVTZ) (Hartree): -227.69932479
Cartesian coordinates (Angs):
  C   0.480462    0.710905    0.000000
  O   -0.790234    0.593453    0.000000
  O   -1.277109   -0.684921    0.000000
  C   1.349635   -0.478579    0.000000
  H   0.807186    1.744095    0.000000
  H   1.102414   -1.094296   -0.871627
  H   1.102414   -1.094296    0.871627
  H   2.400422   -0.195890    0.000000
Rotational constants (GHz):  17.4531507  7.0986646  5.2054191

Population analysis as 298K (%)
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)
Compound      Qtot      Erel  Erel2  n*Q*MB      %
-----
TS.CH3CHO2s.ringclose.freq 3.719e+37 0.00  0.00  7.439e+37 100
Total              7.439e+37 100

TS.CH3CHO2s.ringclose.freq
~~~~~
E(CCSD(T)/AUG-CC-PVTZ) (Hartree): -228.55295804
E(CCSD-T/AUG-CC-PVTZ) (Hartree): -228.55093593
E(CCSD/AUG-CC-PVTZ) (Hartree): -228.50999010
  T1 diagnostic:  0.041834
  D1 diagnostic:  0.190100
E(CCSD[T]/AUG-CC-PVTZ) (Hartree): -228.55909378
E(RHF/AUG-CC-PVTZ) (Hartree): -227.66705423
Point group : C1
Cartesian coordinates (Angs):
  C   0.290825    0.614623    0.226603
  O   -0.888577    0.605766   -0.283125
  O   -1.092938   -0.812475    0.139795
  C   1.402950   -0.318551   -0.098486
  H   0.516133    1.496981    0.836404
  H   1.094673   -1.017406   -0.872265
  H   1.692446   -0.883177    0.791210
  H   2.268622    0.281426   -0.404813
Rotational constants (GHz):  16.3541894  7.1700460  5.4731673
Vibrational harmonic frequencies (cm-1):
  1714.7200    206.5800 ( A)    360.4500 ( A)
  478.9900 ( A)    702.8400 ( A)    850.2800 ( A)
  905.6600 ( A)    1062.8400 ( A)    1135.3500 ( A)
  1328.7000 ( A)    1396.2700 ( A)    1443.7800 ( A)

```



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1468.2200 ( A)      1545.3600 ( A)      3011.5900 ( A)
3060.3500 ( A)      3088.0800 ( A)      3170.2300 ( A)
Zero-point correction (Hartree): 0.057445

TS.CH3CHO2s.ringclose.freq
-----
E (CCSD(T)/AUG-CC-PVTZ) (Hartree): -228.55295804
E (CCSD-T/AUG-CC-PVTZ) (Hartree): -228.55093593
E (CCSD/AUG-CC-PVTZ) (Hartree): -228.50999010
T1 diagnostic: 0.041834
D1 diagnostic: 0.190100
E (CCSD[T]/AUG-CC-PVTZ) (Hartree): -228.55909378
E (RHF/AUG-CC-PVTZ) (Hartree): -227.66705423
Cartesian coordinates (Angs):
C      0.290825      0.614623      0.226603
O     -0.888577      0.605766     -0.283125
O     -1.092938     -0.812475      0.139795
C      1.402950     -0.318551     -0.098486
H      0.516133      1.496981      0.836404
H      1.094673     -1.017406     -0.872265
H      1.692446     -0.883177      0.791210
H      2.268622      0.281426     -0.404813
Rotational constants (GHz): 16.3541894  7.1700460  5.4731673

Population analysis as 298K (%)
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)
Compound      Qtot      Erel      Erel2  n*Q*MB      %
-----
TS.CH3CHO2s.14Hshift.freq 1.925e+37 0.00  0.00  3.851e+37 100
Total                               3.851e+37 100

TS.CH3CHO2s.14Hshift.freq
-----
E (CCSD(T)/AUG-CC-PVTZ) (Hartree): -228.56158301
E (CCSD-T/AUG-CC-PVTZ) (Hartree): -228.56045708
E (CCSD/AUG-CC-PVTZ) (Hartree): -228.51683915
T1 diagnostic: 0.028898
D1 diagnostic: 0.125656
E (CCSD[T]/AUG-CC-PVTZ) (Hartree): -228.56569385
E (RHF/AUG-CC-PVTZ) (Hartree): -227.65471766
Point group : C1
Cartesian coordinates (Angs):
C      0.551831      0.714684      0.041416
O     -0.748815      0.661581      0.022838
O     -1.141460     -0.697163     -0.028651
C      1.237433     -0.513861     -0.013297
H      0.931866      1.720479     -0.102632
H      1.076763     -1.182332      0.834291
H      2.263107     -0.472415     -0.360692
H      0.107202     -1.023563     -0.492479
Rotational constants (GHz): 16.3876764  8.3926552  5.6904369
Vibrational harmonic frequencies (cm-1):
i1703.1200      487.8800 ( A)      531.8000 ( A)
717.6400 ( A)      743.6900 ( A)      854.3300 ( A)
878.4200 ( A)      965.0200 ( A)      1029.7200 ( A)
1205.0400 ( A)      1267.1800 ( A)      1343.7700 ( A)
1490.8900 ( A)      1543.8900 ( A)      1843.1400 ( A)
3091.7900 ( A)      3190.4400 ( A)      3206.3400 ( A)
Zero-point correction (Hartree): 0.055567

TS.CH3CHO2s.14Hshift.freq
-----
E (CCSD(T)/AUG-CC-PVTZ) (Hartree): -228.56158301
E (CCSD-T/AUG-CC-PVTZ) (Hartree): -228.56045708
E (CCSD/AUG-CC-PVTZ) (Hartree): -228.51683915
T1 diagnostic: 0.028898
D1 diagnostic: 0.125656
E (CCSD[T]/AUG-CC-PVTZ) (Hartree): -228.56569385
E (RHF/AUG-CC-PVTZ) (Hartree): -227.65471766
Cartesian coordinates (Angs):
C      0.551831      0.714684      0.041416
O     -0.748815      0.661581      0.022838
O     -1.141460     -0.697163     -0.028651
C      1.237433     -0.513861     -0.013297
H      0.931866      1.720479     -0.102632
H      1.076763     -1.182332      0.834291
H      2.263107     -0.472415     -0.360692
H      0.107202     -1.023563     -0.492479
Rotational constants (GHz): 16.3876764  8.3926552  5.6904369

Population analysis as 298K (%)
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)
Compound      Qtot      Erel      Erel2  n*Q*MB      %
-----
TS.CH3CHO2s.14Hshift.freq 1.925e+37 0.00  0.00  3.851e+37 100
Total                               3.851e+37 100

TS.CH3CHO2s.14Hshift.freq
-----
E (CCSD(T)/AUG-CC-PVTZ) (Hartree): -228.56158301
E (CCSD-T/AUG-CC-PVTZ) (Hartree): -228.56045708
E (CCSD/AUG-CC-PVTZ) (Hartree): -228.51683915
T1 diagnostic: 0.028898
D1 diagnostic: 0.125656
E (CCSD[T]/AUG-CC-PVTZ) (Hartree): -228.56569385
E (RHF/AUG-CC-PVTZ) (Hartree): -227.65471766
Point group : C1
Cartesian coordinates (Angs):
C      0.551831      0.714684      0.041416
O     -0.748815      0.661581      0.022838

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```

O      -1.141460      -0.697163      -0.028651
C      1.237433      -0.513861      -0.013297
H      0.931866      1.720479      -0.102632
H      1.076763      -1.182332      0.834291
H      2.263107      -0.472415      -0.360692
H      0.107202      -1.023563      -0.492479
Rotational constants (GHz): 16.3876764 8.3926552 5.6904369
Vibrational harmonic frequencies (cm-1):
i1703.1200      487.8800 ( A)      531.8000 ( A)
717.6400 ( A)      743.6900 ( A)      854.3300 ( A)
878.4200 ( A)      965.0200 ( A)      1029.7200 ( A)
1205.0400 ( A)      1267.1800 ( A)      1343.7700 ( A)
1490.8900 ( A)      1543.8900 ( A)      1843.1400 ( A)
3091.7900 ( A)      3190.4400 ( A)      3206.3400 ( A)
Zero-point correction (Hartree): 0.055567

```

TS.CH3CHO2s.14Hshift.freq

```

-----
E(CCSD(T)/AUG-CC-PVTZ) (Hartree): -228.56158301
E(CCSD-T/AUG-CC-PVTZ) (Hartree): -228.56045708
E(CCSD/AUG-CC-PVTZ) (Hartree): -228.51683915
T1 diagnostic: 0.028898
D1 diagnostic: 0.125656

```

```

E(CCSD[T]/AUG-CC-PVTZ) (Hartree): -228.56569385
E(RHF/AUG-CC-PVTZ) (Hartree): -227.65471766

```

Cartesian coordinates (Angs):

```

C      0.551831      0.714684      0.041416
O      -0.748815      0.661581      0.022838
O      -1.141460      -0.697163      -0.028651
C      1.237433      -0.513861      -0.013297
H      0.931866      1.720479      -0.102632
H      1.076763      -1.182332      0.834291
H      2.263107      -0.472415      -0.360692
H      0.107202      -1.023563      -0.492479
Rotational constants (GHz): 16.3876764 8.3926552 5.6904369

```

```

#####
Z-nopinone oxide
#####

```

Population analysis as 298K (%)

Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)

Compound	Qtot	Erel	Erel2	n*Q*MB	%
BpineneCI.anti	2.748e+41	0.00	0.00	2.748e+41	100
Total				2.748e+41	100

BpineneCI.anti

~~~~~

```

E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -500.86638278
E(CCSD/Aug-CC-pVTZ) (Hartree): -500.76544814
T1 diagnostic: 0.021764

```

E(MP2/Aug-CC-pVTZ) (Hartree): -500.70336319

E(MP3/Aug-CC-pVTZ) (Hartree): -500.75300931

E(RHF/Aug-CC-pVTZ) (Hartree): -498.67556252

E(RM062X/Aug-CC-pVTZ) (Hartree): -501.63704055

Electronic state : 1-A

Cartesian coordinates (Angs):

```

C      0.963826      -0.640437      0.235540
C      -0.069856      -0.329276      -0.930518
C      -1.138876      0.405231      -0.237648
C      0.658435      1.852576      0.703218
C      1.496083      0.800890      -0.026243
C      0.971654      0.674065      -1.473710
C      1.949975      -1.716610      -0.197429
C      0.408645      -0.999739      1.604258
C      -0.832037      1.773788      0.275455
O      -2.233850      -0.109137      0.064589
H      -0.454109      -1.155304      -1.518068
H      1.039664      2.846774      0.472916
H      0.743810      1.717816      1.780780
H      2.562531      0.962396      0.128008
H      0.602710      1.577788      -1.956212
H      1.673040      0.183670      -2.139078
H      2.375566      -1.534285      -1.182025
H      1.455412      -2.687929      -0.215546
H      2.771437      -1.767836      0.519491
H      -0.131397      -1.944683      1.543376
H      -0.284030      -0.260091      2.003912
H      1.226214      -1.110418      2.318943
H      -1.012288      2.476445      -0.541192
H      -1.518317      2.029043      1.079493
O      -2.453317      -1.422902      -0.316132

```

Rotational constants (GHz): 1.5298900 1.1446700 0.9056100

Vibrational harmonic frequencies (cm-1):

```

78.7864      146.0416      173.9867
219.5288      238.4950      283.2039
298.1706      320.6046      383.7328
386.6057      422.7995      450.5859
458.5897      555.3926      586.1118
651.9078      676.4507      786.9215
804.4593      835.4470      871.1424
906.5125      931.0880      953.2289
963.0641      973.5128      985.8831
1010.8613      1023.0074      1066.8329
1081.7015      1095.3764      1119.4424
1171.6907      1200.4113      1217.8169
1244.1949      1251.7519      1262.3525
1275.4979      1301.6345      1323.5252
1342.2497      1359.2938      1396.1176
1410.2347      1426.8447      1469.0214

```

|           |           |           |
|-----------|-----------|-----------|
| 1486.3928 | 1487.4077 | 1505.5827 |
| 1508.6014 | 1520.4850 | 1528.3571 |
| 1663.4093 | 3059.4976 | 3062.9094 |
| 3070.0291 | 3084.9287 | 3098.5079 |
| 3104.6162 | 3124.4810 | 3126.2794 |
| 3131.5979 | 3141.2064 | 3145.6330 |
| 3148.5863 | 3175.0688 | 3179.9354 |

Zero-point correction (Hartree): 0.218125

Population analysis as 298K (%)

Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)

| Compound                   | Qtot      | Erel | Erel2 | n*Q*MB    | %   |
|----------------------------|-----------|------|-------|-----------|-----|
| BpineneCI.anti.ringclose.a | 1.916e+41 | 0.00 | 0.00  | 1.916e+41 | 67  |
| BpineneCI.anti.ringclose.b | 2.214e+41 | 0.51 | 0.51  | 9.433e+40 | 33  |
| Total                      |           |      |       | 2.859e+41 | 100 |

BpineneCI.anti.ringclose.a

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E (CCSD(T)/Aug-CC-pVTZ) (Hartree): -500.83748544

E (CCSD/Aug-CC-pVTZ) (Hartree): -500.73583320

T1 diagnostic: 0.024192

E (MP2/Aug-CC-pVTZ) (Hartree): -500.66979990

E (MP3/Aug-CC-pVTZ) (Hartree): -500.72178488

E (RHF/Aug-CC-pVTZ) (Hartree): -498.64912289

E (RM062X/Aug-CC-pVTZ) (Hartree): -501.60548445

Electronic state : 1-A

Cartesian coordinates (Angs):

C	1.105924	-0.491945	0.181967
C	-0.040739	-0.396485	-0.885228
C	-1.246261	0.163955	-0.244088
C	0.363962	1.878956	0.747000
C	1.328624	1.026857	-0.073845
C	0.727574	0.825215	-1.478852
C	2.260949	-1.335683	-0.341770
C	0.739498	-0.964619	1.578452
H	-0.276096	-1.265725	-1.487960
H	0.481004	2.925499	0.466750
H	0.609941	1.803357	1.805801
H	2.351398	1.394280	0.004642
H	0.138100	1.641104	-1.896826
H	1.449913	0.497060	-2.218278
H	2.582760	-1.045148	-1.340232
H	1.972595	-2.386862	-0.370900
H	3.117719	-1.238802	0.327315
H	0.457601	-2.016586	1.550023
H	-0.103251	-0.428657	2.011553
H	1.597484	-0.850961	2.244590
C	-1.098544	1.442349	0.519888
H	-1.673024	2.186647	-0.040555
H	-1.646694	1.304995	1.452862
O	-2.064850	-1.641274	0.081397
O	-2.423321	-0.285201	-0.397637

Rotational constants (GHz): 1.5881000 1.1103100 0.9155700

Vibrational harmonic frequencies (cm-1):

i477.3561	93.2639	168.9975
186.8277	212.8374	233.5906
280.4337	309.2343	357.6202
385.5860	394.6133	420.6876
452.6528	470.3238	526.6564
608.6062	658.8030	773.4899
788.9140	836.7144	849.5038
878.5384	900.8293	930.5568
962.7456	972.1409	983.7706
1006.4833	1017.7116	1048.6716
1078.9731	1106.0437	1133.7006
1168.3627	1207.7184	1216.6910
1238.1717	1250.0960	1259.0947
1276.5114	1297.4992	1315.5775
1328.5093	1361.4675	1379.3288
1409.0683	1425.1928	1439.8159
1479.9520	1485.6664	1502.4872
1504.5942	1513.9448	1520.7358
1590.6979	3058.1080	3058.5512
3061.7300	3081.6852	3090.0466
3100.9419	3105.9270	3123.9370
3124.8097	3132.8768	3144.3551
3148.9200	3173.6284	3179.7680

Zero-point correction (Hartree): 0.215938

BpineneCI.anti.ringclose.b

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E (CCSD(T)/Aug-CC-pVTZ) (Hartree): -500.83696617

E (CCSD/Aug-CC-pVTZ) (Hartree): -500.73543151

T1 diagnostic: 0.024239

E (MP2/Aug-CC-pVTZ) (Hartree): -500.66941459

E (MP3/Aug-CC-pVTZ) (Hartree): -500.72137656

E (RHF/Aug-CC-pVTZ) (Hartree): -498.64929652

E (RM062X/Aug-CC-pVTZ) (Hartree): -501.60468811

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 1.234441  | -0.383837 | 0.246266  |
| C | -0.124712 | -0.770255 | -0.453743 |
| C | -1.185120 | 0.017050  | 0.209476  |
| C | 0.411302  | 1.988701  | -0.075555 |
| C | 1.239801  | 0.860441  | -0.683175 |
| C | 0.364813  | 0.058251  | -1.672963 |
| C | 2.318635  | -1.386615 | -0.128318 |
| C | 1.246954  | -0.189540 | 1.755184  |
| H | -0.394452 | -1.813317 | -0.560566 |
| H | 0.344784  | 2.816806  | -0.780424 |

|                                                                               |           |           |                     |
|-------------------------------------------------------------------------------|-----------|-----------|---------------------|
| H                                                                             | 0.906494  | 2.370507  | 0.817256            |
| H                                                                             | 2.211921  | 1.215800  | -1.023833           |
| H                                                                             | -0.397639 | 0.599281  | -2.230798           |
| H                                                                             | 0.939747  | -0.552969 | -2.359360           |
| H                                                                             | 2.371550  | -1.572799 | -1.198988           |
| H                                                                             | 2.141464  | -2.339693 | 0.371374            |
| H                                                                             | 3.291214  | -1.011535 | 0.195654            |
| H                                                                             | 1.093144  | -1.147155 | 2.254698            |
| H                                                                             | 0.480552  | 0.494286  | 2.117856            |
| H                                                                             | 2.215567  | 0.200221  | 2.074215            |
| C                                                                             | -1.004501 | 1.496012  | 0.279021            |
| H                                                                             | -1.744270 | 1.852982  | -0.448373           |
| H                                                                             | -1.370644 | 1.842133  | 1.246284            |
| O                                                                             | -2.675942 | -1.170340 | -0.442797           |
| O                                                                             | -2.211447 | -0.466634 | 0.776277            |
| Rotational constants (GHz):                                                   |           | 1.6768200 | 0.9921500 0.8995400 |
| Vibrational harmonic frequencies (cm-1):                                      |           |           |                     |
| i460.6678                                                                     | 83.2963   |           | 173.2229            |
| 192.1124                                                                      | 208.5442  |           | 225.7522            |
| 266.7220                                                                      | 295.1260  |           | 370.3539            |
| 388.3189                                                                      | 412.5241  |           | 424.8020            |
| 455.5340                                                                      | 471.0263  |           | 512.1841            |
| 591.2105                                                                      | 670.9524  |           | 779.7562            |
| 791.1694                                                                      | 829.1189  |           | 850.2733            |
| 876.9848                                                                      | 905.2819  |           | 936.5263            |
| 960.7234                                                                      | 971.8360  |           | 983.2190            |
| 1004.1429                                                                     | 1019.4869 |           | 1061.3274           |
| 1079.2304                                                                     | 1099.6998 |           | 1132.3251           |
| 1164.3769                                                                     | 1202.6072 |           | 1219.5162           |
| 1237.3478                                                                     | 1251.8316 |           | 1264.1009           |
| 1270.9170                                                                     | 1302.5710 |           | 1316.8577           |
| 1326.1040                                                                     | 1365.3915 |           | 1380.3113           |
| 1408.7027                                                                     | 1425.7423 |           | 1436.2803           |
| 1485.6180                                                                     | 1489.1888 |           | 1504.5989           |
| 1507.7737                                                                     | 1517.4246 |           | 1523.8798           |
| 1595.6279                                                                     | 3037.7080 |           | 3056.7766           |
| 3060.3672                                                                     | 3080.2360 |           | 3097.5638           |
| 3105.5905                                                                     | 3107.8512 |           | 3119.5502           |
| 3121.9923                                                                     | 3124.2573 |           | 3139.2045           |
| 3148.9089                                                                     | 3181.1931 |           | 3189.0875           |
| Zero-point correction (Hartree): 0.215947                                     |           |           |                     |
| #####                                                                         |           |           |                     |
| E-nopinone oxide                                                              |           |           |                     |
| #####                                                                         |           |           |                     |
| Population analysis as 298K (%)                                               |           |           |                     |
| Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T) |           |           |                     |
| Compound                                                                      | Qtot      | Erel      | Erel2 n*Q*MB %      |
| -----                                                                         |           |           |                     |
| BpineneCI.syn                                                                 | 2.943e+41 | 0.00      | 0.00 2.943e+41 100  |
| Total                                                                         |           |           | 2.943e+41 100       |
| BpineneCI.syn                                                                 |           |           |                     |
| ~~~~~                                                                         |           |           |                     |
| E (CCSD(T)/Aug-CC-pVTZ) (Hartree): -500.86947783                              |           |           |                     |
| E (CCSD/Aug-CC-pVTZ) (Hartree): -500.76875817                                 |           |           |                     |
| T1 diagnostic: 0.021965                                                       |           |           |                     |
| E (MP2/Aug-CC-pVTZ) (Hartree): -500.70624118                                  |           |           |                     |
| E (MP3/Aug-CC-pVTZ) (Hartree): -500.75627843                                  |           |           |                     |
| E (RHF/Aug-CC-pVTZ) (Hartree): -498.67941601                                  |           |           |                     |
| E (RM062X/Aug-CC-pVTZ) (Hartree): -501.64038541                               |           |           |                     |
| Electronic state : 1-A                                                        |           |           |                     |
| Cartesian coordinates (Angs):                                                 |           |           |                     |
| C                                                                             | 1.322233  | -0.408205 | 0.215725            |
| C                                                                             | 0.222264  | -0.542627 | -0.895128           |
| C                                                                             | -1.083682 | -0.200493 | -0.291063           |
| C                                                                             | 0.111598  | 1.781456  | 0.701825            |
| C                                                                             | 1.255558  | 1.121367  | -0.067229           |
| C                                                                             | 0.775186  | 0.781633  | -1.495285           |
| C                                                                             | 2.640470  | -1.019754 | -0.241722           |
| C                                                                             | 0.995997  | -0.918813 | 1.609707            |
| C                                                                             | -1.234300 | 1.061671  | 0.468762            |
| O                                                                             | -2.047223 | -0.977143 | -0.450914           |
| H                                                                             | 0.174558  | -1.449861 | -1.492785           |
| H                                                                             | 0.027873  | 2.822226  | 0.390205            |
| H                                                                             | 0.344794  | 1.790337  | 1.766552            |
| H                                                                             | 2.185353  | 1.678765  | 0.042094            |
| H                                                                             | 0.053799  | 1.455451  | -1.955183           |
| H                                                                             | 1.584747  | 0.594658  | -2.192056           |
| H                                                                             | 2.939012  | -0.693677 | -1.236060           |
| H                                                                             | 2.570182  | -2.108295 | -0.249902           |
| H                                                                             | 3.433860  | -0.740344 | 0.453492            |
| H                                                                             | 0.950486  | -2.008953 | 1.607880            |
| H                                                                             | 0.046939  | -0.551919 | 1.997193            |
| H                                                                             | 1.779511  | -0.620869 | 2.308900            |
| H                                                                             | -1.957609 | 1.663384  | -0.090548           |
| H                                                                             | -1.774322 | 0.815101  | 1.385449            |
| O                                                                             | -3.251668 | -0.595784 | 0.104816            |
| Rotational constants (GHz):                                                   |           | 1.8908200 | 0.8880000 0.8245500 |
| Vibrational harmonic frequencies (cm-1):                                      |           |           |                     |
| 77.8162                                                                       | 177.4091  |           | 180.4626            |
| 200.9436                                                                      | 227.6051  |           | 275.0679            |
| 290.8870                                                                      | 312.0728  |           | 375.0300            |
| 389.2499                                                                      | 414.0991  |           | 431.4525            |
| 463.5538                                                                      | 542.3298  |           | 587.7999            |
| 631.6900                                                                      | 688.0446  |           | 788.8739            |
| 795.5134                                                                      | 846.6514  |           | 880.0626            |
| 900.8988                                                                      | 914.6141  |           | 958.5285            |
| 965.4007                                                                      | 973.3336  |           | 986.5825            |
| 1012.0469                                                                     | 1021.4860 |           | 1065.4651           |

|           |           |           |
|-----------|-----------|-----------|
| 1081.5071 | 1107.7431 | 1134.5213 |
| 1172.6203 | 1201.6713 | 1214.8801 |
| 1249.0232 | 1254.0085 | 1257.4930 |
| 1274.2062 | 1310.2306 | 1328.6013 |
| 1331.3629 | 1372.9899 | 1393.1288 |
| 1410.2114 | 1427.4049 | 1445.9392 |
| 1486.4500 | 1490.2052 | 1504.5352 |
| 1508.4649 | 1517.4107 | 1522.5843 |
| 1659.0316 | 3058.2183 | 3061.6835 |
| 3061.7723 | 3079.9296 | 3091.3171 |
| 3097.5990 | 3102.4305 | 3119.3957 |
| 3120.1951 | 3124.7731 | 3134.5396 |
| 3145.0970 | 3146.7061 | 3178.6640 |

Zero-point correction (Hartree): 0.217687

Population analysis as 298K (%)

Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)

| Compound                  | Qtot      | Erel | Erel2 | n*Q*MB    | %    |
|---------------------------|-----------|------|-------|-----------|------|
| BpineneCI.syn.ringclose.a | 1.614e+41 | 0.00 | 0.00  | 1.614e+41 | 73.6 |
| BpineneCI.syn.ringclose.b | 1.659e+41 | 0.62 | 0.62  | 5.805e+40 | 26.4 |
| Total                     |           |      |       | 2.195e+41 | 100  |

BpineneCI.syn.ringclose.a

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E (CCSD(T)/Aug-CC-pVTZ) (Hartree): -500.83522220

E (CCSD/Aug-CC-pVTZ) (Hartree): -500.73333139

T1 diagnostic: 0.023840

E (MP2/Aug-CC-pVTZ) (Hartree): -500.66836654

E (MP3/Aug-CC-pVTZ) (Hartree): -500.71927161

E (RHF/Aug-CC-pVTZ) (Hartree): -498.64568249

E (RM062X/Aug-CC-pVTZ) (Hartree): -501.60280673

Electronic state : 1-A

Cartesian coordinates (Angs):

C	1.280303	-0.399948	0.146998
C	0.142696	-0.391205	-0.967262
C	-1.108428	-0.223893	-0.198303
C	0.076288	1.700994	0.906642
C	1.210776	1.149429	0.046344
C	0.696570	0.983728	-1.401007
C	2.574193	-0.967306	-0.421502
C	0.986272	-1.073586	1.477614
H	0.095387	-1.229270	-1.656804
H	0.028060	2.783479	0.792629
H	0.277082	1.500268	1.958874
H	2.144164	1.688337	0.206345
H	-0.022332	1.714386	-1.765676
H	1.492632	0.874113	-2.128801
H	2.845794	-0.530806	-1.380189
H	2.489842	-2.046768	-0.550885
H	3.390124	-0.775313	0.277592
H	0.904503	-2.152722	1.340845
H	0.064026	-0.735294	1.947003
H	1.806252	-0.884096	2.172789
C	-1.289424	1.094393	0.493131
H	-1.780701	1.758039	-0.217816
H	-1.987953	0.960559	1.314741
O	-3.066731	-0.519711	-0.357769
O	-1.828564	-1.250357	0.006947

Rotational constants (GHz): 1.8301700 0.9620200 0.8635500

Vibrational harmonic frequencies (cm-1):

i495.4352	99.8761	173.8332
184.7963	211.6174	235.1121
312.0973	325.1058	372.8157
388.1596	413.2320	432.9357
458.8794	493.6098	544.2146
606.3030	652.7000	768.5414
801.4181	839.5113	844.1162
869.4867	910.5300	933.6055
961.0716	970.4884	984.9902
1006.2566	1022.7901	1069.5690
1080.4981	1082.5118	1108.6835
1163.6927	1194.7592	1213.8270
1242.4488	1243.5655	1259.5234
1271.1021	1297.1071	1317.3273
1330.9639	1357.9572	1374.1706
1410.3142	1427.1554	1452.7995
1484.1812	1487.6541	1504.5115
1507.4385	1519.8272	1526.2804
1593.3508	3059.0390	3062.8753
3081.5517	3096.4180	3098.9172
3112.4355	3122.3261	3122.6723
3127.4868	3144.8396	3145.8991
3151.8686	3159.6398	3182.1682

Zero-point correction (Hartree): 0.216443

BpineneCI.syn.ringclose.b

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E (CCSD(T)/Aug-CC-pVTZ) (Hartree): -500.83401884

E (CCSD/Aug-CC-pVTZ) (Hartree): -500.73206914

T1 diagnostic: 0.023702

E (MP2/Aug-CC-pVTZ) (Hartree): -500.66674231

E (MP3/Aug-CC-pVTZ) (Hartree): -500.71836911

E (RHF/Aug-CC-pVTZ) (Hartree): -498.64461277

E (RM062X/Aug-CC-pVTZ) (Hartree): -501.60180398

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 1.144457  | -0.513266 | 0.153110  |
| C | 0.223716  | -0.128491 | -1.091641 |
| C | -1.128807 | 0.082047  | -0.538885 |
| C | 0.028146  | 1.531525  | 1.167574  |

|                                                                               |           |           |                     |
|-------------------------------------------------------------------------------|-----------|-----------|---------------------|
| C                                                                             | 1.243345  | 1.018641  | 0.393256            |
| C                                                                             | 0.994462  | 1.216809  | -1.117614           |
| C                                                                             | 2.458113  | -1.112237 | -0.334692           |
| C                                                                             | 0.578050  | -1.398601 | 1.249594            |
| H                                                                             | 0.215196  | -0.796774 | -1.948950           |
| H                                                                             | 0.119504  | 2.605389  | 1.328209            |
| H                                                                             | -0.012089 | 1.062156  | 2.149766            |
| H                                                                             | 2.178861  | 1.383709  | 0.815833            |
| H                                                                             | 0.445907  | 2.102552  | -1.431024           |
| H                                                                             | 1.896157  | 1.132759  | -1.712874           |
| H                                                                             | 2.941681  | -0.526226 | -1.113207           |
| H                                                                             | 2.291697  | -2.118801 | -0.719361           |
| H                                                                             | 3.149493  | -1.186359 | 0.506509            |
| H                                                                             | 0.465143  | -2.419828 | 0.883983            |
| H                                                                             | -0.400740 | -1.084536 | 1.601615            |
| H                                                                             | 1.276156  | -1.415510 | 2.089661            |
| C                                                                             | -1.275775 | 1.247671  | 0.392708            |
| H                                                                             | -1.461022 | 2.085129  | -0.292456           |
| H                                                                             | -2.147922 | 1.134372  | 1.021766            |
| O                                                                             | -2.472729 | -1.087720 | 0.378401            |
| O                                                                             | -2.096305 | -0.615107 | -0.980893           |
| Rotational constants (GHz):                                                   |           |           |                     |
| Vibrational harmonic frequencies (cm-1):                                      |           |           |                     |
| i499.4805                                                                     | 106.3458  | 140.5547  |                     |
| 174.4500                                                                      | 217.3193  | 238.0460  |                     |
| 318.2154                                                                      | 351.4367  | 384.0859  |                     |
| 392.3878                                                                      | 404.9012  | 434.2575  |                     |
| 461.0722                                                                      | 484.5638  | 545.8721  |                     |
| 618.6276                                                                      | 660.0723  | 753.2236  |                     |
| 797.2012                                                                      | 820.2657  | 850.4190  |                     |
| 871.2635                                                                      | 912.9281  | 940.2563  |                     |
| 959.8369                                                                      | 974.1611  | 988.2230  |                     |
| 1004.8072                                                                     | 1019.8465 | 1066.3654 |                     |
| 1076.8678                                                                     | 1085.1862 | 1109.9702 |                     |
| 1162.9411                                                                     | 1193.9178 | 1214.2837 |                     |
| 1236.2571                                                                     | 1247.1603 | 1260.9801 |                     |
| 1274.7872                                                                     | 1296.5799 | 1321.0522 |                     |
| 1331.0990                                                                     | 1358.4228 | 1376.3510 |                     |
| 1409.9009                                                                     | 1431.7110 | 1457.0511 |                     |
| 1478.9034                                                                     | 1486.8750 | 1503.3790 |                     |
| 1507.1346                                                                     | 1517.9129 | 1528.4631 |                     |
| 1584.3223                                                                     | 3022.2368 | 3056.1541 |                     |
| 3062.3898                                                                     | 3084.4850 | 3101.0250 |                     |
| 3112.1645                                                                     | 3121.5842 | 3125.8617 |                     |
| 3127.2179                                                                     | 3138.2972 | 3148.9250 |                     |
| 3166.8297                                                                     | 3184.5865 | 3207.9264 |                     |
| Zero-point correction (Hartree): 0.216431                                     |           |           |                     |
| Population analysis as 298K (%)                                               |           |           |                     |
| Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T) |           |           |                     |
| Compound                                                                      | Qtot      | Erel      | Erel2 n*Q*MB %      |
| BpineneCI.syn.14Hshift.a                                                      | 1.383e+41 | 0.00      | 0.00 1.383e+41 86.6 |
| BpineneCI.syn.14Hshift.b                                                      | 1.368e+41 | 1.10      | 1.10 2.140e+40 13.4 |
| Total                                                                         |           |           | 1.597e+41 100       |
| BpineneCI.syn.14Hshift.a                                                      |           |           |                     |
| E (CCSD(T)/Aug-CC-pVTZ) (Hartree): -500.84100779                              |           |           |                     |
| E (CCSD/Aug-CC-pVTZ) (Hartree): -500.73689338                                 |           |           |                     |
| T1 diagnostic: 0.018868                                                       |           |           |                     |
| E (MP2/Aug-CC-pVTZ) (Hartree): -500.68507774                                  |           |           |                     |
| E (MP3/Aug-CC-pVTZ) (Hartree): -500.72694154                                  |           |           |                     |
| E (RHF/Aug-CC-pVTZ) (Hartree): -498.63076869                                  |           |           |                     |
| E (RM062X/Aug-CC-pVTZ) (Hartree): -501.61224663                               |           |           |                     |
| Electronic state : 1-A                                                        |           |           |                     |
| Cartesian coordinates (Angs):                                                 |           |           |                     |
| C                                                                             | 1.255304  | -0.457922 | 0.193067            |
| C                                                                             | 0.312816  | -0.284229 | -1.060935           |
| C                                                                             | -1.041143 | -0.027041 | -0.521179           |
| C                                                                             | -0.007399 | 1.618449  | 0.990582            |
| C                                                                             | 1.236852  | 1.099061  | 0.259483            |
| C                                                                             | 0.969223  | 1.103844  | -1.264015           |
| C                                                                             | 2.617191  | -1.001252 | -0.223167           |
| C                                                                             | 0.750259  | -1.258880 | 1.381068            |
| H                                                                             | 0.325014  | -1.047346 | -1.835986           |
| H                                                                             | -0.052376 | 2.702823  | 0.884840            |
| H                                                                             | 0.082704  | 1.409354  | 2.058684            |
| H                                                                             | 2.144463  | 1.581037  | 0.622106            |
| H                                                                             | 0.327045  | 1.892689  | -1.651483           |
| H                                                                             | 1.873868  | 1.045898  | -1.858637           |
| H                                                                             | 3.043486  | -0.481038 | -1.078112           |
| H                                                                             | 2.540469  | -2.059900 | -0.474986           |
| H                                                                             | 3.316577  | -0.905397 | 0.609162            |
| H                                                                             | 0.681033  | -2.315906 | 1.119153            |
| H                                                                             | -0.227302 | -0.938753 | 1.735589            |
| H                                                                             | 1.455396  | -1.168523 | 2.209547            |
| C                                                                             | -1.280444 | 0.980805  | 0.436575            |
| H                                                                             | -2.104687 | 1.650153  | 0.196848            |
| H                                                                             | -2.213148 | 0.163459  | 0.906859            |
| O                                                                             | -3.044883 | -0.617472 | 0.134004            |
| O                                                                             | -1.963679 | -0.903222 | -0.708062           |
| Rotational constants (GHz):                                                   |           |           |                     |
| Vibrational harmonic frequencies (cm-1):                                      |           |           |                     |
| i1585.0946                                                                    | 104.5968  | 175.0236  |                     |
| 190.6700                                                                      | 228.8686  | 253.9944  |                     |
| 290.5622                                                                      | 340.0363  | 380.3811  |                     |
| 389.6484                                                                      | 410.8711  | 428.4719  |                     |
| 456.5083                                                                      | 495.7592  | 585.7069  |                     |
| 630.1519                                                                      | 679.9998  | 729.4554  |                     |
| 793.1787                                                                      | 845.0898  | 865.4832  |                     |

|           |           |           |
|-----------|-----------|-----------|
| 877.7257  | 895.3374  | 933.3724  |
| 969.1320  | 978.3113  | 991.3937  |
| 999.8018  | 1008.6752 | 1031.4585 |
| 1068.7144 | 1091.8828 | 1106.7614 |
| 1128.7599 | 1167.8905 | 1202.6917 |
| 1235.4806 | 1242.2323 | 1252.7166 |
| 1264.4520 | 1306.3419 | 1309.8625 |
| 1318.7039 | 1367.3971 | 1406.3167 |
| 1410.0961 | 1426.0428 | 1474.8127 |
| 1486.4537 | 1490.0663 | 1498.3804 |
| 1506.1221 | 1518.8584 | 1520.0046 |
| 1580.7622 | 1864.2452 | 3057.4495 |
| 3061.4631 | 3064.0071 | 3095.6582 |
| 3102.2442 | 3105.6229 | 3118.1090 |
| 3123.5776 | 3129.7823 | 3130.5399 |
| 3147.9817 | 3153.2627 | 3182.1645 |

Zero-point correction (Hartree): 0.213413

BpineneCI.syn.14Hshift.b

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E (CCSD(T)/Aug-CC-pVTZ) (Hartree): -500.83934124

E (CCSD/Aug-CC-pVTZ) (Hartree): -500.73540947

T1 diagnostic: 0.018863

E (MP2/Aug-CC-pVTZ) (Hartree): -500.68309845

E (MP3/Aug-CC-pVTZ) (Hartree): -500.72550109

E (RHF/Aug-CC-pVTZ) (Hartree): -498.63002768

E (RM062X/Aug-CC-pVTZ) (Hartree): -501.61061278

Electronic state : 1-A

Cartesian coordinates (Angs):

C	1.423317	-0.217730	0.277027
C	0.230274	-0.928117	-0.436908
C	-1.049568	-0.393593	0.083288
C	-0.039344	1.851731	-0.064661
C	1.097238	1.001500	-0.641381
C	0.517057	-0.001136	-1.664011
C	2.751456	-0.870766	-0.090167
C	1.371585	-0.036747	1.785273
H	0.221070	-2.008623	-0.562084
H	-0.333290	2.600984	-0.801855
H	0.318522	2.396986	0.810234
H	1.940263	1.616745	-0.954560
H	-0.344399	0.315545	-2.248628
H	1.265032	-0.431227	-2.320737
H	2.869456	-1.032520	-1.159573
H	2.847188	-1.836558	0.408462
H	3.576080	-0.239566	0.244504
H	1.484272	-1.001494	2.283124
H	0.444649	0.412910	2.132607
H	2.197419	0.599120	2.109811
C	-1.239679	0.984827	0.310621
H	-2.466477	0.783009	-0.141359
H	-1.730493	1.222898	1.252867
O	-3.233873	-0.332846	0.183865
O	-2.099041	-1.134407	0.015221

Rotational constants (GHz): 2.0333000 0.8588100 0.8245200

Vibrational harmonic frequencies (cm-1):

i1597.4564	112.7557	175.7230
199.3276	217.8200	250.6226
284.1785	327.8516	369.8413
391.9459	424.5116	434.1629
463.9839	491.2292	587.3502
615.2334	690.1131	745.6747
811.1869	835.6471	866.6930
883.9100	911.0698	922.8846
953.4897	971.7483	985.8419
1000.9544	1020.9619	1025.5445
1071.1825	1088.3712	1105.8020
1138.0841	1167.9842	1210.7587
1226.8772	1242.3398	1253.7981
1263.3798	1303.3187	1310.1522
1331.4892	1369.5626	1406.4049
1409.7032	1425.3323	1476.9867
1488.0125	1491.4047	1499.1840
1507.0310	1518.7665	1525.5929
1583.8315	1866.4989	3057.4983
3061.5095	3064.6454	3097.1555
3098.0728	3108.2744	3116.2201
3122.7482	3127.0576	3132.3243
3147.3701	3160.1250	3181.6133

Zero-point correction (Hartree): 0.213530

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Z-pinonaldehyde-K-oxide

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Population analysis as 298K (%)

Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)

Compound	Qtot	Erel	Erel2	n*Q*MB	%
ApineneCI.A.b.mpt	1.581e+44	0.00	0.00	1.581e+44	48.1
ApineneCI.A.b.mmt	1.644e+44	0.58	0.58	6.204e+43	18.9
ApineneCI.A.b.mpm	2.772e+44	0.92	0.92	5.873e+43	17.9
ApineneCI.A.b.mmp	1.412e+44	1.05	1.05	2.409e+43	7.33
ApineneCI.A.b.mpp	2.744e+44	1.88	1.88	1.149e+43	3.5
ApineneCI.A.b.mmm	2.704e+44	2.03	2.03	8.753e+42	2.66
ApineneCI.A.b.mtt	4.475e+43	1.64	1.64	2.807e+42	0.854
ApineneCI.A.b.cmt	4.714e+43	2.05	2.05	1.475e+42	0.449
ApineneCI.A.b.mtm	1.302e+44	3.19	3.19	5.951e+41	0.181
ApineneCI.A.b.cpt	7.467e+43	3.28	3.28	2.940e+41	0.0894
ApineneCI.A.b.pmt	1.067e+44	3.79	3.79	1.765e+41	0.0537
ApineneCI.A.b.pmp	1.307e+44	4.66	4.66	4.968e+40	0.0151

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ApineneCI.A.b.cpp 1.619e+44 5.28 5.28 2.166e+40 0.00659
ApineneCI.A.b.ppt 1.607e+44 5.31 5.31 2.062e+40 0.00627
ApineneCI.A.b.ppp 3.225e+44 5.92 5.92 1.466e+40 0.00446
ApineneCI.A.b.ppm 3.055e+44 5.90 5.90 1.435e+40 0.00436
ApineneCI.A.b.cmp 1.927e+44 5.69 5.69 1.297e+40 0.00395
ApineneCI.A.b.cmm 5.523e+44 6.61 6.61 7.838e+39 0.00238
ApineneCI.A.b.cpm 4.929e+44 6.75 6.75 5.551e+39 0.00169
ApineneCI.A.b.pmm 2.534e+44 6.42 6.42 4.968e+39 0.00151
ApineneCI.A.b.ptm 1.732e+44 6.91 6.91 1.495e+39 0.000455
ApineneCI.A.b.ptt 8.753e+43 7.06 7.06 5.831e+38 0.000177
ApineneCI.A.b.ctm 1.108e+44 7.31 7.31 4.841e+38 0.000147
ApineneCI.A.b.ctt 1.939e+44 10.27 10.27 5.658e+36 1.72e-06
Total 3.287e+44 100

ApineneCI.A.b.cmm
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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.15930466
Electronic state : 1-A
Cartesian coordinates (Angs):
C -1.142719 -0.242249 -0.727443
H -1.567731 0.379446 -1.519295
C -2.264611 -1.050227 -0.081760
C -3.330204 -0.123375 0.433504
H -2.710101 -1.709575 -0.826757
H -1.862881 -1.650649 0.736484
H -3.137512 0.340088 1.421563
C -0.211676 0.645614 0.149658
C 0.089059 -1.002098 -1.251472
C -0.535445 2.126988 0.171148
C 0.001985 0.110222 1.558537
H 0.294696 -0.938704 1.558512
H 0.796171 0.672225 2.056027
H -0.904372 0.237205 2.153449
H 0.247165 2.698541 0.674550
H -1.465720 2.299771 0.717324
H -0.660779 2.522992 -0.837123
H 0.106222 -1.249717 -2.309741
H 0.319968 -1.877678 -0.657690
C 0.952988 0.203377 -0.826007
H 0.992924 0.937705 -1.632825
C 2.309315 0.155599 -0.235988
C 3.160992 1.377418 -0.308601
H 2.597780 2.233095 0.068694
H 4.072438 1.248283 0.267002
H 3.407258 1.589710 -1.350210
O -4.324507 0.161812 -0.176547
O 2.826423 -0.795726 0.388782
O 2.160130 -1.983630 0.561588
Rotational constants (GHz): 1.5421100 0.4682900 0.4216500
Vibrational harmonic frequencies (cm-1):
19.3317 55.5202 65.9831
86.2812 152.1753 161.6696
183.5340 228.3425 236.4163
260.1194 278.7772 285.3187
299.1134 304.6328 342.5228
374.0549 415.6555 426.0062
480.8887 530.9538 567.4101
610.9202 627.2205 727.2363
772.8204 881.1847 897.1419
932.0102 949.5343 957.2797
968.8075 994.5360 1007.0275
1015.2204 1034.8537 1039.9906
1074.6873 1110.0512 1127.3176
1153.0636 1173.3473 1192.6200
1204.4858 1244.3629 1260.5386
1272.4086 1284.0763 1302.1825
1333.6697 1384.5647 1401.1359
1411.1550 1423.6946 1435.5329
1448.0661 1467.4987 1474.2273
1474.6551 1486.1274 1494.2113
1503.4195 1506.1088 1515.3667
1651.6935 1856.2119 2933.9986
3045.2184 3050.0717 3062.0384
3063.8649 3074.6298 3079.1950
3108.0848 3111.8805 3119.0046
3121.7004 3125.4590 3132.0397
3148.1978 3182.5293 3205.5359
Zero-point correction (Hartree): 0.246954

ApineneCI.A.b.cmp
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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.16080229
Electronic state : 1-A
Cartesian coordinates (Angs):
C 1.088437 -0.299761 0.970144
H 1.421463 0.277574 1.838046
C 2.267061 -1.068006 0.386139
C 3.383457 -0.112341 0.076428
H 2.620235 -1.788239 1.129488
H 1.982565 -1.603626 -0.518073
H 3.847630 0.371013 0.960347
C 0.269308 0.642314 0.041143
C -0.198446 -1.070460 1.313550
C 0.613192 2.116473 0.130628
C 0.220332 0.177410 -1.408193
H -0.103983 -0.859640 -1.491723
H -0.488027 0.790379 -1.970903
H 1.200831 0.291665 -1.872476
H -0.093180 2.726701 -0.435761
H 1.604010 2.290808 -0.295349
H 0.618982 2.464247 1.164736
H -0.338430 -1.371406 2.348862

```


H	-0.365846	-1.912159	0.653493
C	-1.002074	0.164163	0.853743
H	-1.135955	0.858411	1.685932
C	-2.274323	0.162398	0.098310
C	-3.091397	1.409825	0.082753
H	-2.460570	2.250923	-0.210755
H	-3.927113	1.314704	-0.603746
H	-3.459493	1.619201	1.088346
O	3.753383	0.176680	-1.028956
O	-2.735819	-0.763269	-0.603217
O	-2.089614	-1.969993	-0.710118
Rotational constants (GHz): 1.4404600 0.4970200 0.4523300			
Vibrational harmonic frequencies (cm-1):			
49.6724	57.2404	74.3357	
88.9752	144.5993	156.9774	
176.4951	235.9858	242.6217	
256.3146	281.6817	289.4960	
304.8468	319.0448	348.0251	
375.3344	418.5067	432.1827	
473.9221	534.7982	569.3974	
607.3825	628.0417	724.1196	
768.9409	871.7992	894.9997	
918.6766	935.7092	966.8610	
983.6004	993.3088	1007.6779	
1026.1369	1037.7672	1043.8651	
1063.4418	1108.4297	1125.7966	
1160.3561	1171.2845	1193.9468	
1200.1783	1244.2912	1256.9508	
1268.9989	1278.6702	1297.2496	
1329.7507	1390.7975	1402.1185	
1410.5110	1429.5753	1431.2991	
1448.6945	1466.7124	1470.7126	
1474.3794	1486.9247	1495.3467	
1501.9224	1512.9507	1516.3139	
1652.1214	1857.0559	2926.6603	
3043.5999	3045.8059	3050.5180	
3059.3482	3063.9066	3075.1539	
3111.2044	3115.8527	3116.7114	
3120.6395	3122.9390	3139.4741	
3147.0338	3182.3587	3205.8372	
Zero-point correction (Hartree): 0.246983			

ApineneCI.A.b.cmt

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E (RM062X/Aug-CC-pVTZ) (Hartree): -616.16696054
Electronic state : 1-A
Cartesian coordinates (Angs):
  C 1.054126 0.018749 0.949247
  H 1.761877 0.635355 1.504016
  C 1.803048 -1.169590 0.386404
  C 3.036596 -0.786800 -0.371362
  H 2.112685 -1.846451 1.190985
  H 1.165852 -1.774852 -0.264843
  H 3.639479 -1.629166 -0.760079
  C 0.229934 0.903884 -0.037884
  C -0.224049 -0.299807 1.756872
  C 0.553532 2.378685 0.136974
  C 0.236860 0.538140 -1.512903
  H -0.000012 -0.511370 -1.676313
  H -0.494997 1.147987 -2.049508
  H 1.216637 0.756511 -1.937959
  H -0.152416 3.004123 -0.414061
  H 1.559831 2.570077 -0.238592
  H 0.521769 2.668694 1.188886
  H -0.239188 0.140397 2.751579
  H -0.477394 -1.351359 1.811621
  C -1.088309 0.520006 0.762239
  H -1.527035 1.408315 1.214873
  C -2.164400 -0.109590 -0.027473
  C -3.388606 0.670501 -0.361074
  H -3.090336 1.600638 -0.849614
  H -4.048004 0.103464 -1.010964
  H -3.910603 0.943480 0.557073
  O 3.389418 0.346925 -0.571286
  O -2.143215 -1.266793 -0.504510
  O -1.037520 -2.061496 -0.312121
Rotational constants (GHz): 1.3248000 0.5928200 0.5185700
Vibrational harmonic frequencies (cm-1):
  65.8419 80.2259 100.6746
  129.7383 163.3035 172.4975
  184.5270 228.0078 241.7476
  262.5729 288.8337 294.8365
  309.4946 332.2952 351.3687
  375.9281 409.4356 414.6523
  458.5744 587.1452 604.6381
  639.7373 673.2245 748.4874
  752.2233 831.3932 844.0425
  907.0873 940.3186 957.7755
  966.2817 986.2683 1011.9018
  1024.2435 1032.9374 1042.2930
  1061.1344 1080.9902 1114.8674
  1180.8885 1188.9052 1190.0117
  1217.0666 1254.4245 1261.7295
  1280.6595 1285.6456 1301.8842
  1345.1623 1395.1939 1397.4175
  1409.7695 1415.0345 1424.4444
  1444.7429 1452.3695 1467.0923
  1469.7478 1473.8537 1487.4771
  1496.7421 1504.9627 1530.6239
  1649.8434 1841.8446 2953.4850
  3041.8685 3042.5373 3049.9193
  3061.5014 3077.0421 3090.4189

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3096.3274	3107.9437	3112.5323
3119.9912	3120.6822	3127.6833
3158.9639	3182.4090	3189.3215

Zero-point correction (Hartree): 0.247345

ApineneCI.A.b.cpm

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.15874425

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -1.176038 | 0.548377  | -0.401622 |
| H | -1.450378 | 1.233941  | -1.209356 |
| C | -2.382692 | 0.307707  | 0.492183  |
| C | -3.558078 | -0.135040 | -0.334566 |
| H | -2.178043 | -0.447051 | 1.249919  |
| H | -2.661181 | 1.244219  | 0.988506  |
| H | -3.856210 | 0.569364  | -1.138409 |
| C | 0.145805  | 1.058025  | 0.237818  |
| C | -0.423821 | -0.669424 | -0.972165 |
| C | 0.405804  | 2.546110  | 0.110585  |
| C | 0.346995  | 0.587252  | 1.671109  |
| H | 0.228140  | -0.490933 | 1.766831  |
| H | 1.354274  | 0.839802  | 2.010960  |
| H | -0.357960 | 1.092503  | 2.333499  |
| H | 1.403345  | 2.809511  | 0.467938  |
| H | -0.312900 | 3.101377  | 0.717768  |
| H | 0.307667  | 2.882818  | -0.922246 |
| H | -0.663555 | -0.978617 | -1.986468 |
| H | -0.456192 | -1.523037 | -0.306221 |
| C | 0.888090  | 0.126829  | -0.802138 |
| H | 1.077373  | 0.727601  | -1.694058 |
| C | 2.200671  | -0.406164 | -0.372800 |
| C | 3.427817  | 0.376429  | -0.697814 |
| H | 3.295869  | 1.408984  | -0.368776 |
| H | 4.300644  | -0.057721 | -0.219821 |
| H | 3.571022  | 0.399757  | -1.779317 |
| O | -4.149067 | -1.167929 | -0.188755 |
| O | 2.411096  | -1.436759 | 0.302379  |
| O | 1.381817  | -2.251952 | 0.699589  |

Rotational constants (GHz): 1.2981700 0.4886100 0.4177100

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| 35.1489   | 47.6283   | 67.6524   |
| 78.5465   | 141.3862  | 159.7203  |
| 168.8773  | 202.2499  | 231.1142  |
| 266.4031  | 272.3378  | 284.5742  |
| 306.9429  | 310.8793  | 327.9914  |
| 374.6251  | 412.8957  | 440.9217  |
| 462.8335  | 548.4388  | 569.3849  |
| 618.5870  | 627.0449  | 739.8484  |
| 769.2856  | 847.3622  | 894.2634  |
| 926.1494  | 939.9521  | 945.7470  |
| 967.0364  | 1001.4751 | 1004.9658 |
| 1028.4807 | 1034.7006 | 1044.2909 |
| 1073.9220 | 1096.5237 | 1138.9404 |
| 1155.4762 | 1177.3393 | 1193.5161 |
| 1222.0710 | 1245.3852 | 1249.2631 |
| 1271.7815 | 1275.4516 | 1300.2940 |
| 1329.0342 | 1392.6460 | 1402.2790 |
| 1409.9759 | 1426.7284 | 1429.6559 |
| 1449.1817 | 1464.0582 | 1468.3569 |
| 1474.8783 | 1485.2237 | 1493.1345 |
| 1502.6820 | 1506.4522 | 1514.7341 |
| 1652.1935 | 1864.1498 | 2917.8599 |
| 3039.4079 | 3043.3459 | 3045.1014 |
| 3050.8051 | 3063.3043 | 3076.7881 |
| 3108.5603 | 3112.7498 | 3116.7821 |
| 3121.0250 | 3122.5248 | 3134.0837 |
| 3150.1277 | 3181.0320 | 3201.6277 |

Zero-point correction (Hartree): 0.246612

ApineneCI.A.b.cpp

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.16175942

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-1.063312	0.644786	-0.394964
H	-1.632983	1.450888	-0.861003
C	-1.992291	-0.130803	0.535005
C	-3.137812	-0.702585	-0.245922
H	-1.434327	-0.956515	0.982049
H	-2.394644	0.512608	1.317205
H	-2.855793	-1.406149	-1.053782
C	0.264292	1.196119	0.212574
C	-0.261134	-0.182155	-1.430864
C	0.453440	2.674368	-0.090025
C	0.531032	0.919559	1.682567
H	0.432461	-0.136845	1.923565
H	1.537665	1.251610	1.949404
H	-0.169651	1.486319	2.297842
H	1.465542	2.998748	0.161333
H	-0.249860	3.266699	0.498190
H	0.275405	2.889148	-1.145053
H	-0.382329	0.152390	-2.458629
H	-0.407124	-1.253468	-1.370509
C	1.077712	0.310800	-0.821669
H	1.638106	0.950106	-1.502765
C	2.062348	-0.629534	-0.246911
C	3.517772	-0.335147	-0.360881
H	3.708282	0.663547	0.038048
H	4.107725	-1.070110	0.178058
H	3.807271	-0.320947	-1.412629
O	-4.295027	-0.436385	-0.060196

O	1.793161	-1.675647	0.384843	
O	0.482112	-2.021778	0.603506	
Rotational constants (GHz):	1.2591100	0.5390100	0.4558000	
Vibrational harmonic frequencies (cm ⁻¹):				
44.7730	54.7158		75.5237	
116.7734	168.2295		170.4660	
179.5416	204.3839		234.4486	
262.7030	278.6251		299.1469	
307.4190	332.3105		336.0496	
374.3100	412.7745		429.7555	
464.8407	536.4280		590.8767	
616.4710	642.8942		750.0426	
814.9922	841.0412		865.0653	
924.0952	942.3615		958.4127	
966.1205	993.2482		1012.6115	
1030.7522	1036.7962		1043.3588	
1073.8008	1108.3301		1117.3805	
1170.8074	1189.0466		1193.8960	
1233.8181	1252.3555		1262.8601	
1270.5026	1289.3626		1305.7964	
1322.1321	1381.6186		1398.6235	
1403.8341	1419.4770		1431.8976	
1442.6485	1464.9819		1467.3615	
1474.1331	1477.4563		1486.7795	
1494.2411	1502.0131		1526.6646	
1651.3850	1853.8097		2938.0899	
3042.7312	3048.0881		3061.3877	
3064.7160	3075.3354		3095.1998	
3109.7355	3111.0205		3115.9025	
3120.6322	3120.9680		3136.5006	
3154.0955	3182.1905		3192.5502	
Zero-point correction (Hartree):	0.247292			

ApineneCI.A.b.cpt

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.16482166

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -1.146837 | 0.652754  | -0.208350 |
| H | -1.769105 | 1.434737  | -0.644600 |
| C | -1.971416 | -0.105052 | 0.809362  |
| C | -3.218878 | -0.682350 | 0.208112  |
| H | -1.400848 | -0.929400 | 1.245241  |
| H | -2.280622 | 0.532201  | 1.645701  |
| H | -3.852510 | -1.269622 | 0.899351  |
| C | 0.236007  | 1.216258  | 0.239875  |
| C | -0.462559 | -0.213547 | -1.288878 |
| C | 0.401145  | 2.678387  | -0.145188 |
| C | 0.651825  | 1.002701  | 1.685904  |
| H | 0.570392  | -0.040999 | 1.982126  |
| H | 1.682820  | 1.334319  | 1.834465  |
| H | 0.022510  | 1.605457  | 2.343538  |
| H | 1.435594  | 3.004070  | -0.015137 |
| H | -0.234072 | 3.303060  | 0.485833  |
| H | 0.114382  | 2.848133  | -1.184212 |
| H | -0.691263 | 0.088462  | -2.307461 |
| H | -0.620726 | -1.279139 | -1.178083 |
| C | 0.937803  | 0.284292  | -0.835318 |
| H | 1.432428  | 0.892656  | -1.591600 |
| C | 1.967365  | -0.646969 | -0.331249 |
| C | 3.404403  | -0.390282 | -0.627994 |
| H | 3.657959  | 0.619421  | -0.298022 |
| H | 4.041802  | -1.115533 | -0.131618 |
| H | 3.566368  | -0.425132 | -1.706255 |
| O | -3.546773 | -0.544671 | -0.940623 |
| O | 1.760088  | -1.657404 | 0.377865  |
| O | 0.478153  | -1.970404 | 0.760643  |

|                             |           |           |           |
|-----------------------------|-----------|-----------|-----------|
| Rotational constants (GHz): | 1.1942900 | 0.5875100 | 0.4998500 |
|-----------------------------|-----------|-----------|-----------|

|                                                       |           |  |           |
|-------------------------------------------------------|-----------|--|-----------|
| Vibrational harmonic frequencies (cm <sup>-1</sup> ): |           |  |           |
| 51.3039                                               | 68.8141   |  | 108.8305  |
| 135.5020                                              | 164.6690  |  | 174.4412  |
| 180.6453                                              | 214.2194  |  | 234.8840  |
| 240.1264                                              | 275.1804  |  | 298.2926  |
| 306.4042                                              | 329.0389  |  | 337.3190  |
| 374.4224                                              | 410.5957  |  | 426.5850  |
| 460.3559                                              | 585.8637  |  | 603.8692  |
| 639.0512                                              | 673.3543  |  | 722.7401  |
| 769.9849                                              | 844.8324  |  | 875.0624  |
| 929.4194                                              | 941.7294  |  | 944.6122  |
| 960.6028                                              | 967.7544  |  | 994.4658  |
| 1013.5904                                             | 1028.7200 |  | 1043.1178 |
| 1057.1360                                             | 1095.6716 |  | 1123.2787 |
| 1170.5992                                             | 1187.4979 |  | 1194.1368 |
| 1232.0399                                             | 1250.4699 |  | 1263.0959 |
| 1270.5058                                             | 1285.8595 |  | 1310.3872 |
| 1337.6004                                             | 1394.1430 |  | 1402.5927 |
| 1409.4167                                             | 1418.7475 |  | 1423.5848 |
| 1440.9764                                             | 1446.9574 |  | 1466.8846 |
| 1470.8556                                             | 1474.0070 |  | 1488.0272 |
| 1494.2759                                             | 1502.6279 |  | 1525.6976 |
| 1651.0195                                             | 1846.5220 |  | 2948.4951 |
| 3040.3554                                             | 3041.5512 |  | 3047.0713 |
| 3061.8989                                             | 3079.8312 |  | 3094.6195 |
| 3096.8111                                             | 3104.9583 |  | 3114.2409 |
| 3119.3370                                             | 3120.3433 |  | 3121.3854 |
| 3157.3076                                             | 3182.7440 |  | 3195.6953 |
| Zero-point correction (Hartree):                      | 0.247162  |  |           |

ApineneCI.A.b.ctm

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.15839791

Electronic state : 1-A

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Cartesian coordinates (Angs):
C      1.002622      1.005840      0.890033
H      1.102444      1.976524      1.378500
C      2.407230      0.505783      0.585548
C      2.533514     -0.860194     -0.047397
H      2.957264      1.210822     -0.039684
H      2.950407      0.437010      1.535805
H      1.824234     -1.636167      0.289171
C      -0.045753      1.140297     -0.257426
C      0.038118      0.109936      1.698644
C      -0.373384      2.575649     -0.630395
C      0.234787      0.323146     -1.510137
H      0.350666     -0.738123     -1.296305
H      -0.588746      0.435662     -2.219872
H      1.139560      0.687394     -1.999729
H      -1.236605      2.623097     -1.297810
H      0.473576      3.025668     -1.152752
H      -0.587036      3.179849      0.252201
H      -0.140780      0.421549      2.724978
H      0.276435     -0.944203      1.669270
C      -1.103118      0.479464      0.721464
H      -1.732351      1.269289      1.132520
C      -2.021956     -0.503501      0.106272
C      -3.377923     -0.055179     -0.319656
H      -3.275569      0.823296     -0.960494
H      -3.899511     -0.844802     -0.851626
H      -3.954651      0.250518      0.554460
O      3.381153     -1.117606     -0.860505
O      -1.769674     -1.699827     -0.157752
O      -0.539499     -2.245670      0.125715
Rotational constants (GHz):      1.1343400      0.6292500      0.5141100
Vibrational harmonic frequencies (cm-1):
42.9648      60.6185      85.8400
127.3830      161.3541      172.3526
191.3411      222.7588      238.7369
260.4265      282.6181      297.8907
311.1813      330.8417      346.4245
373.9192      412.4117      416.7752
451.9315      573.3506      599.0022
611.4007      635.5967      702.6822
755.9464      812.4008      878.8410
917.3955      934.6631      958.9617
963.9463      987.9473      1011.5780
1027.3579      1036.3607      1039.4337
1069.8222      1106.0761      1131.4232
1154.5090      1172.8331      1197.5712
1226.8527      1247.7392      1252.6215
1275.0552      1291.4135      1321.1072
1337.4058      1384.5266      1398.1932
1406.1881      1423.0676      1441.2162
1446.9934      1448.4374      1466.2581
1473.9255      1488.8360      1493.3807
1494.5560      1504.5335      1530.5337
1650.2850      1845.2941      2995.0642
3033.2324      3042.9332      3048.0125
3061.4483      3072.2907      3089.8375
3104.9174      3109.2398      3113.4929
3114.5542      3120.2148      3121.9919
3149.9082      3182.6333      3215.0358
Zero-point correction (Hartree): 0.247159

ApineneCI.A.b.ctt
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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.15308620
Electronic state : 1-A
Cartesian coordinates (Angs):
C      1.192528      0.798030      0.824441
H      1.164159      1.645944      1.514924
C      2.641571      0.628562      0.401037
C      3.103079     -0.647296     -0.254502
H      2.932653      1.446543     -0.268808
H      3.303282      0.744632      1.268063
H      4.155440     -0.601923     -0.602080
C      0.086704      1.062548     -0.233484
C      0.330882     -0.336380      1.419547
C      -0.180599      2.522126     -0.547930
C      0.239217      0.246794     -1.509909
H      0.333105     -0.817806     -1.306174
H      -0.631150      0.397906     -2.153340
H      1.116193      0.583148     -2.068332
H      -1.047078      2.639465     -1.201580
H      0.676637      2.952009     -1.071928
H      -0.348703      3.104101      0.359330
H      0.316705     -0.433253      2.502548
H      0.515978     -1.293636      0.954299
C      -0.893358      0.364347      0.789761
H      -1.259915      1.145282      1.460563
C      -2.093829     -0.273194      0.203738
C      -3.319849      0.557125      0.020626
H      -3.061434      1.475578     -0.509394
H      -4.076715      0.009249     -0.532513
H      -3.713825      0.848624      0.995651
O      2.470485     -1.654968     -0.392789
O      -2.196903     -1.443618     -0.221258
O      -1.150258     -2.324143     -0.138600
Rotational constants (GHz):      1.1931900      0.6315800      0.5004000
Vibrational harmonic frequencies (cm-1):
44.9336      61.6970      75.9879
113.3260      142.6971      153.5545
183.8098      198.1855      219.3546
234.8162      271.8393      284.7363
302.7530      305.2045      324.4717

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376.1150	413.9254	423.1707
470.5391	557.1291	596.4006
626.3326	687.2302	748.2416
754.5340	783.9110	885.2077
908.2275	929.5808	945.7751
967.1395	990.4642	1000.0409
1005.1866	1031.0178	1037.7377
1061.1191	1088.4339	1126.4744
1165.2921	1172.6899	1195.3697
1229.6574	1245.5133	1256.8579
1273.6743	1301.2005	1331.6783
1370.3840	1397.7718	1407.2907
1412.6364	1427.8227	1434.4282
1442.8111	1454.3926	1468.4322
1475.4723	1483.5994	1492.4399
1505.7696	1506.2004	1516.9834
1653.6362	1871.3525	2920.1411
3025.6647	3042.2454	3043.8950
3048.0403	3053.3887	3062.2666
3067.3236	3100.2102	3108.0994
3116.3396	3120.0250	3122.2362
3163.3412	3179.1820	3236.5515

Zero-point correction (Hartree): 0.246574

ApineneCI.A.b.mmm

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.16644184

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -1.163545 | -0.466201 | -0.614007 |
| H | -1.532937 | -0.073452 | -1.563721 |
| C | -2.341549 | -0.968516 | 0.213155  |
| C | -3.369108 | 0.112595  | 0.404448  |
| H | -2.820096 | -1.813308 | -0.282670 |
| H | -1.987836 | -1.292149 | 1.196107  |
| H | -3.045134 | 0.981734  | 1.010136  |
| C | -0.152276 | 0.565535  | -0.023317 |
| C | -0.006959 | -1.445503 | -0.878399 |
| C | -0.356944 | 1.993029  | -0.490407 |
| C | 0.001715  | 0.501623  | 1.488639  |
| H | 0.126889  | -0.521121 | 1.853158  |
| H | 0.875903  | 1.086133  | 1.781248  |
| H | -0.870467 | 0.926894  | 1.988252  |
| H | 0.434498  | 2.639161  | -0.120411 |
| H | -1.321558 | 2.361163  | -0.131088 |
| H | -0.363338 | 2.048212  | -1.579538 |
| H | -0.014808 | -1.989620 | -1.819812 |
| H | 0.092901  | -2.159812 | -0.060152 |
| C | 0.974871  | -0.269156 | -0.742177 |
| H | 1.217267  | 0.220610  | -1.689160 |
| C | 2.249758  | -0.498546 | -0.035090 |
| C | 2.702955  | -1.829298 | 0.446289  |
| H | 2.633178  | -2.560169 | -0.360006 |
| H | 3.722494  | -1.770193 | 0.815278  |
| H | 2.046376  | -2.172039 | 1.248758  |
| O | -4.470942 | 0.088550  | -0.070604 |
| O | 3.031874  | 0.452542  | 0.186474  |
| O | 2.635713  | 1.698230  | -0.228519 |

Rotational constants (GHz): 1.5881800 0.4615000 0.4051900

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| 27.0666   | 60.6951   | 72.3996   |
| 85.8279   | 156.7744  | 187.8749  |
| 199.2836  | 225.6540  | 252.4118  |
| 260.2033  | 274.0292  | 290.1590  |
| 300.1409  | 331.9045  | 349.0846  |
| 377.9471  | 411.4430  | 434.2881  |
| 505.8697  | 527.8487  | 565.3894  |
| 608.9070  | 629.7359  | 729.3324  |
| 773.2401  | 852.3028  | 902.6583  |
| 917.6373  | 954.3427  | 962.1854  |
| 966.8151  | 971.6344  | 1004.4667 |
| 1011.5116 | 1034.6261 | 1045.7762 |
| 1075.4579 | 1099.4390 | 1129.5199 |
| 1151.9045 | 1173.0632 | 1191.4695 |
| 1199.5147 | 1248.5063 | 1265.9478 |
| 1284.0007 | 1288.2153 | 1312.0419 |
| 1331.0597 | 1363.9533 | 1393.7147 |
| 1406.3463 | 1415.2597 | 1420.8483 |
| 1432.2332 | 1465.6564 | 1469.3687 |
| 1471.2806 | 1480.1599 | 1496.0458 |
| 1496.6797 | 1506.8958 | 1515.6509 |
| 1640.9043 | 1859.8603 | 2940.3520 |
| 3043.2736 | 3052.3926 | 3057.9842 |
| 3063.2559 | 3071.7348 | 3072.8554 |
| 3085.4618 | 3110.9228 | 3116.5344 |
| 3122.4526 | 3122.7727 | 3124.5885 |
| 3144.5814 | 3172.2633 | 3182.2170 |

Zero-point correction (Hartree): 0.246794

ApineneCI.A.b.mmp

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.16805834

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-1.111296	-0.611409	-0.824444
H	-1.386326	-0.269093	-1.825615
C	-2.352677	-1.105744	-0.096745
C	-3.393233	-0.021666	-0.043455
H	-2.774696	-1.952664	-0.647037
H	-2.126080	-1.427929	0.919020
H	-3.736104	0.350276	-1.029998
C	-0.226253	0.488583	-0.166280

C	0.112458	-1.538342	-0.919657
C	-0.469535	1.889005	-0.690868
C	-0.243550	0.466421	1.355179
H	-0.087207	-0.537351	1.758381
H	0.547877	1.118363	1.729495
H	-1.199427	0.829449	1.735403
H	0.223588	2.597959	-0.246221
H	-1.493343	2.189927	-0.450484
H	-0.348172	1.926467	-1.774267
H	0.234974	-2.121857	-1.829257
H	0.161111	-2.209180	-0.061241
C	1.011312	-0.301974	-0.738386
H	1.316019	0.167181	-1.677604
C	2.219012	-0.422089	0.099164
C	2.680417	-1.692928	0.715142
H	2.736858	-2.474743	-0.043047
H	3.648714	-1.554288	1.186634
H	1.956117	-2.021148	1.463516
O	-3.831202	0.455231	0.967083
O	2.931257	0.581258	0.326263
O	2.520715	1.774697	-0.211544
Rotational constants (GHz): 1.4744100 0.4959400 0.4384500			
Vibrational harmonic frequencies (cm-1):			
52.1213	58.6853	69.4576	
101.4533	148.8996	183.5910	
191.1514	232.5218	241.8282	
253.1272	276.7112	291.4647	
303.9097	339.6901	351.5595	
381.4143	419.7035	439.8296	
501.0607	538.2513	564.4752	
611.7603	628.7390	724.3456	
763.8702	855.5620	897.8220	
915.1334	951.9345	955.3021	
970.1533	984.5426	1005.3025	
1021.5223	1039.0246	1047.9628	
1064.6606	1103.4666	1125.7402	
1156.8702	1171.4971	1194.3718	
1198.4160	1250.9678	1260.4616	
1280.1811	1287.3991	1310.7397	
1329.8850	1367.7170	1399.8824	
1410.1329	1419.7842	1422.9013	
1429.3811	1464.2806	1465.9650	
1471.9438	1479.7769	1495.2819	
1498.1883	1510.5158	1514.9216	
1641.2584	1859.0365	2933.2677	
3044.2957	3046.4444	3050.3276	
3058.7743	3063.2222	3073.8953	
3085.2876	3112.4098	3113.1005	
3121.7583	3129.7281	3130.8974	
3142.8046	3163.7493	3181.7041	
Zero-point correction (Hartree): 0.246842			
ApineneCI.A.b.mmt			
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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.16845852			
Electronic state : 1-A			
Cartesian coordinates (Angs):			
C	-1.193014	-0.566705	-0.697679
H	-1.627549	-0.160154	-1.611405
C	-2.282841	-1.205642	0.135402
C	-3.448359	-0.311210	0.449579
H	-2.688598	-2.088876	-0.372179
H	-1.896657	-1.581056	1.089102
H	-4.236771	-0.765711	1.080006
C	-0.256825	0.516534	-0.070928
C	0.030777	-1.446637	-1.012868
C	-0.513873	1.933094	-0.545186
C	-0.159755	0.458758	1.444687
H	0.032805	-0.551959	1.815103
H	0.651511	1.108992	1.776525
H	-1.088028	0.812480	1.897659
H	0.264598	2.600372	-0.184321
H	-1.489133	2.263269	-0.187582
H	-0.524953	1.976944	-1.635399
H	0.075793	-1.910352	-1.995795
H	0.160943	-2.222837	-0.257153
C	0.945285	-0.235199	-0.766045
H	1.220284	0.315070	-1.669523
C	2.185555	-0.442228	0.004722
C	2.656874	-1.767659	0.485634
H	2.675567	-2.478802	-0.340907
H	3.644784	-1.677915	0.927343
H	1.960578	-2.157901	1.230690
O	-3.561389	0.819473	0.062762
O	2.926338	0.525553	0.289998
O	2.520287	1.769949	-0.118520
Rotational constants (GHz): 1.4859900 0.5204300 0.4454700			
Vibrational harmonic frequencies (cm-1):			
36.0466	59.8570	82.9333	
115.0742	157.1281	159.3110	
198.1062	210.4674	241.2247	
262.5219	269.7608	284.5221	
300.3316	330.2830	348.9076	
364.3745	418.1025	447.4019	
485.9059	550.2896	602.3136	
627.0414	680.1669	726.4743	
747.4928	799.4321	897.4119	
904.9039	929.6085	955.9494	
966.3482	969.9236	987.5200	
1005.8383	1034.6300	1045.6095	
1060.8834	1102.6448	1109.3913	
1154.3180	1170.6860	1194.2517	

1206.8024	1252.2182	1269.1960
1286.7707	1288.5781	1316.7922
1344.5434	1366.7872	1396.8712
1410.5862	1415.1067	1419.3051
1424.5324	1447.6730	1466.2904
1471.0491	1484.8172	1494.1746
1496.8847	1508.9015	1514.4407
1638.6568	1858.3440	2942.6178
3034.8963	3039.1101	3062.9382
3063.4998	3065.3915	3073.0849
3079.4069	3095.6325	3105.4980
3122.2974	3123.9558	3130.5371
3138.5985	3164.2203	3181.4280

Zero-point correction (Hartree): 0.246493

ApineneCI.A.b.mpm

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.16806673

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 1.220966  | -0.502846 | -0.434402 |
| H | 1.451648  | -1.050791 | -1.351568 |
| C | 2.420448  | -0.546378 | 0.504885  |
| C | 3.595152  | 0.075904  | -0.193335 |
| H | 2.223645  | 0.011182  | 1.419653  |
| H | 2.654125  | -1.584824 | 0.755101  |
| H | 4.026519  | -0.517076 | -1.024119 |
| C | -0.169400 | -0.982831 | 0.078134  |
| C | 0.621948  | 0.871048  | -0.784896 |
| C | -0.551454 | -2.378593 | -0.369496 |
| C | -0.370022 | -0.816606 | 1.576162  |
| H | -0.077250 | 0.175397  | 1.928474  |
| H | -1.423306 | -0.976058 | 1.813524  |
| H | 0.219178  | -1.551290 | 2.127248  |
| H | -1.549619 | -2.638693 | -0.027679 |
| H | 0.167929  | -3.095038 | 0.037099  |
| H | -0.530667 | -2.458958 | -1.456947 |
| H | 0.922429  | 1.330376  | -1.723540 |
| H | 0.792013  | 1.585516  | 0.021332  |
| C | -0.776763 | 0.231514  | -0.719850 |
| H | -1.143718 | -0.135431 | -1.682201 |
| C | -1.874552 | 1.000402  | -0.103023 |
| C | -1.746886 | 2.408994  | 0.350991  |
| H | -1.325602 | 3.019987  | -0.448014 |
| H | -2.714280 | 2.797694  | 0.654534  |
| H | -1.053551 | 2.460875  | 1.193039  |
| O | 4.032855  | 1.164245  | 0.063068  |
| O | -2.998474 | 0.475446  | 0.060781  |
| O | -3.141395 | -0.831756 | -0.332217 |

Rotational constants (GHz): 1.4008100 0.4898700 0.4110800

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| 38.6776   | 53.5778   | 72.9683   |
| 87.0309   | 134.5722  | 176.5392  |
| 187.4004  | 209.0665  | 244.3175  |
| 254.1485  | 279.3004  | 292.0682  |
| 304.8640  | 327.1227  | 334.2384  |
| 367.4717  | 437.7266  | 454.5418  |
| 487.0439  | 541.1966  | 567.9602  |
| 609.1505  | 632.3915  | 740.6329  |
| 777.6471  | 868.1425  | 900.4585  |
| 917.6700  | 938.8484  | 955.3195  |
| 968.2784  | 983.7900  | 998.5560  |
| 1008.0300 | 1038.4326 | 1045.3784 |
| 1065.4396 | 1093.7113 | 1134.0576 |
| 1150.8125 | 1168.4297 | 1191.7072 |
| 1213.0296 | 1250.6448 | 1253.7150 |
| 1276.5037 | 1294.6451 | 1305.4811 |
| 1326.6370 | 1366.5598 | 1395.5598 |
| 1406.7886 | 1415.3333 | 1421.5247 |
| 1426.6152 | 1464.5933 | 1469.7052 |
| 1472.7840 | 1479.0105 | 1495.1386 |
| 1497.3805 | 1507.1851 | 1514.1159 |
| 1640.7462 | 1855.8839 | 2936.8195 |
| 3044.5421 | 3047.0301 | 3059.3540 |
| 3059.8531 | 3063.6361 | 3072.1286 |
| 3088.4366 | 3112.6764 | 3113.9188 |
| 3122.1568 | 3125.6280 | 3135.1814 |
| 3146.2663 | 3167.3071 | 3181.9002 |

Zero-point correction (Hartree): 0.246646

ApineneCI.A.b.mpp

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.16656483

Electronic state : 1-A

Cartesian coordinates (Angs):

C	1.227707	-0.209998	-0.376026
H	1.540103	-0.693873	-1.303985
C	2.408713	-0.151032	0.582990
C	3.529520	0.646133	-0.020856
H	2.102081	0.347151	1.507929
H	2.775714	-1.148230	0.825720
H	3.276574	1.695158	-0.276596
C	-0.098669	-0.879457	0.090502
C	0.456668	1.083783	-0.704370
C	-0.278727	-2.305076	-0.389010
C	-0.357098	-0.770061	1.584895
H	-0.207513	0.244844	1.962182
H	-1.386049	-1.070163	1.790972
H	0.309006	-1.432230	2.139979
H	-1.236748	-2.707252	-0.071161
H	0.526423	-2.923278	0.017235
H	-0.229336	-2.359241	-1.477008

H	0.714480	1.613078	-1.618878
H	0.495458	1.786412	0.129846
C	-0.843194	0.259819	-0.702594
H	-1.122113	-0.129509	-1.685474
C	-2.056187	0.856953	-0.112179
C	-2.139879	2.258709	0.373265
H	-1.778302	2.941182	-0.396611
H	-3.162295	2.503957	0.644682
H	-1.493706	2.384356	1.244569
O	4.626996	0.219729	-0.251517
O	-3.102432	0.180043	0.000126
O	-3.051676	-1.123648	-0.422747
Rotational constants (GHz): 1.5299000 0.4470100 0.3895000			
Vibrational harmonic frequencies (cm-1):			
41.3442	54.6724	62.6138	
93.8464	140.9279	176.1340	
191.2417	208.1211	242.3439	
256.4322	272.5179	294.0429	
304.9127	332.1216	333.5884	
369.6104	430.8842	445.9436	
491.0684	531.1845	570.3875	
610.0166	633.6235	742.3145	
783.8747	857.1316	901.5994	
914.4402	934.7231	955.6293	
968.1766	977.5814	1003.8947	
1007.3063	1037.3174	1045.8442	
1075.7031	1098.4284	1142.2082	
1146.0210	1173.7795	1192.3584	
1214.0443	1252.3084	1263.3587	
1277.6776	1296.4788	1310.6784	
1330.8716	1366.1426	1393.5118	
1407.1488	1416.0479	1421.4796	
1434.3565	1465.5583	1467.0392	
1471.8527	1479.4968	1493.9348	
1497.9489	1507.0869	1513.9229	
1641.3655	1862.2407	2929.0668	
3043.3716	3049.4890	3052.0048	
3062.5304	3069.4736	3071.3457	
3080.6073	3111.2979	3116.3487	
3121.8085	3125.6481	3126.5303	
3139.4348	3167.4334	3180.3863	
Zero-point correction (Hartree): 0.246674			

ApineneCI.A.b.mpt

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E (CCSD(T)/Aug-CC-pVTZ) (Hartree): -615.23990238

E (CCSD/Aug-CC-pVTZ) (Hartree): -615.12080376

T1 diagnostic: 0.021625

E (MP2/Aug-CC-pVTZ) (Hartree): -615.04873251

E (MP3/Aug-CC-pVTZ) (Hartree): -615.10460812

E (RHF/Aug-CC-pVTZ) (Hartree): -612.61560640

E (RM062X/Aug-CC-pVTZ) (Hartree): -616.16933612

Electronic state : 1-A

Cartesian coordinates (Angs):

|                                                           |           |           |           |
|-----------------------------------------------------------|-----------|-----------|-----------|
| C                                                         | -1.287512 | 0.341659  | -0.293244 |
| H                                                         | -1.617227 | 0.767979  | -1.242141 |
| C                                                         | -2.418328 | 0.421267  | 0.704715  |
| C                                                         | -3.661413 | -0.291689 | 0.247992  |
| H                                                         | -2.139237 | -0.010543 | 1.672369  |
| H                                                         | -2.696209 | 1.459134  | 0.920862  |
| H                                                         | -4.518468 | -0.252814 | 0.947035  |
| C                                                         | 0.099504  | 0.947990  | 0.067928  |
| C                                                         | -0.625933 | -1.021166 | -0.557942 |
| C                                                         | 0.359838  | 2.317031  | -0.526406 |
| C                                                         | 0.419619  | 0.931541  | 1.555178  |
| H                                                         | 0.215244  | -0.039143 | 2.014632  |
| H                                                         | 1.475835  | 1.168079  | 1.695752  |
| H                                                         | -0.170120 | 1.681070  | 2.085641  |
| H                                                         | 1.361864  | 2.663716  | -0.288480 |
| H                                                         | -0.372077 | 3.025890  | -0.128741 |
| H                                                         | 0.252747  | 2.296442  | -1.611409 |
| H                                                         | -0.973893 | -1.581452 | -1.420852 |
| H                                                         | -0.681162 | -1.663495 | 0.322792  |
| C                                                         | 0.729078  | -0.297608 | -0.662709 |
| H                                                         | 0.995761  | -0.001769 | -1.681138 |
| C                                                         | 1.919686  | -0.937859 | -0.073085 |
| C                                                         | 1.922457  | -2.308925 | 0.499874  |
| H                                                         | 1.480293  | -3.008420 | -0.210247 |
| H                                                         | 2.934400  | -2.612453 | 0.750809  |
| H                                                         | 1.303270  | -2.330565 | 1.399075  |
| O                                                         | -3.757922 | -0.879594 | -0.794582 |
| O                                                         | 3.015157  | -0.334026 | -0.037332 |
| O                                                         | 3.043641  | 0.941734  | -0.543057 |
| Rotational constants (GHz): 1.4173000 0.4939300 0.4245200 |           |           |           |
| Vibrational harmonic frequencies (cm-1):                  |           |           |           |
| 45.5987                                                   | 59.0743   | 79.9774   |           |
| 115.0743                                                  | 150.8024  | 167.8153  |           |
| 193.9951                                                  | 210.3167  | 235.3990  |           |
| 248.2379                                                  | 264.8768  | 287.0392  |           |
| 302.0145                                                  | 328.7378  | 332.1495  |           |
| 367.5068                                                  | 428.8205  | 445.4397  |           |
| 488.6835                                                  | 548.8619  | 606.2694  |           |
| 624.1967                                                  | 678.0085  | 721.2834  |           |
| 752.2533                                                  | 841.0941  | 903.6107  |           |
| 915.4214                                                  | 932.6952  | 943.5745  |           |
| 954.6841                                                  | 967.5122  | 984.4051  |           |
| 1003.2278                                                 | 1022.4019 | 1043.3109 |           |
| 1046.9951                                                 | 1097.0798 | 1139.0598 |           |
| 1152.9900                                                 | 1168.9005 | 1192.3842 |           |
| 1213.4706                                                 | 1246.3049 | 1264.4488 |           |
| 1279.3988                                                 | 1296.8408 | 1322.7374 |           |
| 1338.0076                                                 | 1368.4639 | 1398.5936 |           |



|           |           |           |
|-----------|-----------|-----------|
| 1412.5682 | 1415.6443 | 1420.6500 |
| 1425.5117 | 1450.1214 | 1465.6244 |
| 1470.6684 | 1478.2258 | 1495.0652 |
| 1497.6254 | 1505.9471 | 1514.3610 |
| 1640.4116 | 1854.1189 | 2948.5011 |
| 3036.5127 | 3041.6249 | 3046.5873 |
| 3063.5119 | 3065.0133 | 3069.2529 |
| 3078.5468 | 3088.2623 | 3108.4350 |
| 3114.5739 | 3122.6848 | 3123.5152 |
| 3156.6481 | 3168.3850 | 3180.9673 |

Zero-point correction (Hartree): 0.246451

ApineneCI.A.b.mtm

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.16459146

Electronic state : 1-A

Cartesian coordinates (Angs):

C	1.124719	0.443060	1.095366
H	1.080156	1.151996	1.924242
C	2.587555	0.298441	0.693860
C	2.910937	-0.774430	-0.309425
H	2.977274	1.243461	0.312717
H	3.168030	0.044161	1.588726
H	2.487066	-1.776801	-0.102196
C	0.060108	0.895461	0.055280
C	0.249986	-0.774103	1.460229
C	-0.218033	2.384686	0.053426
C	0.311231	0.388534	-1.356517
H	0.528978	-0.682841	-1.387299
H	-0.574838	0.575931	-1.966024
H	1.156671	0.906758	-1.811075
H	-0.996911	2.637723	-0.660683
H	0.699198	2.919029	-0.209202
H	-0.537661	2.722976	1.039688
H	0.176987	-1.039713	2.512442
H	0.516297	-1.665434	0.894451
C	-0.946044	-0.038586	0.827860
H	-1.512856	0.574911	1.533081
C	-1.922989	-0.819581	0.046483
C	-1.883754	-2.298014	-0.096298
H	-1.813694	-2.765354	0.886537
H	-2.768020	-2.650291	-0.618909
H	-0.992419	-2.588706	-0.656509
O	3.619163	-0.614377	-1.265070
O	-2.861188	-0.241619	-0.546246
O	-2.912545	1.125921	-0.451381

Rotational constants (GHz): 1.2902900 0.5276300 0.4718300

Vibrational harmonic frequencies (cm-1):

47.1633	58.3685	85.6736
102.1342	145.2290	194.6040
202.2840	219.7511	234.5200
250.5424	272.5590	293.7053
305.0570	334.9793	358.3195
366.9614	421.2646	451.7126
485.4171	553.4882	588.7439
620.3517	632.8396	710.6235
752.1670	821.0324	896.5160
919.0768	923.7488	955.2760
965.8516	988.3012	993.0764
1007.7064	1038.9793	1046.6494
1064.3106	1109.5532	1136.9400
1140.3905	1172.6076	1191.7993
1223.6428	1250.6387	1253.9832
1289.2504	1306.1161	1322.2319
1336.9783	1369.7284	1396.6259
1409.3049	1417.7828	1422.0673
1440.9504	1451.4863	1465.5293
1471.4258	1478.5137	1493.8748
1500.0919	1505.2989	1515.2871
1640.9788	1858.2976	2936.5106
3033.1128	3041.6693	3048.2047
3063.1195	3072.5812	3073.3536
3098.9591	3108.4826	3110.3964
3115.4103	3122.1761	3128.4724
3149.5994	3165.2797	3181.1901

Zero-point correction (Hartree): 0.246791

ApineneCI.A.b.mtt

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.16745486

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 1.266589  | 0.875659  | 0.790825  |
| H | 1.396069  | 1.747287  | 1.433522  |
| C | 2.608639  | 0.633409  | 0.118480  |
| C | 2.886412  | -0.674239 | -0.568565 |
| H | 2.811043  | 1.415858  | -0.622578 |
| H | 3.422824  | 0.739620  | 0.846080  |
| H | 3.897591  | -0.731344 | -1.016083 |
| C | -0.018882 | 1.102679  | -0.067364 |
| C | 0.569506  | -0.255646 | 1.582777  |
| C | -0.538078 | 2.527591  | 0.003970  |
| C | 0.040322  | 0.642545  | -1.515845 |
| H | 0.376080  | -0.388012 | -1.615847 |
| H | -0.954699 | 0.734662  | -1.953150 |
| H | 0.721300  | 1.277269  | -2.087483 |
| H | -1.515081 | 2.595463  | -0.469664 |
| H | 0.158106  | 3.199404  | -0.505331 |
| H | -0.630775 | 2.860555  | 1.038982  |
| H | 0.574205  | -0.136975 | 2.663623  |
| H | 0.939139  | -1.244738 | 1.334331  |
| C | -0.763186 | 0.096988  | 0.893751  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| H | -1.479625 | 0.644608  | 1.509729  |
| C | -1.518820 | -0.981678 | 0.231327  |
| C | -1.099164 | -2.404365 | 0.204481  |
| H | -0.122529 | -2.480796 | -0.278826 |
| H | -0.980299 | -2.772374 | 1.224917  |
| H | -1.832541 | -3.004310 | -0.325726 |
| O | 2.148582  | -1.620025 | -0.650545 |
| O | -2.585996 | -0.713481 | -0.367271 |
| O | -2.985190 | 0.604276  | -0.384624 |

Rotational constants (GHz): 1.1672200 0.6732200 0.5364700

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| 51.0161   | 86.7734   | 116.8605  |
| 134.1246  | 162.2617  | 184.6326  |
| 215.3669  | 228.0170  | 234.3206  |
| 248.0058  | 288.3738  | 294.3563  |
| 308.9174  | 312.2423  | 326.9088  |
| 370.9863  | 420.8734  | 450.2508  |
| 476.7032  | 561.5137  | 607.4732  |
| 629.3918  | 679.4282  | 746.3580  |
| 766.9976  | 776.7195  | 888.3740  |
| 899.6668  | 932.8225  | 951.5901  |
| 957.9996  | 965.7312  | 997.7555  |
| 1008.6391 | 1022.3134 | 1044.2941 |
| 1061.3465 | 1092.7439 | 1137.9718 |
| 1141.7774 | 1170.3334 | 1201.2036 |
| 1225.4384 | 1252.9153 | 1269.1079 |
| 1288.4157 | 1310.0571 | 1326.7422 |
| 1361.2474 | 1376.6964 | 1396.2425 |
| 1403.1842 | 1414.1088 | 1425.9490 |
| 1429.1485 | 1446.2856 | 1468.7588 |
| 1470.7546 | 1481.4402 | 1498.1043 |
| 1499.3511 | 1508.8603 | 1521.7226 |
| 1637.3888 | 1852.5378 | 2944.3359 |
| 3028.8299 | 3043.7483 | 3052.7419 |
| 3056.1333 | 3062.1529 | 3076.6302 |
| 3080.2259 | 3108.5247 | 3113.5680 |
| 3120.8766 | 3121.6542 | 3151.7972 |
| 3157.1670 | 3181.0393 | 3183.4502 |

Zero-point correction (Hartree): 0.247183

ApineneCI.A.b.pmm

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E(RM062X/Aug-CC-pVT2) (Hartree): -616.15984979

Electronic state : 1-A

Cartesian coordinates (Angs):

C	1.077835	-0.668950	0.114463
H	1.333515	-1.056464	1.103450
C	2.303172	-0.762340	-0.788059
C	3.469784	-0.031157	-0.184864
H	2.583565	-1.806760	-0.923306
H	2.078656	-0.330151	-1.766662
H	3.372153	1.072135	-0.132606
C	0.302709	0.675665	0.304442
C	-0.226970	-1.337191	-0.354994
C	0.631066	1.475974	1.552115
C	0.395885	1.558998	-0.935228
H	0.064748	1.046432	-1.840044
H	-0.193788	2.466949	-0.819704
H	1.429514	1.871060	-1.092046
H	-0.090791	2.282870	1.698370
H	1.621407	1.929478	1.477104
H	0.615061	0.842528	2.439174
H	-0.447488	-2.346394	-0.029662
H	-0.350747	-1.266386	-1.435825
C	-0.978560	-0.203081	0.385924
H	-1.134342	-0.558677	1.411477
C	-2.316060	0.204719	-0.082253
C	-2.714534	1.552078	-0.571944
H	-2.349005	2.319307	0.110960
H	-2.275359	1.747553	-1.550162
H	-3.796958	1.606001	-0.646828
O	4.450717	-0.564331	0.254730
O	-3.250318	-0.630497	-0.030839
O	-2.966161	-1.881142	0.445947

Rotational constants (GHz): 1.5536100 0.4332800 0.3844800

Vibrational harmonic frequencies (cm-1):

29.5347	48.0157	77.9017
89.6632	171.7454	195.2320
209.5664	233.7804	239.8522
255.7992	280.5555	291.2507
309.4894	337.9857	367.0209
370.8556	395.7696	462.0341
523.1660	535.9443	563.7038
617.3719	622.9699	723.1201
761.3782	858.6230	923.1010
939.3030	945.0469	960.5815
966.9665	983.4946	1001.1203
1015.7728	1030.6157	1038.9145
1067.5007	1103.1872	1126.2760
1141.2603	1172.3822	1191.5538
1203.1473	1240.0726	1263.9057
1284.3453	1298.3133	1313.7348
1326.8490	1370.5221	1399.9591
1410.4064	1420.3654	1426.7232
1437.8956	1465.0418	1471.0732
1475.1952	1489.2617	1494.5438
1500.6091	1511.8219	1523.0218
1620.9699	1860.8838	2928.2193
3038.7318	3047.1319	3058.3876
3062.9438	3070.6702	3072.7175
3096.6914	3111.7830	3123.9959
3127.6686	3129.3813	3135.4152

3142.3174 3177.4428 3194.1415
 Zero-point correction (Hartree): 0.247194

ApineneCI.A.b.pmp

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.16273834

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.991549  | -0.935964 | 0.213405  |
| H | 1.146811  | -1.364024 | 1.207772  |
| C | 2.244592  | -1.141230 | -0.627664 |
| C | 3.426122  | -0.522296 | 0.063528  |
| H | 2.424835  | -2.215243 | -0.728068 |
| H | 2.141592  | -0.708896 | -1.621788 |
| H | 3.702213  | -0.986724 | 1.031470  |
| C | 0.394098  | 0.495801  | 0.388877  |
| C | -0.364227 | -1.423368 | -0.327027 |
| C | 0.781454  | 1.226398  | 1.661832  |
| C | 0.674181  | 1.370222  | -0.829824 |
| H | 0.313289  | 0.920443  | -1.756744 |
| H | 0.213249  | 2.351066  | -0.723715 |
| H | 1.748850  | 1.526186  | -0.931243 |
| H | 0.194281  | 2.139416  | 1.783955  |
| H | 1.834692  | 1.513789  | 1.632905  |
| H | 0.619319  | 0.599785  | 2.539594  |
| H | -0.732761 | -2.397216 | -0.028489 |
| H | -0.425834 | -1.325303 | -1.410829 |
| C | -0.994465 | -0.205202 | 0.396028  |
| H | -1.249508 | -0.546250 | 1.406594  |
| C | -2.239863 | 0.380407  | -0.133222 |
| C | -2.426793 | 1.773874  | -0.618968 |
| H | -2.000260 | 2.476424  | 0.097324  |
| H | -1.907577 | 1.918655  | -1.566179 |
| H | -3.486006 | 1.974268  | -0.753162 |
| O | 4.033328  | 0.431819  | -0.341267 |
| O | -3.277901 | -0.323341 | -0.145052 |
| O | -3.187561 | -1.607006 | 0.323670  |

Rotational constants (GHz): 1.5855800      0.4544800      0.4040900

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| 46.5481   | 60.4905   | 75.3704   |
| 95.5598   | 158.3659  | 174.4077  |
| 221.8196  | 234.1179  | 242.5489  |
| 259.0065  | 283.0152  | 287.5621  |
| 313.4911  | 343.1499  | 372.8703  |
| 384.4001  | 403.5294  | 469.4001  |
| 524.9279  | 535.8054  | 560.4799  |
| 619.4012  | 622.1810  | 721.8123  |
| 754.8519  | 867.1119  | 917.5984  |
| 927.7263  | 945.9729  | 962.7267  |
| 966.6482  | 995.7808  | 1008.3645 |
| 1014.4942 | 1035.6326 | 1042.0966 |
| 1058.2728 | 1098.7264 | 1122.1662 |
| 1145.9869 | 1173.4075 | 1188.9169 |
| 1203.1624 | 1239.1854 | 1257.0836 |
| 1278.7775 | 1295.7676 | 1309.2640 |
| 1326.1158 | 1374.0023 | 1404.4769 |
| 1412.3132 | 1424.4765 | 1427.9782 |
| 1431.2293 | 1465.1111 | 1470.2130 |
| 1474.5683 | 1490.3055 | 1497.5041 |
| 1500.9880 | 1516.1587 | 1527.8106 |
| 1622.7096 | 1855.0664 | 2931.2001 |
| 3036.4928 | 3044.7330 | 3053.5125 |
| 3058.9299 | 3061.4114 | 3073.4235 |
| 3098.1451 | 3110.9986 | 3124.2129 |
| 3128.2912 | 3135.7341 | 3136.6123 |
| 3141.3648 | 3178.0418 | 3191.6202 |

Zero-point correction (Hartree): 0.247285

ApineneCI.A.b.pmt

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.16393867

Electronic state : 1-A

Cartesian coordinates (Angs):

C	1.068853	-0.848121	0.178872
H	1.336507	-1.167884	1.187399
C	2.224835	-1.121215	-0.757839
C	3.519546	-0.463799	-0.378101
H	2.415680	-2.198460	-0.820924
H	1.997425	-0.817711	-1.785736
H	4.378604	-0.686841	-1.039360
C	0.421144	0.573728	0.271944
C	-0.300752	-1.433975	-0.211295
C	0.803578	1.428079	1.466880
C	0.615958	1.355370	-1.021938
H	0.237289	0.822958	-1.897012
H	0.129885	2.328774	-0.976733
H	1.681306	1.539740	-1.172222
H	0.123379	2.279037	1.558231
H	1.820044	1.804779	1.366314
H	0.747586	0.850994	2.390461
H	-0.613163	-2.380293	0.213458
H	-0.433996	-1.463065	-1.293644
C	-0.939742	-0.168849	0.408820
H	-1.138561	-0.405998	1.461072
C	-2.225580	0.323723	-0.117626
C	-2.482104	1.666288	-0.705549
H	-2.051859	2.437993	-0.066869
H	-2.007986	1.750124	-1.683296
H	-3.552357	1.821022	-0.809271
O	3.659226	0.263822	0.567693
O	-3.237245	-0.412795	-0.033855
O	-3.085006	-1.648845	0.536553

Rotational constants (GHz): 1.5539200 0.4711200 0.4194100
 Vibrational harmonic frequencies (cm-1):
 45.6179 55.4203 84.6387
 121.7622 157.0464 192.0292
 213.5014 234.0171 246.0940
 249.1002 273.1886 292.6924
 313.6150 319.6030 374.6336
 379.3136 398.4710 460.1415
 518.8458 546.2003 612.6902
 620.3296 678.4678 716.5212
 753.9274 789.8441 914.4600
 926.7951 940.9111 947.5476
 963.6633 977.3184 998.3404
 1012.0687 1032.2895 1039.5184
 1054.4284 1095.4174 1114.8540
 1145.5086 1173.4134 1195.5089
 1208.1957 1239.7127 1271.2983
 1288.0966 1294.6404 1318.3955
 1342.8109 1377.1868 1403.0236
 1413.8492 1420.8866 1422.7805
 1430.4606 1449.4690 1464.8548
 1472.9792 1487.8353 1495.2927
 1499.8815 1512.7226 1523.7658
 1621.6195 1854.4090 2949.6925
 3036.2672 3040.9559 3048.0940
 3053.3263 3065.3127 3073.9879
 3082.3361 3092.4774 3114.9392
 3117.2423 3136.9998 3138.3908
 3152.5905 3178.0547 3188.5167
 Zero-point correction (Hartree): 0.247097

ApineneCI.A.b.ppm

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.16057493

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 1.198313  | 0.164108  | 0.512127  |
| H | 1.390502  | 0.056703  | 1.583391  |
| C | 2.509479  | 0.412394  | -0.216825 |
| C | 3.485804  | -0.689003 | 0.093525  |
| H | 2.373909  | 0.457340  | -1.296558 |
| H | 2.946809  | 1.356937  | 0.125085  |
| H | 3.722104  | -0.821460 | 1.168457  |
| C | 0.006583  | 1.154810  | 0.332424  |
| C | 0.292495  | -0.992705 | 0.049452  |
| C | -0.156181 | 2.200145  | 1.420074  |
| C | 0.040290  | 1.818389  | -1.039861 |
| H | 0.065516  | 1.092875  | -1.854433 |
| H | -0.818297 | 2.471754  | -1.186931 |
| H | 0.933922  | 2.438793  | -1.122514 |
| H | -1.090200 | 2.753040  | 1.297478  |
| H | 0.662020  | 2.922618  | 1.383774  |
| H | -0.161601 | 1.740576  | 2.408701  |
| H | 0.355494  | -1.950995 | 0.550958  |
| H | 0.352031  | -1.142636 | -1.028742 |
| C | -0.909905 | -0.096287 | 0.445626  |
| H | -1.125088 | -0.320367 | 1.496987  |
| C | -2.196983 | -0.272706 | -0.251026 |
| C | -2.896191 | 0.732473  | -1.095627 |
| H | -2.946409 | 1.687254  | -0.571479 |
| H | -2.348626 | 0.897183  | -2.023473 |
| H | -3.898247 | 0.381291  | -1.325097 |
| O | 3.979405  | -1.409841 | -0.728004 |
| O | -2.815389 | -1.353689 | -0.101558 |
| O | -2.246025 | -2.312798 | 0.691444  |

Rotational constants (GHz): 1.1533600 0.4853200 0.3994100  
 Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| 34.7146   | 46.1841   | 71.1257   |
| 104.2715  | 126.5004  | 170.4487  |
| 217.7641  | 233.7877  | 243.5072  |
| 258.4216  | 267.7971  | 288.7284  |
| 303.3504  | 330.2497  | 369.7857  |
| 379.5632  | 420.3374  | 447.8057  |
| 527.6606  | 552.7296  | 575.6053  |
| 616.8635  | 625.7018  | 728.4074  |
| 767.2266  | 845.8395  | 919.5466  |
| 928.3415  | 945.2210  | 953.2487  |
| 963.4391  | 994.3657  | 1001.8249 |
| 1015.5493 | 1026.5206 | 1046.0773 |
| 1067.1437 | 1092.3223 | 1137.2410 |
| 1143.0279 | 1174.6063 | 1200.8317 |
| 1215.5789 | 1238.1884 | 1252.6834 |
| 1282.3700 | 1298.9573 | 1309.7870 |
| 1326.5918 | 1374.6427 | 1404.1718 |
| 1412.9454 | 1422.8854 | 1427.3503 |
| 1431.2102 | 1463.8776 | 1467.6085 |
| 1475.3168 | 1491.2426 | 1494.9824 |
| 1502.1616 | 1514.5473 | 1522.6126 |
| 1621.2225 | 1862.4314 | 2930.8609 |
| 3041.3387 | 3041.6915 | 3045.4719 |
| 3054.9559 | 3060.5658 | 3072.6796 |
| 3098.0264 | 3110.3880 | 3124.4491 |
| 3126.6129 | 3132.3692 | 3135.2885 |
| 3141.4829 | 3177.6586 | 3191.4055 |

Zero-point correction (Hartree): 0.247095

ApineneCI.A.b.ppp

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.16037795

Electronic state : 1-A

Cartesian coordinates (Angs):

C	1.193495	0.015255	0.343051

H	1.466195	-0.182775	1.382513
C	2.455302	0.264414	-0.470417
C	3.375401	-0.920879	-0.375127
H	2.192197	0.395805	-1.524521
H	2.991989	1.150213	-0.129333
H	2.937110	-1.885862	-0.697941
C	0.045352	1.071977	0.338437
C	0.189004	-1.058022	-0.122918
C	0.029617	2.036087	1.509910
C	-0.000175	1.836797	-0.979584
H	-0.095058	1.176705	-1.843667
H	-0.825725	2.546525	-0.998519
H	0.919504	2.411024	-1.099744
H	-0.882697	2.636790	1.512562
H	0.877388	2.721839	1.453976
H	0.086875	1.501607	2.458324
H	0.236437	-2.053509	0.301492
H	0.146940	-1.129510	-1.210629
C	-0.926673	-0.138661	0.434988
H	-1.071898	-0.432365	1.481578
C	-2.273006	-0.188049	-0.165051
C	-2.996982	0.941354	-0.808336
H	-2.931074	1.830134	-0.180370
H	-2.544732	1.185580	-1.769487
H	-4.037490	0.668193	-0.959515
O	4.502973	-0.875153	0.032688
O	-2.922272	-1.258891	-0.100355
O	-2.332447	-2.328710	0.516863
Rotational constants (GHz):			
Vibrational harmonic frequencies (cm-1):			
42.0574	49.3471	52.0700	
99.0128	141.7233	174.6404	
218.4692	228.7837	235.7680	
258.2665	265.2902	290.3945	
300.4648	319.3431	365.2987	
374.7132	424.1898	437.3492	
525.9944	531.9042	575.9387	
616.3580	626.1824	729.9076	
780.1565	850.6910	915.8768	
929.9665	939.1491	951.9843	
962.4526	989.7475	1000.1633	
1015.5500	1031.0792	1042.3374	
1070.4883	1098.9355	1128.5215	
1146.3607	1173.5373	1199.8826	
1212.2835	1237.1251	1259.8550	
1281.0100	1301.0485	1311.5856	
1324.8869	1370.1954	1399.9260	
1411.0635	1422.0842	1428.0272	
1431.1121	1463.5082	1465.6554	
1474.1199	1489.8401	1494.4132	
1498.9970	1513.2799	1521.5314	
1621.9742	1860.9559	2938.2857	
3036.6096	3046.5521	3049.1186	
3058.6527	3065.2941	3073.3373	
3088.5745	3111.9921	3120.5034	
3123.1565	3127.7984	3136.2947	
3140.5687	3177.7073	3189.9536	
Zero-point correction (Hartree): 0.246929			
ApineneCI.A.b.ppt			
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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.16140317			
Electronic state : 1-A			
Cartesian coordinates (Angs):			
C	1.270858	0.118526	0.297216
H	1.576766	-0.136190	1.313385
C	2.496326	0.462687	-0.516159
C	3.559734	-0.602165	-0.458869
H	2.256418	0.623974	-1.572202
H	2.963109	1.395501	-0.177075
H	4.453999	-0.413442	-1.083039
C	0.075201	1.116357	0.367562
C	0.315191	-0.975476	-0.212678
C	0.029467	2.013886	1.590459
C	-0.029662	1.950711	-0.905198
H	-0.098065	1.334201	-1.803374
H	-0.892797	2.614016	-0.878531
H	0.855106	2.581778	-1.002683
H	-0.910826	2.568038	1.638079
H	0.841589	2.743722	1.562640
H	0.127415	1.431481	2.506701
H	0.433036	-1.984780	0.159717
H	0.258297	-0.991527	-1.302041
C	-0.836870	-0.142827	0.410226
H	-0.948605	-0.501770	1.440249
C	-2.188984	-0.225379	-0.170808
C	-2.966635	0.891702	-0.772817
H	-2.943893	1.758599	-0.111948
H	-2.527708	1.193529	-1.723602
H	-3.992994	0.574446	-0.934402
O	3.484597	-1.597478	0.206440
O	-2.798312	-1.320968	-0.128618
O	-2.161110	-2.386518	0.446493
Rotational constants (GHz):			
Vibrational harmonic frequencies (cm-1):			
40.7163	54.6960	87.9542	
109.4046	152.5430	181.6029	
200.7259	228.7542	241.3093	
253.1903	265.7228	286.5047	
298.1268	321.2831	371.4018	
378.3884	406.7470	462.5145	
523.1058	550.1170	615.9974	

618.8946	682.9555	714.4338
737.0862	839.7235	920.0156
932.1836	935.6347	949.9592
953.9305	963.0520	994.2910
1003.8337	1021.8173	1031.5067
1051.0017	1091.4437	1131.0659
1149.8844	1172.4762	1198.3600
1213.9263	1238.5067	1262.9152
1286.8389	1299.0545	1323.5312
1334.7473	1376.2641	1405.7845
1416.1226	1421.0006	1423.4357
1432.3998	1452.6053	1465.1776
1474.9932	1491.2067	1494.6641
1501.8290	1514.5353	1523.3983
1621.5290	1859.5799	2946.9112
3032.7140	3039.1881	3044.2855
3057.7378	3067.6671	3072.5037
3082.2719	3093.5127	3107.9127
3121.1319	3127.8721	3135.2292
3139.7703	3177.2678	3204.9625

Zero-point correction (Hartree): 0.246975

ApineneCI.A.b.ptm

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.15911428

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 1.032267  | -0.485847 | 1.015554  |
| H | 0.915935  | -0.598832 | 2.095260  |
| C | 2.507555  | -0.686253 | 0.684450  |
| C | 2.845982  | -0.893360 | -0.766417 |
| H | 3.108329  | 0.143588  | 1.060328  |
| H | 2.848433  | -1.595030 | 1.193330  |
| H | 2.280230  | -1.692219 | -1.282834 |
| C | 0.294322  | 0.825353  | 0.607735  |
| C | -0.085498 | -1.308492 | 0.338921  |
| C | 0.271323  | 1.923658  | 1.654566  |
| C | 0.815198  | 1.368974  | -0.718089 |
| H | 0.753444  | 0.637403  | -1.526859 |
| H | 0.268778  | 2.259787  | -1.024428 |
| H | 1.863235  | 1.652646  | -0.614707 |
| H | -0.385823 | 2.742004  | 1.352001  |
| H | 1.271223  | 2.339233  | 1.795338  |
| H | -0.079144 | 1.544170  | 2.614779  |
| H | -0.436727 | -2.212964 | 0.820590  |
| H | 0.106940  | -1.511949 | -0.713110 |
| C | -0.983040 | -0.055294 | 0.508853  |
| H | -1.462936 | -0.150039 | 1.490142  |
| C | -2.090538 | 0.167616  | -0.438756 |
| C | -2.256969 | 1.334431  | -1.346195 |
| H | -2.090507 | 2.260060  | -0.794722 |
| H | -1.522650 | 1.297264  | -2.150822 |
| H | -3.257158 | 1.327291  | -1.770087 |
| O | 3.696813  | -0.284884 | -1.356335 |
| O | -3.026754 | -0.665914 | -0.476784 |
| O | -2.955712 | -1.747594 | 0.359629  |

Rotational constants (GHz): 1.2454000 0.4841900 0.4540200

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| 36.7856   | 51.0333   | 84.2982   |
| 99.8716   | 151.7410  | 183.6481  |
| 226.4138  | 233.1767  | 246.6690  |
| 259.0943  | 280.8106  | 284.8416  |
| 299.3141  | 312.5014  | 384.9629  |
| 397.0061  | 416.1706  | 453.3394  |
| 521.1561  | 548.6512  | 588.1846  |
| 620.9032  | 628.9716  | 714.0138  |
| 737.2358  | 828.1710  | 908.3506  |
| 923.5277  | 945.1568  | 952.3431  |
| 961.8977  | 995.2597  | 1001.0724 |
| 1012.3225 | 1036.6154 | 1043.9599 |
| 1059.7828 | 1101.9240 | 1120.8644 |
| 1145.6517 | 1175.3035 | 1198.7258 |
| 1218.1008 | 1237.3814 | 1257.6065 |
| 1298.2421 | 1310.0522 | 1319.6419 |
| 1329.7878 | 1376.5810 | 1402.7626 |
| 1411.4570 | 1423.7521 | 1428.6915 |
| 1438.7000 | 1456.3402 | 1463.4279 |
| 1474.5635 | 1490.5568 | 1495.5417 |
| 1504.0631 | 1515.0941 | 1524.5660 |
| 1621.9140 | 1855.2580 | 2949.5144 |
| 3037.5833 | 3038.7994 | 3045.7595 |
| 3056.7629 | 3072.1160 | 3072.6718 |
| 3107.6477 | 3111.0526 | 3111.2629 |
| 3124.7279 | 3125.8017 | 3135.5351 |
| 3138.7839 | 3177.1148 | 3191.9358 |

Zero-point correction (Hartree): 0.247233

ApineneCI.A.b.ptt

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.15885782

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-1.170312	-0.115018	-1.038035
H	-1.078777	0.031375	-2.117001
C	-2.648549	-0.308688	-0.745616
C	-3.099812	-0.908837	0.558684
H	-3.184689	0.643054	-0.847691
H	-3.099839	-0.949808	-1.512265
H	-4.202142	-0.980176	0.648134
C	-0.348257	1.028556	-0.367786
C	-0.085919	-1.128852	-0.617144
C	-0.285674	2.330832	-1.146442

C	-0.793694	1.294798	1.065484
H	-0.738717	0.406648	1.691724
H	-0.204829	2.091618	1.518804
H	-1.833654	1.629703	1.067026
H	0.430515	3.022248	-0.696799
H	-1.260489	2.824087	-1.149304
H	0.012397	2.158829	-2.181016
H	0.202281	-1.903317	-1.318055
H	-0.282241	-1.559171	0.360270
C	0.877802	0.085773	-0.527271
H	1.325802	0.201479	-1.520924
C	2.021096	0.015163	0.398920
C	2.248601	0.866718	1.596894
H	2.132188	1.917784	1.331262
H	1.511835	0.641341	2.367480
H	3.247340	0.689594	1.985791
O	-2.403866	-1.312576	1.449177
O	2.936630	-0.808565	0.160009
O	2.808651	-1.607354	-0.945883

Rotational constants (GHz): 1.1651100 0.5348600 0.4953100
 Vibrational harmonic frequencies (cm-1):
 46.8883 64.8203 102.6553
 124.7635 154.2099 185.4722
 199.3497 229.4563 243.5790
 247.6255 265.2088 289.7418
 297.0067 313.9632 368.4045
 388.0133 399.0074 462.7796
 522.0937 549.4793 612.7619
 617.5728 685.6339 735.3447
 755.5725 782.4640 901.2746
 930.8676 933.6158 949.0423
 963.8826 966.7356 1000.3689
 1005.7491 1019.6109 1043.2654
 1056.7223 1091.2599 1100.9403
 1157.5934 1180.6198 1200.2607
 1225.9193 1240.5665 1264.9338
 1302.4772 1314.1594 1329.1187
 1361.5600 1387.8298 1406.2264
 1413.1741 1422.5552 1426.8954
 1434.3353 1448.8332 1465.3753
 1475.0375 1489.3473 1494.6525
 1506.7766 1512.6283 1518.6392
 1622.6006 1861.6192 2931.0596
 3028.2973 3040.0290 3043.7591
 3052.7029 3059.0686 3062.8532
 3073.6018 3107.3809 3119.4534
 3125.2289 3131.8510 3137.0014
 3159.2188 3177.5564 3197.5715
 Zero-point correction (Hartree): 0.247221

Population analysis as 298K (%)

Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)

Compound	Qtot	Erel	Erel2	n*Q*MB	%
ApineneCI.A.b.14Hshift.a.mt	9.474e+43	0.00	0.00	9.474e+43	35.7
ApineneCI.A.b.14Hshift.a.pt	1.453e+44	0.41	0.41	7.291e+43	27.5
ApineneCI.A.b.14Hshift.a.pm	2.918e+44	1.11	1.11	4.494e+43	16.9
ApineneCI.A.b.14Hshift.a.mp	1.220e+44	1.00	1.00	2.253e+43	8.5
ApineneCI.A.b.14Hshift.a.pp	2.612e+44	1.89	1.89	1.076e+43	4.06
ApineneCI.A.b.14Hshift.a.tt	3.362e+43	0.96	0.96	6.611e+42	2.49
ApineneCI.A.b.14Hshift.a.mm	2.160e+44	2.18	2.18	5.479e+42	2.07
ApineneCI.A.b.14Hshift.b.mt	6.396e+43	1.74	1.74	3.366e+42	1.27
ApineneCI.A.b.14Hshift.b.mp	8.764e+43	2.52	2.52	1.242e+42	0.468
ApineneCI.A.b.14Hshift.b.pt	8.818e+43	2.78	2.78	8.075e+41	0.305
ApineneCI.A.b.14Hshift.a.tm	1.190e+44	3.15	3.15	5.802e+41	0.219
ApineneCI.A.b.14Hshift.b.pm	1.702e+44	3.42	3.42	5.251e+41	0.198
ApineneCI.A.b.14Hshift.b.pp	1.799e+44	3.65	3.65	3.786e+41	0.143
ApineneCI.A.b.14Hshift.b.mm	1.749e+44	3.97	3.97	2.161e+41	0.0815
ApineneCI.A.b.14Hshift.b.tm	8.387e+43	4.79	4.79	2.593e+40	0.00978
ApineneCI.A.b.14Hshift.b.tt	5.837e+43	4.95	4.95	1.358e+40	0.00512
Total				2.651e+44	100

ApineneCI.A.b.14Hshift.a.mm

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 E(RM062X/Aug-CC-pVTZ) (Hartree): -616.13523566

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -1.125973 | -0.430714 | -0.602791 |
| H | -1.430471 | 0.044478  | -1.537204 |
| C | -2.354550 | -1.016399 | 0.085098  |
| C | -3.412569 | 0.031559  | 0.291451  |
| H | -2.777864 | -1.815946 | -0.523230 |
| H | -2.071901 | -1.427254 | 1.058148  |
| H | -3.161783 | 0.833074  | 1.014290  |
| C | -0.183885 | 0.552874  | 0.155890  |
| C | 0.059762  | -1.373736 | -0.873037 |
| C | -0.387981 | 2.014201  | -0.197363 |
| C | -0.161519 | 0.360294  | 1.666307  |
| H | -0.046728 | -0.689605 | 1.942409  |
| H | 0.675918  | 0.918225  | 2.088224  |
| H | -1.078753 | 0.735259  | 2.126371  |
| H | 0.328491  | 2.653649  | 0.313180  |
| H | -1.397539 | 2.317455  | 0.091083  |
| H | -0.283350 | 2.174566  | -1.270925 |
| H | 0.132709  | -1.787193 | -1.877151 |
| H | 0.094882  | -2.195935 | -0.152148 |
| C | 1.010956  | -0.237544 | -0.514924 |
| H | 1.565331  | 0.806122  | -1.118045 |
| C | 2.282822  | -0.469724 | 0.032379  |
| C | 2.882235  | -1.775265 | 0.404049  |
| H | 2.752766  | -2.475592 | -0.421817 |

|                                           |           |           |                               |
|-------------------------------------------|-----------|-----------|-------------------------------|
| H                                         | 2.359853  | -2.190559 | 1.267240                      |
| H                                         | 3.940009  | -1.665825 | 0.626862                      |
| O                                         | -4.464182 | 0.053634  | -0.286699                     |
| O                                         | 3.095397  | 0.536528  | 0.034749                      |
| O                                         | 2.461615  | 1.638814  | -0.536755                     |
| Rotational constants (GHz):               |           |           | 1.6125800 0.4539600 0.4028400 |
| Vibrational harmonic frequencies (cm-1):  |           |           |                               |
| i1575.9991                                | 29.9935   |           | 59.5279                       |
| 78.2247                                   | 106.3991  |           | 135.1196                      |
| 148.9294                                  | 199.5166  |           | 229.5174                      |
| 253.1967                                  | 265.9380  |           | 271.3680                      |
| 288.5895                                  | 321.7356  |           | 332.5905                      |
| 366.5672                                  | 379.9424  |           | 428.2039                      |
| 480.5695                                  | 526.6223  |           | 537.2281                      |
| 607.8662                                  | 639.8888  |           | 691.4251                      |
| 715.2260                                  | 766.3076  |           | 857.1492                      |
| 938.4173                                  | 950.0259  |           | 954.4563                      |
| 966.9571                                  | 987.6623  |           | 1008.9781                     |
| 1011.8831                                 | 1035.4752 |           | 1045.8267                     |
| 1060.4951                                 | 1100.0344 |           | 1105.9259                     |
| 1159.0679                                 | 1169.2944 |           | 1189.0955                     |
| 1190.2292                                 | 1252.7042 |           | 1260.5913                     |
| 1269.1530                                 | 1293.7654 |           | 1318.7386                     |
| 1335.6280                                 | 1384.0861 |           | 1394.8955                     |
| 1403.9914                                 | 1416.5963 |           | 1434.6079                     |
| 1438.3640                                 | 1469.6420 |           | 1471.0812                     |
| 1481.4981                                 | 1487.0291 |           | 1492.0358                     |
| 1497.6188                                 | 1502.7480 |           | 1510.3813                     |
| 1564.1583                                 | 1859.7955 |           | 1888.6632                     |
| 2937.4566                                 | 3043.7529 |           | 3046.4242                     |
| 3054.4927                                 | 3059.2539 |           | 3066.9678                     |
| 3077.3967                                 | 3112.9650 |           | 3119.4889                     |
| 3120.1844                                 | 3122.4189 |           | 3124.4365                     |
| 3128.6255                                 | 3155.8006 |           | 3176.0095                     |
| Zero-point correction (Hartree): 0.242317 |           |           |                               |

ApineneCI.A.b.14Hshift.a.mp

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.13715720

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-1.064271	-0.538425	-0.833836
H	-1.265414	-0.091713	-1.810684
C	-2.350241	-1.120149	-0.264665
C	-3.415817	-0.062618	-0.193368
H	-2.704059	-1.912095	-0.932373
H	-2.201880	-1.542313	0.728506
H	-3.689335	0.394952	-1.165635
C	-0.259565	0.492653	0.009416
C	0.178048	-1.440390	-0.936209
C	-0.498464	1.938925	-0.378852
C	-0.413384	0.306699	1.513751
H	-0.263028	-0.732923	1.811595
H	0.326649	0.919976	2.030220
H	-1.407329	0.614341	1.844914
H	0.121634	2.617758	0.202212
H	-1.548249	2.186044	-0.198566
H	-0.284291	2.102336	-1.435891
H	0.383393	-1.882389	-1.909613
H	0.163086	-2.235461	-0.185207
C	1.034568	-0.250477	-0.513989
H	1.596149	0.804858	-1.092283
C	2.253317	-0.403351	0.165151
C	2.869243	-1.664851	0.645513
H	2.852980	-2.399664	-0.160099
H	2.281158	-2.072095	1.469441
H	3.893701	-1.498031	0.966795
O	-3.941162	0.312795	0.818767
O	3.015061	0.641039	0.211374
O	2.394130	1.693457	-0.460242
Rotational constants (GHz):			1.5415100 0.4822100 0.4295900
Vibrational harmonic frequencies (cm-1):			
i1574.8754	48.2800		63.8563
81.9504	113.1249		128.9658
135.5885	190.9310		235.4584
263.3722	269.0174		275.3553
291.6328	328.3293		337.4739
371.8927	385.2453		429.8516
476.9697	533.7879		539.7167
604.1867	641.2919		690.0934
713.7663	756.0020		856.1309
923.9593	949.4449		960.8501
972.1836	989.4019		1001.9997
1020.0800	1046.3748		1048.6747
1062.7651	1086.1173		1108.0917
1157.4492	1176.1056		1188.9303
1191.6697	1244.5646		1261.2847
1265.7789	1288.2615		1312.1368
1335.0183	1389.4017		1400.3018
1407.4747	1420.9009		1427.0556
1437.7236	1466.5620		1472.3142
1482.2225	1487.6485		1493.0475
1498.6245	1508.1807		1509.6404
1563.8940	1857.5796		1890.6919
2928.1216	3045.4209		3047.2703
3049.8516	3050.9556		3064.2564
3066.4755	3115.4853		3116.5311
3119.8626	3124.5599		3128.1595
3132.0469	3154.6323		3175.4659
Zero-point correction (Hartree): 0.242365			

ApineneCI.A.b.14Hshift.a.mt


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E(CCSd(T)/Aug-CC-pVTZ) (Hartree): -615.20945972
E(CCSd(Aug-CC-pVTZ) (Hartree): -615.08623556
T1 diagnostic: 0.018757
E(MP2/Aug-CC-pVTZ) (Hartree): -615.02730090
E(MP3/Aug-CC-pVTZ) (Hartree): -615.07210470
E(RHF/Aug-CC-pVTZ) (Hartree): -612.56206796
E(RM062X/Aug-CC-pVTZ) (Hartree): -616.13869603
Electronic state : 1-A
Cartesian coordinates (Angs):
  C    1.168511    -0.269709    0.921339
  H    1.897790    0.199754    1.580460
  C    1.875355    -1.279059    0.043249
  C    3.057276    -0.721306    -0.701695
  H    2.254441    -2.111679    0.648017
  H    1.199305    -1.741084    -0.684135
  H    3.555839    -1.420903    -1.399461
  C    0.267920    0.779874    0.188559
  C   -0.075152    -0.854751    1.628737
  C    0.362971    2.136179    0.866771
  C    0.387759    0.930827    -1.316655
  H    0.390871    -0.030482    -1.833564
  H   -0.462506    1.504162    -1.685125
  H    1.305220    1.461274    -1.570920
  H   -0.410057    2.805954    0.489998
  H    1.341548    2.574419    0.663901
  H    0.246576    2.042596    1.947868
  H   -0.167599    -0.540661    2.666965
  H   -0.167470    -1.941694    1.587573
  C   -0.976893    -0.058377    0.698229
  H   -1.827437    0.941020    0.777655
  C   -1.898023    -0.652283    -0.171958
  C   -2.200003    -2.094118    -0.369915
  H   -2.432013    -2.547073    0.594588
  H   -1.331536    -2.613330    -0.775642
  H   -3.050216    -2.216136    -1.035586
  O    3.477645    0.394195    -0.560848
  O   -2.730968    0.161592    -0.745570
  O   -2.516814    1.460488    -0.280152
Rotational constants (GHz):    1.2925200    0.5731900    0.5011200
Vibrational harmonic frequencies (cm-1):
i1565.5749    37.0318    85.9626
  97.9213    113.6858    130.2138
 151.4571    178.8905    220.8345
 260.0025    270.3823    287.0532
 294.6946    318.0709    327.8268
 379.9810    386.5873    416.4918
 473.1366    506.5456    593.7241
 665.2064    679.0213    700.6863
 730.4424    743.0421    833.6238
 864.5502    921.1994    953.1248
 965.9020    980.6370    993.6547
1013.4810    1030.8013    1041.7283
1049.9673    1058.2495    1092.3348
1160.8324    1166.4926    1196.1187
1208.9207    1245.1620    1266.1414
1268.0288    1290.4194    1306.1674
1336.8261    1391.6447    1396.0403
1407.4366    1413.3716    1424.6606
1433.0981    1451.5874    1472.8997
1483.4436    1485.7585    1494.8735
1498.2451    1508.2587    1516.4484
1575.0485    1856.7232    1894.6310
2950.1809    3034.3236    3051.7900
3057.4809    3066.7442    3068.4847
3070.9277    3101.9214    3121.8363
3124.1428    3128.3239    3132.2686
3136.8281    3145.6534    3173.3260
Zero-point correction (Hartree): 0.242310

ApineneCI.A.b.14Hshift.a.pm
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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.13676054
Electronic state : 1-A
Cartesian coordinates (Angs):
  C    1.199230    -0.449533    -0.417397
  H    1.369059    -0.964136    -1.366142
  C    2.472243    -0.484158    0.418930
  C    3.577330    0.171913    -0.358079
  H    2.345062    0.049495    1.359790
  H    2.748591    -1.522297    0.625875
  H    3.913979    -0.375637    -1.260951
  C   -0.123353    -0.993160    0.195776
  C    0.535431    0.914588    -0.680817
  C   -0.490132    -2.388748    -0.270214
  C   -0.186350    -0.898438    1.713774
  H    0.103163    0.090942    2.072103
  H   -1.205784    -1.099519    2.046620
  H    0.473018    -1.635301    2.177740
  H   -1.433010    -2.721312    0.157959
  H    0.298388    -3.081892    0.034913
  H   -0.576053    -2.429344    -1.356675
  H    0.722198    1.371755    -1.650773
  H    0.783892    1.641092    0.098146
  C   -0.824930    0.256487    -0.471015
  H   -1.704995    -0.432433    -1.187249
  C   -1.932385    0.962052    0.024988
  C   -1.976548    2.376086    0.471716
  H   -1.502094    3.003931    -0.283211
  H   -1.404921    2.490636    1.393964
  H   -3.001615    2.701587    0.625955
  O    4.057413    1.237561    -0.083912

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O      -3.081093      0.379605      -0.097899
O      -2.905332      -0.853428      -0.724943
Rotational constants (GHz):      1.3639400      0.4845800      0.4093000
Vibrational harmonic frequencies (cm-1):
i1585.7206      36.7548      51.4084
68.3533      105.3815      132.7838
135.3142      177.2101      206.2053
255.0342      265.1352      273.9867
288.0776      329.5702      334.5196
340.7173      389.2673      456.9429
478.7741      514.4257      545.7440
616.1967      639.1958      693.6048
719.0880      777.1751      861.2933
933.3132      937.7343      953.3359
963.4473      985.6730      1003.1221
1015.3267      1042.2478      1051.5053
1063.3037      1080.1021      1111.3789
1151.0367      1174.7576      1188.7271
1203.7522      1245.7633      1261.8276
1275.7174      1281.6975      1312.0166
1334.6987      1386.9035      1396.7636
1403.6027      1416.2287      1426.0795
1437.0086      1469.5911      1471.8497
1480.9120      1488.0770      1490.5991
1498.0752      1504.1200      1508.9944
1563.0527      1857.1651      1888.5855
2932.5648      3045.0042      3049.1887
3050.9584      3054.9940      3064.7094
3067.4811      3114.2960      3116.6106
3122.3733      3122.7919      3129.0008
3135.9461      3155.0155      3175.9818
Zero-point correction (Hartree): 0.242140

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ApineneCI.A.b.14Hshift.a.pp

E(RM062X/Aug-CC-pVTZ) (Hartree): -616.13555214

Electronic state : 1-A

Cartesian coordinates (Angs):

```

C      -1.203676      0.183524      -0.339831
H      -1.456062      0.655867      -1.291139
C      -2.451666      0.099061      0.527880
C      -3.506742      -0.720844      -0.158391
H      -2.206746      -0.395884      1.472764
H      -2.859468      1.086626      0.744029
H      -3.205684      -1.757080      -0.413170
C      0.060623      0.891338      0.226324
C      -0.381994      -1.094106      -0.604998
C      0.235694      2.318434      -0.255013
C      0.185158      0.815191      1.741631
H      0.033160      -0.199883      2.113746
H      1.182648      1.141884      2.039386
H      -0.543831      1.468791      2.225392
H      1.143036      2.768660      0.141118
H      -0.623362      2.909221      0.073045
H      0.280730      2.361942      -1.343694
H      -0.541464      -1.594489      -1.558525
H      -0.500273      -1.828539      0.198228
C      0.890982      -0.267218      -0.458434
H      1.641659      0.516663      -1.220407
C      2.099940      -0.819228      -0.005955
C      2.344168      -2.208735      0.453692
H      1.922614      -2.904657      -0.272424
H      1.833581      -2.379643      1.402678
H      3.408276      -2.398029      0.564959
O      -4.600938      -0.323800      -0.450081
O      3.158169      -0.098337      -0.187477
O      2.799802      1.092643      -0.817120

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Rotational constants (GHz): 1.4823200 0.4447700 0.3914400

Vibrational harmonic frequencies (cm-1):

```

i1586.0404      38.7897      55.3714
68.0858      103.8612      132.8918
139.5411      181.8915      205.9292
252.9090      268.5505      274.4045
288.9997      326.9792      334.2324
341.2258      391.0660      453.4544
476.6579      512.1808      537.2092
616.3534      640.9346      693.3990
720.2630      783.2523      853.8702
926.2857      934.0427      952.7538
964.1275      984.9549      1009.1981
1015.3744      1041.3211      1047.9630
1061.0448      1099.9743      1111.7804
1153.8148      1172.9441      1190.6027
1201.6995      1253.1025      1262.5203
1277.7350      1282.8583      1317.0897
1333.5201      1384.4907      1395.2083
1404.5484      1418.3475      1431.7882
1438.2209      1465.5956      1471.6883
1481.0744      1487.6973      1491.6058
1497.9229      1503.6928      1510.0929
1563.3746      1861.3324      1889.0810
2930.5084      3038.5335      3044.7381
3051.0662      3052.7337      3066.7403
3077.3330      3113.9990      3118.3599
3119.2729      3122.6332      3124.3875
3128.0827      3155.8817      3175.7300

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Zero-point correction (Hartree): 0.242176

ApineneCI.A.b.14Hshift.a.pt

E(RM062X/Aug-CC-pVTZ) (Hartree): -616.13778744

Electronic state : 1-A

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Cartesian coordinates (Angs):
C      -1.270515      0.298154      -0.274639
H      -1.540440      0.687685      -1.257032
C      -2.478064      0.356956      0.630967
C      -3.656935      -0.406759      0.093138
H      -2.263458      -0.047382      1.626360
H      -2.809465      1.387710      0.802490
H      -4.563169      -0.393689      0.728525
C      0.053469      0.973862      0.181782
C      -0.541217      -1.044962      -0.451650
C      0.300988      2.334079      -0.441544
C      0.231925      1.035955      1.693066
H      0.028367      0.073323      2.166451
H      1.259332      1.320085      1.925916
H      -0.433163      1.781562      2.134814
H      1.249910      2.758560      -0.121447
H      -0.505206      3.010506      -0.144956
H      0.305048      2.270314      -1.530130
H      -0.776833      -1.603122      -1.354266
H      -0.681560      -1.703418      0.411602
C      0.787296      -0.295960      -0.409196
H      1.566089      0.366982      -1.254333
C      1.971037      -0.884421      0.059159
C      2.138868      -2.246887      0.622971
H      1.653737      -2.967271      -0.036523
H      1.643794      -2.310305      1.593147
H      3.191396      -2.496578      0.725242
O      -3.656930      -1.006268      -0.947069
O      3.069502      -0.252743      -0.205686
O      2.769242      0.902129      -0.927268
Rotational constants (GHz):      1.3577400      0.4940300      0.4287200
Vibrational harmonic frequencies (cm-1):
i1584.5443      43.3763      56.7297
103.6032      109.4606      139.5995
154.1713      172.4726      208.9123
234.3046      261.3643      271.9535
287.5691      325.0548      335.7504
340.3814      384.9270      438.4288
488.3120      509.5855      597.6717
630.2692      675.4172      700.2897
716.1096      733.9160      843.6869
931.6602      933.8160      943.0631
955.6702      964.1449      992.1419
1010.2652      1022.2302      1044.3533
1059.5319      1077.9451      1118.5135
1149.5759      1173.6355      1191.9942
1203.9478      1256.9981      1259.0074
1281.1785      1285.4202      1330.2928
1339.2984      1391.1410      1400.3261
1411.4564      1416.0118      1424.7461
1436.6222      1450.3771      1472.2339
1480.6087      1487.3225      1491.4957
1497.7053      1503.5114      1509.8637
1564.7355      1855.6947      1884.9971
2945.9166      3036.2418      3039.0121
3043.0091      3049.0617      3066.0727
3067.4495      3091.6024      3111.0666
3116.4381      3120.3121      3128.1754
3137.6227      3154.5510      3175.2465
Zero-point correction (Hartree): 0.242052

ApineneCI.A.b.14Hshift.a.tm
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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.13364988
Electronic state : 1-A
Cartesian coordinates (Angs):
C      1.067759      0.410329      1.070214
H      0.943114      1.118047      1.891178
C      2.562429      0.269596      0.807972
C      2.985171      -0.803295      -0.157348
H      2.986488      1.215043      0.466183
H      3.053250      0.016807      1.755435
H      2.552388      -1.807982      0.014363
C      0.111890      0.865227      -0.067265
C      0.164410      -0.807865      1.355743
C      -0.152968      2.357799      -0.094285
C      0.512207      0.365655      -1.448904
H      0.721635      -0.706689      -1.453218
H      -0.301371      0.552299      -2.151653
H      1.402565      0.883413      -1.811350
H      -0.848805      2.629667      -0.884725
H      0.791883      2.880570      -0.264151
H      -0.566016      2.700474      0.855102
H      -0.022137      -1.036976      2.403478
H      0.497388      -1.720028      0.855742
C      -0.951093      -0.104998      0.586525
H      -1.874513      0.818341      0.826665
C      -1.968620      -0.810591      -0.074818
C      -2.107905      -2.281241      -0.214342
H      -1.982152      -2.746839      0.763769
H      -1.319773      -2.667154      -0.862833
H      -3.082303      -2.540947      -0.618880
O      3.776100      -0.638892      -1.045557
O      -2.997409      -0.117059      -0.439996
O      -2.815106      1.211983      -0.060204
Rotational constants (GHz):      1.3486800      0.5134800      0.4534300
Vibrational harmonic frequencies (cm-1):
i1580.4750      44.2043      71.8480
84.8871      108.4131      133.6049
145.1696      199.7563      224.0752
246.9922      260.4264      266.1965
286.7403      324.4437      357.2071

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360.7426	399.0429	431.2828
461.4155	522.2943	589.9538
609.1915	640.9347	688.5856
709.6472	736.5560	822.2585
914.2253	945.6899	954.3302
960.8593	977.5689	1000.4611
1015.4151	1044.7098	1050.4066
1062.0378	1093.0428	1111.8567
1152.8723	1166.9207	1190.0272
1208.8929	1245.7571	1262.9935
1277.8161	1312.7437	1318.7005
1340.5708	1387.9640	1396.7375
1407.3481	1419.0861	1436.7012
1440.4198	1450.9193	1471.4552
1481.0811	1489.9342	1490.0940
1499.8965	1503.0920	1510.1578
1563.0275	1856.4626	1892.1387
2944.0543	3033.7389	3042.8011
3050.6580	3065.1056	3066.4148
3078.9947	3107.9400	3111.9895
3116.7586	3122.1939	3122.6761
3128.5036	3155.0066	3174.9941

Zero-point correction (Hartree): 0.242288

ApineneCI.A.b.14Hshift.a.tt

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.13773714

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -1.308403 | -0.886791 | 0.777789  |
| H | -1.556257 | -1.770915 | 1.365759  |
| C | -2.600685 | -0.453105 | 0.102734  |
| C | -2.686860 | 0.896165  | -0.546796 |
| H | -2.895078 | -1.177380 | -0.666609 |
| H | -3.426906 | -0.475257 | 0.823541  |
| H | -3.687978 | 1.134206  | -0.955572 |
| C | -0.044011 | -1.179523 | -0.095243 |
| C | -0.518029 | 0.149371  | 1.618605  |
| C | 0.493765  | -2.575891 | 0.186673  |
| C | -0.137716 | -0.953844 | -1.593518 |
| H | -0.526255 | 0.032048  | -1.838330 |
| H | 0.859084  | -1.046497 | -2.026094 |
| H | -0.775915 | -1.711426 | -2.055273 |
| H | 1.458418  | -2.723056 | -0.296435 |
| H | -0.206077 | -3.322535 | -0.195718 |
| H | 0.611738  | -2.739415 | 1.259227  |
| H | -0.353224 | -0.169411 | 2.646607  |
| H | -0.933830 | 1.155019  | 1.625199  |
| C | 0.693247  | -0.042414 | 0.713854  |
| H | 1.863528  | -0.648655 | 0.758492  |
| C | 1.388714  | 1.026745  | 0.130594  |
| C | 1.145555  | 2.482939  | 0.280376  |
| H | 1.041269  | 2.715353  | 1.340994  |
| H | 0.212370  | 2.753669  | -0.209640 |
| H | 1.977710  | 3.048410  | -0.130141 |
| O | -1.798000 | 1.699422  | -0.643723 |
| O | 2.510701  | 0.717141  | -0.444195 |
| O | 2.760291  | -0.646072 | -0.274133 |

Rotational constants (GHz): 1.0979600 0.7375900 0.5596300

Vibrational harmonic frequencies (cm-1):

|            |           |           |
|------------|-----------|-----------|
| i1568.1378 | 64.4989   | 89.5886   |
| 116.8757   | 135.7918  | 152.4624  |
| 171.6983   | 175.8124  | 227.8313  |
| 242.3325   | 261.3182  | 288.1276  |
| 300.6359   | 306.5929  | 329.4217  |
| 364.2522   | 388.8747  | 425.8314  |
| 478.0569   | 509.0937  | 596.6577  |
| 662.0665   | 676.9220  | 697.2065  |
| 731.5946   | 766.9961  | 779.1037  |
| 895.5065   | 923.5483  | 942.7818  |
| 960.6670   | 976.8696  | 990.1916  |
| 1012.7080  | 1021.0120 | 1048.0383 |
| 1062.8583  | 1090.0596 | 1119.5049 |
| 1146.3984  | 1178.2293 | 1186.1705 |
| 1205.9633  | 1250.2275 | 1274.4650 |
| 1290.9614  | 1312.2582 | 1328.9287 |
| 1363.2077  | 1392.6019 | 1396.4729 |
| 1404.4952  | 1414.8305 | 1428.1677 |
| 1436.1724  | 1443.7078 | 1470.5030 |
| 1482.3026  | 1487.5225 | 1499.8458 |
| 1500.8615  | 1507.1739 | 1522.9206 |
| 1570.9452  | 1855.5080 | 1887.3959 |
| 2944.2305  | 3030.2958 | 3047.2738 |
| 3053.2749  | 3056.5312 | 3077.2027 |
| 3078.8612  | 3090.2665 | 3112.6332 |
| 3121.8675  | 3139.2274 | 3146.5028 |
| 3147.5611  | 3167.1531 | 3179.9302 |

Zero-point correction (Hartree): 0.242886

ApineneCI.A.b.14Hshift.b.mm

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.13265066

Electronic state : 1-A

Cartesian coordinates (Angs):

C	1.079979	-0.667280	0.011612
H	1.269949	-1.153288	0.970777
C	2.369795	-0.625926	-0.798265
C	3.470578	0.054118	-0.033410
H	2.695004	-1.636819	-1.044096
H	2.204471	-0.078519	-1.730558
H	3.288571	1.117013	0.224408
C	0.245375	0.627542	0.279203

C	-0.155196	-1.316450	-0.638108
C	0.415668	1.257495	1.651345
C	0.421989	1.671465	-0.820822
H	0.218335	1.259885	-1.811032
H	-0.244336	2.519108	-0.663196
H	1.441238	2.062709	-0.822492
H	-0.340035	2.027969	1.820571
H	1.396155	1.729097	1.747559
H	0.314438	0.508692	2.436250
H	-0.363666	-2.359096	-0.418158
H	-0.169080	-1.165004	-1.718843
C	-1.005340	-0.249152	0.101064
H	-1.574801	-1.134397	0.901648
C	-2.312528	0.174567	-0.195536
C	-2.812066	1.535727	-0.523334
H	-2.466382	1.841781	-1.509932
H	-2.413777	2.246712	0.201341
H	-3.898157	1.554518	-0.486311
O	4.485406	-0.480510	0.318924
O	-3.246217	-0.687354	0.052607
O	-2.697620	-1.846260	0.590915
Rotational constants (GHz): 1.5753900 0.4348500 0.3901800			
Vibrational harmonic frequencies (cm-1):			
i1572.9419	26.3648	73.7030	
76.8757	115.1041	160.4312	
176.7391	201.9791	221.5321	
228.6503	260.1112	285.5028	
296.1583	311.9699	322.5146	
355.6193	378.3289	412.9542	
483.5416	534.8341	566.9293	
595.2205	625.3117	702.9972	
730.2926	760.6945	846.4613	
933.2039	952.9122	963.2702	
971.1039	986.3967	1007.2431	
1016.1420	1035.1880	1058.1705	
1073.3407	1085.8509	1104.6640	
1142.0899	1154.6058	1186.3426	
1201.9085	1251.9466	1258.7363	
1284.4191	1291.5125	1319.7892	
1327.4850	1385.1316	1396.7570	
1402.7686	1416.3920	1435.1482	
1436.1129	1468.2049	1474.3369	
1483.9189	1486.1972	1494.3689	
1507.3120	1508.3895	1514.1595	
1567.5770	1860.7599	1886.1084	
2930.7357	3045.5344	3053.4496	
3059.9288	3069.7928	3073.3569	
3079.1663	3108.6456	3118.3982	
3124.5454	3132.7198	3133.1824	
3139.1601	3158.8993	3173.8592	
Zero-point correction (Hartree): 0.242584			
ApineneCI.A.b.14Hshift.b.mp			
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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.13511815			
Electronic state : 1-A			
Cartesian coordinates (Angs):			
C	0.999835	-0.936596	0.088515
H	1.091302	-1.440556	1.054048
C	2.319549	-1.031864	-0.664536
C	3.425753	-0.452599	0.171017
H	2.544100	-2.086922	-0.847455
H	2.281402	-0.511198	-1.620278
H	3.618594	-0.980535	1.126651
C	0.340350	0.457174	0.327840
C	-0.286829	-1.419787	-0.603593
C	0.568341	1.060133	1.703430
C	0.702770	1.460381	-0.765875
H	0.460918	1.081751	-1.760944
H	0.167050	2.398582	-0.622853
H	1.770353	1.684694	-0.739475
H	-0.053109	1.946492	1.849250
H	1.610994	1.365222	1.820174
H	0.323017	0.343785	2.487336
H	-0.640987	-2.424191	-0.391033
H	-0.245542	-1.271406	-1.683695
C	-1.010350	-0.244067	0.108350
H	-1.727634	-1.043724	0.882929
C	-2.235074	0.352504	-0.236086
C	-2.528097	1.769261	-0.576216
H	-2.106166	2.022283	-1.548056
H	-2.059116	2.417874	0.164441
H	-3.601429	1.940287	-0.578207
O	4.057827	0.528304	-0.113119
O	-3.287232	-0.373485	-0.027567
O	-2.921999	-1.596028	0.526947
Rotational constants (GHz): 1.5986300 0.4588900 0.4098100			
Vibrational harmonic frequencies (cm-1):			
i1568.7965	52.7793	68.1427	
82.7119	119.5629	150.0122	
159.5279	199.8614	223.8743	
244.2054	265.8584	281.0386	
297.7365	312.7868	337.9492	
364.3602	390.0539	412.9675	
494.5041	541.4445	560.7578	
594.1858	625.1308	702.6138	
729.8631	753.5740	860.9010	
924.1052	957.6534	967.4186	
969.2348	985.3125	1015.7027	
1017.8977	1046.4120	1056.3707	
1063.9467	1086.5684	1099.3416	
1142.2011	1157.1454	1187.9523	

1203.0847	1246.8444	1255.4057
1281.2986	1291.4213	1317.6698
1325.7597	1390.2631	1400.0028
1404.7355	1420.6078	1428.1389
1434.4472	1468.0376	1474.3428
1485.7339	1487.2171	1495.4464
1506.6694	1511.5467	1520.2543
1568.3154	1855.7057	1882.8477
2930.4235	3043.8210	3053.9707
3056.6510	3062.0123	3073.4923
3078.1629	3108.3313	3123.0560
3128.8576	3132.2409	3135.6585
3139.4910	3155.9125	3173.0875

Zero-point correction (Hartree): 0.242749

ApineneCI.A.b.14Hshift.b.mt

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.13618125

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 1.084375  | -0.851066 | 0.049121  |
| H | 1.293977  | -1.266302 | 1.035597  |
| C | 2.315132  | -0.972094 | -0.821774 |
| C | 3.548388  | -0.318316 | -0.269493 |
| H | 2.559328  | -2.026220 | -0.996021 |
| H | 2.149813  | -0.554010 | -1.820995 |
| H | 4.461867  | -0.430889 | -0.884516 |
| C | 0.367050  | 0.526261  | 0.237169  |
| C | -0.219777 | -1.448263 | -0.511783 |
| C | 0.585003  | 1.219189  | 1.571507  |
| C | 0.649107  | 1.482945  | -0.917592 |
| H | 0.395285  | 1.045666  | -1.885697 |
| H | 0.083790  | 2.407989  | -0.807189 |
| H | 1.707234  | 1.752844  | -0.927858 |
| H | -0.120881 | 2.045236  | 1.689517  |
| H | 1.598322  | 1.612640  | 1.641771  |
| H | 0.427136  | 0.523639  | 2.395538  |
| H | -0.519364 | -2.438489 | -0.180848 |
| H | -0.245374 | -1.413338 | -1.602760 |
| C | -0.961235 | -0.239234 | 0.115526  |
| H | -1.620087 | -0.988637 | 0.983387  |
| C | -2.218548 | 0.280562  | -0.231746 |
| C | -2.578902 | 1.653627  | -0.673543 |
| H | -2.187600 | 1.849352  | -1.670982 |
| H | -2.126023 | 2.376515  | 0.005930  |
| H | -3.658590 | 1.778459  | -0.664229 |
| O | 3.587745  | 0.296537  | 0.761734  |
| O | -3.235663 | -0.462560 | 0.072767  |
| O | -2.804881 | -1.618492 | 0.716123  |

Rotational constants (GHz): 1.5542600 0.4763900 0.4303500

Vibrational harmonic frequencies (cm-1):

|            |           |           |
|------------|-----------|-----------|
| i1564.4049 | 49.2254   | 74.9794   |
| 108.7497   | 119.9770  | 163.8182  |
| 177.0490   | 200.4318  | 209.0506  |
| 239.4979   | 259.6059  | 292.7357  |
| 293.8039   | 308.8991  | 322.4092  |
| 348.4280   | 383.3784  | 406.2239  |
| 497.4352   | 545.2569  | 585.1290  |
| 623.1041   | 679.8280  | 704.2180  |
| 722.0685   | 755.7210  | 785.5930  |
| 919.5700   | 936.2691  | 959.3158  |
| 966.2202   | 973.5575  | 1010.5733 |
| 1015.8646  | 1032.0798 | 1052.9756 |
| 1059.5068  | 1087.0356 | 1092.8295 |
| 1138.4801  | 1157.1521 | 1191.5339 |
| 1204.1242  | 1252.9708 | 1265.7508 |
| 1281.5967  | 1302.0010 | 1320.9466 |
| 1344.2198  | 1393.1289 | 1397.3570 |
| 1409.9264  | 1417.0339 | 1422.8219 |
| 1434.9427  | 1448.4101 | 1474.6387 |
| 1482.8881  | 1488.0330 | 1493.5169 |
| 1505.3931  | 1509.1749 | 1514.3022 |
| 1569.8781  | 1854.8422 | 1882.1217 |
| 2944.8173  | 3038.9863 | 3048.3943 |
| 3050.8552  | 3064.2830 | 3066.6564 |
| 3073.1666  | 3093.2164 | 3114.6031 |
| 3118.7717  | 3130.9907 | 3138.8831 |
| 3148.8276  | 3152.3925 | 3173.4398 |

Zero-point correction (Hartree): 0.242574

ApineneCI.A.b.14Hshift.b.pm

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.13351214

Electronic state : 1-A

Cartesian coordinates (Angs):

C	1.188561	0.119167	0.497555
H	1.322690	-0.099255	1.560014
C	2.525307	0.502215	-0.119996
C	3.521529	-0.598792	0.113977
H	2.442710	0.671521	-1.192760
H	2.901801	1.413149	0.357172
H	3.743416	-0.817078	1.177922
C	-0.036398	1.072758	0.349777
C	0.377277	-1.017658	-0.152082
C	-0.336656	1.938634	1.560649
C	0.049773	1.925049	-0.913539
H	0.181613	1.315193	-1.808903
H	-0.850217	2.526047	-1.041217
H	0.893509	2.614625	-0.848708
H	-1.285274	2.466179	1.438988
H	0.444581	2.689740	1.699345
H	-0.400708	1.333175	2.464274

H	0.452686	-2.015535	0.269783
H	0.547309	-1.070074	-1.228652
C	-0.893750	-0.193811	0.194118
H	-1.329723	-1.073634	1.081069
C	-2.170949	-0.294056	-0.384197
C	-2.970483	0.742274	-1.088600
H	-2.522146	0.979200	-2.052620
H	-2.974626	1.655870	-0.493037
H	-3.992057	0.397723	-1.226376
O	4.039527	-1.242481	-0.755960
O	-2.833880	-1.365707	-0.087015
O	-2.093251	-2.162003	0.780192
Rotational constants (GHz): 1.2224900 0.4790800 0.4048500			
Vibrational harmonic frequencies (cm-1):			
i1563.0036	38.2060		58.1939
82.4263	122.8827		129.6207
165.1130	205.7598		213.0001
235.6430	268.7273		278.8575
299.9095	310.3035		319.0433
347.2947	391.7246		423.9705
483.4445	552.4497		566.6517
605.4188	627.9586		703.1885
736.0890	769.6240		846.6983
933.6669	940.2839		957.6792
967.1803	979.7217		1011.3550
1019.6119	1049.4626		1058.3614
1065.8882	1082.6961		1097.8404
1146.3236	1152.8125		1202.4315
1202.8656	1240.9424		1259.8373
1282.3649	1290.2351		1316.0663
1324.0068	1389.6082		1398.8839
1404.0107	1418.2308		1426.3987
1436.1483	1467.1253		1474.6940
1484.9720	1486.5615		1495.2630
1506.0515	1509.3081		1516.4592
1567.8323	1860.5366		1887.9706
2931.9100	3044.2644		3045.3428
3054.6788	3061.4702		3073.8493
3078.6052	3107.6014		3119.5887
3131.2045	3132.5085		3135.4760
3139.8354	3156.9303		3174.0026
Zero-point correction (Hartree): 0.242582			
ApineneCI.A.b.14Hshift.b.pp			
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E(RM062X/Aug-CC-pVT2) (Hartree): -616.13299836			
Electronic state : 1-A			
Cartesian coordinates (Angs):			
C	1.184167	-0.024861	0.306035
H	1.393554	-0.358261	1.324552
C	2.485078	0.371957	-0.376494
C	3.435190	-0.792070	-0.402492
H	2.282056	0.657550	-1.413300
H	2.969847	1.207761	0.128590
H	3.046484	-1.706859	-0.893026
C	0.000297	0.989295	0.361779
C	0.260623	-1.051987	-0.379974
C	-0.152301	1.737925	1.674149
C	0.021030	1.962191	-0.814034
H	0.040799	1.443181	-1.774184
H	-0.854176	2.611151	-0.799044
H	0.901701	2.604636	-0.759007
H	-1.082386	2.310318	1.691916
H	0.672887	2.439640	1.814462
H	-0.165379	1.045987	2.515612
H	0.315728	-2.091428	-0.069974
H	0.330842	-0.997604	-1.468413
C	-0.931918	-0.216399	0.158496
H	-1.334563	-1.166326	0.986497
C	-2.257571	-0.201876	-0.309204
C	-3.062169	0.937328	-0.823278
H	-2.688890	1.260710	-1.794148
H	-2.967926	1.779283	-0.136527
H	-4.108025	0.652029	-0.901396
O	4.535741	-0.785668	0.075828
O	-2.944594	-1.272284	-0.068034
O	-2.172035	-2.187147	0.639393
Rotational constants (GHz): 1.3312800 0.4513400 0.3858200			
Vibrational harmonic frequencies (cm-1):			
i1570.2844	43.4264		52.5286
80.1765	121.6424		136.4611
167.1950	194.4501		213.8114
234.5312	258.1274		282.2843
299.4858	309.9128		312.5859
337.5793	381.9673		429.0796
476.5842	533.7429		570.3554
602.6212	628.0861		703.1114
736.6843	778.0856		850.5403
924.1982	939.3075		958.1889
967.4131	977.7977		1009.2668
1017.9792	1042.1958		1058.7679
1074.2183	1087.0483		1103.5962
1143.6311	1157.6839		1196.0749
1203.5827	1245.8518		1263.5024
1285.9946	1291.3218		1319.9166
1327.2755	1384.6964		1395.9117
1402.5388	1417.5924		1430.6783
1435.2371	1464.3388		1473.3762
1484.0165	1486.6170		1494.5051
1505.1373	1509.2832		1513.0742
1567.6907	1860.8776		1884.7517
2932.5700	3045.4473		3049.6252

3054.3764	3064.0685	3072.4849
3076.0535	3109.1995	3118.6147
3122.3837	3131.7327	3133.3226
3138.4340	3153.0479	3172.5931

Zero-point correction (Hartree): 0.242429

ApineneCI.A.b.14Hshift.b.pt

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.13438596

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 1.259821  | 0.109435  | 0.304903  |
| H | 1.498769  | -0.242781 | 1.309263  |
| C | 2.524633  | 0.584488  | -0.370527 |
| C | 3.608117  | -0.459825 | -0.395504 |
| H | 2.347126  | 0.886894  | -1.408170 |
| H | 2.943247  | 1.469880  | 0.122565  |
| H | 4.545440  | -0.160293 | -0.902379 |
| C | 0.019546  | 1.049863  | 0.382609  |
| C | 0.402930  | -0.957720 | -0.399183 |
| C | -0.181201 | 1.756871  | 1.711905  |
| C | -0.018876 | 2.051687  | -0.769344 |
| H | 0.036807  | 1.557115  | -1.741077 |
| H | -0.933163 | 2.644070  | -0.743928 |
| H | 0.818676  | 2.748191  | -0.696136 |
| H | -1.144442 | 2.271350  | 1.741005  |
| H | 0.599218  | 2.504646  | 1.872295  |
| H | -0.153051 | 1.044995  | 2.536150  |
| H | 0.533388  | -1.992088 | -0.099940 |
| H | 0.470986  | -0.884698 | -1.486620 |
| C | -0.841730 | -0.201959 | 0.147726  |
| H | -1.190755 | -1.189382 | 0.952224  |
| C | -2.164336 | -0.249950 | -0.323652 |
| C | -3.030472 | 0.853505  | -0.817177 |
| H | -2.673758 | 1.218036  | -1.779628 |
| H | -2.987199 | 1.684685  | -0.112521 |
| H | -4.058144 | 0.510811  | -0.905963 |
| O | 3.504695  | -1.553221 | 0.088025  |
| O | -2.794368 | -1.360487 | -0.107456 |
| O | -1.975794 | -2.247517 | 0.583471  |

Rotational constants (GHz): 1.2183900 0.5141100 0.4182600

Vibrational harmonic frequencies (cm-1):

|            |           |           |
|------------|-----------|-----------|
| i1566.4005 | 49.0373   | 69.4404   |
| 102.9060   | 121.0445  | 149.2461  |
| 175.1807   | 204.5010  | 213.8203  |
| 220.2108   | 267.5519  | 272.6712  |
| 292.1255   | 310.9429  | 312.8409  |
| 343.0637   | 388.3125  | 408.2945  |
| 498.1368   | 548.8593  | 586.7428  |
| 621.8685   | 685.6125  | 703.5038  |
| 720.4698   | 738.3224  | 837.1392  |
| 931.0630   | 939.7411  | 943.7689  |
| 957.2098   | 969.0384  | 986.8880  |
| 1010.6709  | 1021.8540 | 1051.9868 |
| 1064.6841  | 1083.8379 | 1094.9867 |
| 1141.6678  | 1161.2022 | 1195.4569 |
| 1204.8821  | 1247.5923 | 1265.7039 |
| 1283.2793  | 1303.5248 | 1317.4212 |
| 1336.5598  | 1392.2327 | 1398.8944 |
| 1412.2975  | 1416.6508 | 1425.2931 |
| 1436.3097  | 1450.0809 | 1475.8574 |
| 1484.4846  | 1486.0292 | 1495.3393 |
| 1505.5737  | 1508.7439 | 1515.2655 |
| 1568.6258  | 1858.2251 | 1885.6708 |
| 2947.2715  | 3034.6524 | 3042.8564 |
| 3052.1820  | 3065.2767 | 3067.3830 |
| 3072.9020  | 3092.7559 | 3105.2007 |
| 3116.0862  | 3131.9899 | 3133.1074 |
| 3138.6123  | 3171.0865 | 3172.2077 |

Zero-point correction (Hartree): 0.242429

ApineneCI.A.b.14Hshift.b.tm

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.13144109

Electronic state : 1-A

Cartesian coordinates (Angs):

C	1.005127	-0.769622	0.785989
H	0.811009	-1.197010	1.771045
C	2.508823	-0.830375	0.541988
C	2.982349	-0.532234	-0.854154
H	3.040366	-0.168735	1.227891
H	2.845889	-1.852922	0.748646
H	2.476877	-1.090235	-1.665543
C	0.237750	0.584456	0.713233
C	-0.009628	-1.388418	-0.199373
C	0.045255	1.295639	2.041230
C	0.838407	1.532788	-0.321185
H	0.905645	1.073201	-1.310080
H	0.239680	2.438654	-0.414538
H	1.844400	1.835517	-0.026035
H	-0.623581	2.152352	1.933168
H	1.000358	1.667598	2.418902
H	-0.384297	0.623117	2.783217
H	-0.355618	-2.400010	-0.008432
H	0.295619	-1.306681	-1.242030
C	-0.961387	-0.225678	0.196163
H	-1.820174	-1.023877	0.812107
C	-2.074385	0.256223	-0.513780
C	-2.335807	1.622063	-1.038048
H	-1.678184	1.838892	-1.879004
H	-2.121343	2.351356	-0.256142
H	-3.374997	1.714577	-1.342723

O	3.879684	0.221558	-1.116445
O	-3.103727	-0.529211	-0.536446
O	-2.841041	-1.682954	0.195039
Rotational constants (GHz):	1.3423100	0.4755200	0.4468300
Vibrational harmonic frequencies (cm-1):			
i1561.3629	51.6283		69.4718
89.8964	122.9534		142.9892
173.4381	199.2135		217.1457
251.8907	265.7781		276.1105
293.0131	309.0918		320.8375
362.0399	388.8739		441.0198
469.7831	549.2111		578.1992
608.5402	629.8427		703.2955
719.1316	739.1612		822.1751
915.9769	943.5527		955.4671
967.1749	975.8153		1012.9539
1018.9846	1049.4606		1057.5885
1065.6137	1085.7277		1102.5897
1142.3055	1156.0060		1198.3776
1207.4360	1240.8072		1264.5992
1294.2748	1315.4063		1324.3611
1329.3830	1390.3913		1398.5724
1404.9940	1419.7603		1434.5172
1437.0002	1453.2259		1473.7120
1485.1058	1485.7067		1495.3773
1508.4730	1509.0348		1517.5338
1568.5436	1854.8146		1884.8094
2946.5928	3034.7914		3044.2151
3051.5624	3072.6423		3077.1034
3092.7061	3106.6697		3107.9184
3119.2783	3130.8932		3131.8288
3138.5039	3157.6572		3172.4113
Zero-point correction (Hartree): 0.242682			

ApineneCI.A.b.14Hshift.b.tt

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.13120603

Electronic state : 1-A

Cartesian coordinates (Angs):

|                                           |           |           |           |
|-------------------------------------------|-----------|-----------|-----------|
| C                                         | -1.143037 | -0.320971 | -0.986570 |
| H                                         | -0.981561 | -0.411516 | -2.062709 |
| C                                         | -2.645108 | -0.347324 | -0.762153 |
| C                                         | -3.212697 | -0.599928 | 0.608418  |
| H                                         | -3.096276 | 0.588476  | -1.114164 |
| H                                         | -3.105943 | -1.116865 | -1.393617 |
| H                                         | -4.319524 | -0.548665 | 0.638759  |
| C                                         | -0.271977 | 0.881163  | -0.510318 |
| C                                         | -0.176660 | -1.299830 | -0.287480 |
| C                                         | -0.017682 | 1.943500  | -1.567535 |
| C                                         | -0.787592 | 1.523318  | 0.774854  |
| H                                         | -0.854336 | 0.805871  | 1.590681  |
| H                                         | -0.143541 | 2.348326  | 1.080117  |
| H                                         | -1.785080 | 1.941285  | 0.615494  |
| H                                         | 0.722596  | 2.668433  | -1.221922 |
| H                                         | -0.936494 | 2.491536  | -1.791303 |
| H                                         | 0.352742  | 1.496108  | -2.489493 |
| H                                         | 0.097888  | -2.205376 | -0.820729 |
| H                                         | -0.488891 | -1.543236 | 0.723903  |
| C                                         | 0.859410  | -0.137911 | -0.299700 |
| H                                         | 1.671126  | -0.748596 | -1.150649 |
| C                                         | 1.991626  | 0.008752  | 0.516771  |
| C                                         | 2.337635  | 1.105798  | 1.458135  |
| H                                         | 1.671961  | 1.090591  | 2.320063  |
| H                                         | 2.202739  | 2.063749  | 0.954696  |
| H                                         | 3.371281  | 1.011018  | 1.780637  |
| O                                         | -2.602601 | -0.861684 | 1.608365  |
| O                                         | 2.966679  | -0.809558 | 0.272721  |
| O                                         | 2.638147  | -1.637576 | -0.796874 |
| Rotational constants (GHz):               | 1.2249400 | 0.5248800 | 0.4986700 |
| Vibrational harmonic frequencies (cm-1):  |           |           |           |
| i1570.2566                                | 52.6027   |           | 90.7520   |
| 106.5045                                  | 128.7370  |           | 149.3664  |
| 174.6798                                  | 191.0591  |           | 204.6852  |
| 227.9443                                  | 257.7337  |           | 273.0794  |
| 292.5969                                  | 308.5240  |           | 320.6479  |
| 352.4225                                  | 395.8406  |           | 409.4898  |
| 495.7547                                  | 547.1530  |           | 580.6989  |
| 622.0610                                  | 690.7760  |           | 702.3371  |
| 736.8754                                  | 757.1473  |           | 781.7945  |
| 901.5197                                  | 938.7601  |           | 959.4739  |
| 968.4679                                  | 973.7328  |           | 986.2123  |
| 1014.6619                                 | 1026.3427 |           | 1054.9352 |
| 1066.5330                                 | 1078.3747 |           | 1099.9636 |
| 1133.5870                                 | 1166.1520 |           | 1200.9371 |
| 1214.3665                                 | 1245.9365 |           | 1275.3034 |
| 1293.0817                                 | 1314.9197 |           | 1328.2734 |
| 1368.6300                                 | 1393.8202 |           | 1401.2510 |
| 1407.7376                                 | 1419.6035 |           | 1430.5356 |
| 1433.2637                                 | 1447.2172 |           | 1473.9420 |
| 1484.7089                                 | 1486.8527 |           | 1495.7067 |
| 1509.4945                                 | 1511.6008 |           | 1516.0358 |
| 1570.1050                                 | 1861.8081 |           | 1885.7741 |
| 2929.6179                                 | 3026.7823 |           | 3041.6497 |
| 3050.6936                                 | 3052.4954 |           | 3069.4454 |
| 3073.3162                                 | 3104.3996 |           | 3114.1526 |
| 3116.0354                                 | 3129.8124 |           | 3139.5906 |
| 3153.1814                                 | 3172.2730 |           | 3175.3658 |
| Zero-point correction (Hartree): 0.242715 |           |           |           |

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Population analysis as 298K (%)
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)

Compound	Qtot	Erel	Erel2	n*Q*MB	%
ApineneCI.A.b.14Hshift.b.mt	6.396e+43	0.00	0.00	6.396e+43	51.2
ApineneCI.A.b.14Hshift.b.mp	8.764e+43	0.78	0.78	2.360e+43	18.9
ApineneCI.A.b.14Hshift.b.pt	8.818e+43	1.04	1.04	1.534e+43	12.3
ApineneCI.A.b.14Hshift.b.pm	1.702e+44	1.68	1.68	9.978e+42	7.99
ApineneCI.A.b.14Hshift.b.pp	1.799e+44	1.91	1.91	7.193e+42	5.76
ApineneCI.A.b.14Hshift.b.mm	1.749e+44	2.22	2.22	4.107e+42	3.29
ApineneCI.A.b.14Hshift.b.tm	8.387e+43	3.04	3.04	4.926e+41	0.394
ApineneCI.A.b.14Hshift.b.tt	5.837e+43	3.21	3.21	2.580e+41	0.207
Total				1.249e+44	100

ApineneCI.A.b.14Hshift.b.mm

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.13265066

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 1.079979  | -0.667280 | 0.011612  |
| H | 1.269949  | -1.153288 | 0.970777  |
| C | 2.369795  | -0.625926 | -0.798265 |
| C | 3.470578  | 0.054118  | -0.033410 |
| H | 2.695004  | -1.636819 | -1.044096 |
| H | 2.204471  | -0.078519 | -1.730558 |
| H | 3.288571  | 1.117013  | 0.224408  |
| C | 0.245375  | 0.627542  | 0.279203  |
| C | -0.155196 | -1.316450 | -0.638108 |
| C | 0.415668  | 1.257495  | 1.651345  |
| C | 0.421989  | 1.671465  | -0.820822 |
| H | 0.218335  | 1.259885  | -1.811032 |
| H | -0.244336 | 2.519108  | -0.663196 |
| H | 1.441238  | 2.062709  | -0.822492 |
| H | -0.340035 | 2.027969  | 1.820571  |
| H | 1.396155  | 1.729097  | 1.747559  |
| H | 0.314438  | 0.508692  | 2.436250  |
| H | -0.363666 | -2.359096 | -0.418158 |
| H | -0.169080 | -1.165004 | -1.718843 |
| C | -1.005340 | -0.249152 | 0.101064  |
| H | -1.574801 | -1.134397 | 0.901648  |
| C | -2.312528 | 0.174567  | -0.195536 |
| C | -2.812066 | 1.535727  | -0.523334 |
| H | -2.466382 | 1.841781  | -1.509932 |
| H | -2.413777 | 2.246712  | 0.201341  |
| H | -3.898157 | 1.554518  | -0.486311 |
| O | 4.485406  | -0.480510 | 0.318924  |
| O | -3.246217 | -0.687354 | 0.052607  |
| O | -2.697620 | -1.846260 | 0.590915  |

Rotational constants (GHz): 1.5753900 0.4348500 0.3901800

Vibrational harmonic frequencies (cm-1):

|            |           |           |
|------------|-----------|-----------|
| i1572.9419 | 26.3648   | 73.7030   |
| 76.8757    | 115.1041  | 160.4312  |
| 176.7391   | 201.9791  | 221.5321  |
| 228.6503   | 260.1112  | 285.5028  |
| 296.1583   | 311.9699  | 322.5146  |
| 355.6193   | 378.3289  | 412.9542  |
| 483.5416   | 534.8341  | 566.9293  |
| 595.2205   | 625.3117  | 702.9972  |
| 730.2926   | 760.6945  | 846.4613  |
| 933.2039   | 952.9122  | 963.2702  |
| 971.1039   | 986.3967  | 1007.2431 |
| 1016.1420  | 1035.1880 | 1058.1705 |
| 1073.3407  | 1085.8509 | 1104.6640 |
| 1142.0899  | 1154.6058 | 1186.3426 |
| 1201.9085  | 1251.9466 | 1258.7363 |
| 1284.4191  | 1291.5125 | 1319.7892 |
| 1327.4850  | 1385.1316 | 1396.7570 |
| 1402.7686  | 1416.3920 | 1435.1482 |
| 1436.1129  | 1468.2049 | 1474.3369 |
| 1483.9189  | 1486.1972 | 1494.3689 |
| 1507.3120  | 1508.3895 | 1514.1595 |
| 1567.5770  | 1860.7599 | 1886.1084 |
| 2930.7357  | 3045.5344 | 3053.4496 |
| 3059.9288  | 3069.7928 | 3073.3569 |
| 3079.1663  | 3108.6456 | 3118.3982 |
| 3124.5454  | 3132.7198 | 3133.1824 |
| 3139.1601  | 3158.8993 | 3173.8592 |

Zero-point correction (Hartree): 0.242584

ApineneCI.A.b.14Hshift.b.mp

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.13511815

Electronic state : 1-A

Cartesian coordinates (Angs):

C	0.999835	-0.936596	0.088515
H	1.091302	-1.440556	1.054048
C	2.319549	-1.031864	-0.664536
C	3.425753	-0.452599	0.171017
H	2.544100	-2.086922	-0.847455
H	2.281402	-0.511198	-1.620278
H	3.618594	-0.980535	1.126651
C	0.340350	0.457174	0.327840
C	-0.286829	-1.419787	-0.603593
C	0.568341	1.060133	1.703430
C	0.702770	1.460381	-0.765875
H	0.460918	1.081751	-1.760944
H	0.167050	2.398582	-0.622853
H	1.770353	1.684694	-0.739475
H	-0.053109	1.946492	1.849250
H	1.610994	1.365222	1.820174
H	0.323017	0.343785	2.487336
H	-0.640987	-2.424191	-0.391033
H	-0.245542	-1.271406	-1.683695
C	-1.010350	-0.244067	0.108350

H	-1.727634	-1.043724	0.882929
C	-2.235074	0.352504	-0.236086
C	-2.528097	1.769261	-0.576216
H	-2.106166	2.022283	-1.548056
H	-2.059116	2.417874	0.164441
H	-3.601429	1.940287	-0.578207
O	4.057827	0.528304	-0.113119
O	-3.287232	-0.373485	-0.027567
O	-2.921999	-1.596028	0.526947
Rotational constants (GHz): 1.5986300 0.4588900 0.4098100			
Vibrational harmonic frequencies (cm-1):			
i1568.7965	52.7793	68.1427	
82.7119	119.5629	150.0122	
159.5279	199.8614	223.8743	
244.2054	265.8584	281.0386	
297.7365	312.7868	337.9492	
364.3602	390.0539	412.9675	
494.5041	541.4445	560.7578	
594.1858	625.1308	702.6138	
729.8631	753.5740	860.9010	
924.1052	957.6534	967.4186	
969.2348	985.3125	1015.7027	
1017.8977	1046.4120	1056.3707	
1063.9467	1086.5684	1099.3416	
1142.2011	1157.1454	1187.9523	
1203.0847	1246.8444	1255.4057	
1281.2986	1291.4213	1317.6698	
1325.7597	1390.2631	1400.0028	
1404.7355	1420.6078	1428.1389	
1434.4472	1468.0376	1474.3428	
1485.7339	1487.2171	1495.4464	
1506.6694	1511.5467	1520.2543	
1568.3154	1855.7057	1882.8477	
2930.4235	3043.8210	3053.9707	
3056.6510	3062.0123	3073.4923	
3078.1629	3108.3313	3123.0560	
3128.8576	3132.2409	3135.6585	
3139.4910	3155.9125	3173.0875	
Zero-point correction (Hartree): 0.242749			
ApineneCI.A.b.14Hshift.b.mt			
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E(RM062X/Aug-CC-pVT2) (Hartree): -616.13618125			
Electronic state : 1-A			
Cartesian coordinates (Angs):			
C	1.084375	-0.851066	0.049121
H	1.293977	-1.266302	1.035597
C	2.315132	-0.972094	-0.821774
C	3.548388	-0.318316	-0.269493
H	2.559328	-2.026220	-0.996021
H	2.149813	-0.554010	-1.820995
H	4.461867	-0.430889	-0.884516
C	0.367050	0.526261	0.237169
C	-0.219777	-1.448263	-0.511783
C	0.585003	1.219189	1.571507
C	0.649107	1.482945	-0.917592
H	0.395285	1.045666	-1.885697
H	0.083790	2.407989	-0.807189
H	1.707234	1.752844	-0.927858
H	-0.120881	2.045236	1.689517
H	1.598322	1.612640	1.641771
H	0.427136	0.523639	2.395538
H	-0.519364	-2.438489	-0.180848
H	-0.245374	-1.413338	-1.602760
C	-0.961235	-0.239234	0.115526
H	-1.620087	-0.988637	0.983387
C	-2.218548	0.280562	-0.231746
C	-2.578902	1.653627	-0.673543
H	-2.187600	1.849352	-1.670982
H	-2.126023	2.376515	0.005930
H	-3.658590	1.778459	-0.664229
O	3.587745	0.296537	0.761734
O	-3.235663	-0.462560	0.072767
O	-2.804881	-1.618492	0.716123
Rotational constants (GHz): 1.5542600 0.4763900 0.4303500			
Vibrational harmonic frequencies (cm-1):			
i1564.4049	49.2254	74.9794	
108.7497	119.9770	163.8182	
177.0490	200.4318	209.0506	
239.4979	259.6059	292.7357	
293.8039	308.8991	322.4092	
348.4280	383.3784	406.2239	
497.4352	545.2569	585.1290	
623.1041	679.8280	704.2180	
722.0685	755.7210	785.5930	
919.5700	936.2691	959.3158	
966.2202	973.5575	1010.5733	
1015.8646	1032.0798	1052.9756	
1059.5068	1087.0356	1092.8295	
1138.4801	1157.1521	1191.5339	
1204.1242	1252.9708	1265.7508	
1281.5967	1302.0010	1320.9466	
1344.2198	1393.1289	1397.3570	
1409.9264	1417.0339	1422.8219	
1434.9427	1448.4101	1474.6387	
1482.8881	1488.0330	1493.5169	
1505.3931	1509.1749	1514.3022	
1569.8781	1854.8422	1882.1217	
2944.8173	3038.9863	3048.3943	
3050.8552	3064.2830	3066.6564	
3073.1666	3093.2164	3114.6031	
3118.7717	3130.9907	3138.8831	

3148.8276 3152.3925 3173.4398
Zero-point correction (Hartree): 0.242574

ApineneCI.A.b.14Hshift.b.pm

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.13351214

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 1.188561  | 0.119167  | 0.497555  |
| H | 1.322690  | -0.099255 | 1.560014  |
| C | 2.525307  | 0.502215  | -0.119996 |
| C | 3.521529  | -0.598792 | 0.113977  |
| H | 2.442710  | 0.671521  | -1.192760 |
| H | 2.901801  | 1.413149  | 0.357172  |
| H | 3.743416  | -0.817078 | 1.177922  |
| C | -0.036398 | 1.072758  | 0.349777  |
| C | 0.377277  | -1.017658 | -0.152082 |
| C | -0.336656 | 1.938634  | 1.560649  |
| C | 0.049773  | 1.925049  | -0.913539 |
| H | 0.181613  | 1.315193  | -1.808903 |
| H | -0.850217 | 2.526047  | -1.041217 |
| H | 0.893509  | 2.614625  | -0.848708 |
| H | -1.285274 | 2.466179  | 1.438988  |
| H | 0.444581  | 2.689740  | 1.699345  |
| H | -0.400708 | 1.333175  | 2.464274  |
| H | 0.452686  | -2.015535 | 0.269783  |
| H | 0.547309  | -1.070074 | -1.228652 |
| C | -0.893750 | -0.193811 | 0.194118  |
| H | -1.329723 | -1.073634 | 1.081069  |
| C | -2.170949 | -0.294056 | -0.384197 |
| C | -2.970483 | 0.742274  | -1.088600 |
| H | -2.522146 | 0.979200  | -2.052620 |
| H | -2.974626 | 1.655870  | -0.493037 |
| H | -3.992057 | 0.397723  | -1.226376 |
| O | 4.039527  | -1.242481 | -0.755960 |
| O | -2.833880 | -1.365707 | -0.087015 |
| O | -2.093251 | -2.162003 | 0.780192  |

Rotational constants (GHz): 1.2224900 0.4790800 0.4048500

Vibrational harmonic frequencies (cm-1):

|            |           |           |
|------------|-----------|-----------|
| i1563.0036 | 38.2060   | 58.1939   |
| 82.4263    | 122.8827  | 129.6207  |
| 165.1130   | 205.7598  | 213.0001  |
| 235.6430   | 268.7273  | 278.8575  |
| 299.9095   | 310.3035  | 319.0433  |
| 347.2947   | 391.7246  | 423.9705  |
| 483.4445   | 552.4497  | 566.6517  |
| 605.4188   | 627.9586  | 703.1885  |
| 736.0890   | 769.6240  | 846.6983  |
| 933.6669   | 940.2839  | 957.6792  |
| 967.1803   | 979.7217  | 1011.3550 |
| 1019.6119  | 1049.4626 | 1058.3614 |
| 1065.8882  | 1082.6961 | 1097.8404 |
| 1146.3236  | 1152.8125 | 1202.4315 |
| 1202.8656  | 1240.9424 | 1259.8373 |
| 1282.3649  | 1290.2351 | 1316.0663 |
| 1324.0068  | 1389.6082 | 1398.8839 |
| 1404.0107  | 1418.2308 | 1426.3987 |
| 1436.1483  | 1467.1253 | 1474.6940 |
| 1484.9720  | 1486.5615 | 1495.2630 |
| 1506.0515  | 1509.3081 | 1516.4592 |
| 1567.8323  | 1860.5366 | 1887.9706 |
| 2931.9100  | 3044.2644 | 3045.3428 |
| 3054.6788  | 3061.4702 | 3073.8493 |
| 3078.6052  | 3107.6014 | 3119.5887 |
| 3131.2045  | 3132.5085 | 3135.4760 |
| 3139.8354  | 3156.9303 | 3174.0026 |

Zero-point correction (Hartree): 0.242582

ApineneCI.A.b.14Hshift.b.pp

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.13299836

Electronic state : 1-A

Cartesian coordinates (Angs):

C	1.184167	-0.024861	0.306035
H	1.393554	-0.358261	1.324552
C	2.485078	0.371957	-0.376494
C	3.435190	-0.792070	-0.402492
H	2.282056	0.657550	-1.413300
H	2.969847	1.207761	0.128590
H	3.046484	-1.706859	-0.893026
C	0.000297	0.989295	0.361779
C	0.260623	-1.051987	-0.379974
C	-0.152301	1.737925	1.674149
C	0.021030	1.962191	-0.814034
H	0.040799	1.443181	-1.774184
H	-0.854176	2.611151	-0.799044
H	0.901701	2.604636	-0.759007
H	-1.082386	2.310318	1.691916
H	0.672887	2.439640	1.814462
H	-0.165379	1.045987	2.515612
H	0.315728	-2.091428	-0.069974
H	0.330842	-0.997604	-1.468413
C	-0.931918	-0.216399	0.158496
H	-1.334563	-1.166326	0.986497
C	-2.257571	-0.201876	-0.309204
C	-3.062169	0.937328	-0.823278
H	-2.688890	1.260710	-1.794148
H	-2.967926	1.779283	-0.136527
H	-4.108025	0.652029	-0.901396
O	4.535741	-0.785668	0.075828
O	-2.944594	-1.272284	-0.068034
O	-2.172035	-2.187147	0.639393

Rotational constants (GHz): 1.3312800 0.4513400 0.3858200
 Vibrational harmonic frequencies (cm-1):
 i1570.2844 43.4264 52.5286
 80.1765 121.6424 136.4611
 167.1950 194.4501 213.8114
 234.5312 258.1274 282.2843
 299.4858 309.9128 312.5859
 337.5793 381.9673 429.0796
 476.5842 533.7429 570.3554
 602.6212 628.0861 703.1114
 736.6843 778.0856 850.5403
 924.1982 939.3075 958.1889
 967.4131 977.7977 1009.2668
 1017.9792 1042.1958 1058.7679
 1074.2183 1087.0483 1103.5962
 1143.6311 1157.6839 1196.0749
 1203.5827 1245.8518 1263.5024
 1285.9946 1291.3218 1319.9166
 1327.2755 1384.6964 1395.9117
 1402.5388 1417.5924 1430.6783
 1435.2371 1464.3388 1473.3762
 1484.0165 1486.6170 1494.5051
 1505.1373 1509.2832 1513.0742
 1567.6907 1860.8776 1884.7517
 2932.5700 3045.4473 3049.6252
 3054.3764 3064.0685 3072.4849
 3076.0535 3109.1995 3118.6147
 3122.3837 3131.7327 3133.3226
 3138.4340 3153.0479 3172.5931
 Zero-point correction (Hartree): 0.242429

ApineneCI.A.b.14Hshift.b.pt

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.13438596

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 1.259821  | 0.109435  | 0.304903  |
| H | 1.498769  | -0.242781 | 1.309263  |
| C | 2.524633  | 0.584488  | -0.370527 |
| C | 3.608117  | -0.459825 | -0.395504 |
| H | 2.347126  | 0.886894  | -1.408170 |
| H | 2.943247  | 1.469880  | 0.122565  |
| H | 4.545440  | -0.160293 | -0.902379 |
| C | 0.019546  | 1.049863  | 0.382609  |
| C | 0.402930  | -0.957720 | -0.399183 |
| C | -0.181201 | 1.756871  | 1.711905  |
| C | -0.018876 | 2.051687  | -0.769344 |
| H | 0.036807  | 1.557115  | -1.741077 |
| H | -0.933163 | 2.644070  | -0.743928 |
| H | 0.818676  | 2.748191  | -0.696136 |
| H | -1.144442 | 2.271350  | 1.741005  |
| H | 0.599218  | 2.504646  | 1.872295  |
| H | -0.153051 | 1.044995  | 2.536150  |
| H | 0.533388  | -1.992088 | -0.099940 |
| H | 0.470986  | -0.884698 | -1.486620 |
| C | -0.841730 | -0.201959 | 0.147726  |
| H | -1.190755 | -1.189382 | 0.952224  |
| C | -2.164336 | -0.249950 | -0.323652 |
| C | -3.030472 | 0.853505  | -0.817177 |
| H | -2.673758 | 1.218036  | -1.779628 |
| H | -2.987199 | 1.684685  | -0.112521 |
| H | -4.058144 | 0.510811  | -0.905963 |
| O | 3.504695  | -1.553221 | 0.088025  |
| O | -2.794368 | -1.360487 | -0.107456 |
| O | -1.975794 | -2.247517 | 0.583471  |

Rotational constants (GHz): 1.2183900 0.5141100 0.4182600  
 Vibrational harmonic frequencies (cm-1):  
 i1566.4005 49.0373 69.4404  
 102.9060 121.0445 149.2461  
 175.1807 204.5010 213.8203  
 220.2108 267.5519 272.6712  
 292.1255 310.9429 312.8409  
 343.0637 388.3125 408.2945  
 498.1368 548.8593 586.7428  
 621.8685 685.6125 703.5038  
 720.4698 738.3224 837.1392  
 931.0630 939.7411 943.7689  
 957.2098 969.0384 986.8880  
 1010.6709 1021.8540 1051.9868  
 1064.6841 1083.8379 1094.9867  
 1141.6678 1161.2022 1195.4569  
 1204.8821 1247.5923 1265.7039  
 1283.2793 1303.5248 1317.4212  
 1336.5598 1392.2327 1398.8944  
 1412.2975 1416.6508 1425.2931  
 1436.3097 1450.0809 1475.8574  
 1484.4846 1486.0292 1495.3393  
 1505.5737 1508.7439 1515.2655  
 1568.6258 1858.2251 1885.6708  
 2947.2715 3034.6524 3042.8564  
 3052.1820 3065.2767 3067.3830  
 3072.9020 3092.7559 3105.2007  
 3116.0862 3131.9899 3133.1074  
 3138.6123 3171.0865 3172.2077  
 Zero-point correction (Hartree): 0.242429

ApineneCI.A.b.14Hshift.b.tm

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.13144109

Electronic state : 1-A

Cartesian coordinates (Angs):

C	1.005127	-0.769622	0.785989

H	0.811009	-1.197010	1.771045
C	2.508823	-0.830375	0.541988
C	2.982349	-0.532234	-0.854154
H	3.040366	-0.168735	1.227891
H	2.845889	-1.852922	0.748646
H	2.476877	-1.090235	-1.665543
C	0.237750	0.584456	0.713233
C	-0.009628	-1.388418	-0.199373
C	0.045255	1.295639	2.041230
C	0.838407	1.532788	-0.321185
H	0.905645	1.073201	-1.310080
H	0.239680	2.438654	-0.414538
H	1.844400	1.835517	-0.026035
H	-0.623581	2.152352	1.933168
H	1.000358	1.667598	2.418902
H	-0.384297	0.623117	2.783217
H	-0.355618	-2.400010	-0.008432
H	0.295619	-1.306681	-1.242030
C	-0.961387	-0.225678	0.196163
H	-1.820174	-1.023877	0.812107
C	-2.074385	0.256223	-0.513780
C	-2.335807	1.622063	-1.038048
H	-1.678184	1.838892	-1.879004
H	-2.121343	2.351356	-0.256142
H	-3.374997	1.714577	-1.342723
O	3.879684	0.221558	-1.116445
O	-3.103727	-0.529211	-0.536446
O	-2.841041	-1.682954	0.195039
Rotational constants (GHz):			
Vibrational harmonic frequencies (cm-1):			
i1561.3629	51.6283	69.4718	
89.8964	122.9534	142.9892	
173.4381	199.2135	217.1457	
251.8907	265.7781	276.1105	
293.0131	309.0918	320.8375	
362.0399	388.8739	441.0198	
469.7831	549.2111	578.1992	
608.5402	629.8427	703.2955	
719.1316	739.1612	822.1751	
915.9769	943.5527	955.4671	
967.1749	975.8153	1012.9539	
1018.9846	1049.4606	1057.5885	
1065.6137	1085.7277	1102.5897	
1142.3055	1156.0060	1198.3776	
1207.4360	1240.8072	1264.5992	
1294.2748	1315.4063	1324.3611	
1329.3830	1390.3913	1398.5724	
1404.9940	1419.7603	1434.5172	
1437.0002	1453.2259	1473.7120	
1485.1058	1485.7067	1495.3773	
1508.4730	1509.0348	1517.5338	
1568.5436	1854.8146	1884.8094	
2946.5928	3034.7914	3044.2151	
3051.5624	3072.6423	3077.1034	
3092.7061	3106.6697	3107.9184	
3119.2783	3130.8932	3131.8288	
3138.5039	3157.6572	3172.4113	
Zero-point correction (Hartree): 0.242682			
ApineneCI.A.b.14Hshift.b.tt			
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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.13120603			
Electronic state : 1-A			
Cartesian coordinates (Angs):			
C	-1.143037	-0.320971	-0.986570
H	-0.981561	-0.411516	-2.062709
C	-2.645108	-0.347324	-0.762153
C	-3.212697	-0.599928	0.608418
H	-3.096276	0.588476	-1.114164
H	-3.105943	-1.116865	-1.393617
H	-4.319524	-0.548665	0.638759
C	-0.271977	0.881163	-0.510318
C	-0.176660	-1.299830	-0.287480
C	-0.017682	1.943500	-1.567535
C	-0.787592	1.523318	0.774854
H	-0.854336	0.805871	1.590681
H	-0.143541	2.348326	1.080117
H	-1.785080	1.941285	0.615494
H	0.722596	2.668433	-1.221922
H	-0.936494	2.491536	-1.791303
H	0.352742	1.496108	-2.489493
H	0.097888	-2.205376	-0.820729
H	-0.488891	-1.543236	0.723903
C	0.859410	-0.137911	-0.299700
H	1.671126	-0.748596	-1.150649
C	1.991626	0.008752	0.516771
C	2.337635	1.105798	1.458135
H	1.671961	1.090591	2.320063
H	2.202739	2.063749	0.954696
H	3.371281	1.011018	1.780637
O	-2.602601	-0.861684	1.608365
O	2.966679	-0.809558	0.272721
O	2.638147	-1.637576	-0.796874
Rotational constants (GHz):			
Vibrational harmonic frequencies (cm-1):			
i1570.2566	52.6027	90.7520	
106.5045	128.7370	149.3664	
174.6798	191.0591	204.6852	
227.9443	257.7337	273.0794	
292.5969	308.5240	320.6479	
352.4225	395.8406	409.4898	
495.7547	547.1530	580.6989	

622.0610	690.7760	702.3371
736.8754	757.1473	781.7945
901.5197	938.7601	959.4739
968.4679	973.7328	986.2123
1014.6619	1026.3427	1054.9352
1066.5330	1078.3747	1099.9636
1133.5870	1166.1520	1200.9371
1214.3665	1245.9365	1275.3034
1293.0817	1314.9197	1328.2734
1368.6300	1393.8202	1401.2510
1407.7376	1419.6035	1430.5356
1433.2637	1447.2172	1473.9420
1484.7089	1486.8527	1495.7067
1509.4945	1511.6008	1516.0358
1570.1050	1861.8081	1885.7741
2929.6179	3026.7823	3041.6497
3050.6936	3052.4954	3069.4454
3073.3162	3104.3996	3114.1526
3116.0354	3129.8124	3139.5906
3153.1814	3172.2730	3175.3658

Zero-point correction (Hartree): 0.242715

Population analysis as 298K (%)

Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)

Compound	Qtot	Erel	Erel2	n*Q*MB	%
ApineneCI.A.b.ringclose.cmtm	1.568e+44	0.00	0.00	1.568e+44	30
ApineneCI.A.b.ringclose.mptm	1.061e+44	0.23	0.23	7.251e+43	13.9
ApineneCI.A.b.ringclose.cptm	1.700e+44	0.57	0.57	6.517e+43	12.5
ApineneCI.A.b.ringclose.mmtm	8.460e+43	0.17	0.17	6.322e+43	12.1
ApineneCI.A.b.ringclose.cmtm	1.396e+44	0.76	0.76	3.886e+43	7.43
ApineneCI.A.b.ringclose.cmpm	4.008e+44	1.67	1.67	2.372e+43	4.54
ApineneCI.A.b.ringclose.mpm	2.196e+44	1.55	1.55	1.602e+43	3.06
ApineneCI.A.b.ringclose.mptm	2.239e+44	1.81	1.81	1.051e+43	2.01
ApineneCI.A.b.ringclose.mmtm	2.138e+44	1.82	1.82	9.929e+42	1.9
ApineneCI.A.b.ringclose.cpm	3.889e+44	2.25	2.25	8.731e+42	1.67
ApineneCI.A.b.ringclose.mmpm	9.930e+43	1.46	1.46	8.482e+42	1.62
ApineneCI.A.b.ringclose.cmm	4.755e+44	2.41	2.41	8.138e+42	1.56
ApineneCI.A.b.ringclose.cppm	3.920e+44	2.30	2.30	8.103e+42	1.55
ApineneCI.A.b.ringclose.cptm	1.871e+44	1.86	1.86	8.088e+42	1.55
ApineneCI.A.b.ringclose.mppm	2.074e+44	2.15	2.15	5.468e+42	1.05
ApineneCI.A.b.ringclose.mmpm	1.808e+44	2.12	2.12	5.025e+42	0.961
ApineneCI.A.b.ringclose.cmpm	1.743e+44	2.30	2.30	3.568e+42	0.682
ApineneCI.A.b.ringclose.mmpm	2.936e+44	2.75	2.75	2.806e+42	0.536
ApineneCI.A.b.ringclose.mpm	4.067e+44	3.08	3.08	2.254e+42	0.431
ApineneCI.A.b.ringclose.cppm	4.025e+44	3.35	3.35	1.415e+42	0.27
ApineneCI.A.b.ringclose.cpm	4.199e+44	3.45	3.45	1.236e+42	0.236
ApineneCI.A.b.ringclose.mtm	9.012e+43	2.83	2.83	7.545e+41	0.144
ApineneCI.A.b.ringclose.mmm	4.301e+44	3.84	3.84	6.576e+41	0.126
ApineneCI.A.b.ringclose.mppm	3.855e+44	3.78	3.78	6.515e+41	0.125
ApineneCI.A.b.ringclose.ctm	1.827e+44	3.79	3.79	3.012e+41	0.0576
ApineneCI.A.b.ringclose.mtm	8.174e+43	3.52	3.52	2.128e+41	0.0407
ApineneCI.A.b.ringclose.mtm	1.723e+44	4.26	4.26	1.286e+41	0.0246
ApineneCI.A.b.ringclose.ctpm	9.501e+43	3.98	3.98	1.137e+41	0.0217
ApineneCI.A.b.ringclose.ctm	9.474e+43	3.99	3.99	1.132e+41	0.0216
ApineneCI.A.b.ringclose.ctpm	1.581e+44	4.60	4.60	6.711e+40	0.0128
ApineneCI.A.b.ringclose.mtm	2.593e+44	5.02	5.02	5.356e+40	0.0102
ApineneCI.A.b.ringclose.ctpm	1.409e+44	5.52	5.52	1.260e+40	0.00241
Total				5.231e+44	100

ApineneCI.A.b.ringclose.cmm

E(RM062X/Aug-CC-pVTZ) (Hartree): -616.13026345

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-1.241083	-0.370048	-0.677613
H	-1.659782	0.151987	-1.541320
C	-2.374364	-1.047930	0.085328
C	-3.400915	-0.024682	0.487864
H	-2.855955	-1.785669	-0.556595
H	-1.978925	-1.544877	0.973168
H	-3.158951	0.581120	1.383338
C	-0.255463	0.589075	0.051815
C	-0.040281	-1.219228	-1.124920
C	-0.518942	2.074456	-0.090006
C	-0.018667	0.211074	1.505738
H	0.220766	-0.843955	1.631633
H	0.820532	0.769730	1.916449
H	-0.912347	0.438144	2.090362
H	0.325055	2.654988	0.287202
H	-1.400420	2.358782	0.488849
H	-0.695255	2.350559	-1.130057
H	-0.063288	-1.648929	-2.122842
H	0.201614	-1.991446	-0.397253
C	0.859074	0.017768	-0.925501
H	0.881741	0.647464	-1.814130
C	2.224270	-0.143885	-0.386770
C	3.290771	0.792971	-0.832927
H	3.280703	0.819620	-1.926223
H	3.059066	1.801109	-0.484717
H	4.254601	0.493535	-0.440380
O	-4.412912	0.185171	-0.122870
O	2.453750	-1.167455	0.340256
O	3.025967	-0.333916	1.418174

Rotational constants (GHz): 1.7227800 0.4261800 0.4183700

Vibrational harmonic frequencies (cm-1):

1508.0513	20.9913	33.7658
68.7129	80.4364	148.6339
178.1190	226.4065	235.5625
248.3903	263.6885	287.8882
308.9036	321.8523	356.3062

378.0938	395.3706	407.0446
479.6956	531.0275	566.9082
570.1970	609.2685	724.8591
779.8055	838.3684	879.2341
888.1368	941.9289	958.6565
960.0684	966.6664	986.2691
1007.0580	1010.0393	1028.2772
1068.1419	1109.8811	1123.7866
1154.6323	1170.5825	1186.6280
1205.7424	1220.8380	1259.9479
1264.4280	1285.9568	1302.9764
1333.0727	1379.1913	1396.8839
1409.4336	1424.7066	1430.5470
1436.2348	1446.2507	1461.7681
1473.0218	1482.6014	1488.7432
1495.9776	1504.6584	1506.3567
1580.3656	1858.1249	2937.0451
3047.6483	3051.4113	3062.7487
3065.8449	3075.1183	3103.2305
3105.9960	3112.1522	3115.4857
3127.0626	3131.8182	3138.4305
3153.0987	3163.5891	3209.9806

Zero-point correction (Hartree): 0.245470

ApineneCI.A.b.ringclose.cmpmp

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Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -1.226366 | -0.512279 | -0.569989 |
| H | -1.641453 | -0.154124 | -1.515552 |
| C | -2.348046 | -1.158824 | 0.240779  |
| C | -3.446782 | -0.152020 | 0.443819  |
| H | -2.749824 | -2.001830 | -0.322042 |
| H | -1.962075 | -1.505249 | 1.200955  |
| H | -3.373465 | 0.474226  | 1.355962  |
| C | -0.361286 | 0.627328  | 0.040408  |
| C | 0.055585  | -1.316256 | -0.847010 |
| C | -0.762921 | 2.042532  | -0.321780 |
| C | -0.149187 | 0.485091  | 1.541439  |
| H | 0.153290  | -0.522513 | 1.827283  |
| H | 0.626450  | 1.172993  | 1.885417  |
| H | -1.067727 | 0.734013  | 2.076282  |
| H | -0.025629 | 2.769661  | 0.025067  |
| H | -1.716201 | 2.292691  | 0.151351  |
| H | -0.882665 | 2.157228  | -1.399680 |
| H | 0.108210  | -1.886056 | -1.770969 |
| H | 0.324753  | -1.957601 | -0.009046 |
| C | 0.840769  | 0.000062  | -0.789490 |
| H | 0.887968  | 0.504842  | -1.755193 |
| C | 2.163264  | 0.062871  | -0.129604 |
| C | 2.969528  | 1.301529  | -0.291712 |
| H | 2.296626  | 2.158212  | -0.177711 |
| H | 3.783564  | 1.321836  | 0.424159  |
| H | 3.381199  | 1.345141  | -1.300682 |
| O | -4.335204 | 0.036122  | -0.341336 |
| O | 2.465914  | -0.862375 | 0.687661  |
| O | 3.800494  | -1.071707 | 0.079079  |

Rotational constants (GHz): 1.7966915 0.4249893 0.3920567

ApineneCI.A.b.ringclose.cmpmp

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E(RM062X/Aug-CC-pVT2) (Hartree): -616.13136146

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-1.190495	-0.644294	-0.794045
H	-1.523692	-0.396043	-1.806098
C	-2.379028	-1.112742	0.033149
C	-3.453932	-0.062175	0.015058
H	-2.782605	-2.025591	-0.414875
H	-2.094473	-1.320945	1.063244
H	-3.888745	0.147496	-0.983621
C	-0.307394	0.523422	-0.267297
C	0.064943	-1.527689	-0.875356
C	-0.593103	1.896603	-0.839954
C	-0.228598	0.570384	1.251172
H	0.050428	-0.389479	1.684640
H	0.528582	1.284641	1.570529
H	-1.196906	0.871153	1.654531
H	0.184667	2.606986	-0.553797
H	-1.541181	2.272297	-0.448517
H	-0.656494	1.871167	-1.928756
H	0.154675	-2.211629	-1.715420
H	0.241087	-2.064236	0.054737
C	0.915759	-0.244732	-0.931436
H	1.029491	0.125866	-1.949965
C	2.213473	-0.184120	-0.228779
C	3.256839	0.751856	-0.730771
H	3.378147	0.582429	-1.804192
H	2.914127	1.780262	-0.603106
H	4.184908	0.617804	-0.188939
O	-3.822376	0.558286	0.974045
O	2.424829	-1.034629	0.698779
O	2.800947	0.032438	1.649571

Rotational constants (GHz): 1.5674200 0.4539000 0.4500500

Vibrational harmonic frequencies (cm-1):

i517.1421	16.5640	50.9829
66.2049	83.2011	144.9885
170.3529	226.2390	234.7872
256.3530	266.2820	281.5151
324.7917	331.1024	363.0075
382.9959	397.6821	412.5424
472.0378	535.2070	561.1913
572.2965	610.7879	718.9500


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771.8611      839.0119      862.8534
889.9850      922.3827      956.6151
967.9172      973.5981      989.6585
1008.0951     1016.6900     1038.7480
1059.6319     1110.3491     1123.1797
1160.4714     1169.1169     1188.1064
1199.7245     1219.0885     1256.7224
1260.4855     1279.8914     1296.3557
1329.5929     1383.7917     1401.0461
1408.1640     1429.2488     1432.7730
1434.4284     1446.2406     1462.4596
1468.4107     1482.5713     1489.8487
1496.0364     1504.9441     1512.5638
1579.2682     1859.2128     2927.0410
3045.4003     3049.2024     3051.7299
3057.1574     3066.6501     3101.4214
3104.3623     3111.9599     3116.0718
3122.2603     3139.6331     3141.7977
3149.6926     3162.8791     3208.5141
Zero-point correction (Hartree): 0.245397

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ApineneCI.A.b.ringclose.cmp

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.13024563
Electronic state : 1-A
Cartesian coordinates (Angs):
C      -1.173763      -0.612813      -0.808814
H      -1.511716      -0.321744      -1.807505
C      -2.332038      -1.235787      -0.039947
C      -3.485526      -0.273136      -0.009998
H      -2.647313      -2.146858      -0.555637
H      -2.044899      -1.487931      0.979719
H      -3.968920      -0.084476      -0.989758
C      -0.408222      0.591526      -0.188281
C      0.152358      -1.384096      -0.925090
C      -0.807476      1.963658      -0.692534
C      -0.372039      0.558082      1.333774
H      -0.051180      -0.409900      1.719158
H      0.321376      1.311144      1.713627
H      -1.362522      0.777252      1.734143
H      -0.129888      2.736582      -0.325479
H      -1.809155      2.211870      -0.334320
H      -0.813170      2.000073      -1.782515
H      0.314153      -1.982633      -1.817193
H      0.352212      -1.988823      -0.042441
C      0.895104      -0.044441      -0.838939
H      1.055878      0.416864      -1.813816
C      2.124863      0.078343      -0.026227
C      2.895683      1.347371      -0.112736
H      2.181717      2.176902      -0.111426
H      3.604481      1.415536      0.704349
H      3.439352      1.385820      -1.056726
O      -3.862304      0.310556      0.969374
O      2.361898      -0.822469      0.838414
O      3.767398      -0.980827      0.397033
Rotational constants (GHz): 1.6727700 0.4453900 0.4148000
Vibrational harmonic frequencies (cm-1):
i498.5723      41.9910      54.8407
65.4919      83.2766      130.9376
171.4864      232.3228      245.5192
251.1985      265.6660      276.4650
316.8508      332.2384      361.4412
374.5182      388.3331      425.0156
464.7125      533.6405      558.1069
575.1425      603.3316      712.4363
760.9396      841.6581      871.5785
895.2682      921.1823      960.5644
965.4380      976.0418      979.9632
1001.3292     1011.2918     1038.1074
1059.5990     1107.6105     1122.3410
1149.9625     1162.1595     1188.7834
1193.8646     1226.0819     1257.6574
1261.5630     1277.3454     1296.3685
1327.2493     1380.3023     1399.6470
1409.2317     1426.4605     1427.8993
1429.0642     1441.5963     1466.4432
1472.9928     1486.5715     1493.8299
1498.4511     1509.4775     1514.6996
1597.6538     1857.0168     2930.2176
3047.4751     3050.0195     3052.7260
3056.0009     3062.6288     3097.2106
3107.4366     3115.5231     3120.7961
3123.3916     3126.3544     3138.1614
3139.9077     3166.0549     3202.4308
Zero-point correction (Hartree): 0.245283

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ApineneCI.A.b.ringclose.cmtm

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E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -615.20780131
E(CCSD/Aug-CC-pVTZ) (Hartree): -615.08749046
T1 diagnostic: 0.023409
E(MP2/Aug-CC-pVTZ) (Hartree): -615.01290597
E(MP3/Aug-CC-pVTZ) (Hartree): -615.06945931
E(RHF/Aug-CC-pVTZ) (Hartree): -612.58448914
E(RM062X/Aug-CC-pVTZ) (Hartree): -616.13406529
Electronic state : 1-A
Cartesian coordinates (Angs):
C      -1.257481      -0.425059      -0.796159
H      -1.708435      0.111206      -1.632792
C      -2.322831      -1.211447      -0.066170
C      -3.480583      -0.387321      0.417829
H      -2.732386      -1.997536      -0.710820

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H	-1.911106	-1.739935	0.799763
H	-4.265922	-0.942268	0.964954
C	-0.340048	0.562187	-0.011763
C	-0.005891	-1.191166	-1.256095
C	-0.639936	2.040961	-0.145739
C	-0.156345	0.170066	1.444915
H	0.157409	-0.866610	1.566130
H	0.612875	0.781172	1.914189
H	-1.097705	0.325077	1.976685
H	0.196747	2.633431	0.230999
H	-1.530519	2.297249	0.426506
H	-0.818780	2.315036	-1.186207
H	0.020714	-1.560462	-2.278287
H	0.246154	-1.999498	-0.571533
C	0.840917	0.056206	-0.953604
H	0.896273	0.734759	-1.804205
C	2.174643	-0.085967	-0.339172
C	3.182994	0.987663	-0.556847
H	3.248468	1.179691	-1.631244
H	2.838959	1.909920	-0.085275
H	4.139510	0.707413	-0.133319
O	-3.587157	0.796734	0.243637
O	2.445491	-1.188570	0.245899
O	2.858554	-0.481338	1.476875
Rotational constants (GHz): 1.6045600 0.4749200 0.4554700			
Vibrational harmonic frequencies (cm-1):			
i514.2831	26.8032		49.1770
77.6190	121.3307		158.8613
171.6704	228.3400		231.4964
251.8969	259.4944		291.7762
320.2057	328.2748		356.2700
368.1778	390.8116		407.6693
476.4428	555.4129		557.4055
605.0551	676.2411		728.8785
750.0685	804.0738		841.1743
885.5833	913.8601		946.3644
959.7712	967.3606		979.8600
998.9296	1011.4149		1029.3606
1058.7404	1103.7043		1118.0738
1159.7289	1167.6028		1186.7216
1210.7918	1222.0679		1260.3796
1267.4491	1288.5159		1311.5139
1348.1863	1386.7816		1407.0613
1410.1974	1423.6162		1430.0777
1434.1965	1445.9021		1452.5706
1462.4209	1480.7635		1489.9439
1493.4686	1501.5015		1509.4081
1575.8994	1853.4907		2955.5757
3042.3496	3052.1300		3052.8546
3057.5063	3070.4247		3086.4616
3099.1972	3103.2638		3112.4447
3119.1584	3131.9780		3146.6532
3147.3973	3157.3226		3209.7978
Zero-point correction (Hartree): 0.245433			
ApineneCI.A.b.ringclose.cmp			
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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.13258182			
Electronic state : 1-A			
Cartesian coordinates (Angs):			
C	-1.230649	-0.539964	-0.734653
H	-1.683314	-0.148301	-1.646944
C	-2.265854	-1.318533	0.047128
C	-3.501377	-0.542733	0.399938
H	-2.585664	-2.202342	-0.516102
H	-1.853274	-1.715500	0.980905
H	-4.277796	-1.106439	0.950654
C	-0.432959	0.613026	-0.051944
C	0.093814	-1.258531	-1.049285
C	-0.832282	2.028284	-0.417378
C	-0.318292	0.450194	1.455944
H	0.020388	-0.544763	1.745523
H	0.388948	1.172160	1.868891
H	-1.289440	0.639117	1.916919
H	-0.088144	2.745342	-0.064163
H	-1.791118	2.274857	0.036629
H	-0.931903	2.140827	-1.497449
H	0.198020	-1.726034	-2.024666
H	0.362741	-1.976715	-0.275881
C	0.841499	0.061840	-0.834594
H	0.959544	0.643118	-1.748673
C	2.101173	0.087003	-0.063851
C	2.914024	1.331924	-0.087101
H	2.229660	2.181469	0.002593
H	3.654845	1.316160	0.703751
H	3.421812	1.423225	-1.047336
O	-3.675296	0.614071	0.125017
O	2.337016	-0.879919	0.728386
O	3.719544	-1.058058	0.225362
Rotational constants (GHz): 1.6937200 0.4637600 0.4207800			
Vibrational harmonic frequencies (cm-1):			
i491.1429	43.6044		43.8143
76.7823	114.2592		143.0705
162.9473	230.3337		232.9943
242.5484	261.0135		277.3850
318.5419	334.0238		358.8609
361.1371	387.8481		411.0136
465.7328	551.5834		566.6409
596.2802	671.2146		718.7248
749.6227	792.5344		845.2680
885.9323	913.8623		946.5674
960.7681	967.1829		978.3397

993.9885	1002.9550	1027.6095
1057.6775	1106.5543	1113.5804
1150.6410	1164.2693	1186.7771
1206.2635	1227.6137	1260.9020
1267.3793	1285.1933	1308.1708
1349.1243	1382.5280	1404.7354
1409.0410	1422.5101	1423.9569
1429.8753	1440.1874	1448.5875
1465.6640	1485.3294	1491.6560
1496.5552	1508.8606	1512.0688
1595.2893	1853.2797	2957.1724
3043.3965	3047.6968	3052.8137
3055.2694	3068.5137	3087.5482
3099.2974	3105.0300	3118.0800
3119.8799	3122.3768	3135.8467
3146.4970	3159.6637	3202.8157

Zero-point correction (Hartree): 0.245156

ApineneCI.A.b.ringclose.cpm

E(RM062X/Aug-CC-pVTZ) (Hartree): -616.13035249

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-1.312216	0.452674	-0.418452
H	-1.624435	1.016048	-1.302763
C	-2.488101	0.305345	0.536971
C	-3.638880	-0.322419	-0.198393
H	-2.229858	-0.320141	1.389883
H	-2.797401	1.292780	0.893171
H	-4.079794	0.298646	-1.004377
C	0.025779	1.052209	0.097581
C	-0.550161	-0.810259	-0.855740
C	0.275008	2.513683	-0.212665
C	0.277941	0.754991	1.567243
H	0.157482	-0.300227	1.807655
H	1.295998	1.022718	1.844559
H	-0.420600	1.333240	2.174757
H	1.299555	2.793808	0.038663
H	-0.393496	3.141175	0.380671
H	0.102666	2.733878	-1.266874
H	-0.837855	-1.289878	-1.787527
H	-0.515697	-1.551986	-0.060001
C	0.744168	0.030473	-0.882614
H	0.882977	0.524872	-1.843473
C	2.018957	-0.564853	-0.434010
C	3.284018	-0.139994	-1.092652
H	3.147042	-0.227753	-2.174202
H	3.471789	0.913207	-0.876486
H	4.119291	-0.730585	-0.737293
O	-4.056150	-1.427807	0.008465
O	1.959657	-1.515335	0.414840
O	2.921901	-0.841971	1.311699

Rotational constants (GHz): 1.3950500 0.4532400 0.4168000

Vibrational harmonic frequencies (cm-1):

1506.7500	33.6450	34.1811
63.6580	88.7917	131.5860
165.3262	211.0946	231.3016
241.3758	268.5558	277.3971
311.5218	336.4881	343.1453
363.2322	395.2209	435.8100
474.0247	542.1822	558.7029
581.8534	610.1524	742.9217
779.3419	837.5426	859.3439
887.8269	930.2589	944.6270
958.8393	967.3139	995.1746
1006.5884	1016.5234	1032.9745
1068.1858	1092.6658	1134.8464
1154.2330	1176.8903	1186.8260
1217.7878	1225.2458	1249.5800
1263.0818	1274.7384	1301.3375
1328.1070	1382.5743	1400.4578
1407.9268	1426.7731	1431.4896
1433.5565	1446.3043	1462.9481
1469.6299	1482.9089	1486.5287
1496.2569	1504.0206	1508.1991
1582.6554	1861.7399	2926.7124
3046.6221	3050.7135	3051.1040
3053.0801	3064.4566	3103.1611
3105.8724	3112.3596	3115.6360
3124.5650	3137.7394	3139.8934
3154.6681	3164.3914	3208.7793

Zero-point correction (Hartree): 0.245303

ApineneCI.A.b.ringclose.cmp

E(RM062X/Aug-CC-pVTZ) (Hartree): -616.12815556

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-1.317242	0.402639	-0.451215
H	-1.632447	0.880548	-1.383226
C	-2.517535	0.239958	0.469673
C	-3.605516	-0.510924	-0.247915
H	-2.257954	-0.303117	1.377204
H	-2.907090	1.226618	0.741693
H	-3.998050	-0.014675	-1.158653
C	-0.054613	1.147293	0.065456
C	-0.448720	-0.828300	-0.771546
C	0.080134	2.595669	-0.357502
C	0.154851	0.993208	1.565134
H	0.088611	-0.045159	1.888880
H	1.137137	1.370265	1.856359
H	-0.596239	1.570245	2.106438

H	1.045615	3.010788	-0.063129
H	-0.693998	3.196411	0.125418
H	-0.028383	2.705914	-1.436742
H	-0.657190	-1.376384	-1.686008
H	-0.408716	-1.526096	0.063185
C	0.781264	0.089393	-0.774728
H	0.989766	0.515911	-1.756291
C	2.048964	-0.344558	-0.146595
C	3.254689	0.502213	-0.352391
H	2.951755	1.550217	-0.262576
H	4.029024	0.236708	0.358002
H	3.638210	0.358997	-1.362646
O	-4.027612	-1.581971	0.086625
O	2.005715	-1.304507	0.684777
O	3.152183	-1.998114	0.053833
Rotational constants (GHz): 1.3097900 0.4649000 0.3896700			
Vibrational harmonic frequencies (cm-1):			
i501.3159	33.8799		40.8005
60.5224	84.2377		114.5985
168.4352	201.9091		227.8061
251.7866	267.8639		280.6664
326.0384	334.1348		339.7928
361.6485	394.4835		430.9680
456.3159	543.5211		566.9496
580.2477	599.4918		725.6353
771.5478	838.2220		852.7488
892.1952	931.1243		942.8297
960.5535	968.8939		986.7589
1000.3146	1009.0913		1035.9653
1069.1377	1097.6222		1137.4994
1151.9460	1158.8837		1188.0395
1216.9307	1225.8056		1247.5881
1264.6135	1275.4323		1300.5273
1326.5218	1381.2645		1401.2696
1408.2086	1424.8852		1427.2150
1428.8425	1442.2670		1465.8750
1467.0174	1484.9370		1491.7693
1498.4816	1508.6741		1510.7632
1598.8022	1864.3091		2925.5460
3045.3568	3046.7868		3048.3567
3052.3514	3056.6451		3097.6352
3106.9977	3113.2654		3120.4242
3121.1149	3128.6403		3134.0440
3141.2641	3165.6279		3201.5051
Zero-point correction (Hartree): 0.245023			
ApineneCI.A.b.ringclose.cppm			
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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.13029061			
Electronic state : 1-A			
Cartesian coordinates (Angs):			
C	-1.305476	0.231504	-0.371249
H	-1.691629	0.740447	-1.257797
C	-2.440808	0.018768	0.621005
C	-3.508952	-0.830639	-0.007405
H	-2.059431	-0.504845	1.501804
H	-2.881787	0.966140	0.931063
H	-3.198409	-1.861060	-0.271995
C	-0.014021	0.962893	0.092794
C	-0.439714	-0.967438	-0.803100
C	0.089599	2.432238	-0.259740
C	0.307269	0.727729	1.559804
H	0.304269	-0.328632	1.825871
H	1.300261	1.103330	1.800450
H	-0.427706	1.247675	2.176730
H	1.091065	2.812430	-0.050267
H	-0.615921	3.010611	0.340175
H	-0.136115	2.607189	-1.312182
H	-0.704522	-1.492897	-1.717066
H	-0.309699	-1.684789	0.005812
C	0.769890	-0.016280	-0.883210
H	0.842338	0.467537	-1.856651
C	2.103904	-0.479839	-0.450748
C	3.312205	0.109497	-1.089160
H	3.188148	0.043927	-2.173677
H	3.377384	1.169228	-0.836095
H	4.209582	-0.392716	-0.749623
O	-4.622325	-0.455393	-0.251908
O	2.152116	-1.461650	0.363212
O	3.028810	-0.712228	1.287383
Rotational constants (GHz): 1.5511700 0.4217300 0.3998200			
Vibrational harmonic frequencies (cm-1):			
i512.0536	29.5338		44.9451
51.2411	89.8549		138.7688
170.8731	217.5014		229.3834
237.3417	268.4418		275.7628
313.4304	332.6043		340.9952
361.5147	394.8472		441.3580
464.3242	525.6832		562.5929
580.4266	609.9896		742.5731
787.6212	838.5671		867.7198
883.5213	929.2970		947.0714
959.0571	967.0859		992.4151
1005.0635	1010.8230		1029.5280
1071.1968	1101.6719		1138.3216
1151.6661	1174.0059		1187.1471
1220.4308	1222.7712		1258.1926
1265.0790	1275.0675		1307.2043
1330.7872	1379.4845		1396.8955
1408.3159	1428.4442		1430.7038
1431.5799	1445.9117		1462.1656
1469.1801	1480.4820		1487.2836

1496.0562	1504.7302	1506.1378
1579.8007	1860.9362	2935.4439
3048.6567	3052.1163	3056.0248
3064.7367	3066.1483	3098.7600
3104.9171	3112.7946	3117.9479
3126.3900	3127.6011	3139.0367
3151.7354	3157.9091	3209.0865

Zero-point correction (Hartree): 0.245319

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.12839958

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -1.311764 | 0.189272  | -0.380006 |
| H | -1.700374 | 0.596110  | -1.316591 |
| C | -2.464872 | -0.023757 | 0.591732  |
| C | -3.456206 | -0.986016 | -0.001135 |
| H | -2.083636 | -0.456710 | 1.520748  |
| H | -2.977114 | 0.911755  | 0.817154  |
| H | -3.068828 | -2.006085 | -0.192629 |
| C | -0.099812 | 1.059575  | 0.057266  |
| C | -0.349094 | -0.976082 | -0.683993 |
| C | -0.102984 | 2.492528  | -0.434041 |
| C | 0.175202  | 0.995085  | 1.552558  |
| H | 0.211996  | -0.028080 | 1.926254  |
| H | 1.131469  | 1.466632  | 1.787218  |
| H | -0.602650 | 1.532897  | 2.096254  |
| H | 0.836671  | 2.996602  | -0.201253 |
| H | -0.904255 | 3.050383  | 0.055313  |
| H | -0.264285 | 2.542133  | -1.511025 |
| H | -0.537159 | -1.578163 | -1.568605 |
| H | -0.213583 | -1.631405 | 0.175480  |
| C | 0.796834  | 0.039894  | -0.769275 |
| H | 0.937313  | 0.438596  | -1.774066 |
| C | 2.114019  | -0.262491 | -0.167336 |
| C | 3.243837  | 0.659815  | -0.457709 |
| H | 2.864278  | 1.685275  | -0.406298 |
| H | 4.059926  | 0.489051  | 0.234778  |
| H | 3.602286  | 0.495766  | -1.474018 |
| O | -4.586728 | -0.704908 | -0.288505 |
| O | 2.171185  | -1.178948 | 0.711473  |
| O | 3.345166  | -1.820106 | 0.074896  |

Rotational constants (GHz): 1.4676200 0.4302400 0.3767500

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i499.0982 | 39.1392   | 43.3951   |
| 50.3496   | 83.1299   | 120.6906  |
| 174.0402  | 210.3160  | 222.6384  |
| 246.0191  | 267.9351  | 271.4944  |
| 321.1083  | 331.9089  | 337.4413  |
| 359.8476  | 393.0519  | 436.2952  |
| 452.1701  | 525.0921  | 570.7792  |
| 579.1068  | 600.2883  | 726.3754  |
| 782.1029  | 842.5201  | 863.3624  |
| 886.9951  | 929.4293  | 943.7349  |
| 961.4766  | 969.9709  | 991.4300  |
| 998.1257  | 1004.3165 | 1030.4957 |
| 1074.0018 | 1102.0234 | 1140.7412 |
| 1144.3962 | 1162.0042 | 1187.7430 |
| 1217.8844 | 1226.3825 | 1256.0188 |
| 1265.4727 | 1274.7507 | 1305.4765 |
| 1327.8102 | 1378.8765 | 1396.2903 |
| 1409.8083 | 1425.0287 | 1426.8306 |
| 1431.1053 | 1440.2219 | 1465.7666 |
| 1468.3279 | 1485.0203 | 1491.4877 |
| 1497.8675 | 1507.7154 | 1509.9387 |
| 1597.9332 | 1861.4690 | 2942.5708 |
| 3047.9164 | 3050.1991 | 3054.6443 |
| 3057.9363 | 3068.6087 | 3098.9189 |
| 3103.2857 | 3115.6158 | 3120.9273 |
| 3122.1835 | 3125.5053 | 3130.3816 |
| 3139.1611 | 3161.2148 | 3202.2405 |

Zero-point correction (Hartree): 0.245100

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.13302754

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-1.374148	0.252060	-0.325410
H	-1.785358	0.520711	-1.300318
C	-2.464812	0.337758	0.715742
C	-3.659564	-0.512160	0.379097
H	-2.109170	0.024057	1.702542
H	-2.824485	1.364712	0.848316
H	-4.475873	-0.505330	1.125744
C	-0.038329	1.014650	-0.107374
C	-0.578027	-1.055849	-0.460515
C	0.113220	2.336186	-0.832604
C	0.335446	1.152872	1.360360
H	0.285790	0.205207	1.895233
H	1.356665	1.514343	1.467107
H	-0.343849	1.860970	1.838885
H	1.138206	2.704474	-0.759097
H	-0.540629	3.086947	-0.383493
H	-0.149438	2.244230	-1.886994
H	-0.914336	-1.775808	-1.200205
H	-0.443347	-1.549914	0.500536
C	0.667523	-0.216836	-0.820502
H	0.714947	-0.006726	-1.888346
C	1.997329	-0.624566	-0.328276
C	3.191200	-0.373292	-1.180469

H	2.982541	-0.771900	-2.177355
H	3.340927	0.702288	-1.289390
H	4.077461	-0.814261	-0.741415
O	-3.759756	-1.168552	-0.621464
O	2.046016	-1.296970	0.755936
O	3.032606	-0.368096	1.346521

Rotational constants (GHz): 1.4350600 0.4591500 0.4343100

Vibrational harmonic frequencies (cm-1):

i504.7522	34.4410	48.6555
78.3551	116.8172	139.9296
171.8380	207.4162	235.5807
241.3834	262.2829	270.3637
316.2368	335.2614	343.2266
363.5550	393.5613	414.7030
483.0960	553.7064	563.7299
606.3929	672.5029	717.9913
761.3961	838.3634	845.2747
881.8296	931.1154	936.7055
951.9359	959.0862	967.0029
1001.9558	1007.2060	1025.5750
1038.9958	1093.7090	1141.8728
1152.5518	1175.8191	1188.8822
1218.2485	1222.9555	1254.7160
1269.1798	1278.2351	1321.6297
1337.3684	1386.1136	1406.9761
1407.9512	1420.8395	1431.8589
1434.9017	1446.7078	1453.2532
1463.1187	1483.9223	1488.3416
1495.5363	1504.3313	1508.5392
1580.3105	1853.9069	2950.6067
3040.2236	3046.7370	3050.4140
3061.7815	3069.7934	3084.2272
3102.7115	3107.3544	3112.1079
3114.9632	3125.5187	3136.6242
3153.6140	3169.7593	3208.6760

Zero-point correction (Hartree): 0.245300

ApineneCI.A.b.ringclose.cptp

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.13065692

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -1.383711 | 0.250224  | -0.292826 |
| H | -1.804281 | 0.578199  | -1.245005 |
| C | -2.491462 | 0.144151  | 0.728932  |
| C | -3.618007 | -0.744521 | 0.273091  |
| H | -2.129212 | -0.251579 | 1.683214  |
| H | -2.928513 | 1.122008  | 0.963292  |
| H | -4.433278 | -0.895020 | 1.005437  |
| C | -0.128568 | 1.109919  | 0.021784  |
| C | -0.477217 | -0.969234 | -0.535697 |
| C | -0.099247 | 2.494694  | -0.592465 |
| C | 0.205053  | 1.165021  | 1.506167  |
| H | 0.217341  | 0.176862  | 1.965707  |
| H | 1.187116  | 1.614849  | 1.664961  |
| H | -0.529165 | 1.779687  | 2.029248  |
| H | 0.867224  | 2.979388  | -0.442041 |
| H | -0.857793 | 3.125589  | -0.123375 |
| H | -0.304625 | 2.457134  | -1.662374 |
| H | -0.735960 | -1.626000 | -1.359964 |
| H | -0.331166 | -1.560310 | 0.367543  |
| C | 0.701298  | -0.008741 | -0.746702 |
| H | 0.815619  | 0.300290  | -1.785755 |
| C | 2.029721  | -0.301494 | -0.167904 |
| C | 3.180410  | 0.537161  | -0.598495 |
| H | 2.841732  | 1.577242  | -0.642125 |
| H | 4.018744  | 0.406238  | 0.075814  |
| H | 3.487763  | 0.252650  | -1.604879 |
| O | -3.666418 | -1.269822 | -0.804975 |
| O | 2.092409  | -1.119760 | 0.803489  |
| O | 3.212613  | -1.872955 | 0.193361  |

Rotational constants (GHz): 1.3461300 0.4736700 0.4094100

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i496.9798 | 41.9214   | 46.6137   |
| 72.8180   | 110.5591  | 139.8879  |
| 164.8160  | 208.6902  | 224.1867  |
| 245.5882  | 250.6639  | 270.3872  |
| 318.0259  | 332.4379  | 338.9071  |
| 361.3332  | 391.7972  | 415.1912  |
| 468.4736  | 554.8305  | 566.3310  |
| 598.2172  | 673.2692  | 716.2743  |
| 740.1716  | 838.3880  | 848.4073  |
| 884.3458  | 930.0141  | 937.9665  |
| 951.1418  | 959.0512  | 969.3422  |
| 991.3886  | 1000.5028 | 1020.2607 |
| 1042.5132 | 1099.4933 | 1144.0916 |
| 1148.7949 | 1159.6464 | 1188.5853 |
| 1216.3418 | 1225.1048 | 1254.7884 |
| 1267.3818 | 1277.4340 | 1321.1736 |
| 1335.0153 | 1382.6496 | 1406.6903 |
| 1408.9973 | 1420.5509 | 1425.4724 |
| 1430.7600 | 1441.0241 | 1453.4035 |
| 1465.7000 | 1484.4501 | 1492.1187 |
| 1497.6272 | 1507.6621 | 1509.3375 |
| 1596.5730 | 1856.2277 | 2952.7039 |
| 3036.9769 | 3046.9590 | 3048.1693 |
| 3054.9931 | 3070.1116 | 3086.2520 |
| 3099.1174 | 3106.3043 | 3112.1545 |
| 3119.3472 | 3120.5584 | 3129.4702 |
| 3138.2920 | 3172.8152 | 3201.8154 |

Zero-point correction (Hartree): 0.244989

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ApineneCI.A.b.ringclose.ctmm
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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.12793999
Electronic state : 1-A
Cartesian coordinates (Angs):
C 1.202827 0.969186 0.726092
H 1.242114 2.006037 1.067600
C 2.635038 0.498452 0.516875
C 2.841984 -0.964712 0.223714
H 3.123256 1.070002 -0.273951
H 3.193592 0.688118 1.441321
H 2.276885 -1.676061 0.854956
C 0.165518 0.898312 -0.428683
C 0.213033 0.206283 1.628790
C -0.005373 2.153654 -1.258915
C 0.343229 -0.322435 -1.317705
H 0.390056 -1.253001 -0.751622
H -0.497960 -0.426109 -2.001132
H 1.261891 -0.219680 -1.897689
H -0.866796 2.066479 -1.923489
H 0.876979 2.310308 -1.882812
H -0.139127 3.034338 -0.629564
H 0.150802 0.498180 2.674058
H 0.316007 -0.873472 1.559414
C -0.924870 0.690621 0.708094
H -1.294305 1.673060 1.000578
C -2.059075 -0.204090 0.402880
C -3.385342 0.396579 0.093638
H -3.628099 1.109268 0.886718
H -3.320600 0.961122 -0.838248
H -4.140360 -0.372949 -0.009355
O 3.608328 -1.374275 -0.604081
O -1.876216 -1.459011 0.544558
O -2.370382 -1.732557 -0.821159
Rotational constants (GHz): 1.2849700 0.5197600 0.4701600
Vibrational harmonic frequencies (cm-1):
1512.4998 25.5569 55.6331
 85.6915 98.0557 139.7258
188.2705 222.3613 232.7661
253.1145 255.4937 270.3194
318.7066 343.7137 359.5762
365.2150 393.1588 408.1978
460.4784 555.0971 563.0700
595.7238 633.2118 700.5113
758.5938 815.0096 837.8131
880.1262 918.9076 953.0842
963.1704 964.8868 984.5080
1003.5323 1013.0350 1033.9487
1060.7665 1110.2204 1133.1157
1152.2535 1169.1859 1188.2929
1219.7350 1227.1558 1252.1192
1262.4638 1294.1270 1321.2755
1337.3821 1385.0131 1400.0129
1406.8993 1428.2446 1433.0122
1440.5805 1447.1340 1448.2098
1462.6406 1480.7184 1487.8601
1497.3097 1505.2886 1506.6456
1580.2737 1857.4839 2953.0838
3032.3497 3047.6247 3050.8764
3063.8598 3065.8767 3103.2298
3107.7015 3110.8099 3111.5753
3117.2810 3124.2900 3137.9104
3147.3755 3170.8159 3208.0644
Zero-point correction (Hartree): 0.245355

ApineneCI.A.b.ringclose.ctmp
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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.12654745
Electronic state : 1-A
Cartesian coordinates (Angs):
C      1.236765      0.536270      1.038097
H      1.310022      1.338338      1.775647
C      2.652609      0.071545      0.721643
C      2.786518     -1.162393     -0.130856
H      3.229678      0.869158      0.251208
H      3.147797     -0.173080      1.668602
H      2.180157     -2.035512      0.175939
C      0.298102      1.041740     -0.092706
C      0.135220     -0.439802      1.500549
C      0.280880      2.539953     -0.317045
C      0.479276      0.296798     -1.407572
H      0.452906     -0.786557     -1.283189
H     -0.312791      0.562859     -2.110490
H      1.433991      0.563297     -1.862570
H     -0.492902      2.829428     -1.030172
H      1.239876      2.863136     -0.727845
H      0.110835      3.079303      0.615140
H      0.001847     -0.578030      2.569913
H      0.186806     -1.412722      1.018106
C     -0.888855      0.448312      0.780749
H     -1.282169      1.243644      1.414433
C     -1.993199     -0.160541      0.007653
C     -3.059529      0.735723     -0.513240
H     -2.580420      1.638568     -0.904893
H     -3.648642      0.224713     -1.265910
H     -3.715535      1.041758      0.301751
O      3.529883     -1.247176     -1.069605
O     -1.882859     -1.380742     -0.330181
O     -3.250548     -1.711323      0.133622
Rotational constants (GHz):  1.2698600      0.5081500      0.4477600
Vibrational harmonic frequencies (cm-1):
1498.4686      38.5483      51.6572

```

|           |           |           |
|-----------|-----------|-----------|
| 86.4117   | 92.3180   | 119.4216  |
| 199.0837  | 216.4098  | 238.5863  |
| 244.5038  | 257.4190  | 271.7206  |
| 325.5830  | 345.6264  | 359.7586  |
| 366.6223  | 390.7497  | 409.8458  |
| 459.4822  | 552.4263  | 565.3164  |
| 590.4377  | 620.0676  | 700.8473  |
| 742.9784  | 821.1965  | 842.3738  |
| 882.3854  | 919.7765  | 959.1907  |
| 960.6223  | 968.0429  | 978.5725  |
| 1000.6680 | 1002.1462 | 1035.8929 |
| 1061.9182 | 1112.7590 | 1130.8909 |
| 1144.7903 | 1163.4479 | 1188.2850 |
| 1218.7857 | 1227.4290 | 1251.7811 |
| 1264.1737 | 1291.7019 | 1319.6073 |
| 1337.7060 | 1382.1478 | 1399.7844 |
| 1409.6017 | 1423.5807 | 1428.6655 |
| 1439.3455 | 1440.9564 | 1451.5114 |
| 1466.3351 | 1485.4562 | 1492.3799 |
| 1500.3552 | 1509.1740 | 1511.3050 |
| 1597.8027 | 1856.6819 | 2952.0227 |
| 3036.6129 | 3047.4684 | 3049.3381 |
| 3055.1415 | 3068.6341 | 3098.3587 |
| 3107.9395 | 3114.4406 | 3115.1710 |
| 3119.9497 | 3122.0380 | 3128.1546 |
| 3136.6086 | 3171.2529 | 3201.0744 |

Zero-point correction (Hartree): 0.245243

ApineneCI.A.b.ringclose.ctpm

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.12805819

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-1.336905	0.834642	-0.700072
H	-1.413745	1.723031	-1.330793
C	-2.738970	0.520448	-0.173989
C	-2.890251	-0.849978	0.442151
H	-3.036257	1.287259	0.544414
H	-3.436622	0.554102	-1.013261
H	-3.038832	-0.900312	1.535840
C	-0.158369	1.053340	0.285383
C	-0.492265	-0.221445	-1.433825
C	0.143813	2.485784	0.675817
C	-0.243271	0.161411	1.514579
H	-0.412269	-0.885058	1.262337
H	0.684365	0.193963	2.083639
H	-1.060267	0.509980	2.150784
H	1.081283	2.546617	1.231458
H	-0.647929	2.873916	1.320360
H	0.215664	3.131460	-0.200186
H	-0.564711	-0.269537	-2.516959
H	-0.621066	-1.216425	-1.016128
C	0.769053	0.463152	-0.856922
H	1.098984	1.289245	-1.485780
C	1.928715	-0.351203	-0.445688
C	3.300498	0.173697	-0.684386
H	3.363911	0.483645	-1.731485
H	3.461714	1.064576	-0.074980
H	4.046012	-0.570229	-0.432318
O	-2.866761	-1.858548	-0.210000
O	1.700573	-1.528956	-0.012676
O	2.489623	-1.291911	1.214522

Rotational constants (GHz): 1.2363400 0.5655000 0.4947700

Vibrational harmonic frequencies (cm-1):

i498.5729	40.5524	62.9072
74.9241	117.0844	141.7906
184.4363	227.7570	237.3672
249.0562	254.2895	273.4636
315.0613	344.0806	355.2649
371.8632	393.4638	411.6451
494.5791	557.1985	564.0495
595.6229	624.1675	726.5983
771.7123	837.2795	864.0854
892.3457	933.2117	944.1190
960.9605	966.5478	988.1719
1004.6606	1017.6772	1024.7629
1056.8696	1064.0811	1127.1827
1154.1197	1172.3488	1192.0802
1219.8489	1229.6884	1249.0970
1261.5991	1297.8897	1315.2053
1340.5959	1381.3541	1396.7807
1407.6261	1424.9881	1430.0629
1437.8621	1446.4872	1463.1080
1469.8096	1484.9649	1487.4030
1499.2231	1506.4547	1509.4938
1584.9519	1852.0898	2965.3372
3046.3845	3049.3903	3055.9651
3058.3832	3069.6103	3103.2069
3111.4093	3111.5396	3115.0895
3115.2259	3124.6363	3133.9638
3150.5635	3177.3697	3208.4811

Zero-point correction (Hartree): 0.245775

ApineneCI.A.b.ringclose.cttm

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.12805818

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -1.336924 | 0.834691  | -0.700082 |
| H | -1.413795 | 1.723089  | -1.330784 |
| C | -2.738978 | 0.520420  | -0.173986 |
| C | -2.890144 | -0.850050 | 0.442085  |



|                                                           |           |           |           |
|-----------------------------------------------------------|-----------|-----------|-----------|
| H                                                         | -3.036300 | 1.287205  | 0.544423  |
| H                                                         | -3.436612 | 0.554024  | -1.013275 |
| H                                                         | -3.038463 | -0.900463 | 1.535799  |
| C                                                         | -0.158401 | 1.053332  | 0.285401  |
| C                                                         | -0.492263 | -0.221385 | -1.433840 |
| C                                                         | 0.143853  | 2.485734  | 0.675925  |
| C                                                         | -0.243449 | 0.161353  | 1.514556  |
| H                                                         | -0.412923 | -0.885040 | 1.262272  |
| H                                                         | 0.684292  | 0.193463  | 2.083467  |
| H                                                         | -1.060182 | 0.510250  | 2.150911  |
| H                                                         | 1.081275  | 2.546458  | 1.231661  |
| H                                                         | -0.647922 | 2.873914  | 1.320395  |
| H                                                         | 0.215852  | 3.131434  | -0.200048 |
| H                                                         | -0.564647 | -0.269414 | -2.516981 |
| H                                                         | -0.621110 | -1.216380 | -1.016199 |
| C                                                         | 0.769056  | 0.463175  | -0.856867 |
| H                                                         | 1.099002  | 1.289268  | -1.485716 |
| C                                                         | 1.928685  | -0.351240 | -0.445668 |
| C                                                         | 3.300504  | 0.173275  | -0.684985 |
| H                                                         | 3.363652  | 0.482813  | -1.732222 |
| H                                                         | 3.462094  | 1.064355  | -0.075973 |
| H                                                         | 4.045938  | -0.570711 | -0.432867 |
| O                                                         | -2.866821 | -1.858569 | -0.210160 |
| O                                                         | 1.700434  | -1.528769 | -0.012107 |
| O                                                         | 2.489913  | -1.291424 | 1.214756  |
| Rotational constants (GHz): 1.2363700 0.5654800 0.4947800 |           |           |           |
| Vibrational harmonic frequencies (cm-1):                  |           |           |           |
| i498.5255                                                 | 40.5982   | 62.9081   |           |
| 74.9931                                                   | 117.1030  | 141.8058  |           |
| 184.4537                                                  | 227.8154  | 237.4266  |           |
| 249.0934                                                  | 254.2667  | 273.4799  |           |
| 315.2124                                                  | 344.1245  | 355.3295  |           |
| 371.9662                                                  | 393.4722  | 411.6749  |           |
| 494.5975                                                  | 557.2029  | 564.0685  |           |
| 595.6144                                                  | 624.1566  | 726.6073  |           |
| 771.7231                                                  | 837.2874  | 864.0887  |           |
| 892.3329                                                  | 933.2044  | 944.1169  |           |
| 960.9663                                                  | 966.5566  | 988.1808  |           |
| 1004.6721                                                 | 1017.6841 | 1024.7628 |           |
| 1056.8576                                                 | 1064.0739 | 1127.1607 |           |
| 1154.1223                                                 | 1172.3674 | 1192.0882 |           |
| 1219.8505                                                 | 1229.6926 | 1249.0979 |           |
| 1261.5985                                                 | 1297.8936 | 1315.1850 |           |
| 1340.5768                                                 | 1381.3389 | 1396.7706 |           |
| 1407.6291                                                 | 1424.9797 | 1430.0647 |           |
| 1437.8516                                                 | 1446.4845 | 1463.1050 |           |
| 1469.8075                                                 | 1485.0527 | 1487.3773 |           |
| 1499.2223                                                 | 1506.4447 | 1509.5860 |           |
| 1584.9635                                                 | 1852.0648 | 2965.4032 |           |
| 3046.3892                                                 | 3049.3919 | 3055.9767 |           |
| 3058.4004                                                 | 3069.6324 | 3103.2217 |           |
| 3111.4113                                                 | 3111.5624 | 3115.0970 |           |
| 3115.2329                                                 | 3124.6371 | 3133.9561 |           |
| 3150.5285                                                 | 3177.3857 | 3208.4863 |           |
| Zero-point correction (Hartree): 0.245777                 |           |           |           |
| ApineneCI.A.b.ringclose.cttp                              |           |           |           |
| ~~~~~                                                     |           |           |           |
| E(RM062X/Aug-CC-pVTZ) (Hartree): -616.12494315            |           |           |           |
| Electronic state : 1-A                                    |           |           |           |
| Cartesian coordinates (Angs):                             |           |           |           |
| C                                                         | 1.387041  | 0.515156  | 0.898425  |
| H                                                         | 1.483803  | 1.256480  | 1.695828  |
| C                                                         | 2.797507  | 0.159545  | 0.458343  |
| C                                                         | 3.053124  | -1.082271 | -0.354182 |
| H                                                         | 3.238800  | 0.992904  | -0.101721 |
| H                                                         | 3.448088  | 0.054020  | 1.334728  |
| H                                                         | 4.115804  | -1.203842 | -0.644293 |
| C                                                         | 0.356520  | 1.097809  | -0.108549 |
| C                                                         | 0.343373  | -0.528172 | 1.349560  |
| C                                                         | 0.313685  | 2.611076  | -0.191704 |
| C                                                         | 0.429765  | 0.478956  | -1.497434 |
| H                                                         | 0.395721  | -0.607961 | -1.468688 |
| H                                                         | -0.396030 | 0.837155  | -2.115876 |
| H                                                         | 1.358299  | 0.775757  | -1.990333 |
| H                                                         | -0.512067 | 2.956905  | -0.815669 |
| H                                                         | 1.237106  | 2.983545  | -0.641963 |
| H                                                         | 0.212265  | 3.062017  | 0.795874  |
| H                                                         | 0.296116  | -0.763285 | 2.409355  |
| H                                                         | 0.392535  | -1.443858 | 0.769563  |
| C                                                         | -0.743947 | 0.405507  | 0.799787  |
| H                                                         | -1.090912 | 1.134623  | 1.534048  |
| C                                                         | -1.912829 | -0.141202 | 0.074761  |
| C                                                         | -2.970562 | 0.813350  | -0.357628 |
| H                                                         | -2.480451 | 1.707753  | -0.753819 |
| H                                                         | -3.622719 | 0.347600  | -1.087394 |
| H                                                         | -3.565923 | 1.119628  | 0.502394  |
| O                                                         | 2.248611  | -1.912581 | -0.672052 |
| O                                                         | -1.875695 | -1.354564 | -0.299415 |
| O                                                         | -3.226979 | -1.631351 | 0.240179  |
| Rotational constants (GHz): 1.2297300 0.5709800 0.4697900 |           |           |           |
| Vibrational harmonic frequencies (cm-1):                  |           |           |           |
| i504.5811                                                 | 35.6205   | 56.6300   |           |
| 87.7201                                                   | 113.3576  | 125.7254  |           |
| 187.6381                                                  | 203.5656  | 226.0849  |           |
| 237.2440                                                  | 248.7083  | 271.8523  |           |
| 321.4840                                                  | 325.0117  | 342.4912  |           |
| 363.7649                                                  | 391.0721  | 411.8885  |           |
| 468.7691                                                  | 544.9204  | 562.9151  |           |
| 597.2019                                                  | 677.9380  | 736.6162  |           |
| 754.5450                                                  | 782.7722  | 841.9302  |           |
| 886.4227                                                  | 907.7865  | 939.2899  |           |

|           |           |           |
|-----------|-----------|-----------|
| 961.0834  | 968.3245  | 977.3317  |
| 988.5316  | 1001.1383 | 1017.0655 |
| 1053.6171 | 1088.8996 | 1127.1794 |
| 1157.9747 | 1163.7280 | 1190.8835 |
| 1223.4348 | 1230.8816 | 1256.4043 |
| 1265.4113 | 1298.1137 | 1330.6051 |
| 1370.2306 | 1384.6876 | 1408.0749 |
| 1409.4152 | 1422.6081 | 1427.2191 |
| 1435.6668 | 1440.7628 | 1449.6286 |
| 1466.0717 | 1485.7430 | 1492.1080 |
| 1503.4846 | 1511.9736 | 1512.5841 |
| 1598.6032 | 1866.3737 | 2933.5639 |
| 3028.2035 | 3045.8208 | 3050.8139 |
| 3052.0698 | 3053.5415 | 3058.4474 |
| 3086.1756 | 3107.7804 | 3111.8468 |
| 3120.8595 | 3121.9638 | 3127.5710 |
| 3161.9886 | 3191.9542 | 3200.6873 |

Zero-point correction (Hartree): 0.245108

ApineneCI.A.b.ringclose.mmmm

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E(RM062X/Aug-CC-pVT2) (Hartree): -616.12726903

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-1.255632	-0.556299	-0.502955
H	-1.568712	-0.334821	-1.525797
C	-2.476541	-0.937489	0.325741
C	-3.508734	0.155753	0.284955
H	-2.925923	-1.850880	-0.063731
H	-2.179285	-1.105113	1.364272
H	-3.227935	1.101049	0.790503
C	-0.289718	0.579135	-0.035469
C	-0.067559	-1.538280	-0.540730
C	-0.471829	1.940187	-0.677269
C	-0.196827	0.699092	1.480911
H	-0.019486	-0.264436	1.963605
H	0.617549	1.369087	1.754865
H	-1.120934	1.111366	1.889329
H	0.380636	2.582377	-0.454285
H	-1.373171	2.427395	-0.299676
H	-0.562330	1.854496	-1.760596
H	-0.029561	-2.255860	-1.355934
H	0.031790	-2.068000	0.406712
C	0.856169	-0.313354	-0.615061
H	1.036600	-0.020273	-1.656702
C	2.193078	-0.264876	0.016492
C	2.919051	-1.512443	0.359330
H	2.249738	-2.143804	0.950468
H	3.155266	-2.062849	-0.552790
H	3.837107	-1.283436	0.886354
O	-4.567017	0.064616	-0.272752
O	2.614418	0.898721	0.315610
O	3.888838	0.716057	-0.406892

Rotational constants (GHz): 1.8611900 0.4083800 0.3733900

Vibrational harmonic frequencies (cm-1):

i489.0875	27.4196	36.5167
67.0941	83.2889	139.0835
180.5118	208.9444	228.2419
231.9374	265.0226	282.5818
305.8579	318.7630	347.0444
378.1929	396.3545	409.4294
468.1740	515.9458	527.3512
588.4278	599.6970	715.1754
757.6700	839.8524	856.3048
892.4481	925.4906	954.9434
964.2483	968.9147	985.4034
1005.8917	1023.3789	1029.0817
1072.5594	1105.0563	1131.0069
1143.4509	1168.6449	1192.4009
1197.2307	1247.8181	1265.1718
1269.2512	1281.5897	1302.4687
1329.2077	1353.9609	1394.9400
1407.2118	1411.4740	1420.8235
1433.6027	1437.2755	1459.9110
1468.7396	1485.0049	1495.5279
1499.7605	1507.9533	1514.5093
1576.7700	1861.5525	2940.3042
3036.2737	3051.7155	3053.0881
3054.0670	3061.3111	3071.2094
3091.6704	3112.7776	3118.9917
3121.4575	3126.8247	3134.0494
3138.7965	3153.9573	3209.0815

Zero-point correction (Hartree): 0.244755

ApineneCI.A.b.ringclose.mmmmp

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E(RM062X/Aug-CC-pVT2) (Hartree): -616.13048381

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 1.257883  | 0.569381  | -0.527262 |
| H | 1.629386  | 0.333573  | -1.527372 |
| C | 2.435021  | 0.888289  | 0.385699  |
| C | 3.407917  | -0.258253 | 0.415675  |
| H | 2.958283  | 1.776910  | 0.032928  |
| H | 2.074354  | 1.070526  | 1.401305  |
| H | 3.032995  | -1.192778 | 0.878577  |
| C | 0.208675  | -0.513477 | -0.129623 |
| C | 0.117028  | 1.600209  | -0.646347 |
| C | 0.333289  | -1.892789 | -0.740825 |
| C | -0.012499 | -0.609739 | 1.374850  |
| H | -0.108519 | 0.369031  | 1.847315  |
| H | -0.920103 | -1.177398 | 1.581282  |

|                                                           |           |           |           |
|-----------------------------------------------------------|-----------|-----------|-----------|
| H                                                         | 0.833737  | -1.117783 | 1.841062  |
| H                                                         | -0.594403 | -2.448180 | -0.592271 |
| H                                                         | 1.143174  | -2.452455 | -0.268501 |
| H                                                         | 0.535740  | -1.834944 | -1.810696 |
| H                                                         | 0.180557  | 2.336733  | -1.443396 |
| H                                                         | -0.051648 | 2.110322  | 0.302042  |
| C                                                         | -0.849333 | 0.426349  | -0.842263 |
| H                                                         | -0.907722 | 0.106385  | -1.884856 |
| C                                                         | -2.209747 | 0.367157  | -0.282052 |
| C                                                         | -2.736418 | 1.441302  | 0.596375  |
| H                                                         | -2.549928 | 2.399968  | 0.102955  |
| H                                                         | -3.789157 | 1.278711  | 0.794410  |
| H                                                         | -2.195196 | 1.454959  | 1.543163  |
| O                                                         | 4.514749  | -0.217867 | -0.045625 |
| O                                                         | -2.920072 | -0.612275 | -0.690871 |
| O                                                         | -3.217482 | -1.060378 | 0.683581  |
| Rotational constants (GHz): 1.7422700 0.4320900 0.3995800 |           |           |           |
| Vibrational harmonic frequencies (cm-1):                  |           |           |           |
| i498.2286                                                 | 32.0176   | 56.3481   |           |
| 67.9745                                                   | 92.5529   | 133.5788  |           |
| 193.2200                                                  | 226.8704  | 247.1320  |           |
| 255.5329                                                  | 264.6911  | 290.6251  |           |
| 308.9579                                                  | 334.4406  | 357.7064  |           |
| 375.4711                                                  | 384.5039  | 421.8716  |           |
| 471.7221                                                  | 513.5911  | 531.5361  |           |
| 589.5920                                                  | 599.8978  | 722.4577  |           |
| 768.1818                                                  | 850.2261  | 851.5057  |           |
| 877.6215                                                  | 927.0204  | 945.8913  |           |
| 965.8376                                                  | 971.3896  | 993.8476  |           |
| 1007.8976                                                 | 1014.8539 | 1031.4417 |           |
| 1075.2757                                                 | 1106.8833 | 1132.1195 |           |
| 1143.6294                                                 | 1168.2558 | 1185.8010 |           |
| 1195.2962                                                 | 1244.9675 | 1265.1650 |           |
| 1280.9506                                                 | 1286.6505 | 1301.8111 |           |
| 1326.9645                                                 | 1365.5279 | 1397.0112 |           |
| 1408.0630                                                 | 1414.4059 | 1420.3911 |           |
| 1432.6031                                                 | 1439.4285 | 1460.6770 |           |
| 1469.4057                                                 | 1484.1228 | 1493.1168 |           |
| 1498.3857                                                 | 1507.7228 | 1516.4605 |           |
| 1578.6856                                                 | 1861.1788 | 2935.7655 |           |
| 3049.3380                                                 | 3049.9390 | 3053.0644 |           |
| 3061.5720                                                 | 3070.3398 | 3081.7509 |           |
| 3092.2655                                                 | 3117.1687 | 3120.3955 |           |
| 3122.4229                                                 | 3127.3296 | 3130.2174 |           |
| 3137.1666                                                 | 3151.5252 | 3205.5564 |           |
| Zero-point correction (Hartree): 0.245233                 |           |           |           |
| ApineneCI.A.b.ringclose.mmpm                              |           |           |           |
| ~~~~~                                                     |           |           |           |
| E(RM062X/Aug-CC-pVTZ) (Hartree): -616.12906840            |           |           |           |
| Electronic state : 1-A                                    |           |           |           |
| Cartesian coordinates (Angs):                             |           |           |           |
| C                                                         | 1.213534  | 0.731782  | -0.695385 |
| H                                                         | 1.451387  | 0.573802  | -1.750843 |
| C                                                         | 2.476473  | 1.115000  | 0.062632  |
| C                                                         | 3.516575  | 0.042274  | -0.106517 |
| H                                                         | 2.871522  | 2.047023  | -0.352073 |
| H                                                         | 2.282222  | 1.257575  | 1.124841  |
| H                                                         | 3.860062  | -0.121619 | -1.147758 |
| C                                                         | 0.364164  | -0.480449 | -0.205569 |
| C                                                         | -0.029119 | 1.637564  | -0.588569 |
| C                                                         | 0.592105  | -1.796262 | -0.921305 |
| C                                                         | 0.415094  | -0.668030 | 1.306433  |
| H                                                         | 0.205239  | 0.259080  | 1.844827  |
| H                                                         | -0.320923 | -1.410569 | 1.614505  |
| H                                                         | 1.402617  | -1.015908 | 1.612130  |
| H                                                         | -0.174325 | -2.520525 | -0.644640 |
| H                                                         | 1.565520  | -2.210081 | -0.648332 |
| H                                                         | 0.564885  | -1.665867 | -2.003999 |
| H                                                         | -0.180995 | 2.384815  | -1.363150 |
| H                                                         | -0.079061 | 2.119590  | 0.387289  |
| C                                                         | -0.881763 | 0.360311  | -0.646897 |
| H                                                         | -1.133917 | 0.099198  | -1.681125 |
| C                                                         | -2.144108 | 0.188693  | 0.104948  |
| C                                                         | -2.859747 | 1.353226  | 0.681041  |
| H                                                         | -2.146331 | 1.924356  | 1.282189  |
| H                                                         | -3.200596 | 2.010400  | -0.120604 |
| H                                                         | -3.711830 | 1.024059  | 1.262710  |
| O                                                         | 3.946808  | -0.636581 | 0.784826  |
| O                                                         | -2.499094 | -1.018263 | 0.298082  |
| O                                                         | -3.852055 | -0.802653 | -0.253012 |
| Rotational constants (GHz): 1.7321800 0.4378600 0.4002300 |           |           |           |
| Vibrational harmonic frequencies (cm-1):                  |           |           |           |
| i484.3405                                                 | 28.6859   | 54.8769   |           |
| 61.8234                                                   | 87.6978   | 133.3051  |           |
| 158.6676                                                  | 213.0038  | 229.9996  |           |
| 243.4729                                                  | 270.2894  | 273.0233  |           |
| 316.1226                                                  | 328.0444  | 351.4186  |           |
| 386.4062                                                  | 400.8690  | 410.7973  |           |
| 473.9518                                                  | 510.4828  | 539.5263  |           |
| 584.2370                                                  | 601.0588  | 712.1345  |           |
| 749.9857                                                  | 839.8018  | 858.9723  |           |
| 887.9582                                                  | 917.9703  | 947.1674  |           |
| 967.4251                                                  | 975.3380  | 998.3301  |           |
| 1013.3919                                                 | 1018.8665 | 1040.4738 |           |
| 1057.3114                                                 | 1106.7937 | 1125.8868 |           |
| 1149.1402                                                 | 1166.3461 | 1193.4611 |           |
| 1197.7893                                                 | 1247.8100 | 1262.3463 |           |
| 1267.6006                                                 | 1279.1240 | 1297.0923 |           |
| 1326.2868                                                 | 1355.8978 | 1400.8484 |           |
| 1407.6994                                                 | 1414.3242 | 1425.5336 |           |
| 1427.1902                                                 | 1437.4408 | 1459.0342 |           |

|           |           |           |
|-----------|-----------|-----------|
| 1468.7588 | 1486.5690 | 1495.6940 |
| 1499.0214 | 1511.8951 | 1515.9281 |
| 1577.6367 | 1858.7028 | 2930.7478 |
| 3045.3253 | 3049.3115 | 3051.6158 |
| 3052.5359 | 3057.1552 | 3058.5660 |
| 3094.4149 | 3112.3071 | 3119.0783 |
| 3120.9620 | 3132.6484 | 3134.5359 |
| 3138.8634 | 3152.5361 | 3210.5635 |

Zero-point correction (Hartree): 0.244825

ApineneCI.A.b.ringclose.mmp

E(RM062X/Aug-CC-pVTZ) (Hartree): -616.13177562

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -1.222404 | 0.803616  | 0.638913  |
| H | -1.512935 | 0.730338  | 1.690787  |
| C | -2.457112 | 1.037903  | -0.218539 |
| C | -3.446001 | -0.074455 | -0.002864 |
| H | -2.927159 | 1.978511  | 0.083829  |
| H | -2.210128 | 1.093225  | -1.277696 |
| H | -3.822621 | -0.175125 | 1.035172  |
| C | -0.279589 | -0.391000 | 0.311768  |
| C | -0.020464 | 1.761459  | 0.516982  |
| C | -0.445475 | -1.662963 | 1.114817  |
| C | -0.213888 | -0.702029 | -1.178675 |
| H | -0.092107 | 0.195813  | -1.786613 |
| H | 0.626672  | -1.366032 | -1.381123 |
| H | -1.139971 | -1.186591 | -1.491731 |
| H | 0.409804  | -2.320723 | 0.951718  |
| H | -1.347056 | -2.193454 | 0.800539  |
| H | -0.521478 | -1.451485 | 2.182228  |
| H | 0.032463  | 2.602752  | 1.203832  |
| H | 0.091054  | 2.123357  | -0.504808 |
| C | 0.891597  | 0.560024  | 0.798630  |
| H | 1.023497  | 0.381706  | 1.867887  |
| C | 2.189941  | 0.329635  | 0.144564  |
| C | 2.684134  | 1.214968  | -0.939530 |
| H | 2.591619  | 2.250002  | -0.596894 |
| H | 3.704925  | 0.956620  | -1.194863 |
| H | 2.059277  | 1.110576  | -1.827208 |
| O | -3.805138 | -0.842175 | -0.852250 |
| O | 2.887774  | -0.614038 | 0.647681  |
| O | 3.036077  | -1.292841 | -0.654363 |

Rotational constants (GHz): 1.5766700 0.4689300 0.4320700

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i498.9382 | 55.3888   | 60.6090   |
| 68.5873   | 91.3445   | 130.7023  |
| 170.2790  | 235.6587  | 255.0675  |
| 259.3003  | 269.3225  | 287.8829  |
| 321.3614  | 349.7905  | 366.8785  |
| 378.1528  | 395.4817  | 419.8157  |
| 476.6123  | 511.3930  | 541.6482  |
| 584.8410  | 604.3226  | 717.4722  |
| 761.2685  | 847.1923  | 860.0980  |
| 870.1498  | 922.0395  | 941.1410  |
| 970.5914  | 972.1486  | 1005.4673 |
| 1010.9247 | 1017.6819 | 1041.5050 |
| 1062.4116 | 1109.4983 | 1126.5595 |
| 1149.7367 | 1167.7920 | 1189.4236 |
| 1196.6605 | 1244.9620 | 1260.5312 |
| 1277.4738 | 1288.1082 | 1298.1275 |
| 1326.1535 | 1367.7648 | 1403.4873 |
| 1408.2517 | 1417.4448 | 1427.3831 |
| 1429.2487 | 1440.7828 | 1461.6937 |
| 1469.0506 | 1487.0437 | 1494.3562 |
| 1499.3442 | 1514.2404 | 1519.0369 |
| 1578.8199 | 1860.0206 | 2929.3857 |
| 3047.3293 | 3049.9906 | 3054.0664 |
| 3055.9017 | 3058.1239 | 3082.8723 |
| 3094.2598 | 3119.2708 | 3119.8430 |
| 3126.9174 | 3127.9129 | 3137.1806 |
| 3140.9534 | 3150.7794 | 3204.1505 |

Zero-point correction (Hartree): 0.245465

ApineneCI.A.b.ringclose.mmtm

E(RM062X/Aug-CC-pVTZ) (Hartree): -616.13047660

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 1.285102  | 0.649512  | -0.601379 |
| H | 1.635927  | 0.367033  | -1.594952 |
| C | 2.444737  | 1.174750  | 0.215429  |
| C | 3.604066  | 0.226511  | 0.332914  |
| H | 2.831852  | 2.104676  | -0.216555 |
| H | 2.137084  | 1.441271  | 1.232118  |
| H | 4.457383  | 0.590203  | 0.936238  |
| C | 0.391869  | -0.510332 | -0.052314 |
| C | 0.038647  | 1.551465  | -0.709016 |
| C | 0.621799  | -1.893911 | -0.626114 |
| C | 0.347506  | -0.553365 | 1.469108  |
| H | 0.115507  | 0.420400  | 1.907749  |
| H | -0.409100 | -1.262292 | 1.804517  |
| H | 1.312359  | -0.881630 | 1.860308  |
| H | -0.214875 | -2.545909 | -0.372206 |
| H | 1.541708  | -2.323000 | -0.231811 |
| H | 0.709032  | -1.854425 | -1.712653 |
| H | -0.054553 | 2.188542  | -1.585008 |
| H | -0.080795 | 2.162081  | 0.186497  |
| C | -0.819147 | 0.280138  | -0.656957 |
| H | -1.017554 | -0.107815 | -1.662964 |
| C | -2.125079 | 0.212669  | 0.032728  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -2.869597 | 1.446342  | 0.388088  |
| H | -2.193793 | 2.101376  | 0.945224  |
| H | -3.154695 | 1.979545  | -0.520215 |
| H | -3.759176 | 1.201162  | 0.954886  |
| O | 3.643108  | -0.859240 | -0.178304 |
| O | -2.501273 | -0.953741 | 0.378229  |
| O | -3.813801 | -0.822506 | -0.285688 |

Rotational constants (GHz): 1.7488800 0.4545300 0.4072900

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i483.1951 | 28.9672   | 47.0339   |
| 79.1544   | 107.3886  | 149.6317  |
| 161.3908  | 211.0706  | 216.9150  |
| 238.9144  | 259.0277  | 286.0446  |
| 318.2647  | 333.2814  | 343.7212  |
| 368.8412  | 398.1165  | 404.8404  |
| 479.3119  | 501.4818  | 572.5135  |
| 594.2076  | 678.3105  | 709.6010  |
| 746.8175  | 789.2522  | 841.6383  |
| 888.6125  | 911.3263  | 931.8991  |
| 966.5539  | 969.3105  | 974.7572  |
| 1001.3464 | 1017.9995 | 1029.2029 |
| 1056.1086 | 1110.6628 | 1114.8067 |
| 1146.1703 | 1167.5118 | 1195.4231 |
| 1203.9842 | 1248.7954 | 1266.5886 |
| 1273.7077 | 1284.7681 | 1306.2392 |
| 1345.9400 | 1357.3706 | 1403.8096 |
| 1406.6924 | 1416.5366 | 1422.9049 |
| 1425.6435 | 1436.8828 | 1450.4277 |
| 1460.5634 | 1486.2983 | 1492.8983 |
| 1498.2702 | 1509.3167 | 1515.0917 |
| 1576.4782 | 1856.7062 | 2951.9125 |
| 3040.8541 | 3044.0299 | 3046.8530 |
| 3052.4791 | 3059.6061 | 3068.7303 |
| 3084.8998 | 3092.9725 | 3111.8974 |
| 3112.6775 | 3128.7061 | 3135.2968 |
| 3146.8324 | 3147.3415 | 3210.3773 |

Zero-point correction (Hartree): 0.244741

ApineneCI.A.b.ringclose.mmtf

E(RM062X/Aug-CC-pVTZ) (Hartree): -616.13354133

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 1.293485  | 0.680065  | -0.582408 |
| H | 1.698620  | 0.414669  | -1.560235 |
| C | 2.416802  | 1.116646  | 0.330702  |
| C | 3.510784  | 0.099099  | 0.490704  |
| H | 2.882894  | 2.036780  | -0.039781 |
| H | 2.052312  | 1.365305  | 1.332702  |
| H | 4.334674  | 0.386889  | 1.170952  |
| C | 0.313264  | -0.449350 | -0.138490 |
| C | 0.093031  | 1.633813  | -0.746793 |
| C | 0.497547  | -1.836935 | -0.713596 |
| C | 0.129876  | -0.513742 | 1.371443  |
| H | -0.031784 | 0.469271  | 1.817974  |
| H | -0.726929 | -1.141014 | 1.617506  |
| H | 1.025663  | -0.943906 | 1.824170  |
| H | -0.412077 | -2.419553 | -0.555691 |
| H | 1.332342  | -2.342769 | -0.230360 |
| H | 0.702793  | -1.793354 | -1.783809 |
| H | 0.103814  | 2.329508  | -1.582717 |
| H | -0.098565 | 2.185614  | 0.174122  |
| C | -0.811273 | 0.402879  | -0.867133 |
| H | -0.873234 | 0.028296  | -1.890889 |
| C | -2.152642 | 0.303308  | -0.272633 |
| C | -2.709109 | 1.386664  | 0.577342  |
| H | -2.581828 | 2.332616  | 0.042325  |
| H | -3.747790 | 1.182100  | 0.807912  |
| H | -2.147526 | 1.463713  | 1.509008  |
| O | 3.528246  | -0.964921 | -0.065497 |
| O | -2.830781 | -0.720290 | -0.625634 |
| O | -3.072962 | -1.125895 | 0.772629  |

Rotational constants (GHz): 1.6187100 0.4867000 0.4401000

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i497.7373 | 48.0443   | 54.8629   |
| 83.1633   | 113.4702  | 146.6715  |
| 168.3956  | 225.3475  | 244.6302  |
| 259.1343  | 266.1507  | 289.4970  |
| 318.8403  | 335.0038  | 359.9803  |
| 377.2030  | 393.6151  | 404.8097  |
| 481.9445  | 504.5493  | 576.8029  |
| 589.1797  | 676.7427  | 722.3761  |
| 748.3325  | 793.2959  | 852.5479  |
| 867.2785  | 913.7796  | 931.5847  |
| 961.1346  | 971.5995  | 975.3480  |
| 1004.6719 | 1010.5893 | 1032.3204 |
| 1059.1670 | 1109.9911 | 1114.6551 |
| 1143.4267 | 1165.8152 | 1185.0289 |
| 1202.3905 | 1246.4798 | 1270.7237 |
| 1281.3952 | 1288.1152 | 1306.6075 |
| 1345.5114 | 1368.5119 | 1405.2105 |
| 1407.8029 | 1417.1454 | 1422.1123 |
| 1426.0565 | 1440.3328 | 1450.6714 |
| 1461.8742 | 1486.4382 | 1489.5730 |
| 1497.4783 | 1509.9885 | 1515.9802 |
| 1577.3008 | 1856.2103 | 2948.8902 |
| 3041.3314 | 3048.5941 | 3049.5829 |
| 3056.6516 | 3070.0267 | 3081.3923 |
| 3086.4667 | 3090.3755 | 3113.9162 |
| 3119.7839 | 3126.5637 | 3137.2124 |
| 3144.0721 | 3147.6106 | 3205.9950 |

Zero-point correction (Hartree): 0.245184

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ApineneCI.A.b.ringclose.mppmm
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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.12843738
Electronic state : 1-A
Cartesian coordinates (Angs):
 C -1.344233 0.368594 -0.479696
 H -1.571041 0.714912 -1.491610
 C -2.594405 0.450073 0.386913
 C -3.669946 -0.387522 -0.245576
 H -2.403480 0.071499 1.390049
 H -2.933598 1.487844 0.448490
 H -4.097101 0.013753 -1.186034
 C -0.034230 1.071836 -0.010820
 C -0.591648 -0.975920 -0.554747
 C 0.263154 2.420843 -0.632142
 C 0.095165 1.130049 1.505875
 H -0.071288 0.157098 1.972928
 H 1.090547 1.473980 1.785131
 H -0.633551 1.828305 1.920158
 H 1.274771 2.742163 -0.383311
 H -0.435415 3.172628 -0.258346
 H 0.173599 2.382540 -1.718366
 H -0.814841 -1.640775 -1.384869
 H -0.692583 -1.530464 0.378076
 C 0.711498 -0.162917 -0.614347
 H 0.987232 0.064299 -1.651482
 C 1.975860 -0.607365 0.012134
 C 2.201480 -2.034908 0.344726
 H 1.350660 -2.383431 0.936990
 H 2.216575 -2.628022 -0.571083
 H 3.142163 -2.158183 0.867058
 O -4.032738 -1.449815 0.178800
 O 2.788995 0.323797 0.317328
 O 3.911390 -0.299572 -0.412092
Rotational constants (GHz): 1.4858000 0.4415800 0.3806100
Vibrational harmonic frequencies (cm-1):
i486.5689 36.3242 39.6415
 62.7782 89.0211 119.5267
168.2404 192.1613 219.8958
226.6880 263.7338 281.3962
314.7787 331.3388 342.1485
355.4904 400.6278 429.1460
479.4588 502.3929 549.3249
590.4704 601.9963 721.2332
769.3156 840.5473 864.0183
893.0611 922.5108 932.2412
966.8031 976.8032 991.9463
1003.1140 1019.1790 1033.3429
1064.5677 1097.4108 1136.7763
1146.3474 1162.1004 1195.3824
1214.6174 1248.3376 1249.9254
1270.0496 1281.6186 1299.5888
1322.9881 1355.5694 1398.8936
1406.5336 1412.6833 1421.7064
1426.2231 1437.6812 1460.2291
1473.4105 1485.2335 1494.3504
1499.2448 1508.5640 1513.8449
1576.5271 1858.6175 2932.8161
3037.4472 3050.0157 3053.3622
3054.1763 3058.4399 3059.2854
3093.1494 3113.5815 3118.6159
3120.5658 3133.8264 3136.5442
3139.6753 3153.5838 3209.5118
Zero-point correction (Hartree): 0.244708

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ApineneCI.A.b.ringclose.mppmp
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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.13138758
Electronic state : 1-A
Cartesian coordinates (Angs):
  C   -1.320917    0.434066   -0.444172
  H   -1.591130    0.906988   -1.392474
  C   -2.497470    0.501711    0.520888
  C   -3.677242   -0.176578   -0.116535
  H   -2.268164   -0.003591    1.457715
  H   -2.748136    1.546630    0.723426
  H   -4.134628    0.363297   -0.969493
  C    0.067274    0.983492   -0.006441
  C   -0.672357   -0.937379   -0.725603
  C    0.460512    2.365825   -0.479056
  C    0.319073    0.834216    1.488258
  H    0.044453   -0.153527    1.860805
  H    1.374327    0.999389    1.706043
  H   -0.276420    1.568364    2.033489
  H    1.523497    2.532804   -0.297725
  H   -0.101392    3.127624    0.065444
  H    0.266996    2.490881   -1.544950
  H   -1.022259   -1.502211   -1.585995
  H   -0.710721   -1.575418    0.157237
  C    0.671680   -0.209312   -0.856046
  H    0.841684    0.171707   -1.865354
  C    1.954233   -0.735099   -0.358718
  C    2.031920   -2.009444    0.397337
  H    1.484907   -2.769130   -0.169152
  H    3.067135   -2.283956    0.561031
  H    1.533972   -1.907741    1.362298
  O   -4.094309   -1.253068    0.211227
  O    2.984368   -0.069547   -0.715500
  O    3.446896    0.094978    0.676546
Rotational constants (GHz):    1.5243500    0.4516300    0.4020400
Vibrational harmonic frequencies (cm-1):

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|           |           |           |
|-----------|-----------|-----------|
| i497.5989 | 36.8707   | 49.1525   |
| 69.7251   | 101.0930  | 114.5073  |
| 162.2974  | 207.0257  | 242.4856  |
| 255.6494  | 269.7968  | 281.5784  |
| 323.4615  | 336.1007  | 351.0441  |
| 375.7532  | 392.7663  | 433.7962  |
| 479.4994  | 503.2272  | 547.6170  |
| 590.7522  | 600.3962  | 735.2950  |
| 772.0866  | 847.3385  | 866.9729  |
| 872.1179  | 923.8713  | 930.9173  |
| 967.7264  | 977.8673  | 996.5119  |
| 1008.4041 | 1011.8344 | 1038.1348 |
| 1068.5768 | 1095.0420 | 1137.9841 |
| 1147.4144 | 1161.0621 | 1186.5429 |
| 1215.4550 | 1246.1189 | 1251.0202 |
| 1277.4683 | 1288.9657 | 1299.5722 |
| 1322.8559 | 1367.3701 | 1401.0908 |
| 1407.9165 | 1415.5160 | 1423.1717 |
| 1426.8095 | 1440.2589 | 1460.8126 |
| 1472.2170 | 1485.2993 | 1493.0030 |
| 1497.9884 | 1509.4752 | 1517.8550 |
| 1578.1581 | 1858.7709 | 2932.9740 |
| 3047.8503 | 3050.0809 | 3055.0540 |
| 3057.7931 | 3060.5568 | 3082.7404 |
| 3094.9044 | 3118.4897 | 3119.3482 |
| 3124.6214 | 3129.8021 | 3138.6373 |
| 3141.2774 | 3153.2348 | 3207.1013 |

Zero-point correction (Hartree): 0.245226

ApineneCI.A.b.ringclose.mppm

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.12736860

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-1.329738	0.117047	-0.378093
H	-1.621961	0.373922	-1.398842
C	-2.553394	0.165556	0.526095
C	-3.586943	-0.814765	0.046910
H	-2.266860	-0.115272	1.543836
H	-2.995335	1.161733	0.545258
H	-3.264723	-1.875588	0.042268
C	-0.071324	0.960706	-0.010725
C	-0.456756	-1.157400	-0.405064
C	0.074060	2.291538	-0.719353
C	0.116454	1.120990	1.492456
H	0.060829	0.167274	2.022090
H	1.087368	1.567686	1.704262
H	-0.654269	1.776071	1.900905
H	1.061863	2.715755	-0.538197
H	-0.674294	2.998242	-0.354898
H	-0.059194	2.180432	-1.795929
H	-0.648011	-1.894707	-1.180502
H	-0.455956	-1.654275	0.565766
C	0.760408	-0.235368	-0.578604
H	0.963777	-0.049952	-1.640441
C	2.088334	-0.524384	0.005753
C	2.464092	-1.904257	0.400590
H	1.677330	-2.298053	1.050243
H	2.498698	-2.543112	-0.483363
H	3.433615	-1.909224	0.883311
O	-4.683923	-0.517092	-0.336224
O	2.822229	0.493372	0.220834
O	3.964941	-0.066143	-0.527805

Rotational constants (GHz): 1.6749200 0.4041200 0.3622000

Vibrational harmonic frequencies (cm-1):

i488.1088	38.2742	44.1802
51.8583	89.8848	125.7626
172.0301	200.4500	220.8203
227.6061	269.8929	273.1650
319.2814	331.6771	343.9769
351.5474	398.7152	430.7346
471.4377	502.6834	535.5391
594.5325	602.1310	722.8346
774.1683	840.1095	859.6272
890.9856	919.8207	930.2952
967.2136	977.7448	983.3321
1003.9500	1024.7787	1030.9052
1074.1621	1101.9044	1140.4558
1144.9640	1165.5956	1196.4137
1213.8118	1249.1880	1255.0618
1271.8093	1281.3854	1304.7911
1327.1700	1355.0466	1396.2456
1407.6483	1412.9222	1423.2675
1429.6539	1437.3226	1460.7914
1469.4032	1486.0016	1495.1555
1499.4317	1509.3749	1515.3816
1576.9414	1863.2160	2928.2029
3038.6465	3051.0329	3052.4375
3053.3573	3056.1480	3069.8702
3087.2808	3113.3397	3118.8858
3121.7445	3126.6027	3134.3105
3139.7208	3149.2065	3209.7817

Zero-point correction (Hartree): 0.244760

ApineneCI.A.b.ringclose.mppm

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.13038215

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |          |           |
|---|-----------|----------|-----------|
| C | -1.316128 | 0.165236 | -0.380018 |
| H | -1.657784 | 0.543117 | -1.346581 |
| C | -2.470122 | 0.198172 | 0.612255  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -3.590811 | -0.675861 | 0.124067  |
| H | -2.132855 | -0.189954 | 1.577566  |
| H | -2.847345 | 1.211344  | 0.750009  |
| H | -3.338284 | -1.749970 | 0.015878  |
| C | 0.020192  | 0.878918  | -0.025079 |
| C | -0.532485 | -1.148498 | -0.599742 |
| C | 0.251834  | 2.262675  | -0.591080 |
| C | 0.333530  | 0.848018  | 1.465014  |
| H | 0.178921  | -0.138605 | 1.904857  |
| H | 1.371952  | 1.134209  | 1.632622  |
| H | -0.318288 | 1.548459  | 1.989521  |
| H | 1.297465  | 2.547149  | -0.463004 |
| H | -0.367555 | 2.994772  | -0.069198 |
| H | 0.008902  | 2.301885  | -1.653340 |
| H | -0.842934 | -1.802756 | -1.410883 |
| H | -0.466736 | -1.727869 | 0.321885  |
| C | 0.721508  | -0.294860 | -0.825251 |
| H | 0.815887  | 0.037079  | -1.861423 |
| C | 2.067685  | -0.653994 | -0.348583 |
| C | 2.305344  | -1.870955 | 0.467250  |
| H | 1.824921  | -2.713807 | -0.038826 |
| H | 3.368838  | -2.026131 | 0.604447  |
| H | 1.832824  | -1.769005 | 1.444954  |
| O | -4.686791 | -0.283154 | -0.165131 |
| O | 3.008962  | 0.096588  | -0.774285 |
| O | 3.493928  | 0.379938  | 0.590480  |

Rotational constants (GHz): 1.6924000 0.4169300 0.3824700  
 Vibrational harmonic frequencies (cm-1):  
 i498.4976 41.1449 50.8837  
 61.7965 102.8031 116.8509  
 167.0995 215.0738 237.0314  
 254.9031 273.2498 275.8872  
 324.7052 336.9642 347.6570  
 376.3522 387.5755 438.0542  
 474.3566 500.6240 534.3639  
 594.8526 599.3577 736.9004  
 777.5875 849.7155 860.8037  
 871.8369 917.6868 928.3262  
 967.8406 980.8275 989.1647  
 1007.2809 1013.6740 1033.9485  
 1077.2253 1100.4255 1139.9242  
 1146.6255 1164.5734 1187.3960  
 1213.3915 1246.4461 1259.0417  
 1277.1410 1288.5538 1305.2389  
 1325.2793 1366.5938 1397.1122  
 1407.6264 1414.7616 1424.1594  
 1430.8595 1439.5609 1460.4247  
 1469.0036 1485.2321 1492.8498  
 1497.4299 1510.4222 1517.2586  
 1578.7321 1862.9887 2930.1381  
 3049.3659 3049.7435 3052.9430  
 3057.2458 3068.4037 3081.3307  
 3087.5938 3117.3873 3121.0874  
 3122.8947 3129.0083 3130.9777  
 3139.1635 3146.1043 3205.2678

Zero-point correction (Hartree): 0.245181

ApineneCI.A.b.ringclose.mptm

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E(RM062X/Aug-CC-pVT2) (Hartree): -616.13030556

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-1.398615	0.224465	-0.330664
H	-1.707106	0.385114	-1.365166
C	-2.589794	0.409231	0.579345
C	-3.738305	-0.499228	0.232824
H	-2.335450	0.220333	1.627852
H	-2.966714	1.437923	0.552441
H	-4.634732	-0.401354	0.873763
C	-0.091399	1.030553	-0.068714
C	-0.598820	-1.090876	-0.251899
C	0.112023	2.277153	-0.905475
C	0.137804	1.325672	1.409039
H	0.039654	0.431731	2.029219
H	1.136100	1.733937	1.562803
H	-0.586189	2.060722	1.764261
H	1.125567	2.660078	-0.783519
H	-0.587208	3.058485	-0.599371
H	-0.051730	2.070420	-1.963574
H	-0.862000	-1.877426	-0.952184
H	-0.604875	-1.496864	0.760519
C	0.663604	-0.257682	-0.529512
H	0.854987	-0.187174	-1.607814
C	1.986423	-0.565916	0.054012
C	2.305000	-1.934569	0.530133
H	1.511364	-2.249381	1.213420
H	2.293533	-2.627715	-0.312481
H	3.281528	-1.955826	0.998042
O	-3.721328	-1.292557	-0.668099
O	2.771585	0.427439	0.193959
O	3.870462	-0.231860	-0.539953

Rotational constants (GHz): 1.5098500 0.4488300 0.3924200
 Vibrational harmonic frequencies (cm-1):
 i487.9116 35.6902 49.5061
 78.7035 104.6706 144.6884
 164.1591 198.4136 213.1065
 216.0866 256.5018 271.1586
 314.4249 329.3597 344.3597
 353.8708 399.8304 409.4852
 475.4101 508.3490 571.4293
 598.0255 675.8217 714.0695
 734.2265 835.9107 842.4629

895.2357	921.2329	932.4522
938.3348	966.7777	978.7126
991.3752	1011.9886	1027.9228
1039.5703	1101.2397	1138.0996
1150.9996	1161.6561	1196.7421
1212.1006	1243.7600	1254.5140
1272.1813	1284.4822	1315.9920
1335.1642	1357.4719	1405.0784
1407.3106	1415.7721	1423.1796
1425.6356	1436.7548	1451.7251
1460.5685	1485.5798	1495.5449
1500.2329	1508.7615	1516.2580
1574.7737	1855.0572	2950.1953
3033.8927	3040.2546	3049.6482
3052.2942	3054.1770	3068.8874
3082.5144	3091.3760	3113.7784
3115.7565	3119.2112	3134.2413
3138.8774	3164.9931	3209.3804

Zero-point correction (Hartree): 0.244560

ApineneCI.A.b.ringclose.mptp

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.13336522

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -1.376338 | 0.278635  | -0.308930 |
| H | -1.739402 | 0.570629  | -1.296076 |
| C | -2.481828 | 0.461527  | 0.703747  |
| C | -3.724235 | -0.314869 | 0.361273  |
| H | -2.172487 | 0.149552  | 1.706854  |
| H | -2.771442 | 1.513772  | 0.803507  |
| H | -4.560765 | -0.217591 | 1.078710  |
| C | 0.009445  | 0.940908  | -0.068356 |
| C | -0.682937 | -1.093526 | -0.425595 |
| C | 0.303837  | 2.246181  | -0.775086 |
| C | 0.376766  | 1.035885  | 1.407522  |
| H | 0.176368  | 0.108730  | 1.947184  |
| H | 1.436437  | 1.267945  | 1.515138  |
| H | -0.209586 | 1.825785  | 1.880291  |
| H | 1.368296  | 2.476469  | -0.706715 |
| H | -0.251768 | 3.063847  | -0.310815 |
| H | 0.026094  | 2.196689  | -1.828320 |
| H | -1.076036 | -1.790332 | -1.159827 |
| H | -0.620076 | -1.589636 | 0.543722  |
| C | 0.612374  | -0.346354 | -0.769143 |
| H | 0.690018  | -0.120634 | -1.834939 |
| C | 1.950721  | -0.739219 | -0.300252 |
| C | 2.144820  | -1.882938 | 0.625689  |
| H | 1.597006  | -2.738685 | 0.219792  |
| H | 3.201287  | -2.090247 | 0.747117  |
| H | 1.712433  | -1.656822 | 1.601047  |
| O | -3.839477 | -1.006844 | -0.613163 |
| O | 2.921354  | -0.096349 | -0.826758 |
| O | 3.467857  | 0.292336  | 0.488437  |

Rotational constants (GHz): 1.5617900 0.4578800 0.4142000

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i496.0347 | 43.7774   | 60.9859   |
| 92.9669   | 107.1642  | 130.6979  |
| 169.6442  | 201.3425  | 240.1152  |
| 254.4068  | 260.7641  | 277.0794  |
| 313.3746  | 337.2938  | 347.4815  |
| 374.8407  | 392.3796  | 415.6618  |
| 477.4342  | 511.6790  | 576.3317  |
| 592.6900  | 672.8234  | 718.9051  |
| 748.4220  | 836.4127  | 852.3887  |
| 873.8708  | 920.8805  | 929.9259  |
| 937.8089  | 965.8840  | 984.2942  |
| 998.0708  | 1008.2810 | 1025.3889 |
| 1046.0036 | 1098.3382 | 1139.6564 |
| 1152.9135 | 1160.8475 | 1187.6344 |
| 1214.6489 | 1241.0768 | 1262.5458 |
| 1280.6850 | 1288.6617 | 1318.2187 |
| 1336.2868 | 1369.2655 | 1405.6523 |
| 1408.1643 | 1417.3763 | 1422.6118 |
| 1427.7425 | 1439.2015 | 1452.8252 |
| 1460.5291 | 1484.9135 | 1493.6860 |
| 1498.8243 | 1509.0647 | 1516.8620 |
| 1577.2000 | 1854.7955 | 2950.5969 |
| 3040.5931 | 3047.9135 | 3050.1382 |
| 3053.0942 | 3069.8136 | 3081.3123 |
| 3084.7630 | 3093.3170 | 3116.4128 |
| 3118.4082 | 3120.9308 | 3131.0636 |
| 3138.5960 | 3161.6654 | 3206.7154 |

Zero-point correction (Hartree): 0.245092

ApineneCI.A.b.ringclose.mtmm

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.12543897

Electronic state : 1-A

Cartesian coordinates (Angs):

C	1.247022	0.322896	1.104083
H	1.220840	0.959619	1.990597
C	2.708744	0.105426	0.732631
C	2.992009	-0.929358	-0.322483
H	3.170009	1.042800	0.418408
H	3.242627	-0.237393	1.626613
H	2.514243	-1.917247	-0.173588
C	0.249998	0.933035	0.075597
C	0.271985	-0.854166	1.338449
C	0.061290	2.434814	0.133353
C	0.509384	0.473698	-1.353743
H	0.601048	-0.612743	-1.433563

H	-0.308427	0.787200	-2.002609
H	1.433193	0.911300	-1.733868
H	-0.778210	2.740688	-0.491129
H	0.958123	2.941703	-0.229055
H	-0.131217	2.768663	1.153565
H	0.161459	-1.221876	2.355362
H	0.467149	-1.696633	0.678082
C	-0.836069	0.054187	0.781387
H	-1.301399	0.645310	1.578687
C	-1.968915	-0.446259	-0.027637
C	-2.325190	-1.886059	-0.044817
H	-1.422481	-2.455273	-0.285040
H	-2.645510	-2.199029	0.950224
H	-3.123186	-2.069911	-0.753448
O	3.721998	-0.754474	-1.258632
O	-2.531743	0.424460	-0.766023
O	-3.880231	0.125455	-0.244113
Rotational constants (GHz):			
	1.4422200	0.4618800	0.4315600
Vibrational harmonic frequencies (cm-1):			
i484.7155	26.4902		53.7252
83.7627	86.8766		125.0628
182.1132	211.4204		218.5160
243.7024	259.3785		269.1207
329.8604	338.8532		346.2511
369.9852	401.6311		411.4046
472.4380	496.7178		577.5705
587.8145	618.4098		704.1040
732.8201	819.4892		839.3849
888.9185	909.8561		928.5561
964.2119	974.9012		998.1183
999.0775	1020.2637		1034.6423
1058.5280	1112.9382		1128.3934
1143.2898	1168.3226		1194.5474
1219.3524	1246.0339		1257.4377
1269.8415	1294.5659		1319.1487
1335.4827	1358.8585		1399.6913
1406.3042	1413.3510		1423.8963
1437.9764	1441.8163		1452.8852
1460.2872	1484.0368		1494.5271
1501.9266	1506.6997		1515.2398
1577.7849	1859.2117		2939.4493
3035.9100	3043.1065		3049.2536
3051.9550	3052.3785		3072.4263
3105.5898	3110.7271		3113.6446
3117.5612	3120.7492		3134.2263
3136.9363	3158.5411		3210.6360
Zero-point correction (Hartree): 0.244814			
ApineneCI.A.b.ringclose.mtmp			
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E(RM062X/Aug-CC-pVT2) (Hartree): -616.12834211			
Electronic state : 1-A			
Cartesian coordinates (Angs):			
C	1.245100	0.588790	1.011371
H	1.252150	1.407889	1.733569
C	2.682743	0.346093	0.570408
C	2.943449	-0.889413	-0.248199
H	3.067509	1.204393	0.017859
H	3.301877	0.233293	1.468213
H	2.515150	-1.831589	0.146183
C	0.138256	0.906514	-0.032684
C	0.352145	-0.536408	1.585095
C	-0.165703	2.360543	-0.319855
C	0.301307	0.127068	-1.331098
H	0.510793	-0.931341	-1.163873
H	-0.610293	0.198204	-1.924937
H	1.134834	0.536079	-1.903925
H	-1.097910	2.442438	-0.881062
H	0.632458	2.803042	-0.919247
H	-0.264163	2.934755	0.602029
H	0.361060	-0.690279	2.661510
H	0.511179	-1.491296	1.087691
C	-0.850791	0.207024	0.988875
H	-1.226332	0.988340	1.652848
C	-2.012758	-0.450165	0.369267
C	-2.069955	-1.921386	0.180789
H	-1.813663	-2.392968	1.134278
H	-3.052514	-2.213359	-0.170411
H	-1.324593	-2.239453	-0.549124
O	3.611358	-0.907709	-1.244714
O	-2.991106	0.325911	0.102631
O	-3.030290	-0.091965	-1.312344
Rotational constants (GHz):			
	1.3580700	0.4896500	0.4697100
Vibrational harmonic frequencies (cm-1):			
i496.1923	53.3892		62.9762
86.6623	103.1904		117.7639
187.5943	230.1406		245.7247
254.4528	266.1204		276.0745
322.3239	344.2205		371.2209
378.2230	404.0658		407.9668
472.4276	499.6644		580.1418
582.9116	625.7659		703.0166
748.0761	817.0038		848.5682
867.9538	908.2408		928.7730
965.6937	975.9465		998.4498
1004.7839	1011.2922		1038.7096
1062.9455	1112.5026		1129.9249
1145.0604	1168.2841		1187.2638
1218.2838	1243.6494		1253.1323
1288.7393	1294.8318		1318.8421
1335.0194	1369.5859		1400.5646
1407.6313	1415.4077		1425.4142

1436.9782	1440.7142	1450.2862
1461.7589	1484.4767	1493.7162
1499.6857	1508.5559	1520.3242
1578.4860	1859.2945	2937.6177
3034.9014	3048.6808	3049.8563
3054.6147	3070.3126	3084.0252
3102.8201	3111.0238	3116.4628
3120.4030	3123.4978	3129.8409
3138.6982	3156.3531	3205.7866

Zero-point correction (Hartree): 0.245326

ApineneCI.A.b.ringclose.mttm

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.12676297

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 1.383669  | 0.559730  | 0.905339  |
| H | 1.415418  | 1.286676  | 1.719990  |
| C | 2.812515  | 0.363211  | 0.427009  |
| C | 3.178472  | -0.830942 | -0.413559 |
| H | 3.147308  | 1.247782  | -0.127472 |
| H | 3.495450  | 0.311719  | 1.283852  |
| H | 4.231333  | -0.817802 | -0.757678 |
| C | 0.277273  | 1.046560  | -0.076403 |
| C | 0.476677  | -0.611589 | 1.345843  |
| C | 0.028076  | 2.541282  | -0.105843 |
| C | 0.420591  | 0.497121  | -1.489758 |
| H | 0.521182  | -0.587271 | -1.503402 |
| H | -0.447105 | 0.777546  | -2.087555 |
| H | 1.305909  | 0.918783  | -1.971256 |
| H | -0.878450 | 2.767520  | -0.667663 |
| H | 0.863371  | 3.054429  | -0.588586 |
| H | -0.083494 | 2.944042  | 0.901380  |
| H | 0.457810  | -0.852605 | 2.405768  |
| H | 0.673129  | -1.509874 | 0.770456  |
| C | -0.711961 | 0.189164  | 0.791671  |
| H | -1.163081 | 0.833769  | 1.552406  |
| C | -1.846396 | -0.439227 | 0.079937  |
| C | -2.016277 | -1.911160 | 0.046470  |
| H | -1.074553 | -2.345458 | -0.303866 |
| H | -2.183809 | -2.288374 | 1.056541  |
| H | -2.851813 | -2.181884 | -0.586560 |
| O | 2.470929  | -1.757578 | -0.700254 |
| O | -2.570734 | 0.363934  | -0.592324 |
| O | -3.830749 | -0.104343 | 0.022504  |

Rotational constants (GHz): 1.3579900 0.5304700 0.4587000

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i473.8706 | 31.0359   | 49.8190   |
| 97.8834   | 111.5793  | 130.9801  |
| 180.2992  | 198.6032  | 223.7866  |
| 229.8932  | 247.9657  | 272.2495  |
| 322.0065  | 327.2470  | 337.6669  |
| 366.8608  | 402.8639  | 410.3509  |
| 479.1954  | 499.5939  | 571.9883  |
| 592.4865  | 677.4709  | 730.8914  |
| 753.4158  | 781.7465  | 841.8341  |
| 885.4752  | 895.4174  | 939.4949  |
| 946.4630  | 967.8059  | 983.3992  |
| 1001.9799 | 1016.2818 | 1021.0262 |
| 1055.2060 | 1087.0130 | 1126.2840 |
| 1157.8422 | 1167.8080 | 1195.8154 |
| 1228.5981 | 1250.6828 | 1259.8513 |
| 1276.5569 | 1297.1307 | 1329.1155 |
| 1354.8028 | 1376.7840 | 1405.9475 |
| 1406.7406 | 1412.5929 | 1423.7842 |
| 1433.1725 | 1437.9178 | 1446.9552 |
| 1459.2379 | 1485.2393 | 1493.4906 |
| 1505.0018 | 1510.7937 | 1513.1877 |
| 1577.0702 | 1859.3301 | 2936.3833 |
| 3029.4478 | 3046.8436 | 3047.7683 |
| 3054.7566 | 3056.8077 | 3060.0335 |
| 3065.5392 | 3111.6368 | 3116.0219 |
| 3116.3655 | 3121.1273 | 3134.1315 |
| 3149.7696 | 3189.5860 | 3212.6552 |

Zero-point correction (Hartree): 0.244926

ApineneCI.A.b.ringclose.mtpp

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.12933370

Electronic state : 1-A

Cartesian coordinates (Angs):

C	1.369307	0.673108	0.828399
H	1.418064	1.460599	1.584361
C	2.759552	0.539891	0.228709
C	3.152626	-0.700162	-0.529561
H	2.962746	1.389500	-0.433066
H	3.520719	0.624904	1.014266
H	4.146072	-0.620368	-1.013307
C	0.148568	1.000600	-0.077320
C	0.583682	-0.514314	1.431174
C	-0.238074	2.456613	-0.228548
C	0.203066	0.319490	-1.438226
H	0.450362	-0.737390	-1.363905
H	-0.757979	0.420924	-1.942378
H	0.972408	0.794904	-2.051750
H	-1.226101	2.533109	-0.685339
H	0.474618	2.974266	-0.874714
H	-0.261238	2.965531	0.735741
H	0.701518	-0.704172	2.495538
H	0.752687	-1.429894	0.873468
C	-0.702925	0.196889	0.990546
H	-1.058763	0.921223	1.726421

C	-1.880271	-0.494895	0.441187
C	-1.870541	-1.954996	0.179484
H	-1.520464	-2.452613	1.089176
H	-2.856985	-2.288842	-0.118597
H	-1.154762	-2.194587	-0.607703
O	2.529421	-1.722386	-0.616829
O	-2.923391	0.231914	0.311662
O	-3.070135	-0.108334	-1.117743

Rotational constants (GHz): 1.3172500 0.5555000 0.4914000

Vibrational harmonic frequencies (cm-1):

i494.3045	47.2947	69.7973
83.5314	112.3944	116.6693
188.6309	200.3192	239.1294
245.9025	253.3728	275.4558
320.8811	326.8540	345.6095
375.8105	395.1530	405.1924
481.9271	504.2472	575.2846
589.6190	677.3444	744.4550
755.8065	783.8309	850.9575
870.2657	898.5389	939.2538
941.7324	969.7614	983.1495
1006.6087	1011.1076	1022.8456
1057.5719	1085.7414	1128.2760
1159.0390	1167.8768	1190.1152
1225.4202	1247.0568	1259.8505
1289.2100	1298.9442	1326.9929
1363.4093	1379.1128	1406.0109
1408.2341	1414.8440	1424.0925
1434.6243	1437.5573	1448.5312
1460.1281	1485.0845	1492.7120
1504.9437	1511.9267	1518.1349
1576.6556	1860.1199	2935.2584
3029.8221	3046.1824	3048.3312
3053.7306	3059.0592	3061.1452
3080.0199	3110.5615	3116.0499
3116.8392	3126.3113	3130.0228
3161.1430	3182.6790	3209.0147

Zero-point correction (Hartree): 0.245215

Population analysis as 298K (%)

Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)

Compound	Qtot	Erel	Erel2	n*Q*MB	%
TS.SOZ.b.CI.A.b	3.477e+42	0.00	0.00	3.477e+42	94.7
TS.SOZ.a.CI.A.b	3.057e+42	1.64	1.64	1.930e+41	5.26
Total				3.670e+42	100

TS.SOZ.a.CI.A.b

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E(RM062X/Aug-CC-pVT2) (Hartree): -616.14514449

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 1.211713  | 0.772957  | -0.930877 |
| H | 2.105138  | 1.148762  | -1.432963 |
| C | 0.309994  | 1.959101  | -0.583733 |
| C | -1.153613 | 1.692595  | -0.258943 |
| H | 0.277790  | 2.627407  | -1.451193 |
| H | 0.746551  | 2.537772  | 0.231792  |
| H | -1.653549 | 2.533967  | 0.238818  |
| C | 1.518954  | -0.222408 | 0.227314  |
| C | 0.483248  | -0.381797 | -1.661729 |
| C | 2.767059  | -1.049868 | -0.123540 |
| C | 1.723525  | 0.257415  | 1.661901  |
| H | 1.201490  | 1.175724  | 1.891460  |
| H | 1.370376  | -0.495347 | 2.368554  |
| H | 2.789717  | 0.404511  | 1.842569  |
| H | 2.907744  | -1.835559 | 0.621259  |
| H | 3.647248  | -0.406924 | -0.099375 |
| H | 2.720609  | -1.519846 | -1.103952 |
| H | 1.153948  | -0.961497 | -2.287030 |
| H | -0.421457 | -0.140377 | -2.201330 |
| C | 0.295810  | -1.069544 | -0.268933 |
| H | 0.504497  | -2.144595 | -0.286753 |
| C | -1.109032 | -1.018267 | 0.246886  |
| C | -2.042678 | -2.065958 | -0.250633 |
| H | -1.713536 | -3.050711 | 0.083085  |
| H | -2.015136 | -2.050450 | -1.339921 |
| H | -3.052568 | -1.867122 | 0.092533  |
| O | -1.832942 | 0.876768  | -0.897119 |
| O | -0.924403 | 0.828101  | 1.486189  |
| O | -1.567497 | -0.355002 | 1.221701  |

Rotational constants (GHz): 1.1346400 0.8167600 0.7324900

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i237.9597 | 92.9630   | 112.0365  |
| 123.0148  | 181.7651  | 223.1985  |
| 226.0170  | 253.7382  | 267.5231  |
| 282.2527  | 309.8027  | 329.6924  |
| 382.1066  | 401.4805  | 424.9827  |
| 443.5105  | 469.5835  | 480.7095  |
| 512.9380  | 559.3064  | 635.0212  |
| 660.4276  | 730.7750  | 769.4572  |
| 795.8667  | 861.9333  | 872.9091  |
| 913.3538  | 921.0461  | 954.1390  |
| 971.8689  | 987.8774  | 996.9443  |
| 1021.7462 | 1037.9930 | 1055.0332 |
| 1071.9791 | 1093.8071 | 1106.8406 |
| 1127.5917 | 1166.1369 | 1175.2477 |
| 1208.4970 | 1235.6723 | 1250.7296 |
| 1264.1827 | 1281.1797 | 1311.5467 |
| 1338.3263 | 1384.0070 | 1392.6963 |
| 1397.3915 | 1405.5298 | 1420.9843 |

|           |           |           |
|-----------|-----------|-----------|
| 1429.0875 | 1457.3271 | 1464.5443 |
| 1477.0527 | 1484.3061 | 1491.3761 |
| 1495.5146 | 1512.0771 | 1516.6344 |
| 1595.4899 | 1644.8594 | 3016.2872 |
| 3037.9110 | 3043.0400 | 3056.6892 |
| 3062.5659 | 3070.3924 | 3075.5015 |
| 3102.0665 | 3114.8725 | 3123.0600 |
| 3133.8263 | 3141.7972 | 3153.5556 |
| 3192.3938 | 3215.7781 | 3216.7355 |

Zero-point correction (Hartree): 0.248822

TS.SOZ.b.CI.A.b

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E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -615.22084543
E(CCSD/Aug-CC-pVTZ) (Hartree): -615.09711984
T1 diagnostic: 0.021172
E(MP2/Aug-CC-pVTZ) (Hartree): -615.03208773
E(MP3/Aug-CC-pVTZ) (Hartree): -615.08050313
E(RHF/Aug-CC-pVTZ) (Hartree): -612.57572571
E(RM062X/Aug-CC-pVTZ) (Hartree): -616.14730661
Electronic state : 1-A

Cartesian coordinates (Angs):

C	-1.103771	-1.277563	-0.333008
H	-1.953417	-1.951211	-0.463143
C	-0.025813	-2.037472	0.446505
C	1.238268	-1.331507	0.911245
H	0.275349	-2.896855	-0.155975
H	-0.464786	-2.440451	1.366772
H	2.101054	-1.997367	1.039650
C	-1.516221	0.150850	0.143835
C	-0.568407	-0.633943	-1.630479
C	-2.892552	0.502283	-0.434391
C	-1.562429	0.519296	1.617664
H	-0.630022	0.342707	2.135977
H	-1.846989	1.568600	1.731306
H	-2.348111	-0.072174	2.093895
H	-3.098094	1.564790	-0.294625
H	-3.661177	-0.058315	0.099286
H	-2.989327	0.275411	-1.493780
H	-1.350130	-0.526516	-2.376470
H	0.311526	-1.062893	-2.083470
C	-0.415753	0.694809	-0.855216
H	-0.756487	1.589086	-1.388805
C	0.929821	1.114036	-0.356248
C	1.057843	2.457966	0.268855
H	0.430978	2.462837	1.161399
H	0.693508	3.231784	-0.406583
H	2.088580	2.649255	0.549508
O	1.213092	-0.251680	1.502653
O	2.041243	0.577920	-0.645928
O	2.039619	-0.780142	-0.880165

Rotational constants (GHz): 1.1391100 0.8273800 0.7218300

Vibrational harmonic frequencies (cm-1):

i221.6340	91.7349	130.8309
142.1123	173.3756	186.8268
189.8277	246.3416	259.9707
273.6449	302.0069	353.3750
368.2885	381.9508	407.8298
430.7738	460.1624	491.6397
508.6556	550.4250	617.3526
650.1096	720.4658	760.7904
784.5267	851.2543	877.0516
925.0963	935.3088	945.5972
961.0907	983.9475	1000.1681
1008.8580	1029.0155	1039.9369
1065.8773	1089.8075	1112.0338
1144.1677	1159.4466	1171.0892
1221.6378	1234.0561	1255.6586
1268.1112	1285.0906	1310.3059
1335.7491	1385.6523	1392.7712
1399.0211	1405.7772	1419.9363
1424.6970	1456.1096	1458.9238
1472.9984	1481.3278	1494.8101
1497.2491	1516.4598	1531.1872
1579.8134	1679.6895	3024.1595
3036.3422	3037.4040	3046.3773
3060.3057	3064.7196	3075.5731
3093.7903	3096.9652	3122.7897
3129.8852	3140.6175	3156.6977
3189.6551	3226.1645	3233.7071

Zero-point correction (Hartree): 0.248377

E-pinonaldehyde-K-oxide
#####

Population analysis as 298K (%)
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)

Compound	Qtot	Erel	Erel2	n*Q*MB	%
ApineneCI.A.a.pmt	2.083e+44	0.00	0.00	2.083e+44	57.8
ApineneCI.A.a.ppt	2.847e+44	0.87	0.87	6.578e+43	18.3
ApineneCI.A.a.pmp	2.804e+44	1.45	1.45	2.427e+43	6.74
ApineneCI.A.a.ppm	6.958e+44	2.41	2.41	1.188e+43	3.3
ApineneCI.A.a.ppp	5.938e+44	2.42	2.42	9.978e+42	2.77
ApineneCI.A.a.pmm	8.065e+44	2.61	2.61	9.834e+42	2.73
ApineneCI.A.a.mpt	3.607e+44	2.28	2.28	7.679e+42	2.13
ApineneCI.A.a.mmt	3.088e+44	2.23	2.23	7.094e+42	1.97
ApineneCI.A.a.tmt	1.947e+44	2.20	2.20	4.732e+42	1.31
ApineneCI.A.a.tpt	2.654e+44	2.61	2.61	3.260e+42	0.905
ApineneCI.A.a.mpm	7.230e+44	3.69	3.69	1.421e+42	0.395

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ApineneCI.A.a.mmp 4.488e+44 3.42 3.42 1.384e+42 0.384
ApineneCI.A.a.tmp 2.872e+44 3.31 3.31 1.077e+42 0.299
ApineneCI.A.a.tpm 5.544e+44 3.72 3.72 1.041e+42 0.289
ApineneCI.A.a.mpp 6.855e+44 4.26 4.26 5.123e+41 0.142
ApineneCI.A.a.mmm 6.848e+44 4.41 4.41 3.992e+41 0.111
ApineneCI.A.a.ptm 2.369e+44 3.83 3.83 3.653e+41 0.101
ApineneCI.A.a.tpp 5.787e+44 4.40 4.40 3.431e+41 0.0953
ApineneCI.A.a.tmm 4.776e+44 4.49 4.49 2.439e+41 0.0677
ApineneCI.A.a.ptt 2.146e+44 4.50 4.50 1.074e+41 0.0298
ApineneCI.A.a.ptp 2.145e+44 4.50 4.50 1.074e+41 0.0298
ApineneCI.A.a.mtp 3.343e+44 5.07 5.07 6.387e+40 0.0177
ApineneCI.A.a.mtt 3.335e+44 5.07 5.07 6.364e+40 0.0177
ApineneCI.A.a.ttt 1.752e+44 4.73 4.73 5.935e+40 0.0165
ApineneCI.A.a.ttp 1.752e+44 4.73 4.73 5.935e+40 0.0165
ApineneCI.A.a.ttm 2.416e+44 5.56 5.56 2.032e+40 0.00564
ApineneCI.A.a.mtm 3.148e+44 5.73 5.73 1.987e+40 0.00552
Total 3.601e+44 100

ApineneCI.A.a.mmm
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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.16351459
Electronic state : 1-A
Cartesian coordinates (Angs):
C -1.302313 0.645373 0.378294
H -1.697817 0.639118 1.396782
C -2.451070 0.851780 -0.602305
C -3.497415 -0.212343 -0.415180
H -2.914758 1.823943 -0.435325
H -2.074335 0.808506 -1.627058
H -3.213846 -1.231145 -0.745756
C -0.317506 -0.557275 0.228661
C -0.103691 1.610944 0.311224
C -0.578106 -1.766349 1.105903
C -0.115024 -0.974794 -1.222694
H 0.134302 -0.130673 -1.868386
H 0.689547 -1.703447 -1.302666
H -1.024925 -1.435396 -1.610897
H 0.273016 -2.448219 1.076832
H -1.458252 -2.312973 0.761551
H -0.748448 -1.471953 2.142214
H -0.119526 2.486806 0.954848
H 0.097704 1.921584 -0.714576
C 0.788003 0.425329 0.727515
H 0.843482 0.376371 1.819823
C 2.173862 0.343418 0.198621
C 3.032043 1.510935 -0.062703
H 2.530157 2.440043 0.188291
H 3.962824 1.383310 0.494254
H 3.332681 1.487265 -1.113612
O -4.569977 -0.021232 0.087813
O 2.619211 -0.806743 -0.012070
O 3.902703 -0.908930 -0.488285
Rotational constants (GHz): 1.8287900 0.4040200 0.3692200
Vibrational harmonic frequencies (cm-1):
28.7222 31.6119 67.5869
76.3753 129.3067 169.3207
206.8445 223.8552 231.4423
255.2906 281.6974 303.0758
311.7617 327.1339 342.4504
389.4604 407.0700 432.1507
505.2814 532.0634 535.7773
591.0682 675.6973 723.6641
775.0580 866.1071 907.6280
929.5382 937.4583 957.3310
966.9884 977.0489 1005.4471
1010.9525 1030.7124 1042.7407
1077.7573 1104.5397 1132.2166
1152.6784 1179.0490 1194.3431
1203.7324 1254.9984 1269.8298
1280.7300 1285.3044 1305.2069
1329.9047 1366.6512 1388.3309
1400.9737 1413.2812 1421.9207
1435.7030 1441.1809 1473.1361
1481.3967 1486.0049 1496.1820
1501.2013 1508.3140 1516.1714
1626.8056 1860.4242 2936.9325
3047.6460 3051.4342 3056.8204
3057.8627 3063.9333 3071.8344
3086.1447 3105.7098 3120.8003
3122.5687 3128.0065 3129.2063
3148.4784 3149.9696 3184.7154
Zero-point correction (Hartree): 0.246579

ApineneCI.A.a.mmp
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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.16502079
Electronic state : 1-A
Cartesian coordinates (Angs):
C -1.268353 0.873941 0.500866
H -1.589358 0.977341 1.541292
C -2.464811 1.050389 -0.422844
C -3.529106 0.046364 -0.076109
H -2.879362 2.052800 -0.280056
H -2.188692 0.930333 -1.469425
H -3.942048 0.133316 0.949327
C -0.387033 -0.407098 0.388312
C -0.013070 1.737524 0.274924
C -0.685546 -1.518186 1.375423
C -0.326437 -0.950906 -1.034247
H -0.050084 -0.183168 -1.759944
H 0.408018 -1.751649 -1.103114
H -1.299755 -1.350440 -1.322056

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H	0.092372	-2.281970	1.338459
H	-1.637177	-1.996253	1.133293
H	-0.743709	-1.135531	2.395657
H	0.081832	2.660403	0.841958
H	0.134837	1.949329	-0.784376
C	0.820582	0.522805	0.728200
H	0.956021	0.553129	1.814026
C	2.149748	0.283862	0.107928
C	3.045381	1.344063	-0.383671
H	2.621990	2.331007	-0.226509
H	4.013555	1.229491	0.108680
H	3.249054	1.157286	-1.441589
O	-3.911658	-0.823809	-0.808621
O	2.511224	-0.911309	0.026692
O	3.740982	-1.161379	-0.529108
Rotational constants (GHz): 1.6529200 0.4357100 0.3954300			
Vibrational harmonic frequencies (cm-1):			
29.9594	53.2388	60.3724	
84.6699	122.8781	148.2434	
200.7853	226.4376	239.4192	
263.8110	271.2258	307.9134	
314.3982	325.2509	343.3918	
397.9134	410.7418	440.9135	
504.4958	522.2940	543.2542	
593.4904	675.4254	717.5654	
769.9433	858.4921	906.5006	
917.2681	935.0784	956.9596	
969.2486	990.2979	1007.4875	
1019.2543	1035.6532	1046.0633	
1064.1498	1106.6252	1128.2339	
1158.0924	1179.1707	1196.0015	
1202.6728	1252.5687	1266.1220	
1280.2315	1284.0029	1303.2820	
1328.1879	1368.9579	1389.7833	
1405.1566	1414.2153	1426.7154	
1428.4628	1441.9992	1468.8732	
1481.6599	1487.0203	1495.7683	
1501.1376	1511.5222	1515.8076	
1625.3658	1859.2931	2927.9711	
3047.9417	3050.6608	3052.9624	
3055.4647	3056.4415	3058.1670	
3086.2831	3105.4130	3118.9070	
3124.5353	3126.4349	3135.3021	
3146.5250	3147.8048	3184.6529	
Zero-point correction (Hartree): 0.246513			
ApineneCI.A.a.mmt			
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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.16676369			
Electronic state : 1-A			
Cartesian coordinates (Angs):			
C	1.327602	0.772551	-0.418130
H	1.756679	0.744868	-1.421021
C	2.411130	1.091527	0.587429
C	3.584342	0.153855	0.554102
H	2.803475	2.102216	0.426050
H	2.024782	1.096944	1.611871
H	4.378219	0.357430	1.297576
C	0.418764	-0.486878	-0.237443
C	0.070024	1.663267	-0.402742
C	0.733743	-1.696408	-1.095798
C	0.267728	-0.887329	1.223894
H	-0.043482	-0.053447	1.857027
H	-0.471922	-1.678289	1.331993
H	1.221382	-1.263919	1.598943
H	-0.099421	-2.400859	-1.066299
H	1.631995	-2.198174	-0.739661
H	0.902918	-1.405276	-2.133560
H	0.029238	2.504373	-1.090877
H	-0.153600	2.015862	0.605485
C	-0.751593	0.408381	-0.752738
H	-0.822298	0.308843	-1.840894
C	-2.122988	0.276071	-0.198845
C	-3.049469	1.406103	-0.013013
H	-2.607052	2.342230	-0.339034
H	-3.974960	1.181177	-0.547342
H	-3.339191	1.443729	1.040369
O	3.694046	-0.763849	-0.212598
O	-2.496771	-0.879224	0.102374
O	-3.768832	-1.019996	0.601358
Rotational constants (GHz): 1.7103200 0.4461800 0.4022700			
Vibrational harmonic frequencies (cm-1):			
31.2264	47.2422	73.4123	
105.7307	143.8749	149.8954	
195.4621	219.2340	239.0429	
247.6679	286.4556	304.3031	
313.7249	328.4976	333.5563	
379.2896	395.5713	443.4083	
507.9628	518.9434	582.6305	
654.0065	686.8292	733.0924	
751.0444	797.3237	907.9148	
911.3673	932.6590	940.1158	
967.2033	971.5854	993.0734	
1008.4048	1031.4676	1042.9261	
1058.6407	1109.4263	1115.0093	
1154.8967	1178.8458	1196.7345	
1209.8309	1253.2442	1272.2677	
1282.5383	1289.6585	1307.8419	
1344.5608	1371.8404	1390.0733	
1405.9618	1415.9982	1422.8088	
1426.4326	1440.7944	1450.7252	
1481.1159	1484.6784	1493.1685	

1499.0978	1507.5430	1514.0851
1628.8614	1856.3025	2948.5529
3041.4199	3046.0503	3050.7339
3056.1409	3057.6384	3070.3489
3076.7637	3089.6208	3106.8569
3114.1799	3122.7399	3141.6611
3146.3127	3147.7821	3184.1874

Zero-point correction (Hartree): 0.246361

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.16451757

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -1.398915 | 0.352266  | -0.466249 |
| H | -1.723129 | 0.667707  | -1.461963 |
| C | -2.570030 | 0.427462  | 0.504853  |
| C | -3.685353 | -0.428036 | -0.026267 |
| H | -2.287654 | 0.061960  | 1.490977  |
| H | -2.915865 | 1.461784  | 0.585792  |
| H | -4.197825 | -0.037515 | -0.928101 |
| C | -0.065463 | 1.086809  | -0.133530 |
| C | -0.624382 | -0.975684 | -0.579020 |
| C | 0.142438  | 2.432497  | -0.798593 |
| C | 0.189992  | 1.179150  | 1.365229  |
| H | 0.106585  | 0.210510  | 1.861387  |
| H | 1.187554  | 1.568636  | 1.560225  |
| H | -0.534367 | 1.854117  | 1.823560  |
| H | 1.162618  | 2.784761  | -0.640567 |
| H | -0.538985 | 3.174798  | -0.377708 |
| H | -0.039131 | 2.374776  | -1.872684 |
| H | -0.911128 | -1.672927 | -1.362092 |
| H | -0.606438 | -1.501965 | 0.375891  |
| C | 0.649275  | -0.133927 | -0.793484 |
| H | 0.784062  | 0.063404  | -1.861851 |
| C | 1.943135  | -0.629335 | -0.256256 |
| C | 2.314928  | -2.050409 | -0.159176 |
| H | 1.529830  | -2.696184 | -0.539346 |
| H | 3.259001  | -2.194220 | -0.689173 |
| H | 2.547088  | -2.273056 | 0.885816  |
| O | -3.996360 | -1.492421 | 0.432528  |
| O | 2.755962  | 0.246703  | 0.114960  |
| O | 3.965902  | -0.180700 | 0.603111  |

Rotational constants (GHz): 1.4454100 0.4365400 0.3771400

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| 30.9254   | 37.9953   | 62.9509   |
| 85.1807   | 110.7676  | 167.0156  |
| 171.0927  | 212.3184  | 231.4061  |
| 258.3164  | 285.2934  | 306.3266  |
| 316.5095  | 324.1230  | 334.9868  |
| 367.2895  | 420.8568  | 450.6737  |
| 504.2251  | 530.2580  | 559.4098  |
| 584.1367  | 672.2536  | 740.7923  |
| 779.1458  | 866.3759  | 907.2719  |
| 925.3922  | 927.7764  | 944.7454  |
| 967.8933  | 989.9429  | 1005.4485 |
| 1006.4729 | 1034.3792 | 1047.1284 |
| 1066.5058 | 1099.3830 | 1136.8029 |
| 1150.7497 | 1180.0276 | 1197.2850 |
| 1217.6715 | 1247.9531 | 1257.7494 |
| 1277.6538 | 1288.6777 | 1302.1923 |
| 1323.9454 | 1367.9955 | 1389.3900 |
| 1402.8057 | 1412.8184 | 1424.2463 |
| 1427.7577 | 1441.7851 | 1473.0781 |
| 1481.6406 | 1485.5805 | 1495.3935 |
| 1499.9714 | 1508.6634 | 1515.7517 |
| 1626.0938 | 1859.4077 | 2932.2318 |
| 3047.5052 | 3049.5231 | 3055.4522 |
| 3056.5648 | 3058.4589 | 3059.9453 |
| 3088.5242 | 3105.5851 | 3118.2683 |
| 3123.5996 | 3129.1345 | 3138.1962 |
| 3147.5536 | 3150.8133 | 3184.9933 |

Zero-point correction (Hartree): 0.246435

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.16359400

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-1.375229	0.096040	-0.377265
H	-1.754197	0.276564	-1.386049
C	-2.523648	0.193631	0.617524
C	-3.575332	-0.826775	0.285078
H	-2.152818	-0.014949	1.625051
H	-2.977391	1.184610	0.604467
H	-3.243870	-1.883005	0.345626
C	-0.099836	0.968503	-0.173460
C	-0.487373	-1.166917	-0.389391
C	-0.034552	2.254627	-0.972486
C	0.197534	1.230494	1.297207
H	0.220006	0.312891	1.888337
H	1.161907	1.721767	1.411757
H	-0.568647	1.882991	1.718280
H	0.956614	2.703565	-0.895765
H	-0.762011	2.975397	-0.594190
H	-0.251328	2.075684	-2.026374
H	-0.734423	-1.964658	-1.085628
H	-0.378258	-1.586463	0.611946
C	0.696344	-0.245574	-0.745287
H	0.766993	-0.147961	-1.833493
C	2.049449	-0.579206	-0.231063
C	2.559370	-1.950873	-0.068233

H	1.826580	-2.689242	-0.378158
H	3.492479	-2.038233	-0.629045
H	2.850444	-2.086982	0.976786
O	-4.696396	-0.566305	-0.053396
O	2.787081	0.389442	0.057107
O	4.047761	0.106154	0.520128

Rotational constants (GHz): 1.6496500 0.3998300 0.3574100

Vibrational harmonic frequencies (cm-1):

32.1865	44.5630	51.2904
84.4669	117.4481	171.0937
179.6541	214.6546	226.6665
261.5586	274.1754	306.3209
316.0353	321.4591	336.7759
368.4067	421.6869	437.0327
506.9807	525.2462	549.5188
587.9748	674.6797	742.4043
783.7004	863.7251	907.3746
921.6889	928.6941	942.6779
967.2267	985.3579	1003.6341
1009.6112	1032.3040	1044.4213
1077.2617	1101.6355	1143.0326
1147.2865	1181.1585	1197.2399
1217.5157	1254.1351	1261.7467
1277.3988	1288.6924	1306.7166
1327.0663	1366.8178	1388.9005
1399.9183	1412.3308	1424.5926
1430.8657	1441.6516	1470.7381
1481.7084	1485.3614	1494.6121
1500.2000	1508.2071	1514.9889
1627.3942	1862.7119	2931.3508
3047.7435	3050.8521	3054.6230
3056.1435	3059.4807	3067.8139
3081.6065	3105.5180	3120.4533
3122.5443	3127.2171	3129.2601
3145.3066	3149.9239	3183.2084

Zero-point correction (Hartree): 0.246424

ApineneCI.A.a.mpt

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.16664586

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -1.442971 | 0.216933  | -0.317105 |
| H | -1.846701 | 0.334791  | -1.324449 |
| C | -2.549206 | 0.425274  | 0.689619  |
| C | -3.715790 | -0.500878 | 0.476828  |
| H | -2.199905 | 0.273595  | 1.716447  |
| H | -2.936552 | 1.450181  | 0.663055  |
| H | -4.549886 | -0.391350 | 1.195275  |
| C | -0.121426 | 1.033568  | -0.205982 |
| C | -0.626200 | -1.087838 | -0.264136 |
| C | -0.008287 | 2.255626  | -1.095771 |
| C | 0.230041  | 1.382764  | 1.235322  |
| H | 0.217082  | 0.508649  | 1.889446  |
| H | 1.222734  | 1.825035  | 1.293928  |
| H | -0.487001 | 2.106282  | 1.626674  |
| H | 1.006888  | 2.654482  | -1.074066 |
| H | -0.685740 | 3.041104  | -0.754114 |
| H | -0.262248 | 2.015158  | -2.128906 |
| H | -0.948832 | -1.907050 | -0.899572 |
| H | -0.514606 | -1.448445 | 0.759813  |
| C | 0.596561  | -0.257831 | -0.706937 |
| H | 0.645308  | -0.240740 | -1.800754 |
| C | 1.942423  | -0.629309 | -0.202041 |
| C | 2.384052  | -2.015588 | 0.025265  |
| H | 1.606002  | -2.728151 | -0.229777 |
| H | 3.298468  | -2.182253 | -0.548061 |
| H | 2.690342  | -2.111071 | 1.070338  |
| O | -3.775010 | -1.319473 | -0.399624 |
| O | 2.735352  | 0.313268  | 0.018413  |
| O | 3.990842  | -0.010863 | 0.473006  |

Rotational constants (GHz): 1.4992500 0.4426800 0.3851700

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| 32.8903   | 49.3447   | 74.5053   |
| 102.0808  | 137.7625  | 152.9624  |
| 188.4870  | 205.4384  | 222.0722  |
| 257.5963  | 267.0297  | 304.0455  |
| 311.7578  | 321.5436  | 336.3146  |
| 367.8604  | 406.8944  | 443.6294  |
| 505.3631  | 531.5611  | 583.6568  |
| 650.6776  | 687.7083  | 721.1416  |
| 757.9355  | 839.6752  | 909.1309  |
| 924.1018  | 933.8479  | 935.4125  |
| 945.6034  | 966.8830  | 991.9097  |
| 1007.6300 | 1023.0949 | 1037.1739 |
| 1049.7293 | 1101.4791 | 1139.8967 |
| 1154.9744 | 1179.8381 | 1198.3564 |
| 1219.5010 | 1250.0283 | 1263.9658 |
| 1277.7427 | 1292.0224 | 1316.8188 |
| 1337.2495 | 1372.4072 | 1390.3113 |
| 1406.7645 | 1417.4428 | 1423.9322 |
| 1427.7307 | 1441.3353 | 1451.8556 |
| 1481.3930 | 1485.9268 | 1496.4108 |
| 1501.4670 | 1508.8166 | 1515.5424 |
| 1627.9379 | 1854.2246 | 2950.8065 |
| 3040.5398 | 3046.5042 | 3048.6644 |
| 3055.8241 | 3057.0112 | 3068.8145 |
| 3079.3472 | 3088.4119 | 3106.4627 |
| 3116.9863 | 3119.2756 | 3127.7610 |
| 3147.9150 | 3160.7215 | 3184.9589 |

Zero-point correction (Hartree): 0.246315

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ApineneCI.A.a.mtm
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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.16146362
Electronic state : 1-A
Cartesian coordinates (Angs):
C -1.339666 0.231553 -1.102200
H -1.422246 0.802560 -2.029474
C -2.751143 -0.039731 -0.598116
C -2.891108 -1.010979 0.543289
H -3.244141 0.890226 -0.311050
H -3.332134 -0.474615 -1.419914
H -2.344155 -1.967838 0.437341
C -0.296330 0.959469 -0.204975
C -0.317435 -0.902983 -1.338602
C -0.206228 2.463637 -0.366167
C -0.422263 0.582162 1.265553
H -0.426959 -0.499352 1.421689
H 0.408368 0.991430 1.838243
H -1.350369 0.981152 1.676751
H 0.658334 2.856029 0.170763
H -1.099585 2.943395 0.038567
H -0.115486 2.743595 -1.416642
H -0.272439 -1.346849 -2.330198
H -0.389662 -1.696792 -0.596706
C 0.778434 0.111501 -0.953496
H 1.105571 0.654544 -1.845979
C 1.990564 -0.368543 -0.240798
C 2.605097 -1.691998 -0.437139
H 2.069460 -2.276003 -1.178851
H 3.652963 -1.545871 -0.708285
H 2.637898 -2.201743 0.529613
O -3.583132 -0.821793 1.505053
O 2.511549 0.437476 0.562183
O 3.642214 0.027018 1.222768
Rotational constants (GHz): 1.3202000 0.4576900 0.4423200
Vibrational harmonic frequencies (cm-1):
29.4929 52.6411 85.6383
91.7601 116.8071 169.3611
199.6239 224.3900 247.3640
260.0325 262.8162 310.6559
322.1774 339.8982 344.1180
368.5233 401.7872 456.1360
502.5420 512.3150 581.8441
617.1452 670.9848 705.3946
758.9859 818.5037 905.3045
909.4410 931.2673 943.6776
967.1042 994.3692 999.2835
1008.4298 1035.2027 1046.5025
1064.9300 1113.6766 1139.2103
1143.8756 1183.7754 1196.5847
1223.7331 1248.9079 1265.4919
1283.1617 1302.4040 1321.9335
1333.6662 1372.9170 1388.9676
1403.3501 1414.4800 1427.7373
1439.8173 1442.2209 1452.2922
1482.1067 1485.3876 1496.3429
1503.4676 1508.1406 1517.7090
1625.2990 1858.8266 2946.3293
3034.2300 3048.9157 3049.9101
3055.3236 3056.1256 3068.8730
3098.0288 3105.3901 3110.0992
3119.0846 3122.0339 3128.2399
3146.0499 3152.1037 3183.7319
Zero-point correction (Hartree): 0.246626

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ApineneCI.A.a.mtp
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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.16225478
Electronic state : 1-A
Cartesian coordinates (Angs):
C      1.482796      0.449977      0.891361
H      1.610982      1.106823      1.755272
C      2.860830      0.230049      0.290610
C      3.106149     -0.911766     -0.659534
H      3.192559      1.140812     -0.221056
H      3.603219      0.083715      1.084986
H      4.113357     -0.890309     -1.120536
C      0.330615      1.059055      0.040054
C      0.543225     -0.702335      1.310987
C      0.182394      2.566619      0.103914
C      0.331850      0.580377     -1.406035
H      0.341907     -0.506020     -1.483101
H      -0.546392      0.955657     -1.929580
H      1.216437      0.959263     -1.923352
H      -0.746969      2.880393     -0.373156
H      1.008506      3.053814     -0.419187
H      0.177003      2.921717      1.135407
H      0.603306     -1.051087      2.339342
H      0.613692     -1.546023      0.631000
C      -0.631951      0.225695      0.943997
H      -0.923001      0.828077      1.810244
C      -1.865283     -0.360646      0.356868
C      -2.348347     -1.727831      0.609390
H      -1.708139     -2.255541      1.308646
H      -3.381553     -1.666960      0.957609
H      -2.408150     -2.250288     -0.349454
O      2.353683     -1.811086     -0.915181
O      -2.521635      0.394491     -0.395201
O      -3.672102     -0.110806     -0.951214
Rotational constants (GHz): 1.2849300 0.5208300 0.4629000
Vibrational harmonic frequencies (cm-1):
26.7044      55.5407      86.5407

```

|           |           |           |
|-----------|-----------|-----------|
| 105.5682  | 122.5125  | 156.2627  |
| 194.0997  | 209.4409  | 225.7411  |
| 248.6897  | 261.2043  | 304.2442  |
| 311.7742  | 317.7406  | 330.6194  |
| 367.7634  | 402.4370  | 452.8696  |
| 496.3479  | 521.9101  | 583.3492  |
| 661.4824  | 679.3584  | 747.9693  |
| 765.9820  | 784.8163  | 895.9196  |
| 907.4354  | 931.5528  | 941.6937  |
| 954.2094  | 967.7237  | 998.1985  |
| 1004.8552 | 1024.5269 | 1038.3735 |
| 1063.4622 | 1086.3581 | 1136.0130 |
| 1157.1256 | 1183.9799 | 1197.3456 |
| 1230.6711 | 1252.5388 | 1268.6068 |
| 1285.1622 | 1304.2002 | 1329.5877 |
| 1360.1023 | 1382.3955 | 1389.1728 |
| 1406.3906 | 1413.0418 | 1424.0856 |
| 1434.4670 | 1440.3895 | 1448.7957 |
| 1480.3496 | 1484.3558 | 1493.7297 |
| 1506.6637 | 1507.9121 | 1514.0093 |
| 1624.6592 | 1861.9841 | 2937.5824 |
| 3029.0048 | 3046.8138 | 3048.8681 |
| 3055.6622 | 3056.5225 | 3058.2886 |
| 3059.4164 | 3105.9679 | 3108.2065 |
| 3114.9472 | 3126.0401 | 3128.6454 |
| 3151.6515 | 3175.9730 | 3188.2795 |

Zero-point correction (Hartree): 0.246372

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.16225479

Electronic state : 1-A

Cartesian coordinates (Angs):

C	1.482790	0.449701	0.891461
H	1.610988	1.106342	1.755527
C	2.860833	0.229792	0.290728
C	3.106095	-0.911828	-0.659668
H	3.192673	1.140647	-0.220700
H	3.603164	0.083193	1.085110
H	4.113282	-0.890291	-1.120711
C	0.330701	1.059069	0.040225
C	0.543100	-0.702622	1.310789
C	0.182629	2.566636	0.104404
C	0.332025	0.580711	-1.405971
H	0.341928	-0.505669	-1.483283
H	-0.546094	0.956232	-1.929542
H	1.216736	0.959583	-1.923089
H	-0.746663	2.880612	-0.372671
H	1.008832	3.053860	-0.418526
H	0.177197	2.921510	1.135974
H	0.603099	-1.051592	2.339075
H	0.613506	-1.546176	0.630628
C	-0.631969	0.225615	0.943941
H	-0.922964	0.827807	1.810346
C	-1.865368	-0.360546	0.356797
C	-2.348958	-1.727425	0.609985
H	-1.708976	-2.255008	1.309546
H	-3.382157	-1.665997	0.958128
H	-2.408907	-2.250349	-0.348594
O	2.353607	-1.811089	-0.915456
O	-2.521324	0.394425	-0.395779
O	-3.671897	-0.110753	-0.951685

Rotational constants (GHz): 1.2848600 0.5208200 0.4629100

Vibrational harmonic frequencies (cm-1):

26.7785	55.5409	86.5132
105.5781	122.5096	156.2724
194.1027	209.4703	225.7307
248.6952	261.1989	304.2619
311.7904	317.7671	330.6032
367.7634	402.4306	452.8347
496.4034	521.8922	583.3597
661.4958	679.3624	747.9684
765.9804	784.8188	895.9203
907.4482	931.5559	941.6975
954.2221	967.7297	998.2043
1004.8747	1024.5340	1038.3754
1063.4640	1086.3501	1135.9867
1157.1214	1183.9883	1197.3473
1230.6640	1252.5315	1268.6138
1285.1381	1304.1990	1329.5824
1360.1091	1382.4034	1389.1907
1406.3908	1413.0407	1424.0908
1434.4638	1440.3935	1448.7911
1480.3604	1484.3565	1493.7361
1506.6711	1507.9119	1514.0181
1624.6888	1861.9857	2937.5739
3028.9948	3046.8082	3048.8252
3055.6634	3056.5253	3058.2890
3059.4139	3105.9727	3108.2118
3114.9471	3126.0492	3128.6433
3151.6735	3175.9749	3188.2655

Zero-point correction (Hartree): 0.246373

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.16646192

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -1.273327 | -0.444999 | -0.626803 |
| H | -1.742346 | -0.031347 | -1.522462 |
| C | -2.343755 | -1.133810 | 0.214126  |
| C | -3.430593 | -0.151138 | 0.555593  |

|                                                           |           |           |           |
|-----------------------------------------------------------|-----------|-----------|-----------|
| H                                                         | -2.783650 | -1.951425 | -0.356931 |
| H                                                         | -1.901474 | -1.532005 | 1.129350  |
| H                                                         | -3.232419 | 0.515943  | 1.418032  |
| C                                                         | -0.357901 | 0.649736  | -0.003486 |
| C                                                         | -0.018332 | -1.244139 | -1.024807 |
| C                                                         | -0.748231 | 2.090293  | -0.267362 |
| C                                                         | -0.069273 | 0.420951  | 1.473812  |
| H                                                         | 0.249910  | -0.600311 | 1.683332  |
| H                                                         | 0.722207  | 1.090567  | 1.815654  |
| H                                                         | -0.956873 | 0.630721  | 2.072813  |
| H                                                         | 0.036507  | 2.775679  | 0.059169  |
| H                                                         | -1.657946 | 2.347159  | 0.279811  |
| H                                                         | -0.935587 | 2.260221  | -1.328047 |
| H                                                         | -0.021755 | -1.744655 | -1.989024 |
| H                                                         | 0.271643  | -1.954888 | -0.253132 |
| C                                                         | 0.787388  | 0.058332  | -0.913311 |
| H                                                         | 0.802303  | 0.608342  | -1.856165 |
| C                                                         | 2.149132  | 0.058083  | -0.337501 |
| C                                                         | 2.986437  | 1.266125  | -0.241577 |
| H                                                         | 2.496151  | 2.124670  | -0.690872 |
| H                                                         | 3.222780  | 1.437170  | 0.811582  |
| H                                                         | 3.949789  | 1.058060  | -0.712952 |
| O                                                         | -4.446883 | -0.032790 | -0.071868 |
| O                                                         | 2.567606  | -1.019820 | 0.141650  |
| O                                                         | 3.803215  | -1.003704 | 0.738685  |
| Rotational constants (GHz): 1.7620900 0.4147400 0.3853700 |           |           |           |
| Vibrational harmonic frequencies (cm-1):                  |           |           |           |
| 20.0414                                                   | 42.2893   | 61.6095   |           |
| 79.8379                                                   | 119.8414  | 170.8905  |           |
| 205.8101                                                  | 225.2811  | 231.4679  |           |
| 250.1435                                                  | 282.1239  | 305.0163  |           |
| 311.4743                                                  | 317.9661  | 337.6728  |           |
| 385.9038                                                  | 403.4053  | 461.9592  |           |
| 483.7333                                                  | 530.8501  | 556.7990  |           |
| 597.9691                                                  | 665.7130  | 720.9277  |           |
| 778.7561                                                  | 879.3711  | 894.8482  |           |
| 931.8424                                                  | 946.9566  | 961.0193  |           |
| 969.0032                                                  | 993.1972  | 998.4687  |           |
| 1003.2673                                                 | 1032.6397 | 1045.3526 |           |
| 1068.4459                                                 | 1113.5371 | 1124.3990 |           |
| 1150.2287                                                 | 1173.1752 | 1192.0867 |           |
| 1200.5730                                                 | 1242.6967 | 1264.7584 |           |
| 1270.4963                                                 | 1283.5942 | 1302.5270 |           |
| 1332.6517                                                 | 1380.4177 | 1390.1885 |           |
| 1406.3703                                                 | 1416.1706 | 1422.6484 |           |
| 1433.9953                                                 | 1440.0662 | 1474.6310 |           |
| 1485.7075                                                 | 1486.2261 | 1493.5292 |           |
| 1501.7700                                                 | 1508.3246 | 1512.8232 |           |
| 1633.4791                                                 | 1859.0132 | 2936.1169 |           |
| 3046.4313                                                 | 3056.1616 | 3057.0146 |           |
| 3066.6617                                                 | 3075.0761 | 3081.3304 |           |
| 3107.1259                                                 | 3107.3878 | 3112.4624 |           |
| 3121.0364                                                 | 3125.5227 | 3130.9129 |           |
| 3135.3135                                                 | 3164.4689 | 3179.0145 |           |
| Zero-point correction (Hartree): 0.246657                 |           |           |           |
| ApineneCI.A.a.pmp                                         |           |           |           |
| ~~~~~                                                     |           |           |           |
| E(RM062X/Aug-CC-pVTZ) (Hartree): -616.16838060            |           |           |           |
| Electronic state : 1-A                                    |           |           |           |
| Cartesian coordinates (Angs):                             |           |           |           |
| C                                                         | -1.233947 | -0.583647 | -0.831377 |
| H                                                         | -1.622927 | -0.262644 | -1.801928 |
| C                                                         | -2.351888 | -1.225935 | -0.020488 |
| C                                                         | -3.491128 | -0.255176 | 0.113887  |
| H                                                         | -2.708346 | -2.113964 | -0.549600 |
| H                                                         | -2.009107 | -1.518978 | 0.970717  |
| H                                                         | -4.018269 | -0.012162 | -0.830812 |
| C                                                         | -0.426416 | 0.596390  | -0.215673 |
| C                                                         | 0.081426  | -1.356902 | -1.040285 |
| C                                                         | -0.848998 | 1.989237  | -0.638555 |
| C                                                         | -0.294524 | 0.501647  | 1.298690  |
| H                                                         | 0.059434  | -0.477707 | 1.623202  |
| H                                                         | 0.415624  | 1.246572  | 1.662577  |
| H                                                         | -1.257080 | 0.692545  | 1.774481  |
| H                                                         | -0.137825 | 2.739653  | -0.287911 |
| H                                                         | -1.822476 | 2.234360  | -0.208310 |
| H                                                         | -0.924171 | 2.067763  | -1.724106 |
| H                                                         | 0.194705  | -1.929798 | -1.956576 |
| H                                                         | 0.316030  | -1.993277 | -0.189067 |
| C                                                         | 0.825467  | -0.015730 | -0.952241 |
| H                                                         | 0.923808  | 0.460027  | -1.930553 |
| C                                                         | 2.121341  | 0.077850  | -0.246233 |
| C                                                         | 2.878810  | 1.333880  | -0.112077 |
| H                                                         | 2.381529  | 2.152336  | -0.624191 |
| H                                                         | 3.012118  | 1.540976  | 0.952501  |
| H                                                         | 3.889334  | 1.171603  | -0.494165 |
| O                                                         | -3.815071 | 0.279945  | 1.138701  |
| O                                                         | 2.553345  | -0.962734 | 0.298375  |
| O                                                         | 3.730071  | -0.863085 | 0.997905  |
| Rotational constants (GHz): 1.6081700 0.4375900 0.4132100 |           |           |           |
| Vibrational harmonic frequencies (cm-1):                  |           |           |           |
| 43.2775                                                   | 54.6553   | 61.8754   |           |
| 83.7898                                                   | 123.3763  | 162.0207  |           |
| 210.0589                                                  | 229.0999  | 238.9902  |           |
| 256.5292                                                  | 275.8759  | 301.9071  |           |
| 316.6228                                                  | 326.3827  | 339.7141  |           |
| 391.4583                                                  | 408.5985  | 467.8831  |           |
| 477.8521                                                  | 533.6196  | 551.0288  |           |
| 600.3928                                                  | 666.9268  | 717.3540  |           |
| 775.8918                                                  | 870.3361  | 890.5488  |           |
| 919.2766                                                  | 944.6526  | 965.0014  |           |

|           |           |           |
|-----------|-----------|-----------|
| 978.3060  | 991.0568  | 1004.7612 |
| 1014.5505 | 1037.3292 | 1046.1272 |
| 1058.1631 | 1114.4649 | 1119.5451 |
| 1158.7872 | 1172.1499 | 1194.5443 |
| 1199.1304 | 1243.4183 | 1260.0873 |
| 1269.3153 | 1280.3181 | 1298.6302 |
| 1329.9949 | 1382.3316 | 1393.4236 |
| 1406.3987 | 1417.7756 | 1426.2659 |
| 1428.2130 | 1440.9074 | 1471.9396 |
| 1486.0019 | 1486.7918 | 1494.7667 |
| 1502.2482 | 1511.0954 | 1515.4612 |
| 1634.2295 | 1857.2319 | 2929.8372 |
| 3045.6137 | 3051.5866 | 3056.0216 |
| 3057.6764 | 3061.8312 | 3076.0170 |
| 3105.4543 | 3108.3586 | 3114.5298 |
| 3121.6206 | 3123.4433 | 3136.3289 |
| 3138.9517 | 3161.8780 | 3180.1415 |

Zero-point correction (Hartree): 0.246726

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E (CCSD(T)/Aug-CC-pVTZ) (Hartree): -615.24144453

E (CCSD/Aug-CC-pVTZ) (Hartree): -615.12234779

T1 diagnostic: 0.021687

E (MP2/Aug-CC-pVTZ) (Hartree): -615.05080978

E (MP3/Aug-CC-pVTZ) (Hartree): -615.10596959

E (RHF/Aug-CC-pVTZ) (Hartree): -612.61783580

E (RM062X/Aug-CC-pVTZ) (Hartree): -616.17056879

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-1.289640	-0.520474	-0.737026
H	-1.786773	-0.103973	-1.614549
C	-2.286020	-1.314441	0.078548
C	-3.497702	-0.541484	0.511884
H	-2.640595	-2.183610	-0.486826
H	-1.827333	-1.733991	0.980376
H	-4.242015	-1.111209	1.099643
C	-0.445664	0.608643	-0.068431
C	0.013519	-1.237149	-1.140748
C	-0.865019	2.038846	-0.342968
C	-0.222280	0.379400	1.418767
H	0.150526	-0.622637	1.636345
H	0.503732	1.093680	1.811440
H	-1.157118	0.528609	1.962026
H	-0.086864	2.734127	-0.019820
H	-1.784207	2.276509	0.190283
H	-1.044595	2.195456	-1.407483
H	0.062773	-1.685843	-2.129388
H	0.313929	-1.976965	-0.400170
C	0.764174	0.085101	-0.938106
H	0.811773	0.674979	-1.855375
C	2.092561	0.102829	-0.290736
C	2.879409	1.332772	-0.095041
H	2.381848	2.194083	-0.530456
H	3.052841	1.461627	0.976108
H	3.873023	1.179499	-0.522350
O	-3.685786	0.618247	0.260282
O	2.525950	-0.981775	0.159763
O	3.729714	-0.952047	0.821623

Rotational constants (GHz): 1.6586900 0.4540200 0.4161000

Vibrational harmonic frequencies (cm-1):

42.6847	46.2665	77.3413
105.7208	141.8201	157.9463
210.0940	220.7751	243.4163
247.2778	279.6579	301.8975
315.7140	324.3130	336.1365
375.4204	397.1335	466.4105
472.0958	546.5592	588.6446
653.5712	674.1494	736.8635
750.9022	800.0557	889.0952
912.7077	931.3251	961.1362
966.7704	980.2580	994.5520
1004.6812	1033.3088	1047.3550
1055.5077	1104.3084	1119.7870
1157.4700	1173.2036	1193.1768
1210.1748	1244.3567	1267.9946
1270.9290	1287.5544	1311.2338
1350.4178	1385.4622	1399.2687
1405.3592	1419.3768	1422.2014
1426.5873	1441.9003	1447.6956
1485.2123	1486.6883	1492.7415
1501.1166	1509.2745	1513.3303
1632.4512	1853.5220	2953.4240
3042.3381	3049.6756	3052.2228
3057.5346	3067.8105	3081.7651
3086.5817	3100.1378	3107.7705
3115.8474	3119.1923	3126.9340
3145.7972	3156.2679	3181.2997

Zero-point correction (Hartree): 0.246605

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E (RM062X/Aug-CC-pVTZ) (Hartree): -616.16655595

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -1.366385 | 0.441380  | -0.408874 |
| H | -1.731712 | 0.991577  | -1.280768 |
| C | -2.516163 | 0.190856  | 0.556122  |
| C | -3.631349 | -0.512170 | -0.167275 |
| H | -2.204425 | -0.423034 | 1.399882  |
| H | -2.896522 | 1.147444  | 0.928869  |
| H | -4.093080 | 0.063929  | -0.994702 |

|                                                |           |           |           |
|------------------------------------------------|-----------|-----------|-----------|
| C                                              | -0.077930 | 1.145929  | 0.102046  |
| C                                              | -0.512028 | -0.754393 | -0.874707 |
| C                                              | 0.032691  | 2.629088  | -0.186732 |
| C                                              | 0.219463  | 0.848741  | 1.564930  |
| H                                              | 0.187427  | -0.218160 | 1.787021  |
| H                                              | 1.212323  | 1.213940  | 1.833859  |
| H                                              | -0.504323 | 1.352407  | 2.207108  |
| H                                              | 1.019252  | 3.010886  | 0.082798  |
| H                                              | -0.704800 | 3.184097  | 0.397203  |
| H                                              | -0.141861 | 2.840734  | -1.242309 |
| H                                              | -0.765200 | -1.227644 | -1.819327 |
| H                                              | -0.437075 | -1.519684 | -0.104156 |
| C                                              | 0.708624  | 0.178642  | -0.862679 |
| H                                              | 0.845369  | 0.679692  | -1.823285 |
| C                                              | 2.023813  | -0.299638 | -0.384804 |
| C                                              | 3.231463  | 0.543829  | -0.369092 |
| H                                              | 3.034393  | 1.525257  | -0.790415 |
| H                                              | 3.592041  | 0.607650  | 0.660482  |
| H                                              | 4.024680  | 0.023306  | -0.910727 |
| O                                              | -4.003951 | -1.625712 | 0.075472  |
| O                                              | 2.079254  | -1.461092 | 0.077573  |
| O                                              | 3.285988  | -1.878944 | 0.578812  |
| Rotational constants (GHz):                    |           |           |           |
|                                                | 1.3032100 | 0.4568100 | 0.3847900 |
| Vibrational harmonic frequencies (cm-1):       |           |           |           |
| 33.2748                                        | 41.6107   |           | 59.7506   |
| 82.3096                                        | 107.9239  |           | 164.3411  |
| 186.6893                                       | 209.0403  |           | 228.0095  |
| 253.1941                                       | 276.7083  |           | 303.6045  |
| 315.9434                                       | 329.0945  |           | 331.1336  |
| 367.2592                                       | 415.7421  |           | 465.8418  |
| 479.6906                                       | 541.6520  |           | 568.9691  |
| 590.9401                                       | 663.6740  |           | 743.3340  |
| 777.3499                                       | 853.3280  |           | 890.3602  |
| 924.6724                                       | 930.3933  |           | 961.5840  |
| 974.6330                                       | 991.0481  |           | 1000.6748 |
| 1009.3941                                      | 1037.3715 |           | 1045.1696 |
| 1067.6944                                      | 1102.6431 |           | 1135.8493 |
| 1153.0786                                      | 1175.0268 |           | 1192.9360 |
| 1219.3701                                      | 1244.2737 |           | 1247.9505 |
| 1273.0157                                      | 1278.3240 |           | 1300.0608 |
| 1327.4998                                      | 1383.5897 |           | 1394.5728 |
| 1405.4043                                      | 1418.7446 |           | 1424.0686 |
| 1427.9394                                      | 1440.8024 |           | 1468.5023 |
| 1484.9317                                      | 1486.3232 |           | 1493.1834 |
| 1501.2611                                      | 1508.2993 |           | 1512.4584 |
| 1634.3860                                      | 1863.4890 |           | 2926.2506 |
| 3046.2396                                      | 3047.8399 |           | 3052.4342 |
| 3056.6051                                      | 3057.1442 |           | 3078.2002 |
| 3106.7058                                      | 3107.2963 |           | 3112.8042 |
| 3122.4560                                      | 3124.1937 |           | 3133.4765 |
| 3136.9496                                      | 3163.5701 |           | 3178.2169 |
| Zero-point correction (Hartree): 0.246433      |           |           |           |
| ApineneCI.A.a.ppp                              |           |           |           |
| ~~~~~                                          |           |           |           |
| E(RM062X/Aug-CC-pVTZ) (Hartree): -616.16667266 |           |           |           |
| Electronic state : 1-A                         |           |           |           |
| Cartesian coordinates (Angs):                  |           |           |           |
| C                                              | -1.353599 | 0.219880  | -0.361995 |
| H                                              | -1.785592 | 0.701330  | -1.242565 |
| C                                              | -2.459604 | -0.078087 | 0.641489  |
| C                                              | -3.478871 | -0.990083 | 0.018017  |
| H                                              | -2.034862 | -0.585496 | 1.512247  |
| H                                              | -2.958949 | 0.834235  | 0.968137  |
| H                                              | -3.102421 | -1.990433 | -0.274091 |
| C                                              | -0.118538 | 1.050651  | 0.089243  |
| C                                              | -0.406767 | -0.914657 | -0.807638 |
| C                                              | -0.143194 | 2.525271  | -0.257617 |
| C                                              | 0.239180  | 0.838043  | 1.553092  |
| H                                              | 0.308276  | -0.218014 | 1.816229  |
| H                                              | 1.202528  | 1.298144  | 1.780451  |
| H                                              | -0.509866 | 1.302381  | 2.195790  |
| H                                              | 0.815480  | 2.998130  | -0.035703 |
| H                                              | -0.907823 | 3.038796  | 0.328801  |
| H                                              | -0.367089 | 2.678901  | -1.313795 |
| H                                              | -0.636428 | -1.443053 | -1.728939 |
| H                                              | -0.240124 | -1.640562 | -0.012927 |
| C                                              | 0.727949  | 0.118761  | -0.860590 |
| H                                              | 0.800272  | 0.592701  | -1.841535 |
| C                                              | 2.087742  | -0.230992 | -0.397034 |
| C                                              | 3.221847  | 0.707899  | -0.438654 |
| H                                              | 2.936847  | 1.653123  | -0.891195 |
| H                                              | 3.595093  | 0.840206  | 0.579833  |
| H                                              | 4.044884  | 0.233508  | -0.978155 |
| O                                              | -4.620821 | -0.689001 | -0.194240 |
| O                                              | 2.246475  | -1.365889 | 0.106197  |
| O                                              | 3.492211  | -1.666862 | 0.596485  |
| Rotational constants (GHz):                    |           |           |           |
|                                                | 1.4768900 | 0.4202100 | 0.3704500 |
| Vibrational harmonic frequencies (cm-1):       |           |           |           |
| 40.7427                                        | 45.2234   |           | 49.1029   |
| 82.1022                                        | 111.7493  |           | 172.0976  |
| 195.2930                                       | 209.0003  |           | 226.3573  |
| 254.6889                                       | 271.0738  |           | 301.8731  |
| 317.4017                                       | 327.9886  |           | 331.8498  |
| 368.8232                                       | 416.0927  |           | 462.4964  |
| 482.3504                                       | 528.8425  |           | 566.3039  |
| 594.0743                                       | 663.9868  |           | 742.8700  |
| 786.6768                                       | 864.8424  |           | 890.1349  |
| 922.2124                                       | 930.0543  |           | 962.6064  |
| 971.9556                                       | 994.6007  |           | 1000.5886 |
| 1004.4716                                      | 1034.4564 |           | 1045.8439 |
| 1071.1994                                      | 1107.6749 |           | 1139.4023 |

|           |           |           |
|-----------|-----------|-----------|
| 1148.8674 | 1176.0775 | 1193.3259 |
| 1220.7578 | 1243.6978 | 1257.4276 |
| 1273.4594 | 1278.6607 | 1306.3513 |
| 1330.6492 | 1380.8851 | 1390.5920 |
| 1405.4152 | 1416.3568 | 1425.1605 |
| 1429.1476 | 1440.0302 | 1470.1360 |
| 1485.6531 | 1486.5566 | 1493.3182 |
| 1500.3908 | 1509.5149 | 1512.3882 |
| 1633.5079 | 1861.2081 | 2936.5405 |
| 3047.9721 | 3053.9343 | 3057.1079 |
| 3057.7239 | 3067.1983 | 3080.7013 |
| 3100.8176 | 3107.5674 | 3115.2012 |
| 3123.3921 | 3124.9293 | 3125.8856 |
| 3134.0146 | 3158.1320 | 3179.7853 |

Zero-point correction (Hartree): 0.246565

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.16907826

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-1.424218	0.279569	-0.260599
H	-1.889214	0.691554	-1.157951
C	-2.479837	0.086287	0.802390
C	-3.631799	-0.760626	0.331759
H	-2.071415	-0.389526	1.699978
H	-2.898865	1.040893	1.141686
H	-4.413804	-0.965127	1.087009
C	-0.144672	1.099273	0.064870
C	-0.540981	-0.918640	-0.656614
C	-0.133312	2.541060	-0.401325
C	0.276881	0.993574	1.524165
H	0.318485	-0.039722	1.870345
H	1.266859	1.429789	1.670418
H	-0.421844	1.539480	2.159877
H	0.850795	2.993292	-0.262730
H	-0.850136	3.131196	0.173942
H	-0.402369	2.616430	-1.455403
H	-0.846551	-1.500433	-1.520396
H	-0.363367	-1.589402	0.182962
C	0.626454	0.063098	-0.841493
H	0.669821	0.454556	-1.859683
C	1.994358	-0.290906	-0.407605
C	3.156129	0.594985	-0.597939
H	2.881289	1.497535	-1.135752
H	3.581024	0.818966	0.383605
H	3.936805	0.035850	-1.118788
O	-3.732692	-1.201652	-0.780093
O	2.140790	-1.371531	0.206661
O	3.399211	-1.663239	0.672836

Rotational constants (GHz): 1.3644600 0.4602400 0.4020400

Vibrational harmonic frequencies (cm-1):

41.2879	49.5747	72.1904
102.3868	136.0637	159.2809
201.7423	207.0368	220.8023
252.6539	257.8209	304.5487
316.7172	328.6492	332.6465
368.9232	405.6099	465.0126
478.7472	552.3014	589.0449
656.2373	674.4774	718.5788
761.9567	841.0058	889.3471
925.1935	932.4168	938.0902
961.7431	977.1988	995.3467
1001.6250	1023.7868	1042.3657
1045.9056	1103.7691	1146.7626
1148.2141	1174.2240	1194.4328
1220.7648	1241.8338	1257.6916
1274.2717	1281.0587	1323.8393
1334.8527	1385.2686	1400.7317
1406.7543	1418.5987	1424.6508
1427.7406	1440.3494	1452.6609
1485.9038	1486.5346	1493.8567
1501.6344	1509.2264	1513.4164
1633.2666	1856.0097	2950.4396
3037.0603	3045.9481	3054.6147
3056.5407	3069.2637	3082.0914
3085.6806	3105.1450	3107.1500
3111.5334	3120.2263	3125.1825
3132.4256	3171.0481	3178.6633

Zero-point correction (Hartree): 0.246497

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.16459769

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 1.317166  | 0.629853  | 0.962690  |
| H | 1.454212  | 1.499629  | 1.608790  |
| C | 2.699156  | 0.086960  | 0.622464  |
| C | 2.751001  | -1.230743 | -0.104298 |
| H | 3.270043  | 0.812966  | 0.041557  |
| H | 3.241090  | -0.076695 | 1.561285  |
| H | 2.137352  | -2.047396 | 0.320931  |
| C | 0.327596  | 1.045175  | -0.162160 |
| C | 0.215028  | -0.256909 | 1.582710  |
| C | 0.346114  | 2.507045  | -0.560726 |
| C | 0.398586  | 0.145921  | -1.388375 |
| H | 0.332895  | -0.913822 | -1.135705 |
| H | -0.423124 | 0.368927  | -2.071606 |
| H | 1.333424  | 0.306882  | -1.926421 |
| H | -0.470680 | 2.739324  | -1.246751 |
| H | 1.281135  | 2.746985  | -1.071166 |

|                                                           |           |           |           |
|-----------------------------------------------------------|-----------|-----------|-----------|
| H                                                         | 0.258720  | 3.156224  | 0.311388  |
| H                                                         | 0.137868  | -0.282986 | 2.666270  |
| H                                                         | 0.219490  | -1.275924 | 1.204033  |
| C                                                         | -0.814406 | 0.597397  | 0.826503  |
| H                                                         | -1.129304 | 1.464694  | 1.410929  |
| C                                                         | -2.009573 | -0.027919 | 0.220921  |
| C                                                         | -3.029012 | 0.732343  | -0.522042 |
| H                                                         | -2.804733 | 1.794982  | -0.526312 |
| H                                                         | -3.089594 | 0.325158  | -1.534303 |
| H                                                         | -4.006268 | 0.526920  | -0.079047 |
| O                                                         | 3.440359  | -1.436164 | -1.065260 |
| O                                                         | -2.114104 | -1.271694 | 0.312141  |
| O                                                         | -3.195314 | -1.857217 | -0.296881 |
| Rotational constants (GHz): 1.2194800 0.5059300 0.4432600 |           |           |           |
| Vibrational harmonic frequencies (cm-1):                  |           |           |           |
| 41.5168                                                   | 49.7888   | 84.8062   |           |
| 90.8807                                                   | 115.0033  | 186.2556  |           |
| 202.0775                                                  | 219.6538  | 244.0950  |           |
| 252.8378                                                  | 261.8146  | 301.7434  |           |
| 319.6026                                                  | 347.3910  | 352.0813  |           |
| 367.7674                                                  | 400.5580  | 466.0833  |           |
| 471.9190                                                  | 543.7230  | 581.9101  |           |
| 619.2901                                                  | 666.2357  | 700.7591  |           |
| 763.5806                                                  | 820.0939  | 888.1171  |           |
| 913.9041                                                  | 930.8925  | 962.6497  |           |
| 980.0602                                                  | 986.4015  | 1000.1742 |           |
| 1004.7066                                                 | 1036.9710 | 1048.0283 |           |
| 1061.0149                                                 | 1115.6886 | 1132.5379 |           |
| 1149.0769                                                 | 1174.5312 | 1193.8608 |           |
| 1224.1072                                                 | 1242.3930 | 1254.8741 |           |
| 1272.8159                                                 | 1294.3478 | 1320.3152 |           |
| 1338.4217                                                 | 1383.6891 | 1394.7704 |           |
| 1405.0037                                                 | 1416.0168 | 1427.2286 |           |
| 1439.4652                                                 | 1440.2804 | 1452.8736 |           |
| 1485.9513                                                 | 1486.8953 | 1494.5229 |           |
| 1504.1716                                                 | 1510.3511 | 1514.9080 |           |
| 1634.0920                                                 | 1856.4584 | 2954.0172 |           |
| 3034.9332                                                 | 3047.4067 | 3054.6193 |           |
| 3056.9703                                                 | 3066.7512 | 3076.8326 |           |
| 3107.7875                                                 | 3108.7090 | 3114.5280 |           |
| 3115.2842                                                 | 3121.3793 | 3123.8580 |           |
| 3132.9664                                                 | 3169.1298 | 3178.9446 |           |
| Zero-point correction (Hartree): 0.246744                 |           |           |           |

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.16333481

Electronic state : 1-A

Cartesian coordinates (Angs):

C	1.470464	0.552684	0.831811
H	1.643232	1.341065	1.568921
C	2.836228	0.110898	0.333457
C	2.994629	-1.192542	-0.403693
H	3.269190	0.886422	-0.309694
H	3.538457	0.037991	1.172659
H	4.026666	-1.366677	-0.767992
C	0.399205	1.103410	-0.151305
C	0.417531	-0.415249	1.415402
C	0.406347	2.606285	-0.354043
C	0.356684	0.375855	-1.487677
H	0.269691	-0.702426	-1.369918
H	-0.487934	0.730251	-2.081867
H	1.265138	0.579588	-2.058908
H	-0.453517	2.930533	-0.943079
H	1.305111	2.909936	-0.896048
H	0.390797	3.136302	0.599162
H	0.424963	-0.576494	2.490085
H	0.405283	-1.370319	0.901106
C	-0.660496	0.530203	0.861152
H	-0.918126	1.316947	1.575100
C	-1.913913	-0.005620	0.287589
C	-2.951363	0.849792	-0.315115
H	-2.682376	1.900255	-0.252862
H	-3.101830	0.529060	-1.348675
H	-3.901729	0.645293	0.183101
O	2.147591	-2.020066	-0.592529
O	-2.068311	-1.246870	0.292737
O	-3.219894	-1.735815	-0.271028
Rotational constants (GHz): 1.1940500 0.5671800 0.4633100			
Vibrational harmonic frequencies (cm-1):			
36.9144	54.3207	91.4316	
109.6162	125.7681	173.0557	
194.6514	212.1790	225.8729	
244.2322	256.2070	297.4871	
315.4083	323.8476	327.5263	
370.0928	399.0678	468.9894	
473.5811	541.4745	587.2379	
662.7651	675.2147	747.8358	
766.8939	783.5406	890.3173	
901.6646	939.6741	942.6671	
965.2034	985.8461	997.7691	
1004.2003	1021.2356	1040.4514	
1057.5787	1090.1199	1131.1057	
1160.1369	1174.5925	1195.8547	
1231.1662	1244.8118	1257.7055	
1273.7954	1300.1211	1331.8962	
1369.8570	1385.1283	1401.4487	
1407.2485	1416.5439	1425.5698	
1434.2563	1441.1277	1446.8908	
1483.8067	1486.3770	1493.5601	
1505.1488	1509.6990	1514.1514	
1636.2985	1866.2788	2931.8832	

3028.6613	3045.1081	3051.8929
3054.3074	3057.3116	3057.9515
3065.5954	3108.7174	3109.6956
3113.0743	3119.2203	3123.3072
3156.6290	3179.0796	3190.9443

Zero-point correction (Hartree): 0.246543

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.16333481

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 1.470464  | 0.552681  | 0.831812  |
| H | 1.643233  | 1.341061  | 1.568923  |
| C | 2.836227  | 0.110896  | 0.333455  |
| C | 2.994628  | -1.192547 | -0.403689 |
| H | 3.269183  | 0.886417  | -0.309703 |
| H | 3.538462  | 0.037998  | 1.172654  |
| H | 4.026668  | -1.366688 | -0.767980 |
| C | 0.399206  | 1.103411  | -0.151303 |
| C | 0.417530  | -0.415251 | 1.415401  |
| C | 0.406352  | 2.606286  | -0.354039 |
| C | 0.356686  | 0.375858  | -1.487677 |
| H | 0.269698  | -0.702423 | -1.369920 |
| H | -0.487935 | 0.730251  | -2.081864 |
| H | 1.265137  | 0.579598  | -2.058910 |
| H | -0.453504 | 2.930538  | -0.943084 |
| H | 1.305123  | 2.909936  | -0.896033 |
| H | 0.390794  | 3.136302  | 0.599167  |
| H | 0.424960  | -0.576497 | 2.490084  |
| H | 0.405281  | -1.370321 | 0.901105  |
| C | -0.660496 | 0.530202  | 0.861151  |
| H | -0.918128 | 1.316944  | 1.575100  |
| C | -1.913912 | -0.005619 | 0.287586  |
| C | -2.951361 | 0.849795  | -0.315118 |
| H | -2.682362 | 1.900256  | -0.252882 |
| H | -3.101848 | 0.529048  | -1.348669 |
| H | -3.901723 | 0.645316  | 0.183116  |
| O | 2.147587  | -2.020067 | -0.592532 |
| O | -2.068314 | -1.246869 | 0.292734  |
| O | -3.219897 | -1.735815 | -0.271025 |

Rotational constants (GHz): 1.1940500 0.5671800 0.4633100

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| 36.9147   | 54.3203   | 91.4320   |
| 109.6151  | 125.7667  | 173.0554  |
| 194.6498  | 212.1721  | 225.8714  |
| 244.2314  | 256.2054  | 297.4868  |
| 315.4087  | 323.8480  | 327.5247  |
| 370.0912  | 399.0675  | 468.9891  |
| 473.5813  | 541.4742  | 587.2376  |
| 662.7647  | 675.2143  | 747.8359  |
| 766.8936  | 783.5402  | 890.3183  |
| 901.6651  | 939.6736  | 942.6673  |
| 965.2031  | 985.8464  | 997.7691  |
| 1004.2003 | 1021.2358 | 1040.4506 |
| 1057.5787 | 1090.1199 | 1131.1056 |
| 1160.1370 | 1174.5924 | 1195.8550 |
| 1231.1658 | 1244.8120 | 1257.7054 |
| 1273.7955 | 1300.1211 | 1331.8961 |
| 1369.8568 | 1385.1279 | 1401.4485 |
| 1407.2484 | 1416.5436 | 1425.5697 |
| 1434.2561 | 1441.1266 | 1446.8907 |
| 1483.8070 | 1486.3767 | 1493.5602 |
| 1505.1490 | 1509.6994 | 1514.1516 |
| 1636.2970 | 1866.2787 | 2931.8836 |
| 3028.6624 | 3045.1085 | 3051.8934 |
| 3054.3078 | 3057.3126 | 3057.9522 |
| 3065.5947 | 3108.7180 | 3109.6960 |
| 3113.0746 | 3119.2214 | 3123.3078 |
| 3156.6310 | 3179.0801 | 3190.9450 |

Zero-point correction (Hartree): 0.246543

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.16371972

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-1.321515	-0.418805	-0.632274
H	-1.665320	0.024454	-1.569457
C	-2.521988	-0.947872	0.142590
C	-3.522569	0.148688	0.384099
H	-3.011600	-1.746292	-0.414781
H	-2.193112	-1.342657	1.107745
H	-3.185452	0.966244	1.052525
C	-0.308276	0.563938	0.029497
C	-0.154522	-1.381889	-0.924554
C	-0.453146	2.037662	-0.292737
C	-0.152874	0.354345	1.529585
H	-0.029907	-0.695135	1.798957
H	0.717136	0.900976	1.898228
H	-1.028112	0.734357	2.059023
H	0.444440	2.582515	0.006237
H	-1.302216	2.471899	0.239041
H	-0.604701	2.193068	-1.361077
H	-0.159363	-1.915392	-1.871381
H	-0.029555	-2.097869	-0.113250
C	0.802262	-0.182831	-0.796796
H	0.913927	0.328068	-1.752874
C	2.147235	-0.304977	-0.181929
C	2.581327	-1.308925	0.803773
H	1.817754	-2.051766	1.002869
H	3.502072	-1.765418	0.432370

H	2.880951	-0.785929	1.715708
O	-4.612204	0.192993	-0.115525
O	2.961746	0.587005	-0.524875
O	4.195140	0.575361	0.065724
Rotational constants (GHz):		1.9314000	0.3867600 0.3668700
Vibrational harmonic frequencies (cm-1):			
27.0577	36.2135	73.8879	
79.0875	132.7242	187.9006	
216.1101	230.8918	237.5562	
272.0654	276.8204	299.6704	
307.5964	337.2205	355.3436	
386.3999	399.0142	452.6156	
487.1551	528.0915	561.9811	
593.4503	666.8072	723.6274	
783.3302	853.6565	887.9848	
930.0662	937.9533	959.7883	
964.8596	980.4318	1002.7559	
1007.6039	1036.8561	1042.9365	
1075.9239	1108.2253	1131.9397	
1159.8074	1178.6326	1191.4866	
1208.8704	1251.9540	1267.7000	
1284.2023	1302.1410	1321.8396	
1333.9504	1366.0650	1390.4513	
1402.5934	1413.7848	1421.4911	
1435.4871	1438.4209	1470.5290	
1479.6077	1487.0386	1491.2575	
1498.1204	1510.2626	1511.5244	
1611.2973	1862.5689	2931.8037	
3048.8979	3054.5441	3058.4520	
3060.1788	3072.1804	3097.7336	
3102.2875	3106.0416	3117.1854	
3121.2005	3126.1748	3128.8611	
3131.9556	3156.2340	3202.1601	
Zero-point correction (Hartree): 0.246909			

ApineneCI.A.a.tmp

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.16571925
Electronic state : 1-A
Cartesian coordinates (Angs):
C      -1.293063      -0.634190      -0.781068
H      -1.560958      -0.351943      -1.802836
C      -2.542140      -1.068633      -0.027239
C      -3.551919      0.045266      -0.046067
H      -2.975680      -1.940380      -0.525539
H      -2.318173      -1.328242      1.006583
H      -3.949379      0.305684      -1.047583
C      -0.388580      0.484949      -0.187648
C      -0.069390      -1.569474      -0.818692
C      -0.578166      1.884048      -0.737606
C      -0.383676      0.504417      1.335360
H      -0.232262      -0.485001      1.768058
H      0.412814      1.155954      1.699535
H      -1.333845      0.889056      1.707899
H      0.240433      2.533852      -0.422745
H      -1.510823      2.316120      -0.368540
H      -0.606911      1.878550      -1.827819
H      0.038510      -2.237910      -1.669109
H      0.007162      -2.147471      0.101122
C      0.823601      -0.313806      -0.792133
H      1.003129      0.053828      -1.802287
C      2.112423      -0.279497      -0.058278
C      2.477831      -1.076015      1.124905
H      1.713947      -1.796550      1.392283
H      3.436412      -1.558415      0.918829
H      2.685740      -0.388614      1.948970
O      -3.901545      0.663735      0.921423
O      2.941411      0.556357      -0.495224
O      4.123679      0.684794      0.180548

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Rotational constants (GHz):		1.7635800	0.4137400 0.3954900
Vibrational harmonic frequencies (cm-1):			
36.4123	49.2414	65.5477	
83.7616	132.3276	161.3486	
224.5793	234.1238	247.1021	
264.0551	276.1952	299.3239	
319.4701	350.7195	359.4160	
389.2559	409.9973	451.3874	
487.1608	535.2433	560.8408	
595.4258	667.4709	716.8810	
778.7986	867.0758	885.6861	
917.5517	934.6249	964.9138	
970.2003	979.5136	1006.9711	
1015.9500	1041.1506	1046.7874	
1060.5928	1110.5551	1126.1609	
1164.0938	1178.2093	1194.6108	
1207.6797	1250.3050	1263.9630	
1279.7490	1298.4238	1322.0710	
1332.6922	1368.6235	1391.0714	
1405.5139	1415.8265	1425.7253	
1427.8595	1439.0496	1471.7970	
1479.7795	1487.9996	1493.1971	
1498.7731	1512.1444	1517.3276	
1612.2357	1858.3665	2931.9118	
3047.5386	3055.3474	3057.5937	
3058.9345	3059.5755	3096.7044	
3103.5584	3105.1376	3118.0828	
3125.1557	3126.3081	3133.8418	
3135.4768	3154.0547	3201.9933	
Zero-point correction (Hartree): 0.247027			

ApineneCI.A.a.tmt

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.16728397  
 Electronic state : 1-A  
 Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -1.358153 | -0.517264 | -0.718608 |
| H | -1.728974 | -0.057833 | -1.635937 |
| C | -2.510141 | -1.149899 | 0.029685  |
| C | -3.626281 | -0.202249 | 0.365850  |
| H | -2.945559 | -1.971067 | -0.550804 |
| H | -2.181545 | -1.609827 | 0.967961  |
| H | -4.481648 | -0.645917 | 0.909678  |
| C | -0.414188 | 0.500973  | -0.007814 |
| C | -0.134518 | -1.405005 | -1.019480 |
| C | -0.602911 | 1.972825  | -0.314194 |
| C | -0.317505 | 0.275461  | 1.493712  |
| H | -0.147613 | -0.769449 | 1.756933  |
| H | 0.499400  | 0.864683  | 1.914405  |
| H | -1.242049 | 0.600826  | 1.974207  |
| H | 0.280451  | 2.534395  | -0.002303 |
| H | -1.473998 | 2.367801  | 0.206308  |
| H | -0.747503 | 2.132297  | -1.383135 |
| H | -0.081576 | -1.895103 | -1.988570 |
| H | 0.006384  | -2.151986 | -0.238436 |
| C | 0.761456  | -0.171578 | -0.810397 |
| H | 0.889056  | 0.378564  | -1.742226 |
| C | 2.085594  | -0.264348 | -0.150274 |
| C | 2.502898  | -1.254893 | 0.856803  |
| H | 1.746235  | -2.010135 | 1.033724  |
| H | 3.444584  | -1.695715 | 0.520939  |
| H | 2.759543  | -0.721199 | 1.775488  |
| O | -3.628440 | 0.964764  | 0.082658  |
| O | 2.899846  | 0.635486  | -0.473479 |
| O | 4.114508  | 0.642941  | 0.157079  |

Rotational constants (GHz): 1.7957600 0.4295000 0.4005800  
 Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| 37.7904   | 47.4490   | 72.9505   |
| 117.2022  | 142.0808  | 166.0243  |
| 215.4441  | 226.4247  | 244.6930  |
| 268.7038  | 275.8787  | 296.0126  |
| 315.5035  | 344.5702  | 347.4817  |
| 377.9436  | 398.7079  | 448.2021  |
| 483.9756  | 557.0188  | 586.3622  |
| 648.6041  | 677.3210  | 739.0109  |
| 750.5278  | 801.7127  | 884.4251  |
| 911.3397  | 932.9757  | 942.5780  |
| 964.6668  | 981.5959  | 982.6697  |
| 1007.0556 | 1036.0952 | 1042.2990 |
| 1055.9032 | 1112.9356 | 1115.1030 |
| 1161.4526 | 1178.6536 | 1192.1476 |
| 1216.2723 | 1251.8762 | 1273.3082 |
| 1285.6473 | 1307.3293 | 1326.4271 |
| 1347.8241 | 1371.4274 | 1390.9189 |
| 1404.9852 | 1417.0949 | 1422.5441 |
| 1426.1982 | 1437.4367 | 1450.7637 |
| 1479.3596 | 1486.1619 | 1490.4831 |
| 1497.7446 | 1510.4308 | 1512.5511 |
| 1611.7096 | 1855.9390 | 2949.6216 |
| 3040.6616 | 3051.4546 | 3054.8913 |
| 3059.1251 | 3067.1728 | 3087.9978 |
| 3093.2418 | 3103.3369 | 3105.9442 |
| 3119.2662 | 3122.4897 | 3126.7765 |
| 3147.6060 | 3149.3469 | 3202.1043 |

Zero-point correction (Hartree): 0.246828

ApineneCI.A.a.tpm  
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 E(RM062X/Aug-CC-pVTZ) (Hartree): -616.16477783
 Electronic state : 1-A
 Cartesian coordinates (Angs):

C	-1.399250	0.438910	-0.437300
H	-1.658987	0.949543	-1.368347
C	-2.623777	0.360731	0.465211
C	-3.712155	-0.376311	-0.263727
H	-2.401314	-0.172945	1.388221
H	-2.971212	1.369794	0.704329
H	-4.157903	0.160605	-1.124583
C	-0.077783	1.055163	0.104240
C	-0.635962	-0.861788	-0.758559
C	0.220778	2.487892	-0.285831
C	0.104982	0.856901	1.602242
H	-0.087545	-0.168820	1.917600
H	1.124248	1.115093	1.895401
H	-0.575187	1.508568	2.152496
H	1.251919	2.746019	-0.037826
H	-0.436358	3.176260	0.249799
H	0.080042	2.642131	-1.355942
H	-0.881549	-1.388566	-1.676924
H	-0.697065	-1.560992	0.074353
C	0.666022	-0.038576	-0.746008
H	0.871904	0.378720	-1.731506
C	1.937323	-0.577938	-0.202112
C	2.087200	-1.639429	0.806912
H	1.139141	-2.085273	1.084126
H	2.782436	-2.382558	0.408796
H	2.601709	-1.216695	1.673813
O	-4.067956	-1.490381	0.004749
O	2.971521	-0.012698	-0.635174
O	4.172866	-0.409947	-0.115102

Rotational constants (GHz): 1.5404700 0.4155500 0.3734800
 Vibrational harmonic frequencies (cm-1):

35.0374	37.9774	62.0053
84.4155	120.5618	158.9591
191.8431	222.7174	232.9002

268.1518	279.6948	301.6540
324.6526	332.2669	341.7359
372.5307	408.7979	460.1951
490.5385	540.4485	571.3331
587.5987	661.8379	744.1422
781.8435	864.5007	885.7184
925.2495	927.2388	950.0348
964.2239	990.2243	1000.1005
1009.8356	1038.8730	1044.6443
1064.5056	1098.9817	1139.0503
1157.2880	1181.3095	1192.6766
1222.1523	1251.5140	1257.4335
1279.3217	1301.0480	1318.2512
1331.3664	1367.7914	1388.8357
1403.4797	1414.4851	1422.3460
1426.1317	1439.0362	1470.8114
1480.1129	1486.8204	1491.1597
1498.0997	1511.0473	1511.5841
1611.8194	1859.4274	2934.3718
3047.7026	3054.8264	3057.4044
3058.0144	3060.6433	3099.1908
3101.6483	3104.2337	3116.5714
3122.5213	3127.6289	3131.7463
3136.6181	3156.5038	3203.4068

Zero-point correction (Hartree): 0.246738

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.16375145

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -1.381988 | 0.183701  | -0.373996 |
| H | -1.702428 | 0.620866  | -1.322261 |
| C | -2.580760 | 0.065074  | 0.556755  |
| C | -3.628650 | -0.818018 | -0.061016 |
| H | -2.267785 | -0.392265 | 1.500116  |
| H | -3.021895 | 1.039603  | 0.766005  |
| H | -3.305903 | -1.857653 | -0.270709 |
| C | -0.109166 | 0.939660  | 0.103501  |
| C | -0.507240 | -1.057898 | -0.652974 |
| C | 0.047180  | 2.374163  | -0.356934 |
| C | 0.127141  | 0.828275  | 1.602831  |
| H | 0.037058  | -0.194600 | 1.969909  |
| H | 1.125648  | 1.189514  | 1.855543  |
| H | -0.595388 | 1.442036  | 2.142361  |
| H | 1.056862  | 2.734953  | -0.152511 |
| H | -0.655960 | 3.024000  | 0.167792  |
| H | -0.136431 | 2.465518  | -1.427618 |
| H | -0.721308 | -1.653006 | -1.537144 |
| H | -0.472798 | -1.714729 | 0.216108  |
| C | 0.711735  | -0.119061 | -0.719964 |
| H | 0.847368  | 0.267244  | -1.729858 |
| C | 2.043468  | -0.514437 | -0.198231 |
| C | 2.321757  | -1.496160 | 0.863297  |
| H | 1.426762  | -2.002684 | 1.205241  |
| H | 3.063920  | -2.200875 | 0.480325  |
| H | 2.828463  | -0.979567 | 1.682609  |
| O | -4.737871 | -0.462219 | -0.346923 |
| O | 3.009429  | 0.107071  | -0.705382 |
| O | 4.257560  | -0.157372 | -0.213386 |

Rotational constants (GHz): 1.7568200 0.3801300 0.3555400

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| 31.6875   | 43.4869   | 50.0651   |
| 89.8532   | 125.0562  | 163.4201  |
| 200.4183  | 224.6560  | 228.8316  |
| 269.5736  | 277.6870  | 299.9004  |
| 325.3275  | 335.4010  | 345.0679  |
| 373.3829  | 406.5666  | 458.0132  |
| 491.9616  | 526.9410  | 570.3124  |
| 590.5956  | 663.8904  | 745.4674  |
| 787.8889  | 857.7125  | 886.1078  |
| 922.7356  | 926.4297  | 948.2877  |
| 964.8259  | 991.8685  | 997.6308  |
| 1006.5224 | 1037.9655 | 1043.6630 |
| 1075.1409 | 1103.7958 | 1146.2850 |
| 1152.3523 | 1181.9780 | 1193.9134 |
| 1224.0313 | 1253.4493 | 1263.2043 |
| 1279.1398 | 1306.7086 | 1319.5110 |
| 1332.8752 | 1366.0501 | 1390.5622 |
| 1401.2557 | 1413.1533 | 1424.0721 |
| 1429.5582 | 1437.4007 | 1468.5717 |
| 1480.3264 | 1487.3777 | 1491.5254 |
| 1498.5108 | 1511.6500 | 1513.1350 |
| 1611.8488 | 1863.1810 | 2930.1565 |
| 3050.0680 | 3053.1731 | 3056.8264 |
| 3058.0360 | 3070.8160 | 3091.5813 |
| 3101.9794 | 3106.5650 | 3119.0812 |
| 3124.2887 | 3125.5627 | 3130.3780 |
| 3132.1819 | 3151.0914 | 3200.9270 |

Zero-point correction (Hartree): 0.246800

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.16655399

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-1.452694	0.259487	-0.312133
H	-1.797397	0.565580	-1.301200
C	-2.610731	0.313946	0.656011
C	-3.775018	-0.536703	0.224457
H	-2.321673	-0.019927	1.658356
H	-2.984601	1.335904	0.786492

H	-4.645613	-0.537109	0.907017
C	-0.131740	1.010553	0.014089
C	-0.650143	-1.048790	-0.446921
C	0.075479	2.358473	-0.645444
C	0.160990	1.094052	1.506260
H	0.039114	0.135886	2.013034
H	1.184646	1.434487	1.673484
H	-0.509072	1.812006	1.981659
H	1.108814	2.689937	-0.527243
H	-0.573210	3.111574	-0.192784
H	-0.147162	2.311711	-1.711573
H	-0.940391	-1.736813	-1.234918
H	-0.615969	-1.586909	0.500329
C	0.609574	-0.192076	-0.677303
H	0.728588	0.045364	-1.734209
C	1.939227	-0.570950	-0.139259
C	2.208331	-1.431903	1.024627
H	1.304463	-1.864850	1.436809
H	2.919870	-2.200668	0.713696
H	2.748342	-0.841310	1.769251
O	-3.795268	-1.187137	-0.784261
O	2.913809	-0.044746	-0.730791
O	4.164160	-0.292042	-0.230512
Rotational constants (GHz): 1.5835500 0.4186400 0.3864800			
Vibrational harmonic frequencies (cm-1):			
35.2510	46.7278	78.4949	
115.9980	128.7144	165.2376	
198.1055	226.0229	229.7745	
249.4518	277.7633	300.5236	
321.6709	335.1518	341.9524	
373.6645	402.2874	447.4855	
490.1870	557.6275	588.1573	
648.4339	676.1540	719.5557	
767.4337	838.4736	886.8841	
925.8520	930.5819	934.4084	
951.1725	964.4885	994.4367	
1001.9227	1026.7300	1041.5722	
1045.2015	1102.7539	1150.4941	
1155.4240	1178.0613	1194.3618	
1225.4701	1247.5420	1265.3978	
1283.3851	1316.3360	1327.7769	
1336.0060	1371.2033	1391.5014	
1406.7765	1417.9600	1423.3692	
1427.8743	1438.9449	1452.3693	
1480.1879	1486.7895	1492.0677	
1498.3324	1511.0061	1513.1465	
1611.7391	1855.8531	2955.4365	
3039.5372	3047.7618	3053.8229	
3058.7205	3068.7638	3087.5465	
3096.8365	3102.8119	3106.6947	
3115.4704	3121.2445	3128.4599	
3129.8410	3165.7266	3202.6443	
Zero-point correction (Hartree): 0.246742			
ApineneCI.A.a.ttm			
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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.16202160			
Electronic state : 1-A			
Cartesian coordinates (Angs):			
C	1.317528	0.748568	0.891415
H	1.326014	1.684637	1.453020
C	2.764773	0.376657	0.592500
C	3.003470	-0.994243	0.020370
H	3.219743	1.106390	-0.078839
H	3.327362	0.402381	1.532992
H	2.537473	-1.836013	0.569216
C	0.282056	0.910498	-0.256442
C	0.343036	-0.220826	1.597739
C	0.074819	2.310330	-0.797294
C	0.485333	-0.077255	-1.396747
H	0.617365	-1.104133	-1.052606
H	-0.374821	-0.060395	-2.068669
H	1.369723	0.190868	-1.975871
H	-0.809935	2.348878	-1.435308
H	0.933836	2.620021	-1.395904
H	-0.057685	3.029629	0.011307
H	0.269335	-0.168035	2.681036
H	0.502681	-1.256209	1.305593
C	-0.793322	0.428992	0.783775
H	-1.183900	1.306581	1.298475
C	-1.946966	-0.355206	0.278653
C	-1.963972	-1.788719	-0.057467
H	-1.029165	-2.282931	0.179985
H	-2.807606	-2.244228	0.466823
H	-2.210840	-1.888762	-1.117595
O	3.685976	-1.213878	-0.941887
O	-2.992542	0.314597	0.091301
O	-4.072199	-0.335900	-0.438496
Rotational constants (GHz): 1.4690500 0.4460800 0.4167500			
Vibrational harmonic frequencies (cm-1):			
35.8599	52.2704	80.4232	
88.7735	126.1411	179.5346	
216.1317	223.3739	235.4170	
258.2576	277.7392	295.3544	
330.8872	346.0437	358.2750	
381.0193	399.8756	450.9627	
478.1306	555.9854	578.9571	
612.5135	665.2230	700.6541	
768.8261	822.9441	883.6926	
909.5564	932.9615	952.0466	
964.1081	983.5348	1000.4275	
1007.9095	1040.6456	1046.6275	

1061.6543	1113.1146	1138.1670
1152.1369	1182.8849	1194.4671
1227.7174	1248.2751	1259.6561
1297.8755	1314.3911	1326.7366
1336.9768	1370.4352	1390.6956
1402.6480	1414.0346	1426.2462
1437.4565	1437.9869	1453.3608
1481.0332	1487.1267	1491.2188
1500.0690	1510.0784	1513.6740
1611.5785	1858.8637	2935.8123
3035.4673	3049.2355	3055.5993
3059.0788	3072.4379	3102.9540
3103.3972	3108.8968	3110.2593
3118.9892	3124.1583	3128.2163
3132.5376	3161.6288	3201.9573

Zero-point correction (Hartree): 0.246913

ApineneCI.A.a.ttp

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.16350311  
Electronic state : 1-A  
Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -1.459857 | 0.728945  | -0.774772 |
| H | -1.545884 | 1.604245  | -1.422268 |
| C | -2.863621 | 0.384253  | -0.305334 |
| C | -3.161487 | -0.970005 | 0.281092  |
| H | -3.206919 | 1.121445  | 0.430266  |
| H | -3.576082 | 0.484254  | -1.133249 |
| H | -4.208494 | -1.075922 | 0.626734  |
| C | -0.325577 | 1.036711  | 0.244598  |
| C | -0.537053 | -0.296268 | -1.469526 |
| C | -0.082967 | 2.502663  | 0.548649  |
| C | -0.410126 | 0.238139  | 1.537059  |
| H | -0.548084 | -0.826028 | 1.365622  |
| H | 0.497527  | 0.383780  | 2.126212  |
| H | -1.250526 | 0.591061  | 2.139205  |
| H | 0.853723  | 2.631171  | 1.094030  |
| H | -0.888559 | 2.904006  | 1.167896  |
| H | -0.027701 | 3.093550  | -0.366051 |
| H | -0.545986 | -0.320942 | -2.556468 |
| H | -0.686988 | -1.297477 | -1.081333 |
| C | 0.662288  | 0.413134  | -0.808989 |
| H | 1.047546  | 1.214747  | -1.438621 |
| C | 1.819405  | -0.358541 | -0.292271 |
| C | 1.796899  | -1.740166 | 0.216627  |
| H | 0.819347  | -2.200217 | 0.126895  |
| H | 2.563667  | -2.305048 | -0.319324 |
| H | 2.139505  | -1.725330 | 1.254391  |
| O | -2.408028 | -1.900328 | 0.375242  |
| O | 2.903884  | 0.274265  | -0.267225 |
| O | 3.996206  | -0.362748 | 0.257391  |

Rotational constants (GHz): 1.3698800 0.5108200 0.4447300  
Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| 37.0298   | 45.3062   | 98.9750   |
| 118.6821  | 135.8793  | 179.2687  |
| 197.3844  | 231.0504  | 236.5105  |
| 242.9874  | 280.2191  | 292.4196  |
| 320.1932  | 331.5485  | 350.6010  |
| 376.8807  | 398.7424  | 442.4859  |
| 487.9831  | 556.3149  | 587.2765  |
| 656.7695  | 674.1668  | 748.8518  |
| 772.7921  | 783.6581  | 886.2107  |
| 898.6017  | 933.2348  | 942.1998  |
| 963.7227  | 970.8098  | 991.6457  |
| 1006.8818 | 1023.0737 | 1045.0926 |
| 1060.6267 | 1089.3346 | 1140.0656 |
| 1161.6897 | 1182.9060 | 1199.6735 |
| 1240.9234 | 1255.8332 | 1262.7268 |
| 1302.4066 | 1319.6725 | 1334.4583 |
| 1360.0069 | 1384.3887 | 1390.6155 |
| 1406.2085 | 1413.5201 | 1424.3064 |
| 1432.9074 | 1443.6064 | 1449.1116 |
| 1480.5530 | 1489.5271 | 1490.6805 |
| 1504.0294 | 1511.3293 | 1518.7663 |
| 1613.1177 | 1858.6974 | 2940.9073 |
| 3029.4127 | 3045.3175 | 3052.9694 |
| 3055.1312 | 3058.4377 | 3065.1910 |
| 3102.9762 | 3103.7190 | 3109.8862 |
| 3114.8965 | 3116.6292 | 3126.5758 |
| 3171.8102 | 3190.9714 | 3203.6175 |

Zero-point correction (Hartree): 0.247080

ApineneCI.A.a.ttt

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.16350311
Electronic state : 1-A
Cartesian coordinates (Angs):

C	-1.459857	0.728944	-0.774772
H	-1.545884	1.604244	-1.422269
C	-2.863621	0.384253	-0.305336
C	-3.161490	-0.970007	0.281087
H	-3.206920	1.121443	0.430266
H	-3.576082	0.484257	-1.133251
H	-4.208498	-1.075925	0.626721
C	-0.325578	1.036712	0.244599
C	-0.537051	-0.296268	-1.469525
C	-0.082969	2.502664	0.548650
C	-0.410129	0.238141	1.537060
H	-0.548088	-0.826027	1.365625
H	0.497524	0.383781	2.126215
H	-1.250529	0.591064	2.139206
H	0.853721	2.631172	1.094032

H	-0.888562	2.904007	1.167896
H	-0.027701	3.093551	-0.366050
H	-0.545983	-0.320942	-2.556467
H	-0.686986	-1.297477	-1.081332
C	0.662289	0.413135	-0.808987
H	1.047547	1.214749	-1.438618
C	1.819406	-0.358540	-0.292269
C	1.796900	-1.740164	0.216632
H	0.819346	-2.200214	0.126904
H	2.563665	-2.305048	-0.319319
H	2.139509	-1.725325	1.254396
O	-2.408030	-1.900329	0.375242
O	2.903886	0.274264	-0.267228
O	3.996209	-0.362751	0.257386

Rotational constants (GHz): 1.3698800 0.5108200 0.4447300

Vibrational harmonic frequencies (cm-1):

37.0298	45.3059	98.9749
118.6817	135.8793	179.2685
197.3841	231.0499	236.5102
242.9871	280.2190	292.4193
320.1933	331.5484	350.5998
376.8808	398.7423	442.4856
487.9834	556.3150	587.2765
656.7695	674.1664	748.8517
772.7919	783.6581	886.2109
898.6017	933.2348	942.1996
963.7224	970.8099	991.6455
1006.8816	1023.0734	1045.0925
1060.6264	1089.3346	1140.0653
1161.6895	1182.9059	1199.6734
1240.9234	1255.8330	1262.7267
1302.4064	1319.6724	1334.4581
1360.0066	1384.3885	1390.6156
1406.2083	1413.5200	1424.3063
1432.9072	1443.6062	1449.1116
1480.5530	1489.5271	1490.6804
1504.0293	1511.3292	1518.7662
1613.1178	1858.6972	2940.9083
3029.4131	3045.3176	3052.9697
3055.1314	3058.4377	3065.1912
3102.9761	3103.7195	3109.8866
3114.8968	3116.6295	3126.5756
3171.8108	3190.9719	3203.6180

Zero-point correction (Hartree): 0.247080

Population analysis as 298K (%)

Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)

Compound	Qtot	Erel	Erel2	n*Q*MB	%
ApineneCI.A.a.14Hshift.b.mtp	1.120e+44	0.00	0.00	1.120e+44	31.2
ApineneCI.A.a.14Hshift.a.mtp	1.009e+44	0.28	0.28	6.273e+43	17.5
ApineneCI.A.a.14Hshift.b.ptt	3.819e+44	1.33	1.33	4.014e+43	11.2
ApineneCI.A.a.14Hshift.b.ptp	1.366e+44	0.79	0.79	3.619e+43	10.1
ApineneCI.A.a.14Hshift.a.ptp	1.334e+44	0.94	0.94	2.716e+43	7.56
ApineneCI.A.a.14Hshift.a.mtt	1.878e+44	1.25	1.25	2.276e+43	6.33
ApineneCI.A.a.14Hshift.b.mtt	1.537e+44	1.14	1.14	2.252e+43	6.27
ApineneCI.A.a.14Hshift.a.ptt	2.060e+44	1.67	1.67	1.227e+43	3.41
ApineneCI.A.a.14Hshift.b.ppp	3.153e+44	2.29	2.29	6.650e+42	1.85
ApineneCI.A.a.14Hshift.b.pmt	4.965e+44	2.60	2.60	6.137e+42	1.71
ApineneCI.A.a.14Hshift.a.pmp	3.105e+44	2.46	2.46	4.859e+42	1.35
ApineneCI.A.a.14Hshift.a.pmt	4.140e+44	2.90	2.90	3.111e+42	0.866
ApineneCI.A.a.14Hshift.b.mmt	4.679e+44	3.18	3.18	2.160e+42	0.601
ApineneCI.A.a.14Hshift.b.tmp	1.160e+44	3.69	3.69	2.271e+41	0.0632
ApineneCI.A.a.14Hshift.b.ttt	1.107e+44	4.08	4.08	1.119e+41	0.0311
ApineneCI.A.a.14Hshift.a.ttt	1.498e+44	4.29	4.29	1.064e+41	0.0296
ApineneCI.A.a.14Hshift.b.ttp	1.133e+44	4.30	4.30	7.946e+40	0.0221
ApineneCI.A.a.14Hshift.a.tmt	1.929e+44	4.66	4.66	7.427e+40	0.0207
ApineneCI.A.a.14Hshift.a.ttp	1.257e+44	4.67	4.67	4.688e+40	0.013
Total				3.593e+44	100

ApineneCI.A.a.14Hshift.a.mtp

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E(CCSDF(T)/Aug-CC-pVTZ) (Hartree): -615.21202409

E(CCSDF(Aug-CC-pVTZ) (Hartree): -615.09018366

T1 diagnostic: 0.018645

E(MP2/Aug-CC-pVTZ) (Hartree): -615.02816731

E(MP3/Aug-CC-pVTZ) (Hartree): -615.07666790

E(RHF/Aug-CC-pVTZ) (Hartree): -612.57051405

E(RM062X/Aug-CC-pVTZ) (Hartree): -616.14233071

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 1.301158  | -0.500521 | 0.747951  |
| H | 1.815601  | -0.064609 | 1.605875  |
| C | 2.285903  | -1.293094 | -0.082668 |
| C | 3.477241  | -0.511620 | -0.555568 |
| H | 2.665836  | -2.150815 | 0.484004  |
| H | 1.809410  | -1.728708 | -0.967356 |
| H | 4.207854  | -1.077809 | -1.163847 |
| C | 0.423520  | 0.606242  | 0.086408  |
| C | 0.018093  | -1.224990 | 1.196562  |
| C | 0.832649  | 2.046472  | 0.320464  |
| C | 0.154951  | 0.348026  | -1.388005 |
| H | -0.199055 | -0.666059 | -1.577961 |
| H | -0.604525 | 1.036186  | -1.763003 |
| H | 1.067898  | 0.512751  | -1.963197 |
| H | 0.033528  | 2.723974  | 0.011654  |
| H | 1.729173  | 2.285580  | -0.249583 |
| H | 1.047018  | 2.225592  | 1.374818  |
| H | 0.002216  | -1.666035 | 2.189868  |
| H | -0.296018 | -1.971683 | 0.469020  |
| C | -0.751434 | 0.092132  | 1.010020  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| H | -0.764734 | 0.687689  | 1.921988  |
| C | -2.099449 | 0.095878  | 0.402736  |
| C | -2.912149 | 1.212865  | 0.124079  |
| H | -3.339404 | 0.548226  | -0.933210 |
| H | -2.453998 | 2.179887  | 0.281800  |
| H | -3.935259 | 1.143078  | 0.490569  |
| O | 3.664277  | 0.650214  | -0.313449 |
| O | -2.465929 | -1.008155 | -0.158871 |
| O | -3.594404 | -0.797757 | -0.950593 |

Rotational constants (GHz): 1.6712600 0.4595100 0.4271500

Vibrational harmonic frequencies (cm-1):

|            |           |           |
|------------|-----------|-----------|
| i1597.1407 | 43.2020   | 47.3728   |
| 79.1041    | 106.0826  | 141.4839  |
| 159.1948   | 224.6839  | 243.6552  |
| 249.7198   | 282.3710  | 296.3651  |
| 319.2276   | 335.7753  | 368.2540  |
| 393.4077   | 471.8160  | 483.1152  |
| 536.4085   | 569.1061  | 615.7997  |
| 668.6230   | 674.9604  | 741.9890  |
| 747.9881   | 780.5115  | 843.4611  |
| 889.4252   | 914.7191  | 929.3936  |
| 948.5566   | 965.9192  | 984.3215  |
| 988.3414   | 1007.8427 | 1030.5405 |
| 1056.6987  | 1062.5075 | 1106.5013 |
| 1121.0641  | 1161.3538 | 1173.6400 |
| 1192.9803  | 1213.7364 | 1252.9253 |
| 1270.5857  | 1286.4056 | 1301.9806 |
| 1316.1399  | 1349.8168 | 1357.8040 |
| 1404.7515  | 1406.4101 | 1420.3088 |
| 1424.7088  | 1427.6617 | 1448.7594 |
| 1485.6914  | 1492.0151 | 1498.9668 |
| 1507.5390  | 1510.5035 | 1521.8394 |
| 1554.1418  | 1853.7644 | 1885.8992 |
| 2949.8328  | 3041.6606 | 3051.3131 |
| 3054.4583  | 3068.1646 | 3086.8325 |
| 3099.6972  | 3106.2500 | 3116.7650 |
| 3118.2619  | 3122.2353 | 3130.3192 |
| 3145.0082  | 3156.2932 | 3223.2102 |

Zero-point correction (Hartree): 0.242899

ApineneCI.A.a.14Hshift.a.mtt

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E(RM062X/Aug-CC-pVT2) (Hartree): -616.14069476

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-1.362707	-0.552890	-0.687144
H	-1.747892	-0.143175	-1.622005
C	-2.496757	-1.173176	0.097800
C	-3.631930	-0.235621	0.395075
H	-2.917054	-2.030848	-0.439576
H	-2.152204	-1.579818	1.054721
H	-4.472148	-0.670447	0.969025
C	-0.434802	0.513942	-0.028681
C	-0.123112	-1.428480	-0.952803
C	-0.657464	1.965919	-0.399937
C	-0.322653	0.353574	1.479583
H	-0.102257	-0.672169	1.779079
H	0.473422	0.990030	1.869894
H	-1.257206	0.660445	1.952998
H	0.211255	2.561867	-0.111938
H	-1.539134	2.361567	0.102041
H	-0.804393	2.074661	-1.474991
H	-0.063522	-1.964173	-1.896921
H	0.041549	-2.128821	-0.134224
C	0.751606	-0.172999	-0.804838
H	0.880579	0.338484	-1.758672
C	2.055448	-0.238213	-0.110519
C	2.611342	-1.254216	0.693745
H	3.792274	-0.803821	0.335131
H	2.135587	-2.222987	0.649769
H	2.884391	-0.941461	1.701243
O	-3.664817	0.914966	0.052338
O	2.852558	0.742046	-0.383043
O	4.100124	0.530941	0.197049

Rotational constants (GHz): 1.8383500 0.4289300 0.3977300

Vibrational harmonic frequencies (cm-1):

i1592.5122	24.7547	46.9475
73.4538	108.1540	136.8907
163.9575	214.0595	241.1234
263.1010	279.5884	287.3031
322.5651	344.2830	369.2508
388.9742	459.7283	480.8324
537.9792	552.3340	593.8652
668.2231	721.2465	741.3332
749.9577	786.0615	830.4985
906.9919	912.9936	927.2075
952.8309	966.8285	988.5585
989.5104	1005.3077	1017.4646
1042.6181	1058.8318	1114.8189
1117.7700	1162.6677	1177.2873
1193.4680	1216.3269	1251.3583
1272.6207	1286.3424	1309.3072
1337.6243	1342.3273	1350.8922
1403.3253	1406.8343	1421.6066
1422.9007	1430.0238	1450.4083
1485.0532	1489.7252	1493.8783
1507.3259	1510.7817	1521.1937
1546.7268	1855.4133	1891.3823
2949.1929	3040.4986	3050.3500
3054.1567	3067.2904	3088.5314
3093.3824	3101.8148	3111.3643
3119.8076	3122.6162	3124.4512

3145.1844 3150.3694 3235.5629
Zero-point correction (Hartree): 0.242806

ApineneCI.A.a.14Hshift.a.pmp

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.13872176  
Electronic state : 1-A

Cartesian coordinates (Angs):  
C -1.368010 0.465992 -0.394950  
H -1.750703 1.057643 -1.231611  
C -2.493294 0.187813 0.591499  
C -3.632763 -0.476792 -0.129490  
H -2.163561 -0.461947 1.400789  
H -2.853233 1.132272 1.012001  
H -4.120573 0.140546 -0.910947  
C -0.055209 1.130067 0.106790  
C -0.542892 -0.717548 -0.935966  
C 0.070346 2.622964 -0.118065  
C 0.283860 0.763822 1.544201  
H 0.229905 -0.309885 1.723670  
H 1.296279 1.089250 1.789598  
H -0.404612 1.260447 2.229353  
H 1.072945 2.974249 0.132632  
H -0.635677 3.161280 0.518116  
H -0.137813 2.886125 -1.155727  
H -0.831942 -1.150078 -1.889883  
H -0.451403 -1.511689 -0.197421  
C 0.689416 0.204854 -0.931902  
H 0.791837 0.743505 -1.873509  
C 2.014432 -0.301079 -0.511027  
C 3.216021 0.428656 -0.407460  
H 3.514102 -0.343353 0.618347  
H 3.132910 1.496944 -0.556488  
H 4.074296 -0.020907 -0.904784  
O -3.997985 -1.602182 0.066629  
O 2.019187 -1.458554 0.058959  
O 3.247023 -1.688876 0.676172

Rotational constants (GHz): 1.3453200 0.4590700 0.3931900

Vibrational harmonic frequencies (cm-1):  
i1587.6767 32.5331 45.6668  
61.7546 84.4987 110.3731  
163.9070 188.7320 229.1461  
256.8406 277.4430 301.6542  
324.0826 334.0877 351.7135  
416.7131 466.9894 498.5912  
535.9381 545.5407 582.6854  
621.8950 677.7105 744.6392  
763.6806 833.2618 858.5405  
891.0177 923.5650 933.3303  
952.3550 964.7234 993.7211  
1002.8027 1006.9073 1038.7297  
1056.6166 1072.2648 1099.8301  
1138.5360 1154.8653 1177.5800  
1192.8507 1221.5710 1249.7246  
1253.7428 1277.7029 1301.0934  
1305.6050 1329.5666 1358.6961  
1400.0917 1406.2642 1423.7453  
1426.1487 1428.1436 1468.9846  
1485.5272 1491.5160 1499.9118  
1506.9909 1510.8543 1522.9416  
1555.1511 1862.4109 1888.1404  
2925.8213 3046.6433 3048.9907  
3052.4050 3058.3781 3101.6170  
3108.3175 3113.5119 3114.5263  
3124.3085 3125.4876 3134.0939  
3139.2893 3164.4570 3220.9029

Zero-point correction (Hartree): 0.242765

ApineneCI.A.a.14Hshift.a.pmt

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.13810045
Electronic state : 1-A

Cartesian coordinates (Angs):
C -1.411439 0.417740 -0.439607
H -1.686229 0.898015 -1.382567
C -2.630157 0.335740 0.470031
C -3.712075 -0.429527 -0.238825
H -2.394588 -0.176238 1.401981
H -2.993058 1.343572 0.691783
H -4.157211 0.079252 -1.117155
C -0.102534 1.077636 0.080454
C -0.618265 -0.871836 -0.728550
C 0.157481 2.507195 -0.347125
C 0.089762 0.918153 1.581397
H -0.055069 -0.110049 1.913817
H 1.098649 1.221665 1.866248
H -0.616179 1.552780 2.119092
H 1.180248 2.800639 -0.104126
H -0.520289 3.190329 0.169213
H 0.014346 2.629443 -1.421127
H -0.854652 -1.431797 -1.629408
H -0.649454 -1.545319 0.127077
C 0.664278 -0.021284 -0.743543
H 0.870959 0.371586 -1.739335
C 1.921017 -0.535723 -0.154673
C 2.159247 -1.686761 0.621476
H 3.386432 -1.668481 0.155054
H 1.377172 -2.431682 0.638067
H 2.613396 -1.498921 1.594104
O -4.065709 -1.535794 0.062584
O 2.978259 0.114996 -0.513923
O 4.122655 -0.515802 -0.034777

Rotational constants (GHz): 1.5380700 0.4178900 0.3707900
 Vibrational harmonic frequencies (cm-1):
 i1588.0301 29.0520 35.7079
 62.6797 88.0959 108.1915
 161.3195 191.9115 234.9219
 267.6631 275.4338 294.1876
 329.1250 338.8323 350.6303
 407.3515 466.7919 497.6218
 538.1157 540.1559 565.4070
 597.6906 734.1510 739.8284
 764.7613 828.8241 863.0785
 908.0191 921.6786 933.2093
 961.9161 970.5173 990.5906
 1001.3796 1007.6661 1021.7666
 1050.0611 1068.3078 1099.9972
 1141.2722 1157.6243 1181.4029
 1193.9955 1222.9889 1251.6132
 1256.4276 1279.0209 1301.6498
 1325.3385 1337.7428 1344.0292
 1396.1342 1407.6614 1423.2694
 1425.5036 1428.0296 1471.2284
 1485.7519 1491.3376 1497.1616
 1508.5021 1510.0377 1521.5237
 1548.7318 1859.7306 1890.1421
 2933.3638 3047.7280 3054.9413
 3056.1266 3059.9852 3095.4774
 3099.9152 3110.8672 3116.6951
 3123.5238 3127.4365 3132.3982
 3136.7322 3157.0053 3236.1689
 Zero-point correction (Hartree): 0.242836

ApineneCI.A.a.14Hshift.a.ptp

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.14110955

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -1.423766 | 0.295090  | -0.257398 |
| H | -1.904390 | 0.740183  | -1.130467 |
| C | -2.454899 | 0.089583  | 0.827044  |
| C | -3.630344 | -0.730094 | 0.367563  |
| H | -2.030208 | -0.412986 | 1.702239  |
| H | -2.851106 | 1.041305  | 1.200203  |
| H | -4.396528 | -0.939337 | 1.137786  |
| C | -0.121511 | 1.082133  | 0.056695  |
| C | -0.570585 | -0.903755 | -0.710394 |
| C | -0.094763 | 2.537385  | -0.364755 |
| C | 0.339812  | 0.924881  | 1.498686  |
| H | 0.357507  | -0.117331 | 1.818178  |
| H | 1.348692  | 1.322766  | 1.622066  |
| H | -0.322471 | 1.477818  | 2.166590  |
| H | 0.903237  | 2.962994  | -0.243432 |
| H | -0.779865 | 3.122956  | 0.252388  |
| H | -0.394974 | 2.651899  | -1.406745 |
| H | -0.910035 | -1.459247 | -1.578912 |
| H | -0.377667 | -1.595767 | 0.107984  |
| C | 0.606084  | 0.068548  | -0.910747 |
| H | 0.615202  | 0.486430  | -1.916794 |
| C | 1.982234  | -0.312508 | -0.526119 |
| C | 3.147154  | 0.476078  | -0.617073 |
| H | 3.555060  | -0.125558 | 0.483439  |
| H | 2.996246  | 1.506232  | -0.910760 |
| H | 3.992891  | -0.003328 | -1.107868 |
| O | -3.765622 | -1.146657 | -0.750195 |
| O | 2.089292  | -1.374444 | 0.200160  |
| O | 3.366569  | -1.456785 | 0.752922  |

Rotational constants (GHz): 1.4155000 0.4605900 0.4094200

Vibrational harmonic frequencies (cm-1):

|            |           |           |
|------------|-----------|-----------|
| i1592.8301 | 42.7564   | 52.4647   |
| 74.3913    | 104.2497  | 135.6231  |
| 159.8756   | 201.5594  | 217.6819  |
| 249.4409   | 260.3520  | 294.8339  |
| 323.5550   | 334.6565  | 353.4177  |
| 404.0214   | 468.4640  | 492.9040  |
| 536.9209   | 568.3709  | 617.3748  |
| 669.4863   | 680.5609  | 723.5345  |
| 744.1927   | 826.0794  | 852.4590  |
| 885.7561   | 923.4635  | 935.3795  |
| 939.7303   | 955.2925  | 965.1951  |
| 994.9486   | 1004.4337 | 1019.6243 |
| 1044.3431  | 1062.8511 | 1101.2752 |
| 1149.8395  | 1150.6762 | 1177.1732 |
| 1194.1574  | 1224.8607 | 1248.2325 |
| 1264.3378  | 1280.1473 | 1304.0033 |
| 1326.1927  | 1336.5707 | 1358.2478 |
| 1405.7031  | 1408.2571 | 1420.4329 |
| 1424.8089  | 1429.7653 | 1453.1597 |
| 1486.0217  | 1491.0982 | 1499.3043 |
| 1506.2998  | 1509.7693 | 1522.1685 |
| 1553.7012  | 1855.3080 | 1886.8053 |
| 2949.0131  | 3037.3382 | 3046.1888 |
| 3056.4381  | 3068.9758 | 3085.3188 |
| 3102.4343  | 3108.4120 | 3112.2756 |
| 3115.4400  | 3122.7492 | 3125.7063 |
| 3135.2460  | 3171.1799 | 3221.1774 |

Zero-point correction (Hartree): 0.242731

ApineneCI.A.a.14Hshift.a.ptt

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.13993614

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-1.463787	0.252191	-0.306700

H	-1.825168	0.542230	-1.294730
C	-2.610956	0.294744	0.674799
C	-3.766812	-0.576647	0.263365
H	-2.303656	-0.028027	1.675306
H	-2.999797	1.311396	0.803697
H	-4.626899	-0.589196	0.959185
C	-0.153179	1.030048	-0.001578
C	-0.637989	-1.041491	-0.435487
C	0.019729	2.374747	-0.677388
C	0.152694	1.131262	1.486424
H	0.071737	0.169754	1.995016
H	1.167418	1.503024	1.639806
H	-0.535065	1.830013	1.965312
H	1.045570	2.731329	-0.568188
H	-0.644338	3.117036	-0.229129
H	-0.208066	2.311072	-1.741647
H	-0.923095	-1.745271	-1.211275
H	-0.574695	-1.564126	0.519159
C	0.604183	-0.168006	-0.685208
H	0.726888	0.057846	-1.744698
C	1.917904	-0.530699	-0.109065
C	2.264626	-1.554322	0.795180
H	3.464929	-1.528948	0.263440
H	1.530973	-2.332167	0.948946
H	2.750409	-1.214943	1.709666
O	-3.792249	-1.230623	-0.743034
O	2.914601	0.124253	-0.606991
O	4.118195	-0.373877	-0.114464
Rotational constants (GHz):			
	1.5887400	0.4227200	0.3839200
Vibrational harmonic frequencies (cm-1):			
i1588.6910	29.3828		46.7220
78.5335	103.2408		127.4444
162.8945	199.2371		222.9128
251.7126	270.8647		292.8824
326.9766	341.8825		352.3604
397.8364	459.4120		490.1193
540.3456	552.6009		595.5505
663.2706	716.6093		739.0509
746.1980	820.6230		846.4030
905.4491	920.5609		933.6997
939.2870	962.4455		972.6588
990.1039	1004.0925		1013.9412
1031.9954	1054.6336		1103.4532
1150.9950	1155.7774		1176.3503
1195.6379	1223.5565		1246.8248
1265.3151	1282.3130		1319.8786
1334.8307	1337.4804		1345.3027
1406.6224	1407.0958		1420.7824
1424.2879	1430.6327		1452.2812
1486.4028	1491.8382		1496.8833
1509.3448	1511.2230		1520.8826
1546.2845	1855.6129		1890.7487
2953.0826	3038.8743		3047.7622
3053.5316	3068.4499		3085.7232
3093.5535	3101.2919		3110.0169
3115.7859	3121.6313		3128.8461
3129.3582	3165.8687		3234.5971
Zero-point correction (Hartree): 0.242718			
ApineneCI.A.a.14Hshift.a.tmt			
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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.13547553			
Electronic state : 1-A			
Cartesian coordinates (Angs):			
C	1.339035	0.669748	0.936584
H	1.372664	1.563093	1.563307
C	2.775461	0.280610	0.610304
C	2.977984	-1.045704	-0.071131
H	3.255702	1.048678	0.002306
H	3.334359	0.212664	1.551045
H	2.472721	-1.913423	0.395639
C	0.308221	0.939195	-0.194873
C	0.339411	-0.321484	1.572395
C	0.139777	2.378763	-0.635067
C	0.482263	0.025166	-1.399183
H	0.558041	-1.027704	-1.122021
H	-0.370293	0.124749	-2.073427
H	1.383687	0.293714	-1.951266
H	-0.740865	2.485701	-1.270830
H	1.009541	2.706626	-1.207937
H	0.023514	3.042176	0.222464
H	0.266660	-0.346555	2.656661
H	0.466877	-1.335605	1.200535
C	-0.780269	0.409379	0.809243
H	-1.165874	1.253547	1.381310
C	-1.914382	-0.342184	0.227486
C	-2.106459	-1.729574	0.072261
H	-3.396616	-1.491660	0.117299
H	-1.447130	-2.377284	0.631423
H	-2.282059	-2.056132	-0.952486
O	3.673637	-1.207137	-1.035681
O	-2.934654	0.390948	-0.074296
O	-4.002380	-0.404571	-0.479041
Rotational constants (GHz):			
	1.4602000	0.4483500	0.4180500
Vibrational harmonic frequencies (cm-1):			
i1593.0062	24.0026		54.0957
87.6739	90.3897		113.6287
179.2885	216.8366		238.5272
259.8126	271.7330		289.9540
344.5673	357.9860		368.5888
396.5701	461.4359		476.6086
537.4091	549.4038		583.1827

626.2150	697.3090	737.5203
745.9267	814.6318	834.1189
901.7986	912.0540	926.4072
963.6924	977.9733	989.5521
992.2522	1007.2812	1021.3110
1048.9124	1067.4784	1112.7168
1141.7909	1153.3457	1180.7305
1195.8022	1229.0647	1247.7975
1259.7586	1297.6931	1320.2378
1331.7372	1339.0060	1347.5210
1398.1445	1407.5682	1424.9223
1427.2013	1441.0414	1451.5085
1487.0739	1491.8044	1499.2579
1508.1827	1513.4491	1521.7858
1548.0298	1858.3027	1890.5336
2942.5452	3035.2192	3048.9140
3053.8993	3072.5600	3099.1619
3108.5441	3109.2223	3111.3489
3118.9436	3121.7586	3127.1249
3131.6864	3163.1684	3234.9911

Zero-point correction (Hartree): 0.243015

ApineneCI.A.a.14Hshift.a.ttp

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.13525539

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 1.480211  | 0.628313  | 0.777915  |
| H | 1.674546  | 1.467187  | 1.451280  |
| C | 2.828154  | 0.165771  | 0.250687  |
| C | 2.972757  | -1.187291 | -0.394237 |
| H | 3.219462  | 0.897072  | -0.466418 |
| H | 3.569304  | 0.161733  | 1.059310  |
| H | 3.981320  | -1.364364 | -0.818390 |
| C | 0.363399  | 1.098430  | -0.194832 |
| C | 0.461037  | -0.304062 | 1.468078  |
| C | 0.342476  | 2.581147  | -0.510799 |
| C | 0.271326  | 0.270818  | -1.468585 |
| H | 0.212825  | -0.796695 | -1.266412 |
| H | -0.610704 | 0.561596  | -2.042033 |
| H | 1.147539  | 0.449234  | -2.096106 |
| H | -0.551029 | 2.850104  | -1.076928 |
| H | 1.208542  | 2.849286  | -1.120627 |
| H | 0.368526  | 3.182306  | 0.398864  |
| H | 0.516516  | -0.395678 | 2.549697  |
| H | 0.434486  | -1.289056 | 1.015159  |
| C | -0.649353 | 0.603459  | 0.906879  |
| H | -0.869251 | 1.434681  | 1.577375  |
| C | -1.921260 | 0.033009  | 0.411804  |
| C | -2.978004 | 0.720908  | -0.220510 |
| H | -3.184959 | -0.381775 | -0.914829 |
| H | -2.782197 | 1.754995  | -0.471089 |
| H | -3.962864 | 0.551289  | 0.212172  |
| O | 2.141199  | -2.049267 | -0.453415 |
| O | -1.974291 | -1.253075 | 0.334132  |
| O | -3.091473 | -1.647024 | -0.399394 |

Rotational constants (GHz): 1.2105700 0.5787300 0.4750300

Vibrational harmonic frequencies (cm-1):

|            |           |           |
|------------|-----------|-----------|
| i1589.3409 | 33.4109   | 55.4284   |
| 87.0379    | 108.2140  | 123.9285  |
| 175.6322   | 198.6632  | 225.8607  |
| 242.4839   | 258.4426  | 293.8952  |
| 321.7083   | 326.2064  | 354.2376  |
| 397.6846   | 473.3109  | 484.3231  |
| 535.4104   | 567.5348  | 614.8213  |
| 663.7108   | 693.7837  | 745.1450  |
| 751.2335   | 782.6663  | 842.7871  |
| 883.5809   | 904.1295  | 929.7784  |
| 941.9179   | 967.0033  | 977.2123  |
| 995.4086   | 1007.2346 | 1020.3539 |
| 1052.9861  | 1064.0164 | 1089.3897 |
| 1134.3721  | 1163.1423 | 1175.1813 |
| 1196.5216  | 1235.3150 | 1251.0706 |
| 1260.9629  | 1298.9838 | 1306.7388 |
| 1332.8269  | 1358.0802 | 1374.7760 |
| 1407.4017  | 1409.6400 | 1423.8141 |
| 1428.0128  | 1435.5381 | 1449.2831 |
| 1485.5507  | 1491.7269 | 1504.5725 |
| 1507.9527  | 1511.9793 | 1523.8083 |
| 1552.5733  | 1865.7292 | 1889.4045 |
| 2932.9218  | 3027.7149 | 3045.4444 |
| 3052.5194  | 3055.1389 | 3057.4661 |
| 3094.0741  | 3110.5940 | 3114.7086 |
| 3115.1055  | 3118.3356 | 3124.8381 |
| 3160.2813  | 3193.4305 | 3219.9541 |

Zero-point correction (Hartree): 0.242825

ApineneCI.A.a.14Hshift.a.ttt

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.13599601

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-1.461918	0.670361	-0.805331
H	-1.528011	1.514736	-1.495380
C	-2.880547	0.336165	-0.375599
C	-3.193931	-0.991637	0.261222
H	-3.256043	1.106051	0.308668
H	-3.560028	0.390014	-1.235202
H	-4.243187	-1.073926	0.607486
C	-0.372830	1.036388	0.242383
C	-0.494549	-0.368206	-1.412395
C	-0.187471	2.514591	0.525014

C	-0.482185	0.253204	1.541617
H	-0.546937	-0.819725	1.377744
H	0.384412	0.453625	2.174141
H	-1.372285	0.567112	2.092019
H	0.721067	2.684350	1.105555
H	-1.029865	2.902711	1.102285
H	-0.113166	3.088521	-0.399186
H	-0.469805	-0.463990	-2.494971
H	-0.622661	-1.344789	-0.958595
C	0.664428	0.416545	-0.763740
H	1.029152	1.204565	-1.423063
C	1.824840	-0.306121	-0.198337
C	1.942226	-1.643600	0.226087
H	3.221649	-1.556176	-0.072612
H	1.145152	-2.315707	-0.056602
H	2.277143	-1.766903	1.255626
O	-2.451055	-1.925888	0.388238
O	2.933050	0.361496	-0.225867
O	3.994884	-0.445183	0.170948
Rotational constants (GHz): 1.3931300 0.5009700 0.4368200			
Vibrational harmonic frequencies (cm-1):			
i1596.8989	27.7484	50.1864	
92.3535	113.4776	126.8183	
176.3017	196.1905	231.5385	
242.8497	273.2075	282.7961	
328.9798	339.7949	351.1190	
391.8102	448.0837	489.3507	
546.0430	558.8727	592.8864	
671.6945	737.4926	745.7081	
750.2668	782.8392	830.9624	
896.7335	910.8105	930.7470	
940.4273	965.7554	990.8970	
996.9127	1003.5502	1010.8317	
1030.8122	1065.8372	1087.0424	
1139.0995	1161.9965	1183.8111	
1198.9534	1242.1027	1251.5010	
1263.4811	1301.4872	1326.7325	
1339.1752	1341.4800	1373.0596	
1404.7354	1406.9844	1423.7845	
1425.4184	1435.0334	1450.5893	
1485.7559	1489.7330	1498.4303	
1507.3023	1509.5521	1522.2520	
1552.6265	1861.0721	1887.8149	
2936.9362	3028.1847	3045.5516	
3052.7383	3055.4083	3062.2009	
3097.2704	3111.2067	3112.2293	
3115.2735	3116.8921	3125.6987	
3164.1880	3191.6780	3236.6404	
Zero-point correction (Hartree): 0.242957			
ApineneCI.A.a.14Hshift.b.mmt			
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E(RM062X/Aug-CC-pVT2) (Hartree): -616.13745264			
Electronic state : 1-A			
Cartesian coordinates (Angs):			
C	-1.329626	-0.539991	-0.550092
H	-1.734307	-0.272995	-1.529036
C	-2.476190	-0.910120	0.383297
C	-3.462117	0.220676	0.483176
H	-2.997485	-1.792162	0.011637
H	-2.083209	-1.125347	1.380459
H	-3.093066	1.135460	0.988579
C	-0.282798	0.541883	-0.143346
C	-0.181276	-1.552352	-0.734132
C	-0.463198	1.932280	-0.718048
C	-0.025554	0.603610	1.356362
H	0.137442	-0.383223	1.792670
H	0.860267	1.207664	1.559928
H	-0.869436	1.065068	1.871768
H	0.439183	2.525983	-0.563114
H	-1.294105	2.449164	-0.233561
H	-0.667043	1.891729	-1.788631
H	-0.243499	-2.246546	-1.567852
H	-0.004918	-2.112095	0.183671
C	0.776331	-0.359843	-0.868810
H	0.860240	-0.037350	-1.908236
C	2.139439	-0.401766	-0.285760
C	2.743639	-1.367815	0.542205
H	3.381752	-0.384673	1.121171
H	2.109347	-2.161290	0.909047
H	3.723286	-1.706312	0.206488
O	-4.573762	0.190983	0.032515
O	2.770377	0.722438	-0.369706
O	3.908841	0.705023	0.434179
Rotational constants (GHz): 1.8803500 0.4056200 0.3776700			
Vibrational harmonic frequencies (cm-1):			
i1597.3392	24.1625	29.7378	
63.4569	82.7479	113.0569	
188.4215	219.6049	229.6859	
263.6539	278.8508	299.2301	
305.4338	322.4565	383.2378	
399.0094	454.5742	501.9491	
527.8997	539.8647	575.0321	
613.5105	670.9872	734.2151	
746.9808	844.6248	857.7831	
900.8001	927.2764	950.0643	
962.4293	968.5634	985.4640	
998.5690	1006.9046	1025.7942	
1042.7121	1078.2243	1107.1902	
1134.9759	1156.3337	1176.3749	
1192.8628	1201.0559	1251.4217	
1267.5428	1281.5057	1299.1537	

1323.8012	1331.8925	1340.1351
1389.0290	1408.9303	1420.2790
1425.2551	1432.6422	1470.1330
1484.8127	1492.6866	1496.4060
1505.1565	1509.0499	1520.6183
1543.6134	1860.8739	1889.5265
2934.5387	3049.5019	3053.2234
3060.0699	3070.1995	3085.8922
3096.9541	3113.7986	3119.2257
3124.1455	3124.6137	3127.2717
3128.5112	3156.0008	3236.0190

Zero-point correction (Hartree): 0.242648

ApineneCI.A.a.14Hshift.b.mtp

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E (CCSD(T)/Aug-CC-pVTZ) (Hartree): -615.21228697

E (CCSD/Aug-CC-pVTZ) (Hartree): -615.09063686

T1 diagnostic: 0.018677

E (MP2/Aug-CC-pVTZ) (Hartree): -615.02837215

E (MP3/Aug-CC-pVTZ) (Hartree): -615.07705005

E (RHF/Aug-CC-pVTZ) (Hartree): -612.57190607

E (RM062X/Aug-CC-pVTZ) (Hartree): -616.14258621

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -1.302140 | -0.519748 | -0.731236 |
| H | -1.777595 | -0.102531 | -1.620424 |
| C | -2.319382 | -1.309960 | 0.061474  |
| C | -3.533344 | -0.527862 | 0.471981  |
| H | -2.669644 | -2.175269 | -0.512464 |
| H | -1.882032 | -1.734040 | 0.971730  |
| H | -4.291740 | -1.091218 | 1.048042  |
| C | -0.471756 | 0.608172  | -0.044454 |
| C | 0.010505  | -1.235849 | -1.106562 |
| C | -0.873245 | 2.042966  | -0.318695 |
| C | -0.273787 | 0.373876  | 1.445637  |
| H | 0.086394  | -0.631974 | 1.666789  |
| H | 0.453330  | 1.081460  | 1.847640  |
| H | -1.215839 | 0.530232  | 1.974291  |
| H | -0.070188 | 2.719671  | -0.016773 |
| H | -1.776005 | 2.303951  | 0.231369  |
| H | -1.069904 | 2.196846  | -1.380563 |
| H | 0.080212  | -1.690117 | -2.091541 |
| H | 0.297572  | -1.970759 | -0.355707 |
| C | 0.749539  | 0.093759  | -0.894864 |
| H | 0.804937  | 0.682408  | -1.811707 |
| C | 2.071155  | 0.139472  | -0.240491 |
| C | 2.987679  | 1.210606  | -0.209172 |
| H | 3.933883  | 0.306141  | -0.055614 |
| H | 2.811319  | 2.008223  | -0.917432 |
| H | 3.259340  | 1.553697  | 0.788532  |
| O | -3.709210 | 0.632412  | 0.214503  |
| O | 2.496782  | -0.967759 | 0.269096  |
| O | 3.806755  | -0.819566 | 0.720417  |

Rotational constants (GHz): 1.7352400 0.4449300 0.4102300

Vibrational harmonic frequencies (cm-1):

|            |           |           |
|------------|-----------|-----------|
| i1592.1906 | 42.2489   | 52.1949   |
| 72.2770    | 104.0185  | 139.3843  |
| 158.3359   | 217.8209  | 242.4803  |
| 253.4674   | 279.0766  | 289.2164  |
| 318.3369   | 327.7010  | 367.8744  |
| 393.4348   | 464.7774  | 477.6451  |
| 536.7444   | 569.1795  | 588.7918  |
| 668.4961   | 719.6492  | 740.7403  |
| 750.5579   | 786.3158  | 833.7046  |
| 901.0452   | 913.4527  | 928.4730  |
| 946.8637   | 966.4199  | 981.7116  |
| 990.4950   | 1012.3575 | 1016.2424 |
| 1051.5663  | 1069.4059 | 1102.9755 |
| 1119.3777  | 1155.6187 | 1170.6892 |
| 1193.3064  | 1208.2906 | 1250.2439 |
| 1272.1449  | 1283.2050 | 1299.7531 |
| 1312.0112  | 1348.4239 | 1356.4498 |
| 1403.8268  | 1409.2955 | 1421.4867 |
| 1422.9194  | 1429.5203 | 1448.6986 |
| 1485.3519  | 1491.1686 | 1497.9261 |
| 1508.0147  | 1511.6863 | 1520.3906 |
| 1554.5084  | 1853.8074 | 1889.1008 |
| 2953.2502  | 3042.0626 | 3048.6518 |
| 3052.2439  | 3067.6074 | 3086.4485 |
| 3091.3797  | 3099.2142 | 3112.5230 |
| 3115.5058  | 3120.5933 | 3126.5934 |
| 3144.9423  | 3155.1583 | 3226.7275 |

Zero-point correction (Hartree): 0.242706

ApineneCI.A.a.14Hshift.b.mtt

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E (RM062X/Aug-CC-pVTZ) (Hartree): -616.14067087

Electronic state : 1-A

Cartesian coordinates (Angs):

C	1.373062	0.623557	-0.631767
H	1.806261	0.297005	-1.578331
C	2.470158	1.128726	0.278431
C	3.565275	0.134973	0.541963
H	2.941243	2.024938	-0.141145
H	2.076745	1.444234	1.250695
H	4.373886	0.483411	1.212272
C	0.384270	-0.478579	-0.139820
C	0.175091	1.561738	-0.883645
C	0.595536	-1.889996	-0.647878
C	0.182778	-0.472264	1.368079
H	-0.017432	0.525916	1.761768
H	-0.660370	-1.110205	1.639086

H	1.072949	-0.864809	1.863095
H	-0.299166	-2.488262	-0.464658
H	1.442500	-2.357267	-0.147656
H	0.795071	-1.891576	-1.720261
H	0.188757	2.180280	-1.777658
H	-0.014807	2.196811	-0.018387
C	-0.736285	0.327846	-0.892545
H	-0.841149	-0.084648	-1.896988
C	-2.077830	0.358698	-0.264106
C	-2.644974	1.293101	0.625980
H	-3.278638	0.289213	1.179477
H	-1.990531	2.063412	1.006665
H	-3.628935	1.657633	0.332993
O	3.599895	-0.971707	0.076873
O	-2.725450	-0.754291	-0.374407
O	-3.835553	-0.760613	0.468893
Rotational constants (GHz): 1.7438200 0.4502900 0.4132800			
Vibrational harmonic frequencies (cm-1):			
i1600.3382	32.9560	46.5148	
71.9839	101.9344	133.0678	
163.5633	220.7917	243.7004	
259.3531	278.3223	290.7940	
315.7170	340.2951	367.8137	
391.4164	468.2082	479.3726	
538.7108	570.2269	603.8937	
659.5008	677.0632	737.0562	
747.9525	777.5113	849.6593	
895.6380	910.3449	931.3693	
953.8730	966.9132	982.9495	
990.9348	999.3730	1021.7706	
1042.8900	1057.4360	1111.4767	
1119.5468	1158.5157	1174.3331	
1193.0523	1207.8294	1251.6677	
1273.2716	1284.1702	1304.9870	
1327.2517	1340.1079	1349.1669	
1402.5657	1407.6625	1421.6395	
1422.0084	1429.7137	1450.6053	
1485.4502	1490.9698	1494.3370	
1507.1853	1508.3022	1521.3474	
1543.5549	1855.5093	1890.0227	
2948.1514	3040.3630	3049.2210	
3055.0505	3067.2375	3086.6179	
3090.9901	3094.9856	3114.7710	
3120.3801	3121.1886	3122.8101	
3146.5347	3148.9250	3236.1695	
Zero-point correction (Hartree): 0.242603			
ApineneCI.A.a.14Hshift.b.pmt			
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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.13831309			
Electronic state : 1-A			
Cartesian coordinates (Angs):			
C	-1.400015	0.436890	-0.432216
H	-1.714832	0.948482	-1.345867
C	-2.559267	0.384903	0.554468
C	-3.716573	-0.318423	-0.096439
H	-2.284795	-0.157410	1.458147
H	-2.862181	1.401806	0.820129
H	-4.200169	0.231214	-0.928664
C	-0.034579	1.034893	0.013590
C	-0.686206	-0.880656	-0.799625
C	0.252170	2.462582	-0.402093
C	0.253844	0.832777	1.494538
H	0.080665	-0.195487	1.815366
H	1.294725	1.078950	1.711052
H	-0.380151	1.485414	2.096337
H	1.297216	2.712542	-0.212824
H	-0.369629	3.158724	0.164903
H	0.051522	2.611837	-1.463741
H	-1.002996	-1.403170	-1.698292
H	-0.703644	-1.577633	0.037407
C	0.626473	-0.084663	-0.863773
H	0.800604	0.309682	-1.866618
C	1.899343	-0.662509	-0.367711
C	2.141599	-1.859987	0.332156
H	3.098783	-1.227269	0.960074
H	1.276347	-2.416402	0.661204
H	2.932134	-2.481081	-0.087671
O	-4.092199	-1.418924	0.199935
O	2.884342	0.173831	-0.385722
O	3.961066	-0.324286	0.345997
Rotational constants (GHz): 1.5604900 0.4298200 0.3803600			
Vibrational harmonic frequencies (cm-1):			
i1585.0266	27.3704	34.9768	
60.9116	86.0235	98.7577	
159.8969	188.3313	232.2721	
264.2814	277.2783	301.5581	
319.7033	334.3358	351.4244	
415.1132	467.5056	498.6878	
539.0459	545.0272	575.2256	
620.1711	666.9946	739.4498	
761.6902	834.9535	868.8588	
902.0878	923.2985	929.9741	
962.0656	970.1221	986.1572	
1000.1822	1006.0135	1033.2696	
1041.1264	1067.3352	1100.8059	
1139.0684	1156.8979	1175.3607	
1194.4396	1217.2276	1249.4709	
1256.2024	1280.7174	1300.0909	
1319.8693	1331.2458	1339.7098	
1394.9916	1406.7875	1422.5096	
1424.5170	1428.1685	1471.9077	

1484.5068	1492.5003	1496.9618
1505.9673	1510.0508	1520.6576
1544.6724	1859.3058	1889.8670
2930.2852	3047.9181	3054.4095
3056.0551	3057.8820	3085.8410
3098.9648	3113.2128	3117.4935
3125.6975	3127.5418	3128.3056
3136.2202	3156.0857	3237.8345

Zero-point correction (Hartree): 0.242579

ApineneCI.A.a.14Hshift.b.ppp

E(RM062X/Aug-CC-pVTZ) (Hartree): -616.13891063

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-1.367845	0.212848	-0.364272
H	-1.787032	0.665990	-1.265809
C	-2.490812	-0.074611	0.623236
C	-3.482971	-1.019605	0.005906
H	-2.077017	-0.551746	1.516219
H	-3.010261	0.838178	0.915293
H	-3.081731	-2.017561	-0.260766
C	-0.151191	1.069338	0.089651
C	-0.397453	-0.920299	-0.762289
C	-0.170008	2.534085	-0.294949
C	0.180438	0.897263	1.564899
H	0.246921	-0.151231	1.857339
H	1.139062	1.365893	1.793692
H	-0.581493	1.376508	2.180979
H	0.801576	2.994769	-0.105074
H	-0.916129	3.074509	0.290853
H	-0.409485	2.661406	-1.351219
H	-0.602745	-1.476762	-1.672889
H	-0.237283	-1.621984	0.055324
C	0.722770	0.131292	-0.821122
H	0.805488	0.582152	-1.811270
C	2.084994	-0.172742	-0.339371
C	3.267170	0.564926	-0.554798
H	3.920600	-0.567987	-0.404306
H	3.226038	1.314134	-1.333292
H	3.777003	0.891353	0.351050
O	-4.628547	-0.748097	-0.226212
O	2.241350	-1.309369	0.250781
O	3.589190	-1.531607	0.520748

Rotational constants (GHz): 1.5127300 0.4136600 0.3670800

Vibrational harmonic frequencies (cm-1):

i1596.4074	40.9894	47.3895
49.3762	83.5791	108.2700
169.2708	196.6362	224.9986
260.1829	270.1880	289.2293
317.0484	333.9046	350.2857
411.8443	462.7597	498.9114
526.6497	536.4608	580.9205
595.5451	732.1945	739.8840
769.8186	835.3016	862.9345
899.9612	920.5046	930.5270
950.0750	966.5251	988.4673
1002.8306	1012.7656	1019.3874
1061.9225	1073.9006	1105.5824
1141.3235	1147.5231	1172.4744
1193.5691	1219.0140	1250.9168
1259.2356	1278.0178	1301.4494
1307.0202	1328.1926	1354.3909
1392.2298	1408.3064	1423.5134
1426.1468	1430.2155	1469.9370
1486.2713	1491.5315	1499.1725
1508.2534	1511.0772	1520.9336
1554.6872	1861.1678	1888.2244
2935.6185	3047.3189	3053.4863
3057.6237	3067.5622	3090.4858
3100.0058	3110.4691	3115.7478
3124.4666	3125.1428	3125.5610
3132.7025	3157.0088	3225.6005

Zero-point correction (Hartree): 0.242672

ApineneCI.A.a.14Hshift.b.ptp

E(RM062X/Aug-CC-pVTZ) (Hartree): -616.14122458

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-1.440691	0.265790	-0.271002
H	-1.892782	0.635221	-1.193179
C	-2.516196	0.091030	0.775105
C	-3.639753	-0.798475	0.315284
H	-2.118462	-0.339701	1.699903
H	-2.962469	1.048908	1.067184
H	-4.434606	-0.987340	1.061370
C	-0.182737	1.120245	0.050714
C	-0.526056	-0.928728	-0.604196
C	-0.171247	2.543357	-0.468180
C	0.209293	1.074987	1.521337
H	0.252160	0.056168	1.907935
H	1.192633	1.525645	1.666964
H	-0.507376	1.638452	2.120782
H	0.821932	2.985027	-0.362990
H	-0.872449	3.163197	0.094721
H	-0.453774	2.580637	-1.520773
H	-0.802816	-1.549352	-1.450610
H	-0.353719	-1.563147	0.264368
C	0.624145	0.073379	-0.802717
H	0.678683	0.429791	-1.832494
C	1.996468	-0.224266	-0.347883

C	3.189878	0.443776	-0.693017
H	3.815846	-0.687234	-0.439615
H	3.135891	1.101851	-1.549207
H	3.748066	0.852972	0.148352
O	-3.707180	-1.288034	-0.778694
O	2.146008	-1.291862	0.361354
O	3.498000	-1.527312	0.600417
Rotational constants (GHz):			1.3882900 0.4539000 0.3985500
Vibrational harmonic frequencies (cm-1):			
i1574.4181	45.9155		54.0498
73.6819	99.0909		134.0785
159.6905	198.3399		216.8881
251.5443	260.5981		291.0986
318.0361	334.0290		353.8898
401.7333	459.5875		492.4811
537.4921	571.4939		590.1013
667.2835	715.7824		739.1594
742.0956	825.2917		845.8354
900.9027	920.7395		934.5713
937.3600	953.9411		965.6438
994.4440	1010.8837		1014.5692
1027.9624	1072.3741		1098.5049
1145.7295	1149.9710		1169.4652
1194.2737	1217.5573		1247.1600
1261.6205	1281.1848		1301.5673
1321.5107	1334.7943		1356.0785
1405.5758	1410.7515		1421.1581
1423.8050	1430.3407		1451.8378
1485.8997	1491.1663		1499.4243
1508.4023	1512.0885		1521.3397
1555.1343	1855.9712		1889.2498
2948.9205	3037.2187		3045.4158
3054.9943	3068.9606		3085.2407
3091.5692	3104.6279		3111.4967
3112.1622	3121.5127		3125.0042
3132.1472	3169.3670		3225.3011
Zero-point correction (Hartree): 0.242598			
ApineneCI.A.a.14Hshift.b.ptt			
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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.14019427			
Electronic state : 1-A			
Cartesian coordinates (Angs):			
C	-1.449081	0.268093	-0.300744
H	-1.856483	0.583502	-1.262921
C	-2.531414	0.349678	0.749605
C	-3.747461	-0.466778	0.405686
H	-2.177155	0.004827	1.727000
H	-2.866356	1.380980	0.909627
H	-4.563212	-0.446046	1.152936
C	-0.090835	0.989208	-0.069687
C	-0.693601	-1.062191	-0.491004
C	0.089558	2.335912	-0.739342
C	0.312380	1.056225	1.397666
H	0.220383	0.090094	1.897465
H	1.349986	1.380430	1.490239
H	-0.313328	1.773684	1.930772
H	1.129586	2.659516	-0.674992
H	-0.530250	3.092165	-0.252585
H	-0.191809	2.291524	-1.792104
H	-1.055345	-1.739525	-1.258230
H	-0.607538	-1.603326	0.451502
C	0.567465	-0.236114	-0.791862
H	0.645619	-0.019072	-1.859226
C	1.900535	-0.674334	-0.312178
C	2.261248	-1.791029	0.466755
H	3.198190	-1.045413	0.992081
H	1.453197	-2.376042	0.880499
H	3.073618	-2.389526	0.055994
O	-3.863840	-1.112393	-0.599845
O	2.821459	0.221779	-0.448136
O	3.964647	-0.140610	0.263303
Rotational constants (GHz):			1.6124200 0.4356000 0.3914000
Vibrational harmonic frequencies (cm-1):			
i1588.5769	16.2406		48.0298
75.8607	94.9121		127.9382
161.7362	200.1888		220.8501
252.9138	269.2469		302.2715
309.6616	331.3891		354.8941
401.6994	464.8326		495.2528
541.0050	564.3976		609.7011
663.4784	676.7718		721.0280
740.8670	821.8160		854.9792
900.3161	923.3106		934.9701
937.3238	962.4225		972.8546
986.6069	1001.3642		1021.1927
1040.3031	1045.3229		1104.3270
1144.1730	1157.9517		1173.2788
1195.9365	1216.6781		1248.6434
1264.4262	1283.3128		1313.3696
1329.1224	1335.7684		1341.0663
1405.2241	1407.0014		1420.0622
1422.6753	1430.6988		1452.0947
1484.7472	1493.8128		1498.1070
1505.9247	1510.2614		1520.8945
1542.3281	1854.8729		1888.8357
2949.1104	3038.6909		3047.1732
3052.8715	3067.6590		3081.6096
3084.2062	3095.4467		3113.0366
3116.1628	3122.4930		3125.8862
3128.0309	3166.0288		3236.9659
Zero-point correction (Hartree): 0.242440			

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ApineneCI.A.a.14Hshift.b.tmp
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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.13689822
Electronic state : 1-A
Cartesian coordinates (Angs):
C      1.327601      0.640243      0.952171
H      1.453883      1.517009      1.590982
C      2.714662      0.090414      0.644972
C      2.776453     -1.236967     -0.062422
H      3.297604      0.807359      0.064863
H      3.239240     -0.062169      1.595503
H      2.151275     -2.045198      0.362391
C      0.358781      1.043458     -0.194906
C      0.211018     -0.236760      1.561803
C      0.370650      2.498631     -0.615296
C      0.449363      0.128373     -1.407976
H      0.386457     -0.928177     -1.141774
H     -0.366979      0.339158     -2.101096
H      1.389920      0.287482     -1.936506
H     -0.470382      2.715847     -1.276866
H      1.288902      2.732675     -1.157575
H      0.306387      3.160311      0.249430
H      0.114617     -0.252077      2.644162
H      0.219825     -1.259411      1.192961
C     -0.800222      0.616697      0.776643
H     -1.120459      1.491823      1.344633
C     -1.995124      0.009104      0.157775
C     -3.127404      0.664450     -0.368191
H     -3.804022     -0.431092     -0.094605
H     -3.240119      1.706662     -0.103179
H     -3.340537      0.445312     -1.413942
O      3.483981     -1.459514     -1.006316
O     -2.075163     -1.277388      0.211760
O     -3.311354     -1.704518     -0.266297
Rotational constants (GHz):      1.2636700      0.4950100      0.4361300
Vibrational harmonic frequencies (cm-1):
i1584.1235      46.0796      53.7861
84.9119      91.9979      108.8074
180.1836      209.5039      244.3401
257.1312      263.4276      289.2615
335.5314      349.8917      362.1979
400.5074      464.8940      476.4342
535.8681      568.5533      582.1466
622.8827      700.8635      738.7133
741.6101      815.7071      837.4560
899.1345      909.5577      929.2958
957.3710      965.8366      991.6462
997.5860      1016.6744      1019.4400
1056.2305      1071.1927      1114.0924
1133.2482      1147.9761      1173.5143
1193.6953      1222.7682      1247.7649
1257.8301      1295.1452      1303.6879
1319.3621      1336.4696      1356.2332
1397.7642      1408.7434      1425.6399
1426.3208      1439.2196      1452.4965
1486.5370      1492.4728      1502.2760
1508.7525      1513.8648      1521.6598
1555.2024      1856.2291      1889.6445
2952.0556      3034.8213      3046.1139
3055.3686      3066.9205      3089.5086
3108.8717      3111.9705      3113.6073
3115.2441      3122.6270      3123.1596
3132.8926      3168.3134      3225.3951
Zero-point correction (Hartree): 0.242903

ApineneCI.A.a.14Hshift.b.ttp
~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -616.13570910
Electronic state : 1-A
Cartesian coordinates (Angs):
C      1.477828      0.567155      0.826859
H      1.636680      1.364429      1.557540
C      2.852273      0.118743      0.359163
C      3.025668     -1.195169     -0.355353
H      3.295983      0.885245     -0.287341
H      3.540136      0.057792      1.211339
H      4.061561     -1.366417     -0.710337
C      0.424275      1.103503     -0.182682
C      0.412587     -0.393342      1.402409
C      0.413133      2.601817     -0.411306
C      0.406904      0.354572     -1.507788
H      0.330071     -0.722577     -1.373933
H     -0.435121      0.690645     -2.115644
H      1.320838      0.559896     -2.069765
H     -0.476579      2.899583     -0.969822
H      1.285837      2.908019     -0.992666
H      0.423988      3.147883      0.532923
H      0.400591     -0.543007      2.478888
H      0.410047     -1.353756      0.898090
C     -0.652632      0.550992      0.817372
H     -0.919275      1.347125      1.515781
C     -1.903296      0.032249      0.228049
C     -3.046666      0.766765     -0.153126
H     -3.740356     -0.330994      0.067449
H     -3.102207      1.782438      0.214162
H     -3.335498      0.655367     -1.197617
O      2.187792     -2.034332     -0.534577
O     -2.025629     -1.249682      0.172614
O     -3.306806     -1.594157     -0.250618
Rotational constants (GHz):      1.2311000      0.5554200      0.4573900
Vibrational harmonic frequencies (cm-1):

```

11589.6349	42.8278	55.1815
88.1545	107.8007	116.7193
173.2671	191.6890	224.6979
242.6630	261.9040	284.4657
318.2514	326.4359	355.0251
397.5925	463.9605	484.2239
534.1519	566.3445	588.0684
674.6001	737.0336	741.2209
750.0468	782.2006	839.4468
894.7665	904.2217	930.1508
941.5935	967.3181	973.1218
997.5128	1006.2331	1018.4987
1040.5573	1069.8404	1091.8299
1129.3546	1160.5504	1174.4295
1195.2685	1230.3680	1250.1824
1261.9719	1298.6996	1304.7656
1330.1650	1354.9732	1373.6193
1406.1013	1409.9221	1424.6110
1426.3160	1434.5237	1447.6183
1485.0547	1490.8072	1504.6837
1509.8336	1511.7409	1522.6534
1552.8214	1865.3363	1889.6266
2929.9077	3027.8092	3044.2214
3052.1570	3054.4547	3057.3117
3080.1925	3110.2833	3111.5122
3114.0571	3118.2028	3121.5913
3158.6014	3191.7493	3223.7101

Zero-point correction (Hartree): 0.242683

ApineneCI.A.a.14Hshift.b.ttt

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.13622582

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 1.488148  | 0.701670  | 0.763541  |
| H | 1.616005  | 1.558157  | 1.429559  |
| C | 2.854988  | 0.385101  | 0.179485  |
| C | 3.121099  | -0.948337 | -0.467130 |
| H | 3.134095  | 1.147777  | -0.557017 |
| H | 3.627422  | 0.467854  | 0.954078  |
| H | 4.129412  | -1.019840 | -0.920818 |
| C | 0.283415  | 1.034660  | -0.162410 |
| C | 0.620985  | -0.348643 | 1.493828  |
| C | 0.024156  | 2.505601  | -0.421735 |
| C | 0.265979  | 0.252077  | -1.467237 |
| H | 0.398409  | -0.816390 | -1.313389 |
| H | -0.681887 | 0.411646  | -1.984798 |
| H | 1.065791  | 0.600180  | -2.124928 |
| H | -0.947869 | 2.643578  | -0.898030 |
| H | 0.785850  | 2.917324  | -1.088018 |
| H | 0.034960  | 3.079671  | 0.505572  |
| H | 0.715432  | -0.409849 | 2.575231  |
| H | 0.736087  | -1.336462 | 1.061202  |
| C | -0.617904 | 0.375226  | 0.943155  |
| H | -0.968654 | 1.155420  | 1.620311  |
| C | -1.796656 | -0.389257 | 0.470145  |
| C | -1.914845 | -1.748037 | 0.122049  |
| H | -2.784700 | -1.370878 | -0.786065 |
| H | -1.000748 | -2.323083 | 0.085095  |
| H | -2.749398 | -2.267739 | 0.591186  |
| O | 2.385073  | -1.896004 | -0.502882 |
| O | -2.786441 | 0.361454  | 0.108820  |
| O | -3.734431 | -0.385167 | -0.589853 |

Rotational constants (GHz): 1.3500700 0.5294800 0.4611200

Vibrational harmonic frequencies (cm-1):

|            |           |           |
|------------|-----------|-----------|
| i1588.9727 | 41.7552   | 44.6378   |
| 91.9302    | 113.9780  | 118.0479  |
| 181.6792   | 198.1568  | 232.0081  |
| 244.4839   | 270.8195  | 291.1753  |
| 325.6943   | 342.1843  | 350.6939  |
| 395.6272   | 464.2084  | 482.9114  |
| 544.4966   | 572.9777  | 603.7112  |
| 657.5544   | 691.2263  | 744.2088  |
| 751.8093   | 780.2452  | 850.5058  |
| 889.0167   | 903.7656  | 938.3234  |
| 940.6420   | 966.0224  | 986.0111  |
| 997.1094   | 1001.8026 | 1007.8204 |
| 1045.3502  | 1059.6204 | 1087.6456 |
| 1142.3233  | 1159.1057 | 1178.6044 |
| 1197.4274  | 1232.3018 | 1253.0373 |
| 1262.2221  | 1299.6153 | 1321.7454 |
| 1332.5188  | 1338.9867 | 1372.0629 |
| 1405.2841  | 1406.9422 | 1423.0224 |
| 1424.5531  | 1433.8568 | 1448.2644 |
| 1487.4596  | 1491.6594 | 1498.0470 |
| 1507.5412  | 1512.6917 | 1522.5904 |
| 1547.8388  | 1859.8267 | 1887.2565 |
| 2934.7022  | 3028.9105 | 3045.6187 |
| 3052.8206  | 3055.8702 | 3061.7459 |
| 3091.3416  | 3112.0599 | 3114.0909 |
| 3115.5300  | 3116.0059 | 3126.5646 |
| 3162.8359  | 3191.3118 | 3234.3177 |

Zero-point correction (Hartree): 0.242854

Population analysis as 298K (%)

Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)

| Compound                     | Qtot      | Erel | Erel2 | n*Q*MB    | %    |
|------------------------------|-----------|------|-------|-----------|------|
| ApineneCI.A.a.ringclose.pmtm | 1.568e+44 | 0.00 | 0.00  | 1.568e+44 | 30   |
| ApineneCI.A.a.ringclose.tptp | 1.061e+44 | 0.23 | 0.23  | 7.251e+43 | 13.9 |
| ApineneCI.A.a.ringclose.pptm | 1.700e+44 | 0.57 | 0.57  | 6.517e+43 | 12.5 |

|                              |           |      |      |           |         |
|------------------------------|-----------|------|------|-----------|---------|
| ApineneCI.A.a.ringclose.tmtt | 8.460e+43 | 0.17 | 0.17 | 6.322e+43 | 12.1    |
| ApineneCI.A.a.ringclose.pmtt | 1.396e+44 | 0.76 | 0.76 | 3.886e+43 | 7.43    |
| ApineneCI.A.a.ringclose.pmpm | 4.008e+44 | 1.67 | 1.67 | 2.372e+43 | 4.54    |
| ApineneCI.A.a.ringclose.tpm  | 2.196e+44 | 1.55 | 1.55 | 1.602e+43 | 3.06    |
| ApineneCI.A.a.ringclose.tptm | 2.239e+44 | 1.81 | 1.81 | 1.051e+43 | 2.01    |
| ApineneCI.A.a.ringclose.tmtm | 2.138e+44 | 1.82 | 1.82 | 9.929e+42 | 1.9     |
| ApineneCI.A.a.ringclose.ppm  | 3.889e+44 | 2.25 | 2.25 | 8.731e+42 | 1.67    |
| ApineneCI.A.a.ringclose.tmp  | 9.930e+43 | 1.46 | 1.46 | 8.482e+42 | 1.62    |
| ApineneCI.A.a.ringclose.pmm  | 4.755e+44 | 2.41 | 2.41 | 8.139e+42 | 1.56    |
| ApineneCI.A.a.ringclose.ppp  | 3.920e+44 | 2.30 | 2.30 | 8.103e+42 | 1.55    |
| ApineneCI.A.a.ringclose.ppt  | 1.871e+44 | 1.86 | 1.86 | 8.088e+42 | 1.55    |
| ApineneCI.A.a.ringclose.tpp  | 2.074e+44 | 2.15 | 2.15 | 5.468e+42 | 1.05    |
| ApineneCI.A.a.ringclose.tmt  | 1.808e+44 | 2.12 | 2.12 | 5.025e+42 | 0.961   |
| ApineneCI.A.a.ringclose.pmp  | 1.743e+44 | 2.30 | 2.30 | 3.568e+42 | 0.682   |
| ApineneCI.A.a.ringclose.tpm  | 2.936e+44 | 2.75 | 2.75 | 2.806e+42 | 0.537   |
| ApineneCI.A.a.ringclose.tpm  | 4.067e+44 | 3.08 | 3.08 | 2.254e+42 | 0.431   |
| ApineneCI.A.a.ringclose.ppp  | 4.025e+44 | 3.35 | 3.35 | 1.415e+42 | 0.27    |
| ApineneCI.A.a.ringclose.pmp  | 4.199e+44 | 3.45 | 3.45 | 1.236e+42 | 0.236   |
| ApineneCI.A.a.ringclose.ttt  | 9.012e+43 | 2.83 | 2.83 | 7.545e+41 | 0.144   |
| ApineneCI.A.a.ringclose.tmm  | 4.301e+44 | 3.84 | 3.84 | 6.576e+41 | 0.126   |
| ApineneCI.A.a.ringclose.tpm  | 3.855e+44 | 3.78 | 3.78 | 6.515e+41 | 0.125   |
| ApineneCI.A.a.ringclose.ptm  | 1.827e+44 | 3.79 | 3.79 | 3.012e+41 | 0.0576  |
| ApineneCI.A.a.ringclose.ttm  | 8.174e+43 | 3.52 | 3.52 | 2.128e+41 | 0.0407  |
| ApineneCI.A.a.ringclose.ttm  | 1.723e+44 | 4.26 | 4.26 | 1.286e+41 | 0.0246  |
| ApineneCI.A.a.ringclose.ptm  | 9.501e+43 | 3.98 | 3.98 | 1.137e+41 | 0.0218  |
| ApineneCI.A.a.ringclose.ptm  | 1.581e+44 | 4.60 | 4.60 | 6.711e+40 | 0.0128  |
| ApineneCI.A.a.ringclose.ttm  | 2.593e+44 | 5.02 | 5.02 | 5.356e+40 | 0.0102  |
| ApineneCI.A.a.ringclose.ptt  | 1.409e+44 | 5.52 | 5.52 | 1.260e+40 | 0.00241 |
| Total                        |           |      |      | 5.230e+44 | 100     |

ApineneCI.A.a.ringclose.pmm

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.13026345

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-1.241082	-0.370043	-0.677616
H	-1.659783	0.151996	-1.541320
C	-2.374362	-1.047929	0.085323
C	-3.400914	-0.024686	0.487865
H	-2.855953	-1.785667	-0.556602
H	-1.978922	-1.544881	0.973161
H	-3.158951	0.581115	1.383340
C	-0.255463	0.589077	0.051817
C	-0.040280	-1.219220	-1.124929
C	-0.518943	2.074459	-0.089999
C	-0.018666	0.211071	1.505738
H	0.220770	-0.843958	1.631628
H	0.820531	0.769727	1.916452
H	-0.912347	0.438135	2.090363
H	0.325052	2.654990	0.287213
H	-1.400422	2.358780	0.488858
H	-0.695257	2.350565	-1.130048
H	-0.063288	-1.648914	-2.122852
H	0.201615	-1.991443	-0.397266
C	0.859075	0.017775	-0.925502
H	0.881743	0.647476	-1.814127
C	2.224270	-0.143883	-0.386770
C	3.290769	0.792982	-0.832913
H	3.280703	0.819647	-1.926209
H	3.059062	1.801115	-0.484689
H	4.254600	0.493542	-0.440370
O	-4.412914	0.185166	-0.122866
O	2.453752	-1.167461	0.340242
O	3.025964	-0.333934	1.418172

Rotational constants (GHz): 1.7227800 0.4261800 0.4183700

Vibrational harmonic frequencies (cm-1):

1508.0521	20.9904	33.7650
68.7130	80.4365	148.6343
178.1193	226.4063	235.5624
248.3902	263.6886	287.8879
308.9029	321.8519	356.3059
378.0939	395.3707	407.0448
479.6952	531.0273	566.9081
570.1969	609.2686	724.8590
779.8055	838.3686	879.2338
888.1367	941.9289	958.6564
960.0683	966.6665	986.2692
1007.0579	1010.0391	1028.2771
1068.1419	1109.8811	1123.7867
1154.6325	1170.5824	1186.6280
1205.7422	1220.8379	1259.9479
1264.4281	1285.9568	1302.9765
1333.0728	1379.1914	1396.8839
1409.4336	1424.7065	1430.5470
1436.2348	1446.2506	1461.7681
1473.0218	1482.6013	1488.7432
1495.9777	1504.6584	1506.3566
1580.3652	1858.1249	2937.0454
3047.6485	3051.4114	3062.7489
3065.8450	3075.1185	3103.2308
3105.9961	3112.1524	3115.4858
3127.0629	3131.8180	3138.4306
3153.0986	3163.5894	3209.9806

Zero-point correction (Hartree): 0.245470

ApineneCI.A.a.ringclose.pmpm

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.13136146

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -1.190495 | -0.644294 | -0.794044 |
| H | -1.523692 | -0.396044 | -1.806098 |

|                                                           |           |           |           |
|-----------------------------------------------------------|-----------|-----------|-----------|
| C                                                         | -2.379028 | -1.112742 | 0.033150  |
| C                                                         | -3.453932 | -0.062175 | 0.015058  |
| H                                                         | -2.782604 | -2.025591 | -0.414874 |
| H                                                         | -2.094473 | -1.320945 | 1.063245  |
| H                                                         | -3.888745 | 0.147496  | -0.983621 |
| C                                                         | -0.307394 | 0.523422  | -0.267297 |
| C                                                         | 0.064943  | -1.527690 | -0.875356 |
| C                                                         | -0.593103 | 1.896602  | -0.839954 |
| C                                                         | -0.228598 | 0.570384  | 1.251172  |
| H                                                         | 0.050428  | -0.389478 | 1.684640  |
| H                                                         | 0.528582  | 1.284642  | 1.570529  |
| H                                                         | -1.196906 | 0.871154  | 1.654531  |
| H                                                         | 0.184667  | 2.606986  | -0.553798 |
| H                                                         | -1.541181 | 2.272296  | -0.448518 |
| H                                                         | -0.656494 | 1.871167  | -1.928757 |
| H                                                         | 0.154675  | -2.211629 | -1.715419 |
| H                                                         | 0.241087  | -2.064236 | 0.054738  |
| C                                                         | 0.915759  | -0.244732 | -0.931436 |
| H                                                         | 1.029491  | 0.125865  | -1.949965 |
| C                                                         | 2.213473  | -0.184120 | -0.228779 |
| C                                                         | 3.256840  | 0.751855  | -0.730771 |
| H                                                         | 3.378147  | 0.582427  | -1.804192 |
| H                                                         | 2.914128  | 1.780261  | -0.603107 |
| H                                                         | 4.184908  | 0.617804  | -0.188939 |
| O                                                         | -3.822376 | 0.558286  | 0.974045  |
| O                                                         | 2.424829  | -1.034628 | 0.698779  |
| O                                                         | 2.800947  | 0.032439  | 1.649571  |
| Rotational constants (GHz): 1.5674200 0.4539000 0.4500500 |           |           |           |
| Vibrational harmonic frequencies (cm-1):                  |           |           |           |
| i517.1421                                                 | 16.5640   |           | 50.9829   |
| 66.2049                                                   | 83.2011   |           | 144.9885  |
| 170.3529                                                  | 226.2390  |           | 234.7872  |
| 256.3530                                                  | 266.2820  |           | 281.5151  |
| 324.7917                                                  | 331.1024  |           | 363.0076  |
| 382.9959                                                  | 397.6821  |           | 412.5424  |
| 472.0378                                                  | 535.2070  |           | 561.1913  |
| 572.2965                                                  | 610.7879  |           | 718.9500  |
| 771.8611                                                  | 839.0119  |           | 862.8534  |
| 889.9850                                                  | 922.3827  |           | 956.6151  |
| 967.9172                                                  | 973.5981  |           | 989.6585  |
| 1008.0951                                                 | 1016.6900 |           | 1038.7480 |
| 1059.6319                                                 | 1110.3491 |           | 1123.1797 |
| 1160.4714                                                 | 1169.1170 |           | 1188.1064 |
| 1199.7245                                                 | 1219.0885 |           | 1256.7224 |
| 1260.4855                                                 | 1279.8914 |           | 1296.3558 |
| 1329.5929                                                 | 1383.7917 |           | 1401.0461 |
| 1408.1640                                                 | 1429.2488 |           | 1432.7730 |
| 1434.4284                                                 | 1446.2406 |           | 1462.4596 |
| 1468.4107                                                 | 1482.5713 |           | 1489.8487 |
| 1496.0364                                                 | 1504.9441 |           | 1512.5638 |
| 1579.2682                                                 | 1859.2128 |           | 2927.0410 |
| 3045.4003                                                 | 3049.2024 |           | 3051.7298 |
| 3057.1574                                                 | 3066.6501 |           | 3101.4214 |
| 3104.3623                                                 | 3111.9599 |           | 3116.0718 |
| 3122.2603                                                 | 3139.6331 |           | 3141.7977 |
| 3149.6926                                                 | 3162.8791 |           | 3208.5141 |
| Zero-point correction (Hartree): 0.245397                 |           |           |           |
| ApineneCI.A.a.ringclose.pmpp                              |           |           |           |
| ~~~~~                                                     |           |           |           |
| E (RM062X/Aug-CC-pVT2) (Hartree): -616.13024563           |           |           |           |
| Electronic state : 1-A                                    |           |           |           |
| Cartesian coordinates (Angs):                             |           |           |           |
| C                                                         | -1.173763 | -0.612813 | -0.808814 |
| H                                                         | -1.511716 | -0.321744 | -1.807505 |
| C                                                         | -2.332038 | -1.235787 | -0.039947 |
| C                                                         | -3.485526 | -0.273136 | -0.009998 |
| H                                                         | -2.647313 | -2.146858 | -0.555637 |
| H                                                         | -2.044899 | -1.487931 | 0.979719  |
| H                                                         | -3.968920 | -0.084476 | -0.989758 |
| C                                                         | -0.408222 | 0.591526  | -0.188281 |
| C                                                         | 0.152358  | -1.384096 | -0.925090 |
| C                                                         | -0.807476 | 1.963657  | -0.692534 |
| C                                                         | -0.372039 | 0.558082  | 1.333774  |
| H                                                         | -0.051180 | -0.409900 | 1.719158  |
| H                                                         | 0.321376  | 1.311144  | 1.713626  |
| H                                                         | -1.362522 | 0.777252  | 1.734143  |
| H                                                         | -0.129888 | 2.736582  | -0.325479 |
| H                                                         | -1.809155 | 2.211869  | -0.334320 |
| H                                                         | -0.813170 | 2.000073  | -1.782515 |
| H                                                         | 0.314153  | -1.982634 | -1.817193 |
| H                                                         | 0.352212  | -1.988823 | -0.042441 |
| C                                                         | 0.895104  | -0.044441 | -0.838939 |
| H                                                         | 1.055878  | 0.416864  | -1.813816 |
| C                                                         | 2.124863  | 0.078343  | -0.026227 |
| C                                                         | 2.895683  | 1.347371  | -0.112736 |
| H                                                         | 2.181717  | 2.176902  | -0.111427 |
| H                                                         | 3.604481  | 1.415536  | 0.704349  |
| H                                                         | 3.439352  | 1.385820  | -1.056726 |
| O                                                         | -3.862303 | 0.310556  | 0.969374  |
| O                                                         | 2.361898  | -0.822468 | 0.838414  |
| O                                                         | 3.767398  | -0.980827 | 0.397033  |
| Rotational constants (GHz): 1.6727700 0.4453900 0.4148000 |           |           |           |
| Vibrational harmonic frequencies (cm-1):                  |           |           |           |
| i498.5723                                                 | 41.9910   |           | 54.8407   |
| 65.4919                                                   | 83.2766   |           | 130.9377  |
| 171.4864                                                  | 232.3228  |           | 245.5192  |
| 251.1985                                                  | 265.6660  |           | 276.4650  |
| 316.8509                                                  | 332.2384  |           | 361.4412  |
| 374.5182                                                  | 388.3331  |           | 425.0156  |
| 464.7126                                                  | 533.6405  |           | 558.1069  |
| 575.1425                                                  | 603.3316  |           | 712.4363  |

|           |           |           |
|-----------|-----------|-----------|
| 760.9396  | 841.6581  | 871.5786  |
| 895.2682  | 921.1823  | 960.5644  |
| 965.4380  | 976.0418  | 979.9631  |
| 1001.3292 | 1011.2918 | 1038.1074 |
| 1059.5990 | 1107.6105 | 1122.3410 |
| 1149.9625 | 1162.1595 | 1188.7834 |
| 1193.8646 | 1226.0819 | 1257.6574 |
| 1261.5630 | 1277.3454 | 1296.3685 |
| 1327.2493 | 1380.3023 | 1399.6470 |
| 1409.2317 | 1426.4605 | 1427.8993 |
| 1429.0642 | 1441.5963 | 1466.4432 |
| 1472.9928 | 1486.5715 | 1493.8299 |
| 1498.4511 | 1509.4775 | 1514.6996 |
| 1597.6538 | 1857.0168 | 2930.2176 |
| 3047.4751 | 3050.0195 | 3052.7261 |
| 3056.0009 | 3062.6288 | 3097.2106 |
| 3107.4366 | 3115.5231 | 3120.7961 |
| 3123.3916 | 3126.3544 | 3138.1614 |
| 3139.9077 | 3166.0549 | 3202.4309 |

Zero-point correction (Hartree): 0.245283

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E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -615.20780131
E(CCSD/Aug-CC-pVTZ) (Hartree): -615.08749046
T1 diagnostic: 0.023409
E(MP2/Aug-CC-pVTZ) (Hartree): -615.01290597
E(MP3/Aug-CC-pVTZ) (Hartree): -615.06945931
E(RHF/Aug-CC-pVTZ) (Hartree): -612.58448914
E(RM062X/Aug-CC-pVTZ) (Hartree): -616.13406529

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-1.257481	-0.425059	-0.796159
H	-1.708435	0.111206	-1.632792
C	-2.322831	-1.211447	-0.066170
C	-3.480583	-0.387321	0.417829
H	-2.732386	-1.997536	-0.710820
H	-1.911106	-1.739935	0.799763
H	-4.265922	-0.942268	0.964954
C	-0.340048	0.562187	-0.011763
C	-0.005891	-1.191166	-1.256095
C	-0.639936	2.040961	-0.145739
C	-0.156345	0.170066	1.444915
H	0.157409	-0.866610	1.566130
H	0.612875	0.781172	1.914189
H	-1.097705	0.325077	1.976685
H	0.196747	2.633431	0.230999
H	-1.530519	2.297249	0.426506
H	-0.818780	2.315036	-1.186207
H	0.020714	-1.560462	-2.278287
H	0.246154	-1.999498	-0.571533
C	0.840917	0.056206	-0.953604
H	0.896273	0.734759	-1.804205
C	2.174643	-0.085967	-0.339172
C	3.182994	0.987663	-0.556847
H	3.248468	1.179691	-1.631244
H	2.838959	1.909920	-0.085275
H	4.139510	0.707413	-0.133319
O	-3.587157	0.796734	0.243637
O	2.445491	-1.188570	0.245899
O	2.858554	-0.481338	1.476875

Rotational constants (GHz): 1.6045600 0.4749200 0.4554700

Vibrational harmonic frequencies (cm-1):

i514.2831	26.8033	49.1770
77.6190	121.3307	158.8612
171.6704	228.3400	231.4964
251.8969	259.4944	291.7762
320.2057	328.2748	356.2700
368.1778	390.8116	407.6693
476.4428	555.4129	557.4055
605.0551	676.2411	728.8785
750.0685	804.0738	841.1743
885.5833	913.8601	946.3644
959.7712	967.3606	979.8600
998.9296	1011.4149	1029.3606
1058.7404	1103.7043	1118.0738
1159.7289	1167.6028	1186.7216
1210.7918	1222.0679	1260.3796
1267.4491	1288.5159	1311.5139
1348.1863	1386.7816	1407.0613
1410.1973	1423.6162	1430.0777
1434.1965	1445.9021	1452.5706
1462.4209	1480.7635	1489.9439
1493.4686	1501.5015	1509.4081
1575.8994	1853.4907	2955.5757
3042.3496	3052.1300	3052.8546
3057.5063	3070.4247	3086.4616
3099.1973	3103.2638	3112.4447
3119.1584	3131.9780	3146.6532
3147.3973	3157.3226	3209.7978

Zero-point correction (Hartree): 0.245433

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.13258182

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -1.230649 | -0.539964 | -0.734653 |
| H | -1.683314 | -0.148301 | -1.646944 |
| C | -2.265854 | -1.318533 | 0.047128  |
| C | -3.501377 | -0.542733 | 0.399938  |
| H | -2.585664 | -2.202342 | -0.516102 |

|                                                |           |           |                               |
|------------------------------------------------|-----------|-----------|-------------------------------|
| H                                              | -1.853274 | -1.715500 | 0.980905                      |
| H                                              | -4.277796 | -1.106439 | 0.950654                      |
| C                                              | -0.432959 | 0.613026  | -0.051944                     |
| C                                              | 0.093814  | -1.258531 | -1.049285                     |
| C                                              | -0.832282 | 2.028284  | -0.417378                     |
| C                                              | -0.318292 | 0.450194  | 1.455944                      |
| H                                              | 0.020388  | -0.544763 | 1.745523                      |
| H                                              | 0.388948  | 1.172160  | 1.868891                      |
| H                                              | -1.289440 | 0.639117  | 1.916919                      |
| H                                              | -0.088144 | 2.745342  | -0.064163                     |
| H                                              | -1.791118 | 2.274857  | 0.036629                      |
| H                                              | -0.931903 | 2.140827  | -1.497449                     |
| H                                              | 0.198020  | -1.726034 | -2.024666                     |
| H                                              | 0.362741  | -1.976715 | -0.275881                     |
| C                                              | 0.841499  | 0.061840  | -0.834594                     |
| H                                              | 0.959544  | 0.643118  | -1.748673                     |
| C                                              | 2.101173  | 0.087003  | -0.063851                     |
| C                                              | 2.914024  | 1.331924  | -0.087101                     |
| H                                              | 2.229660  | 2.181469  | 0.002593                      |
| H                                              | 3.654845  | 1.316160  | 0.703751                      |
| H                                              | 3.421812  | 1.423225  | -1.047336                     |
| O                                              | -3.675295 | 0.614071  | 0.125017                      |
| O                                              | 2.337016  | -0.879919 | 0.728386                      |
| O                                              | 3.719544  | -1.058058 | 0.225362                      |
| Rotational constants (GHz):                    |           |           | 1.6937200 0.4637600 0.4207800 |
| Vibrational harmonic frequencies (cm-1):       |           |           |                               |
| i491.1429                                      | 43.6044   | 43.8143   |                               |
| 76.7823                                        | 114.2592  | 143.0705  |                               |
| 162.9473                                       | 230.3337  | 232.9944  |                               |
| 242.5484                                       | 261.0135  | 277.3850  |                               |
| 318.5419                                       | 334.0238  | 358.8609  |                               |
| 361.1371                                       | 387.8481  | 411.0136  |                               |
| 465.7328                                       | 551.5834  | 566.6409  |                               |
| 596.2802                                       | 671.2146  | 718.7248  |                               |
| 749.6227                                       | 792.5344  | 845.2680  |                               |
| 885.9323                                       | 913.8623  | 946.5674  |                               |
| 960.7681                                       | 967.1829  | 978.3397  |                               |
| 993.9885                                       | 1002.9550 | 1027.6095 |                               |
| 1057.6775                                      | 1106.5543 | 1113.5804 |                               |
| 1150.6410                                      | 1164.2693 | 1186.7771 |                               |
| 1206.2635                                      | 1227.6137 | 1260.9020 |                               |
| 1267.3793                                      | 1285.1933 | 1308.1708 |                               |
| 1349.1243                                      | 1382.5280 | 1404.7354 |                               |
| 1409.0410                                      | 1422.5101 | 1423.9569 |                               |
| 1429.8753                                      | 1440.1874 | 1448.5875 |                               |
| 1465.6640                                      | 1485.3294 | 1491.6560 |                               |
| 1496.5552                                      | 1508.8606 | 1512.0688 |                               |
| 1595.2893                                      | 1853.2797 | 2957.1724 |                               |
| 3043.3965                                      | 3047.6968 | 3052.8137 |                               |
| 3055.2694                                      | 3068.5137 | 3087.5482 |                               |
| 3099.2974                                      | 3105.0300 | 3118.0800 |                               |
| 3119.8799                                      | 3122.3768 | 3135.8467 |                               |
| 3146.4970                                      | 3159.6637 | 3202.8157 |                               |
| Zero-point correction (Hartree): 0.245156      |           |           |                               |
| ApineneCI.A.a.ringclose.ppm                    |           |           |                               |
| ~~~~~                                          |           |           |                               |
| E(RM062X/Aug-CC-pVTZ) (Hartree): -616.13035249 |           |           |                               |
| Electronic state : 1-A                         |           |           |                               |
| Cartesian coordinates (Angs):                  |           |           |                               |
| C                                              | -1.312216 | 0.452674  | -0.418452                     |
| H                                              | -1.624435 | 1.016049  | -1.302763                     |
| C                                              | -2.488101 | 0.305344  | 0.536971                      |
| C                                              | -3.638880 | -0.322419 | -0.198393                     |
| H                                              | -2.229858 | -0.320142 | 1.389883                      |
| H                                              | -2.797400 | 1.292779  | 0.893172                      |
| H                                              | -4.079794 | 0.298647  | -1.004376                     |
| C                                              | 0.025779  | 1.052209  | 0.097581                      |
| C                                              | -0.550161 | -0.810258 | -0.855740                     |
| C                                              | 0.275008  | 2.513683  | -0.212664                     |
| C                                              | 0.277941  | 0.754990  | 1.567243                      |
| H                                              | 0.157483  | -0.300228 | 1.807655                      |
| H                                              | 1.295998  | 1.022717  | 1.844559                      |
| H                                              | -0.420600 | 1.333239  | 2.174758                      |
| H                                              | 1.299555  | 2.793809  | 0.038665                      |
| H                                              | -0.393497 | 3.141175  | 0.380673                      |
| H                                              | 0.102666  | 2.733879  | -1.266873                     |
| H                                              | -0.837855 | -1.289877 | -1.787528                     |
| H                                              | -0.515697 | -1.551986 | -0.060002                     |
| C                                              | 0.744168  | 0.030473  | -0.882614                     |
| H                                              | 0.882977  | 0.524873  | -1.843473                     |
| C                                              | 2.018957  | -0.564852 | -0.434011                     |
| C                                              | 3.284019  | -0.139991 | -1.092650                     |
| H                                              | 3.147043  | -0.227749 | -2.174201                     |
| H                                              | 3.471788  | 0.913209  | -0.876483                     |
| H                                              | 4.119292  | -0.730583 | -0.737293                     |
| O                                              | -4.056150 | -1.427807 | 0.008464                      |
| O                                              | 1.959657  | -1.515336 | 0.414838                      |
| O                                              | 2.921900  | -0.841973 | 1.311699                      |
| Rotational constants (GHz):                    |           |           | 1.3950500 0.4532400 0.4168000 |
| Vibrational harmonic frequencies (cm-1):       |           |           |                               |
| i506.7501                                      | 33.6450   | 34.1810   |                               |
| 63.6580                                        | 88.7917   | 131.5860  |                               |
| 165.3263                                       | 211.0946  | 231.3016  |                               |
| 241.3759                                       | 268.5558  | 277.3971  |                               |
| 311.5218                                       | 336.4881  | 343.1453  |                               |
| 363.2321                                       | 395.2209  | 435.8099  |                               |
| 474.0247                                       | 542.1821  | 558.7029  |                               |
| 581.8534                                       | 610.1524  | 742.9216  |                               |
| 779.3419                                       | 837.5426  | 859.3439  |                               |
| 887.8270                                       | 930.2589  | 944.6270  |                               |
| 958.8393                                       | 967.3140  | 995.1746  |                               |

|           |           |           |
|-----------|-----------|-----------|
| 1006.5884 | 1016.5234 | 1032.9745 |
| 1068.1857 | 1092.6659 | 1134.8464 |
| 1154.2330 | 1176.8903 | 1186.8260 |
| 1217.7878 | 1225.2458 | 1249.5800 |
| 1263.0818 | 1274.7384 | 1301.3375 |
| 1328.1070 | 1382.5744 | 1400.4578 |
| 1407.9268 | 1426.7731 | 1431.4896 |
| 1433.5565 | 1446.3043 | 1462.9481 |
| 1469.6299 | 1482.9088 | 1486.5287 |
| 1496.2569 | 1504.0206 | 1508.1991 |
| 1582.6554 | 1861.7398 | 2926.7123 |
| 3046.6221 | 3050.7135 | 3051.1040 |
| 3053.0801 | 3064.4565 | 3103.1610 |
| 3105.8724 | 3112.3596 | 3115.6360 |
| 3124.5650 | 3137.7394 | 3139.8934 |
| 3154.6681 | 3164.3913 | 3208.7793 |

Zero-point correction (Hartree): 0.245303

ApineneCI.A.a.ringclose.pppm

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.12815556

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-1.317242	0.402639	-0.451215
H	-1.632446	0.880547	-1.383226
C	-2.517535	0.239958	0.469672
C	-3.605516	-0.510923	-0.247916
H	-2.257954	-0.303117	1.377204
H	-2.907090	1.226618	0.741693
H	-3.998049	-0.014675	-1.158655
C	-0.054613	1.147292	0.065456
C	-0.448719	-0.828300	-0.771546
C	0.080134	2.595668	-0.357502
C	0.154851	0.993208	1.565134
H	0.088611	-0.045159	1.888880
H	1.137137	1.370265	1.856359
H	-0.596239	1.570244	2.106438
H	1.045615	3.010788	-0.063129
H	-0.693998	3.196410	0.125418
H	-0.028383	2.705914	-1.436742
H	-0.657189	-1.376385	-1.686007
H	-0.408715	-1.526096	0.063186
C	0.781264	0.089392	-0.774728
H	0.989766	0.515910	-1.756291
C	2.048964	-0.344558	-0.146595
C	3.254689	0.502214	-0.352391
H	2.951755	1.550217	-0.262575
H	4.029024	0.236709	0.358002
H	3.638210	0.358999	-1.362646
O	-4.027615	-1.581969	0.086625
O	2.005716	-1.304507	0.684777
O	3.152184	-1.998114	0.053832

Rotational constants (GHz): 1.3097900 0.4649000 0.3896700

Vibrational harmonic frequencies (cm-1):

1501.3160	33.8799	40.8005
60.5224	84.2378	114.5985
168.4352	201.9091	227.8061
251.7867	267.8639	280.6665
326.0384	334.1348	339.7928
361.6485	394.4835	430.9680
456.3158	543.5211	566.9496
580.2477	599.4918	725.6353
771.5476	838.2219	852.7486
892.1952	931.1243	942.8297
960.5535	968.8939	986.7589
1000.3146	1009.0913	1035.9653
1069.1378	1097.6222	1137.4995
1151.9460	1158.8838	1188.0395
1216.9307	1225.8056	1247.5881
1264.6135	1275.4323	1300.5274
1326.5218	1381.2645	1401.2696
1408.2087	1424.8852	1427.2151
1428.8425	1442.2670	1465.8750
1467.0173	1484.9370	1491.7693
1498.4816	1508.6741	1510.7633
1598.8022	1864.3091	2925.5458
3045.3566	3046.7868	3048.3567
3052.3514	3056.6451	3097.6351
3106.9977	3113.2653	3120.4241
3121.1149	3128.6403	3134.0440
3141.2640	3165.6279	3201.5051

Zero-point correction (Hartree): 0.245023

ApineneCI.A.a.ringclose.pppm

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.13029061

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -1.305476 | 0.231504  | -0.371249 |
| H | -1.691629 | 0.740447  | -1.257797 |
| C | -2.440808 | 0.018768  | 0.621005  |
| C | -3.508952 | -0.830639 | -0.007405 |
| H | -2.059431 | -0.504845 | 1.501804  |
| H | -2.881787 | 0.966140  | 0.931063  |
| H | -3.198409 | -1.861060 | -0.271995 |
| C | -0.014021 | 0.962893  | 0.092794  |
| C | -0.439714 | -0.967438 | -0.803100 |
| C | 0.089599  | 2.432238  | -0.259740 |
| C | 0.307269  | 0.727729  | 1.559804  |
| H | 0.304269  | -0.328632 | 1.825871  |
| H | 1.300261  | 1.103330  | 1.800450  |
| H | -0.427706 | 1.247675  | 2.176730  |



|                                                           |           |           |           |
|-----------------------------------------------------------|-----------|-----------|-----------|
| H                                                         | 1.091065  | 2.812430  | -0.050267 |
| H                                                         | -0.615921 | 3.010611  | 0.340175  |
| H                                                         | -0.136115 | 2.607189  | -1.312182 |
| H                                                         | -0.704522 | -1.492897 | -1.717066 |
| H                                                         | -0.309699 | -1.684789 | 0.005812  |
| C                                                         | 0.769890  | -0.016280 | -0.883210 |
| H                                                         | 0.842338  | 0.467537  | -1.856651 |
| C                                                         | 2.103904  | -0.479839 | -0.450748 |
| C                                                         | 3.312205  | 0.109497  | -1.089160 |
| H                                                         | 3.188148  | 0.043927  | -2.173677 |
| H                                                         | 3.377384  | 1.169228  | -0.836094 |
| H                                                         | 4.209582  | -0.392716 | -0.749623 |
| O                                                         | -4.622325 | -0.455393 | -0.251908 |
| O                                                         | 2.152116  | -1.461650 | 0.363212  |
| O                                                         | 3.028810  | -0.712228 | 1.287383  |
| Rotational constants (GHz): 1.5511700 0.4217300 0.3998200 |           |           |           |
| Vibrational harmonic frequencies (cm-1):                  |           |           |           |
| i512.0536                                                 | 29.5338   |           | 44.9451   |
| 51.2411                                                   | 89.8549   |           | 138.7688  |
| 170.8731                                                  | 217.5014  |           | 229.3834  |
| 237.3417                                                  | 268.4418  |           | 275.7628  |
| 313.4304                                                  | 332.6043  |           | 340.9952  |
| 361.5147                                                  | 394.8472  |           | 441.3580  |
| 464.3242                                                  | 525.6832  |           | 562.5929  |
| 580.4266                                                  | 609.9896  |           | 742.5731  |
| 787.6212                                                  | 838.5671  |           | 867.7198  |
| 883.5213                                                  | 929.2970  |           | 947.0714  |
| 959.0571                                                  | 967.0859  |           | 992.4151  |
| 1005.0635                                                 | 1010.8230 |           | 1029.5280 |
| 1071.1968                                                 | 1101.6719 |           | 1138.3216 |
| 1151.6661                                                 | 1174.0059 |           | 1187.1471 |
| 1220.4308                                                 | 1222.7712 |           | 1258.1926 |
| 1265.0790                                                 | 1275.0675 |           | 1307.2043 |
| 1330.7872                                                 | 1379.4845 |           | 1396.8955 |
| 1408.3159                                                 | 1428.4442 |           | 1430.7038 |
| 1431.5799                                                 | 1445.9117 |           | 1462.1656 |
| 1469.1801                                                 | 1480.4820 |           | 1487.2836 |
| 1496.0562                                                 | 1504.7302 |           | 1506.1378 |
| 1579.8007                                                 | 1860.9362 |           | 2935.4439 |
| 3048.6567                                                 | 3052.1163 |           | 3056.0248 |
| 3064.7367                                                 | 3066.1483 |           | 3098.7600 |
| 3104.9171                                                 | 3112.7946 |           | 3117.9479 |
| 3126.3900                                                 | 3127.6011 |           | 3139.0367 |
| 3151.7354                                                 | 3157.9091 |           | 3209.0865 |
| Zero-point correction (Hartree): 0.245319                 |           |           |           |
| ApineneCI.A.a.ringclose.pppp                              |           |           |           |
| ~~~~~                                                     |           |           |           |
| E(RM062X/Aug-CC-pVTZ) (Hartree): -616.12839958            |           |           |           |
| Electronic state : 1-A                                    |           |           |           |
| Cartesian coordinates (Angs):                             |           |           |           |
| C                                                         | -1.311764 | 0.189272  | -0.380006 |
| H                                                         | -1.700373 | 0.596110  | -1.316592 |
| C                                                         | -2.464872 | -0.023756 | 0.591731  |
| C                                                         | -3.456206 | -0.986016 | -0.001136 |
| H                                                         | -2.083636 | -0.456710 | 1.520748  |
| H                                                         | -2.977114 | 0.911755  | 0.817153  |
| H                                                         | -3.068828 | -2.006084 | -0.192632 |
| C                                                         | -0.099812 | 1.059575  | 0.057266  |
| C                                                         | -0.349094 | -0.976082 | -0.683993 |
| C                                                         | -0.102983 | 2.492528  | -0.434041 |
| C                                                         | 0.175202  | 0.995085  | 1.552558  |
| H                                                         | 0.211995  | -0.028080 | 1.926254  |
| H                                                         | 1.131469  | 1.466631  | 1.787218  |
| H                                                         | -0.602650 | 1.532896  | 2.096254  |
| H                                                         | 0.836671  | 2.996602  | -0.201253 |
| H                                                         | -0.904254 | 3.050383  | 0.055313  |
| H                                                         | -0.264285 | 2.542133  | -1.511025 |
| H                                                         | -0.537158 | -1.578164 | -1.568605 |
| H                                                         | -0.213583 | -1.631405 | 0.175480  |
| C                                                         | 0.796834  | 0.039894  | -0.769275 |
| H                                                         | 0.937313  | 0.438596  | -1.774066 |
| C                                                         | 2.114019  | -0.262491 | -0.167335 |
| C                                                         | 3.243837  | 0.659816  | -0.457708 |
| H                                                         | 2.864278  | 1.685275  | -0.406297 |
| H                                                         | 4.059925  | 0.489051  | 0.234778  |
| H                                                         | 3.602286  | 0.495766  | -1.474017 |
| O                                                         | -4.586729 | -0.704908 | -0.288503 |
| O                                                         | 2.171185  | -1.178949 | 0.711473  |
| O                                                         | 3.345167  | -1.820106 | 0.074896  |
| Rotational constants (GHz): 1.4676200 0.4302400 0.3767500 |           |           |           |
| Vibrational harmonic frequencies (cm-1):                  |           |           |           |
| i499.0982                                                 | 39.1392   |           | 43.3951   |
| 50.3496                                                   | 83.1300   |           | 120.6906  |
| 174.0402                                                  | 210.3160  |           | 222.6384  |
| 246.0192                                                  | 267.9352  |           | 271.4944  |
| 321.1084                                                  | 331.9089  |           | 337.4414  |
| 359.8476                                                  | 393.0519  |           | 436.2952  |
| 452.1700                                                  | 525.0921  |           | 570.7792  |
| 579.1068                                                  | 600.2883  |           | 726.3754  |
| 782.1029                                                  | 842.5201  |           | 863.3622  |
| 886.9950                                                  | 929.4293  |           | 943.7348  |
| 961.4766                                                  | 969.9709  |           | 991.4300  |
| 998.1257                                                  | 1004.3166 |           | 1030.4957 |
| 1074.0018                                                 | 1102.0234 |           | 1140.7413 |
| 1144.3962                                                 | 1162.0042 |           | 1187.7430 |
| 1217.8844                                                 | 1226.3825 |           | 1256.0189 |
| 1265.4727                                                 | 1274.7507 |           | 1305.4765 |
| 1327.8102                                                 | 1378.8765 |           | 1396.2903 |
| 1409.8083                                                 | 1425.0287 |           | 1426.8306 |
| 1431.1053                                                 | 1440.2219 |           | 1465.7666 |
| 1468.3279                                                 | 1485.0203 |           | 1491.4877 |

|           |           |           |
|-----------|-----------|-----------|
| 1497.8675 | 1507.7154 | 1509.9387 |
| 1597.9332 | 1861.4690 | 2942.5707 |
| 3047.9163 | 3050.1990 | 3054.6442 |
| 3057.9362 | 3068.6086 | 3098.9189 |
| 3103.2857 | 3115.6158 | 3120.9273 |
| 3122.1835 | 3125.5053 | 3130.3816 |
| 3139.1610 | 3161.2147 | 3202.2404 |

Zero-point correction (Hartree): 0.245100

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.13302754

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-1.374148	0.252060	-0.325410
H	-1.785358	0.520710	-1.300318
C	-2.464813	0.337758	0.715742
C	-3.659564	-0.512159	0.379097
H	-2.109170	0.024058	1.702542
H	-2.824485	1.364712	0.848316
H	-4.475873	-0.505330	1.125744
C	-0.038329	1.014650	-0.107374
C	-0.578027	-1.055849	-0.460515
C	0.113220	2.336186	-0.832604
C	0.335446	1.152872	1.360360
H	0.285789	0.205208	1.895233
H	1.356665	1.514343	1.467107
H	-0.343849	1.860970	1.838884
H	1.138206	2.704474	-0.759098
H	-0.540629	3.086947	-0.383494
H	-0.149438	2.244230	-1.886995
H	-0.914336	-1.775808	-1.200204
H	-0.443347	-1.549914	0.500536
C	0.667523	-0.216836	-0.820502
H	0.714947	-0.006726	-1.888346
C	1.997329	-0.624566	-0.328275
C	3.191200	-0.373292	-1.180469
H	2.982540	-0.771901	-2.177355
H	3.340927	0.702288	-1.289391
H	4.077461	-0.814262	-0.741415
O	-3.759756	-1.168553	-0.621463
O	2.046016	-1.296970	0.755937
O	3.032606	-0.368095	1.346521

Rotational constants (GHz): 1.4350600 0.4591500 0.4343100

Vibrational harmonic frequencies (cm-1):

i504.7521	34.4411	48.6555
78.3551	116.8172	139.9296
171.8380	207.4162	235.5808
241.3834	262.2829	270.3637
316.2368	335.2614	343.2266
363.5550	393.5613	414.7030
483.0960	553.7064	563.7299
606.3930	672.5029	717.9913
761.3961	838.3634	845.2747
881.8296	931.1154	936.7055
951.9359	959.0862	967.0029
1001.9558	1007.2060	1025.5750
1038.9958	1093.7089	1141.8728
1152.5518	1175.8191	1188.8822
1218.2485	1222.9555	1254.7160
1269.1798	1278.2351	1321.6297
1337.3684	1386.1136	1406.9761
1407.9512	1420.8395	1431.8589
1434.9017	1446.7078	1453.2532
1463.1187	1483.9223	1488.3416
1495.5363	1504.3313	1508.5393
1580.3105	1853.9069	2950.6068
3040.2236	3046.7370	3050.4140
3061.7815	3069.7934	3084.2272
3102.7115	3107.3544	3112.1079
3114.9632	3125.5187	3136.6242
3153.6140	3169.7593	3208.6760

Zero-point correction (Hartree): 0.245300

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.13065692

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -1.383711 | 0.250224  | -0.292826 |
| H | -1.804281 | 0.578199  | -1.245005 |
| C | -2.491462 | 0.144151  | 0.728932  |
| C | -3.618007 | -0.744521 | 0.273091  |
| H | -2.129212 | -0.251579 | 1.683214  |
| H | -2.928513 | 1.122008  | 0.963292  |
| H | -4.433278 | -0.895020 | 1.005437  |
| C | -0.128568 | 1.109919  | 0.021784  |
| C | -0.477217 | -0.969234 | -0.535697 |
| C | -0.099247 | 2.494694  | -0.592465 |
| C | 0.205053  | 1.165021  | 1.506167  |
| H | 0.217341  | 0.176862  | 1.965707  |
| H | 1.187116  | 1.614849  | 1.664961  |
| H | -0.529165 | 1.779687  | 2.029248  |
| H | 0.867224  | 2.979388  | -0.442041 |
| H | -0.857793 | 3.125589  | -0.123375 |
| H | -0.304625 | 2.457134  | -1.662374 |
| H | -0.735960 | -1.626000 | -1.359964 |
| H | -0.331166 | -1.560310 | 0.367543  |
| C | 0.701298  | -0.008741 | -0.746702 |
| H | 0.815619  | 0.300290  | -1.785755 |
| C | 2.029721  | -0.301494 | -0.167904 |
| C | 3.180410  | 0.537161  | -0.598495 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| H | 2.841732  | 1.577242  | -0.642125 |
| H | 4.018744  | 0.406238  | 0.075814  |
| H | 3.487763  | 0.252650  | -1.604879 |
| O | -3.666418 | -1.269822 | -0.804975 |
| O | 2.092409  | -1.119760 | 0.803489  |
| O | 3.212613  | -1.872955 | 0.193361  |

Rotational constants (GHz): 1.3461300 0.4736700 0.4094100  
 Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i496.9798 | 41.9214   | 46.6137   |
| 72.8180   | 110.5591  | 139.8879  |
| 164.8160  | 208.6902  | 224.1867  |
| 245.5882  | 250.6639  | 270.3872  |
| 318.0259  | 332.4379  | 338.9071  |
| 361.3332  | 391.7972  | 415.1912  |
| 468.4736  | 554.8305  | 566.3310  |
| 598.2172  | 673.2692  | 716.2743  |
| 740.1716  | 838.3880  | 848.4073  |
| 884.3458  | 930.0141  | 937.9665  |
| 951.1418  | 959.0512  | 969.3422  |
| 991.3886  | 1000.5028 | 1020.2607 |
| 1042.5132 | 1099.4933 | 1144.0916 |
| 1148.7949 | 1159.6464 | 1188.5853 |
| 1216.3418 | 1225.1048 | 1254.7884 |
| 1267.3818 | 1277.4340 | 1321.1736 |
| 1335.0153 | 1382.6496 | 1406.6903 |
| 1408.9973 | 1420.5509 | 1425.4724 |
| 1430.7600 | 1441.0241 | 1453.4035 |
| 1465.7000 | 1484.4501 | 1492.1187 |
| 1497.6272 | 1507.6621 | 1509.3375 |
| 1596.5730 | 1856.2277 | 2952.7039 |
| 3036.9769 | 3046.9590 | 3048.1693 |
| 3054.9931 | 3070.1116 | 3086.2520 |
| 3099.1174 | 3106.3043 | 3112.1545 |
| 3119.3472 | 3120.5584 | 3129.4702 |
| 3138.2920 | 3172.8152 | 3201.8154 |

Zero-point correction (Hartree): 0.244989

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 E(RM062X/Aug-CC-pVTZ) (Hartree): -616.12793999

Electronic state : 1-A

Cartesian coordinates (Angs):

C	1.202827	0.969186	0.726093
H	1.242114	2.006037	1.067600
C	2.635038	0.498452	0.516875
C	2.841984	-0.964712	0.223714
H	3.123256	1.070002	-0.273951
H	3.193592	0.688118	1.441321
H	2.276885	-1.676061	0.854956
C	0.165518	0.898312	-0.428683
C	0.213033	0.206283	1.628790
C	-0.005373	2.153654	-1.258915
C	0.343229	-0.322435	-1.317705
H	0.390056	-1.253001	-0.751622
H	-0.497960	-0.426108	-2.001133
H	1.261891	-0.219680	-1.897689
H	-0.866797	2.066480	-1.923488
H	0.876979	2.310308	-1.882811
H	-0.139127	3.034338	-0.629563
H	0.150802	0.498179	2.674058
H	0.316007	-0.873472	1.559414
C	-0.924870	0.690621	0.708094
H	-1.294305	1.673060	1.000579
C	-2.059075	-0.204090	0.402880
C	-3.385342	0.396579	0.093637
H	-3.628099	1.109268	0.886717
H	-3.320599	0.961122	-0.838249
H	-4.140360	-0.372949	-0.009355
O	3.608328	-1.374275	-0.604082
O	-1.876216	-1.459011	0.544558
O	-2.370382	-1.732557	-0.821159

Rotational constants (GHz): 1.2849700 0.5197600 0.4701600
 Vibrational harmonic frequencies (cm-1):

i512.4998	25.5568	55.6331
85.6915	98.0557	139.7258
188.2705	222.3613	232.7661
253.1145	255.4937	270.3194
318.7066	343.7137	359.5762
365.2150	393.1588	408.1978
460.4784	555.0971	563.0700
595.7238	633.2118	700.5113
758.5938	815.0096	837.8132
880.1262	918.9076	953.0842
963.1704	964.8868	984.5080
1003.5323	1013.0350	1033.9487
1060.7665	1110.2204	1133.1157
1152.2535	1169.1859	1188.2929
1219.7350	1227.1558	1252.1192
1262.4638	1294.1270	1321.2755
1337.3821	1385.0131	1400.0129
1406.8993	1428.2446	1433.0122
1440.5805	1447.1340	1448.2098
1462.6406	1480.7184	1487.8601
1497.3097	1505.2887	1506.6456
1580.2736	1857.4839	2953.0838
3032.3497	3047.6247	3050.8764
3063.8598	3065.8766	3103.2297
3107.7015	3110.8099	3111.5752
3117.2810	3124.2899	3137.9104
3147.3755	3170.8159	3208.0644

Zero-point correction (Hartree): 0.245355

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.12654745
Electronic state : 1-A
Cartesian coordinates (Angs):
C      1.236765      0.536270      1.038097
H      1.310022      1.338338      1.775647
C      2.652609      0.071545      0.721643
C      2.786518     -1.162393     -0.130856
H      3.229678      0.869158      0.251208
H      3.147797     -0.173080      1.668602
H      2.180157     -2.035512      0.175939
C      0.298102      1.041740     -0.092706
C      0.135220     -0.439802      1.500549
C      0.280880      2.539953     -0.317045
C      0.479276      0.296798     -1.407572
H      0.452906     -0.786557     -1.283189
H      -0.312791      0.562859     -2.110490
H      1.433991      0.563297     -1.862570
H      -0.492902      2.829428     -1.030172
H      1.239876      2.863136     -0.727845
H      0.110835      3.079303      0.615140
H      0.001847     -0.578030      2.569913
H      0.186806     -1.412722      1.018106
C      -0.888855      0.448312      0.780749
H      -1.282169      1.243644      1.414433
C      -1.993199     -0.160541      0.007653
C      -3.059529      0.735723     -0.513240
H      -2.580420      1.638568     -0.904893
H      -3.648642      0.224713     -1.265910
H      -3.715535      1.041758      0.301751
O      3.529883     -1.247176     -1.069605
O      -1.882859     -1.380742     -0.330181
O      -3.250548     -1.711323      0.133622
Rotational constants (GHz):  1.2698600    0.5081500    0.4477600
Vibrational harmonic frequencies (cm-1):
i498.4686      38.5483      51.6572
   86.4117      92.3180      119.4216
  199.0837      216.4098      238.5863
  244.5038      257.4190      271.7206
  325.5830      345.6264      359.7586
  366.6223      390.7497      409.8458
  459.4822      552.4263      565.3164
  590.4377      620.0676      700.8473
  742.9784      821.1965      842.3738
  882.3854      919.7765      959.1907
  960.6223      968.0429      978.5725
 1000.6680      1002.1462      1035.8929
 1061.9182      1112.7590      1130.8909
 1144.7903      1163.4479      1188.2850
 1218.7857      1227.4290      1251.7811
 1264.1737      1291.7019      1319.6073
 1337.7060      1382.1478      1399.7844
 1409.6017      1423.5807      1428.6655
 1439.3455      1440.9564      1451.5114
 1466.3351      1485.4562      1492.3799
 1500.3552      1509.1740      1511.3050
 1597.8027      1856.6819      2952.0227
 3036.6129      3047.4684      3049.3381
 3055.1415      3068.6341      3098.3587
 3107.9395      3114.4406      3115.1710
 3119.9497      3122.0380      3128.1546
 3136.6086      3171.2529      3201.0744
Zero-point correction (Hartree): 0.245243

ApineneCI.A.a.ringclose.ptpm
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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.12805819
Electronic state : 1-A
Cartesian coordinates (Angs):
C      -1.336905      0.834642     -0.700072
H      -1.413745      1.723031     -1.330794
C      -2.738970      0.520448     -0.173989
C      -2.890251     -0.849978      0.442151
H      -3.036257      1.287259      0.544415
H      -3.436622      0.554103     -1.013261
H      -3.038832     -0.900312      1.535840
C      -0.158369      1.053340      0.285383
C      -0.492265     -0.221445     -1.433825
C      0.143813      2.485783      0.675817
C      -0.243271      0.161411      1.514579
H      -0.412269     -0.885058      1.262337
H      0.684365      0.193962      2.083639
H      -1.060267      0.509980      2.150784
H      1.081283      2.546616      1.231458
H      -0.647929      2.873916      1.320360
H      0.215664      3.131460     -0.200186
H      -0.564711     -0.269537     -2.516959
H      -0.621066     -1.216425     -1.016128
C      0.769053      0.463152     -0.856922
H      1.098984      1.289245     -1.485780
C      1.928715     -0.351203     -0.445688
C      3.300498      0.173696     -0.684387
H      3.363911      0.483644     -1.731486
H      3.461714      1.064576     -0.074981
H      4.046012     -0.570229     -0.432319
O      -2.866762     -1.858548     -0.210001
O      1.700573     -1.528955     -0.012675
O      2.489624     -1.291911      1.214522
Rotational constants (GHz):  1.2363400    0.5655000    0.4947700
Vibrational harmonic frequencies (cm-1):
i498.5728      40.5524      62.9072

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74.9242	117.0843	141.7906
184.4364	227.7571	237.3673
249.0562	254.2895	273.4636
315.0613	344.0807	355.2649
371.8633	393.4638	411.6452
494.5791	557.1985	564.0495
595.6229	624.1675	726.5983
771.7123	837.2795	864.0854
892.3457	933.2117	944.1190
960.9605	966.5478	988.1719
1004.6606	1017.6772	1024.7629
1056.8696	1064.0810	1127.1827
1154.1197	1172.3488	1192.0802
1219.8489	1229.6884	1249.0970
1261.5990	1297.8896	1315.2053
1340.5959	1381.3541	1396.7807
1407.6261	1424.9881	1430.0629
1437.8621	1446.4872	1463.1080
1469.8096	1484.9649	1487.4030
1499.2231	1506.4547	1509.4939
1584.9519	1852.0898	2965.3371
3046.3845	3049.3903	3055.9651
3058.3831	3069.6103	3103.2069
3111.4093	3111.5396	3115.0895
3115.2259	3124.6363	3133.9638
3150.5635	3177.3697	3208.4811

Zero-point correction (Hartree): 0.245775

ApineneCI.A.a.ringclose.pttp

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.12494315

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 1.387041  | 0.515156  | 0.898425  |
| H | 1.483803  | 1.256480  | 1.695828  |
| C | 2.797507  | 0.159545  | 0.458343  |
| C | 3.053124  | -1.082271 | -0.354182 |
| H | 3.238800  | 0.992904  | -0.101721 |
| H | 3.448088  | 0.054020  | 1.334728  |
| H | 4.115804  | -1.203842 | -0.644293 |
| C | 0.356520  | 1.097809  | -0.108549 |
| C | 0.343373  | -0.528172 | 1.349560  |
| C | 0.313685  | 2.611076  | -0.191704 |
| C | 0.429765  | 0.478956  | -1.497434 |
| H | 0.395721  | -0.607961 | -1.468688 |
| H | -0.396030 | 0.837155  | -2.115876 |
| H | 1.358299  | 0.775757  | -1.990333 |
| H | -0.512067 | 2.956905  | -0.815669 |
| H | 1.237106  | 2.983545  | -0.641963 |
| H | 0.212265  | 3.062017  | 0.795874  |
| H | 0.296116  | -0.763285 | 2.409355  |
| H | 0.392535  | -1.443858 | 0.769563  |
| C | -0.743947 | 0.405507  | 0.799787  |
| H | -1.090912 | 1.134623  | 1.534048  |
| C | -1.912829 | -0.141202 | 0.074761  |
| C | -2.970562 | 0.813350  | -0.357628 |
| H | -2.480451 | 1.707753  | -0.753819 |
| H | -3.622719 | 0.347600  | -1.087394 |
| H | -3.565923 | 1.119628  | 0.502394  |
| O | 2.248611  | -1.912581 | -0.672052 |
| O | -1.875695 | -1.354564 | -0.299415 |
| O | -3.226979 | -1.631351 | 0.240179  |

Rotational constants (GHz): 1.2297300 0.5709800 0.4697900

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i504.5811 | 35.6205   | 56.6300   |
| 87.7201   | 113.3576  | 125.7254  |
| 187.6381  | 203.5656  | 226.0849  |
| 237.2440  | 248.7083  | 271.8523  |
| 321.4840  | 325.0117  | 342.4912  |
| 363.7649  | 391.0721  | 411.8885  |
| 468.7691  | 544.9204  | 562.9151  |
| 597.2019  | 677.9380  | 736.6162  |
| 754.5450  | 782.7722  | 841.9302  |
| 886.4227  | 907.7865  | 939.2899  |
| 961.0834  | 968.3245  | 977.3317  |
| 988.5316  | 1001.1383 | 1017.0655 |
| 1053.6171 | 1088.8996 | 1127.1794 |
| 1157.9747 | 1163.7280 | 1190.8835 |
| 1223.4348 | 1230.8816 | 1256.4043 |
| 1265.4113 | 1298.1137 | 1330.6051 |
| 1370.2306 | 1384.6876 | 1408.0749 |
| 1409.4152 | 1422.6081 | 1427.2191 |
| 1435.6668 | 1440.7628 | 1449.6286 |
| 1466.0717 | 1485.7430 | 1492.1080 |
| 1503.4846 | 1511.9736 | 1512.5841 |
| 1598.6032 | 1866.3737 | 2933.5639 |
| 3028.2035 | 3045.8208 | 3050.8139 |
| 3052.0698 | 3053.5415 | 3058.4474 |
| 3086.1756 | 3107.7804 | 3111.8468 |
| 3120.8595 | 3121.9638 | 3127.5710 |
| 3161.9886 | 3191.9542 | 3200.6873 |

Zero-point correction (Hartree): 0.245108

ApineneCI.A.a.ringclose.tmmm

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.12726903

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-1.255632	-0.556299	-0.502955
H	-1.568712	-0.334821	-1.525797
C	-2.476541	-0.937489	0.325741
C	-3.508734	0.155753	0.284955

H	-2.925922	-1.850880	-0.063731
H	-2.179285	-1.105113	1.364272
H	-3.227935	1.101049	0.790503
C	-0.289718	0.579135	-0.035469
C	-0.067559	-1.538280	-0.540730
C	-0.471829	1.940187	-0.677269
C	-0.196827	0.699092	1.480911
H	-0.019486	-0.264436	1.963605
H	0.617549	1.369087	1.754865
H	-1.120934	1.111366	1.889329
H	0.380636	2.582377	-0.454285
H	-1.373170	2.427396	-0.299676
H	-0.562329	1.854496	-1.760596
H	-0.029561	-2.255860	-1.355934
H	0.031790	-2.068000	0.406712
C	0.856169	-0.313354	-0.615061
H	1.036600	-0.020272	-1.656702
C	2.193078	-0.264876	0.016492
C	2.919051	-1.512443	0.359330
H	2.249738	-2.143804	0.950468
H	3.155266	-2.062850	-0.552790
H	3.837107	-1.283436	0.886355
O	-4.567017	0.064616	-0.272752
O	2.614418	0.898721	0.315610
O	3.888838	0.716056	-0.406892
Rotational constants (GHz): 1.8611900 0.4083800 0.3733900			
Vibrational harmonic frequencies (cm-1):			
i489.0875	27.4196	36.5167	
67.0941	83.2889	139.0836	
180.5118	208.9444	228.2419	
231.9374	265.0226	282.5818	
305.8579	318.7630	347.0444	
378.1929	396.3545	409.4294	
468.1740	515.9458	527.3512	
588.4278	599.6970	715.1754	
757.6700	839.8524	856.3047	
892.4481	925.4906	954.9434	
964.2483	968.9147	985.4034	
1005.8917	1023.3789	1029.0817	
1072.5595	1105.0563	1131.0069	
1143.4509	1168.6449	1192.4009	
1197.2307	1247.8181	1265.1718	
1269.2512	1281.5897	1302.4687	
1329.2077	1353.9609	1394.9400	
1407.2118	1411.4740	1420.8235	
1433.6027	1437.2755	1459.9110	
1468.7396	1485.0049	1495.5279	
1499.7605	1507.9533	1514.5093	
1576.7700	1861.5525	2940.3042	
3036.2737	3051.7155	3053.0881	
3054.0670	3061.3111	3071.2094	
3091.6704	3112.7776	3118.9917	
3121.4575	3126.8247	3134.0494	
3138.7965	3153.9573	3209.0815	
Zero-point correction (Hartree): 0.244755			
ApineneCI.A.a.ringclose.ttmp			
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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.13048381			
Electronic state : 1-A			
Cartesian coordinates (Angs):			
C	1.257882	0.569379	-0.527266
H	1.629383	0.333572	-1.527377
C	2.435020	0.888287	0.385694
C	3.407918	-0.258253	0.415670
H	2.958281	1.776909	0.032925
H	2.074354	1.070522	1.401301
H	3.032989	-1.192785	0.878554
C	0.208674	-0.513479	-0.129627
C	0.117027	1.600207	-0.646349
C	0.333285	-1.892791	-0.740832
C	-0.012498	-0.609744	1.374846
H	-0.108516	0.369025	1.847313
H	-0.920102	-1.177402	1.581278
H	0.833738	-1.117789	1.841055
H	-0.594408	-2.448180	-0.592279
H	1.143170	-2.452458	-0.268510
H	0.535735	-1.834943	-1.810704
H	0.180555	2.336732	-1.443397
H	-0.051647	2.110320	0.302041
C	-0.849335	0.426349	-0.842263
H	-0.907727	0.106385	-1.884856
C	-2.209748	0.367158	-0.282049
C	-2.736417	1.441305	0.596376
H	-2.549927	2.399970	0.102953
H	-3.789155	1.278715	0.794412
H	-2.195194	1.454964	1.543163
O	4.514758	-0.217860	-0.045608
O	-2.920074	-0.612275	-0.690865
O	-3.217482	-1.060374	0.683589
Rotational constants (GHz): 1.7422700 0.4320900 0.3995800			
Vibrational harmonic frequencies (cm-1):			
i498.2290	32.0193	56.3477	
67.9745	92.5530	133.5791	
193.2197	226.8708	247.1320	
255.5330	264.6910	290.6249	
308.9574	334.4402	357.7061	
375.4710	384.5034	421.8715	
471.7219	513.5905	531.5361	
589.5921	599.8979	722.4578	
768.1819	850.2254	851.5044	
877.6211	927.0202	945.8917	

965.8374	971.3895	993.8480
1007.8975	1014.8542	1031.4417
1075.2760	1106.8834	1132.1196
1143.6298	1168.2558	1185.8010
1195.2965	1244.9676	1265.1651
1280.9505	1286.6503	1301.8110
1326.9645	1365.5277	1397.0112
1408.0630	1414.4058	1420.3911
1432.6033	1439.4284	1460.6769
1469.4052	1484.1227	1493.1168
1498.3856	1507.7226	1516.4604
1578.6856	1861.1790	2935.7653
3049.3384	3049.9390	3053.0645
3061.5719	3070.3398	3081.7505
3092.2656	3117.1689	3120.3959
3122.4232	3127.3298	3130.2175
3137.1668	3151.5254	3205.5566

Zero-point correction (Hartree): 0.245233

ApineneCI.A.a.ringclose.tmpm

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E(RM062X/Aug-CC-pVT2) (Hartree): -616.12906840

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 1.213534  | 0.731782  | -0.695385 |
| H | 1.451387  | 0.573802  | -1.750843 |
| C | 2.476473  | 1.115000  | 0.062632  |
| C | 3.516575  | 0.042274  | -0.106517 |
| H | 2.871522  | 2.047023  | -0.352073 |
| H | 2.282222  | 1.257575  | 1.124841  |
| H | 3.860062  | -0.121619 | -1.147758 |
| C | 0.364164  | -0.480449 | -0.205569 |
| C | -0.029119 | 1.637564  | -0.588569 |
| C | 0.592105  | -1.796262 | -0.921305 |
| C | 0.415094  | -0.668030 | 1.306433  |
| H | 0.205239  | 0.259081  | 1.844827  |
| H | -0.320924 | -1.410569 | 1.614505  |
| H | 1.402617  | -1.015908 | 1.612130  |
| H | -0.174325 | -2.520525 | -0.644639 |
| H | 1.565520  | -2.210081 | -0.648332 |
| H | 0.564885  | -1.665867 | -2.003999 |
| H | -0.180995 | 2.384815  | -1.363151 |
| H | -0.079061 | 2.119590  | 0.387289  |
| C | -0.881763 | 0.360311  | -0.646897 |
| H | -1.133917 | 0.099198  | -1.681125 |
| C | -2.144108 | 0.188693  | 0.104948  |
| C | -2.859747 | 1.353226  | 0.681041  |
| H | -2.146331 | 1.924356  | 1.282189  |
| H | -3.200596 | 2.010400  | -0.120604 |
| H | -3.711830 | 1.024059  | 1.262710  |
| O | 3.946808  | -0.636581 | 0.784826  |
| O | -2.499094 | -1.018263 | 0.298082  |
| O | -3.852055 | -0.802653 | -0.253012 |

Rotational constants (GHz): 1.7321800 0.4378600 0.4002300

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i484.3405 | 28.6859   | 54.8769   |
| 61.8234   | 87.6977   | 133.3050  |
| 158.6675  | 213.0037  | 229.9996  |
| 243.4729  | 270.2894  | 273.0233  |
| 316.1226  | 328.0444  | 351.4186  |
| 386.4062  | 400.8690  | 410.7973  |
| 473.9518  | 510.4828  | 539.5263  |
| 584.2370  | 601.0588  | 712.1345  |
| 749.9857  | 839.8018  | 858.9722  |
| 887.9582  | 917.9703  | 947.1674  |
| 967.4251  | 975.3380  | 998.3301  |
| 1013.3919 | 1018.8665 | 1040.4738 |
| 1057.3114 | 1106.7937 | 1125.8868 |
| 1149.1402 | 1166.3461 | 1193.4611 |
| 1197.7893 | 1247.8100 | 1262.3463 |
| 1267.6006 | 1279.1240 | 1297.0923 |
| 1326.2868 | 1355.8978 | 1400.8484 |
| 1407.6994 | 1414.3242 | 1425.5336 |
| 1427.1902 | 1437.4408 | 1459.0342 |
| 1468.7588 | 1486.5690 | 1495.6940 |
| 1499.0214 | 1511.8951 | 1515.9281 |
| 1577.6367 | 1858.7028 | 2930.7478 |
| 3045.3253 | 3049.3115 | 3051.6158 |
| 3052.5359 | 3057.1552 | 3058.5660 |
| 3094.4149 | 3112.3071 | 3119.0783 |
| 3120.9620 | 3132.6484 | 3134.5359 |
| 3138.8634 | 3152.5361 | 3210.5635 |

Zero-point correction (Hartree): 0.244825

ApineneCI.A.a.ringclose.tmpm

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E(RM062X/Aug-CC-pVT2) (Hartree): -616.13177562

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-1.222404	0.803616	0.638913
H	-1.512935	0.730338	1.690787
C	-2.457112	1.037903	-0.218539
C	-3.446001	-0.074455	-0.002864
H	-2.927159	1.978511	0.083829
H	-2.210128	1.093225	-1.277696
H	-3.822621	-0.175125	1.035172
C	-0.279589	-0.391000	0.311768
C	-0.020464	1.761459	0.516982
C	-0.445475	-1.662963	1.114817
C	-0.213888	-0.702029	-1.178675
H	-0.092107	0.195813	-1.786613
H	0.626672	-1.366032	-1.381123

H	-1.139971	-1.186591	-1.491731
H	0.409804	-2.320723	0.951718
H	-1.347056	-2.193454	0.800539
H	-0.521478	-1.451485	2.182228
H	0.032463	2.602752	1.203832
H	0.091054	2.123357	-0.504808
C	0.891597	0.560024	0.798630
H	1.023497	0.381706	1.867887
C	2.189941	0.329635	0.144564
C	2.684134	1.214968	-0.939530
H	2.591619	2.250002	-0.596893
H	3.704925	0.956620	-1.194863
H	2.059277	1.110576	-1.827208
O	-3.805138	-0.842175	-0.852250
O	2.887774	-0.614038	0.647681
O	3.036077	-1.292841	-0.654363
Rotational constants (GHz): 1.5766700 0.4689300 0.4320700			
Vibrational harmonic frequencies (cm-1):			
i498.9382	55.3888	60.6090	
68.5873	91.3445	130.7023	
170.2790	235.6587	255.0675	
259.3003	269.3225	287.8829	
321.3614	349.7905	366.8785	
378.1528	395.4817	419.8157	
476.6123	511.3930	541.6482	
584.8410	604.3226	717.4722	
761.2685	847.1923	860.0980	
870.1498	922.0395	941.1410	
970.5914	972.1486	1005.4673	
1010.9247	1017.6819	1041.5050	
1062.4116	1109.4983	1126.5595	
1149.7367	1167.7920	1189.4236	
1196.6605	1244.9620	1260.5312	
1277.4738	1288.1082	1298.1275	
1326.1535	1367.7648	1403.4873	
1408.2517	1417.4447	1427.3831	
1429.2487	1440.7828	1461.6937	
1469.0506	1487.0437	1494.3562	
1499.3442	1514.2404	1519.0369	
1578.8199	1860.0206	2929.3857	
3047.3293	3049.9906	3054.0664	
3055.9017	3058.1239	3082.8723	
3094.2598	3119.2708	3119.8430	
3126.9174	3127.9129	3137.1806	
3140.9534	3150.7794	3204.1505	
Zero-point correction (Hartree): 0.245465			
ApineneCI.A.a.ringclose.tmtm			
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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.13047660			
Electronic state : 1-A			
Cartesian coordinates (Angs):			
C	1.285102	0.649512	-0.601379
H	1.635927	0.367033	-1.594952
C	2.444737	1.174750	0.215429
C	3.604066	0.226511	0.332914
H	2.831852	2.104676	-0.216555
H	2.137084	1.441271	1.232118
H	4.457383	0.590203	0.936238
C	0.391869	-0.510332	-0.052314
C	0.038647	1.551465	-0.709016
C	0.621799	-1.893911	-0.626114
C	0.347506	-0.553364	1.469108
H	0.115507	0.420400	1.907749
H	-0.409100	-1.262292	1.804517
H	1.312359	-0.881630	1.860308
H	-0.214875	-2.545909	-0.372206
H	1.541708	-2.323000	-0.231811
H	0.709032	-1.854426	-1.712653
H	-0.054553	2.188542	-1.585009
H	-0.080795	2.162081	0.186497
C	-0.819147	0.280138	-0.656957
H	-1.017554	-0.107815	-1.662964
C	-2.125079	0.212669	0.032728
C	-2.869597	1.446342	0.388088
H	-2.193793	2.101376	0.945224
H	-3.154695	1.979545	-0.520215
H	-3.759176	1.201162	0.954886
O	3.643108	-0.859240	-0.178304
O	-2.501273	-0.953741	0.378229
O	-3.813801	-0.822506	-0.285688
Rotational constants (GHz): 1.7488800 0.4545300 0.4072900			
Vibrational harmonic frequencies (cm-1):			
i483.1951	28.9672	47.0339	
79.1544	107.3886	149.6317	
161.3908	211.0706	216.9150	
238.9144	259.0277	286.0446	
318.2647	333.2814	343.7212	
368.8412	398.1165	404.8404	
479.3120	501.4818	572.5135	
594.2077	678.3105	709.6011	
746.8175	789.2522	841.6383	
888.6125	911.3263	931.8991	
966.5539	969.3105	974.7572	
1001.3465	1017.9995	1029.2029	
1056.1086	1110.6628	1114.8067	
1146.1703	1167.5118	1195.4231	
1203.9842	1248.7954	1266.5886	
1273.7077	1284.7681	1306.2392	
1345.9400	1357.3706	1403.8096	
1406.6924	1416.5366	1422.9049	
1425.6435	1436.8828	1450.4277	

1460.5634	1486.2983	1492.8983
1498.2702	1509.3167	1515.0917
1576.4782	1856.7062	2951.9125
3040.8541	3044.0298	3046.8530
3052.4791	3059.6061	3068.7303
3084.8998	3092.9725	3111.8974
3112.6775	3128.7061	3135.2968
3146.8324	3147.3415	3210.3773

Zero-point correction (Hartree): 0.244741

ApineneCI.A.a.ringclose.tmp

E(RM062X/Aug-CC-pVTZ) (Hartree): -616.13354133

Electronic state : 1-A

Cartesian coordinates (Angs):

C	1.293485	0.680065	-0.582408
H	1.698620	0.414669	-1.560235
C	2.416802	1.116646	0.330702
C	3.510784	0.099099	0.490704
H	2.882894	2.036780	-0.039781
H	2.052312	1.365305	1.332702
H	4.334674	0.386889	1.170952
C	0.313264	-0.449350	-0.138490
C	0.093031	1.633813	-0.746793
C	0.497547	-1.836935	-0.713596
C	0.129876	-0.513742	1.371443
H	-0.031784	0.469271	1.817974
H	-0.726929	-1.141014	1.617506
H	1.025663	-0.943906	1.824170
H	-0.412077	-2.419553	-0.555691
H	1.332342	-2.342769	-0.230361
H	0.702793	-1.793354	-1.783809
H	0.103814	2.329508	-1.582717
H	-0.098565	2.185614	0.174122
C	-0.811273	0.402879	-0.867133
H	-0.873234	0.028296	-1.890889
C	-2.152642	0.303308	-0.272633
C	-2.709109	1.386664	0.577342
H	-2.581828	2.332616	0.042325
H	-3.747790	1.182100	0.807911
H	-2.147526	1.463713	1.509008
O	3.528246	-0.964921	-0.065497
O	-2.830781	-0.720290	-0.625634
O	-3.072962	-1.125895	0.772629

Rotational constants (GHz): 1.6187100 0.4867000 0.4401000

Vibrational harmonic frequencies (cm-1):

i497.7373	48.0443	54.8629
83.1633	113.4702	146.6715
168.3956	225.3475	244.6303
259.1343	266.1507	289.4970
318.8403	335.0038	359.9803
377.2030	393.6151	404.8097
481.9445	504.5493	576.8029
589.1797	676.7427	722.3761
748.3325	793.2959	852.5479
867.2785	913.7796	931.5847
961.1346	971.5995	975.3480
1004.6719	1010.5893	1032.3204
1059.1670	1109.9911	1114.6551
1143.4267	1165.8152	1185.0289
1202.3905	1246.4798	1270.7237
1281.3952	1288.1152	1306.6075
1345.5114	1368.5119	1405.2105
1407.8029	1417.1454	1422.1123
1426.0565	1440.3328	1450.6714
1461.8742	1486.4382	1489.5730
1497.4783	1509.9885	1515.9802
1577.3008	1856.2103	2948.8902
3041.3314	3048.5941	3049.5829
3056.6516	3070.0267	3081.3923
3086.4667	3090.3755	3113.9162
3119.7839	3126.5637	3137.2124
3144.0721	3147.6106	3205.9950

Zero-point correction (Hartree): 0.245184

ApineneCI.A.a.ringclose.tpm

E(RM062X/Aug-CC-pVTZ) (Hartree): -616.12843738

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-1.344233	0.368594	-0.479696
H	-1.571041	0.714912	-1.491610
C	-2.594405	0.450073	0.386913
C	-3.669946	-0.387522	-0.245576
H	-2.403480	0.071499	1.390049
H	-2.933598	1.487844	0.448490
H	-4.097101	0.013753	-1.186034
C	-0.034230	1.071836	-0.010820
C	-0.591648	-0.975920	-0.554747
C	0.263154	2.420843	-0.632142
C	0.095165	1.130049	1.505875
H	-0.071288	0.157098	1.972928
H	1.090547	1.473980	1.785131
H	-0.633551	1.828305	1.920158
H	1.274771	2.742163	-0.383311
H	-0.435415	3.172628	-0.258346
H	0.173599	2.382540	-1.718366
H	-0.814841	-1.640775	-1.384869
H	-0.692583	-1.530464	0.378076
C	0.711498	-0.162917	-0.614347
H	0.987232	0.064300	-1.651482
C	1.975860	-0.607365	0.012134

C	2.201480	-2.034908	0.344726
H	1.350660	-2.383431	0.936990
H	2.216575	-2.628022	-0.571083
H	3.142163	-2.158183	0.867058
O	-4.032738	-1.449815	0.178800
O	2.788995	0.323797	0.317328
O	3.911390	-0.299572	-0.412092

Rotational constants (GHz): 1.4858000 0.4415800 0.3806100

Vibrational harmonic frequencies (cm-1):

i486.5689	36.3242	39.6415
62.7782	89.0211	119.5267
168.2404	192.1613	219.8958
226.6880	263.7338	281.3962
314.7787	331.3388	342.1485
355.4904	400.6278	429.1460
479.4588	502.3929	549.3249
590.4704	601.9963	721.2332
769.3156	840.5473	864.0183
893.0611	922.5107	932.2412
966.8031	976.8032	991.9463
1003.1140	1019.1790	1033.3429
1064.5677	1097.4108	1136.7763
1146.3474	1162.1004	1195.3824
1214.6174	1248.3376	1249.9254
1270.0496	1281.6186	1299.5889
1322.9881	1355.5694	1398.8936
1406.5336	1412.6833	1421.7064
1426.2231	1437.6812	1460.2291
1473.4105	1485.2335	1494.3504
1499.2448	1508.5640	1513.8449
1576.5271	1858.6175	2932.8161
3037.4472	3050.0157	3053.3622
3054.1763	3058.4399	3059.2854
3093.1495	3113.5815	3118.6159
3120.5658	3133.8264	3136.5442
3139.6753	3153.5838	3209.5118

Zero-point correction (Hartree): 0.244708

ApineneCI.A.a.ringclose.tpm

E(RM062X/Aug-CC-pVTZ) (Hartree): -616.13138758

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-1.320917	0.434066	-0.444172
H	-1.591130	0.906988	-1.392474
C	-2.497470	0.501711	0.520888
C	-3.677242	-0.176578	-0.116535
H	-2.268164	-0.003590	1.457715
H	-2.748136	1.546630	0.723426
H	-4.134628	0.363297	-0.969492
C	0.067274	0.983492	-0.006441
C	-0.672357	-0.937379	-0.725603
C	0.460512	2.365825	-0.479056
C	0.319073	0.834216	1.488258
H	0.044453	-0.153527	1.860805
H	1.374327	0.999389	1.706043
H	-0.276420	1.568364	2.033489
H	1.523497	2.532804	-0.297725
H	-0.101392	3.127624	0.065444
H	0.266996	2.490881	-1.544950
H	-1.022259	-1.502211	-1.585995
H	-0.710721	-1.575418	0.157237
C	0.671680	-0.209312	-0.856046
H	0.841684	0.171707	-1.865354
C	1.954233	-0.735099	-0.358718
C	2.031920	-2.009444	0.397337
H	1.484907	-2.769130	-0.169152
H	3.067135	-2.283956	0.561031
H	1.533972	-1.907741	1.362298
O	-4.094309	-1.253068	0.211227
O	2.984368	-0.069547	-0.715500
O	3.446896	0.094978	0.676546

Rotational constants (GHz): 1.5243500 0.4516300 0.4020400

Vibrational harmonic frequencies (cm-1):

i497.5989	36.8707	49.1525
69.7251	101.0930	114.5073
162.2974	207.0256	242.4856
255.6494	269.7968	281.5784
323.4615	336.1007	351.0441
375.7532	392.7663	433.7962
479.4994	503.2272	547.6170
590.7522	600.3962	735.2950
772.0866	847.3385	866.9729
872.1179	923.8713	930.9173
967.7264	977.8673	996.5119
1008.4041	1011.8344	1038.1348
1068.5768	1095.0420	1137.9841
1147.4144	1161.0621	1186.5429
1215.4550	1246.1189	1251.0202
1277.4683	1288.9657	1299.5722
1322.8559	1367.3701	1401.0908
1407.9165	1415.5161	1423.1717
1426.8095	1440.2589	1460.8126
1472.2170	1485.2993	1493.0030
1497.9884	1509.4752	1517.8550
1578.1581	1858.7709	2932.9740
3047.8503	3050.0809	3055.0540
3057.7931	3060.5568	3082.7404
3094.9044	3118.4897	3119.3482
3124.6214	3129.8021	3138.6373
3141.2774	3153.2348	3207.1013

Zero-point correction (Hartree): 0.245226

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ApineneCI.A.a.ringclose.tppm
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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.12736860
Electronic state : 1-A
Cartesian coordinates (Angs):
  C   -1.329738    0.117047   -0.378093
  H   -1.621961    0.373922   -1.398842
  C   -2.553394    0.165556    0.526095
  C   -3.586943   -0.814765    0.046910
  H   -2.266860   -0.115272    1.543836
  H   -2.995335    1.161733    0.545258
  H   -3.264723   -1.875588    0.042268
  C   -0.071324    0.960706   -0.010725
  C   -0.456756   -1.157400   -0.405064
  C    0.074060    2.291538   -0.719353
  C    0.116454    1.120990    1.492456
  H    0.060829    0.167274    2.022090
  H    1.087368    1.567686    1.704262
  H   -0.654269    1.776071    1.900905
  H    1.061863    2.715755   -0.538197
  H   -0.674294    2.998242   -0.354898
  H   -0.059194    2.180432   -1.795929
  H   -0.648011   -1.894707   -1.180502
  H   -0.455956   -1.654275    0.565766
  C    0.760408   -0.235368   -0.578604
  H    0.963777   -0.049952   -1.640441
  C    2.088334   -0.524384    0.005753
  C    2.464092   -1.904257    0.400590
  H    1.677330   -2.298053    1.050243
  H    2.498698   -2.543112   -0.483363
  H    3.433615   -1.909224    0.883311
  O   -4.683923   -0.517092   -0.336224
  O    2.822229    0.493372    0.220834
  O    3.964941   -0.066143   -0.527805
Rotational constants (GHz):    1.6749200    0.4041200    0.3622000
Vibrational harmonic frequencies (cm-1):
i488.1088      38.2742      44.1801
 51.8583      89.8848      125.7626
172.0301     200.4500     220.8203
227.6061     269.8929     273.1650
319.2814     331.6771     343.9769
351.5474     398.7153     430.7346
471.4377     502.6834     535.5391
594.5325     602.1309     722.8346
774.1683     840.1095     859.6272
890.9856     919.8207     930.2952
967.2136     977.7448     983.3321
1003.9500    1024.7787     1030.9052
1074.1621    1101.9044     1140.4558
1144.9640    1165.5956     1196.4137
1213.8118    1249.1880     1255.0618
1271.8093    1281.3854     1304.7911
1327.1700    1355.0466     1396.2456
1407.6483    1412.9222     1423.2675
1429.6539    1437.3226     1460.7914
1469.4032    1486.0016     1495.1555
1499.4317    1509.3749     1515.3816
1576.9414    1863.2160     2928.2029
3038.6465    3051.0329     3052.4375
3053.3573    3056.1480     3069.8702
3087.2808    3113.3397     3118.8858
3121.7445    3126.6027     3134.3105
3139.7208    3149.2065     3209.7817
Zero-point correction (Hartree): 0.244760

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ApineneCI.A.a.ringclose.tppp
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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.13038215
Electronic state : 1-A
Cartesian coordinates (Angs):
  C   -1.316128    0.165236   -0.380018
  H   -1.657784    0.543117   -1.346581
  C   -2.470122    0.198172    0.612255
  C   -3.590811   -0.675861    0.124067
  H   -2.132855   -0.189953    1.577566
  H   -2.847345    1.211344    0.750009
  H   -3.338284   -1.749970    0.015878
  C    0.020192    0.878918   -0.025079
  C   -0.532485   -1.148498   -0.599742
  C    0.251834    2.262675   -0.591080
  C    0.333530    0.848018    1.465014
  H    0.178921   -0.138605    1.904857
  H    1.371952    1.134209    1.632622
  H   -0.318288    1.548459    1.989520
  H    1.297465    2.547149   -0.463004
  H   -0.367555    2.994772   -0.069198
  H    0.008902    2.301885   -1.653340
  H   -0.842933   -1.802756   -1.410883
  H   -0.466736   -1.727869    0.321885
  C    0.721508   -0.294860   -0.825251
  H    0.815887    0.037079   -1.861423
  C    2.067685   -0.653994   -0.348583
  C    2.305344   -1.870955    0.467250
  H    1.824921   -2.713807   -0.038827
  H    3.368838   -2.026132    0.604447
  H    1.832823   -1.769005    1.444954
  O   -4.686791   -0.283154   -0.165131
  O    3.008962    0.096588   -0.774285
  O    3.493928    0.379937    0.590481
Rotational constants (GHz):    1.6924000    0.4169300    0.3824700
Vibrational harmonic frequencies (cm-1):

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i498.4976	41.1449	50.8837
61.7965	102.8031	116.8509
167.0995	215.0738	237.0314
254.9032	273.2498	275.8872
324.7052	336.9642	347.6571
376.3523	387.5755	438.0542
474.3566	500.6240	534.3639
594.8526	599.3577	736.9004
777.5875	849.7155	860.8036
871.8369	917.6868	928.3262
967.8406	980.8275	989.1647
1007.2809	1013.6740	1033.9485
1077.2253	1100.4255	1139.9242
1146.6255	1164.5734	1187.3960
1213.3915	1246.4461	1259.0417
1277.1410	1288.5538	1305.2389
1325.2793	1366.5938	1397.1122
1407.6264	1414.7616	1424.1594
1430.8596	1439.5609	1460.4247
1469.0036	1485.2321	1492.8498
1497.4299	1510.4222	1517.2586
1578.7321	1862.9887	2930.1381
3049.3659	3049.7435	3052.9430
3057.2457	3068.4037	3081.3307
3087.5938	3117.3873	3121.0874
3122.8947	3129.0083	3130.9777
3139.1635	3146.1043	3205.2678

Zero-point correction (Hartree): 0.245181

ApineneCI.A.a.ringclose.tptm

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.13030556

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -1.398615 | 0.224465  | -0.330664 |
| H | -1.707106 | 0.385114  | -1.365166 |
| C | -2.589794 | 0.409231  | 0.579345  |
| C | -3.738305 | -0.499228 | 0.232824  |
| H | -2.335450 | 0.220333  | 1.627852  |
| H | -2.966714 | 1.437923  | 0.552441  |
| H | -4.634732 | -0.401354 | 0.873763  |
| C | -0.091399 | 1.030553  | -0.068714 |
| C | -0.598820 | -1.090876 | -0.251899 |
| C | 0.112023  | 2.277153  | -0.905475 |
| C | 0.137804  | 1.325672  | 1.409039  |
| H | 0.039654  | 0.431731  | 2.029219  |
| H | 1.136100  | 1.733937  | 1.562803  |
| H | -0.586189 | 2.060722  | 1.764261  |
| H | 1.125567  | 2.660078  | -0.783519 |
| H | -0.587208 | 3.058485  | -0.599371 |
| H | -0.051730 | 2.070420  | -1.963574 |
| H | -0.862000 | -1.877426 | -0.952184 |
| H | -0.604875 | -1.496864 | 0.760519  |
| C | 0.663604  | -0.257682 | -0.529512 |
| H | 0.854987  | -0.187174 | -1.607814 |
| C | 1.986423  | -0.565916 | 0.054012  |
| C | 2.305000  | -1.934569 | 0.530133  |
| H | 1.511364  | -2.249381 | 1.213420  |
| H | 2.293533  | -2.627715 | -0.312481 |
| H | 3.281529  | -1.955826 | 0.998042  |
| O | -3.721328 | -1.292557 | -0.668099 |
| O | 2.771585  | 0.427439  | 0.193959  |
| O | 3.870462  | -0.231860 | -0.539953 |

Rotational constants (GHz): 1.5098500 0.4488300 0.3924200

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i487.9116 | 35.6902   | 49.5060   |
| 78.7035   | 104.6706  | 144.6884  |
| 164.1591  | 198.4136  | 213.1065  |
| 216.0866  | 256.5018  | 271.1586  |
| 314.4249  | 329.3597  | 344.3597  |
| 353.8708  | 399.8304  | 409.4852  |
| 475.4101  | 508.3490  | 571.4293  |
| 598.0255  | 675.8217  | 714.0695  |
| 734.2265  | 835.9107  | 842.4629  |
| 895.2357  | 921.2329  | 932.4522  |
| 938.3347  | 966.7777  | 978.7126  |
| 991.3752  | 1011.9886 | 1027.9228 |
| 1039.5703 | 1101.2397 | 1138.0996 |
| 1150.9996 | 1161.6561 | 1196.7421 |
| 1212.1006 | 1243.7600 | 1254.5140 |
| 1272.1813 | 1284.4822 | 1315.9920 |
| 1335.1642 | 1357.4719 | 1405.0784 |
| 1407.3106 | 1415.7721 | 1423.1796 |
| 1425.6356 | 1436.7548 | 1451.7251 |
| 1460.5685 | 1485.5798 | 1495.5449 |
| 1500.2329 | 1508.7615 | 1516.2580 |
| 1574.7737 | 1855.0572 | 2950.1953 |
| 3033.8928 | 3040.2546 | 3049.6482 |
| 3052.2942 | 3054.1770 | 3068.8874 |
| 3082.5144 | 3091.3760 | 3113.7784 |
| 3115.7565 | 3119.2112 | 3134.2413 |
| 3138.8774 | 3164.9931 | 3209.3804 |

Zero-point correction (Hartree): 0.244560

ApineneCI.A.a.ringclose.tptp

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.13336522

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-1.376338	0.278635	-0.308930
H	-1.739402	0.570629	-1.296076
C	-2.481828	0.461527	0.703747

C	-3.724235	-0.314869	0.361273
H	-2.172487	0.149552	1.706854
H	-2.771442	1.513772	0.803507
H	-4.560765	-0.217591	1.078710
C	0.009445	0.940908	-0.068356
C	-0.682937	-1.093526	-0.425595
C	0.303837	2.246181	-0.775086
C	0.376766	1.035885	1.407522
H	0.176368	0.108730	1.947184
H	1.436437	1.267945	1.515137
H	-0.209586	1.825785	1.880291
H	1.368296	2.476469	-0.706715
H	-0.251768	3.063847	-0.310815
H	0.026094	2.196689	-1.828320
H	-1.076036	-1.790332	-1.159827
H	-0.620076	-1.589636	0.543722
C	0.612374	-0.346354	-0.769143
H	0.690018	-0.120634	-1.834939
C	1.950721	-0.739219	-0.300252
C	2.144820	-1.882938	0.625689
H	1.597006	-2.738685	0.219792
H	3.201287	-2.090247	0.747116
H	1.712433	-1.656822	1.601047
O	-3.839477	-1.006844	-0.613163
O	2.921354	-0.096349	-0.826758
O	3.467857	0.292336	0.488437
Rotational constants (GHz):			1.5617900
Vibrational harmonic frequencies (cm-1):			0.4578800
			0.4142000
i496.0347	43.7774		60.9859
92.9669	107.1642		130.6979
169.6442	201.3425		240.1152
254.4068	260.7641		277.0794
313.3746	337.2938		347.4815
374.8407	392.3796		415.6618
477.4342	511.6790		576.3317
592.6900	672.8234		718.9051
748.4220	836.4127		852.3887
873.8708	920.8805		929.9259
937.8089	965.8840		984.2942
998.0708	1008.2810		1025.3889
1046.0036	1098.3382		1139.6564
1152.9135	1160.8475		1187.6344
1214.6489	1241.0768		1262.5458
1280.6850	1288.6617		1318.2187
1336.2868	1369.2655		1405.6523
1408.1643	1417.3763		1422.6118
1427.7425	1439.2015		1452.8252
1460.5291	1484.9135		1493.6860
1498.8243	1509.0647		1516.8620
1577.2000	1854.7955		2950.5969
3040.5931	3047.9135		3050.1382
3053.0942	3069.8136		3081.3123
3084.7630	3093.3170		3116.4128
3118.4082	3120.9308		3131.0636
3138.5960	3161.6654		3206.7154
Zero-point correction (Hartree):			0.245092
ApineneCI.A.a.ringclose.tttm			
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E(RM062X/Aug-CC-pVT2) (Hartree): -616.12543897			
Electronic state : 1-A			
Cartesian coordinates (Angs):			
C	1.247022	0.322896	1.104083
H	1.220840	0.959619	1.990597
C	2.708744	0.105426	0.732631
C	2.992009	-0.929358	-0.322483
H	3.170009	1.042800	0.418408
H	3.242627	-0.237393	1.626613
H	2.514243	-1.917247	-0.173588
C	0.249998	0.933035	0.075597
C	0.271985	-0.854166	1.338449
C	0.061290	2.434814	0.133353
C	0.509384	0.473697	-1.353743
H	0.601048	-0.612743	-1.433563
H	-0.308427	0.787200	-2.002609
H	1.433193	0.911300	-1.733868
H	-0.778210	2.740688	-0.491130
H	0.958123	2.941703	-0.229055
H	-0.131217	2.768663	1.153564
H	0.161459	-1.221875	2.355362
H	0.467149	-1.696633	0.678082
C	-0.836069	0.054187	0.781387
H	-1.301399	0.645310	1.578686
C	-1.968915	-0.446259	-0.027637
C	-2.325190	-1.886059	-0.044817
H	-1.422480	-2.455273	-0.285040
H	-2.645509	-2.199029	0.950224
H	-3.123186	-2.069911	-0.753448
O	3.721998	-0.754474	-1.258632
O	-2.531743	0.424460	-0.766023
O	-3.880231	0.125455	-0.244113
Rotational constants (GHz):			1.4422200
Vibrational harmonic frequencies (cm-1):			0.4618800
			0.4315600
i484.7155	26.4902		53.7252
83.7628	86.8766		125.0628
182.1132	211.4204		218.5160
243.7024	259.3785		269.1207
329.8604	338.8532		346.2510
369.9852	401.6311		411.4046
472.4380	496.7177		577.5705
587.8145	618.4098		704.1040
732.8201	819.4892		839.3849

888.9185	909.8561	928.5561
964.2119	974.9012	998.1183
999.0775	1020.2637	1034.6423
1058.5280	1112.9382	1128.3934
1143.2898	1168.3226	1194.5473
1219.3524	1246.0339	1257.4377
1269.8415	1294.5659	1319.1487
1335.4827	1358.8585	1399.6913
1406.3042	1413.3510	1423.8963
1437.9764	1441.8163	1452.8852
1460.2872	1484.0368	1494.5271
1501.9266	1506.6997	1515.2398
1577.7849	1859.2117	2939.4493
3035.9100	3043.1065	3049.2535
3051.9550	3052.3785	3072.4263
3105.5898	3110.7271	3113.6446
3117.5612	3120.7492	3134.2263
3136.9363	3158.5411	3210.6360

Zero-point correction (Hartree): 0.244814

ApineneCI.A.a.ringclose.ttmp

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.12834211

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 1.245100  | 0.588790  | 1.011371  |
| H | 1.252150  | 1.407889  | 1.733569  |
| C | 2.682743  | 0.346093  | 0.570408  |
| C | 2.943449  | -0.889413 | -0.248199 |
| H | 3.067510  | 1.204393  | 0.017859  |
| H | 3.301877  | 0.233293  | 1.468213  |
| H | 2.515150  | -1.831589 | 0.146183  |
| C | 0.138256  | 0.906514  | -0.032684 |
| C | 0.352145  | -0.536408 | 1.585095  |
| C | -0.165703 | 2.360543  | -0.319855 |
| C | 0.301307  | 0.127068  | -1.331098 |
| H | 0.510793  | -0.931341 | -1.163873 |
| H | -0.610293 | 0.198204  | -1.924937 |
| H | 1.134834  | 0.536079  | -1.903925 |
| H | -1.097910 | 2.442438  | -0.881062 |
| H | 0.632458  | 2.803042  | -0.919247 |
| H | -0.264163 | 2.934755  | 0.602029  |
| H | 0.361060  | -0.690279 | 2.661510  |
| H | 0.511179  | -1.491296 | 1.087691  |
| C | -0.850791 | 0.207024  | 0.988875  |
| H | -1.226332 | 0.988340  | 1.652848  |
| C | -2.012758 | -0.450165 | 0.369267  |
| C | -2.069955 | -1.921386 | 0.180789  |
| H | -1.813663 | -2.392968 | 1.134278  |
| H | -3.052514 | -2.213359 | -0.170411 |
| H | -1.324593 | -2.239453 | -0.549124 |
| O | 3.611358  | -0.907709 | -1.244714 |
| O | -2.991106 | 0.325911  | 0.102631  |
| O | -3.030290 | -0.091965 | -1.312344 |

Rotational constants (GHz): 1.3580700 0.4896500 0.4697100

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i496.1923 | 53.3892   | 62.9763   |
| 86.6623   | 103.1904  | 117.7639  |
| 187.5943  | 230.1406  | 245.7247  |
| 254.4528  | 266.1204  | 276.0745  |
| 322.3239  | 344.2205  | 371.2209  |
| 378.2230  | 404.0658  | 407.9668  |
| 472.4276  | 499.6644  | 580.1418  |
| 582.9116  | 625.7660  | 703.0166  |
| 748.0761  | 817.0038  | 848.5682  |
| 867.9538  | 908.2408  | 928.7730  |
| 965.6937  | 975.9465  | 998.4498  |
| 1004.7839 | 1011.2922 | 1038.7096 |
| 1062.9455 | 1112.5026 | 1129.9249 |
| 1145.0604 | 1168.2841 | 1187.2638 |
| 1218.2838 | 1243.6494 | 1253.1323 |
| 1288.7393 | 1294.8318 | 1318.8421 |
| 1335.0194 | 1369.5860 | 1400.5646 |
| 1407.6314 | 1415.4077 | 1425.4142 |
| 1436.9782 | 1440.7143 | 1450.2862 |
| 1461.7589 | 1484.4767 | 1493.7162 |
| 1499.6857 | 1508.5559 | 1520.3242 |
| 1578.4860 | 1859.2945 | 2937.6177 |
| 3034.9014 | 3048.6808 | 3049.8563 |
| 3054.6147 | 3070.3126 | 3084.0252 |
| 3102.8201 | 3111.0238 | 3116.4628 |
| 3120.4030 | 3123.4978 | 3129.8409 |
| 3138.6982 | 3156.3531 | 3205.7866 |

Zero-point correction (Hartree): 0.245326

ApineneCI.A.a.ringclose.tttm

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.12676297

Electronic state : 1-A

Cartesian coordinates (Angs):

C	1.383669	0.559730	0.905339
H	1.415418	1.286676	1.719990
C	2.812515	0.363211	0.427009
C	3.178472	-0.830942	-0.413559
H	3.147308	1.247782	-0.127472
H	3.495450	0.311719	1.283852
H	4.231333	-0.817802	-0.757677
C	0.277273	1.046560	-0.076403
C	0.476677	-0.611589	1.345843
C	0.028076	2.541282	-0.105843
C	0.420591	0.497121	-1.489758
H	0.521182	-0.587271	-1.503402

H	-0.447105	0.777546	-2.087555
H	1.305909	0.918783	-1.971256
H	-0.878450	2.767520	-0.667663
H	0.863371	3.054429	-0.588586
H	-0.083494	2.944042	0.901380
H	0.457810	-0.852606	2.405768
H	0.673129	-1.509874	0.770456
C	-0.711961	0.189164	0.791671
H	-1.163081	0.833769	1.552407
C	-1.846397	-0.439227	0.079937
C	-2.016277	-1.911160	0.046470
H	-1.074553	-2.345458	-0.303866
H	-2.183809	-2.288374	1.056541
H	-2.851813	-2.181884	-0.586560
O	2.470929	-1.757578	-0.700254
O	-2.570734	0.363934	-0.592324
O	-3.830749	-0.104343	0.022504
Rotational constants (GHz):			
Vibrational harmonic frequencies (cm-1):			
i473.8706	31.0359	49.8190	
97.8834	111.5793	130.9801	
180.2992	198.6032	223.7866	
229.8932	247.9657	272.2495	
322.0065	327.2470	337.6669	
366.8608	402.8639	410.3509	
479.1954	499.5939	571.9883	
592.4865	677.4709	730.8914	
753.4158	781.7465	841.8341	
885.4752	895.4174	939.4949	
946.4630	967.8059	983.3992	
1001.9799	1016.2818	1021.0262	
1055.2060	1087.0130	1126.2840	
1157.8422	1167.8080	1195.8154	
1228.5981	1250.6828	1259.8513	
1276.5569	1297.1307	1329.1155	
1354.8028	1376.7840	1405.9475	
1406.7406	1412.5929	1423.7842	
1433.1725	1437.9178	1446.9552	
1459.2379	1485.2393	1493.4906	
1505.0018	1510.7937	1513.1877	
1577.0702	1859.3301	2936.3833	
3029.4478	3046.8436	3047.7683	
3054.7566	3056.8077	3060.0335	
3065.5392	3111.6368	3116.0219	
3116.3655	3121.1273	3134.1315	
3149.7696	3189.5860	3212.6552	
Zero-point correction (Hartree): 0.244926			
ApineneCI.A.a.ringclose.ttp			
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E(RM062X/Aug-CC-pVT2) (Hartree): -616.12933370			
Electronic state : 1-A			
Cartesian coordinates (Angs):			
C	1.369307	0.673108	0.828399
H	1.418064	1.460599	1.584361
C	2.759552	0.539891	0.228709
C	3.152626	-0.700162	-0.529561
H	2.962746	1.389500	-0.433066
H	3.520719	0.624904	1.014266
H	4.146072	-0.620368	-1.013306
C	0.148568	1.000600	-0.077320
C	0.583682	-0.514314	1.431174
C	-0.238074	2.456613	-0.228548
C	0.203066	0.319490	-1.438226
H	0.450362	-0.737390	-1.363905
H	-0.757979	0.420924	-1.942378
H	0.972408	0.794904	-2.051750
H	-1.226101	2.533109	-0.685339
H	0.474618	2.974266	-0.874714
H	-0.261238	2.965531	0.735741
H	0.701518	-0.704172	2.495538
H	0.752686	-1.429894	0.873468
C	-0.702925	0.196889	0.990546
H	-1.058763	0.921223	1.726421
C	-1.880271	-0.494895	0.441187
C	-1.870541	-1.954996	0.179484
H	-1.520464	-2.452613	1.089176
H	-2.856985	-2.288842	-0.118597
H	-1.154762	-2.194587	-0.607703
O	2.529421	-1.722386	-0.616829
O	-2.923391	0.231914	0.311662
O	-3.070135	-0.108334	-1.117743
Rotational constants (GHz):			
Vibrational harmonic frequencies (cm-1):			
i494.3045	47.2947	69.7973	
83.5314	112.3944	116.6693	
188.6309	200.3192	239.1294	
245.9026	253.3728	275.4558	
320.8811	326.8540	345.6095	
375.8105	395.1530	405.1924	
481.9271	504.2472	575.2846	
589.6190	677.3444	744.4550	
755.8065	783.8309	850.9575	
870.2657	898.5389	939.2538	
941.7324	969.7614	983.1495	
1006.6087	1011.1076	1022.8456	
1057.5719	1085.7414	1128.2760	
1159.0390	1167.8768	1190.1152	
1225.4202	1247.0569	1259.8505	
1289.2100	1298.9442	1326.9929	
1363.4093	1379.1128	1406.0109	
1408.2341	1414.8440	1424.0925	

1434.6243	1437.5573	1448.5312
1460.1281	1485.0845	1492.7120
1504.9437	1511.9267	1518.1348
1576.6556	1860.1199	2935.2584
3029.8221	3046.1824	3048.3312
3053.7306	3059.0592	3061.1452
3080.0199	3110.5615	3116.0499
3116.8392	3126.3113	3130.0228
3161.1430	3182.6790	3209.0147

Zero-point correction (Hartree): 0.245215

Z-pinonaldehyde-A-oxide
#####

Population analysis as 298K (%)
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)
Compound Qtot Erel Erel2 n*Q*MB %

ApineneCI.J.b.pmm	3.708e+44	0.00	0.00	3.708e+44	41.1
ApineneCI.J.b.ppp	4.377e+44	0.15	0.15	3.415e+44	37.9
ApineneCI.J.b.pmp	3.769e+44	0.99	0.99	7.139e+43	7.92
ApineneCI.J.b.mmm	4.337e+44	1.53	1.53	3.257e+43	3.61
ApineneCI.J.b.mpm	5.938e+44	2.06	2.06	1.835e+43	2.04
ApineneCI.J.b.ppm	5.571e+44	2.09	2.09	1.627e+43	1.8
ApineneCI.J.b.mpp	5.234e+44	2.07	2.07	1.585e+43	1.76
ApineneCI.J.b.ptm	1.947e+44	1.58	1.58	1.346e+43	1.49
ApineneCI.J.b.ptp	1.913e+44	1.89	1.89	7.929e+42	0.88
ApineneCI.J.b.mmp	5.023e+44	2.61	2.61	6.099e+42	0.677
ApineneCI.J.b.mtp	1.598e+44	2.10	2.10	4.608e+42	0.511
ApineneCI.J.b.tpm	1.819e+44	2.64	2.64	2.114e+42	0.234
ApineneCI.J.b.mtm	4.673e+44	4.01	4.01	5.313e+41	0.0589
ApineneCI.J.b.mtt	2.142e+44	4.64	4.64	8.519e+40	0.00945
Total				9.016e+44	100

ApineneCI.J.b.mmm

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.16415811

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.657042 | -0.580662 | -0.101323 |
| H | -1.131685 | -0.707368 | -1.073464 |
| C | -1.734495 | -0.716381 | 0.981447  |
| C | -2.791807 | 0.289902  | 0.788861  |
| H | -2.202086 | -1.698647 | 0.874730  |
| H | -1.303281 | -0.603930 | 1.974652  |
| H | -2.913577 | 1.176456  | 1.403011  |
| C | 0.265932  | 0.672084  | -0.132339 |
| C | 0.586437  | -1.481433 | 0.002493  |
| C | -0.119896 | 1.764114  | -1.110515 |
| C | 0.517157  | 1.255615  | 1.252639  |
| H | 0.840621  | 0.499391  | 1.970722  |
| H | 1.290663  | 2.019133  | 1.205818  |
| H | -0.394960 | 1.717985  | 1.638744  |
| H | 0.683402  | 2.496916  | -1.198280 |
| H | -1.018986 | 2.286922  | -0.773856 |
| H | -0.324489 | 1.351547  | -2.098942 |
| H | 0.577480  | -2.420372 | -0.545315 |
| H | 0.853743  | -1.675594 | 1.042416  |
| C | 1.391762  | -0.300322 | -0.580725 |
| H | 1.394432  | -0.370746 | -1.673270 |
| C | 2.819278  | -0.056384 | -0.165327 |
| C | 3.680580  | -1.277885 | 0.033990  |
| H | 3.557272  | -1.968341 | -0.801553 |
| H | 3.356016  | -1.805799 | 0.932612  |
| H | 4.721449  | -0.987220 | 0.139205  |
| O | 3.249497  | 1.062287  | -0.022719 |
| O | -3.638500 | 0.210920  | -0.124333 |
| O | -3.577678 | -0.863486 | -0.957004 |

Rotational constants (GHz): 1.7211900 0.4281600 0.3969200

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| 34.4543   | 42.8134   | 61.9860   |
| 99.3788   | 128.2513  | 134.3749  |
| 163.4127  | 208.3356  | 225.5752  |
| 270.3175  | 278.4923  | 313.4287  |
| 321.2635  | 354.0876  | 368.1609  |
| 403.5347  | 412.3323  | 498.9903  |
| 517.6509  | 545.8426  | 608.0905  |
| 621.3348  | 679.4727  | 729.0681  |
| 761.9498  | 883.8247  | 888.6188  |
| 913.2551  | 916.5048  | 940.9537  |
| 963.6513  | 970.9475  | 987.2276  |
| 1005.2353 | 1019.1329 | 1035.2923 |
| 1055.8273 | 1089.9251 | 1114.9710 |
| 1140.7031 | 1177.9912 | 1197.1767 |
| 1209.2729 | 1238.0051 | 1246.8272 |
| 1268.3420 | 1293.4973 | 1304.5607 |
| 1330.7184 | 1352.7351 | 1383.7770 |
| 1392.0172 | 1396.2102 | 1409.0716 |
| 1420.6352 | 1456.9233 | 1464.9081 |
| 1477.2195 | 1482.8949 | 1494.5407 |
| 1499.3124 | 1505.2078 | 1514.8617 |
| 1641.8393 | 1830.9636 | 3044.0336 |
| 3047.7294 | 3053.8897 | 3064.5660 |
| 3064.6924 | 3078.7535 | 3107.9709 |
| 3110.8522 | 3112.5008 | 3126.3063 |
| 3130.5806 | 3140.1453 | 3147.0102 |
| 3150.8936 | 3179.7230 | 3187.8663 |

Zero-point correction (Hartree): 0.247057

ApineneCI.J.b.mmp



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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.16231771
Electronic state : 1-A
Cartesian coordinates (Angs):
C -0.454193 0.592526 1.059615
H -0.594388 0.339396 2.113942
C -1.756946 1.136922 0.475797
C -2.822250 0.123245 0.591436
H -2.067797 2.016693 1.048870
H -1.659185 1.415725 -0.569732
H -3.078113 -0.340861 1.540384
C 0.254129 -0.598341 0.353560
C 0.829951 1.428485 0.899271
C 0.024045 -1.975139 0.942828
C 0.019893 -0.610623 -1.152263
H 0.233426 0.357308 -1.610934
H 0.665931 -1.354033 -1.619547
H -1.018695 -0.851386 -1.390382
H 0.733123 -2.687337 0.519061
H -0.985000 -2.329704 0.716998
H 0.154416 -1.967795 2.026250
H 1.112319 2.084538 1.719432
H 0.808262 2.004726 -0.025559
C 1.597092 0.103066 0.734667
H 1.932203 -0.274685 1.702870
C 2.744506 -0.063631 -0.232048
C 3.281599 1.157742 -0.930402
H 3.465510 1.960323 -0.214956
H 2.533142 1.524445 -1.636493
H 4.190486 0.905072 -1.467812
O 3.189318 -1.166209 -0.441891
O -3.496533 -0.319492 -0.358392
O -3.284360 0.164709 -1.613111
Rotational constants (GHz): 1.5102500 0.4432000 0.4323100
Vibrational harmonic frequencies (cm-1):
26.8704 42.9690 62.8477
81.8316 140.6818 148.5802
181.8908 224.0865 227.3024
261.2189 283.4627 315.0927
322.5538 339.4410 366.2268
410.1939 444.9861 485.6875
509.0908 527.0669 602.2915
616.5179 670.6688 715.3411
763.3325 847.9040 886.7365
899.9051 915.9122 936.5104
964.3525 971.6656 1000.3077
1014.3427 1018.9889 1042.6005
1052.5273 1097.3322 1113.8641
1152.7972 1176.4072 1196.6956
1210.0195 1244.9450 1253.9502
1261.3823 1276.2199 1293.3208
1326.2841 1349.8830 1388.4718
1397.0719 1406.0484 1408.8284
1429.7419 1461.5980 1464.9767
1475.5262 1484.0741 1495.7552
1498.6701 1507.1286 1515.5261
1649.6545 1827.7987 3042.8122
3049.9156 3050.5296 3056.8582
3061.6676 3079.3523 3090.1141
3110.9371 3115.5121 3123.7141
3127.1009 3133.6149 3145.6897
3161.9915 3175.8646 3180.9614
Zero-point correction (Hartree): 0.246936

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ApineneCI,J.b.mpm
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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.16332852
Electronic state : 1-A
Cartesian coordinates (Angs):
C      -0.716206      0.582917      -0.498526
H      -0.915529      0.945263      -1.510354
C      -1.926669      0.872845      0.400861
C      -3.177536      0.398775      -0.214601
H      -1.807400      0.357801      1.355009
H      -2.007181      1.949731      0.556807
H      -3.846874      1.036338      -0.783791
C       0.672784      1.132248      -0.055025
C      -0.118563      -0.833710      -0.562291
C       1.102402      2.450075      -0.667426
C       0.826803      1.167209      1.460340
H       0.560940      0.215600      1.923978
H       1.858418      1.390547      1.725168
H       0.185948      1.941030      1.887593
H       2.148550      2.650833      -0.433200
H       0.503324      3.274757      -0.273465
H       0.990719      2.435580      -1.752697
H      -0.455114      -1.491992      -1.358643
H      -0.250646      -1.348524      0.386735
C       1.264609      -0.161591      -0.681847
H       1.501311      0.021321      -1.735315
C       2.491820      -0.788420      -0.071067
C       2.560880      -2.293163      -0.082431
H       2.304338      -2.675796      -1.071403
H       1.818510      -2.692030      0.611375
H       3.552221      -2.624402      0.211606
O       3.377182      -0.106226      0.386124
O      -3.573485      -0.781146      -0.149948
O      -2.806631      -1.681273      0.525409
Rotational constants (GHz):      1.2880400      0.4950900      0.4023200
Vibrational harmonic frequencies (cm-1):
30.5281      35.3347      73.3419
107.3521      120.5337      134.5989

```

|           |           |           |
|-----------|-----------|-----------|
| 165.0527  | 177.7330  | 231.8883  |
| 256.4816  | 279.6573  | 304.5514  |
| 313.0186  | 344.5684  | 363.7990  |
| 413.6111  | 421.0661  | 511.5844  |
| 515.5150  | 539.8703  | 602.5384  |
| 633.2700  | 672.8801  | 730.1244  |
| 776.2649  | 878.0480  | 895.2360  |
| 908.8140  | 922.6690  | 925.9817  |
| 965.5310  | 972.0011  | 985.7169  |
| 1013.2586 | 1018.4765 | 1035.8453 |
| 1043.0270 | 1089.1692 | 1130.9131 |
| 1144.7570 | 1175.7525 | 1197.2872 |
| 1218.2104 | 1239.0183 | 1253.2514 |
| 1264.7415 | 1285.3538 | 1306.6958 |
| 1326.0166 | 1352.3440 | 1390.1941 |
| 1396.9519 | 1399.0222 | 1409.3794 |
| 1420.5548 | 1461.8675 | 1464.0329 |
| 1476.0687 | 1484.4860 | 1494.9140 |
| 1498.7332 | 1506.7844 | 1515.5177 |
| 1649.6237 | 1828.3220 | 3044.2888 |
| 3049.0165 | 3054.6747 | 3057.6171 |
| 3065.0813 | 3070.9056 | 3109.4258 |
| 3111.7220 | 3119.1523 | 3126.1516 |
| 3128.7177 | 3132.4561 | 3149.6487 |
| 3164.1496 | 3181.6817 | 3184.5372 |

Zero-point correction (Hartree): 0.247065

ApineneCI.J.b.mpp

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.16328028

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-0.733157	-0.043310	-0.120854
H	-1.216881	0.108252	-1.085420
C	-1.810793	-0.016988	0.970799
C	-2.873699	-0.981764	0.650308
H	-1.383099	-0.255362	1.943112
H	-2.267869	0.976330	0.984043
H	-2.993694	-1.946411	1.132458
C	0.471989	0.933492	0.003568
C	0.248766	-1.228380	-0.190800
C	0.367722	2.220657	-0.788749
C	0.847504	1.219887	1.452143
H	0.980024	0.306139	2.035619
H	1.781741	1.775696	1.494980
H	0.067946	1.816203	1.930018
H	1.321911	2.749184	-0.778661
H	-0.391844	2.876525	-0.358391
H	0.091045	2.022155	-1.824670
H	0.018420	-2.045374	-0.871182
H	0.457320	-1.636032	0.800141
C	1.324645	-0.207165	-0.618981
H	1.317106	-0.110318	-1.709473
C	2.765422	-0.385645	-0.215704
C	3.294356	-1.798115	-0.208054
H	3.007857	-2.315135	-1.124978
H	2.844589	-2.347726	0.620923
H	4.374251	-1.790897	-0.095075
O	3.460280	0.560234	0.064706
O	-3.725182	-0.773647	-0.238106
O	-3.663266	0.406009	-0.913537

Rotational constants (GHz): 1.5539400 0.4250100 0.3829100

Vibrational harmonic frequencies (cm-1):

34.3989	41.1769	64.2683
105.1497	118.6651	137.1450
160.0085	199.2157	215.3453
257.4604	273.4585	311.2243
315.0743	348.3837	362.1473
411.2591	416.5057	511.5673
518.3208	533.2354	603.2595
631.3868	677.7081	734.2450
773.2518	883.2303	901.9478
915.3745	916.2057	931.9286
963.2969	966.7400	981.7681
1002.3363	1026.7622	1034.9969
1043.1948	1090.5033	1128.2866
1137.6953	1180.1671	1198.3657
1227.2279	1238.1170	1250.8451
1257.3195	1290.0558	1306.3249
1330.6755	1352.8503	1384.3059
1393.2547	1395.6677	1409.5052
1420.0561	1459.4571	1465.1941
1477.9096	1483.8338	1492.7544
1498.8247	1506.6767	1514.3110
1642.5869	1832.4392	3049.7929
3051.6700	3055.3356	3061.5241
3064.3767	3071.9005	3104.8128
3113.4608	3120.0882	3125.7202
3130.2590	3136.3831	3140.6003
3152.3109	3181.1861	3189.8927

Zero-point correction (Hartree): 0.247036

ApineneCI.J.b.mtm

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.16029464

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |          |           |          |
|---|----------|-----------|----------|
| C | 0.463811 | 0.027323  | 1.331136 |
| H | 0.359029 | 0.504571  | 2.307082 |
| C | 1.951275 | -0.286420 | 1.147324 |
| C | 2.272175 | -1.162191 | 0.004605 |
| H | 2.528797 | 0.629269  | 1.041402 |

|                                                           |           |           |           |
|-----------------------------------------------------------|-----------|-----------|-----------|
| H                                                         | 2.300006  | -0.821947 | 2.037426  |
| H                                                         | 1.911533  | -2.183916 | -0.068424 |
| C                                                         | -0.292425 | 0.902137  | 0.293065  |
| C                                                         | -0.632435 | -1.050735 | 1.199334  |
| C                                                         | -0.335512 | 2.389158  | 0.579254  |
| C                                                         | 0.164073  | 0.646166  | -1.137879 |
| H                                                         | 0.103091  | -0.411593 | -1.409253 |
| H                                                         | -0.473674 | 1.190038  | -1.832896 |
| H                                                         | 1.195838  | 0.980119  | -1.276537 |
| H                                                         | -1.040365 | 2.881041  | -0.091731 |
| H                                                         | 0.649220  | 2.835410  | 0.425230  |
| H                                                         | -0.645486 | 2.584628  | 1.607167  |
| H                                                         | -0.933731 | -1.581960 | 2.099417  |
| H                                                         | -0.408317 | -1.777848 | 0.418546  |
| C                                                         | -1.552015 | 0.069666  | 0.667883  |
| H                                                         | -2.071051 | 0.549210  | 1.503533  |
| C                                                         | -2.591668 | -0.197155 | -0.391701 |
| C                                                         | -3.181859 | -1.583230 | -0.451619 |
| H                                                         | -3.432119 | -1.937936 | 0.549044  |
| H                                                         | -2.437258 | -2.271049 | -0.857896 |
| H                                                         | -4.059093 | -1.586099 | -1.091490 |
| O                                                         | -2.934472 | 0.677856  | -1.148036 |
| O                                                         | 3.014958  | -0.850352 | -0.946559 |
| O                                                         | 3.527146  | 0.408716  | -1.006534 |
| Rotational constants (GHz): 1.3275300 0.4788300 0.4573000 |           |           |           |
| Vibrational harmonic frequencies (cm-1):                  |           |           |           |
| 19.1835                                                   | 52.8802   | 74.6970   |           |
| 92.2144                                                   | 134.0871  | 151.5244  |           |
| 180.6473                                                  | 208.9111  | 231.3858  |           |
| 254.3844                                                  | 279.5894  | 318.7835  |           |
| 325.1770                                                  | 346.3881  | 369.6242  |           |
| 408.8673                                                  | 430.1849  | 493.4426  |           |
| 508.0940                                                  | 589.2145  | 607.9481  |           |
| 618.5392                                                  | 671.4236  | 720.3246  |           |
| 749.5047                                                  | 853.0705  | 892.7659  |           |
| 898.7532                                                  | 920.4497  | 924.4323  |           |
| 957.9584                                                  | 972.5306  | 988.7433  |           |
| 999.6065                                                  | 1023.2861 | 1031.1582 |           |
| 1044.1308                                                 | 1118.9557 | 1131.3159 |           |
| 1151.0618                                                 | 1177.7598 | 1195.3238 |           |
| 1215.4889                                                 | 1241.5973 | 1248.2998 |           |
| 1266.8806                                                 | 1298.3280 | 1303.1695 |           |
| 1327.7493                                                 | 1353.3909 | 1387.1692 |           |
| 1392.5818                                                 | 1408.6446 | 1417.5547 |           |
| 1428.2801                                                 | 1457.6722 | 1463.3265 |           |
| 1477.6047                                                 | 1487.4028 | 1496.9451 |           |
| 1501.2857                                                 | 1514.3784 | 1521.0159 |           |
| 1649.8589                                                 | 1833.2464 | 3037.0004 |           |
| 3040.0065                                                 | 3047.8122 | 3056.8170 |           |
| 3062.7690                                                 | 3076.9753 | 3087.0007 |           |
| 3102.0410                                                 | 3116.9766 | 3124.7265 |           |
| 3129.4435                                                 | 3140.1154 | 3141.7845 |           |
| 3149.7612                                                 | 3180.1617 | 3181.8337 |           |
| Zero-point correction (Hartree): 0.247148                 |           |           |           |
| ApineneCI.J.b.mtp                                         |           |           |           |
| ~~~~~                                                     |           |           |           |
| E(RM062X/Aug-CC-pVTZ) (Hartree): -616.16359021            |           |           |           |
| Electronic state : 1-A                                    |           |           |           |
| Cartesian coordinates (Angs):                             |           |           |           |
| C                                                         | -0.700656 | 0.672444  | -0.874134 |
| H                                                         | -0.680116 | 1.065954  | -1.891570 |
| C                                                         | -2.088578 | 0.997180  | -0.292930 |
| C                                                         | -2.455735 | 0.180037  | 0.875245  |
| H                                                         | -2.122936 | 2.050856  | -0.013501 |
| H                                                         | -2.843466 | 0.783522  | -1.052999 |
| H                                                         | -2.422888 | 0.522186  | 1.903906  |
| C                                                         | 0.581278  | 1.163805  | -0.141694 |
| C                                                         | -0.131171 | -0.757211 | -0.879903 |
| C                                                         | 1.144364  | 2.496526  | -0.594349 |
| C                                                         | 0.438498  | 1.133562  | 1.375711  |
| H                                                         | 0.103551  | 0.159620  | 1.739664  |
| H                                                         | 1.394846  | 1.344809  | 1.849578  |
| H                                                         | -0.279076 | 1.891108  | 1.701519  |
| H                                                         | 2.126910  | 2.663628  | -0.151283 |
| H                                                         | 0.491289  | 3.317654  | -0.288535 |
| H                                                         | 1.246622  | 2.531161  | -1.679855 |
| H                                                         | -0.320747 | -1.370457 | -1.755161 |
| H                                                         | -0.436968 | -1.319897 | 0.001478  |
| C                                                         | 1.262139  | -0.116348 | -0.697620 |
| H                                                         | 1.697775  | 0.099635  | -1.678943 |
| C                                                         | 2.332934  | -0.811903 | 0.101779  |
| C                                                         | 2.427476  | -2.306899 | -0.062560 |
| H                                                         | 2.413969  | -2.571440 | -1.120875 |
| H                                                         | 1.551694  | -2.775743 | 0.389876  |
| H                                                         | 3.329544  | -2.679401 | 0.413325  |
| O                                                         | 3.082674  | -0.194507 | 0.819577  |
| O                                                         | -2.878596 | -0.989369 | 0.764298  |
| O                                                         | -2.968240 | -1.518667 | -0.486862 |
| Rotational constants (GHz): 1.1717400 0.5627900 0.4589000 |           |           |           |
| Vibrational harmonic frequencies (cm-1):                  |           |           |           |
| 40.4161                                                   | 64.0702   | 72.6297   |           |
| 125.9204                                                  | 134.6370  | 152.5607  |           |
| 168.2383                                                  | 210.1952  | 232.7042  |           |
| 255.2746                                                  | 278.7323  | 313.6387  |           |
| 323.1139                                                  | 347.2169  | 368.6227  |           |
| 407.9904                                                  | 425.0324  | 495.9774  |           |
| 522.5323                                                  | 590.5354  | 618.4225  |           |
| 624.7251                                                  | 679.9268  | 729.1405  |           |
| 759.7355                                                  | 883.0588  | 896.7208  |           |
| 908.3052                                                  | 916.4816  | 936.7692  |           |
| 962.8684                                                  | 970.7027  | 978.6965  |           |

|           |           |           |
|-----------|-----------|-----------|
| 996.8553  | 1015.1623 | 1038.0812 |
| 1054.4434 | 1069.5398 | 1131.0110 |
| 1147.8709 | 1176.0083 | 1198.3766 |
| 1223.1077 | 1239.7282 | 1247.4083 |
| 1269.0373 | 1299.0081 | 1301.3742 |
| 1324.9831 | 1358.6361 | 1380.1672 |
| 1395.8471 | 1399.9779 | 1410.5475 |
| 1419.6821 | 1458.0085 | 1464.4781 |
| 1477.1022 | 1483.2121 | 1491.0071 |
| 1495.7038 | 1505.9936 | 1513.8616 |
| 1640.4016 | 1828.4381 | 3042.6253 |
| 3045.4907 | 3049.1964 | 3060.8354 |
| 3065.2268 | 3082.4757 | 3101.7075 |
| 3109.4310 | 3112.3807 | 3122.5950 |
| 3126.5371 | 3128.4966 | 3149.5031 |
| 3167.6484 | 3180.9227 | 3196.7191 |

Zero-point correction (Hartree): 0.247392

ApineneCI.J.b.mtt

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.15982933

Electronic state : 1-A

Cartesian coordinates (Angs):

C	0.652861	0.826488	1.025115
H	0.523567	1.602458	1.782072
C	2.176539	0.742131	0.778077
C	2.695870	0.243804	-0.512011
H	2.609964	1.732695	0.913495
H	2.585357	0.061736	1.533791
H	3.159192	0.894485	-1.247162
C	-0.398215	1.096199	-0.090476
C	-0.151942	-0.408329	1.466920
C	-0.818252	2.535902	-0.306913
C	-0.072226	0.426098	-1.417977
H	0.279661	-0.599654	-1.286421
H	-0.961188	0.406415	-2.049814
H	0.690091	0.992103	-1.958283
H	-1.704017	2.576350	-0.942524
H	-0.022800	3.104887	-0.794692
H	-1.056947	3.022652	0.639429
H	-0.223661	-0.588400	2.537424
H	0.206819	-1.303945	0.969319
C	-1.370177	0.216124	0.765380
H	-1.934413	0.866557	1.436151
C	-2.369276	-0.612367	-0.006217
C	-2.212749	-2.108681	-0.001423
H	-2.149110	-2.477897	1.023359
H	-1.272295	-2.378618	-0.487527
H	-3.045618	-2.568790	-0.524155
O	-3.245674	-0.060863	-0.629659
O	2.755969	-0.956666	-0.836338
O	2.179804	-1.868377	-0.002416

Rotational constants (GHz): 1.1919200 0.5924500 0.4964000

Vibrational harmonic frequencies (cm-1):

36.5945	44.9273	53.7753
138.3315	147.4718	161.2326
195.2771	210.7399	236.9302
258.9056	273.3566	296.5232
337.2170	355.4385	387.1931
406.7453	458.2147	485.5097
503.0908	587.7964	610.2351
632.6617	672.2410	722.9082
741.6094	861.1546	885.0608
908.8008	928.6032	943.6537
965.7720	971.5316	987.1520
1000.5212	1015.1029	1032.1788
1057.6823	1084.7832	1143.5816
1148.2713	1177.5612	1193.4640
1221.1640	1256.4972	1257.4540
1268.3271	1292.9012	1320.9986
1336.6584	1352.0963	1389.6248
1392.7716	1404.8893	1416.4360
1421.9524	1462.2090	1464.9234
1474.3587	1487.2489	1495.9854
1510.3802	1519.1944	1521.3930
1655.4810	1822.3481	3037.6611
3042.2639	3045.3955	3060.9327
3069.8743	3083.3169	3107.1974
3109.7661	3113.1818	3116.8822
3121.2542	3127.1243	3128.8589
3180.9740	3182.8044	3183.5813

Zero-point correction (Hartree): 0.247674

ApineneCI.J.b.pmm

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E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -615.23853837

E(CCSD/Aug-CC-pVTZ) (Hartree): -615.11844801

T1 diagnostic: 0.022633

E(MP2/Aug-CC-pVTZ) (Hartree): -615.04732443

E(MP3/Aug-CC-pVTZ) (Hartree): -615.10160447

E(RHF/Aug-CC-pVTZ) (Hartree): -612.61097130

E(RM062X/Aug-CC-pVTZ) (Hartree): -616.16666246

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.689883 | -0.537280 | -0.399200 |
| H | -1.182339 | -0.209285 | -1.312983 |
| C | -1.764873 | -1.053917 | 0.565866  |
| C | -2.727044 | 0.003760  | 0.916522  |
| H | -2.324770 | -1.840066 | 0.051551  |
| H | -1.312184 | -1.445687 | 1.475157  |
| H | -2.775846 | 0.488037  | 1.886725  |
| C | 0.309925  | 0.555748  | 0.067583  |

|                                                           |           |           |           |
|-----------------------------------------------------------|-----------|-----------|-----------|
| C                                                         | 0.492921  | -1.466041 | -0.718846 |
| C                                                         | -0.005880 | 1.968513  | -0.383234 |
| C                                                         | 0.594528  | 0.509680  | 1.562512  |
| H                                                         | 0.852620  | -0.492857 | 1.903924  |
| H                                                         | 1.429137  | 1.166555  | 1.815593  |
| H                                                         | -0.273951 | 0.858305  | 2.126458  |
| H                                                         | 0.812611  | 2.653640  | -0.152276 |
| H                                                         | -0.898996 | 2.340808  | 0.125311  |
| H                                                         | -0.195436 | 2.004787  | -1.455969 |
| H                                                         | 0.425924  | -2.073076 | -1.617526 |
| H                                                         | 0.768343  | -2.097492 | 0.125572  |
| C                                                         | 1.395693  | -0.226588 | -0.762818 |
| H                                                         | 1.459024  | 0.207718  | -1.761761 |
| C                                                         | 2.764849  | -0.303737 | -0.141901 |
| C                                                         | 3.664380  | 0.883848  | -0.374698 |
| H                                                         | 3.128039  | 1.807056  | -0.146983 |
| H                                                         | 3.938412  | 0.928428  | -1.430189 |
| H                                                         | 4.559297  | 0.805518  | 0.235330  |
| O                                                         | 3.104683  | -1.239382 | 0.540280  |
| O                                                         | -3.573705 | 0.445029  | 0.112917  |
| O                                                         | -3.608177 | -0.093935 | -1.135529 |
| Rotational constants (GHz): 1.7459100 0.4318400 0.4120100 |           |           |           |
| Vibrational harmonic frequencies (cm-1):                  |           |           |           |
| 33.5272                                                   | 55.2744   | 60.4412   |           |
| 108.6295                                                  | 121.4225  | 129.2470  |           |
| 156.6435                                                  | 213.9388  | 219.9430  |           |
| 263.1962                                                  | 280.8851  | 309.3467  |           |
| 316.9709                                                  | 348.8465  | 367.7393  |           |
| 381.0494                                                  | 436.8462  | 466.5936  |           |
| 531.7818                                                  | 580.6175  | 601.0893  |           |
| 623.5439                                                  | 682.2141  | 726.0588  |           |
| 776.3970                                                  | 886.6325  | 901.8792  |           |
| 909.8695                                                  | 917.5887  | 952.7428  |           |
| 959.3165                                                  | 970.3995  | 978.8304  |           |
| 999.3202                                                  | 1005.5464 | 1037.7619 |           |
| 1058.6313                                                 | 1090.0227 | 1112.4144 |           |
| 1149.5135                                                 | 1171.6894 | 1192.8084 |           |
| 1205.6009                                                 | 1212.9023 | 1253.1288 |           |
| 1265.6057                                                 | 1287.0588 | 1303.5885 |           |
| 1339.1040                                                 | 1364.7157 | 1382.9513 |           |
| 1392.4596                                                 | 1404.0936 | 1411.8435 |           |
| 1423.2922                                                 | 1455.8391 | 1464.9097 |           |
| 1476.0627                                                 | 1483.6835 | 1489.9287 |           |
| 1499.4027                                                 | 1505.2383 | 1509.5938 |           |
| 1641.6414                                                 | 1834.3915 | 3043.1660 |           |
| 3048.9701                                                 | 3060.3620 | 3062.7476 |           |
| 3087.8423                                                 | 3095.7183 | 3104.6963 |           |
| 3109.6713                                                 | 3113.5597 | 3124.5244 |           |
| 3128.9845                                                 | 3133.0799 | 3139.6768 |           |
| 3158.0374                                                 | 3179.8261 | 3186.9647 |           |
| Zero-point correction (Hartree): 0.247118                 |           |           |           |
| ApineneCI.J.b.pmp                                         |           |           |           |
| ~~~~~                                                     |           |           |           |
| E(RM062X/Aug-CC-pVTZ) (Hartree): -616.16501341            |           |           |           |
| Electronic state : 1-A                                    |           |           |           |
| Cartesian coordinates (Angs):                             |           |           |           |
| C                                                         | -0.486087 | 0.890648  | 0.816714  |
| H                                                         | -0.634779 | 0.919618  | 1.899912  |
| C                                                         | -1.805531 | 1.202804  | 0.107162  |
| C                                                         | -2.854141 | 0.271761  | 0.562678  |
| H                                                         | -2.116887 | 2.215306  | 0.383313  |
| H                                                         | -1.719152 | 1.139086  | -0.973713 |
| H                                                         | -3.130876 | 0.187917  | 1.610599  |
| C                                                         | 0.283975  | -0.411075 | 0.458027  |
| C                                                         | 0.760213  | 1.712977  | 0.446499  |
| C                                                         | 0.094540  | -1.571868 | 1.415134  |
| C                                                         | 0.059377  | -0.848261 | -0.983415 |
| H                                                         | 0.251693  | -0.039576 | -1.689356 |
| H                                                         | 0.730048  | -1.671758 | -1.236962 |
| H                                                         | -0.968863 | -1.184087 | -1.135897 |
| H                                                         | 0.783507  | -2.388003 | 1.189434  |
| H                                                         | -0.918799 | -1.972666 | 1.330159  |
| H                                                         | 0.257555  | -1.264315 | 2.449254  |
| H                                                         | 1.001723  | 2.570959  | 1.068545  |
| H                                                         | 0.758738  | 2.014159  | -0.600078 |
| C                                                         | 1.596910  | 0.440098  | 0.625643  |
| C                                                         | 1.971139  | 0.327047  | 1.645324  |
| C                                                         | 2.702268  | 0.162945  | -0.358984 |
| C                                                         | 3.542380  | -1.058831 | -0.084246 |
| H                                                         | 2.898677  | -1.922265 | 0.092415  |
| H                                                         | 4.123369  | -0.901676 | 0.826271  |
| H                                                         | 4.210401  | -1.251220 | -0.918406 |
| O                                                         | 2.881894  | 0.859380  | -1.327052 |
| O                                                         | -3.488832 | -0.516680 | -0.164275 |
| O                                                         | -3.250677 | -0.533413 | -1.505186 |
| Rotational constants (GHz): 1.5278800 0.4454200 0.4348100 |           |           |           |
| Vibrational harmonic frequencies (cm-1):                  |           |           |           |
| 31.1843                                                   | 64.2171   | 67.4959   |           |
| 80.5873                                                   | 114.3269  | 145.6952  |           |
| 158.5474                                                  | 222.0354  | 233.5496  |           |
| 249.5860                                                  | 285.7560  | 312.9251  |           |
| 322.3181                                                  | 349.5690  | 365.9628  |           |
| 383.1191                                                  | 440.8200  | 470.1714  |           |
| 515.6536                                                  | 578.8360  | 599.4440  |           |
| 623.3961                                                  | 667.0558  | 719.4512  |           |
| 774.2033                                                  | 860.0120  | 896.0282  |           |
| 911.0343                                                  | 919.3816  | 951.5575  |           |
| 961.3708                                                  | 968.3520  | 972.5705  |           |
| 1005.4347                                                 | 1016.7233 | 1046.2624 |           |
| 1053.7395                                                 | 1098.9242 | 1112.6276 |           |
| 1152.7898                                                 | 1178.2681 | 1193.8350 |           |

|           |           |           |
|-----------|-----------|-----------|
| 1205.9447 | 1214.8738 | 1249.4124 |
| 1262.0977 | 1275.6226 | 1291.4326 |
| 1327.1914 | 1368.4633 | 1391.5656 |
| 1404.9878 | 1408.0265 | 1414.0659 |
| 1434.1930 | 1463.1471 | 1464.8645 |
| 1477.6201 | 1484.8365 | 1493.8677 |
| 1500.8329 | 1509.1552 | 1510.8658 |
| 1651.5345 | 1837.1300 | 3042.7855 |
| 3048.2094 | 3051.0706 | 3054.0686 |
| 3063.7644 | 3079.6903 | 3101.0185 |
| 3108.7694 | 3117.2703 | 3120.3340 |
| 3126.4957 | 3130.1735 | 3157.9187 |
| 3164.1376 | 3176.0969 | 3179.0768 |

Zero-point correction (Hartree): 0.247039

ApineneCI.J.b.ppm

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.16322681

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-0.730055	0.536481	-0.419636
H	-0.949115	1.001039	-1.384373
C	-1.895718	0.789381	0.550305
C	-3.205452	0.565359	-0.084807
H	-1.815359	0.103909	1.396834
H	-1.860836	1.823542	0.896400
H	-3.846583	1.364247	-0.443570
C	0.686217	1.000988	0.023531
C	-0.178073	-0.882077	-0.631528
C	1.131921	2.352570	-0.498468
C	0.894188	0.901920	1.528740
H	0.601960	-0.072277	1.919816
H	1.946512	1.053036	1.777711
H	0.320429	1.673064	2.045758
H	2.177592	2.548256	-0.252809
H	0.536839	3.150634	-0.047425
H	1.018160	2.414141	-1.581396
H	-0.556003	-1.449537	-1.475993
H	-0.275007	-1.488494	0.265703
C	1.226107	-0.270732	-0.729834
H	1.490933	0.009702	-1.751407
C	2.383639	-0.976204	-0.073345
C	3.753557	-0.417973	-0.371714
H	3.757247	0.662514	-0.214879
H	3.993130	-0.587568	-1.422893
H	4.499856	-0.893520	0.257674
O	2.223735	-1.902397	0.682069
O	-3.690663	-0.566981	-0.273120
O	-2.962790	-1.644494	0.122974

Rotational constants (GHz): 1.4211500 0.4736800 0.4032900

Vibrational harmonic frequencies (cm-1):

26.2130	49.9795	70.2840
105.9966	120.7218	125.1318
159.9785	182.3673	230.0214
242.9976	288.7773	299.7015
316.5257	337.5973	364.9735
385.8949	438.6001	474.8864
532.9506	585.0909	602.4778
626.1371	670.9485	733.0943
785.9557	875.8609	907.7599
918.3382	923.4257	935.8549
958.3043	963.6245	976.9630
999.1023	1020.8167	1031.4993
1049.4311	1087.4079	1128.9345
1149.1090	1171.9326	1192.5726
1204.4902	1220.9397	1252.6133
1262.3924	1274.1489	1311.4941
1331.9864	1366.8199	1386.3669
1396.7586	1403.4202	1413.9623
1423.6245	1459.0584	1464.5284
1476.7099	1484.8785	1492.1408
1497.1123	1506.9569	1509.0602
1648.5498	1838.1181	3043.3579
3052.8143	3056.4888	3061.8190
3063.7435	3077.3130	3107.0951
3115.4701	3121.6030	3123.0596
3123.1802	3124.7418	3140.1071
3178.4829	3178.7488	3185.7006

Zero-point correction (Hartree): 0.247017

ApineneCI.J.b.ppp

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.16658235

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.745191 | -0.059769 | -0.180792 |
| H | -1.236431 | 0.419799  | -1.026970 |
| C | -1.800449 | -0.327005 | 0.901764  |
| C | -2.946118 | -1.033729 | 0.310147  |
| H | -1.381264 | -0.921374 | 1.711686  |
| H | -2.172142 | 0.631229  | 1.275023  |
| H | -3.140300 | -2.095075 | 0.424417  |
| C | 0.508893  | 0.768368  | 0.208903  |
| C | 0.169694  | -1.204492 | -0.649955 |
| C | 0.460198  | 2.236368  | -0.163540 |
| C | 0.913085  | 0.585544  | 1.665416  |
| H | 0.986525  | -0.465853 | 1.944654  |
| H | 1.887269  | 1.041854  | 1.852087  |
| H | 0.190322  | 1.072074  | 2.322484  |
| H | 1.418688  | 2.725637  | 0.022171  |
| H | -0.296718 | 2.751488  | 0.431707  |
| H | 0.203455  | 2.366305  | -1.214916 |

|                                                           |           |           |           |
|-----------------------------------------------------------|-----------|-----------|-----------|
| H                                                         | -0.107546 | -1.738733 | -1.555417 |
| H                                                         | 0.384494  | -1.922174 | 0.142053  |
| C                                                         | 1.312461  | -0.186244 | -0.752191 |
| H                                                         | 1.374260  | 0.273976  | -1.739706 |
| C                                                         | 2.684173  | -0.589201 | -0.281288 |
| C                                                         | 3.789860  | 0.401867  | -0.543121 |
| H                                                         | 3.482664  | 1.397276  | -0.216972 |
| H                                                         | 3.973495  | 0.462297  | -1.617288 |
| H                                                         | 4.698109  | 0.098624  | -0.030987 |
| O                                                         | 2.878303  | -1.623580 | 0.309326  |
| O                                                         | -3.788360 | -0.458905 | -0.409544 |
| O                                                         | -3.633008 | 0.876536  | -0.626793 |
| Rotational constants (GHz): 1.6557100 0.4224800 0.3886600 |           |           |           |
| Vibrational harmonic frequencies (cm-1):                  |           |           |           |
| 31.5588                                                   | 55.8845   | 62.8472   |           |
| 105.6609                                                  | 120.4568  | 125.7805  |           |
| 154.3166                                                  | 203.9256  | 216.5447  |           |
| 250.5500                                                  | 281.2126  | 316.3875  |           |
| 320.5063                                                  | 346.3651  | 373.8324  |           |
| 385.1458                                                  | 440.4066  | 475.5998  |           |
| 529.2733                                                  | 587.3350  | 598.9582  |           |
| 624.9812                                                  | 676.8462  | 737.0265  |           |
| 784.5201                                                  | 890.0802  | 910.3426  |           |
| 914.0189                                                  | 920.5815  | 936.1969  |           |
| 959.0151                                                  | 966.7429  | 980.4474  |           |
| 1002.0217                                                 | 1010.6440 | 1029.3490 |           |
| 1055.9290                                                 | 1089.5868 | 1127.2068 |           |
| 1146.5325                                                 | 1173.9007 | 1194.1114 |           |
| 1210.1733                                                 | 1235.8356 | 1249.5539 |           |
| 1263.2378                                                 | 1279.2435 | 1305.5949 |           |
| 1336.6886                                                 | 1366.4297 | 1385.2716 |           |
| 1392.9872                                                 | 1404.1140 | 1413.1456 |           |
| 1424.8484                                                 | 1459.9225 | 1464.8102 |           |
| 1476.8242                                                 | 1486.0380 | 1491.6823 |           |
| 1500.9931                                                 | 1509.2902 | 1510.9583 |           |
| 1642.2631                                                 | 1833.9351 | 3047.4475 |           |
| 3053.5541                                                 | 3060.2748 | 3063.4897 |           |
| 3086.3925                                                 | 3090.1612 | 3104.6665 |           |
| 3112.3444                                                 | 3117.7035 | 3125.7304 |           |
| 3129.1529                                                 | 3132.9448 | 3139.8289 |           |
| 3149.4327                                                 | 3178.7486 | 3191.3308 |           |
| Zero-point correction (Hartree): 0.247272                 |           |           |           |
| ApineneCI.J.b.ptm                                         |           |           |           |
| ~~~~~                                                     |           |           |           |
| E(RM062X/Aug-CC-pVTZ) (Hartree): -616.16438308            |           |           |           |
| Electronic state : 1-A                                    |           |           |           |
| Cartesian coordinates (Angs):                             |           |           |           |
| C                                                         | 0.485737  | 0.342502  | 1.320860  |
| H                                                         | 0.379668  | 1.048129  | 2.146752  |
| C                                                         | 1.986695  | 0.094543  | 1.144620  |
| C                                                         | 2.337682  | -0.997413 | 0.216648  |
| H                                                         | 2.495814  | 0.995773  | 0.810611  |
| H                                                         | 2.393926  | -0.202176 | 2.117574  |
| H                                                         | 2.058092  | -2.031243 | 0.396146  |
| C                                                         | -0.370338 | 0.867597  | 0.136799  |
| C                                                         | -0.519696 | -0.807304 | 1.520586  |
| C                                                         | -0.542897 | 2.372136  | 0.075539  |
| C                                                         | 0.075691  | 0.319775  | -1.211949 |
| H                                                         | 0.105809  | -0.771149 | -1.223747 |
| H                                                         | -0.621950 | 0.625586  | -1.994292 |
| H                                                         | 1.063999  | 0.705990  | -1.475155 |
| H                                                         | -1.272030 | 2.656728  | -0.685427 |
| H                                                         | 0.405000  | 2.847447  | -0.185724 |
| H                                                         | -0.875695 | 2.772127  | 1.034311  |
| H                                                         | -0.757529 | -1.099558 | 2.540269  |
| H                                                         | -0.282436 | -1.698065 | 0.940296  |
| C                                                         | -1.552290 | 0.034590  | 0.758853  |
| H                                                         | -2.136907 | 0.677058  | 1.420229  |
| C                                                         | -2.461010 | -0.661378 | -0.219160 |
| C                                                         | -3.517491 | 0.196724  | -0.866913 |
| H                                                         | -3.061890 | 1.099983  | -1.276640 |
| H                                                         | -4.237957 | 0.516889  | -0.112226 |
| H                                                         | -4.025586 | -0.357993 | -1.649933 |
| O                                                         | -2.324273 | -1.827998 | -0.495508 |
| O                                                         | 3.016536  | -0.857875 | -0.819311 |
| O                                                         | 3.412383  | 0.391352  | -1.192474 |
| Rotational constants (GHz): 1.3348900 0.4898800 0.4716100 |           |           |           |
| Vibrational harmonic frequencies (cm-1):                  |           |           |           |
| 47.7118                                                   | 61.7033   | 76.9927   |           |
| 87.9550                                                   | 113.7182  | 145.1694  |           |
| 191.1389                                                  | 202.5103  | 235.3269  |           |
| 244.8302                                                  | 285.1983  | 313.7565  |           |
| 341.5690                                                  | 346.6850  | 373.8228  |           |
| 386.8421                                                  | 436.4565  | 463.6221  |           |
| 571.3090                                                  | 584.5514  | 604.6660  |           |
| 625.7263                                                  | 671.6497  | 716.2864  |           |
| 764.1562                                                  | 855.7034  | 894.0117  |           |
| 906.6591                                                  | 921.3243  | 950.2845  |           |
| 955.4235                                                  | 969.9764  | 974.3774  |           |
| 996.5139                                                  | 1004.8707 | 1023.7327 |           |
| 1054.8716                                                 | 1120.1285 | 1134.9645 |           |
| 1154.0352                                                 | 1172.8511 | 1194.4216 |           |
| 1206.8816                                                 | 1217.2971 | 1254.0125 |           |
| 1264.2011                                                 | 1291.9279 | 1301.4221 |           |
| 1334.4161                                                 | 1369.7240 | 1386.4784 |           |
| 1401.6665                                                 | 1410.3031 | 1421.7574 |           |
| 1431.5588                                                 | 1457.3670 | 1464.5889 |           |
| 1476.9684                                                 | 1488.5408 | 1495.9789 |           |
| 1501.3099                                                 | 1514.4962 | 1521.8233 |           |
| 1650.5545                                                 | 1834.0852 | 3040.6829 |           |
| 3040.7228                                                 | 3046.7456 | 3063.2472 |           |

|           |           |           |
|-----------|-----------|-----------|
| 3075.2969 | 3081.0402 | 3098.4461 |
| 3109.1976 | 3115.3708 | 3120.6583 |
| 3121.7529 | 3125.7281 | 3149.1046 |
| 3153.4363 | 3179.4798 | 3182.8549 |

Zero-point correction (Hartree): 0.247360

ApineneCI.J.b.ptp

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.16396722

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-0.689014	0.796460	-0.752123
H	-0.670930	1.359973	-1.685922
C	-2.017356	1.128582	-0.046171
C	-2.446758	0.099538	0.915053
H	-1.927508	2.085667	0.468990
H	-2.808293	1.179238	-0.797453
H	-2.350609	0.174870	1.992700
C	0.650564	1.052878	-0.009819
C	-0.240397	-0.649839	-1.022665
C	1.311088	2.390498	-0.280629
C	0.559636	0.787350	1.487217
H	0.145682	-0.197978	1.704250
H	1.549908	0.826499	1.945306
H	-0.054322	1.549512	1.972680
H	2.305706	2.441465	0.166908
H	0.717882	3.202371	0.147593
H	1.408224	2.570999	-1.351583
H	-0.499727	-1.080769	-1.983684
H	-0.545116	-1.342015	-0.239576
C	1.207714	-0.192585	-0.794165
H	1.686247	0.152721	-1.712398
C	2.146814	-1.081445	-0.022710
C	3.602511	-0.686764	-0.046127
H	3.703524	0.372261	0.200021
H	3.997149	-0.817017	-1.055267
H	4.170159	-1.293392	0.653110
O	1.751766	-2.023840	0.618765
O	-2.998680	-0.957528	0.545746
O	-3.170183	-1.150187	-0.788615

Rotational constants (GHz): 1.2901100 0.5427300 0.4617000

Vibrational harmonic frequencies (cm-1):

43.0535	61.8029	66.6285
112.6215	121.2807	144.9117
176.6413	199.7495	232.2781
244.6697	287.9600	328.4508
333.6363	344.7622	377.7557
387.2944	439.4457	465.7948
574.1101	589.2406	614.5093
626.2223	676.9458	726.8096
773.9602	880.5924	902.9411
916.2317	921.7919	945.1374
959.2373	967.2196	975.3594
992.8709	1001.1695	1035.6510
1054.3239	1067.1719	1137.8811
1147.0515	1171.2350	1195.1644
1205.0458	1226.5337	1250.8275
1263.5158	1295.9524	1296.7611
1335.0967	1365.9133	1378.7134
1396.9434	1402.4646	1414.6785
1422.0080	1459.0371	1464.0488
1475.5778	1486.1215	1491.0201
1493.3855	1507.0546	1511.0198
1639.1608	1835.0629	3043.1959
3047.6966	3061.4635	3062.6580
3081.9264	3083.5386	3106.3285
3111.0366	3116.9482	3122.7539
3123.2396	3125.5327	3130.3629
3178.9284	3179.1532	3195.7500

Zero-point correction (Hartree): 0.247427

ApineneCI.J.b.tpm

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.16313552

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.664388 | 1.001856  | -0.652678 |
| H | -0.654769 | 1.722420  | -1.471725 |
| C | -2.013535 | 1.108963  | 0.097704  |
| C | -2.970021 | 0.142358  | -0.463853 |
| H | -1.886137 | 0.849984  | 1.147354  |
| H | -2.422259 | 2.113285  | 0.000053  |
| H | -3.641920 | 0.358156  | -1.289027 |
| C | 0.666803  | 1.137880  | 0.147940  |
| C | -0.184010 | -0.368813 | -1.176260 |
| C | 1.348136  | 2.490567  | 0.115753  |
| C | 0.556836  | 0.617369  | 1.574277  |
| H | -0.007009 | -0.315965 | 1.628240  |
| H | 1.553320  | 0.456340  | 1.987408  |
| H | 0.052277  | 1.349007  | 2.207817  |
| H | 2.357997  | 2.409970  | 0.520859  |
| H | 0.796385  | 3.217212  | 0.716346  |
| H | 1.421548  | 2.871025  | -0.903907 |
| H | -0.394593 | -0.602864 | -2.218131 |
| H | -0.539533 | -1.176516 | -0.539322 |
| C | 1.250183  | 0.059420  | -0.825194 |
| H | 1.737093  | 0.565269  | -1.660276 |
| C | 2.254270  | -0.896368 | -0.226365 |
| C | 1.832210  | -2.319221 | 0.021262  |
| H | 1.458140  | -2.765334 | -0.901842 |
| H | 1.004967  | -2.340978 | 0.734194  |
| H | 2.671269  | -2.889878 | 0.407084  |



|                                          |           |           |           |           |
|------------------------------------------|-----------|-----------|-----------|-----------|
| O                                        | 3.354980  | -0.493270 | 0.067288  |           |
| O                                        | -3.074185 | -1.031024 | -0.053415 |           |
| O                                        | -2.276507 | -1.433855 | 0.981048  |           |
| Rotational constants (GHz):              | 1.2134700 |           | 0.5743700 | 0.4666700 |
| Vibrational harmonic frequencies (cm-1): |           |           |           |           |
| 41.5594                                  | 45.6933   |           |           | 62.0044   |
| 125.9187                                 | 151.0193  |           |           | 156.6934  |
| 194.0068                                 | 198.1011  |           |           | 236.7413  |
| 275.3406                                 | 281.4104  |           |           | 314.3748  |
| 336.4362                                 | 357.0366  |           |           | 374.2624  |
| 415.7098                                 | 454.1262  |           |           | 487.8269  |
| 515.6859                                 | 556.2868  |           |           | 599.9460  |
| 624.3534                                 | 661.4780  |           |           | 730.0099  |
| 762.3292                                 | 879.5646  |           |           | 896.1838  |
| 903.8408                                 | 918.5804  |           |           | 923.4246  |
| 965.9387                                 | 969.5419  |           |           | 995.4446  |
| 1006.9989                                | 1020.1906 |           |           | 1043.4749 |
| 1055.0441                                | 1078.1502 |           |           | 1125.2241 |
| 1156.9314                                | 1178.3826 |           |           | 1195.9233 |
| 1224.2204                                | 1259.3825 |           |           | 1262.0057 |
| 1274.7148                                | 1283.3275 |           |           | 1303.6644 |
| 1326.7889                                | 1357.8153 |           |           | 1383.7208 |
| 1392.5745                                | 1400.8560 |           |           | 1407.0317 |
| 1421.5592                                | 1464.1495 |           |           | 1467.9886 |
| 1474.7700                                | 1487.6055 |           |           | 1493.8689 |
| 1505.1086                                | 1515.5432 |           |           | 1519.1107 |
| 1644.7298                                | 1824.0201 |           |           | 3045.7709 |
| 3050.9636                                | 3061.4734 |           |           | 3077.6189 |
| 3088.9445                                | 3093.6616 |           |           | 3094.0062 |
| 3115.0586                                | 3118.8038 |           |           | 3121.5183 |
| 3127.2488                                | 3131.1221 |           |           | 3154.1290 |
| 3156.7030                                | 3181.8681 |           |           | 3184.8859 |
| Zero-point correction (Hartree):         | 0.247795  |           |           |           |

Population analysis as 298K (%)

Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)

| Compound                     | Qtot      | Erel | Erel2 | n*Q*MB    | %        |
|------------------------------|-----------|------|-------|-----------|----------|
| ApineneCI.J.b.14Hshift.ppcdu | 3.091e+44 | 0.00 | 0.00  | 3.091e+44 | 28.6     |
| ApineneCI.J.b.14Hshift.pmcdu | 5.175e+44 | 0.60 | 0.60  | 1.866e+44 | 17.3     |
| ApineneCI.J.b.14Hshift.pmcud | 2.750e+44 | 0.35 | 0.35  | 1.528e+44 | 14.1     |
| ApineneCI.J.b.14Hshift.ppcud | 2.916e+44 | 0.51 | 0.51  | 1.241e+44 | 11.5     |
| ApineneCI.J.b.14Hshift.ptcud | 1.546e+44 | 0.29 | 0.29  | 9.496e+43 | 8.79     |
| ApineneCI.J.b.14Hshift.ptcdu | 1.648e+44 | 0.40 | 0.40  | 8.397e+43 | 7.77     |
| ApineneCI.J.b.14Hshift.mmcdu | 5.270e+44 | 1.74 | 1.74  | 2.787e+43 | 2.58     |
| ApineneCI.J.b.14Hshift.mmcud | 3.883e+44 | 1.56 | 1.56  | 2.765e+43 | 2.56     |
| ApineneCI.J.b.14Hshift.mpcdu | 4.063e+44 | 1.64 | 1.64  | 2.535e+43 | 2.35     |
| ApineneCI.J.b.14Hshift.mpcud | 8.536e+44 | 2.09 | 2.09  | 2.487e+43 | 2.3      |
| ApineneCI.J.b.14Hshift.pppuu | 1.725e+44 | 1.85 | 1.85  | 7.532e+42 | 0.697    |
| ApineneCI.J.b.14Hshift.mtcud | 2.692e+44 | 2.36 | 2.36  | 4.967e+42 | 0.46     |
| ApineneCI.J.b.14Hshift.pmmdd | 2.292e+44 | 2.33 | 2.33  | 4.496e+42 | 0.416    |
| ApineneCI.J.b.14Hshift.mtcdu | 2.086e+44 | 2.35 | 2.35  | 3.915e+42 | 0.362    |
| ApineneCI.J.b.14Hshift.ptpuu | 1.229e+44 | 2.98 | 2.98  | 7.998e+41 | 0.074    |
| ApineneCI.J.b.14Hshift.pmmud | 1.939e+44 | 3.42 | 3.42  | 6.051e+41 | 0.056    |
| ApineneCI.J.b.14Hshift.mmmdd | 3.036e+44 | 3.75 | 3.75  | 5.378e+41 | 0.0498   |
| ApineneCI.J.b.14Hshift.mppuu | 2.769e+44 | 3.85 | 3.85  | 4.191e+41 | 0.0388   |
| ApineneCI.J.b.14Hshift.mtpuu | 1.315e+44 | 3.72 | 3.72  | 2.473e+41 | 0.0229   |
| ApineneCI.J.b.14Hshift.ppmdd | 1.191e+44 | 6.21 | 6.21  | 3.325e+39 | 0.000308 |
| ApineneCI.J.b.14Hshift.mpmdu | 1.172e+44 | 6.45 | 6.45  | 2.183e+39 | 0.000202 |
| Total                        |           |      |       | 1.081e+45 | 100      |

ApineneCI.J.b.14Hshift.mmcdu

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.13578293

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-0.479337	-0.079192	-1.081072
H	-0.537704	0.390480	-2.067309
C	-1.835287	-0.533458	-0.618594
C	-2.806440	0.429013	-0.307768
H	-2.772119	1.497909	-0.496120
O	-3.751842	0.083015	0.490122
O	-3.583243	-1.243111	0.855734
H	-2.244939	-1.157175	0.475861
H	-2.235769	-1.412594	-1.129044
C	0.396904	0.831954	-0.161789
C	0.660351	-1.118162	-1.094058
C	0.401443	2.315081	-0.475415
C	0.133984	0.596803	1.319699
H	0.142496	-0.464370	1.575711
H	0.893811	1.098711	1.916512
H	-0.843390	0.991437	1.604157
H	1.199543	2.812598	0.077090
H	-0.545071	2.779337	-0.186566
H	0.557991	2.493305	-1.540479
H	0.858150	-1.641251	-2.026846
H	0.525529	-1.849379	-0.296842
C	1.616176	0.015600	-0.677969
H	2.025373	0.503305	-1.568184
C	2.779359	-0.224859	0.251006
C	3.376888	-1.607844	0.271463
H	3.511792	-1.982039	-0.744256
H	2.684355	-2.287935	0.771700
H	4.321602	-1.597160	0.806571
O	3.209347	0.669496	0.938523

Rotational constants (GHz):	1.5315800	0.4249800	0.3954700
Vibrational harmonic frequencies (cm-1):			
i1613.7541	24.0830		35.9575
62.0649	85.0201		141.8867
160.3564	169.2018		226.9746
233.1393	271.8733		301.1695

311.2203	333.8412	344.5708
405.5130	426.6750	488.1069
505.3364	531.8632	588.0660
623.4685	651.7595	715.8542
740.3148	790.5772	852.9434
893.5119	924.6657	950.3161
962.6482	970.0848	977.4293
988.7529	1013.4572	1022.7976
1035.9950	1102.3706	1119.2319
1139.8576	1178.6005	1188.5037
1194.6194	1227.3216	1244.8905
1253.4668	1280.1262	1290.4037
1314.2974	1338.6835	1353.7883
1383.8679	1393.4190	1405.2237
1419.9059	1424.0436	1464.0991
1476.0223	1479.3864	1493.8988
1498.3110	1503.9855	1512.2192
1602.4197	1829.1499	1855.4783
3042.1702	3045.6159	3053.5360
3056.2667	3063.4288	3086.5514
3087.0081	3109.2501	3117.0186
3125.3499	3126.9228	3143.8128
3145.8594	3181.4069	3183.2619

Zero-point correction (Hartree): 0.242161

ApineneCI.J.b.14Hshift.mmcud

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E(RM062X/Aug-CC-pVT2) (Hartree): -616.13631770

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.545823 | -0.067503 | -0.691424 |
| H | -0.746500 | 0.266338  | -1.712187 |
| C | -1.836321 | -0.328037 | 0.028083  |
| C | -2.943704 | 0.494880  | -0.231849 |
| H | -2.971485 | 1.413712  | -0.809358 |
| O | -4.107360 | 0.023846  | 0.033789  |
| O | -3.980213 | -1.251584 | 0.558784  |
| H | -2.690114 | -1.329283 | -0.009757 |
| H | -1.739373 | -0.602615 | 1.081505  |
| C | 0.540428  | 0.876203  | -0.077109 |
| C | 0.504171  | -1.196722 | -0.738144 |
| C | 0.564419  | 2.298078  | -0.600997 |
| C | 0.525197  | 0.866548  | 1.445337  |
| H | 0.541112  | -0.146797 | 1.852650  |
| H | 1.395259  | 1.393507  | 1.832319  |
| H | -0.374745 | 1.361007  | 1.815087  |
| H | 1.456153  | 2.817945  | -0.248463 |
| H | -0.309875 | 2.852401  | -0.250369 |
| H | 0.565646  | 2.316357  | -1.692104 |
| H | 0.493558  | -1.862806 | -1.597537 |
| H | 0.470375  | -1.793765 | 0.173675  |
| C | 1.590388  | -0.104861 | -0.666571 |
| H | 1.857020  | 0.214325  | -1.679487 |
| C | 2.889274  | -0.335299 | 0.062594  |
| C | 3.444980  | -1.736173 | 0.042346  |
| H | 3.408788  | -2.144749 | -0.968541 |
| H | 2.821575  | -2.378950 | 0.666889  |
| H | 4.462602  | -1.739380 | 0.421027  |
| O | 3.457816  | 0.572745  | 0.618809  |

Rotational constants (GHz): 1.6595500 0.3883200 0.3514100

Vibrational harmonic frequencies (cm-1):

|            |           |           |
|------------|-----------|-----------|
| i1599.1018 | 33.0923   | 40.2541   |
| 57.8460    | 90.8543   | 135.7221  |
| 155.7714   | 182.0036  | 223.8941  |
| 247.4004   | 264.3860  | 286.4487  |
| 316.8238   | 327.7822  | 331.7429  |
| 412.1813   | 421.9463  | 492.2177  |
| 517.0993   | 535.2110  | 577.1354  |
| 616.9774   | 635.5958  | 728.7972  |
| 749.2892   | 797.3265  | 876.0145  |
| 895.0151   | 921.0019  | 954.4689  |
| 963.4048   | 968.5134  | 977.6469  |
| 987.1587   | 1011.2898 | 1027.8938 |
| 1039.3572  | 1101.9858 | 1114.7054 |
| 1163.5875  | 1178.7413 | 1192.3307 |
| 1198.3381  | 1226.1584 | 1242.7460 |
| 1253.3767  | 1274.4954 | 1287.1441 |
| 1312.2456  | 1337.9064 | 1356.1927 |
| 1388.9196  | 1394.6115 | 1406.0409 |
| 1418.3452  | 1446.1471 | 1465.2917 |
| 1477.6632  | 1483.9919 | 1494.4968 |
| 1499.7225  | 1507.1332 | 1514.5291 |
| 1602.5767  | 1830.2263 | 1853.2670 |
| 3043.1083  | 3049.7570 | 3053.5018 |
| 3062.7314  | 3063.9268 | 3085.1487 |
| 3087.4606  | 3110.2560 | 3115.7495 |
| 3125.4888  | 3126.7664 | 3144.7439 |
| 3148.8281  | 3181.1760 | 3186.6614 |

Zero-point correction (Hartree): 0.242415

ApineneCI.J.b.14Hshift.mmmdd

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E(RM062X/Aug-CC-pVT2) (Hartree): -616.13333100

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-0.695446	-0.354161	-0.142907
H	-1.132877	-0.450901	-1.134690
C	-1.803139	-0.318604	0.908189
C	-2.973785	0.431043	0.699461
H	-3.384491	1.227340	1.312114
O	-3.812251	-0.001455	-0.175241
O	-3.347178	-1.190847	-0.721494

H	-2.493028	-1.311733	0.341606
H	-1.415511	-0.216038	1.916450
C	0.367817	0.788890	-0.177729
C	0.435407	-1.382463	0.026133
C	0.118975	1.885834	-1.191945
C	0.649136	1.381956	1.195423
H	0.861440	0.614853	1.943104
H	1.508854	2.047355	1.149382
H	-0.215636	1.954199	1.537618
H	0.982264	2.549395	-1.258321
H	-0.747415	2.485391	-0.900318
H	-0.075824	1.470808	-2.181626
H	0.335748	-2.334635	-0.489392
H	0.647824	-1.566530	1.080104
C	1.384466	-0.319793	-0.567897
H	1.408955	-0.423257	-1.657574
C	2.818951	-0.220309	-0.117101
C	3.522354	-1.517916	0.191172
H	3.341872	-2.244169	-0.602605
H	3.110324	-1.942136	1.108652
H	4.586899	-1.344627	0.316558
O	3.375952	0.847030	-0.030496

Rotational constants (GHz): 1.6774200 0.4271400 0.3882000
 Vibrational harmonic frequencies (cm-1):

i1607.5421	31.6734	37.5218
67.2982	124.2179	128.4707
140.4217	174.9084	211.5288
229.7190	272.8788	291.6202
315.0288	322.8009	366.1435
403.2406	415.9314	501.9242
517.6866	564.9061	604.9248
620.0604	671.0730	734.3623
786.3232	828.3530	893.1255
913.2493	925.9375	955.7234
965.2454	968.8645	978.1350
993.0682	1010.8558	1023.1964
1035.5020	1076.1942	1115.5298
1125.9906	1164.1718	1182.1769
1194.4587	1233.5111	1243.4308
1252.3399	1285.6250	1309.0577
1317.6075	1334.3922	1341.9728
1366.2592	1393.2395	1405.3725
1416.0684	1431.0781	1463.7208
1476.7245	1482.2886	1492.8979
1500.0361	1505.5226	1514.0900
1570.6957	1830.1438	1858.8619
3042.0888	3050.6611	3054.1063
3065.3057	3082.7134	3109.2946
3112.7071	3117.2416	3126.8844
3127.4971	3146.2981	3150.4521
3163.3871	3180.6130	3188.0847

 Zero-point correction (Hartree): 0.242914

ApineneCI.J.b.14Hshift.mpcdu
 ~~~~~  
 E(RM062X/Aug-CC-pVTZ) (Hartree): -616.13615197  
 Electronic state : 1-A  
 Cartesian coordinates (Angs):  

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.536329  | -0.268775 | 0.662857  |
| H | 0.739354  | -0.171379 | 1.732314  |
| C | 1.825176  | -0.333675 | -0.102169 |
| C | 2.978238  | -0.822152 | 0.531575  |
| H | 3.052996  | -1.306036 | 1.500318  |
| O | 4.114268  | -0.477169 | 0.045094  |
| O | 3.916354  | 0.329549  | -1.063100 |
| H | 2.606974  | 0.600660  | -0.595155 |
| H | 1.737076  | -0.647300 | -1.145638 |
| C | -0.513230 | 0.822078  | 0.277822  |
| C | -0.550485 | -1.346521 | 0.450208  |
| C | -0.492525 | 2.091194  | 1.104104  |
| C | -0.482889 | 1.148164  | -1.210014 |
| H | -0.521023 | 0.250225  | -1.830925 |
| H | -1.335915 | 1.770514  | -1.473679 |
| H | 0.432105  | 1.688013  | -1.457456 |
| H | -1.354869 | 2.714113  | 0.863478  |
| H | 0.413143  | 2.665801  | 0.898211  |
| H | -0.518513 | 1.866530  | 2.171641  |
| H | -0.572114 | -2.190182 | 1.136817  |
| H | -0.529448 | -1.723434 | -0.572768 |
| C | -1.600170 | -0.231551 | 0.628411  |
| H | -1.865209 | -0.141054 | 1.686915  |
| C | -2.899202 | -0.245054 | -0.136193 |
| C | -3.493597 | -1.593708 | -0.453338 |
| H | -3.470729 | -2.236826 | 0.427550  |
| H | -2.887624 | -2.081726 | -1.219223 |
| H | -4.510158 | -1.476708 | -0.816521 |
| O | -3.438361 | 0.784969  | -0.460176 |

 Rotational constants (GHz): 1.6698900 0.3840300 0.3567600  
 Vibrational harmonic frequencies (cm-1):  

|            |           |           |
|------------|-----------|-----------|
| i1581.3815 | 29.5027   | 42.8678   |
| 58.3091    | 94.5687   | 134.5011  |
| 153.7173   | 181.8369  | 224.6124  |
| 243.2697   | 265.6131  | 293.5799  |
| 307.0860   | 314.4807  | 337.2386  |
| 402.7869   | 421.6162  | 498.1543  |
| 526.1871   | 530.1132  | 568.3945  |
| 614.5264   | 638.6664  | 728.6645  |
| 743.3258   | 817.4898  | 871.1322  |
| 897.9710   | 920.1936  | 948.0616  |
| 964.7948   | 967.2972  | 980.0854  |
| 982.9418   | 1008.8694 | 1029.2565 |
| 1040.1390  | 1101.4856 | 1114.3863 |

|           |           |           |
|-----------|-----------|-----------|
| 1162.4031 | 1178.9845 | 1190.0735 |
| 1202.1390 | 1221.4570 | 1242.8874 |
| 1252.0536 | 1272.5590 | 1288.9106 |
| 1312.4020 | 1337.9737 | 1356.2272 |
| 1388.7400 | 1393.3697 | 1405.2568 |
| 1417.0529 | 1446.6127 | 1464.7236 |
| 1477.1784 | 1484.5364 | 1494.5645 |
| 1499.0125 | 1507.5076 | 1513.8956 |
| 1604.0720 | 1830.7214 | 1854.7284 |
| 3046.4624 | 3050.9012 | 3054.9951 |
| 3060.4944 | 3063.9393 | 3083.2567 |
| 3083.9752 | 3115.3298 | 3119.0097 |
| 3125.4035 | 3127.5224 | 3139.9656 |
| 3149.1594 | 3181.3062 | 3190.2096 |

Zero-point correction (Hartree): 0.242374

ApineneCI.J.b.14Hshift.mpcud

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.13540258

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-0.528086	0.363347	-0.953159
H	-0.528236	0.798191	-1.956013
C	-1.917312	0.360079	-0.379344
C	-2.747814	-0.744506	-0.616554
H	-2.573106	-1.578872	-1.288426
O	-3.721630	-0.941703	0.197131
O	-3.722003	0.052213	1.162019
H	-2.367655	0.308861	0.856834
H	-2.446518	1.315710	-0.412060
C	0.628344	1.038622	-0.148807
C	0.286427	-0.947853	-0.973160
C	0.996794	2.450730	-0.555810
C	0.429045	0.946544	1.357536
H	0.164951	-0.063479	1.677951
H	1.343400	1.239041	1.871753
H	-0.374476	1.612513	1.674673
H	1.924500	2.752772	-0.068224
H	0.213331	3.153268	-0.263218
H	1.136640	2.525762	-1.635311
H	0.269228	-1.547256	-1.881343
H	0.027015	-1.582203	-0.124087
C	1.540923	-0.101034	-0.689813
H	1.997814	0.219628	-1.630664
C	2.661983	-0.605542	0.184205
C	2.827179	-2.097257	0.318978
H	2.745863	-2.583267	-0.654129
H	2.019237	-2.489593	0.940319
H	3.781222	-2.324540	0.784883
O	3.393869	0.172577	0.746178

Rotational constants (GHz): 1.3864200 0.4318800 0.3901500

Vibrational harmonic frequencies (cm-1):

i1583.9627	18.2747	30.0691
54.0294	99.6414	141.1764
160.8633	168.3543	215.3541
238.7640	277.4361	309.0184
313.0756	321.8400	336.6835
402.4135	434.4825	493.8439
505.5328	534.8219	587.5362
621.5408	651.6518	725.4677
734.7748	811.4824	873.6672
892.4368	923.4343	931.9993
966.0397	966.5819	979.1818
987.6388	1005.9382	1025.6796
1041.0081	1064.6619	1131.8405
1164.6460	1174.4275	1187.5782
1199.0993	1225.4015	1245.4012
1253.8050	1281.5986	1301.6179
1319.6035	1341.7368	1355.3325
1387.9149	1394.6327	1407.8654
1416.5624	1424.2740	1464.2544
1476.8405	1482.4465	1494.3074
1498.8883	1506.3268	1513.4625
1607.8693	1829.9189	1862.6336
3046.7818	3053.9926	3056.4214
3060.1904	3062.6487	3077.1483
3084.6654	3115.4818	3120.1214
3124.6043	3128.1274	3134.6652
3144.1147	3181.7457	3189.1067

Zero-point correction (Hartree): 0.242343

ApineneCI.J.b.14Hshift.mpmdu

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.12940132

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.719905 | 0.836065  | -0.715957 |
| H | -0.703369 | 1.539953  | -1.551210 |
| C | -2.138412 | 0.933637  | -0.117099 |
| C | -3.133442 | -0.003622 | -0.437863 |
| H | -4.080867 | 0.161311  | -0.942365 |
| O | -3.077000 | -1.162783 | 0.120679  |
| O | -2.010583 | -1.194584 | 1.017350  |
| H | -1.948915 | 0.144919  | 0.959364  |
| H | -2.517806 | 1.948441  | -0.180995 |
| C | 0.557518  | 1.111878  | 0.127378  |
| C | -0.099683 | -0.483767 | -1.210894 |
| C | 1.087923  | 2.531412  | 0.103585  |
| C | 0.475883  | 0.599311  | 1.557974  |
| H | 0.146653  | -0.438703 | 1.610290  |
| H | 1.455121  | 0.673938  | 2.031861  |
| H | -0.225981 | 1.203224  | 2.136064  |

|                                                           |           |           |           |
|-----------------------------------------------------------|-----------|-----------|-----------|
| H                                                         | 2.094578  | 2.562886  | 0.522787  |
| H                                                         | 0.450258  | 3.191498  | 0.696253  |
| H                                                         | 1.131725  | 2.919125  | -0.915217 |
| H                                                         | -0.259862 | -0.737277 | -2.257212 |
| H                                                         | -0.381142 | -1.323704 | -0.583207 |
| C                                                         | 1.274479  | 0.095926  | -0.823197 |
| H                                                         | 1.727526  | 0.644001  | -1.651161 |
| C                                                         | 2.357701  | -0.747057 | -0.195005 |
| C                                                         | 2.120282  | -2.225883 | -0.041541 |
| H                                                         | 1.822657  | -2.662348 | -0.996231 |
| H                                                         | 1.292419  | -2.392318 | 0.651243  |
| H                                                         | 3.018156  | -2.705543 | 0.335851  |
| O                                                         | 3.373180  | -0.219734 | 0.193170  |
| Rotational constants (GHz): 1.2814600 0.5616700 0.4692700 |           |           |           |
| Vibrational harmonic frequencies (cm-1):                  |           |           |           |
| i1631.5625                                                | 37.1636   |           | 45.4437   |
| 76.9852                                                   | 129.0303  |           | 149.3306  |
| 185.8998                                                  | 195.6551  |           | 206.1685  |
| 242.3451                                                  | 267.1851  |           | 288.9034  |
| 327.3324                                                  | 329.7312  |           | 348.9035  |
| 413.0237                                                  | 457.9692  |           | 492.8499  |
| 522.9287                                                  | 533.0235  |           | 594.2469  |
| 621.5155                                                  | 718.6946  |           | 728.5321  |
| 748.8961                                                  | 822.3056  |           | 885.9610  |
| 916.0758                                                  | 930.6469  |           | 942.3579  |
| 965.2595                                                  | 971.6174  |           | 973.8935  |
| 998.3471                                                  | 1006.6218 |           | 1025.9037 |
| 1043.4751                                                 | 1057.2424 |           | 1105.9745 |
| 1140.9762                                                 | 1175.6206 |           | 1191.5470 |
| 1198.5541                                                 | 1228.0342 |           | 1255.8357 |
| 1256.9065                                                 | 1285.3171 |           | 1307.3809 |
| 1317.0704                                                 | 1330.4025 |           | 1348.6833 |
| 1368.5549                                                 | 1390.4956 |           | 1405.4121 |
| 1414.5096                                                 | 1419.5403 |           | 1465.5744 |
| 1474.4064                                                 | 1486.6502 |           | 1493.1684 |
| 1503.2636                                                 | 1510.0958 |           | 1515.9377 |
| 1569.9540                                                 | 1824.0586 |           | 1873.5859 |
| 3044.7796                                                 | 3056.6045 |           | 3058.7279 |
| 3061.4467                                                 | 3084.2618 |           | 3101.6661 |
| 3113.9897                                                 | 3121.8834 |           | 3124.1062 |
| 3127.2800                                                 | 3139.4018 |           | 3153.6878 |
| 3177.6869                                                 | 3181.7646 |           | 3182.4625 |
| Zero-point correction (Hartree): 0.243283                 |           |           |           |
| ApineneCI.J.b.14Hshift.mppuu                              |           |           |           |
| ~~~~~                                                     |           |           |           |
| E(RM062X/Aug-CC-pVTZ) (Hartree): -616.13313223            |           |           |           |
| Electronic state : 1-A                                    |           |           |           |
| Cartesian coordinates (Angs):                             |           |           |           |
| C                                                         | -0.693116 | -0.345273 | -0.232608 |
| H                                                         | -1.135597 | -0.188168 | -1.214197 |
| C                                                         | -1.800561 | -0.588904 | 0.796595  |
| C                                                         | -3.020960 | -1.159816 | 0.402901  |
| H                                                         | -3.505712 | -2.053950 | 0.781140  |
| O                                                         | -3.801788 | -0.446517 | -0.330279 |
| O                                                         | -3.234732 | 0.805183  | -0.538942 |
| H                                                         | -2.402154 | 0.569558  | 0.532637  |
| H                                                         | -1.426812 | -0.980904 | 1.736461  |
| C                                                         | 0.343330  | 0.782523  | 0.030380  |
| C                                                         | 0.460624  | -1.363717 | -0.337377 |
| C                                                         | 0.073680  | 2.105778  | -0.656723 |
| C                                                         | 0.605887  | 0.988643  | 1.516731  |
| H                                                         | 0.850559  | 0.054703  | 2.027595  |
| H                                                         | 1.439084  | 1.673260  | 1.661436  |
| H                                                         | -0.280865 | 1.410084  | 1.993443  |
| H                                                         | 0.931665  | 2.771002  | -0.550462 |
| H                                                         | -0.797670 | 2.594699  | -0.215764 |
| H                                                         | -0.127027 | 1.962246  | -1.719208 |
| H                                                         | 0.377735  | -2.149386 | -1.085414 |
| H                                                         | 0.685338  | -1.813179 | 0.630482  |
| C                                                         | 1.384467  | -0.162050 | -0.632188 |
| H                                                         | 1.408606  | 0.023391  | -1.710992 |
| C                                                         | 2.816929  | -0.155003 | -0.164485 |
| C                                                         | 3.550443  | -1.472346 | -0.210396 |
| H                                                         | 3.382659  | -1.966434 | -1.168428 |
| H                                                         | 3.153206  | -2.133230 | 0.562251  |
| H                                                         | 4.611476  | -1.314197 | -0.042275 |
| O                                                         | 3.350416  | 0.861521  | 0.207261  |
| Rotational constants (GHz): 1.6948600 0.4339300 0.3896700 |           |           |           |
| Vibrational harmonic frequencies (cm-1):                  |           |           |           |
| i1610.7031                                                | 32.0175   |           | 41.2687   |
| 68.9407                                                   | 114.3602  |           | 132.0911  |
| 149.3881                                                  | 172.3625  |           | 213.6895  |
| 227.0350                                                  | 274.8122  |           | 281.7258  |
| 306.4633                                                  | 319.4460  |           | 362.1367  |
| 405.9361                                                  | 411.9331  |           | 513.4749  |
| 522.6323                                                  | 545.9453  |           | 603.6883  |
| 632.4918                                                  | 672.0312  |           | 733.2284  |
| 781.6380                                                  | 831.5793  |           | 894.6679  |
| 917.4657                                                  | 929.2964  |           | 951.9079  |
| 965.2518                                                  | 968.5183  |           | 980.8892  |
| 982.8527                                                  | 1008.7693 |           | 1028.7279 |
| 1036.0818                                                 | 1067.6380 |           | 1103.7756 |
| 1123.3903                                                 | 1168.0991 |           | 1180.2328 |
| 1197.1288                                                 | 1230.7267 |           | 1241.0249 |
| 1251.5886                                                 | 1293.7313 |           | 1295.6470 |
| 1317.2361                                                 | 1333.4667 |           | 1341.8526 |
| 1366.2256                                                 | 1392.4885 |           | 1407.9835 |
| 1419.7457                                                 | 1434.2948 |           | 1464.6303 |
| 1477.1905                                                 | 1482.3611 |           | 1492.7921 |
| 1498.9845                                                 | 1505.9725 |           | 1513.5299 |
| 1572.6299                                                 | 1832.0518 |           | 1856.7443 |

|           |           |           |
|-----------|-----------|-----------|
| 3048.0394 | 3050.3522 | 3053.8693 |
| 3064.5831 | 3081.2983 | 3114.3950 |
| 3115.9964 | 3118.3136 | 3126.5209 |
| 3127.7552 | 3141.2949 | 3151.1014 |
| 3164.1131 | 3179.5014 | 3190.0688 |

Zero-point correction (Hartree): 0.242864

ApineneCI.J.b.14Hshift.mtcdu

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.13526526

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-0.548601	0.330142	-0.889484
H	-0.566211	0.788054	-1.880363
C	-1.959793	0.277818	-0.377543
C	-2.341126	-0.636658	0.616903
H	-1.714427	-1.286844	1.217175
O	-3.589733	-0.921825	0.705869
O	-4.299708	-0.210577	-0.247437
H	-3.099568	-0.024144	-0.963020
H	-2.434319	1.255367	-0.252433
C	0.587713	1.035306	-0.076729
C	0.326034	-0.937863	-0.964295
C	0.862338	2.484003	-0.425744
C	0.416604	0.869740	1.427480
H	0.309090	-0.177078	1.720479
H	1.286402	1.262700	1.950002
H	-0.469394	1.408570	1.767645
H	1.779278	2.823680	0.057518
H	0.043772	3.123392	-0.087643
H	0.972638	2.614864	-1.503270
H	0.309218	-1.510359	-1.888656
H	0.141720	-1.614633	-0.129080
C	1.540862	-0.026516	-0.686148
H	1.937280	0.345296	-1.636902
C	2.722332	-0.527660	0.103176
C	3.132423	-1.960321	-0.128193
H	3.170039	-2.176315	-1.196844
H	2.382360	-2.625448	0.303889
H	4.095856	-2.151665	0.334568
O	3.317386	0.194478	0.865368

Rotational constants (GHz): 1.4941900 0.4165400 0.3777100

Vibrational harmonic frequencies (cm-1):

11599.3411	36.6911	59.2275
68.5121	94.5189	125.2251
154.2439	197.0099	224.6741
239.9276	276.3134	291.9205
310.5931	321.3383	328.8109
405.1026	419.5008	492.4781
516.9213	538.4440	593.7621
629.5925	666.6880	731.3488
753.2789	800.0133	861.3080
897.1049	921.4193	930.2194
964.9244	967.6724	976.9170
988.2476	1010.0678	1018.8683
1043.6820	1049.7273	1126.9052
1155.0871	1179.5845	1187.8432
1200.8054	1228.6855	1242.5414
1246.3154	1289.0686	1311.7022
1316.1724	1355.0623	1368.2943
1387.5031	1395.7621	1411.4594
1416.8896	1425.6207	1463.9833
1476.8188	1483.7059	1493.8127
1500.0795	1505.2096	1514.0047
1607.5329	1832.1387	1861.4301
3046.1967	3049.3528	3054.2633
3064.7030	3070.3037	3076.6556
3085.1223	3114.1738	3116.2387
3126.2069	3127.1299	3143.5097
3150.9660	3180.8211	3202.1712

Zero-point correction (Hartree): 0.242621

ApineneCI.J.b.14Hshift.mtcud

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.13510237

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.492974  | 0.113671  | 1.120149  |
| H | 0.454354  | 0.594116  | 2.098271  |
| C | 1.933331  | -0.130132 | 0.763836  |
| C | 2.285395  | -1.062654 | -0.225077 |
| H | 1.667032  | -1.818528 | -0.696909 |
| O | 3.417601  | -0.905260 | -0.808326 |
| O | 4.060503  | 0.208843  | -0.291156 |
| H | 2.833867  | 0.659267  | 0.210168  |
| H | 2.636892  | -0.132162 | 1.599266  |
| C | -0.417127 | 0.944843  | 0.158813  |
| C | -0.568097 | -1.012028 | 1.100797  |
| C | -0.504700 | 2.429854  | 0.445040  |
| C | -0.087466 | 0.701374  | -1.307710 |
| H | -0.077743 | -0.361844 | -1.561444 |
| H | -0.831872 | 1.177102  | -1.943081 |
| H | 0.893641  | 1.114759  | -1.547880 |
| H | -1.280326 | 2.890883  | -0.167674 |
| H | 0.445492  | 2.917907  | 0.217726  |
| H | -0.739889 | 2.614833  | 1.494333  |
| H | -0.749750 | -1.549688 | 2.028531  |
| H | -0.386115 | -1.735949 | 0.305899  |
| C | -1.588602 | 0.057506  | 0.658286  |
| H | -2.039568 | 0.516520  | 1.544372  |
| C | -2.725357 | -0.287492 | -0.268753 |
| C | -3.356350 | -1.646040 | -0.092905 |

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H      -3.552547      -1.839544      0.962654
H      -2.659790      -2.414809      -0.432773
H      -4.274017      -1.708184      -0.669974
O      -3.118561      0.499157      -1.095060
Rotational constants (GHz):      1.4962500      0.4320700      0.4014400
Vibrational harmonic frequencies (cm-1):
i1607.2685      32.1224      50.8784
69.3216      85.6643      128.2943
151.7728      191.5070      223.0333
237.9139      274.3418      307.6068
315.1407      323.2511      347.3745
401.1660      417.7208      496.2605
514.7598      532.7035      591.1695
625.2725      681.3310      714.9198
740.3451      794.0926      845.5532
895.7526      923.3543      946.2906
960.9678      966.0464      973.9557
984.6604      1010.6388      1017.9910
1041.0289      1061.6861      1125.0029
1136.5719      1177.3629      1190.9108
1192.1175      1225.9740      1241.2065
1251.5617      1290.5905      1302.6954
1315.0772      1353.3885      1367.1615
1388.5596      1395.6854      1410.9999
1414.5726      1425.4454      1464.3622
1476.8577      1484.2479      1493.3939
1498.0024      1506.4350      1513.7161
1600.2625      1832.3213      1855.2273
3047.2913      3048.6921      3051.7612
3064.1937      3081.0780      3087.2263
3094.9151      3112.5303      3117.4447
3125.5922      3127.3608      3142.4950
3150.3779      3180.1725      3197.0090
Zero-point correction (Hartree): 0.242474

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ApineneCI.J.b.14Hshift.mtpuu
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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.13342981
Electronic state : 1-A
Cartesian coordinates (Angs):
C -0.732243 0.576272 -0.824046
H -0.761570 0.925978 -1.857535
C -2.075266 0.898285 -0.163061
C -2.550775 0.168071 0.936419
H -2.805867 0.527479 1.928467
O -2.977970 -1.027371 0.717764
O -2.897717 -1.310822 -0.642604
H -2.779322 0.023708 -0.884818
H -2.203776 1.969460 -0.035462
C 0.565494 1.144373 -0.160274
C -0.111632 -0.830502 -0.782797
C 1.065904 2.470084 -0.696641
C 0.476346 1.175732 1.358898
H 0.141871 0.220559 1.770613
H 1.451083 1.397302 1.788809
H -0.228051 1.946562 1.677900
H 2.058022 2.690013 -0.300194
H 0.396287 3.282593 -0.404591
H 1.126829 2.455353 -1.785799
H -0.307535 -1.491264 -1.621284
H -0.369630 -1.356066 0.136416
C 1.264009 -0.138995 -0.683883
H 1.654895 0.043590 -1.690520
C 2.388978 -0.760858 0.102538
C 2.504533 -2.262459 0.037724
H 2.431217 -2.602809 -0.996161
H 1.668763 -2.711585 0.577408
H 3.441679 -2.584769 0.481428
O 3.164814 -0.083822 0.733098
Rotational constants (GHz): 1.2260500 0.5490200 0.4555100
Vibrational harmonic frequencies (cm-1):
i1616.7736 35.7103 61.5271
71.6818 126.0201 141.5485
162.0537 173.6913 206.8621
235.3375 275.3756 288.3142
314.5335 322.9474 351.3943
413.0145 426.0010 496.2912
522.1934 592.2186 605.1415
629.4812 689.4010 735.3999
776.7731 822.6280 895.3985
908.6588 919.3807 940.9468
964.5041 971.7707 976.3180
984.8431 1009.2777 1017.0266
1039.6336 1054.7058 1098.4985
1132.9931 1175.5006 1184.6708
1201.1245 1227.0897 1244.0630
1252.7311 1281.0651 1306.4998
1316.0918 1317.9532 1347.6455
1374.6491 1394.2101 1406.6517
1416.3186 1420.6151 1464.1250
1476.5240 1482.1149 1492.8639
1496.9782 1504.5391 1513.3772
1574.6397 1828.9578 1871.4504
3044.8011 3047.6154 3050.6132
3065.0957 3074.7937 3097.1591
3110.9545 3113.3103 3126.4839
3126.9388 3145.6415 3149.8205
3163.4649 3180.6995 3186.2500
Zero-point correction (Hartree): 0.242957

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ApineneCI.J.b.14Hshift.pmcdu
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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.13772450
Electronic state : 1-A
Cartesian coordinates (Angs):
  C    0.501948    0.071943    1.077734
  H    0.584972    0.740305    1.940324
  C    1.858632   -0.401203    0.635253
  C    2.840749    0.551070    0.327507
  H    2.815317    1.620211    0.517847
  O    3.786462    0.197389   -0.465788
  O    3.612011   -1.129126   -0.827253
  H    2.269365   -1.036678   -0.448779
  H    2.243002   -1.283269    1.152946
  C   -0.456411    0.742224    0.043013
  C   -0.583461   -0.982931    1.357768
  C   -0.513889    2.256797    0.078760
  C   -0.235603    0.238992   -1.375959
  H   -0.201326   -0.849251   -1.423404
  H   -1.041321    0.577832   -2.030604
  H    0.703820    0.623547   -1.776937
  H   -1.314128    2.639614   -0.557902
  H    0.422877    2.683260   -0.289505
  H   -0.679971    2.622854    1.092840
  H   -0.719435   -1.306514    2.386510
  H   -0.475792   -1.856466    0.716167
  C   -1.622661   -0.023091    0.768366
  H   -2.063452    0.630617    1.523851
  C   -2.703521   -0.582371   -0.118430
  C   -3.763190    0.392907   -0.567074
  H   -3.295464    1.292456   -0.971375
  H   -4.358253    0.702352    0.293961
  H   -4.405703   -0.065738   -1.312708
  O   -2.700982   -1.733409   -0.478817
Rotational constants (GHz):    1.5858800    0.4230500    0.3981100
Vibrational harmonic frequencies (cm-1):
  i1614.2534    18.2378    58.1047
    61.5971    84.6235    112.0638
   157.0308    163.5883    234.0036
   244.5308    277.4538    284.2974
   320.2674    337.2673    361.2275
   384.9133    432.4747    455.7285
   521.6903    575.4701    588.3437
   621.8231    648.3741    715.4977
   745.6290    803.8182    850.2465
   910.1308    938.7109    953.7478
   959.9714    967.1340    974.3403
   976.2353    999.8264   1016.8439
  1041.3206   1102.3942   1126.7459
  1146.7639   1173.7496   1188.8441
  1192.3070   1208.4904   1231.0792
  1260.1507   1270.0073   1284.1761
  1316.8853   1343.8395   1365.5892
  1381.3931   1401.0431   1407.9330
  1425.1665   1428.5251   1464.0248
  1476.6330   1481.2720   1492.7432
  1500.6338   1504.2072   1508.7659
  1601.1836   1837.1049   1854.6564
  3037.0736   3041.9308   3053.2270
  3063.2298   3078.7971   3087.2164
  3098.9180   3104.9572   3116.3997
  3121.4260   3125.5242   3138.0572
  3156.2516   3178.4356   3179.2608
Zero-point correction (Hartree): 0.242291

ApineneCI.J.b.14Hshift.pmcud
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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.13836149
Electronic state : 1-A
Cartesian coordinates (Angs):
 C -0.560156 0.051265 -0.736524
 H -0.760206 0.611252 -1.653120
 C -1.850613 -0.274231 -0.043403
 C -2.907464 0.648813 -0.089719
 H -2.886800 1.668241 -0.462620
 O -4.094283 0.202752 0.106911
 O -4.040498 -1.159603 0.349468
 H -2.765201 -1.192176 -0.265498
 H -1.751350 -0.777375 0.921684
 C 0.593706 0.773584 0.029337
 C 0.413286 -1.101197 -1.051491
 C 0.705475 2.266465 -0.209713
 C 0.597145 0.460352 1.518283
 H 0.542490 -0.610999 1.712961
 H 1.511201 0.832309 1.985590
 H -0.248851 0.944688 2.008508
 H 1.608928 2.677566 0.245455
 H -0.147367 2.785940 0.234664
 H 0.726446 2.495252 -1.276021
 H 0.352199 -1.557167 -2.036053
 H 0.377719 -1.880911 -0.291824
 C 1.582001 -0.148712 -0.773634
 H 1.913779 0.378554 -1.670260
 C 2.771940 -0.664125 -0.008869
 C 3.949574 0.272582 0.094572
 H 3.613913 1.259055 0.419960
 H 4.399171 0.398829 -0.891921
 H 4.686550 -0.123227 0.786918
 O 2.767033 -1.745474 0.525938
Rotational constants (GHz): 1.7277400 0.3902400 0.3576500
Vibrational harmonic frequencies (cm-1):
 i1587.4732 43.4085 52.0526
 56.4539 95.8244 112.0716
 151.6195 168.7645 226.0775

```



|           |           |           |
|-----------|-----------|-----------|
| 251.2783  | 265.5135  | 284.7798  |
| 312.6386  | 322.6114  | 359.1260  |
| 386.3263  | 429.1031  | 469.1275  |
| 522.9351  | 566.3545  | 594.9026  |
| 618.5301  | 624.8452  | 734.0518  |
| 750.3741  | 805.5350  | 877.7641  |
| 909.1814  | 929.7368  | 957.3745  |
| 960.5354  | 967.2708  | 974.8885  |
| 983.5381  | 999.2392  | 1017.6261 |
| 1040.0085 | 1101.4621 | 1120.7830 |
| 1163.3977 | 1179.7985 | 1189.1927 |
| 1194.9386 | 1207.6881 | 1233.6946 |
| 1257.8797 | 1271.6881 | 1273.3470 |
| 1319.6310 | 1341.0421 | 1369.7105 |
| 1386.7995 | 1401.0238 | 1408.4944 |
| 1422.4686 | 1445.8139 | 1464.0360 |
| 1476.3760 | 1485.3595 | 1492.4764 |
| 1499.4422 | 1507.9996 | 1509.0284 |
| 1603.5598 | 1835.6636 | 1853.9631 |
| 3041.3245 | 3053.2682 | 3060.6585 |
| 3062.7912 | 3080.5911 | 3088.9741 |
| 3099.7888 | 3105.3376 | 3117.7365 |
| 3120.8346 | 3125.0133 | 3134.7825 |
| 3158.3220 | 3178.9799 | 3187.3334 |

Zero-point correction (Hartree): 0.242520

ApineneCI,J.b.14Hshift.pmmdd  
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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.13574191

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.717145 | -0.362642 | -0.275377 |
| H | -1.163008 | -0.156453 | -1.246368 |
| C | -1.817377 | -0.535263 | 0.770585  |
| C | -2.911882 | 0.344177  | 0.835253  |
| H | -3.244179 | 0.946636  | 1.674864  |
| O | -3.790851 | 0.277271  | -0.101946 |
| O | -3.442045 | -0.724390 | -0.998424 |
| H | -2.599957 | -1.242621 | -0.046771 |
| H | -1.420692 | -0.781538 | 1.750173  |
| C | 0.415234  | 0.677700  | -0.021206 |
| C | 0.344779  | -1.465262 | -0.402425 |
| C | 0.240567  | 2.006135  | -0.728142 |
| C | 0.724763  | 0.883247  | 1.453672  |
| H | 0.872752  | -0.059981 | 1.979670  |
| H | 1.634956  | 1.474000  | 1.576034  |
| H | -0.090210 | 1.426458  | 1.936010  |
| H | 1.117657  | 2.645126  | -0.605506 |
| H | -0.615952 | 2.542559  | -0.311113 |
| H | 0.062548  | 1.865411  | -1.794528 |
| H | 0.190413  | -2.228641 | -1.160324 |
| H | 0.562540  | -1.942290 | 0.552488  |
| C | 1.380805  | -0.370908 | -0.689684 |
| H | 1.467346  | -0.146962 | -1.754287 |
| C | 2.748531  | -0.483874 | -0.071554 |
| C | 3.765585  | 0.531386  | -0.529651 |
| H | 3.336405  | 1.534277  | -0.487785 |
| H | 4.022493  | 0.338869  | -1.572834 |
| H | 4.658845  | 0.475292  | 0.085278  |
| O | 3.003506  | -1.307672 | 0.772393  |

Rotational constants (GHz): 1.7464400 0.4222800 0.4014400

Vibrational harmonic frequencies (cm-1):

|            |           |           |
|------------|-----------|-----------|
| i1617.3123 | 31.5000   | 57.4527   |
| 62.4072    | 117.3245  | 128.4700  |
| 141.1183   | 164.8607  | 215.2623  |
| 226.6643   | 281.5926  | 286.6628  |
| 311.9299   | 327.8919  | 366.7440  |
| 384.2116   | 442.7065  | 464.7219  |
| 550.2870   | 579.3150  | 606.4688  |
| 625.0918   | 664.3349  | 737.4138  |
| 796.2023   | 829.3322  | 898.8346  |
| 920.7391   | 926.1866  | 956.6122  |
| 963.4214   | 966.9423  | 977.9708  |
| 992.8586   | 998.4681  | 1016.5621 |
| 1041.7317  | 1070.5651 | 1114.8122 |
| 1131.4327  | 1168.2185 | 1178.3079 |
| 1188.6122  | 1208.3095 | 1243.7149 |
| 1258.9628  | 1271.7296 | 1306.9262 |
| 1322.0111  | 1341.6263 | 1349.4216 |
| 1374.2399  | 1400.3057 | 1408.2760 |
| 1421.4617  | 1430.9610 | 1464.9695 |
| 1476.0141  | 1484.5060 | 1490.4508 |
| 1500.2946  | 1507.4644 | 1509.1485 |
| 1569.8141  | 1834.6711 | 1856.0883 |
| 3040.7990  | 3051.1741 | 3062.5298 |
| 3086.8939  | 3098.7545 | 3103.1228 |
| 3113.7221  | 3118.3887 | 3124.1321 |
| 3125.7705  | 3134.2134 | 3158.0394 |
| 3162.0395  | 3179.3276 | 3186.7495 |

Zero-point correction (Hartree): 0.243056

ApineneCI,J.b.14Hshift.pmmud  
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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.13422040

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.660349 | -0.553229 | -0.756621 |
| H | -0.980936 | -0.112259 | -1.699312 |
| C | -1.845603 | -1.235045 | -0.042621 |
| C | -2.615175 | -0.581181 | 0.930691  |
| H | -2.844018 | -0.914672 | 1.937401  |
| O | -3.335835 | 0.416408  | 0.553415  |

|                                                           |           |           |           |
|-----------------------------------------------------------|-----------|-----------|-----------|
| O                                                         | -3.187629 | 0.583604  | -0.819123 |
| H                                                         | -2.729653 | -0.729339 | -0.881831 |
| H                                                         | -1.632865 | -2.264453 | 0.222741  |
| C                                                         | 0.211805  | 0.513478  | -0.028813 |
| C                                                         | 0.599482  | -1.403397 | -0.987731 |
| C                                                         | -0.110139 | 1.956296  | -0.361778 |
| C                                                         | 0.296257  | 0.303636  | 1.474979  |
| H                                                         | 0.472819  | -0.739784 | 1.737922  |
| H                                                         | 1.109453  | 0.895554  | 1.900132  |
| H                                                         | -0.626091 | 0.635432  | 1.955445  |
| H                                                         | 0.620500  | 2.637904  | 0.079366  |
| H                                                         | -1.097712 | 2.218675  | 0.021315  |
| H                                                         | -0.123779 | 2.114994  | -1.440385 |
| H                                                         | 0.690043  | -1.920772 | -1.939376 |
| H                                                         | 0.784207  | -2.104467 | -0.174858 |
| C                                                         | 1.435741  | -0.136616 | -0.779047 |
| H                                                         | 1.610996  | 0.408454  | -1.708019 |
| C                                                         | 2.711916  | -0.236241 | 0.012332  |
| C                                                         | 3.565053  | 1.006732  | 0.047095  |
| H                                                         | 2.949507  | 1.874832  | 0.290041  |
| H                                                         | 3.985161  | 1.182936  | -0.944776 |
| H                                                         | 4.366664  | 0.894722  | 0.771051  |
| O                                                         | 3.012437  | -1.235557 | 0.618487  |
| Rotational constants (GHz): 1.6951700 0.4721400 0.4432800 |           |           |           |
| Vibrational harmonic frequencies (cm-1):                  |           |           |           |
| i1593.1497                                                | 25.7460   | 60.6538   |           |
| 65.2791                                                   | 122.5506  | 133.5187  |           |
| 152.2576                                                  | 188.7212  | 216.6926  |           |
| 227.8417                                                  | 266.5707  | 282.1189  |           |
| 311.6964                                                  | 329.2478  | 362.9250  |           |
| 380.3370                                                  | 440.1310  | 474.3078  |           |
| 572.0297                                                  | 578.5249  | 610.0957  |           |
| 630.2061                                                  | 673.4013  | 731.4964  |           |
| 785.5283                                                  | 830.9836  | 898.0597  |           |
| 914.4218                                                  | 940.1736  | 959.5509  |           |
| 963.7962                                                  | 965.0778  | 978.2554  |           |
| 989.3763                                                  | 998.5698  | 1013.9871 |           |
| 1043.4084                                                 | 1062.0248 | 1110.1330 |           |
| 1132.4058                                                 | 1171.3576 | 1181.7130 |           |
| 1187.9057                                                 | 1208.6005 | 1236.5615 |           |
| 1258.7679                                                 | 1274.7883 | 1303.3815 |           |
| 1315.0045                                                 | 1351.4425 | 1371.6970 |           |
| 1390.8699                                                 | 1402.7041 | 1413.2144 |           |
| 1415.4088                                                 | 1423.9734 | 1465.6498 |           |
| 1476.4559                                                 | 1476.9148 | 1488.1181 |           |
| 1500.2583                                                 | 1501.2872 | 1509.5810 |           |
| 1577.6284                                                 | 1833.4507 | 1867.5053 |           |
| 3047.8101                                                 | 3051.3799 | 3062.4602 |           |
| 3085.8739                                                 | 3095.9455 | 3099.8454 |           |
| 3110.7102                                                 | 3118.1082 | 3124.7096 |           |
| 3128.4986                                                 | 3133.1162 | 3156.3575 |           |
| 3167.7037                                                 | 3179.1975 | 3194.8675 |           |
| Zero-point correction (Hartree): 0.243269                 |           |           |           |
| ApineneCI.J.b.14Hshift.ppcdu                              |           |           |           |
| ~~~~~                                                     |           |           |           |
| E (CCSD(T)/Aug-CC-pVTZ) (Hartree): -615.20937533          |           |           |           |
| E (CCSD/Aug-CC-pVTZ) (Hartree): -615.08703680             |           |           |           |
| T1 diagnostic: 0.019226                                   |           |           |           |
| E (MP2/Aug-CC-pVTZ) (Hartree): -615.02558713              |           |           |           |
| E (MP3/Aug-CC-pVTZ) (Hartree): -615.07326661              |           |           |           |
| E (RHF/Aug-CC-pVTZ) (Hartree): -612.56695676              |           |           |           |
| E (RM062X/Aug-CC-pVTZ) (Hartree): -616.13884217           |           |           |           |
| Electronic state : 1-A                                    |           |           |           |
| Cartesian coordinates (Angs):                             |           |           |           |
| C                                                         | -0.551997 | -0.172574 | -0.740712 |
| H                                                         | -0.757746 | 0.157689  | -1.762071 |
| C                                                         | -1.836901 | -0.300724 | 0.024034  |
| C                                                         | -3.025146 | -0.576544 | -0.669812 |
| H                                                         | -3.140056 | -0.855708 | -1.712458 |
| O                                                         | -4.131457 | -0.259102 | -0.102459 |
| O                                                         | -3.871235 | 0.300386  | 1.137740  |
| H                                                         | -2.550902 | 0.565959  | 0.708581  |
| H                                                         | -1.762460 | -0.825743 | 0.980150  |
| C                                                         | 0.566782  | 0.746755  | -0.162550 |
| C                                                         | 0.461802  | -1.335797 | -0.768947 |
| C                                                         | 0.629181  | 2.145942  | -0.740529 |
| C                                                         | 0.557080  | 0.786130  | 1.359467  |
| H                                                         | 0.524913  | -0.212335 | 1.796425  |
| H                                                         | 1.456323  | 1.278927  | 1.734601  |
| H                                                         | -0.305639 | 1.349254  | 1.717217  |
| H                                                         | 1.500281  | 2.691334  | -0.371802 |
| H                                                         | -0.259899 | 2.710699  | -0.451300 |
| H                                                         | 0.677401  | 2.121277  | -1.829978 |
| H                                                         | 0.431835  | -2.013157 | -1.618996 |
| H                                                         | 0.442675  | -1.916607 | 0.152292  |
| C                                                         | 1.595155  | -0.304858 | -0.718659 |
| H                                                         | 1.922727  | 0.006779  | -1.712515 |
| C                                                         | 2.790732  | -0.585365 | 0.152061  |
| C                                                         | 3.924654  | 0.404606  | 0.058424  |
| H                                                         | 3.540572  | 1.422020  | 0.152495  |
| H                                                         | 4.389496  | 0.329612  | -0.926269 |
| H                                                         | 4.662975  | 0.206176  | 0.829581  |
| O                                                         | 2.822624  | -1.523985 | 0.909393  |
| Rotational constants (GHz): 1.7214000 0.3836100 0.3667000 |           |           |           |
| Vibrational harmonic frequencies (cm-1):                  |           |           |           |
| i1586.0153                                                | 38.5957   | 51.4589   |           |
| 58.0227                                                   | 95.4503   | 113.6866  |           |
| 149.5847                                                  | 169.9199  | 223.1414  |           |
| 248.6940                                                  | 269.7975  | 286.5150  |           |
| 302.2297                                                  | 314.5825  | 363.6886  |           |
| 387.1970                                                  | 418.3181  | 475.7148  |           |

|           |           |           |
|-----------|-----------|-----------|
| 522.2324  | 559.8971  | 598.8955  |
| 615.0623  | 625.5516  | 726.7773  |
| 750.3503  | 821.3354  | 875.3614  |
| 909.1107  | 930.8311  | 953.6963  |
| 958.5575  | 965.6311  | 972.2602  |
| 981.0635  | 999.3624  | 1018.1777 |
| 1040.5184 | 1102.8077 | 1119.3103 |
| 1162.3037 | 1179.5202 | 1189.7776 |
| 1197.7068 | 1206.4843 | 1228.4295 |
| 1257.7377 | 1269.5481 | 1275.3663 |
| 1317.4902 | 1341.2891 | 1370.5444 |
| 1387.2984 | 1401.2336 | 1408.8186 |
| 1422.3560 | 1446.6149 | 1463.8625 |
| 1476.3712 | 1484.6560 | 1492.6378 |
| 1499.5617 | 1507.9447 | 1509.3657 |
| 1603.4629 | 1835.1272 | 1854.5345 |
| 3045.5496 | 3054.4762 | 3057.8310 |
| 3063.5403 | 3081.7663 | 3083.2684 |
| 3096.0453 | 3112.3095 | 3120.3339 |
| 3121.9421 | 3125.9421 | 3135.5485 |
| 3152.6410 | 3179.4877 | 3187.3894 |

Zero-point correction (Hartree): 0.242446

ApineneCI.J.b.14Hshift.ppcud

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.13821770

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.521699 | 0.460973  | -0.976268 |
| H | -0.483860 | 1.046036  | -1.897953 |
| C | -1.923681 | 0.441271  | -0.432163 |
| C | -2.702081 | -0.715256 | -0.594144 |
| H | -2.479043 | -1.591367 | -1.193938 |
| O | -3.687612 | -0.883929 | 0.210366  |
| O | -3.752508 | 0.183839  | 1.090719  |
| H | -2.396865 | 0.471564  | 0.791342  |
| H | -2.498109 | 1.362507  | -0.554731 |
| C | 0.647463  | 0.951699  | -0.064121 |
| C | 0.240059  | -0.862630 | -1.188376 |
| C | 1.077544  | 2.391452  | -0.262991 |
| C | 0.413796  | 0.649660  | 1.408447  |
| H | 0.083984  | -0.376660 | 1.570538  |
| H | 1.332440  | 0.799244  | 1.979558  |
| H | -0.344782 | 1.318167  | 1.816654  |
| H | 1.980959  | 2.618569  | 0.306719  |
| H | 0.294450  | 3.071095  | 0.080031  |
| H | 1.275132  | 2.602865  | -1.314667 |
| H | 0.215920  | -1.310269 | -2.179344 |
| H | -0.022687 | -1.617816 | -0.446943 |
| C | 1.526800  | -0.150050 | -0.761217 |
| H | 2.057640  | 0.295859  | -1.604699 |
| C | 2.496602  | -0.886942 | 0.123878  |
| C | 3.794338  | -0.177792 | 0.418955  |
| H | 3.596181  | 0.846142  | 0.740605  |
| H | 4.387511  | -0.115587 | -0.495187 |
| H | 4.351004  | -0.713012 | 1.182389  |
| O | 2.234530  | -1.965115 | 0.597369  |

Rotational constants (GHz): 1.4533700 0.4364200 0.4002100

Vibrational harmonic frequencies (cm-1):

|            |           |           |
|------------|-----------|-----------|
| 11571.2624 | 31.4892   | 53.1044   |
| 62.4124    | 104.8083  | 115.7080  |
| 157.5958   | 161.1619  | 221.4559  |
| 238.8200   | 282.6116  | 300.8077  |
| 306.6438   | 324.5117  | 356.7591  |
| 385.9914   | 426.4925  | 467.8445  |
| 520.4395   | 577.4191  | 598.4191  |
| 625.6028   | 652.3124  | 723.5848  |
| 745.9241   | 812.4610  | 869.5383  |
| 907.5214   | 936.8387  | 944.2300  |
| 961.2293   | 966.2090  | 973.4601  |
| 983.3916   | 1000.1437 | 1015.2269 |
| 1030.3193  | 1066.7342 | 1142.0182 |
| 1162.1526  | 1173.6513 | 1187.8176 |
| 1193.3063  | 1209.8898 | 1232.5141 |
| 1261.5179  | 1270.8486 | 1302.3639 |
| 1323.4196  | 1353.2675 | 1369.1693 |
| 1387.0341  | 1403.5754 | 1414.3631 |
| 1420.7422  | 1426.3912 | 1464.6060 |
| 1477.1375  | 1480.8522 | 1492.6389 |
| 1501.0171  | 1504.5294 | 1509.0919 |
| 1606.9714  | 1835.8852 | 1867.3892 |
| 3045.5016  | 3055.7914 | 3061.2411 |
| 3063.6210  | 3079.8299 | 3086.5811 |
| 3087.5132  | 3111.4709 | 3121.0245 |
| 3122.2021  | 3126.5522 | 3137.9642 |
| 3144.9636  | 3177.9989 | 3195.8845 |

Zero-point correction (Hartree): 0.242628

ApineneCI.J.b.14Hshift.ppmdd

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.12951694

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.721572 | 0.800318  | -0.703327 |
| H | -0.665075 | 1.511947  | -1.530993 |
| C | -2.137845 | 0.961154  | -0.114601 |
| C | -3.174414 | 0.078399  | -0.466617 |
| H | -4.099002 | 0.294223  | -0.993666 |
| O | -3.189320 | -1.082405 | 0.086096  |
| O | -2.141064 | -1.180265 | 0.996107  |
| H | -2.004390 | 0.153586  | 0.952705  |
| H | -2.465768 | 1.994315  | -0.174701 |

|                                                           |           |           |           |
|-----------------------------------------------------------|-----------|-----------|-----------|
| C                                                         | 0.556386  | 1.019714  | 0.153402  |
| C                                                         | -0.141087 | -0.533223 | -1.206409 |
| C                                                         | 1.096504  | 2.436622  | 0.173023  |
| C                                                         | 0.446620  | 0.459870  | 1.564160  |
| H                                                         | 0.111407  | -0.576507 | 1.570784  |
| H                                                         | 1.415947  | 0.504249  | 2.065095  |
| H                                                         | -0.254799 | 1.055010  | 2.151795  |
| H                                                         | 2.071642  | 2.484804  | 0.661692  |
| H                                                         | 0.420447  | 3.090747  | 0.728617  |
| H                                                         | 1.201883  | 2.834150  | -0.837408 |
| H                                                         | -0.314491 | -0.782811 | -2.250835 |
| H                                                         | -0.403750 | -1.376461 | -0.574645 |
| C                                                         | 1.247248  | 0.003977  | -0.828828 |
| H                                                         | 1.714694  | 0.561468  | -1.643804 |
| C                                                         | 2.252104  | -0.938374 | -0.221286 |
| C                                                         | 3.616735  | -0.356258 | 0.058134  |
| H                                                         | 3.518437  | 0.575021  | 0.618571  |
| H                                                         | 4.106934  | -0.110724 | -0.885577 |
| H                                                         | 4.221371  | -1.067606 | 0.612804  |
| O                                                         | 1.977939  | -2.079656 | 0.053253  |
| Rotational constants (GHz): 1.3486200 0.5422700 0.4634700 |           |           |           |
| Vibrational harmonic frequencies (cm-1):                  |           |           |           |
| i1626.9476                                                | 50.1094   |           | 59.8747   |
| 72.3694                                                   | 108.6399  |           | 127.1204  |
| 157.5115                                                  | 185.8861  |           | 206.0450  |
| 221.5736                                                  | 268.5730  |           | 290.3477  |
| 305.1218                                                  | 325.4298  |           | 345.6590  |
| 385.4223                                                  | 446.3752  |           | 481.0566  |
| 532.5617                                                  | 580.1541  |           | 596.3677  |
| 626.5868                                                  | 720.2485  |           | 733.6804  |
| 754.6696                                                  | 821.4672  |           | 904.5897  |
| 930.9411                                                  | 932.0331  |           | 944.4407  |
| 962.2476                                                  | 965.4217  |           | 975.8918  |
| 979.4457                                                  | 1000.2061 |           | 1023.0472 |
| 1039.7295                                                 | 1059.5518 |           | 1104.1024 |
| 1139.5534                                                 | 1174.1565 |           | 1187.4811 |
| 1196.7981                                                 | 1208.5838 |           | 1226.3229 |
| 1259.9982                                                 | 1280.1103 |           | 1305.3955 |
| 1321.8724                                                 | 1332.9497 |           | 1360.0714 |
| 1376.5131                                                 | 1399.2919 |           | 1407.3080 |
| 1417.5095                                                 | 1422.8719 |           | 1465.0442 |
| 1477.4265                                                 | 1484.5997 |           | 1490.8710 |
| 1503.0566                                                 | 1508.8917 |           | 1512.2451 |
| 1570.2783                                                 | 1839.4512 |           | 1882.1605 |
| 3044.0478                                                 | 3048.2611 |           | 3054.3510 |
| 3063.9933                                                 | 3072.5782 |           | 3107.6340 |
| 3109.3176                                                 | 3114.5071 |           | 3120.9147 |
| 3127.2984                                                 | 3146.2215 |           | 3147.8717 |
| 3178.6974                                                 | 3179.9099 |           | 3181.1372 |
| Zero-point correction (Hartree): 0.243017                 |           |           |           |
| ApineneCI.J.b.14Hshift.pppuu                              |           |           |           |
| ~~~~~                                                     |           |           |           |
| E(RM062X/Aug-CC-pVTZ) (Hartree): -616.13651628            |           |           |           |
| Electronic state : 1-A                                    |           |           |           |
| Cartesian coordinates (Angs):                             |           |           |           |
| C                                                         | -0.718517 | -0.324705 | -0.370807 |
| H                                                         | -1.170833 | 0.110801  | -1.259392 |
| C                                                         | -1.820587 | -0.766035 | 0.599275  |
| C                                                         | -3.100303 | -1.072628 | 0.113920  |
| H                                                         | -3.669140 | -1.989497 | 0.228738  |
| O                                                         | -3.814027 | -0.099929 | -0.336345 |
| O                                                         | -3.122750 | 1.097194  | -0.183810 |
| H                                                         | -2.305032 | 0.468056  | 0.725959  |
| H                                                         | -1.467473 | -1.459145 | 1.354921  |
| C                                                         | 0.387552  | 0.636062  | 0.140066  |
| C                                                         | 0.366700  | -1.342649 | -0.768503 |
| C                                                         | 0.194687  | 2.098948  | -0.206063 |
| C                                                         | 0.676309  | 0.456786  | 1.623878  |
| H                                                         | 0.846773  | -0.587535 | 1.886961  |
| H                                                         | 1.566732  | 1.018643  | 1.913176  |
| H                                                         | -0.161058 | 0.830969  | 2.214768  |
| H                                                         | 1.070471  | 2.691647  | 0.066963  |
| H                                                         | -0.663806 | 2.503571  | 0.334081  |
| H                                                         | 0.007470  | 2.228584  | -1.272393 |
| H                                                         | 0.227844  | -1.890325 | -1.697550 |
| H                                                         | 0.596616  | -2.043138 | 0.033247  |
| C                                                         | 1.379931  | -0.190744 | -0.760635 |
| H                                                         | 1.468040  | 0.297254  | -1.732916 |
| C                                                         | 2.745959  | -0.434328 | -0.178165 |
| C                                                         | 3.734952  | 0.695154  | -0.321766 |
| H                                                         | 3.277853  | 1.632829  | -0.000393 |
| H                                                         | 3.997756  | 0.813755  | -1.374428 |
| H                                                         | 4.628726  | 0.490287  | 0.259967  |
| O                                                         | 3.020398  | -1.453755 | 0.406542  |
| Rotational constants (GHz): 1.7507800 0.4396400 0.3985100 |           |           |           |
| Vibrational harmonic frequencies (cm-1):                  |           |           |           |
| i1607.2056                                                | 41.3700   |           | 58.1547   |
| 62.7534                                                   | 117.0932  |           | 126.3648  |
| 150.7684                                                  | 162.8749  |           | 221.0626  |
| 230.3934                                                  | 270.8842  |           | 283.0604  |
| 304.6520                                                  | 319.3129  |           | 363.2201  |
| 382.7450                                                  | 442.0922  |           | 475.5556  |
| 537.7919                                                  | 588.1704  |           | 602.5858  |
| 625.8898                                                  | 673.4986  |           | 734.5810  |
| 792.0449                                                  | 832.9335  |           | 903.1813  |
| 922.5086                                                  | 933.5749  |           | 958.3224  |
| 961.3441                                                  | 965.8850  |           | 974.8605  |
| 987.0702                                                  | 1002.1455 |           | 1022.7783 |
| 1036.9252                                                 | 1066.0764 |           | 1102.0297 |
| 1132.4318                                                 | 1169.9711 |           | 1174.8182 |
| 1193.4808                                                 | 1208.5717 |           | 1236.8976 |

|           |           |           |
|-----------|-----------|-----------|
| 1256.6168 | 1280.4609 | 1294.6414 |
| 1317.4691 | 1335.3243 | 1350.1570 |
| 1374.3940 | 1400.7149 | 1410.3276 |
| 1424.2039 | 1434.9246 | 1464.8133 |
| 1476.2843 | 1482.9946 | 1490.5438 |
| 1499.1277 | 1506.6610 | 1508.3712 |
| 1572.9723 | 1833.3011 | 1857.5583 |
| 3046.4724 | 3053.8922 | 3063.0764 |
| 3085.4860 | 3096.3225 | 3112.2500 |
| 3116.5449 | 3118.7438 | 3124.9090 |
| 3126.4380 | 3133.9199 | 3154.0760 |
| 3167.8257 | 3179.4677 | 3193.4827 |

Zero-point correction (Hartree): 0.243075

ApineneCI.J.b.14Hshift.ptcdu

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.13852286

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.549905 | 0.553951  | -0.822435 |
| H | -0.576186 | 1.275598  | -1.641087 |
| C | -1.937648 | 0.437346  | -0.258138 |
| C | -2.354879 | -0.732270 | 0.398066  |
| H | -1.762544 | -1.591246 | 0.693903  |
| O | -3.618942 | -0.940343 | 0.478755  |
| O | -4.303203 | 0.101356  | -0.126012 |
| H | -3.123622 | 0.431643  | -0.826849 |
| H | -2.316569 | 1.346216  | 0.218064  |
| C | 0.653815  | 0.938696  | 0.095660  |
| C | 0.232373  | -0.689854 | -1.285567 |
| C | 1.033784  | 2.405897  | 0.103916  |
| C | 0.505344  | 0.408257  | 1.513905  |
| H | 0.285909  | -0.659572 | 1.534461  |
| H | 1.428279  | 0.558246  | 2.077924  |
| H | -0.294166 | 0.937017  | 2.034676  |
| H | 1.962959  | 2.573728  | 0.652470  |
| H | 0.254513  | 2.996503  | 0.591003  |
| H | 1.162651  | 2.785046  | -0.910450 |
| H | 0.164272  | -0.963044 | -2.335305 |
| H | 0.040680  | -1.572029 | -0.676424 |
| C | 1.522508  | -0.011917 | -0.807312 |
| H | 2.000194  | 0.578526  | -1.591131 |
| C | 2.547744  | -0.844951 | -0.085907 |
| C | 3.865669  | -0.172176 | 0.202270  |
| H | 3.692533  | 0.804318  | 0.658673  |
| H | 4.394040  | 0.004848  | -0.736192 |
| H | 4.472230  | -0.792824 | 0.854937  |
| O | 2.309895  | -1.969868 | 0.281581  |

Rotational constants (GHz): 1.5790500 0.4230700 0.3836200

Vibrational harmonic frequencies (cm-1):

|            |           |           |
|------------|-----------|-----------|
| i1593.1298 | 50.1754   | 58.2839   |
| 64.0300    | 99.3257   | 119.1227  |
| 154.7578   | 185.6860  | 217.9586  |
| 244.5250   | 276.4790  | 292.0706  |
| 308.3667   | 319.7031  | 359.8258  |
| 384.1375   | 423.5656  | 464.0241  |
| 526.4772   | 580.1030  | 597.9340  |
| 624.3791   | 662.4321  | 738.3573  |
| 755.6782   | 803.6657  | 864.1032  |
| 899.1532   | 930.8448  | 949.9404  |
| 961.4842   | 968.2009  | 974.0701  |
| 981.1881   | 1000.8053 | 1019.5948 |
| 1023.3949  | 1058.7846 | 1137.4055 |
| 1160.7994  | 1170.2345 | 1187.2239 |
| 1195.8850  | 1209.8714 | 1234.7102 |
| 1258.0036  | 1270.9214 | 1309.0092 |
| 1325.1462  | 1365.1684 | 1368.9613 |
| 1384.8383  | 1403.0368 | 1413.8519 |
| 1420.8000  | 1426.1966 | 1464.4861 |
| 1476.9935  | 1485.3194 | 1491.6538 |
| 1500.7053  | 1506.0993 | 1509.8096 |
| 1605.6625  | 1832.6510 | 1863.1221 |
| 3044.9123  | 3054.1759 | 3062.3352 |
| 3070.5384  | 3075.8490 | 3084.0255 |
| 3102.2962  | 3109.3559 | 3118.1017 |
| 3123.6778  | 3125.0644 | 3134.5093 |
| 3157.3025  | 3178.5311 | 3198.7360 |

Zero-point correction (Hartree): 0.242763

ApineneCI.J.b.14Hshift.ptcud

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.13870922

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.504757  | 0.429044  | 1.104513  |
| H | 0.464840  | 1.165932  | 1.907050  |
| C | 1.944745  | 0.197985  | 0.735862  |
| C | 2.330650  | -0.973620 | 0.063562  |
| H | 1.760680  | -1.882990 | -0.094627 |
| O | 3.409788  | -0.926978 | -0.629256 |
| O | 3.971722  | 0.337725  | -0.539493 |
| H | 2.739998  | 0.832893  | -0.104112 |
| H | 2.684399  | 0.511971  | 1.475364  |
| C | -0.502011 | 0.885498  | 0.002574  |
| C | -0.453931 | -0.730410 | 1.455930  |
| C | -0.728867 | 2.380566  | -0.094909 |
| C | -0.185308 | 0.295260  | -1.363468 |
| H | -0.057323 | -0.787758 | -1.326467 |
| H | -0.997070 | 0.497862  | -2.065040 |
| H | 0.725713  | 0.738984  | -1.767570 |
| H | -1.529176 | 2.618755  | -0.798519 |
| H | 0.178965  | 2.874119  | -0.448794 |

|                                                 |           |           |           |
|-------------------------------------------------|-----------|-----------|-----------|
| H                                               | -0.989682 | 2.803583  | 0.875970  |
| H                                               | -0.571667 | -0.980210 | 2.507218  |
| H                                               | -0.252854 | -1.642395 | 0.895809  |
| C                                               | -1.585970 | 0.046889  | 0.774154  |
| H                                               | -2.120300 | 0.701723  | 1.464830  |
| C                                               | -2.563574 | -0.711241 | -0.083106 |
| C                                               | -3.741525 | 0.075357  | -0.599270 |
| H                                               | -3.398012 | 1.011902  | -1.042606 |
| H                                               | -4.393486 | 0.338951  | 0.235454  |
| H                                               | -4.295275 | -0.508127 | -1.328673 |
| O                                               | -2.389454 | -1.869142 | -0.376292 |
| Rotational constants (GHz):                     | 1.5090900 | 0.4462200 | 0.4135300 |
| Vibrational harmonic frequencies (cm-1):        |           |           |           |
| i1597.6607                                      | 48.3361   |           | 57.9410   |
| 70.8327                                         | 90.2505   |           | 116.0074  |
| 153.9666                                        | 185.6298  |           | 224.9585  |
| 246.1590                                        | 282.3380  |           | 291.5552  |
| 324.5804                                        | 334.8344  |           | 364.6024  |
| 385.6094                                        | 421.1657  |           | 472.8723  |
| 517.1231                                        | 577.5655  |           | 596.1339  |
| 622.8813                                        | 681.1356  |           | 716.7215  |
| 746.6302                                        | 800.1253  |           | 845.7345  |
| 903.5515                                        | 939.3770  |           | 958.8112  |
| 961.4968                                        | 967.2965  |           | 972.6515  |
| 981.4255                                        | 999.7606  |           | 1017.6893 |
| 1031.4967                                       | 1063.6756 |           | 1129.4315 |
| 1146.8823                                       | 1170.7889 |           | 1186.9056 |
| 1193.4766                                       | 1208.7159 |           | 1228.6855 |
| 1258.4222                                       | 1275.0533 |           | 1303.6506 |
| 1320.5443                                       | 1365.7786 |           | 1368.2602 |
| 1387.6959                                       | 1402.9769 |           | 1413.5100 |
| 1419.6429                                       | 1426.5404 |           | 1464.2962 |
| 1476.4450                                       | 1484.9911 |           | 1492.2532 |
| 1498.4879                                       | 1507.8265 |           | 1509.1483 |
| 1599.4358                                       | 1832.8577 |           | 1856.6126 |
| 3045.4594                                       | 3053.3024 |           | 3062.1848 |
| 3082.6679                                       | 3083.5929 |           | 3095.1359 |
| 3101.4850                                       | 3111.7855 |           | 3118.6396 |
| 3122.7587                                       | 3124.4306 |           | 3130.3871 |
| 3155.9887                                       | 3178.8440 |           | 3196.2062 |
| Zero-point correction (Hartree):                | 0.242773  |           |           |
| ApineneCI.J.b.14Hshift.ptpuu                    |           |           |           |
| ~~~~~                                           |           |           |           |
| E (RM062X/Aug-CC-pVT2) (Hartree): -616.13464449 |           |           |           |
| Electronic state : 1-A                          |           |           |           |
| Cartesian coordinates (Angs):                   |           |           |           |
| C                                               | -0.722856 | 0.702158  | -0.715440 |
| H                                               | -0.756088 | 1.239807  | -1.664755 |
| C                                               | -2.009408 | 0.998977  | 0.061875  |
| C                                               | -2.538404 | 0.072465  | 0.975147  |
| H                                               | -2.732528 | 0.198056  | 2.035713  |
| O                                               | -3.093631 | -0.982796 | 0.491659  |
| O                                               | -3.067977 | -0.932555 | -0.897819 |
| H                                               | -2.814588 | 0.402481  | -0.816161 |
| H                                               | -2.022612 | 2.016006  | 0.443411  |
| C                                               | 0.634618  | 1.037494  | -0.022050 |
| C                                               | -0.221460 | -0.731524 | -0.951467 |
| C                                               | 1.231410  | 2.387847  | -0.364601 |
| C                                               | 0.598460  | 0.821603  | 1.483188  |
| H                                               | 0.185281  | -0.152903 | 1.745885  |
| H                                               | 1.605604  | 0.871594  | 1.902201  |
| H                                               | 0.000052  | 1.597644  | 1.963522  |
| H                                               | 2.236749  | 2.495919  | 0.047676  |
| H                                               | 0.618582  | 3.190648  | 0.052501  |
| H                                               | 1.287475  | 2.530531  | -1.444273 |
| H                                               | -0.486926 | -1.204539 | -1.890787 |
| H                                               | -0.480185 | -1.405020 | -0.135912 |
| C                                               | 1.212153  | -0.213607 | -0.780290 |
| H                                               | 1.653697  | 0.114070  | -1.723287 |
| C                                               | 2.202377  | -1.042589 | -0.006528 |
| C                                               | 3.635916  | -0.574775 | -0.052142 |
| H                                               | 3.686012  | 0.492106  | 0.174268  |
| H                                               | 4.026878  | -0.703869 | -1.062882 |
| H                                               | 4.240131  | -1.139569 | 0.651537  |
| O                                               | 1.863561  | -1.996056 | 0.650559  |
| Rotational constants (GHz):                     | 1.3382200 | 0.5317300 | 0.4611000 |
| Vibrational harmonic frequencies (cm-1):        |           |           |           |
| i1611.2776                                      | 48.5580   |           | 59.2261   |
| 65.4115                                         | 112.5781  |           | 136.1586  |
| 155.0638                                        | 178.5499  |           | 203.3825  |
| 235.1260                                        | 269.2794  |           | 289.7842  |
| 313.5514                                        | 335.1604  |           | 353.0098  |
| 385.6737                                        | 441.4171  |           | 471.1748  |
| 571.1865                                        | 585.6101  |           | 612.2103  |
| 628.0411                                        | 684.1612  |           | 741.2722  |
| 784.3121                                        | 823.5534  |           | 890.9426  |
| 917.3749                                        | 927.1846  |           | 950.6756  |
| 962.1382                                        | 965.0030  |           | 978.9214  |
| 982.5326                                        | 998.8185  |           | 1013.8644 |
| 1032.3796                                       | 1050.3728 |           | 1099.2450 |
| 1141.1915                                       | 1167.7563 |           | 1184.0162 |
| 1193.0057                                       | 1206.7585 |           | 1236.8899 |
| 1256.0828                                       | 1267.5828 |           | 1307.2115 |
| 1318.4746                                       | 1326.1406 |           | 1357.5916 |
| 1377.3712                                       | 1400.6028 |           | 1408.7742 |
| 1418.7297                                       | 1421.1779 |           | 1464.5842 |
| 1475.9882                                       | 1483.2712 |           | 1489.8685 |
| 1494.8503                                       | 1504.9667 |           | 1506.6634 |
| 1574.5424                                       | 1834.8624 |           | 1876.4163 |
| 3044.0793                                       | 3051.1812 |           | 3062.4869 |
| 3071.6518                                       | 3082.3094 |           | 3107.6613 |

|           |           |           |
|-----------|-----------|-----------|
| 3112.6235 | 3115.6888 | 3124.0215 |
| 3125.2712 | 3130.9398 | 3146.0373 |
| 3176.3651 | 3178.7712 | 3187.3099 |

Zero-point correction (Hartree): 0.243000

Population analysis as 298K (%)

Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)

| Compound                     | Qtot      | Erel | Erel2 | n*Q*MB    | %        |
|------------------------------|-----------|------|-------|-----------|----------|
| ApineneCI.J.b.ringclose.pmtm | 1.044e+44 | 0.00 | 0.00  | 1.044e+44 | 18.1     |
| ApineneCI.J.b.ringclose.pmpm | 1.139e+44 | 0.10 | 0.10  | 9.646e+43 | 16.7     |
| ApineneCI.J.b.ringclose.pmtp | 2.481e+44 | 0.63 | 0.63  | 8.592e+43 | 14.9     |
| ApineneCI.J.b.ringclose.pppm | 3.127e+44 | 0.90 | 0.90  | 6.881e+43 | 11.9     |
| ApineneCI.J.b.ringclose.pmpm | 3.003e+44 | 1.19 | 1.19  | 4.048e+43 | 7.03     |
| ApineneCI.J.b.ringclose.pmpm | 2.511e+44 | 1.24 | 1.24  | 3.069e+43 | 5.33     |
| ApineneCI.J.b.ringclose.pppm | 2.567e+44 | 1.41 | 1.41  | 2.379e+43 | 4.13     |
| ApineneCI.J.b.ringclose.pppp | 3.612e+44 | 1.72 | 1.72  | 1.969e+43 | 3.42     |
| ApineneCI.J.b.ringclose.mppm | 2.955e+44 | 1.64 | 1.64  | 1.865e+43 | 3.24     |
| ApineneCI.J.b.ringclose.pptp | 1.915e+44 | 1.44 | 1.44  | 1.683e+43 | 2.92     |
| ApineneCI.J.b.ringclose.pptm | 2.064e+44 | 1.69 | 1.69  | 1.186e+43 | 2.06     |
| ApineneCI.J.b.ringclose.pppm | 3.812e+44 | 2.10 | 2.10  | 1.104e+43 | 1.92     |
| ApineneCI.J.b.ringclose.pppm | 3.296e+44 | 2.32 | 2.32  | 6.566e+42 | 1.14     |
| ApineneCI.J.b.ringclose.mppp | 5.311e+44 | 2.65 | 2.65  | 6.066e+42 | 1.05     |
| ApineneCI.J.b.ringclose.mptm | 3.172e+44 | 2.38 | 2.38  | 5.697e+42 | 0.989    |
| ApineneCI.J.b.ringclose.mppm | 9.007e+44 | 3.09 | 3.09  | 4.875e+42 | 0.846    |
| ApineneCI.J.b.ringclose.mmtm | 1.735e+44 | 2.20 | 2.20  | 4.195e+42 | 0.728    |
| ApineneCI.J.b.ringclose.mppm | 4.363e+44 | 2.78 | 2.78  | 3.986e+42 | 0.692    |
| ApineneCI.J.b.ringclose.mppm | 3.207e+44 | 2.73 | 2.73  | 3.218e+42 | 0.559    |
| ApineneCI.J.b.ringclose.mptp | 2.211e+44 | 2.59 | 2.59  | 2.766e+42 | 0.48     |
| ApineneCI.J.b.ringclose.mppp | 7.639e+44 | 3.39 | 3.39  | 2.511e+42 | 0.436    |
| ApineneCI.J.b.ringclose.mppm | 1.427e+44 | 2.45 | 2.45  | 2.283e+42 | 0.396    |
| ApineneCI.J.b.ringclose.ptmm | 1.885e+44 | 2.86 | 2.86  | 1.499e+42 | 0.26     |
| ApineneCI.J.b.ringclose.mmtm | 3.407e+44 | 3.22 | 3.22  | 1.487e+42 | 0.258    |
| ApineneCI.J.b.ringclose.mppm | 4.022e+44 | 3.48 | 3.48  | 1.122e+42 | 0.195    |
| ApineneCI.J.b.ringclose.ptpm | 2.394e+44 | 3.56 | 3.56  | 5.899e+41 | 0.102    |
| ApineneCI.J.b.ringclose.ptpm | 2.579e+44 | 4.29 | 4.29  | 1.844e+41 | 0.032    |
| ApineneCI.J.b.ringclose.ptpp | 2.811e+44 | 4.51 | 4.51  | 1.394e+41 | 0.0242   |
| ApineneCI.J.b.ringclose.mtmm | 2.767e+44 | 4.86 | 4.86  | 7.500e+40 | 0.013    |
| ApineneCI.J.b.ringclose.mtpm | 1.518e+44 | 4.52 | 4.52  | 7.352e+40 | 0.0128   |
| ApineneCI.J.b.ringclose.mtpp | 3.893e+44 | 5.97 | 5.97  | 1.623e+40 | 0.00282  |
| ApineneCI.J.b.ringclose.mtpp | 2.651e+44 | 6.12 | 6.12  | 8.628e+39 | 0.0015   |
| ApineneCI.J.b.ringclose.mtpp | 1.327e+44 | 7.43 | 7.43  | 4.730e+38 | 8.21e-05 |
| ApineneCI.J.b.ringclose.pttp | 2.902e+44 | 8.12 | 8.12  | 3.238e+38 | 5.62e-05 |
| Total                        |           |      |       | 5.760e+44 | 100      |

ApineneCI.J.b.ringclose.mppm

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.12176013

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.528091 | -0.382429 | -0.643153 |
| H | -0.791757 | -0.174116 | -1.683015 |
| C | -1.776969 | -0.776620 | 0.141373  |
| C | -2.789924 | 0.301709  | 0.050087  |
| H | -2.220262 | -1.704302 | -0.213787 |
| H | -1.522049 | -0.922057 | 1.194089  |
| H | -2.435618 | 1.330899  | 0.196938  |
| C | 0.428594  | 0.747526  | -0.138922 |
| C | 0.655964  | -1.369249 | -0.611544 |
| C | 0.305382  | 2.108588  | -0.798274 |
| C | 0.431447  | 0.883165  | 1.379021  |
| H | 0.588151  | -0.074002 | 1.880378  |
| H | 1.228333  | 1.554983  | 1.691555  |
| H | -0.518019 | 1.291962  | 1.731466  |
| H | 1.179344  | 2.715482  | -0.557882 |
| H | -0.579095 | 2.645939  | -0.448783 |
| H | 0.240001  | 2.016293  | -1.883415 |
| H | 0.726368  | -2.101360 | -1.412086 |
| H | 0.705768  | -1.885175 | 0.348068  |
| C | 1.591472  | -0.145692 | -0.654010 |
| H | 1.809514  | 0.111444  | -1.695665 |
| C | 2.914260  | -0.142689 | 0.069876  |
| C | 3.652704  | -1.453915 | 0.146650  |
| H | 3.663262  | -1.941908 | -0.829004 |
| H | 3.127478  | -2.123089 | 0.830937  |
| H | 4.664755  | -1.291360 | 0.504686  |
| O | 3.357831  | 0.874392  | 0.544643  |
| O | -3.978989 | 0.197707  | -0.361568 |
| O | -4.275742 | -0.831099 | 0.654287  |

Rotational constants (GHz): 1.7919100 0.3842600 0.3536800

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| 1750.8606 | 33.2526   | 50.1965   |
| 62.2959   | 82.1160   | 140.4928  |
| 150.7440  | 167.8790  | 227.7478  |
| 235.0312  | 249.8490  | 277.8367  |
| 305.3883  | 315.0025  | 323.0741  |
| 390.2837  | 407.5018  | 440.0246  |
| 492.1944  | 516.9590  | 534.9233  |
| 604.0685  | 622.6476  | 722.2625  |
| 763.4694  | 770.6963  | 868.8088  |
| 900.8583  | 926.7774  | 959.1755  |
| 963.7334  | 976.8912  | 993.2257  |
| 1011.3599 | 1028.8438 | 1034.5015 |
| 1078.5796 | 1101.6119 | 1120.2979 |
| 1145.0785 | 1178.5490 | 1194.6766 |
| 1206.1081 | 1239.7155 | 1248.4861 |
| 1267.2219 | 1276.2348 | 1295.5480 |
| 1322.5908 | 1350.1656 | 1382.7629 |
| 1390.9431 | 1398.8630 | 1409.3623 |
| 1423.1344 | 1449.5825 | 1464.8848 |
| 1477.4676 | 1482.2144 | 1496.7895 |

|           |           |           |
|-----------|-----------|-----------|
| 1499.6031 | 1504.8513 | 1515.1758 |
| 1623.2293 | 1831.1098 | 3046.6509 |
| 3051.0791 | 3053.6224 | 3057.1086 |
| 3062.3258 | 3064.5495 | 3076.0927 |
| 3085.0998 | 3113.0546 | 3115.0881 |
| 3125.9619 | 3128.0295 | 3147.3444 |
| 3148.2464 | 3151.0035 | 3182.1738 |

Zero-point correction (Hartree): 0.244977

ApineneCI.J.b.ringclose.mmmmp

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.12323022

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.609032 | -0.593695 | -0.235106 |
| H | -1.021154 | -0.658773 | -1.241415 |
| C | -1.755705 | -0.818980 | 0.749103  |
| C | -2.815985 | 0.209391  | 0.641162  |
| H | -2.200774 | -1.796742 | 0.579531  |
| H | -1.365776 | -0.743236 | 1.771467  |
| H | -2.598108 | 1.205013  | 1.048482  |
| C | 0.302590  | 0.666092  | -0.138807 |
| C | 0.639599  | -1.486490 | -0.118902 |
| C | -0.042170 | 1.821291  | -1.058219 |
| C | 0.495496  | 1.153741  | 1.292918  |
| H | 0.782401  | 0.348294  | 1.971859  |
| H | 1.277325  | 1.909542  | 1.328345  |
| H | -0.424793 | 1.601480  | 1.674386  |
| H | 0.765709  | 2.554277  | -1.062670 |
| H | -0.954443 | 2.325734  | -0.730031 |
| H | -0.203793 | 1.474913  | -2.079361 |
| H | 0.668020  | -2.393991 | -0.716914 |
| H | 0.859421  | -1.735376 | 0.920158  |
| C | 1.457401  | -0.267850 | -0.596587 |
| H | 1.505728  | -0.272114 | -1.690377 |
| C | 2.863718  | -0.035743 | -0.108061 |
| C | 3.725477  | -1.259683 | 0.072024  |
| H | 3.649445  | -1.907597 | -0.802405 |
| H | 3.362295  | -1.834894 | 0.925712  |
| H | 4.757278  | -0.967694 | 0.242506  |
| O | 3.277594  | 1.077881  | 0.104942  |
| O | -4.010901 | 0.034207  | 0.269153  |
| O | -3.570083 | -0.541747 | -1.016147 |

Rotational constants (GHz): 1.7947600 0.4096500 0.3813600

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i745.5739 | 37.8065   | 49.0241   |
| 67.7329   | 96.4412   | 120.9348  |
| 139.6459  | 163.6526  | 214.5731  |
| 220.8178  | 272.1623  | 286.2944  |
| 311.2369  | 315.0276  | 357.8050  |
| 380.4963  | 405.6472  | 430.1081  |
| 488.9377  | 526.6830  | 547.3512  |
| 610.2458  | 622.6725  | 725.1067  |
| 761.8445  | 810.9906  | 874.5421  |
| 902.8604  | 929.8592  | 957.1832  |
| 965.5201  | 975.6499  | 989.3417  |
| 1003.4168 | 1028.1691 | 1035.6472 |
| 1076.2927 | 1105.4794 | 1126.4766 |
| 1145.8214 | 1179.6139 | 1197.0554 |
| 1209.5994 | 1238.7419 | 1251.6047 |
| 1275.5113 | 1284.4093 | 1303.1144 |
| 1330.6595 | 1345.8407 | 1378.5348 |
| 1389.9668 | 1394.7609 | 1409.3943 |
| 1422.2561 | 1454.6681 | 1463.4684 |
| 1476.0751 | 1482.0763 | 1494.5696 |
| 1500.4736 | 1504.8524 | 1515.8622 |
| 1617.7342 | 1830.7974 | 3028.8049 |
| 3046.6538 | 3051.5339 | 3054.3389 |
| 3064.1371 | 3064.9413 | 3081.8557 |
| 3109.2085 | 3112.4641 | 3114.3436 |
| 3126.2747 | 3132.0429 | 3146.7454 |
| 3149.6229 | 3152.1893 | 3181.1739 |

Zero-point correction (Hartree): 0.245239

ApineneCI.J.b.ringclose.mmpm

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.12395884

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.560928  | -0.749388 | 0.654193  |
| H | 0.840070  | -0.646769 | 1.706966  |
| C | 1.766137  | -1.237072 | -0.153803 |
| C | 3.037474  | -0.654765 | 0.323890  |
| H | 1.864886  | -2.315904 | 0.032411  |
| H | 1.642620  | -1.050290 | -1.216737 |
| H | 3.364283  | -0.948432 | 1.330655  |
| C | -0.225910 | 0.529698  | 0.239376  |
| C | -0.745032 | -1.559293 | 0.566006  |
| C | 0.109162  | 1.813160  | 0.968500  |
| C | -0.260127 | 0.755596  | -1.266801 |
| H | -0.503532 | -0.155561 | -1.818279 |
| H | -1.016433 | 1.504187  | -1.506645 |
| H | 0.708213  | 1.112814  | -1.614319 |
| H | -0.649977 | 2.568816  | 0.760923  |
| H | 1.081350  | 2.186765  | 0.643702  |
| H | 0.137758  | 1.652465  | 2.047831  |
| H | -0.906511 | -2.342653 | 1.303712  |
| H | -0.878596 | -1.977886 | -0.431796 |
| C | -1.502881 | -0.232061 | 0.736863  |
| H | -1.654442 | -0.001858 | 1.792788  |
| C | -2.794758 | 0.073303  | 0.019812  |
| C | -3.394861 | -0.983393 | -0.871400 |



|   |           |           |           |
|---|-----------|-----------|-----------|
| H | -3.479907 | -1.930372 | -0.336415 |
| H | -2.735699 | -1.156167 | -1.724674 |
| H | -4.367522 | -0.655400 | -1.225091 |
| O | -3.308228 | 1.158091  | 0.151733  |
| O | 3.873090  | 0.026917  | -0.333373 |
| O | 2.841718  | 1.017683  | -0.698967 |

Rotational constants (GHz): 1.7045000 0.4492100 0.4113600

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i732.0117 | 40.3831   | 57.2609   |
| 75.1896   | 95.7486   | 150.2371  |
| 174.9591  | 191.6305  | 203.3834  |
| 249.8049  | 260.1922  | 283.6021  |
| 315.9002  | 335.6006  | 345.8354  |
| 386.5205  | 431.0714  | 458.1829  |
| 500.0162  | 503.6908  | 542.2467  |
| 607.2914  | 622.0643  | 715.8247  |
| 761.9989  | 815.2480  | 874.6037  |
| 889.1741  | 922.0224  | 940.7978  |
| 971.2865  | 987.5267  | 1002.9961 |
| 1015.0468 | 1023.2856 | 1048.9849 |
| 1068.5252 | 1099.2760 | 1120.8052 |
| 1150.7931 | 1176.0517 | 1191.1132 |
| 1207.1938 | 1246.6226 | 1258.0958 |
| 1264.3014 | 1282.7955 | 1294.2391 |
| 1323.7094 | 1354.9199 | 1388.8295 |
| 1390.3026 | 1398.0676 | 1410.7314 |
| 1417.0331 | 1451.9962 | 1466.4731 |
| 1477.0056 | 1488.1574 | 1496.3236 |
| 1500.6942 | 1511.0586 | 1520.6459 |
| 1621.4591 | 1827.4465 | 3003.2750 |
| 3046.0182 | 3048.1187 | 3052.9743 |
| 3054.4117 | 3063.3978 | 3085.1625 |
| 3088.5810 | 3117.6173 | 3119.4426 |
| 3125.2991 | 3128.9648 | 3140.9076 |
| 3148.9036 | 3165.6864 | 3180.7149 |

Zero-point correction (Hartree): 0.245527

ApineneCI.J.b.ringclose.mmp

E(RM062X/Aug-CC-pVTZ) (Hartree): -616.12305240

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.458638  | -0.579300 | 0.886377  |
| H | 0.618411  | -0.397532 | 1.953192  |
| C | 1.755915  | -1.052636 | 0.236646  |
| C | 2.804334  | -0.031006 | 0.467473  |
| H | 2.077930  | -1.986126 | 0.707139  |
| H | 1.663776  | -1.236363 | -0.830139 |
| H | 2.912538  | 0.341855  | 1.495546  |
| C | -0.306618 | 0.638767  | 0.287104  |
| C | -0.807313 | -1.439953 | 0.706513  |
| C | -0.079361 | 1.977444  | 0.960622  |
| C | -0.122919 | 0.759177  | -1.221528 |
| H | -0.328934 | -0.180166 | -1.739007 |
| H | -0.801560 | 1.512559  | -1.617652 |
| H | 0.900309  | 1.053497  | -1.461637 |
| H | -0.802446 | 2.709284  | 0.598826  |
| H | 0.921585  | 2.357938  | 0.738958  |
| H | -0.184149 | 1.897815  | 2.044021  |
| H | -1.043464 | -2.160829 | 1.485648  |
| H | -0.802606 | -1.947151 | -0.258367 |
| C | -1.609872 | -0.123856 | 0.659957  |
| H | -1.918268 | 0.158102  | 1.671415  |
| C | -2.824627 | 0.033991  | -0.220504 |
| C | -3.618381 | -1.207199 | -0.535688 |
| H | -3.776513 | -1.799879 | 0.366348  |
| H | -3.048485 | -1.828903 | -1.229351 |
| H | -4.566904 | -0.937152 | -0.989829 |
| O | -3.138966 | 1.121254  | -0.639183 |
| O | 3.459943  | 0.604456  | -0.404933 |
| O | 3.964024  | -0.651900 | -0.993003 |

Rotational constants (GHz): 1.6632400 0.4185500 0.3917600

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i740.3145 | 22.3764   | 50.4171   |
| 59.9677   | 83.4830   | 137.6645  |
| 158.8293  | 164.5474  | 225.3617  |
| 241.1378  | 268.0209  | 279.5461  |
| 294.3620  | 315.4065  | 327.5304  |
| 391.5599  | 411.8645  | 442.2884  |
| 492.2792  | 524.3227  | 533.1769  |
| 605.9836  | 618.2244  | 717.4818  |
| 751.9041  | 783.6577  | 879.4773  |
| 901.7467  | 921.5657  | 951.1536  |
| 964.7412  | 979.5104  | 998.6988  |
| 1016.7179 | 1031.6907 | 1046.4254 |
| 1050.2579 | 1100.4891 | 1115.6291 |
| 1147.9754 | 1178.7306 | 1197.2432 |
| 1203.9470 | 1241.3136 | 1242.6021 |
| 1261.5067 | 1272.3596 | 1294.0395 |
| 1322.0254 | 1349.1395 | 1387.4422 |
| 1391.3882 | 1399.1551 | 1410.2106 |
| 1423.4803 | 1452.3728 | 1463.8659 |
| 1476.6115 | 1483.2271 | 1496.7478 |
| 1500.5703 | 1507.5326 | 1515.3841 |
| 1620.8047 | 1831.8306 | 3040.1907 |
| 3044.7782 | 3051.0944 | 3054.6400 |
| 3057.5861 | 3063.4868 | 3063.7200 |
| 3088.9356 | 3107.3642 | 3118.8623 |
| 3124.8984 | 3127.6461 | 3145.9513 |
| 3147.6015 | 3166.2455 | 3181.9321 |

Zero-point correction (Hartree): 0.244939

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ApineneCI.J.b.ringclose.mmtm
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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.12381800
Electronic state : 1-A
Cartesian coordinates (Angs):
C      0.616179      0.801521     -0.441496
H      1.004851      0.741474     -1.454256
C      1.684339      1.353828      0.476824
C      2.865309      0.515683      0.784517
H      2.064556      2.310684      0.100050
H      1.268579      1.593050      1.466308
H      3.477589      0.848957      1.632318
C     -0.102390     -0.541402     -0.098238
C     -0.749456      1.518228     -0.425320
C      0.354567     -1.776336     -0.850030
C     -0.162041     -0.807391      1.401502
H     -0.548307      0.047342      1.961953
H     -0.812731     -1.654831      1.606721
H      0.833990     -1.045265      1.781875
H     -0.374623     -2.577384     -0.716695
H      1.324841     -2.118749     -0.491943
H      0.453664     -1.566475     -1.915459
H     -0.929120      2.286365     -1.174263
H     -0.979828      1.924068      0.561448
C     -1.396991      0.133863     -0.631157
H     -1.488901     -0.066780     -1.703686
C     -2.737367     -0.184830     -0.022618
C     -3.758342      0.926437     -0.025797
H     -3.797274      1.402681     -1.006484
H     -3.458480      1.694746      0.689227
H     -4.733914      0.536502      0.248614
O     -2.985663     -1.278431      0.423470
O      3.176914     -0.615862      0.317828
O      3.185282     -0.104956     -1.065655
Rotational constants (GHz):  1.7103800    0.4711600    0.4338300
Vibrational harmonic frequencies (cm-1):
i724.3611      35.3366      66.7414
  72.2729      108.9453      127.7719
 155.4944      176.6703      219.1591
 232.2976      263.5225      282.4188
 309.3202      313.8911      337.9064
 368.3704      401.8076      409.7098
 503.6952      521.7461      587.0166
 619.8979      674.8051      714.9095
 752.3401      785.8154      841.6117
 899.9059      917.2747      934.7380
 966.2307      971.2515      982.1497
1002.4812      1025.8231      1035.9780
1041.9589      1108.6531      1115.4238
1143.5820      1176.7718      1196.1964
1205.2004      1236.9684      1251.7879
1272.5941      1290.8832      1305.4737
1341.8396      1365.9375      1385.9720
1392.4688      1405.0966      1419.1653
1424.3098      1437.6351      1465.3524
1476.8319      1480.5988      1491.6391
1498.7642      1502.9955      1513.8479
1617.0636      1831.2654      3008.0501
3047.2917      3050.2972      3051.2999
3058.1748      3059.0141      3065.0273
3072.8388      3108.0848      3126.4656
3127.7953      3132.1831      3142.3737
3147.3977      3149.0495      3180.1120
Zero-point correction (Hartree): 0.244997

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ApineneCI.J.b.ringclose.mmtp
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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.12202489
Electronic state : 1-A
Cartesian coordinates (Angs):
C -0.672271 -0.631300 -0.381490
H -1.116524 -0.499817 -1.368218
C -1.702995 -1.189233 0.580850
C -3.131797 -0.871653 0.383094
H -1.684342 -2.290786 0.558480
H -1.459913 -0.947141 1.621869
H -3.841742 -1.459398 0.979450
C 0.184029 0.635658 -0.038329
C 0.628839 -1.457136 -0.474108
C -0.145942 1.938127 -0.741826
C 0.316942 0.860409 1.460731
H 0.646567 -0.036807 1.991852
H 1.045523 1.644072 1.658616
H -0.648111 1.170793 1.865942
H 0.724489 2.595504 -0.691577
H -0.994792 2.438402 -0.280769
H -0.391725 1.764880 -1.790510
H 0.703496 -2.204358 -1.261906
H 0.859426 -1.929450 0.483082
C 1.392140 -0.132914 -0.645410
H 1.469733 0.110926 -1.710235
C 2.773583 0.040942 -0.069742
C 3.671061 -1.172426 -0.082025
H 3.630643 -1.665619 -1.054250
H 3.313750 -1.893195 0.655820
H 4.689830 -0.883667 0.158532
O 3.147391 1.104965 0.359879
O -3.655346 -0.136659 -0.497727
O -2.845526 1.027046 -0.082983
Rotational constants (GHz): 1.7258300 0.4602700 0.4105400
Vibrational harmonic frequencies (cm-1):
i717.3244 26.8909 44.7953

```

|           |           |           |
|-----------|-----------|-----------|
| 76.1535   | 82.8755   | 134.8906  |
| 154.6942  | 169.9352  | 221.2437  |
| 258.0086  | 271.7054  | 288.8673  |
| 313.7646  | 321.7734  | 353.7960  |
| 370.6638  | 406.7952  | 410.7071  |
| 503.4319  | 517.6212  | 589.6489  |
| 618.6117  | 670.4626  | 708.7949  |
| 758.5639  | 769.8866  | 843.7764  |
| 899.9181  | 919.3099  | 944.3434  |
| 961.8525  | 968.3871  | 981.0512  |
| 1005.3620 | 1029.1043 | 1034.3890 |
| 1048.5447 | 1106.2959 | 1113.8794 |
| 1157.5578 | 1171.6514 | 1193.5746 |
| 1204.5462 | 1239.3283 | 1250.9451 |
| 1268.6426 | 1289.4697 | 1299.2838 |
| 1341.7976 | 1362.5018 | 1384.4275 |
| 1391.1485 | 1400.8368 | 1416.0648 |
| 1422.0794 | 1434.9039 | 1464.7074 |
| 1478.1606 | 1482.1555 | 1492.8529 |
| 1496.1692 | 1506.7541 | 1513.5811 |
| 1625.6234 | 1831.3984 | 2985.3705 |
| 3042.7713 | 3049.0146 | 3052.8499 |
| 3054.9598 | 3059.3113 | 3064.0741 |
| 3069.4509 | 3098.3905 | 3108.2519 |
| 3121.1276 | 3125.9302 | 3132.1406 |
| 3149.1272 | 3150.2698 | 3178.9594 |

Zero-point correction (Hartree): 0.244819

ApineneCI.J.b.ringclose.mppmm

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.12217156

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.577051 | 0.417074  | -0.654818 |
| H | -0.723174 | 0.778711  | -1.676748 |
| C | -1.872200 | 0.555462  | 0.140891  |
| C | -2.948303 | -0.160744 | -0.582064 |
| H | -1.801506 | 0.159082  | 1.149840  |
| H | -2.149665 | 1.611566  | 0.214670  |
| H | -3.046840 | 0.046638  | -1.656621 |
| C | 0.726823  | 1.061498  | -0.093717 |
| C | 0.133583  | -0.951541 | -0.688435 |
| C | 1.108890  | 2.409778  | -0.669873 |
| C | 0.753043  | 1.100625  | 1.429208  |
| H | 0.524606  | 0.129286  | 1.872319  |
| H | 1.740037  | 1.400987  | 1.775788  |
| H | 0.021251  | 1.819096  | 1.801897  |
| H | 2.113865  | 2.684823  | -0.347693 |
| H | 0.418995  | 3.185123  | -0.329110 |
| H | 1.091040  | 2.392461  | -1.760654 |
| H | -0.063320 | -1.612679 | -1.529771 |
| H | -0.036060 | -1.500125 | 0.238866  |
| C | 1.468589  | -0.180355 | -0.665774 |
| H | 1.790384  | 0.031150  | -1.690392 |
| C | 2.677470  | -0.715863 | 0.060179  |
| C | 2.827450  | -2.213019 | 0.136487  |
| H | 2.637986  | -2.665688 | -0.837822 |
| H | 2.079785  | -2.613744 | 0.823908  |
| H | 3.820400  | -2.470097 | 0.492600  |
| O | 3.488377  | 0.037319  | 0.541419  |
| O | -3.641712 | -1.125737 | -0.156253 |
| O | -4.122609 | -0.325842 | 0.988135  |

Rotational constants (GHz): 1.4144100 0.4143200 0.3662700

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i741.6424 | 26.2086   | 39.4500   |
| 53.7933   | 89.3653   | 118.7618  |
| 138.7315  | 166.2263  | 195.1752  |
| 234.4521  | 271.3009  | 276.0879  |
| 293.6192  | 321.9282  | 327.0100  |
| 359.7079  | 420.8955  | 470.3009  |
| 484.7687  | 510.9428  | 541.2384  |
| 597.1870  | 631.5452  | 730.0212  |
| 758.2598  | 795.6162  | 860.9205  |
| 897.0479  | 923.1388  | 944.8911  |
| 967.1870  | 982.0591  | 992.0486  |
| 1010.1805 | 1020.8268 | 1041.6176 |
| 1065.4578 | 1095.5863 | 1128.0304 |
| 1151.7002 | 1176.7076 | 1197.6536 |
| 1213.0319 | 1234.6884 | 1243.1111 |
| 1256.8879 | 1278.8739 | 1293.3595 |
| 1319.5517 | 1348.9767 | 1386.2880 |
| 1390.8165 | 1398.4295 | 1410.3581 |
| 1421.5490 | 1453.1191 | 1463.4226 |
| 1475.6551 | 1484.5057 | 1495.3160 |
| 1498.8793 | 1507.6233 | 1516.3770 |
| 1621.1978 | 1831.2238 | 3044.3928 |
| 3046.9224 | 3053.3625 | 3053.6211 |
| 3057.1074 | 3059.1686 | 3063.8046 |
| 3081.9912 | 3115.0761 | 3119.6352 |
| 3125.0655 | 3129.4985 | 3138.7308 |
| 3151.1885 | 3166.5867 | 3181.6109 |

Zero-point correction (Hartree): 0.244763

ApineneCI.J.b.ringclose.mppmp

~~~~~  
E(RM062X/Aug-CC-pVTZ) (Hartree): -616.12486140

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |          |           |
|---|-----------|----------|-----------|
| C | -0.689360 | 0.526868 | -0.509350 |
| H | -0.909829 | 0.873248 | -1.523264 |
| C | -1.899847 | 0.760962 | 0.396186  |
| C | -3.154533 | 0.290737 | -0.223411 |

|                                                           |           |           |           |
|-----------------------------------------------------------|-----------|-----------|-----------|
| H                                                         | -1.767523 | 0.276073  | 1.359246  |
| H                                                         | -2.021566 | 1.845565  | 0.523954  |
| H                                                         | -3.538848 | 0.869537  | -1.073877 |
| C                                                         | 0.685677  | 1.117542  | -0.076478 |
| C                                                         | -0.061829 | -0.875053 | -0.559738 |
| C                                                         | 1.087921  | 2.429446  | -0.719582 |
| C                                                         | 0.834461  | 1.192445  | 1.438021  |
| H                                                         | 0.597612  | 0.243376  | 1.922455  |
| H                                                         | 1.857779  | 1.453233  | 1.700430  |
| H                                                         | 0.168290  | 1.955110  | 1.846363  |
| H                                                         | 2.129021  | 2.658862  | -0.489279 |
| H                                                         | 0.470106  | 3.249828  | -0.346148 |
| H                                                         | 0.978074  | 2.386692  | -1.804309 |
| H                                                         | -0.376787 | -1.542380 | -1.356536 |
| H                                                         | -0.192936 | -1.387558 | 0.392501  |
| C                                                         | 1.309668  | -0.176020 | -0.670768 |
| H                                                         | 1.555494  | -0.008775 | -1.724690 |
| C                                                         | 2.541970  | -0.767880 | -0.035782 |
| C                                                         | 2.639635  | -2.271229 | -0.016772 |
| H                                                         | 2.389812  | -2.679469 | -0.997118 |
| H                                                         | 1.906231  | -2.669830 | 0.686682  |
| H                                                         | 3.637206  | -2.577165 | 0.283554  |
| O                                                         | 3.410237  | -0.060808 | 0.416116  |
| O                                                         | -3.921108 | -0.622916 | 0.195570  |
| O                                                         | -2.819719 | -1.605432 | 0.196574  |
| Rotational constants (GHz): 1.3456200 0.4727100 0.3908300 |           |           |           |
| Vibrational harmonic frequencies (cm-1):                  |           |           |           |
| i732.8220                                                 | 32.0943   | 56.2403   |           |
| 73.3871                                                   | 108.1341  | 128.3066  |           |
| 142.0769                                                  | 172.1973  | 186.6534  |           |
| 238.1441                                                  | 259.0030  | 278.5528  |           |
| 303.2284                                                  | 319.3679  | 346.6282  |           |
| 369.4054                                                  | 416.6785  | 459.8571  |           |
| 503.6672                                                  | 520.2050  | 544.5716  |           |
| 602.4995                                                  | 632.0092  | 729.9994  |           |
| 779.7666                                                  | 825.3980  | 862.1989  |           |
| 898.6562                                                  | 920.4036  | 952.1398  |           |
| 967.4871                                                  | 980.4996  | 993.3605  |           |
| 1012.1425                                                 | 1017.8508 | 1042.5294 |           |
| 1058.7308                                                 | 1095.9817 | 1131.6296 |           |
| 1146.0049                                                 | 1177.8427 | 1196.9464 |           |
| 1219.3811                                                 | 1238.5549 | 1244.6670 |           |
| 1252.1767                                                 | 1284.7472 | 1301.2624 |           |
| 1317.8088                                                 | 1351.6801 | 1386.5879 |           |
| 1390.4527                                                 | 1397.5089 | 1409.9396 |           |
| 1420.0199                                                 | 1453.0879 | 1463.8403 |           |
| 1476.4833                                                 | 1483.9937 | 1494.3394 |           |
| 1499.0434                                                 | 1505.6572 | 1514.7335 |           |
| 1617.2273                                                 | 1828.5309 | 3008.0224 |           |
| 3043.9863                                                 | 3048.9138 | 3049.4529 |           |
| 3054.8075                                                 | 3055.7609 | 3064.9956 |           |
| 3101.7890                                                 | 3111.3877 | 3117.7456 |           |
| 3126.2065                                                 | 3128.3943 | 3148.7342 |           |
| 3161.9101                                                 | 3164.1044 | 3181.5355 |           |
| Zero-point correction (Hartree): 0.245135                 |           |           |           |
| ApineneCI.J.b.ringclose.mppm                              |           |           |           |
| ~~~~~                                                     |           |           |           |
| E(RM062X/Aug-CC-pVTZ) (Hartree): -616.12303283            |           |           |           |
| Electronic state : 1-A                                    |           |           |           |
| Cartesian coordinates (Angs):                             |           |           |           |
| C                                                         | -0.698888 | 0.119140  | -0.250477 |
| H                                                         | -1.110117 | 0.302706  | -1.242579 |
| C                                                         | -1.844018 | 0.221171  | 0.755092  |
| C                                                         | -2.847846 | -0.841756 | 0.538003  |
| H                                                         | -1.443743 | 0.046103  | 1.761725  |
| H                                                         | -2.327466 | 1.193148  | 0.694960  |
| H                                                         | -2.550965 | -1.866845 | 0.797047  |
| C                                                         | 0.575190  | 0.990154  | -0.046033 |
| C                                                         | 0.186809  | -1.143475 | -0.274880 |
| C                                                         | 0.629707  | 2.285048  | -0.831793 |
| C                                                         | 0.891496  | 1.239416  | 1.423036  |
| H                                                         | 0.910287  | 0.316536  | 2.007017  |
| H                                                         | 1.867394  | 1.710244  | 1.521659  |
| H                                                         | 0.141863  | 1.901555  | 1.860493  |
| H                                                         | 1.626789  | 2.722771  | -0.768541 |
| H                                                         | -0.086133 | 3.007719  | -0.434772 |
| H                                                         | 0.392021  | 2.116649  | -1.882771 |
| H                                                         | -0.071441 | -1.936008 | -0.973978 |
| H                                                         | 0.303292  | -1.570783 | 0.723260  |
| C                                                         | 1.366486  | -0.213890 | -0.629527 |
| H                                                         | 1.431045  | -0.111357 | -1.717577 |
| C                                                         | 2.762118  | -0.510305 | -0.144508 |
| C                                                         | 3.169038  | -1.961645 | -0.098758 |
| H                                                         | 2.889042  | -2.463579 | -1.026012 |
| H                                                         | 2.631461  | -2.462173 | 0.708803  |
| H                                                         | 4.238124  | -2.043517 | 0.072425  |
| O                                                         | 3.516510  | 0.377529  | 0.169815  |
| O                                                         | -4.062259 | -0.698933 | 0.221500  |
| O                                                         | -3.702001 | 0.075616  | -0.984076 |
| Rotational constants (GHz): 1.5515800 0.4113500 0.3690800 |           |           |           |
| Vibrational harmonic frequencies (cm-1):                  |           |           |           |
| i737.2125                                                 | 35.7037   | 42.1120   |           |
| 64.8030                                                   | 108.6328  | 122.5532  |           |
| 132.7332                                                  | 161.9464  | 206.7753  |           |
| 220.4840                                                  | 256.3957  | 276.7335  |           |
| 312.2298                                                  | 323.0158  | 347.3189  |           |
| 396.6193                                                  | 400.7435  | 431.8272  |           |
| 502.2290                                                  | 521.0640  | 538.7739  |           |
| 602.7916                                                  | 631.0865  | 733.4214  |           |
| 770.1949                                                  | 819.6449  | 877.4077  |           |
| 900.4017                                                  | 927.1782  | 938.7837  |           |

|           |           |           |
|-----------|-----------|-----------|
| 966.1649  | 978.8204  | 986.4700  |
| 1003.6268 | 1029.9195 | 1036.4800 |
| 1064.4711 | 1104.3593 | 1138.9359 |
| 1151.2631 | 1178.9078 | 1197.1647 |
| 1214.8772 | 1237.0571 | 1254.9885 |
| 1263.3887 | 1284.6714 | 1303.6208 |
| 1331.3629 | 1346.0642 | 1374.7854 |
| 1390.5958 | 1394.8223 | 1407.7615 |
| 1418.6507 | 1454.9863 | 1464.4812 |
| 1477.3690 | 1484.1539 | 1493.1077 |
| 1498.3967 | 1506.6873 | 1514.1711 |
| 1621.9247 | 1832.3215 | 3023.3025 |
| 3049.2936 | 3051.0557 | 3054.6211 |
| 3054.9986 | 3064.4170 | 3070.3105 |
| 3107.3575 | 3113.1320 | 3119.4712 |
| 3125.7043 | 3130.0026 | 3137.0870 |
| 3151.7779 | 3155.1311 | 3181.5755 |

Zero-point correction (Hartree): 0.245130

ApineneCI.J.b.ringclose.mppp

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E(RM062X/Aug-CC-pVT2) (Hartree): -616.12178705

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.591539 | 0.092997  | -0.531758 |
| H | -0.847814 | 0.281242  | -1.577195 |
| C | -1.844380 | 0.189526  | 0.334688  |
| C | -2.827832 | -0.814035 | -0.131815 |
| H | -1.591254 | -0.039852 | 1.373333  |
| H | -2.307780 | 1.173416  | 0.319103  |
| H | -2.445253 | -1.824253 | -0.333008 |
| C | 0.642655  | 0.975946  | -0.168775 |
| C | 0.304978  | -1.161395 | -0.442205 |
| C | 0.792337  | 2.268540  | -0.945165 |
| C | 0.760014  | 1.230312  | 1.328530  |
| H | 0.704690  | 0.308735  | 1.912054  |
| H | 1.714352  | 1.703739  | 1.550609  |
| H | -0.041327 | 1.890246  | 1.664200  |
| H | 1.769981  | 2.711583  | -0.751796 |
| H | 0.026970  | 2.988458  | -0.648172 |
| H | 0.699501  | 2.096325  | -2.018431 |
| H | 0.156423  | -1.956114 | -1.170241 |
| H | 0.282494  | -1.590026 | 0.561309  |
| C | 1.514186  | -0.223513 | -0.634880 |
| H | 1.729426  | -0.120819 | -1.703292 |
| C | 2.834140  | -0.495387 | 0.041820  |
| C | 3.218650  | -1.939597 | 0.237196  |
| H | 3.043448  | -2.507889 | -0.677384 |
| H | 2.586218  | -2.378634 | 1.011323  |
| H | 4.259427  | -2.010116 | 0.538352  |
| O | 3.548590  | 0.412474  | 0.389798  |
| O | -4.015494 | -0.606052 | -0.505442 |
| O | -4.352941 | 0.010277  | 0.793572  |

Rotational constants (GHz): 1.6061200 0.3835300 0.3463800

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i747.8751 | 25.8187   | 47.3015   |
| 52.5239   | 108.8191  | 109.7042  |
| 128.1005  | 163.8448  | 214.6815  |
| 231.1253  | 246.3490  | 280.1985  |
| 298.5904  | 316.5385  | 328.2132  |
| 368.4614  | 412.1533  | 473.5699  |
| 481.0889  | 513.5589  | 532.9820  |
| 599.2419  | 631.8157  | 733.1710  |
| 766.9427  | 792.8328  | 867.0832  |
| 898.6353  | 923.4920  | 938.5407  |
| 966.5854  | 980.9972  | 989.3572  |
| 1006.5333 | 1028.9101 | 1038.2456 |
| 1070.4562 | 1102.0109 | 1134.5972 |
| 1149.7569 | 1176.4366 | 1196.4074 |
| 1209.9888 | 1237.1819 | 1250.5654 |
| 1257.9971 | 1279.5031 | 1296.4329 |
| 1321.0927 | 1348.9372 | 1383.5011 |
| 1391.7082 | 1398.4163 | 1411.3456 |
| 1420.9734 | 1450.6422 | 1463.2318 |
| 1477.2350 | 1485.2420 | 1494.9251 |
| 1499.2792 | 1507.7539 | 1515.3957 |
| 1625.4015 | 1833.0939 | 3048.8683 |
| 3049.2351 | 3052.8256 | 3055.6636 |
| 3060.9696 | 3063.8206 | 3070.6786 |
| 3076.6810 | 3117.4994 | 3119.4680 |
| 3125.2745 | 3129.8026 | 3136.4233 |
| 3151.3057 | 3151.6868 | 3180.5216 |

Zero-point correction (Hartree): 0.244849

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E(RM062X/Aug-CC-pVT2) (Hartree): -616.12316454

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.789817 | 0.244284  | -0.248575 |
| H | -1.191133 | 0.300729  | -1.262209 |
| C | -1.869622 | 0.618282  | 0.742941  |
| C | -3.261424 | 0.206668  | 0.456854  |
| H | -1.629137 | 0.274506  | 1.755769  |
| H | -1.943252 | 1.712846  | 0.841458  |
| H | -4.039158 | 0.678987  | 1.070495  |
| C | 0.552144  | 1.041288  | -0.183823 |
| C | 0.002046  | -1.064033 | -0.095785 |
| C | 0.694298  | 2.202057  | -1.148030 |
| C | 0.905951  | 1.475627  | 1.234759  |
| H | 0.836045  | 0.650859  | 1.947204  |
| H | 1.925715  | 1.853438  | 1.266899  |

|                                                           |           |           |           |
|-----------------------------------------------------------|-----------|-----------|-----------|
| H                                                         | 0.236670  | 2.269900  | 1.570827  |
| H                                                         | 1.718980  | 2.576257  | -1.142792 |
| H                                                         | 0.032728  | 3.024840  | -0.865286 |
| H                                                         | 0.443279  | 1.899960  | -2.165735 |
| H                                                         | -0.342307 | -1.913592 | -0.675072 |
| H                                                         | 0.084079  | -1.356316 | 0.952205  |
| C                                                         | 1.246543  | -0.288675 | -0.579416 |
| H                                                         | 1.309997  | -0.354876 | -1.670915 |
| C                                                         | 2.621089  | -0.613052 | -0.057665 |
| C                                                         | 2.917703  | -2.069794 | 0.193144  |
| H                                                         | 2.588609  | -2.674225 | -0.653218 |
| H                                                         | 2.349418  | -2.407774 | 1.061685  |
| H                                                         | 3.979081  | -2.209408 | 0.374984  |
| O                                                         | 3.445213  | 0.250181  | 0.128064  |
| O                                                         | -3.690535 | -0.485065 | -0.507060 |
| O                                                         | -2.813812 | -1.620371 | -0.157596 |
| Rotational constants (GHz): 1.4170100 0.4691200 0.3972800 |           |           |           |
| Vibrational harmonic frequencies (cm-1):                  |           |           |           |
| i722.7002                                                 | 36.1985   | 51.2473   |           |
| 70.2520                                                   | 111.7231  | 125.4060  |           |
| 133.2131                                                  | 177.3873  | 193.5048  |           |
| 221.0338                                                  | 258.7119  | 274.0222  |           |
| 306.8142                                                  | 317.0857  | 333.8786  |           |
| 355.1950                                                  | 409.1065  | 418.0149  |           |
| 507.1464                                                  | 517.9029  | 585.9167  |           |
| 613.7497                                                  | 668.3737  | 729.8772  |           |
| 753.1735                                                  | 793.1968  | 843.6355  |           |
| 902.3716                                                  | 921.8980  | 933.5350  |           |
| 963.3232                                                  | 972.7749  | 980.2101  |           |
| 1002.8512                                                 | 1015.0547 | 1028.5853 |           |
| 1047.1924                                                 | 1094.9081 | 1124.4101 |           |
| 1149.1640                                                 | 1177.7160 | 1198.3680 |           |
| 1215.1145                                                 | 1234.4872 | 1241.7085 |           |
| 1256.6177                                                 | 1286.5603 | 1307.5448 |           |
| 1348.3744                                                 | 1362.4862 | 1383.7307 |           |
| 1393.3080                                                 | 1403.7579 | 1418.8720 |           |
| 1419.7158                                                 | 1437.0911 | 1463.4470 |           |
| 1476.2063                                                 | 1484.3655 | 1495.6385 |           |
| 1499.9721                                                 | 1507.0336 | 1515.6460 |           |
| 1620.8729                                                 | 1828.3247 | 2990.9284 |           |
| 3043.3511                                                 | 3045.7782 | 3047.9714 |           |
| 3053.9695                                                 | 3058.2247 | 3065.3311 |           |
| 3078.6075                                                 | 3088.2388 | 3110.4150 |           |
| 3114.5737                                                 | 3126.9068 | 3127.6792 |           |
| 3152.2226                                                 | 3174.0734 | 3180.1290 |           |
| Zero-point correction (Hartree): 0.244624                 |           |           |           |
| ApineneCI.J.b.ringclose.mptp                              |           |           |           |
| ~~~~~                                                     |           |           |           |
| E(RM062X/Aug-CC-pVTZ) (Hartree): -616.12312253            |           |           |           |
| Electronic state : 1-A                                    |           |           |           |
| Cartesian coordinates (Angs):                             |           |           |           |
| C                                                         | -0.790748 | 0.460109  | -0.320349 |
| H                                                         | -1.126204 | 0.592999  | -1.345812 |
| C                                                         | -1.907861 | 0.846450  | 0.620759  |
| C                                                         | -3.014884 | -0.120497 | 0.795852  |
| H                                                         | -1.537953 | 0.986867  | 1.647353  |
| H                                                         | -2.354789 | 1.811716  | 0.356234  |
| H                                                         | -3.698937 | 0.079380  | 1.630418  |
| C                                                         | 0.621304  | 1.104970  | -0.155085 |
| C                                                         | -0.154063 | -0.934209 | -0.187499 |
| C                                                         | 0.931501  | 2.278406  | -1.063864 |
| C                                                         | 0.968411  | 1.443836  | 1.289527  |
| H                                                         | 0.782445  | 0.607713  | 1.967603  |
| H                                                         | 2.021769  | 1.704059  | 1.370214  |
| H                                                         | 0.377554  | 2.296174  | 1.631403  |
| H                                                         | 1.992423  | 2.527171  | -1.012173 |
| H                                                         | 0.361396  | 3.161400  | -0.765835 |
| H                                                         | 0.681594  | 2.047914  | -2.100231 |
| H                                                         | -0.564996 | -1.720901 | -0.814149 |
| H                                                         | -0.135820 | -1.272500 | 0.850721  |
| C                                                         | 1.182905  | -0.277244 | -0.590580 |
| H                                                         | 1.279446  | -0.300495 | -1.681166 |
| C                                                         | 2.492216  | -0.776500 | -0.039278 |
| C                                                         | 2.620892  | -2.267970 | 0.141315  |
| H                                                         | 2.269918  | -2.788527 | -0.750795 |
| H                                                         | 1.981258  | -2.587987 | 0.965879  |
| H                                                         | 3.652259  | -2.530123 | 0.357226  |
| O                                                         | 3.395934  | -0.019170 | 0.221617  |
| O                                                         | -3.174972 | -1.240078 | 0.233605  |
| O                                                         | -3.180887 | -0.635623 | -1.111683 |
| Rotational constants (GHz): 1.3116500 0.4922400 0.4178700 |           |           |           |
| Vibrational harmonic frequencies (cm-1):                  |           |           |           |
| i718.5847                                                 | 37.9608   | 55.7702   |           |
| 79.5889                                                   | 117.1813  | 129.8067  |           |
| 139.9733                                                  | 170.5630  | 188.2785  |           |
| 230.5838                                                  | 262.8682  | 281.0501  |           |
| 313.7856                                                  | 329.2495  | 338.6273  |           |
| 352.3228                                                  | 409.6340  | 421.7389  |           |
| 503.0680                                                  | 517.5814  | 581.5794  |           |
| 613.7968                                                  | 665.1215  | 736.7092  |           |
| 749.0049                                                  | 807.7516  | 844.1626  |           |
| 901.1663                                                  | 924.6595  | 945.2443  |           |
| 951.5978                                                  | 965.7652  | 982.7959  |           |
| 994.5828                                                  | 1014.1594 | 1032.3025 |           |
| 1045.9080                                                 | 1088.4807 | 1131.1760 |           |
| 1162.8945                                                 | 1174.4525 | 1195.1729 |           |
| 1208.0425                                                 | 1237.9404 | 1247.8955 |           |
| 1265.7043                                                 | 1289.8899 | 1308.3074 |           |
| 1348.4561                                                 | 1363.1797 | 1384.3607 |           |
| 1393.3702                                                 | 1404.5195 | 1418.7985 |           |
| 1419.3843                                                 | 1439.8215 | 1464.1970 |           |

|           |           |           |
|-----------|-----------|-----------|
| 1476.7966 | 1485.7840 | 1495.2560 |
| 1497.6321 | 1508.6808 | 1516.4966 |
| 1615.5735 | 1828.5769 | 3007.9243 |
| 3045.8418 | 3048.0947 | 3051.7470 |
| 3052.6368 | 3062.4691 | 3064.9625 |
| 3072.1317 | 3109.0976 | 3114.3904 |
| 3126.5234 | 3127.5730 | 3132.5233 |
| 3150.8998 | 3154.9769 | 3180.2264 |

Zero-point correction (Hartree): 0.244923

ApineneCI.J.b.ringclose.mtmm  
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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.11963109

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.475415  | 0.262269  | 1.175057  |
| H | 0.383549  | 0.812686  | 2.113515  |
| C | 1.972428  | 0.059054  | 0.937413  |
| C | 2.300291  | -0.845638 | -0.191560 |
| H | 2.498292  | 1.000261  | 0.786557  |
| H | 2.406765  | -0.396461 | 1.833074  |
| H | 1.716600  | -1.769341 | -0.284081 |
| C | -0.423534 | 0.979614  | 0.126326  |
| C | -0.535170 | -0.906021 | 1.217538  |
| C | -0.585582 | 2.477299  | 0.293481  |
| C | -0.038249 | 0.642256  | -1.308654 |
| H | 0.034690  | -0.435830 | -1.479592 |
| H | -0.789055 | 1.023405  | -1.998263 |
| H | 0.923517  | 1.091969  | -1.560716 |
| H | -1.366888 | 2.849475  | -0.370154 |
| H | 0.343933  | 2.995156  | 0.047790  |
| H | -0.856307 | 2.731419  | 1.319380  |
| H | -0.730930 | -1.367927 | 2.182373  |
| H | -0.312671 | -1.689792 | 0.493912  |
| C | -1.577762 | 0.085765  | 0.656963  |
| H | -2.077613 | 0.594872  | 1.487426  |
| C | -2.666310 | -0.374074 | -0.279160 |
| C | -3.241160 | -1.746258 | -0.034665 |
| H | -3.451708 | -1.887305 | 1.026372  |
| H | -2.504855 | -2.501467 | -0.316469 |
| H | -4.141987 | -1.882983 | -0.625188 |
| O | -3.064469 | 0.339884  | -1.166563 |
| O | 3.094286  | -0.621145 | -1.148531 |
| O | 4.200491  | -0.340457 | -0.211451 |

Rotational constants (GHz): 1.4322300 0.4378800 0.4150600

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i742.1090 | 32.3059   | 57.3170   |
| 71.2030   | 97.8583   | 126.0899  |
| 151.8693  | 189.3651  | 217.9975  |
| 236.7848  | 263.3283  | 269.2496  |
| 285.3362  | 323.3562  | 338.9056  |
| 368.2915  | 409.8002  | 462.0318  |
| 474.5907  | 519.1775  | 587.2996  |
| 613.8134  | 622.5905  | 711.0150  |
| 739.2514  | 775.8002  | 865.5020  |
| 898.6057  | 917.7555  | 923.8011  |
| 963.9449  | 977.6769  | 994.6620  |
| 1005.8574 | 1030.6896 | 1040.2102 |
| 1049.8953 | 1116.3984 | 1133.2691 |
| 1142.5101 | 1179.2781 | 1195.8188 |
| 1214.2722 | 1239.0784 | 1242.5692 |
| 1261.6898 | 1296.9373 | 1298.1503 |
| 1322.9762 | 1356.0824 | 1391.0117 |
| 1392.9535 | 1401.2172 | 1412.4534 |
| 1422.3529 | 1435.8977 | 1464.2243 |
| 1476.9231 | 1484.4035 | 1495.8476 |
| 1500.9981 | 1507.0027 | 1516.2421 |
| 1620.7030 | 1832.5250 | 3045.0746 |
| 3048.5011 | 3051.5010 | 3052.4387 |
| 3064.2368 | 3068.8941 | 3074.1551 |
| 3093.3932 | 3112.8589 | 3117.1571 |
| 3125.5731 | 3129.0869 | 3138.0229 |
| 3145.5066 | 3149.1024 | 3181.2908 |

Zero-point correction (Hartree): 0.245048

ApineneCI.J.b.ringclose.mtmm  
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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.11826551

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.510903  | -0.258041 | 1.220031  |
| H | 0.454931  | 0.136867  | 2.235976  |
| C | 1.966982  | -0.689216 | 1.014513  |
| C | 2.393823  | -0.943435 | -0.377512 |
| H | 2.662181  | 0.008536  | 1.467943  |
| H | 2.065531  | -1.672492 | 1.502396  |
| H | 1.816951  | -1.672466 | -0.960261 |
| C | -0.256040 | 0.748569  | 0.309845  |
| C | -0.651495 | -1.254320 | 1.056312  |
| C | -0.170261 | 2.208921  | 0.699165  |
| C | -0.004226 | 0.584189  | -1.185685 |
| H | -0.112321 | -0.452683 | -1.515706 |
| H | -0.737410 | 1.173213  | -1.738197 |
| H | 0.991998  | 0.938025  | -1.451574 |
| H | -0.908976 | 2.791222  | 0.147289  |
| H | 0.822977  | 2.599014  | 0.468096  |
| H | -0.357010 | 2.343044  | 1.765655  |
| H | -0.909617 | -1.872630 | 1.913751  |
| H | -0.522838 | -1.896530 | 0.183966  |
| C | -1.539832 | -0.037204 | 0.736643  |
| H | -1.932872 | 0.401071  | 1.656691  |
| C | -2.676610 | -0.094653 | -0.253995 |

|                                                           |           |           |           |
|-----------------------------------------------------------|-----------|-----------|-----------|
| C                                                         | -3.098483 | -1.440694 | -0.784070 |
| H                                                         | -3.218007 | -2.155625 | 0.030959  |
| H                                                         | -2.314148 | -1.829039 | -1.437825 |
| H                                                         | -4.020615 | -1.342333 | -1.348706 |
| O                                                         | -3.209716 | 0.926612  | -0.614205 |
| O                                                         | 3.485455  | -0.576670 | -0.904300 |
| O                                                         | 3.145597  | 0.844823  | -0.672986 |
| Rotational constants (GHz): 1.4521900 0.4730500 0.4459600 |           |           |           |
| Vibrational harmonic frequencies (cm-1):                  |           |           |           |
| i736.3206                                                 | 21.9930   | 27.5530   |           |
| 88.6275                                                   | 113.6852  | 148.7392  |           |
| 177.6716                                                  | 183.6452  | 196.2126  |           |
| 241.1017                                                  | 257.3601  | 287.2729  |           |
| 330.5087                                                  | 347.5355  | 352.1017  |           |
| 387.5606                                                  | 415.2368  | 457.3027  |           |
| 486.1595                                                  | 495.8343  | 585.5007  |           |
| 615.2525                                                  | 646.2628  | 715.2331  |           |
| 749.7454                                                  | 816.2789  | 835.3684  |           |
| 887.0321                                                  | 919.5863  | 930.6136  |           |
| 970.1316                                                  | 987.3114  | 996.1973  |           |
| 1005.4629                                                 | 1017.1743 | 1046.3621 |           |
| 1053.9085                                                 | 1113.9697 | 1132.8337 |           |
| 1151.6449                                                 | 1177.0996 | 1187.7681 |           |
| 1214.6401                                                 | 1251.3971 | 1253.2224 |           |
| 1265.8835                                                 | 1292.4823 | 1312.5111 |           |
| 1330.0849                                                 | 1354.4885 | 1384.5515 |           |
| 1388.9837                                                 | 1400.5573 | 1413.6678 |           |
| 1422.2497                                                 | 1441.9659 | 1465.3497 |           |
| 1476.5127                                                 | 1488.6718 | 1495.5876 |           |
| 1501.1699                                                 | 1514.6442 | 1528.3083 |           |
| 1613.9885                                                 | 1829.5685 | 2978.7889 |           |
| 3041.9981                                                 | 3049.4011 | 3061.3666 |           |
| 3063.0629                                                 | 3074.7754 | 3077.6284 |           |
| 3083.6804                                                 | 3111.7047 | 3121.4383 |           |
| 3123.5549                                                 | 3129.2028 | 3132.9607 |           |
| 3136.7019                                                 | 3175.3133 | 3180.6715 |           |
| Zero-point correction (Hartree): 0.245449                 |           |           |           |
| ApineneCI.J.b.ringclose.mtpm                              |           |           |           |
| ~~~~~                                                     |           |           |           |
| E(RM062X/Aug-CC-pVTZ) (Hartree): -616.12099903            |           |           |           |
| Electronic state : 1-A                                    |           |           |           |
| Cartesian coordinates (Angs):                             |           |           |           |
| C                                                         | 0.602084  | 0.836293  | 0.993796  |
| H                                                         | 0.461092  | 1.592714  | 1.768264  |
| C                                                         | 2.116459  | 0.790503  | 0.719588  |
| C                                                         | 2.622138  | 0.189252  | -0.536991 |
| H                                                         | 2.480213  | 1.825331  | 0.683142  |
| H                                                         | 2.593361  | 0.262554  | 1.545013  |
| H                                                         | 2.580658  | 0.797688  | -1.445839 |
| C                                                         | -0.484613 | 1.086421  | -0.093657 |
| C                                                         | -0.141439 | -0.439329 | 1.423390  |
| C                                                         | -0.970615 | 2.511539  | -0.266093 |
| C                                                         | -0.170861 | 0.461696  | -1.448387 |
| H                                                         | 0.293677  | -0.523456 | -1.354010 |
| H                                                         | -1.087843 | 0.356118  | -2.030370 |
| H                                                         | 0.493229  | 1.109930  | -2.022816 |
| H                                                         | -1.868287 | 2.529517  | -0.885984 |
| H                                                         | -0.209130 | 3.127059  | -0.751199 |
| H                                                         | -1.214179 | 2.962816  | 0.696310  |
| H                                                         | -0.176270 | -0.655195 | 2.488875  |
| H                                                         | 0.233809  | -1.307489 | 0.889794  |
| C                                                         | -1.400528 | 0.152103  | 0.767860  |
| H                                                         | -1.968076 | 0.768991  | 1.466446  |
| C                                                         | -2.391383 | -0.694174 | 0.005662  |
| C                                                         | -2.157077 | -2.178348 | -0.072688 |
| H                                                         | -2.024807 | -2.594123 | 0.927262  |
| H                                                         | -1.229173 | -2.371875 | -0.615957 |
| H                                                         | -2.988931 | -2.656708 | -0.580405 |
| O                                                         | -3.324120 | -0.162867 | -0.549779 |
| O                                                         | 3.316639  | -0.866713 | -0.640591 |
| O                                                         | 2.243190  | -1.660371 | -0.026305 |
| Rotational constants (GHz): 1.2409800 0.5594900 0.4733000 |           |           |           |
| Vibrational harmonic frequencies (cm-1):                  |           |           |           |
| i735.8716                                                 | 36.6076   | 50.0889   |           |
| 59.5203                                                   | 138.1356  | 152.3581  |           |
| 165.8305                                                  | 190.8424  | 220.7833  |           |
| 240.4817                                                  | 264.1247  | 280.8180  |           |
| 317.2523                                                  | 342.8521  | 362.6731  |           |
| 395.1155                                                  | 422.6182  | 462.8981  |           |
| 486.1710                                                  | 500.5979  | 586.1870  |           |
| 612.3387                                                  | 640.9036  | 716.9063  |           |
| 744.9634                                                  | 827.1718  | 849.4235  |           |
| 886.5534                                                  | 929.0758  | 954.9503  |           |
| 968.2542                                                  | 981.3596  | 998.9704  |           |
| 1008.8556                                                 | 1019.1381 | 1040.3130 |           |
| 1071.6393                                                 | 1075.9732 | 1143.6775 |           |
| 1155.7547                                                 | 1179.4664 | 1193.7165 |           |
| 1225.3325                                                 | 1255.0195 | 1258.5262 |           |
| 1264.6918                                                 | 1292.0319 | 1306.7309 |           |
| 1331.2246                                                 | 1352.6178 | 1384.2154 |           |
| 1391.0378                                                 | 1401.6392 | 1411.3498 |           |
| 1418.6376                                                 | 1452.3024 | 1464.0294 |           |
| 1473.9334                                                 | 1488.6498 | 1496.1738 |           |
| 1504.4599                                                 | 1520.8840 | 1523.3538 |           |
| 1603.7760                                                 | 1822.5080 | 3015.5451 |           |
| 3040.7367                                                 | 3045.3164 | 3060.5435 |           |
| 3072.6122                                                 | 3086.0725 | 3086.6266 |           |
| 3109.5355                                                 | 3112.7851 | 3115.2800 |           |
| 3119.2855                                                 | 3121.7842 | 3127.4963 |           |
| 3129.0459                                                 | 3179.7926 | 3182.4372 |           |
| Zero-point correction (Hartree): 0.245868                 |           |           |           |



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ApineneCI.J.b.ringclose.mtpp
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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.11781364
Electronic state : 1-A
Cartesian coordinates (Angs):
C      -0.537325      0.490003      -0.923253
H      -0.475892      0.972619      -1.900453
C      -2.009039      0.563975      -0.500189
C      -2.382927      -0.474065      0.493423
H      -2.208106      1.546240      -0.060534
H      -2.686442      0.461827      -1.344428
H      -1.713076      -0.639838      1.343367
C      0.618317      1.080044      -0.061792
C      0.233150      -0.845479      -1.010489
C      1.002677      2.514449      -0.368238
C      0.421646      0.898471      1.439962
H      0.316231      -0.150151      1.724616
H      1.285865      1.283933      1.976917
H      -0.463122      1.442111      1.778956
H      1.932540      2.774224      0.138917
H      0.226743      3.203171      -0.025942
H      1.140747      2.664835      -1.439820
H      0.198244      -1.394885      -1.948093
H      -0.023181      -1.526335      -0.196763
C      1.505667      -0.034370      -0.680516
H      1.951116      0.330596      -1.611887
C      2.627852      -0.640128      0.122891
C      2.945537      -2.089350      -0.143574
H      3.008687      -2.271838      -1.217313
H      2.134878      -2.713604      0.237112
H      3.875210      -2.363619      0.345660
O      3.246959      0.018032      0.922718
O      -3.315838      -1.319543      0.379991
O      -4.312841      -0.248561      0.196084
Rotational constants (GHz):      1.3878000      0.4372200      0.3858300
Vibrational harmonic frequencies (cm-1):
i752.3126      37.1927      51.0149
74.2018      99.8307      135.0607
152.9147      186.4521      201.7212
238.6487      261.9503      273.5188
285.1628      317.5499      347.6512
362.7480      417.6061      468.2369
473.1550      519.8871      587.8290
610.6861      623.2910      725.7427
754.5065      765.1568      859.5017
897.2560      924.5269      946.4440
965.4992      973.8117      995.6276
1003.6699      1026.4414      1040.7724
1064.3709      1085.6994      1129.8614
1153.7365      1178.7397      1197.7522
1225.2402      1228.4588      1241.7242
1260.8481      1298.4564      1303.6014
1320.0560      1357.2850      1388.8600
1394.5408      1400.3283      1410.8556
1421.5173      1446.1749      1464.6780
1477.6851      1487.1132      1495.7560
1500.6844      1507.9635      1519.1561
1618.3841      1832.4469      3046.4459
3048.8616      3051.8941      3058.4046
3064.4261      3071.2965      3079.2222
3098.6856      3114.3546      3116.1949
3125.8946      3129.2797      3142.2172
3148.3824      3150.2735      3180.9714
Zero-point correction (Hartree): 0.245231

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ApineneCI.J.b.ringclose.mtpp
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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.11592765
Electronic state : 1-A
Cartesian coordinates (Angs):
C 0.689972 0.805726 0.974052
H 0.572130 1.622234 1.692672
C 2.193292 0.766533 0.725741
C 2.941710 -0.068394 -0.248260
H 2.529452 1.782714 0.465781
H 2.710059 0.573495 1.676495
H 3.987159 0.249381 -0.364206
C -0.360035 1.069209 -0.142238
C -0.165238 -0.367064 1.489547
C -0.715308 2.519302 -0.406196
C -0.077751 0.343868 -1.449852
H 0.186023 -0.700948 -1.289734
H -0.957077 0.394666 -2.093567
H 0.748229 0.821123 -1.980934
H -1.607421 2.577819 -1.031412
H 0.097708 3.030615 -0.927860
H -0.916837 3.053062 0.523626
H -0.238576 -0.482140 2.568989
H 0.132925 -1.304910 1.035745
C -1.361523 0.274914 0.762139
H -1.896105 0.980713 1.400216
C -2.395754 -0.547717 0.032892
C -2.274005 -2.047452 0.064923
H -2.216976 -2.397629 1.096877
H -1.342276 -2.349389 -0.418501
H -3.120642 -2.496661 -0.445086
O -3.275109 0.009702 -0.581291
O 2.587431 -0.973650 -1.051418
O 1.997686 -1.767014 0.042010
Rotational constants (GHz): 1.2243100 0.5881500 0.5015600
Vibrational harmonic frequencies (cm-1):

```

|           |           |           |
|-----------|-----------|-----------|
| i720.9885 | 45.0340   | 49.8714   |
| 62.1389   | 135.5087  | 143.0481  |
| 186.0907  | 201.7997  | 207.3698  |
| 225.5975  | 248.4858  | 278.1479  |
| 301.3805  | 325.9557  | 352.9362  |
| 380.7725  | 403.8719  | 459.2072  |
| 488.0506  | 516.3741  | 587.5033  |
| 606.9509  | 694.7892  | 718.0496  |
| 740.4374  | 761.8408  | 845.6030  |
| 890.4034  | 896.3386  | 934.5816  |
| 963.9174  | 970.3240  | 996.2032  |
| 1005.1681 | 1019.9357 | 1028.8481 |
| 1055.9336 | 1084.1512 | 1143.9657 |
| 1151.9884 | 1185.2788 | 1196.6325 |
| 1234.9522 | 1257.5392 | 1261.3721 |
| 1275.0882 | 1298.8827 | 1331.6607 |
| 1350.1777 | 1381.1110 | 1392.5374 |
| 1397.8834 | 1405.4334 | 1418.9963 |
| 1432.1243 | 1433.8254 | 1465.8284 |
| 1474.5266 | 1486.3999 | 1494.3328 |
| 1506.3686 | 1513.0866 | 1516.4353 |
| 1629.9336 | 1822.1183 | 2987.2725 |
| 3021.3695 | 3042.4307 | 3045.9181 |
| 3050.3644 | 3055.5390 | 3061.7085 |
| 3084.0391 | 3107.7524 | 3110.7038 |
| 3118.3925 | 3122.0039 | 3126.8184 |
| 3149.1601 | 3180.9907 | 3196.5915 |

Zero-point correction (Hartree): 0.245432

ApineneCI.J.b.ringclose.pmmm

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.12371327

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.553785 | -0.246239 | -0.754137 |
| H | -0.829125 | 0.219904  | -1.703404 |
| C | -1.809444 | -0.733066 | -0.033486 |
| C | -2.754216 | 0.393007  | 0.152426  |
| H | -2.315176 | -1.530145 | -0.573882 |
| H | -1.541953 | -1.129551 | 0.949112  |
| H | -2.334538 | 1.338960  | 0.521335  |
| C | 0.487169  | 0.670136  | -0.037131 |
| C | 0.558855  | -1.283732 | -0.992906 |
| C | 0.451418  | 2.145084  | -0.392374 |
| C | 0.517946  | 0.472047  | 1.472468  |
| H | 0.600037  | -0.579228 | 1.748298  |
| H | 1.374327  | 0.991908  | 1.906500  |
| H | -0.381559 | 0.881526  | 1.936660  |
| H | 1.342355  | 2.656925  | -0.022850 |
| H | -0.412911 | 2.639658  | 0.056464  |
| H | 0.401263  | 2.288815  | -1.472218 |
| H | 0.570064  | -1.797709 | -1.950110 |
| H | 0.610615  | -2.016952 | -0.188807 |
| C | 1.594992  | -0.178130 | -0.765411 |
| H | 1.878591  | 0.326018  | -1.691025 |
| C | 2.823560  | -0.498497 | 0.046332  |
| C | 3.890946  | 0.565504  | 0.086347  |
| H | 3.447791  | 1.528457  | 0.347383  |
| H | 4.329848  | 0.676579  | -0.906691 |
| H | 4.662089  | 0.298996  | 0.802836  |
| O | 2.925745  | -1.530581 | 0.662184  |
| O | -3.952564 | 0.458598  | -0.239367 |
| O | -4.303976 | -0.756872 | 0.520638  |

Rotational constants (GHz): 1.8180600 0.3875700 0.3613300

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i748.0510 | 46.0044   | 54.4976   |
| 63.6930   | 82.3550   | 110.8062  |
| 144.7829  | 159.8141  | 230.2079  |
| 235.3026  | 250.8754  | 283.2836  |
| 290.6449  | 322.9205  | 340.1323  |
| 377.8990  | 403.0573  | 433.2636  |
| 492.9963  | 509.7845  | 581.2426  |
| 599.3500  | 623.7760  | 721.2996  |
| 764.7526  | 783.1534  | 872.5678  |
| 907.5066  | 941.1583  | 957.6270  |
| 964.5992  | 969.4308  | 986.9602  |
| 1002.2586 | 1017.6071 | 1037.7085 |
| 1082.4983 | 1101.6840 | 1118.8620 |
| 1150.7302 | 1175.3042 | 1193.0972 |
| 1203.1116 | 1211.5065 | 1253.7582 |
| 1261.6562 | 1273.0401 | 1291.2027 |
| 1325.6389 | 1366.2896 | 1382.4179 |
| 1391.0677 | 1406.9093 | 1414.7636 |
| 1428.0549 | 1449.5957 | 1462.9206 |
| 1476.7016 | 1485.5872 | 1493.1703 |
| 1500.1929 | 1507.4572 | 1509.8498 |
| 1623.4097 | 1836.0372 | 3046.2387 |
| 3052.4048 | 3052.6933 | 3061.3608 |
| 3063.1558 | 3076.5529 | 3083.9343 |
| 3099.7811 | 3109.4940 | 3115.1088 |
| 3124.2757 | 3126.2734 | 3135.6151 |
| 3149.2802 | 3159.9456 | 3179.7187 |

Zero-point correction (Hartree): 0.245075

ApineneCI.J.b.ringclose.pmp

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.12566754

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.642700 | -0.509419 | -0.483537 |
| H | -1.071058 | -0.165864 | -1.424067 |
| C | -1.796124 | -1.008358 | 0.387100  |

|                                                |           |           |           |
|------------------------------------------------|-----------|-----------|-----------|
| C                                              | -2.769871 | 0.051020  | 0.736196  |
| H                                              | -2.322966 | -1.805172 | -0.133595 |
| H                                              | -1.390574 | -1.372130 | 1.338826  |
| H                                              | -2.479052 | 0.770205  | 1.512721  |
| C                                              | 0.351772  | 0.564505  | 0.039329  |
| C                                              | 0.541473  | -1.454796 | -0.743697 |
| C                                              | 0.077689  | 1.988576  | -0.403301 |
| C                                              | 0.585872  | 0.492386  | 1.543072  |
| H                                              | 0.804335  | -0.520970 | 1.879833  |
| H                                              | 1.433382  | 1.119532  | 1.827188  |
| H                                              | -0.283893 | 0.861526  | 2.090086  |
| H                                              | 0.897232  | 2.655715  | -0.127874 |
| H                                              | -0.830090 | 2.371140  | 0.070221  |
| H                                              | -0.065355 | 2.043072  | -1.482386 |
| H                                              | 0.506176  | -2.066479 | -1.641113 |
| H                                              | 0.772194  | -2.084652 | 0.114769  |
| C                                              | 1.459299  | -0.225958 | -0.754192 |
| H                                              | 1.560165  | 0.209134  | -1.749847 |
| C                                              | 2.806649  | -0.319894 | -0.089206 |
| C                                              | 3.727287  | 0.857297  | -0.289189 |
| H                                              | 3.195674  | 1.786170  | -0.073659 |
| H                                              | 4.033826  | 0.903042  | -1.335658 |
| H                                              | 4.602145  | 0.765352  | 0.347431  |
| O                                              | 3.112862  | -1.261750 | 0.600166  |
| O                                              | -3.971800 | 0.138733  | 0.354907  |
| O                                              | -3.567339 | 0.112794  | -1.063615 |
| Rotational constants (GHz):                    |           |           | 1.8110800 |
| Vibrational harmonic frequencies (cm-1):       |           |           | 0.4134500 |
|                                                |           |           | 0.3940800 |
| 1747.0095                                      | 43.0261   |           | 58.9837   |
| 62.1717                                        | 105.1890  |           | 116.6316  |
| 139.8319                                       | 158.2383  |           | 215.9222  |
| 226.2224                                       | 262.3768  |           | 284.4392  |
| 305.2534                                       | 315.6911  |           | 356.3448  |
| 375.7063                                       | 412.5558  |           | 438.1205  |
| 460.5517                                       | 535.1767  |           | 582.7075  |
| 603.7426                                       | 624.7752  |           | 721.7990  |
| 775.0594                                       | 813.2851  |           | 878.6997  |
| 906.4115                                       | 945.7622  |           | 955.0434  |
| 964.1540                                       | 970.1707  |           | 987.5724  |
| 999.8933                                       | 1005.3158 |           | 1038.9377 |
| 1082.0946                                      | 1106.0394 |           | 1123.5022 |
| 1150.3363                                      | 1173.1400 |           | 1191.9438 |
| 1207.4131                                      | 1213.0995 |           | 1257.6382 |
| 1268.0103                                      | 1281.3982 |           | 1301.4475 |
| 1332.2204                                      | 1361.5791 |           | 1379.3698 |
| 1391.4056                                      | 1403.8302 |           | 1411.7488 |
| 1425.5559                                      | 1453.5466 |           | 1464.1752 |
| 1475.8019                                      | 1482.7288 |           | 1489.8999 |
| 1500.5885                                      | 1504.4276 |           | 1510.4030 |
| 1616.6181                                      | 1834.9542 |           | 3029.7547 |
| 3044.2165                                      | 3052.4357 |           | 3061.5642 |
| 3062.4332                                      | 3086.5249 |           | 3097.9593 |
| 3105.4073                                      | 3111.4813 |           | 3113.5902 |
| 3124.1268                                      | 3130.3472 |           | 3136.1103 |
| 3146.6926                                      | 3158.5149 |           | 3179.6848 |
| Zero-point correction (Hartree):               |           |           | 0.245317  |
| ApineneCI.J.b.ringclose.pmpm                   |           |           |           |
| ~~~~~                                          |           |           |           |
| E(RM062X/Aug-CC-pVT2) (Hartree): -616.12770046 |           |           |           |
| Electronic state : 1-A                         |           |           |           |
| Cartesian coordinates (Angs):                  |           |           |           |
| C                                              | -0.589792 | -0.776777 | -0.628618 |
| H                                              | -0.872092 | -0.674699 | -1.680718 |
| C                                              | -1.814261 | -1.186234 | 0.196133  |
| C                                              | -3.063696 | -0.585619 | -0.312805 |
| H                                              | -1.945779 | -2.268597 | 0.059880  |
| H                                              | -1.685759 | -0.955915 | 1.249856  |
| H                                              | -3.408018 | -0.929255 | -1.297739 |
| C                                              | 0.260290  | 0.468352  | -0.234508 |
| C                                              | 0.670250  | -1.651482 | -0.528305 |
| C                                              | -0.015631 | 1.738305  | -1.013285 |
| C                                              | 0.280299  | 0.734457  | 1.264536  |
| H                                              | 0.510529  | -0.164824 | 1.837686  |
| H                                              | 1.046945  | 1.474820  | 1.502281  |
| H                                              | -0.684161 | 1.124418  | 1.586949  |
| H                                              | 0.726843  | 2.506199  | -0.786181 |
| H                                              | -1.000075 | 2.126901  | -0.748866 |
| H                                              | 0.008421  | 1.552438  | -2.088657 |
| H                                              | 0.796837  | -2.442395 | -1.263749 |
| H                                              | 0.806725  | -2.062944 | 0.471194  |
| C                                              | 1.509437  | -0.380378 | -0.688994 |
| H                                              | 1.730977  | -0.156066 | -1.734353 |
| C                                              | 2.754820  | -0.232691 | 0.143409  |
| C                                              | 3.597635  | 0.985515  | -0.137724 |
| H                                              | 2.970957  | 1.879020  | -0.140048 |
| H                                              | 4.035269  | 0.900631  | -1.133995 |
| H                                              | 4.385443  | 1.077853  | 0.603902  |
| O                                              | 3.041899  | -1.024146 | 1.007787  |
| O                                              | -3.867580 | 0.172534  | 0.299997  |
| O                                              | -2.794214 | 1.143077  | 0.592656  |
| Rotational constants (GHz):                    |           |           | 1.7080500 |
| Vibrational harmonic frequencies (cm-1):       |           |           | 0.4517000 |
|                                                |           |           | 0.4145300 |
| 1729.7722                                      | 61.1096   |           | 68.5527   |
| 70.8029                                        | 99.2134   |           | 118.2370  |
| 163.0592                                       | 174.4117  |           | 214.0882  |
| 240.1187                                       | 262.1227  |           | 289.5665  |
| 309.6821                                       | 323.5583  |           | 351.8066  |
| 377.7445                                       | 425.2286  |           | 442.2686  |
| 466.1234                                       | 533.6567  |           | 583.5774  |
| 603.0920                                       | 625.9653  |           | 719.8472  |
| 772.3383                                       | 817.0971  |           | 886.9589  |

|           |           |           |
|-----------|-----------|-----------|
| 908.2667  | 923.2828  | 956.8418  |
| 969.4236  | 972.5276  | 990.5007  |
| 1003.2853 | 1022.0959 | 1052.2463 |
| 1067.8354 | 1102.6594 | 1119.6742 |
| 1150.6661 | 1176.1073 | 1189.0975 |
| 1201.1198 | 1214.2180 | 1252.6513 |
| 1262.7743 | 1279.5451 | 1292.2767 |
| 1324.0327 | 1371.2468 | 1389.9361 |
| 1394.1660 | 1401.7611 | 1415.4526 |
| 1420.3525 | 1454.7758 | 1464.6525 |
| 1477.4901 | 1484.0776 | 1499.6648 |
| 1500.3036 | 1508.0855 | 1519.9315 |
| 1620.2665 | 1834.2759 | 3007.9624 |
| 3043.8542 | 3046.2145 | 3054.2686 |
| 3057.0902 | 3064.4808 | 3081.3856 |
| 3095.8597 | 3112.7125 | 3119.8434 |
| 3125.2073 | 3127.4201 | 3148.7720 |
| 3152.5887 | 3167.2935 | 3179.4206 |

Zero-point correction (Hartree): 0.245523

ApineneCI.J.b.ringclose.pmpp

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.12549870

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.491896  | -0.494300 | 0.984837  |
| H | 0.657857  | -0.149695 | 2.009795  |
| C | 1.809357  | -0.966267 | 0.372842  |
| C | 2.793931  | 0.135697  | 0.471301  |
| H | 2.187208  | -1.817542 | 0.946281  |
| H | 1.714830  | -1.279934 | -0.662447 |
| H | 2.914101  | 0.601385  | 1.459557  |
| C | -0.357701 | 0.573619  | 0.236746  |
| C | -0.716002 | -1.448464 | 0.954750  |
| C | -0.216032 | 1.998505  | 0.735523  |
| C | -0.187457 | 0.507080  | -1.275994 |
| H | -0.326415 | -0.503207 | -1.660820 |
| H | -0.921059 | 1.149208  | -1.767467 |
| H | 0.805825  | 0.852580  | -1.567559 |
| H | -0.950691 | 2.657971  | 0.269419  |
| H | 0.773199  | 2.392838  | 0.487275  |
| H | -0.345402 | 2.054040  | 1.817329  |
| H | -0.899499 | -2.056168 | 1.836878  |
| H | -0.715070 | -2.085452 | 0.071425  |
| C | -1.618721 | -0.229893 | 0.724867  |
| H | -1.979867 | 0.203470  | 1.659715  |
| C | -2.752801 | -0.348752 | -0.259417 |
| C | -3.675879 | 0.839845  | -0.353066 |
| H | -3.094118 | 1.756162  | -0.468434 |
| H | -4.239148 | 0.934744  | 0.576997  |
| H | -4.360641 | 0.719909  | -1.187201 |
| O | -2.889657 | -1.322783 | -0.957264 |
| O | 3.367907  | 0.740033  | -0.477677 |
| O | 3.941167  | -0.521340 | -0.986945 |

Rotational constants (GHz): 1.6435400 0.4252800 0.4048100

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i738.3857 | 43.2331   | 54.5754   |
| 62.7695   | 82.9925   | 117.4937  |
| 153.6250  | 159.1983  | 224.0242  |
| 246.2592  | 256.3600  | 280.3034  |
| 289.1008  | 320.8537  | 342.5256  |
| 380.8384  | 397.5917  | 436.5050  |
| 495.6357  | 520.2240  | 577.0114  |
| 599.9914  | 624.5267  | 716.9701  |
| 760.8429  | 790.8799  | 892.1576  |
| 908.3819  | 929.3914  | 956.6156  |
| 964.2503  | 971.6548  | 986.5200  |
| 1002.8945 | 1024.3300 | 1046.6364 |
| 1055.6941 | 1101.5698 | 1113.1744 |
| 1150.5309 | 1174.2165 | 1194.4299 |
| 1198.6000 | 1211.0353 | 1244.1126 |
| 1259.0386 | 1268.7938 | 1288.4834 |
| 1324.4058 | 1366.9613 | 1386.7999 |
| 1393.7807 | 1404.5932 | 1414.4319 |
| 1427.7531 | 1454.5111 | 1464.8836 |
| 1476.7485 | 1484.9491 | 1492.9249 |
| 1500.6177 | 1509.4227 | 1511.0897 |
| 1620.2052 | 1837.4509 | 3040.3344 |
| 3041.4313 | 3050.5746 | 3055.8892 |
| 3062.8572 | 3065.7065 | 3080.0860 |
| 3101.4188 | 3105.1249 | 3120.4969 |
| 3121.7113 | 3125.2989 | 3138.2478 |
| 3159.2347 | 3170.4649 | 3179.9037 |

Zero-point correction (Hartree): 0.245056

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.12753196

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.674156 | -0.660980 | -0.697064 |
| H | -1.086905 | -0.284072 | -1.628553 |
| C | -1.763199 | -1.362983 | 0.084520  |
| C | -2.852013 | -0.564205 | 0.688067  |
| H | -2.240209 | -2.136818 | -0.528619 |
| H | -1.342478 | -1.915442 | 0.937782  |
| H | -3.477984 | -1.090158 | 1.420296  |
| C | 0.167261  | 0.467896  | -0.030197 |
| C | 0.621200  | -1.456804 | -0.946333 |
| C | -0.188906 | 1.890522  | -0.414852 |
| C | 0.277749  | 0.316458  | 1.481557  |
| H | 0.574048  | -0.690804 | 1.777023  |

|                                                           |           |           |           |
|-----------------------------------------------------------|-----------|-----------|-----------|
| H                                                         | 1.025632  | 1.004620  | 1.880834  |
| H                                                         | -0.672819 | 0.562546  | 1.958498  |
| H                                                         | 0.578575  | 2.587271  | -0.069340 |
| H                                                         | -1.142220 | 2.182943  | 0.024107  |
| H                                                         | -0.282691 | 1.987524  | -1.496509 |
| H                                                         | 0.716601  | -1.979154 | -1.894993 |
| H                                                         | 0.857061  | -2.143343 | -0.133140 |
| C                                                         | 1.410392  | -0.155111 | -0.772677 |
| H                                                         | 1.557950  | 0.374319  | -1.715389 |
| C                                                         | 2.695633  | -0.190635 | 0.008548  |
| C                                                         | 3.510657  | 1.077946  | 0.002216  |
| H                                                         | 2.873648  | 1.930187  | 0.245684  |
| H                                                         | 3.901828  | 1.251236  | -1.001844 |
| H                                                         | 4.331042  | 1.003218  | 0.709759  |
| O                                                         | 3.033047  | -1.162688 | 0.640325  |
| O                                                         | -3.060558 | 0.679773  | 0.609194  |
| O                                                         | -3.147338 | 0.630829  | -0.863058 |
| Rotational constants (GHz): 1.6618600 0.4855200 0.4486100 |           |           |           |
| Vibrational harmonic frequencies (cm-1):                  |           |           |           |
| i719.7615                                                 | 59.5553   | 63.4291   |           |
| 74.0981                                                   | 111.7428  | 130.7377  |           |
| 160.2152                                                  | 166.4555  | 229.0653  |           |
| 234.0656                                                  | 258.5114  | 279.2495  |           |
| 310.7438                                                  | 325.2355  | 335.5064  |           |
| 364.5537                                                  | 379.0383  | 438.3729  |           |
| 472.5349                                                  | 566.5148  | 586.8731  |           |
| 623.9123                                                  | 669.4818  | 715.1938  |           |
| 755.4276                                                  | 795.8531  | 841.4431  |           |
| 906.3964                                                  | 917.4472  | 952.2687  |           |
| 962.9772                                                  | 972.5166  | 976.8562  |           |
| 992.6369                                                  | 1005.4299 | 1037.8990 |           |
| 1048.6846                                                 | 1107.2071 | 1122.1739 |           |
| 1146.8395                                                 | 1171.7425 | 1193.8976 |           |
| 1203.3337                                                 | 1212.9310 | 1258.2796 |           |
| 1269.6361                                                 | 1276.8120 | 1306.0382 |           |
| 1356.4962                                                 | 1373.0754 | 1383.7425 |           |
| 1399.1076                                                 | 1406.7752 | 1420.8658 |           |
| 1424.8927                                                 | 1436.4598 | 1465.0244 |           |
| 1476.4117                                                 | 1481.2195 | 1489.4958 |           |
| 1499.8993                                                 | 1504.4483 | 1511.4637 |           |
| 1615.2650                                                 | 1830.6474 | 3003.9006 |           |
| 3048.0170                                                 | 3051.3791 | 3053.8962 |           |
| 3059.2225                                                 | 3063.0894 | 3085.9122 |           |
| 3091.3301                                                 | 3114.2472 | 3121.3375 |           |
| 3125.7193                                                 | 3130.2532 | 3137.9682 |           |
| 3145.5968                                                 | 3153.2538 | 3179.3095 |           |
| Zero-point correction (Hartree): 0.245198                 |           |           |           |
| ApineneCI.J.b.ringclose.pmt                               |           |           |           |
| ~~~~~                                                     |           |           |           |
| E(RM062X/Aug-CC-pVT2) (Hartree): -616.12636230            |           |           |           |
| Electronic state : 1-A                                    |           |           |           |
| Cartesian coordinates (Angs):                             |           |           |           |
| C                                                         | -0.710087 | -0.556486 | -0.589055 |
| H                                                         | -1.181589 | -0.201567 | -1.505954 |
| C                                                         | -1.744932 | -1.235026 | 0.289865  |
| C                                                         | -3.146409 | -0.771741 | 0.258684  |
| H                                                         | -1.819688 | -2.299075 | 0.016182  |
| H                                                         | -1.433175 | -1.260173 | 1.340470  |
| H                                                         | -3.889072 | -1.447643 | 0.701806  |
| C                                                         | 0.242397  | 0.556126  | -0.040819 |
| C                                                         | 0.521348  | -1.434875 | -0.889106 |
| C                                                         | 0.017530  | 1.970131  | -0.542254 |
| C                                                         | 0.376154  | 0.529991  | 1.473118  |
| H                                                         | 0.637470  | -0.460753 | 1.849247  |
| H                                                         | 1.158396  | 1.218021  | 1.800187  |
| H                                                         | -0.564344 | 0.850215  | 1.924351  |
| H                                                         | 0.904713  | 2.579186  | -0.350885 |
| H                                                         | -0.836429 | 2.430934  | -0.051594 |
| H                                                         | -0.169412 | 1.975598  | -1.617204 |
| H                                                         | 0.534132  | -1.982106 | -1.829068 |
| H                                                         | 0.738560  | -2.123223 | -0.071366 |
| C                                                         | 1.416164  | -0.200381 | -0.774750 |
| H                                                         | 1.601717  | 0.281358  | -1.736065 |
| C                                                         | 2.703218  | -0.325052 | -0.005174 |
| C                                                         | 3.629391  | 0.863477  | -0.061811 |
| H                                                         | 3.079430  | 1.773826  | 0.183140  |
| H                                                         | 4.004401  | 0.983165  | -1.079680 |
| H                                                         | 4.459654  | 0.727572  | 0.624800  |
| O                                                         | 2.961677  | -1.302811 | 0.654761  |
| O                                                         | -3.627940 | 0.221000  | -0.353898 |
| O                                                         | -2.715414 | 1.154020  | 0.335319  |
| Rotational constants (GHz): 1.7024700 0.4724500 0.4250200 |           |           |           |
| Vibrational harmonic frequencies (cm-1):                  |           |           |           |
| i723.2830                                                 | 31.4647   | 59.3303   |           |
| 68.4075                                                   | 92.5984   | 130.0103  |           |
| 143.4465                                                  | 167.9754  | 222.7833  |           |
| 253.9310                                                  | 262.1054  | 282.6523  |           |
| 316.6862                                                  | 332.5454  | 348.5080  |           |
| 368.5390                                                  | 387.2136  | 435.9811  |           |
| 469.8385                                                  | 570.8524  | 587.1087  |           |
| 624.9563                                                  | 668.9072  | 710.8871  |           |
| 763.1346                                                  | 776.7553  | 850.6967  |           |
| 904.1206                                                  | 925.0646  | 951.1346  |           |
| 963.9879                                                  | 967.9862  | 979.3048  |           |
| 1000.4275                                                 | 1006.5639 | 1035.4691 |           |
| 1053.6107                                                 | 1103.0794 | 1120.1957 |           |
| 1161.8665                                                 | 1170.0608 | 1189.6726 |           |
| 1197.0084                                                 | 1215.7464 | 1257.1168 |           |
| 1263.9983                                                 | 1280.2263 | 1302.5870 |           |
| 1355.3778                                                 | 1374.1802 | 1384.4703 |           |
| 1399.8968                                                 | 1402.8387 | 1418.0710 |           |

|           |           |           |
|-----------|-----------|-----------|
| 1422.0144 | 1432.3559 | 1465.8969 |
| 1476.6793 | 1482.9481 | 1492.3084 |
| 1496.4557 | 1506.9303 | 1515.3599 |
| 1623.6602 | 1830.2154 | 2992.3843 |
| 3048.3645 | 3050.9431 | 3053.8290 |
| 3060.9406 | 3064.4637 | 3083.7223 |
| 3086.8226 | 3093.5661 | 3111.7596 |
| 3116.1595 | 3127.1690 | 3127.9035 |
| 3143.9652 | 3157.8137 | 3179.1235 |

Zero-point correction (Hartree): 0.245029

ApineneCI.J.b.ringclose.ppm

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.12406953

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.574920 | 0.460340  | -0.621572 |
| H | -0.714077 | 0.999516  | -1.563295 |
| C | -1.856813 | 0.521533  | 0.203412  |
| C | -2.976261 | -0.015996 | -0.605432 |
| H | -1.800321 | -0.037311 | 1.133983  |
| H | -2.087143 | 1.561912  | 0.454410  |
| H | -3.047997 | 0.330447  | -1.645869 |
| C | 0.753426  | 0.950678  | 0.022909  |
| C | 0.083588  | -0.905599 | -0.894123 |
| C | 1.180940  | 2.357916  | -0.344035 |
| C | 0.789511  | 0.746195  | 1.531636  |
| H | 0.516074  | -0.269721 | 1.816120  |
| H | 1.793209  | 0.937223  | 1.916584  |
| H | 0.107586  | 1.439520  | 2.026108  |
| H | 2.180006  | 2.579971  | 0.036153  |
| H | 0.495703  | 3.088855  | 0.091305  |
| H | 1.187965  | 2.499496  | -1.425424 |
| H | -0.136564 | -1.401044 | -1.836730 |
| H | -0.076331 | -1.606908 | -0.075612 |
| C | 1.451937  | -0.228173 | -0.750446 |
| H | 1.833729  | 0.146848  | -1.702070 |
| C | 2.543716  | -0.952858 | -0.007267 |
| C | 3.900856  | -0.295648 | -0.018741 |
| H | 3.808331  | 0.757071  | 0.254829  |
| H | 4.309228  | -0.326996 | -1.030444 |
| H | 4.572579  | -0.806002 | 0.664928  |
| O | 2.332746  | -1.976711 | 0.593860  |
| O | -3.750507 | -0.965341 | -0.302249 |
| O | -4.171972 | -0.273349 | 0.931760  |

Rotational constants (GHz): 1.5316500 0.4051300 0.3691800

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i744.3987 | 41.2969   | 53.7818   |
| 61.8646   | 88.8552   | 123.7393  |
| 131.1905  | 162.0355  | 201.0079  |
| 237.8210  | 261.5658  | 280.3757  |
| 293.2826  | 326.9254  | 347.2990  |
| 356.6749  | 397.6575  | 456.6903  |
| 482.8165  | 529.1721  | 583.2691  |
| 597.7863  | 624.8997  | 736.2256  |
| 756.1891  | 805.4899  | 862.5761  |
| 911.5852  | 932.1361  | 953.8605  |
| 962.7777  | 966.7141  | 989.8250  |
| 1002.8493 | 1016.4172 | 1048.2218 |
| 1066.8362 | 1100.6380 | 1128.3955 |
| 1157.5412 | 1176.1214 | 1194.6152 |
| 1206.5961 | 1220.2405 | 1237.2087 |
| 1262.3097 | 1272.4958 | 1291.4519 |
| 1326.1699 | 1368.3876 | 1387.8524 |
| 1393.3916 | 1406.0734 | 1416.6516 |
| 1427.3302 | 1449.6073 | 1465.3108 |
| 1478.2251 | 1486.2586 | 1494.4120 |
| 1500.0129 | 1509.5758 | 1512.1553 |
| 1622.9150 | 1838.4021 | 3044.3232 |
| 3045.3774 | 3049.2927 | 3054.2301 |
| 3055.6027 | 3062.6240 | 3080.8786 |
| 3095.7204 | 3110.8238 | 3119.0925 |
| 3123.1208 | 3125.4828 | 3137.3816 |
| 3152.1076 | 3159.4907 | 3179.1412 |

Zero-point correction (Hartree): 0.245078

ApineneCI.J.b.ringclose.ppm

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.12522319

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.693077 | 0.530614  | -0.453847 |
| H | -0.910146 | 1.020041  | -1.407942 |
| C | -1.877998 | 0.705533  | 0.498845  |
| C | -3.167036 | 0.441297  | -0.171681 |
| H | -1.779802 | 0.057630  | 1.365569  |
| H | -1.917166 | 1.760268  | 0.805136  |
| H | -3.510116 | 1.186138  | -0.902328 |
| C | 0.710446  | 0.996491  | 0.024510  |
| C | -0.131122 | -0.877429 | -0.696647 |
| C | 1.160369  | 2.357037  | -0.469753 |
| C | 0.886286  | 0.877669  | 1.532287  |
| H | 0.599467  | -0.106559 | 1.901854  |
| H | 1.930136  | 1.040504  | 1.808041  |
| H | 0.288354  | 1.632153  | 2.046799  |
| H | 2.201471  | 2.551615  | -0.204640 |
| H | 0.555624  | 3.146422  | -0.016492 |
| H | 1.063944  | 2.434629  | -1.553365 |
| H | -0.481246 | -1.415366 | -1.571887 |
| H | -0.250122 | -1.513908 | 0.178045  |
| C | 1.274054  | -0.260142 | -0.736846 |
| H | 1.570487  | 0.039846  | -1.743957 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 2.410772  | -0.979062 | -0.058988 |
| C | 3.788206  | -0.411336 | -0.298046 |
| H | 3.783068  | 0.665887  | -0.120397 |
| H | 4.064812  | -0.560033 | -1.343294 |
| H | 4.513656  | -0.897280 | 0.347542  |
| O | 2.227719  | -1.923734 | 0.667764  |
| O | -3.996131 | -0.474242 | 0.092218  |
| O | -2.967567 | -1.517778 | -0.085942 |

Rotational constants (GHz): 1.4696500 0.4570600 0.3943200

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i733.4832 | 47.3882   | 55.9883   |
| 65.4585   | 105.0276  | 120.3626  |
| 133.5926  | 166.9873  | 189.4682  |
| 233.1911  | 246.6741  | 286.9211  |
| 304.0536  | 318.7104  | 349.6261  |
| 370.9566  | 404.5204  | 462.9260  |
| 472.2220  | 540.7789  | 586.8529  |
| 597.7706  | 624.3996  | 733.1837  |
| 785.2598  | 822.6953  | 864.6557  |
| 907.4300  | 932.1449  | 956.5519  |
| 962.8944  | 968.3649  | 987.1428  |
| 999.0713  | 1015.0866 | 1048.9726 |
| 1053.8866 | 1098.3756 | 1128.8059 |
| 1152.1619 | 1176.1901 | 1192.2484 |
| 1204.1906 | 1224.4611 | 1242.6749 |
| 1256.3736 | 1274.7389 | 1300.0535 |
| 1324.2274 | 1367.1216 | 1387.8107 |
| 1388.5216 | 1403.4515 | 1414.5462 |
| 1423.4397 | 1451.9981 | 1464.4372 |
| 1476.7259 | 1485.1247 | 1491.7223 |
| 1497.3387 | 1506.9351 | 1508.6969 |
| 1619.7542 | 1837.8753 | 3004.5046 |
| 3043.2834 | 3046.7797 | 3052.3418 |
| 3053.7579 | 3061.6564 | 3080.2670 |
| 3107.6041 | 3114.8987 | 3115.5314 |
| 3122.7138 | 3124.3625 | 3138.8721 |
| 3160.9738 | 3174.0850 | 3178.4976 |

Zero-point correction (Hartree): 0.245134

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.12622128

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.707598 | 0.154363  | -0.259301 |
| H | -1.121557 | 0.636943  | -1.144002 |
| C | -1.828608 | 0.035440  | 0.771828  |
| C | -2.899482 | -0.863231 | 0.291880  |
| H | -1.425492 | -0.444994 | 1.672321  |
| H | -2.252222 | 1.008718  | 1.007021  |
| H | -2.660351 | -1.932945 | 0.230068  |
| C | 0.616500  | 0.859991  | 0.144612  |
| C | 0.098428  | -1.097076 | -0.655793 |
| C | 0.742019  | 2.307691  | -0.287325 |
| C | 0.955893  | 0.700067  | 1.619792  |
| H | 0.910305  | -0.339994 | 1.943923  |
| H | 1.967119  | 1.059759  | 1.820251  |
| H | 0.269362  | 1.287709  | 2.231671  |
| H | 1.747190  | 2.691429  | -0.100731 |
| H | 0.041547  | 2.932243  | 0.271041  |
| H | 0.522504  | 2.421165  | -1.349109 |
| H | -0.205669 | -1.634176 | -1.550938 |
| H | 0.210480  | -1.802497 | 0.168552  |
| C | 1.346196  | -0.210865 | -0.750706 |
| H | 1.491276  | 0.199746  | -1.751294 |
| C | 2.649138  | -0.739730 | -0.213022 |
| C | 3.866727  | 0.109825  | -0.474645 |
| H | 3.661912  | 1.148004  | -0.206703 |
| H | 4.093305  | 0.096054  | -1.542255 |
| H | 4.717019  | -0.265875 | 0.086586  |
| O | 2.706458  | -1.761198 | 0.427018  |
| O | -4.108592 | -0.567480 | 0.075842  |
| O | -3.723117 | 0.503661  | -0.866650 |

Rotational constants (GHz): 1.6589800 0.4072300 0.3750500

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i734.6320 | 43.3853   | 54.1015   |
| 63.1366   | 106.6112  | 117.9989  |
| 126.1919  | 154.5977  | 209.4424  |
| 219.6147  | 251.9452  | 284.8606  |
| 317.2819  | 326.9922  | 350.1923  |
| 381.8104  | 413.0258  | 434.4093  |
| 468.3673  | 535.5863  | 588.7860  |
| 596.4720  | 624.5722  | 735.7949  |
| 779.0473  | 823.6364  | 879.9445  |
| 906.5387  | 932.2593  | 950.9747  |
| 964.9965  | 967.0217  | 991.5875  |
| 1000.9488 | 1005.9088 | 1039.4003 |
| 1071.9878 | 1105.7997 | 1140.3105 |
| 1155.9010 | 1173.5183 | 1194.1060 |
| 1209.9215 | 1217.6315 | 1259.9620 |
| 1263.0359 | 1273.6051 | 1303.2324 |
| 1336.6747 | 1355.8452 | 1378.4368 |
| 1390.0413 | 1403.5441 | 1411.6608 |
| 1423.3436 | 1454.5456 | 1464.2395 |
| 1476.3201 | 1486.0791 | 1491.8424 |
| 1498.1688 | 1508.7526 | 1509.6118 |
| 1621.0150 | 1834.2222 | 3022.5353 |
| 3047.6943 | 3052.8682 | 3059.3118 |
| 3062.7222 | 3084.3696 | 3088.2777 |
| 3106.5296 | 3112.4192 | 3117.3977 |
| 3124.6227 | 3128.6505 | 3132.3016 |
| 3147.3822 | 3153.7006 | 3179.5385 |

```

Zero-point correction (Hartree): 0.245316

ApineneCI.J.b.ringclose.pppp
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E(RM062X/Aug-CC-pVT2) (Hartree): -616.12467231
Electronic state : 1-A
Cartesian coordinates (Angs):
  C    -0.599695      0.160435     -0.544934
  H    -0.856858      0.563740     -1.527306
  C    -1.835168      0.167571      0.352834
  C    -2.871243     -0.694152     -0.259884
  H    -1.580471     -0.254540      1.328780
  H    -2.249655      1.159463      0.517120
  H    -2.543431     -1.678216     -0.621535
  C     0.686334      0.883202     -0.045983
  C     0.218764     -1.136428     -0.710185
  C     0.910155      2.277290     -0.597326
  C     0.824772      0.867095      1.469926
  H     0.703098     -0.133574      1.885145
  H     1.813791      1.224003      1.764000
  H     0.085233      1.526019      1.926896
  H     1.893848      2.659629     -0.317757
  H     0.163647      2.967631     -0.199082
  H     0.836422      2.287432     -1.685294
  H     0.024606     -1.758707     -1.580496
  H     0.196371     -1.755892      0.186936
  C     1.493169     -0.284093     -0.725511
  H     1.779692      0.019150     -1.734188
  C     2.699954     -0.780617      0.026983
  C     3.962755      0.025395     -0.140619
  H     3.751889      1.085922      0.008746
  H     4.328257     -0.085350     -1.163116
  H     4.721313     -0.311863      0.559305
  O     2.644820     -1.743260      0.751808
  O    -4.045106     -0.363615     -0.586607
  O    -4.350531      0.053245      0.797305
Rotational constants (GHz):    1.6998800    0.3808500    0.3542800
Vibrational harmonic frequencies (cm-1):
  i744.8452      45.1245      54.5689
    62.7271      103.2969      114.7055
   120.6298      157.4739      213.4149
   223.1672      246.9617      285.8874
   289.5677      318.8604      347.8282
   364.1601      398.3469      452.9105
   488.6159      510.2305      584.3931
   597.7467      624.3196      738.5163
   770.2800      801.6033      872.3373
   908.3081      929.2543      951.7393
   965.6932      966.8053      993.5879
  1001.1420     1008.6104     1041.8431
  1075.0830     1104.2203     1134.4433
  1155.5709     1173.2822     1193.8935
  1208.2935     1215.3898     1249.4717
  1262.8443     1270.4898     1293.9202
  1327.2104     1364.9591     1383.2963
  1393.4646     1404.8144     1414.8310
  1425.0229     1451.8384     1464.1097
  1476.3862     1485.6510     1492.3449
  1499.1679     1508.6528     1509.8335
  1625.2103     1836.2683     3047.7282
  3052.3284     3055.1144     3060.4717
  3063.5151     3071.4320     3084.1535
  3089.7303     3113.9934     3120.5029
  3124.6507     3126.0943     3135.2138
  3148.0278     3152.1121     3179.8616
Zero-point correction (Hartree): 0.245084

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E(RM062X/Aug-CC-pVT2) (Hartree): -616.12449615
Electronic state : 1-A
Cartesian coordinates (Angs):
 C -0.798119 0.212670 -0.227459
 H -1.209364 0.420715 -1.216591
 C -1.843173 0.513596 0.825363
 C -3.263194 0.261338 0.496839
 H -1.629122 -0.004172 1.767770
 H -1.835260 1.581484 1.096639
 H -3.999443 0.667829 1.202040
 C 0.583970 0.920625 -0.089233
 C -0.077915 -1.143295 -0.246686
 C 0.778882 2.161661 -0.937945
 C 0.976066 1.185833 1.359220
 H 0.851402 0.302318 1.985723
 H 2.024743 1.483510 1.422386
 H 0.381454 1.999550 1.777857
 H 1.809766 2.519005 -0.889756
 H 0.135784 2.971340 -0.583741
 H 0.532467 1.966031 -1.981946
 H -0.465828 -1.888464 -0.931963
 H 0.012212 -1.577090 0.748812
 C 1.216635 -0.413832 -0.629940
 H 1.344516 -0.334824 -1.711186
 C 2.512607 -0.830190 0.011887
 C 3.764397 -0.216031 -0.564356
 H 3.641909 0.865441 -0.650996
 H 3.923265 -0.599275 -1.573849
 H 4.622518 -0.451241 0.058221
 O 2.547646 -1.574633 0.961087
 O -3.748216 -0.207328 -0.568943
 O -2.954674 -1.447590 -0.455339
Rotational constants (GHz): 1.5334500 0.4508000 0.4078700

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Vibrational harmonic frequencies (cm-1):
1722.0493 52.3435 58.2269
 64.3691 114.2917 127.3768
 129.8020 166.5070 202.6393
 226.9694 247.6172 282.1408
 310.8838 321.4163 344.3986
 355.4833 384.8427 440.6925
 474.0157 566.4633 586.0889
 622.0057 656.5618 733.2076
 758.0936 793.6621 850.1214
 904.0662 927.2627 949.7588
 961.3575 967.6313 980.0973
 996.8823 1004.8351 1026.0316
1048.5250 1098.7067 1131.2375
1147.1652 1176.2889 1194.8481
1205.7043 1223.9168 1240.4220
1257.4346 1273.3550 1320.2720
1346.9329 1373.7841 1384.6559
1399.9680 1406.9428 1421.0975
1424.6296 1438.6778 1465.1272
1476.4934 1485.3228 1493.7003
1497.9705 1507.3698 1512.7178
1622.3974 1834.0548 2987.3097
3042.2870 3046.7620 3052.7010
3057.6502 3061.8022 3082.8824
3085.4697 3104.5642 3104.8844
3114.0859 3123.5454 3125.1325
3134.4048 3177.8380 3181.1459
Zero-point correction (Hartree): 0.244858

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.12517896

Electronic state : 1-A

Cartesian coordinates (Angs):

```

C -0.795126 0.453327 -0.255451
H -1.143016 0.798882 -1.225260
C -1.872154 0.704026 0.775234
C -3.040167 -0.206970 0.756872
H -1.481991 0.590492 1.797053
H -2.256609 1.729831 0.735282
H -3.688293 -0.175748 1.641838
C 0.645687 0.989770 -0.006283
C -0.225842 -0.967754 -0.395685
C 0.998462 2.277604 -0.725291
C 1.028422 1.071136 1.465248
H 0.810061 0.146239 2.000180
H 2.098453 1.261582 1.571158
H 0.499885 1.892816 1.952349
H 2.062685 2.505160 -0.633478
H 0.445572 3.117251 -0.297681
H 0.751363 2.214973 -1.785278
H -0.668941 -1.596885 -1.162136
H -0.203936 -1.507264 0.551929
C 1.148301 -0.346053 -0.673779
H 1.317278 -0.170343 -1.737513
C 2.369411 -0.967106 -0.051188
C 3.698348 -0.434598 -0.525887
H 3.692853 0.656822 -0.499228
H 3.852904 -0.725790 -1.566335
H 4.503763 -0.824622 0.089312
O 2.290931 -1.808012 0.811135
O -3.293269 -1.140251 -0.055118
O -3.288173 -0.220947 -1.207884
Rotational constants (GHz): 1.4282100 0.4709500 0.4263000

```

```

Vibrational harmonic frequencies (cm-1):
1722.9126 45.0121 59.0417
 69.4024 118.4250 133.6197
 139.3603 159.6572 198.6065
 231.1218 249.4189 289.5662
 316.1825 337.2688 343.6575
 354.5138 386.0474 442.1653
 469.5847 560.5657 587.0096
 623.7847 655.2979 743.9122
 750.4988 818.2378 845.8471
 904.9905 932.6092 946.6018
 955.5509 964.8239 974.3672
 995.5736 1004.0600 1025.4842
1047.2186 1091.9626 1141.3948
1155.7644 1174.4476 1194.4524
1206.2212 1216.2481 1253.7441
1264.8565 1275.5913 1322.7438
1348.0519 1374.2200 1384.7760
1400.3874 1406.9277 1422.5157
1423.5474 1440.3135 1465.4545
1477.2866 1487.1759 1493.3870
1496.9341 1509.4473 1510.5053
1615.6929 1833.1585 3011.1921
3044.6295 3050.2618 3052.6224
3062.3161 3063.6573 3084.1617
3090.9552 3107.5811 3113.5434
3124.4595 3126.6908 3129.6150
3135.9412 3162.8336 3177.3795
Zero-point correction (Hartree): 0.245140

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ApineneCI.J.b.ringclose.ptmm

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.12308702

Electronic state : 1-A

Cartesian coordinates (Angs):

```

C 0.485057 0.685624 1.053169
H 0.394920 1.545397 1.719862

```

|                                                           |           |           |           |
|-----------------------------------------------------------|-----------|-----------|-----------|
| C                                                         | 1.980925  | 0.489647  | 0.801178  |
| C                                                         | 2.320585  | -0.756017 | 0.069611  |
| H                                                         | 2.429710  | 1.330697  | 0.275534  |
| H                                                         | 2.486610  | 0.425906  | 1.769938  |
| H                                                         | 1.807659  | -1.676271 | 0.372940  |
| C                                                         | -0.505256 | 0.904843  | -0.124434 |
| C                                                         | -0.427075 | -0.437255 | 1.589968  |
| C                                                         | -0.797187 | 2.350208  | -0.477152 |
| C                                                         | -0.139672 | 0.109176  | -1.369873 |
| H                                                         | 0.030201  | -0.947495 | -1.153368 |
| H                                                         | -0.947119 | 0.154344  | -2.103600 |
| H                                                         | 0.756698  | 0.518816  | -1.837745 |
| H                                                         | -1.600492 | 2.425148  | -1.212775 |
| H                                                         | 0.088338  | 2.820679  | -0.909896 |
| H                                                         | -1.088224 | 2.920175  | 0.405874  |
| H                                                         | -0.562454 | -0.498963 | 2.666606  |
| H                                                         | -0.188380 | -1.427598 | 1.206476  |
| C                                                         | -1.572187 | 0.162661  | 0.763059  |
| H                                                         | -2.149882 | 0.901342  | 1.321326  |
| C                                                         | -2.495722 | -0.776748 | 0.033392  |
| C                                                         | -3.695210 | -0.147321 | -0.627379 |
| H                                                         | -3.383794 | 0.713716  | -1.221855 |
| H                                                         | -4.376092 | 0.225651  | 0.139796  |
| H                                                         | -4.206653 | -0.873361 | -1.252118 |
| O                                                         | -2.261753 | -1.957375 | -0.053550 |
| O                                                         | 3.040598  | -0.861492 | -0.964141 |
| O                                                         | 4.169081  | -0.189520 | -0.289338 |
| Rotational constants (GHz): 1.4581000 0.4537000 0.4252600 |           |           |           |
| Vibrational harmonic frequencies (cm-1):                  |           |           |           |
| i740.7053                                                 | 50.4675   |           | 55.8142   |
| 72.2337                                                   | 99.5752   |           | 110.6135  |
| 150.2306                                                  | 192.3917  |           | 218.2809  |
| 240.0203                                                  | 255.4521  |           | 269.0047  |
| 284.3695                                                  | 347.4305  |           | 357.1847  |
| 368.4444                                                  | 391.2868  |           | 439.3394  |
| 475.3067                                                  | 570.7579  |           | 584.0167  |
| 608.5118                                                  | 629.4494  |           | 706.2417  |
| 750.6481                                                  | 783.4917  |           | 868.9528  |
| 901.5537                                                  | 923.5469  |           | 947.6286  |
| 962.2559                                                  | 970.6792  |           | 985.2572  |
| 1001.7447                                                 | 1008.7942 |           | 1046.2565 |
| 1059.8816                                                 | 1118.2148 |           | 1134.9923 |
| 1149.1448                                                 | 1172.5532 |           | 1195.4207 |
| 1207.1217                                                 | 1217.0605 |           | 1246.9947 |
| 1262.0180                                                 | 1288.3295 |           | 1295.2976 |
| 1331.2250                                                 | 1369.3945 |           | 1389.4181 |
| 1397.3881                                                 | 1406.7837 |           | 1415.6115 |
| 1426.0332                                                 | 1436.6608 |           | 1463.7495 |
| 1475.3890                                                 | 1486.2914 |           | 1494.1896 |
| 1502.3697                                                 | 1508.8414 |           | 1512.7405 |
| 1620.1626                                                 | 1834.2193 |           | 3046.5557 |
| 3050.8664                                                 | 3052.9190 |           | 3062.4815 |
| 3071.8125                                                 | 3077.1379 |           | 3085.3423 |
| 3106.4479                                                 | 3112.6156 |           | 3115.6746 |
| 3123.4022                                                 | 3124.8326 |           | 3128.3405 |
| 3137.9106                                                 | 3159.7140 |           | 3180.1312 |
| Zero-point correction (Hartree): 0.245315                 |           |           |           |
| ApineneCI.J.b.ringclose.ptmp                              |           |           |           |
| ~~~~~                                                     |           |           |           |
| E (RM062X/Aug-CC-pVT2) (Hartree): -616.12229411           |           |           |           |
| Electronic state : 1-A                                    |           |           |           |
| Cartesian coordinates (Angs):                             |           |           |           |
| C                                                         | 0.530147  | -0.350879 | 1.207639  |
| H                                                         | 0.460775  | -0.005757 | 2.240937  |
| C                                                         | 2.008237  | -0.686373 | 0.975469  |
| C                                                         | 2.446822  | -0.817039 | -0.429608 |
| H                                                         | 2.667630  | 0.012178  | 1.478519  |
| H                                                         | 2.156904  | -1.695554 | 1.392054  |
| H                                                         | 1.916051  | -1.537057 | -1.064328 |
| C                                                         | -0.298360 | 0.651062  | 0.348243  |
| C                                                         | -0.570030 | -1.403658 | 0.999169  |
| C                                                         | -0.289637 | 2.087092  | 0.831395  |
| C                                                         | -0.031079 | 0.589543  | -1.151463 |
| H                                                         | -0.086219 | -0.428384 | -1.540487 |
| H                                                         | -0.791989 | 1.165772  | -1.683213 |
| H                                                         | 0.941489  | 1.022392  | -1.386165 |
| H                                                         | -1.009361 | 2.696588  | 0.281521  |
| H                                                         | 0.700526  | 2.519595  | 0.673793  |
| H                                                         | -0.529453 | 2.148984  | 1.893792  |
| H                                                         | -0.792061 | -2.071484 | 1.828252  |
| H                                                         | -0.436194 | -1.991926 | 0.091598  |
| C                                                         | -1.538375 | -0.246010 | 0.726501  |
| H                                                         | -1.989083 | 0.137408  | 1.644218  |
| C                                                         | -2.591755 | -0.419725 | -0.334142 |
| C                                                         | -3.589895 | 0.702075  | -0.466259 |
| H                                                         | -3.067356 | 1.658260  | -0.530563 |
| H                                                         | -4.213126 | 0.739701  | 0.428955  |
| H                                                         | -4.212841 | 0.551715  | -1.342842 |
| O                                                         | -2.611658 | -1.384257 | -1.059158 |
| O                                                         | 3.513547  | -0.343300 | -0.923656 |
| O                                                         | 3.076592  | 1.032687  | -0.598149 |
| Rotational constants (GHz): 1.4747900 0.4737800 0.4524800 |           |           |           |
| Vibrational harmonic frequencies (cm-1):                  |           |           |           |
| i733.2736                                                 | 21.5993   |           | 64.2432   |
| 86.0086                                                   | 111.9953  |           | 116.1091  |
| 159.7193                                                  | 184.8171  |           | 196.9509  |
| 239.6943                                                  | 255.1383  |           | 293.0650  |
| 328.0309                                                  | 344.6423  |           | 361.9384  |
| 381.9725                                                  | 413.1962  |           | 427.3301  |
| 461.4595                                                  | 571.9464  |           | 582.2222  |
| 621.9702                                                  | 649.4475  |           | 715.8622  |

|           |           |           |
|-----------|-----------|-----------|
| 763.2983  | 818.6294  | 838.6467  |
| 903.0577  | 931.6580  | 950.2031  |
| 968.7390  | 971.7401  | 987.0326  |
| 1001.6800 | 1007.7046 | 1050.9660 |
| 1058.5347 | 1120.5236 | 1133.3235 |
| 1153.7668 | 1171.5194 | 1189.0133 |
| 1209.4060 | 1215.3994 | 1259.2582 |
| 1266.5205 | 1287.1428 | 1310.9406 |
| 1332.7629 | 1373.2846 | 1380.9264 |
| 1398.6391 | 1403.9790 | 1418.4527 |
| 1425.7814 | 1442.1969 | 1464.2860 |
| 1476.2042 | 1486.8702 | 1497.6985 |
| 1502.9426 | 1511.7846 | 1529.5551 |
| 1610.4598 | 1833.7471 | 2981.5319 |
| 3045.9269 | 3048.6144 | 3063.5327 |
| 3067.2858 | 3072.6079 | 3080.6459 |
| 3094.1459 | 3111.3414 | 3116.3567 |
| 3122.9838 | 3125.6816 | 3135.5346 |
| 3149.3934 | 3175.0190 | 3180.1317 |

Zero-point correction (Hartree): 0.245628

ApineneCI.J.b.ringclose.ptpm

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E(RM062X/Aug-CC-pVT2) (Hartree): -616.12096919

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.623700 | 0.755411  | -0.773995 |
| H | -0.569872 | 1.340375  | -1.693572 |
| C | -2.002354 | 1.029039  | -0.155617 |
| C | -2.523260 | -0.018683 | 0.756071  |
| H | -1.926166 | 1.940794  | 0.454081  |
| H | -2.742771 | 1.171030  | -0.937229 |
| H | -2.040498 | -0.146956 | 1.731768  |
| C | 0.684173  | 1.028758  | 0.018154  |
| C | -0.128686 | -0.672616 | -1.060310 |
| C | 1.312045  | 2.391969  | -0.198620 |
| C | 0.569440  | 0.720663  | 1.505633  |
| H | 0.214017  | -0.293246 | 1.689181  |
| H | 1.544198  | 0.808897  | 1.989513  |
| H | -0.100537 | 1.431999  | 1.994065  |
| H | 2.293776  | 2.458050  | 0.274554  |
| H | 0.685606  | 3.173697  | 0.238270  |
| H | 1.428901  | 2.606774  | -1.261229 |
| H | -0.348132 | -1.097654 | -2.035027 |
| H | -0.437410 | -1.384186 | -0.296865 |
| C | 1.298374  | -0.177421 | -0.785690 |
| H | 1.786201  | 0.208531  | -1.682649 |
| C | 2.246596  | -1.060330 | -0.018318 |
| C | 3.689336  | -0.621363 | 0.004908  |
| H | 3.752062  | 0.432155  | 0.285025  |
| H | 4.110832  | -0.708611 | -0.997998 |
| H | 4.259197  | -1.231847 | 0.698933  |
| O | 1.865682  | -2.033505 | 0.584547  |
| O | -3.597171 | -0.667798 | 0.601828  |
| O | -3.148660 | -1.168993 | -0.711890 |

Rotational constants (GHz): 1.3494000 0.4984600 0.4329600

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i758.2640 | 41.7453   | 52.9046   |
| 64.8519   | 104.3408  | 114.2967  |
| 145.7058  | 183.9041  | 185.0626  |
| 233.1216  | 239.7971  | 283.4038  |
| 325.9969  | 336.1074  | 356.9769  |
| 379.4629  | 408.4525  | 454.4442  |
| 464.8300  | 574.8854  | 590.3820  |
| 608.0325  | 627.9851  | 723.1974  |
| 770.4365  | 812.2558  | 853.9843  |
| 904.9820  | 935.4640  | 956.0075  |
| 965.4265  | 971.3270  | 978.7081  |
| 1000.4714 | 1008.9596 | 1046.1819 |
| 1058.9025 | 1082.7354 | 1141.5938 |
| 1153.7081 | 1173.3053 | 1195.4255 |
| 1205.9397 | 1230.5620 | 1246.9861 |
| 1262.0584 | 1292.4326 | 1312.7495 |
| 1332.5443 | 1368.7360 | 1385.0890 |
| 1395.5865 | 1402.9609 | 1415.7232 |
| 1422.8062 | 1450.2632 | 1464.1020 |
| 1475.5051 | 1488.2259 | 1492.3917 |
| 1499.4202 | 1509.6160 | 1514.8393 |
| 1615.1806 | 1835.3066 | 3003.6032 |
| 3043.8151 | 3049.1758 | 3061.4091 |
| 3076.3972 | 3079.0293 | 3082.5906 |
| 3107.0039 | 3111.2802 | 3112.3743 |
| 3123.1728 | 3125.7679 | 3136.4811 |
| 3160.2190 | 3168.9229 | 3179.2016 |

Zero-point correction (Hartree): 0.245471

ApineneCI.J.b.ringclose.ptpp

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E(RM062X/Aug-CC-pVT2) (Hartree): -616.12039420

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.529454 | 0.666188  | -0.846678 |
| H | -0.465796 | 1.364504  | -1.683094 |
| C | -1.976981 | 0.722687  | -0.345962 |
| C | -2.402314 | -0.517102 | 0.354377  |
| H | -2.091087 | 1.563538  | 0.344946  |
| H | -2.687751 | 0.894275  | -1.151121 |
| H | -1.708101 | -0.974781 | 1.066470  |
| C | 0.677789  | 0.973118  | 0.083766  |
| C | 0.154148  | -0.651230 | -1.267778 |
| C | 1.155575  | 2.412418  | 0.071933  |
| C | 0.498443  | 0.482876  | 1.515505  |

|                                                |           |           |           |
|------------------------------------------------|-----------|-----------|-----------|
| H                                              | 0.303718  | -0.587939 | 1.567924  |
| H                                              | 1.405860  | 0.667781  | 2.093795  |
| H                                              | -0.316055 | 1.017784  | 2.007958  |
| H                                              | 2.091032  | 2.525517  | 0.623327  |
| H                                              | 0.415817  | 3.061621  | 0.546306  |
| H                                              | 1.313544  | 2.766990  | -0.947021 |
| H                                              | 0.075674  | -0.951916 | -2.309121 |
| H                                              | -0.108100 | -1.498732 | -0.634523 |
| C                                              | 1.486093  | -0.052049 | -0.796261 |
| H                                              | 2.000619  | 0.491115  | -1.590910 |
| C                                              | 2.456771  | -0.935780 | -0.058520 |
| C                                              | 3.818226  | -0.347285 | 0.209753  |
| H                                              | 3.713460  | 0.646258  | 0.650100  |
| H                                              | 4.350882  | -0.221611 | -0.734516 |
| H                                              | 4.386501  | -0.995448 | 0.869989  |
| O                                              | 2.144055  | -2.032967 | 0.334706  |
| O                                              | -3.426495 | -1.209875 | 0.091941  |
| O                                              | -4.306308 | -0.043657 | 0.293189  |
| Rotational constants (GHz):                    |           |           |           |
| Vibrational harmonic frequencies (cm-1):       |           |           |           |
| i753.3372                                      | 46.4054   | 51.1210   |           |
| 67.2164                                        | 92.4061   | 119.7619  |           |
| 146.2890                                       | 183.1100  | 197.4719  |           |
| 244.3073                                       | 250.1009  | 267.3004  |           |
| 285.2832                                       | 328.0986  | 356.0514  |           |
| 360.8265                                       | 394.5166  | 445.6228  |           |
| 471.0970                                       | 576.0238  | 585.4066  |           |
| 600.5701                                       | 626.7201  | 722.8442  |           |
| 758.7156                                       | 774.1156  | 858.0652  |           |
| 907.6352                                       | 934.9229  | 956.8960  |           |
| 964.4375                                       | 970.3536  | 979.8561  |           |
| 999.9219                                       | 1008.0619 | 1047.1167 |           |
| 1064.7885                                      | 1086.8511 | 1140.8905 |           |
| 1149.5130                                      | 1173.4758 | 1195.1998 |           |
| 1209.0918                                      | 1224.9027 | 1236.0205 |           |
| 1262.8763                                      | 1289.4218 | 1300.6127 |           |
| 1329.2976                                      | 1368.9026 | 1387.1905 |           |
| 1396.4354                                      | 1404.5005 | 1415.4257 |           |
| 1422.6164                                      | 1442.9961 | 1464.0892 |           |
| 1476.6805                                      | 1489.6706 | 1492.3077 |           |
| 1501.9377                                      | 1507.4323 | 1518.8404 |           |
| 1618.0579                                      | 1834.3262 | 3045.8304 |           |
| 3053.2096                                      | 3057.6864 | 3062.1914 |           |
| 3073.1699                                      | 3084.1577 | 3094.3844 |           |
| 3100.5711                                      | 3110.2192 | 3114.9462 |           |
| 3123.9294                                      | 3126.5418 | 3139.4401 |           |
| 3145.4063                                      | 3153.6741 | 3180.1856 |           |
| Zero-point correction (Hartree): 0.245241      |           |           |           |
| ApineneCI.J.b.ringclose.pttp                   |           |           |           |
| ~~~~~                                          |           |           |           |
| E(RM062X/Aug-CC-pVT2) (Hartree): -616.11452555 |           |           |           |
| Electronic state : 1-A                         |           |           |           |
| Cartesian coordinates (Angs):                  |           |           |           |
| C                                              | 0.689862  | 0.755731  | 0.969341  |
| H                                              | 0.521568  | 1.550646  | 1.703071  |
| C                                              | 2.189092  | 0.843076  | 0.702461  |
| C                                              | 2.979141  | 0.080724  | -0.298681 |
| H                                              | 2.435349  | 1.887984  | 0.459273  |
| H                                              | 2.729271  | 0.670954  | 1.643779  |
| H                                              | 3.976845  | 0.506552  | -0.474382 |
| C                                              | -0.385754 | 0.970949  | -0.130386 |
| C                                              | -0.089698 | -0.474169 | 1.469968  |
| C                                              | -0.778981 | 2.412425  | -0.393313 |
| C                                              | -0.087088 | 0.240921  | -1.431943 |
| H                                              | 0.206337  | -0.793807 | -1.259809 |
| H                                              | -0.967608 | 0.247611  | -2.078336 |
| H                                              | 0.716149  | 0.742562  | -1.975066 |
| H                                              | -1.633040 | 2.473969  | -1.070557 |
| H                                              | 0.045821  | 2.953442  | -0.863939 |
| H                                              | -1.040070 | 2.927641  | 0.532162  |
| H                                              | -0.126699 | -0.629845 | 2.545416  |
| H                                              | 0.206333  | -1.389194 | 0.969733  |
| C                                              | -1.332796 | 0.128392  | 0.799241  |
| H                                              | -1.875109 | 0.810715  | 1.458606  |
| C                                              | -2.311167 | -0.788192 | 0.113265  |
| C                                              | -3.539866 | -0.127000 | -0.464884 |
| H                                              | -3.251260 | 0.720957  | -1.088393 |
| H                                              | -4.155085 | 0.267650  | 0.345690  |
| H                                              | -4.112597 | -0.843637 | -1.046045 |
| O                                              | -2.117693 | -1.972889 | 0.007495  |
| O                                              | 2.686068  | -0.878290 | -1.060369 |
| O                                              | 2.222539  | -1.693989 | 0.076422  |
| Rotational constants (GHz):                    |           |           |           |
| Vibrational harmonic frequencies (cm-1):       |           |           |           |
| i727.2228                                      | 25.2063   | 58.6591   |           |
| 64.9329                                        | 114.1534  | 131.4046  |           |
| 150.4131                                       | 194.8330  | 203.8143  |           |
| 217.6408                                       | 236.4035  | 285.1943  |           |
| 299.5982                                       | 336.0327  | 343.1958  |           |
| 363.5272                                       | 384.1458  | 437.1449  |           |
| 483.2157                                       | 561.4291  | 582.9144  |           |
| 625.0892                                       | 695.4373  | 724.9348  |           |
| 749.8009                                       | 757.3474  | 840.7556  |           |
| 893.8811                                       | 919.7955  | 945.9135  |           |
| 962.0623                                       | 971.7021  | 979.7829  |           |
| 996.9551                                       | 1003.5209 | 1028.5519 |           |
| 1056.2516                                      | 1083.3791 | 1141.9198 |           |
| 1152.4144                                      | 1178.8689 | 1193.3756 |           |
| 1210.3680                                      | 1228.3755 | 1262.7092 |           |
| 1275.5511                                      | 1296.0684 | 1331.5880 |           |
| 1367.8453                                      | 1382.3466 | 1398.1430 |           |

|           |           |           |
|-----------|-----------|-----------|
| 1404.1720 | 1410.0875 | 1424.8360 |
| 1431.4590 | 1439.2274 | 1465.1068 |
| 1478.1564 | 1485.7349 | 1493.2275 |
| 1507.0702 | 1509.7018 | 1516.8324 |
| 1634.9793 | 1841.3851 | 2992.2705 |
| 3024.6739 | 3036.0147 | 3042.4837 |
| 3049.0186 | 3051.1147 | 3062.3672 |
| 3067.8915 | 3105.3379 | 3109.9181 |
| 3114.5838 | 3120.0414 | 3125.6981 |
| 3150.8012 | 3178.0533 | 3197.1842 |

Zero-point correction (Hartree): 0.245126

Population analysis as 298K (%)

Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)

| Compound        | Qtot      | Erel | Erel2 | n*Q*MB    | %      |
|-----------------|-----------|------|-------|-----------|--------|
| TS.SOZ.b.CI.J.b | 2.051e+42 | 0.00 | 0.00  | 2.051e+42 | 99.9   |
| TS.SOZ.a.CI.J.b | 2.838e+42 | 4.48 | 4.48  | 1.461e+39 | 0.0712 |
| Total           |           |      |       | 2.052e+42 | 100    |

TS.SOZ.a.CI.J.b

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.13398648

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -1.087159 | -1.238201 | -0.402918 |
| H | -1.836003 | -2.031483 | -0.429693 |
| C | 0.234760  | -1.897947 | 0.041083  |
| C | 1.628205  | -1.349689 | -0.192810 |
| H | 0.257868  | -2.879706 | -0.435537 |
| H | 0.200616  | -2.048308 | 1.123705  |
| H | 2.292494  | -1.879585 | -0.867018 |
| C | -1.546911 | 0.050231  | 0.340698  |
| C | -0.939634 | -0.381298 | -1.675838 |
| C | -3.040658 | 0.288263  | 0.071969  |
| C | -1.356787 | 0.243645  | 1.838469  |
| H | -2.161703 | -0.270498 | 2.368285  |
| H | -0.405230 | -0.107946 | 2.210789  |
| H | -1.445039 | 1.305445  | 2.081056  |
| H | -3.327307 | 1.266982  | 0.460314  |
| H | -3.631554 | -0.462506 | 0.598766  |
| H | -3.313339 | 0.254315  | -0.979956 |
| H | -1.860294 | -0.317304 | -2.243810 |
| H | -0.119872 | -0.620396 | -2.344052 |
| C | -0.725850 | 0.832234  | -0.740595 |
| H | -1.162007 | 1.791548  | -1.032033 |
| C | 0.770314  | 1.064046  | -0.557120 |
| C | 1.209826  | 2.407501  | -0.058856 |
| H | 0.624927  | 2.698240  | 0.811504  |
| H | 1.035599  | 3.140030  | -0.851619 |
| H | 2.264756  | 2.381818  | 0.193081  |
| O | 1.555236  | 0.340225  | -1.197675 |
| O | 2.261054  | -0.744385 | 0.731995  |
| O | 1.397391  | 0.112491  | 1.384645  |

Rotational constants (GHz): 1.1959100 0.7821600 0.7178700

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i356.1235 | 89.1337   | 124.2400  |
| 152.2505  | 180.6512  | 209.1366  |
| 230.2699  | 240.6188  | 244.0951  |
| 256.1238  | 317.6744  | 330.7180  |
| 372.3042  | 388.7989  | 414.7012  |
| 469.8892  | 482.5512  | 518.3673  |
| 559.5717  | 577.9618  | 614.2948  |
| 661.8367  | 699.9880  | 753.2292  |
| 792.3903  | 859.1444  | 895.1670  |
| 928.8003  | 938.3128  | 953.1668  |
| 968.4047  | 982.2024  | 997.6414  |
| 1006.6057 | 1028.4189 | 1039.8516 |
| 1042.3140 | 1087.7262 | 1118.6153 |
| 1139.8047 | 1156.5091 | 1183.8733 |
| 1203.8845 | 1228.8256 | 1249.2749 |
| 1269.2720 | 1275.3747 | 1320.9385 |
| 1329.1960 | 1354.9994 | 1358.7881 |
| 1399.0249 | 1400.6695 | 1404.2389 |
| 1421.1361 | 1458.0988 | 1463.4915 |
| 1476.5899 | 1481.6061 | 1495.3537 |
| 1500.3602 | 1520.5510 | 1529.9673 |
| 1549.3957 | 1636.4338 | 3050.9618 |
| 3054.0893 | 3056.3361 | 3060.3511 |
| 3062.8554 | 3074.4001 | 3101.8473 |
| 3106.0103 | 3120.8692 | 3135.7614 |
| 3136.8354 | 3157.0016 | 3190.9866 |
| 3191.9564 | 3192.4981 | 3222.4400 |

Zero-point correction (Hartree): 0.248890

TS.SOZ.b.CI.J.b

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E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -615.21544917

E(CCSD/Aug-CC-pVTZ) (Hartree): -615.09077889

T1 diagnostic: 0.022677

E(MP2/Aug-CC-pVTZ) (Hartree): -615.02533277

E(MP3/Aug-CC-pVTZ) (Hartree): -615.07309376

E(RHF/Aug-CC-pVTZ) (Hartree): -612.56749185

E(RM062X/Aug-CC-pVTZ) (Hartree): -616.14121797

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -1.019337 | -0.987547 | -0.816814 |
| H | -1.720340 | -1.677692 | -1.290971 |
| C | 0.104699  | -1.864552 | -0.236408 |
| C | 1.287201  | -1.402960 | 0.585047  |
| H | 0.591773  | -2.355921 | -1.086128 |

```

H -0.372773 -2.640033 0.364546
H 1.472445 -1.909056 1.527332
C -1.656411 0.026226 0.171414
C -0.565648 0.204587 -1.678425
C -3.059688 0.430977 -0.286946
C -1.755135 -0.330637 1.650854
H -0.901622 -0.879114 2.032662
H -1.854245 0.573138 2.254368
H -2.651468 -0.933422 1.811709
H -3.432057 1.242375 0.341158
H -3.745176 -0.411551 -0.183099
H -3.093420 0.767544 -1.321056
H -1.345136 0.501845 -2.373451
H 0.383992 0.127569 -2.188694
C -0.622804 1.060332 -0.385547
H -0.983133 2.085676 -0.501039
C 0.696852 1.115427 0.355388
C 1.536290 2.343566 0.170430
H 1.085291 3.156763 0.745803
H 1.560229 2.635731 -0.877164
H 2.543342 2.156139 0.528767
O 0.908725 0.356821 1.317605
O 2.074614 -0.131458 -0.995338
O 2.364934 -0.976925 0.057895
Rotational constants (GHz): 1.2547200 0.7726600 0.6859700
Vibrational harmonic frequencies (cm-1):
i352.4615 123.1430 142.1259
167.9013 179.9208 218.8065
226.6397 230.0004 251.0464
255.2819 283.0923 322.6342
369.3617 379.7253 424.3110
451.3837 457.5345 511.1343
557.6858 597.6453 608.4177
668.5569 702.9681 775.3255
801.6373 867.9189 882.8841
920.2390 940.7191 954.3352
973.3389 981.9925 988.5071
1011.4118 1022.3585 1037.4755
1047.6561 1083.1051 1127.4473
1152.4818 1161.9642 1175.3679
1207.6288 1225.3514 1250.4483
1268.0121 1283.7763 1320.1533
1339.6346 1362.9629 1374.8853
1401.6310 1404.8315 1410.2101
1423.9824 1457.5136 1463.7280
1478.0034 1484.7123 1490.7053
1497.3349 1514.0374 1515.2660
1550.7804 1650.5527 3042.1629
3054.8258 3056.5725 3059.7808
3066.2398 3068.2823 3102.0193
3113.2189 3118.8832 3129.1851
3139.2211 3152.8267 3180.9652
3186.8744 3190.3759 3214.6378
Zero-point correction (Hartree): 0.248976

```

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#####
E-pinonaldehyde-A-oxide
#####

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Population analysis as 298K (%)
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)
Compound Qtot Erel Erel2 n*Q*MB %

ApineneCI.J.a.pmt 3.584e+44 0.00 0.00 3.584e+44 42.4
ApineneCI.J.a.pmp 4.108e+44 0.50 0.50 1.778e+44 21
ApineneCI.J.a.pmm 9.028e+44 1.51 1.51 7.036e+43 8.32
ApineneCI.J.a.ppt 4.197e+44 1.15 1.15 6.002e+43 7.1
ApineneCI.J.a.ppp 7.223e+44 1.51 1.51 5.612e+43 6.64
ApineneCI.J.a.ppm 9.514e+44 1.72 1.72 5.197e+43 6.15
ApineneCI.J.a.pmt 6.449e+44 2.16 2.16 1.694e+43 2
ApineneCI.J.a.mpm 1.134e+45 2.65 2.65 1.301e+43 1.54
ApineneCI.J.a.mpt 5.113e+44 2.24 2.24 1.172e+43 1.39
ApineneCI.J.a.mmp 7.492e+44 2.47 2.47 1.151e+43 1.36
ApineneCI.J.a.mpp 9.966e+44 3.10 3.10 5.322e+42 0.629
ApineneCI.J.a.ptm 3.362e+44 2.48 2.48 5.098e+42 0.603
ApineneCI.J.a.mmm 9.046e+44 3.17 3.17 4.309e+42 0.51
ApineneCI.J.a.mtt 1.095e+45 3.78 3.78 1.865e+42 0.221
ApineneCI.J.a.ptt 6.189e+44 4.00 4.00 7.236e+41 0.0856
ApineneCI.J.a.mtm 5.678e+44 4.12 4.12 5.374e+41 0.0636
Total 8.457e+44 100

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ApineneCI.J.a.mmm
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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.15792058
Electronic state : 1-A
Cartesian coordinates (Angs):
C      -0.455380      -0.679752      -0.412751
H      -0.823649      -0.640625     -1.439938
C     -1.596834     -1.102825      0.512195
C     -2.725424     -0.148104      0.428352
H     -1.953985     -2.096779      0.243825
H     -1.238705     -1.129522      1.544191
H     -2.675793      0.883042      0.772975
C      0.362548      0.617978     -0.127886
C      0.851512     -1.493820     -0.367483
C     -0.023270      1.853149     -0.918423
C      0.460465      0.937172      1.359479
H      0.788160      0.078131      1.948513
H      1.176404      1.740035      1.521559
H     -0.507357      1.261502      1.747546
H      0.737068      2.626001     -0.799388

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|                                                           |           |           |           |
|-----------------------------------------------------------|-----------|-----------|-----------|
| H                                                         | -0.976201 | 2.261691  | -0.574453 |
| H                                                         | -0.119209 | 1.625871  | -1.980931 |
| H                                                         | 0.965617  | -2.309064 | -1.077669 |
| H                                                         | 1.048342  | -1.866570 | 0.638572  |
| C                                                         | 1.598096  | -0.172285 | -0.642615 |
| H                                                         | 1.694854  | -0.027983 | -1.723588 |
| C                                                         | 2.961491  | 0.089065  | -0.054336 |
| C                                                         | 3.894962  | -1.090428 | 0.042811  |
| H                                                         | 3.900372  | -1.648189 | -0.894766 |
| H                                                         | 3.536089  | -1.772016 | 0.816369  |
| H                                                         | 4.896377  | -0.753457 | 0.292759  |
| O                                                         | 3.285438  | 1.196545  | 0.298251  |
| O                                                         | -3.792293 | -0.501134 | -0.097142 |
| O                                                         | -4.795316 | 0.417969  | -0.195065 |
| Rotational constants (GHz): 1.9174900 0.3685100 0.3399400 |           |           |           |
| Vibrational harmonic frequencies (cm-1):                  |           |           |           |
| 30.0426                                                   | 36.2658   | 54.7671   |           |
| 87.3030                                                   | 127.6332  | 149.8524  |           |
| 163.1000                                                  | 204.6451  | 230.0384  |           |
| 258.5359                                                  | 270.3997  | 306.4360  |           |
| 313.4045                                                  | 316.8891  | 342.9943  |           |
| 384.4339                                                  | 403.6905  | 435.9756  |           |
| 508.5269                                                  | 530.7746  | 588.7945  |           |
| 605.2845                                                  | 624.5883  | 723.7829  |           |
| 766.4191                                                  | 859.5853  | 901.5264  |           |
| 925.3173                                                  | 947.5657  | 962.8350  |           |
| 970.2593                                                  | 980.3179  | 989.0317  |           |
| 1009.5259                                                 | 1025.3837 | 1035.7956 |           |
| 1084.6556                                                 | 1099.7974 | 1124.5665 |           |
| 1146.6913                                                 | 1180.8666 | 1198.2660 |           |
| 1211.3835                                                 | 1239.6333 | 1252.5853 |           |
| 1275.2902                                                 | 1283.4944 | 1301.1060 |           |
| 1326.0918                                                 | 1351.4843 | 1381.2916 |           |
| 1389.3551                                                 | 1397.8077 | 1411.5314 |           |
| 1424.2565                                                 | 1463.7622 | 1470.8123 |           |
| 1476.6781                                                 | 1485.2606 | 1496.7556 |           |
| 1500.2968                                                 | 1506.0983 | 1516.5143 |           |
| 1661.2827                                                 | 1832.9008 | 3048.5857 |           |
| 3052.4335                                                 | 3055.3019 | 3064.4794 |           |
| 3065.7873                                                 | 3075.8913 | 3084.6201 |           |
| 3114.4318                                                 | 3116.7297 | 3125.8324 |           |
| 3128.8600                                                 | 3130.3265 | 3146.5737 |           |
| 3154.3979                                                 | 3161.8622 | 3181.5805 |           |
| Zero-point correction (Hartree): 0.246657                 |           |           |           |
| ApineneCI.J.a.mmp                                         |           |           |           |
| ~~~~~                                                     |           |           |           |
| E(RM062X/Aug-CC-pVTZ) (Hartree): -616.15899272            |           |           |           |
| Electronic state : 1-A                                    |           |           |           |
| Cartesian coordinates (Angs):                             |           |           |           |
| C                                                         | -0.354925 | 0.973164  | 0.602088  |
| H                                                         | -0.573036 | 1.055748  | 1.670091  |
| C                                                         | -1.560416 | 1.460550  | -0.199653 |
| C                                                         | -2.756533 | 0.673896  | 0.176011  |
| H                                                         | -1.745865 | 2.512516  | 0.035065  |
| H                                                         | -1.390336 | 1.369869  | -1.271468 |
| H                                                         | -3.169447 | 0.653278  | 1.183416  |
| C                                                         | 0.232553  | -0.443243 | 0.331040  |
| C                                                         | 1.029345  | 1.586789  | 0.322811  |
| C                                                         | -0.232810 | -1.550126 | 1.256101  |
| C                                                         | 0.096107  | -0.869772 | -1.126694 |
| H                                                         | 0.453057  | -0.103119 | -1.818189 |
| H                                                         | 0.681593  | -1.770206 | -1.302072 |
| H                                                         | -0.945601 | -1.085854 | -1.367760 |
| H                                                         | 0.369833  | -2.446295 | 1.104937  |
| H                                                         | -1.276451 | -1.808393 | 1.056745  |
| H                                                         | -0.146938 | -1.251636 | 2.302307  |
| H                                                         | 1.345525  | 2.426869  | 0.936665  |
| H                                                         | 1.138274  | 1.852202  | -0.729082 |
| C                                                         | 1.621016  | 0.193840  | 0.625396  |
| H                                                         | 1.837978  | 0.111917  | 1.695186  |
| C                                                         | 2.841341  | -0.316486 | -0.099463 |
| C                                                         | 3.861130  | 0.705756  | -0.531768 |
| H                                                         | 4.065632  | 1.407032  | 0.278469  |
| H                                                         | 3.456767  | 1.287568  | -1.362497 |
| H                                                         | 4.773450  | 0.209786  | -0.848935 |
| O                                                         | 2.989063  | -1.496436 | -0.302318 |
| O                                                         | -3.310751 | -0.055181 | -0.660415 |
| O                                                         | -4.370222 | -0.811819 | -0.249529 |
| Rotational constants (GHz): 1.7314400 0.4106300 0.3746700 |           |           |           |
| Vibrational harmonic frequencies (cm-1):                  |           |           |           |
| 27.4725                                                   | 38.8650   | 55.8243   |           |
| 93.6328                                                   | 140.5495  | 155.7761  |           |
| 158.7973                                                  | 200.2493  | 233.3294  |           |
| 254.8866                                                  | 272.0680  | 306.8503  |           |
| 313.5369                                                  | 319.1487  | 350.7439  |           |
| 390.6032                                                  | 408.9876  | 433.3109  |           |
| 505.4728                                                  | 526.4846  | 591.2897  |           |
| 605.6145                                                  | 618.9501  | 720.3216  |           |
| 762.2281                                                  | 865.2655  | 898.5805  |           |
| 922.5995                                                  | 946.0698  | 957.9112  |           |
| 967.2089                                                  | 978.7100  | 997.7651  |           |
| 1019.8528                                                 | 1030.4199 | 1041.6439 |           |
| 1062.3981                                                 | 1100.2459 | 1118.5885 |           |
| 1150.3956                                                 | 1179.4830 | 1197.3814 |           |
| 1211.6372                                                 | 1241.2981 | 1248.7213 |           |
| 1267.7315                                                 | 1281.4824 | 1297.3846 |           |
| 1325.0640                                                 | 1352.4197 | 1382.8340 |           |
| 1391.2412                                                 | 1402.2008 | 1412.9397 |           |
| 1423.7807                                                 | 1464.5713 | 1470.0027 |           |
| 1477.4825                                                 | 1486.1869 | 1496.9482 |           |
| 1500.5952                                                 | 1510.1945 | 1516.0768 |           |

|           |           |           |
|-----------|-----------|-----------|
| 1664.5803 | 1833.3541 | 3041.2677 |
| 3054.1762 | 3056.3237 | 3058.7821 |
| 3060.5993 | 3063.6953 | 3086.3111 |
| 3108.7386 | 3122.4131 | 3125.3145 |
| 3129.0597 | 3136.7040 | 3144.8604 |
| 3151.5278 | 3157.2042 | 3180.1297 |

Zero-point correction (Hartree): 0.246624

ApineneCI.J.a.mmt

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.15920912

Electronic state : 1-A

Cartesian coordinates (Angs):

C	0.482047	0.869150	-0.482607
H	0.875846	0.794326	-1.497343
C	1.512004	1.517497	0.421787
C	2.815669	0.817684	0.482260
H	1.707619	2.548611	0.104188
H	1.139923	1.599932	1.448086
H	3.630179	1.108402	1.142741
C	-0.165352	-0.501401	-0.093842
C	-0.919920	1.506924	-0.505432
C	0.345060	-1.741698	-0.803110
C	-0.198592	-0.720306	1.413337
H	-0.637930	0.124649	1.948850
H	-0.790181	-1.601959	1.650132
H	0.814429	-0.877367	1.791360
H	-0.367175	-2.556412	-0.663613
H	1.312658	-2.057474	-0.413649
H	0.456188	-1.562149	-1.873660
H	-1.137896	2.230313	-1.287814
H	-1.167756	1.946230	0.462386
C	-1.495140	0.083929	-0.646267
H	-1.584758	-0.169675	-1.707732
C	-2.810884	-0.283163	-0.009493
C	-3.883769	0.777113	-0.015236
H	-3.960566	1.234401	-1.002715
H	-3.611289	1.570754	0.682961
H	-4.834990	0.345343	0.280905
O	-2.996219	-1.379012	0.459994
O	3.022500	-0.160328	-0.250129
O	4.232339	-0.789698	-0.164048

Rotational constants (GHz): 1.7691800 0.4302600 0.3877300

Vibrational harmonic frequencies (cm-1):

28.9320	44.5238	63.1843
96.7949	117.9352	133.2044
163.4593	211.8266	242.3341
249.9237	267.0286	299.6831
311.8452	321.1963	330.4465
392.7698	401.4105	439.1868
505.7068	521.5764	595.7994
619.1653	683.1445	714.9790
763.9758	828.1812	899.1087
920.9279	938.4391	963.3032
968.0815	973.1178	993.6356
998.4449	1027.3778	1032.3420
1040.1357	1112.6515	1114.3411
1155.9066	1172.1286	1193.6173
1202.9979	1238.4736	1254.6153
1272.8970	1289.2713	1306.1401
1335.7734	1356.3085	1378.3550
1392.6446	1406.9711	1420.8209
1425.9801	1446.8921	1464.2628
1476.7616	1484.5144	1494.9776
1498.2135	1506.4753	1513.6709
1665.0348	1832.8672	3034.5590
3046.1145	3050.7599	3055.4586
3065.1893	3065.7522	3075.8179
3090.1710	3107.5786	3124.5853
3126.6121	3137.5904	3139.9676
3152.4558	3157.5739	3181.0376

Zero-point correction (Hartree): 0.246334

ApineneCI.J.a.mpm

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.15862772

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.542519  | -0.638090 | -0.502711 |
| H | 0.739189  | -0.973598 | -1.523876 |
| C | 1.726942  | -0.999063 | 0.395267  |
| C | 2.953306  | -0.364214 | -0.134208 |
| H | 1.560140  | -0.652466 | 1.413977  |
| H | 1.863429  | -2.083515 | 0.409189  |
| H | 3.438507  | -0.660344 | -1.062548 |
| C | -0.891009 | -1.096886 | -0.098168 |
| C | 0.057613  | 0.823825  | -0.522032 |
| C | -1.414889 | -2.342765 | -0.783601 |
| C | -1.068944 | -1.198141 | 1.411571  |
| H | -0.747051 | -0.291856 | 1.928557  |
| H | -2.117394 | -1.360595 | 1.652717  |
| H | -0.489727 | -2.035615 | 1.805015  |
| H | -2.477844 | -2.467984 | -0.574209 |
| H | -0.891652 | -3.231894 | -0.424513 |
| H | -1.283000 | -2.283067 | -1.864918 |
| H | 0.437689  | 1.478463  | -1.302497 |
| H | 0.216072  | 1.301265  | 0.445923  |
| C | -1.374940 | 0.268029  | -0.663593 |
| H | -1.620114 | 0.154693  | -1.724531 |
| C | -2.550981 | 0.964989  | -0.026786 |
| C | -2.503112 | 2.469731  | 0.028165  |
| H | -2.196233 | 2.875741  | -0.936778 |



|                                           |           |           |                               |
|-------------------------------------------|-----------|-----------|-------------------------------|
| H                                         | -1.750993 | 2.780139  | 0.756045                      |
| H                                         | -3.472564 | 2.863068  | 0.318427                      |
| O                                         | -3.488244 | 0.333809  | 0.397017                      |
| O                                         | 3.444727  | 0.608992  | 0.457900                      |
| O                                         | 4.535081  | 1.215084  | -0.097343                     |
| Rotational constants (GHz):               |           |           | 1.3298900 0.4167000 0.3512600 |
| Vibrational harmonic frequencies (cm-1):  |           |           |                               |
| 30.6248                                   | 34.1438   | 56.8518   |                               |
| 92.0204                                   | 123.7319  | 137.9765  |                               |
| 166.5021                                  | 179.5769  | 229.8067  |                               |
| 251.2680                                  | 274.7861  | 294.5354  |                               |
| 317.9007                                  | 320.2424  | 344.6498  |                               |
| 364.9856                                  | 411.9068  | 467.8726  |                               |
| 498.7791                                  | 515.4881  | 597.4813  |                               |
| 598.9636                                  | 634.3781  | 732.0544  |                               |
| 786.7988                                  | 850.5364  | 898.4173  |                               |
| 921.5709                                  | 938.5310  | 964.6415  |                               |
| 966.7061                                  | 979.8976  | 992.3312  |                               |
| 1012.4965                                 | 1021.8220 | 1042.2727 |                               |
| 1061.6479                                 | 1095.9367 | 1129.5552 |                               |
| 1151.2475                                 | 1179.9487 | 1199.3262 |                               |
| 1224.8756                                 | 1240.8804 | 1253.1758 |                               |
| 1259.1171                                 | 1284.9546 | 1300.3659 |                               |
| 1320.2322                                 | 1352.1462 | 1381.4387 |                               |
| 1390.9183                                 | 1398.3851 | 1409.9622 |                               |
| 1421.6618                                 | 1463.9362 | 1474.4063 |                               |
| 1475.9681                                 | 1485.4344 | 1495.1332 |                               |
| 1500.4435                                 | 1508.0001 | 1515.5449 |                               |
| 1660.2371                                 | 1831.4368 | 3047.4352 |                               |
| 3051.8735                                 | 3054.6353 | 3063.8484 |                               |
| 3064.3280                                 | 3064.4190 | 3084.4235 |                               |
| 3114.8736                                 | 3116.8892 | 3125.4907 |                               |
| 3130.2564                                 | 3139.0456 | 3146.2690 |                               |
| 3151.6978                                 | 3159.9284 | 3181.8999 |                               |
| Zero-point correction (Hartree): 0.246535 |           |           |                               |

ApineneCI.J.a.mpp

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.15790241

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-0.572607	0.258191	-0.338611
H	-0.920759	0.429935	-1.359140
C	-1.723153	0.510060	0.634307
C	-2.836963	-0.422911	0.357059
H	-1.377342	0.335315	1.656804
H	-2.086686	1.535018	0.562131
H	-2.745723	-1.505423	0.428483
C	0.775121	1.015393	-0.139493
C	0.189103	-1.081562	-0.274444
C	0.978015	2.254286	-0.988385
C	1.069151	1.312690	1.325413
H	0.980590	0.425301	1.955867
H	2.083532	1.691127	1.432356
H	0.376977	2.067240	1.703534
H	2.010652	2.596822	-0.912644
H	0.326019	3.064029	-0.653886
H	0.758753	2.052848	-2.037800
H	-0.122029	-1.881235	-0.942657
H	0.228389	-1.465437	0.746606
C	1.463401	-0.288161	-0.631677
H	1.574366	-0.251014	-1.720205
C	2.809501	-0.683893	-0.079436
C	3.071944	-2.159531	0.079022
H	2.770247	-2.697644	-0.820751
H	2.466479	-2.548086	0.900152
H	4.122837	-2.330122	0.291994
O	3.635751	0.150305	0.198394
O	-3.936574	0.013019	-0.015175
O	-4.922600	-0.889079	-0.294889

Rotational constants (GHz):			1.5712200 0.3657600 0.3249600
Vibrational harmonic frequencies (cm-1):			
36.2759	40.7804	44.2004	
93.4759	132.1129	140.8045	
158.8237	197.8967	223.1144	
254.4027	269.3226	290.4946	
312.4804	317.4499	341.7099	
357.1674	408.8423	475.2253	
496.3457	516.9643	590.0644	
602.0005	632.9723	734.0486	
787.9568	851.8565	898.8515	
922.7900	937.1235	963.6383	
967.1563	979.0000	985.0358	
1005.2507	1029.2218	1038.8015	
1063.3885	1108.3174	1136.6845	
1160.6157	1178.5608	1197.7902	
1217.0152	1238.6647	1255.4589	
1265.6217	1284.6468	1302.7305	
1323.3877	1352.0905	1380.3878	
1390.6889	1397.8641	1411.2017	
1420.9852	1464.4816	1470.7969	
1477.5805	1484.8561	1495.1866	
1499.4010	1507.1504	1516.1215	
1665.3072	1832.8018	3048.7334	
3051.9178	3055.0093	3059.7121	
3063.8449	3072.8656	3080.2812	
3114.7058	3118.0246	3125.0514	
3127.7764	3130.4904	3141.2093	
3153.6757	3156.2669	3181.6045	

Rotational constants (GHz):			1.5712200 0.3657600 0.3249600
Vibrational harmonic frequencies (cm-1):			
36.2759	40.7804	44.2004	
93.4759	132.1129	140.8045	
158.8237	197.8967	223.1144	
254.4027	269.3226	290.4946	
312.4804	317.4499	341.7099	
357.1674	408.8423	475.2253	
496.3457	516.9643	590.0644	
602.0005	632.9723	734.0486	
787.9568	851.8565	898.8515	
922.7900	937.1235	963.6383	
967.1563	979.0000	985.0358	
1005.2507	1029.2218	1038.8015	
1063.3885	1108.3174	1136.6845	
1160.6157	1178.5608	1197.7902	
1217.0152	1238.6647	1255.4589	
1265.6217	1284.6468	1302.7305	
1323.3877	1352.0905	1380.3878	
1390.6889	1397.8641	1411.2017	
1420.9852	1464.4816	1470.7969	
1477.5805	1484.8561	1495.1866	
1499.4010	1507.1504	1516.1215	
1665.3072	1832.8018	3048.7334	
3051.9178	3055.0093	3059.7121	
3063.8449	3072.8656	3080.2812	
3114.7058	3118.0246	3125.0514	
3127.7764	3130.4904	3141.2093	
3153.6757	3156.2669	3181.6045	

Rotational constants (GHz):			1.5712200 0.3657600 0.3249600
Vibrational harmonic frequencies (cm-1):			
36.2759	40.7804	44.2004	
93.4759	132.1129	140.8045	
158.8237	197.8967	223.1144	
254.4027	269.3226	290.4946	
312.4804	317.4499	341.7099	
357.1674	408.8423	475.2253	
496.3457	516.9643	590.0644	
602.0005	632.9723	734.0486	
787.9568	851.8565	898.8515	
922.7900	937.1235	963.6383	
967.1563	979.0000	985.0358	
1005.2507	1029.2218	1038.8015	
1063.3885	1108.3174	1136.6845	
1160.6157	1178.5608	1197.7902	
1217.0152	1238.6647	1255.4589	
1265.6217	1284.6468	1302.7305	
1323.3877	1352.0905	1380.3878	
1390.6889	1397.8641	1411.2017	
1420.9852	1464.4816	1470.7969	
1477.5805	1484.8561	1495.1866	
1499.4010	1507.1504	1516.1215	
1665.3072	1832.8018	3048.7334	
3051.9178	3055.0093	3059.7121	
3063.8449	3072.8656	3080.2812	
3114.7058	3118.0246	3125.0514	
3127.7764	3130.4904	3141.2093	
3153.6757	3156.2669	3181.6045	

Rotational constants (GHz):			1.5712200 0.3657600 0.3249600
Vibrational harmonic frequencies (cm-1):			
36.2759	40.7804	44.2004	
93.4759	132.1129	140.8045	
158.8237	197.8967	223.1144	
254.4027	269.3226	290.4946	
312.4804	317.4499	341.7099	
357.1674	408.8423	475.2253	
496.3457	516.9643	590.0644	
602.0005	632.9723	734.0486	
787.9568	851.8565	898.8515	
922.7900	937.1235	963.6383	
967.1563	979.0000	985.0358	
1005.2507	1029.2218	1038.8015	
1063.3885	1108.3174	1136.6845	
1160.6157	1178.5608	1197.7902	
1217.0152	1238.6647	1255.4589	
1265.6217	1284.6468	1302.7305	
1323.3877	1352.0905	1380.3878	
1390.6889	1397.8641	1411.2017	
1420.9852	1464.4816	1470.7969	
1477.5805	1484.8561	1495.1866	
1499.4010	1507.1504	1516.1215	
1665.3072	1832.8018	3048.7334	
3051.9178	3055.0093	3059.7121	
3063.8449	3072.8656	3080.2812	
3114.7058	3118.0246	3125.0514	
3127.7764	3130.4904	3141.2093	
3153.6757	3156.2669	3181.6045	

Rotational constants (GHz):			1.5712200 0.3657600 0.3249600
Vibrational harmonic frequencies (cm-1):			
36.2759	40.7804	44.2004	
93.4759	132.1129	140.8045	
158.8237	197.8967	223.1144	
254.4027	269.3226	290.4946	
312.4804	317.4499	341.7099	
357.1674	408.8423	475.2253	
496.3457	516.9643	590.0644	
602.0005	632.9723	734.0486	
787.9568	851.8565	898.8515	
922.7900	937.1235	963.6383	
967.1563	979.0000	985.0358	
1005.2507	1029.2218	1038.8015	
1063.3885	1108.3174	1136.6845	
1160.6157	1178.5608	1197.7902	
1217.0152	1238.6647	1255.4589	
1265.6217	1284.6468	1302.7305	
1323.3877	1352.0905	1380.3878	
1390.6889	1397.8641	1411.2017	
1420.9852	1464.4816	1470.7969	
1477.5805	1484.8561	1495.1866	
1499.4010	1507.1504	1516.1215	
1665.3072	1832.8018	3048.7334	
3051.9178	3055.0093	3059.7121	
3063.8449	3072.8656	3080.2812	
3114.7058	3118.0246	3125.0514	
3127.7764	3130.4904	3141.2093	
3153.6757	3156.2669	3181.6045	

Rotational constants (GHz):			1.5712200 0.3657600 0.3249600
Vibrational harmonic frequencies (cm-1):			
36.2759	40.7804	44.2004	
93.4759	132.1129	140.8045	
158.8237	197.8967	223.1144	
254.4027	269.3226	290.4946	
312.4804	317.4499	341.7099	
357.1674	408.8423	475.2253	
496.3457	516.9643	590.0644	
602.0005	632.9723	734.0486	
787.9568	851.8565	898.8515	
922.7900	937.1235	963.6383	
967.1563	979.0000	985.0358	
1005.2507	1029.2218	1038.8015	
1063.3885	1108.3174	1136.6845	
1160.6157	1178.5608	1197.7902	
1217.0152	1238.6647	1255.4589	
1265.6217	1284.6468	1302.7305	
1323.3877	1352.0905	1380.3878	
1390.6889	1397.8641	1411.2017	
1420.9852	1464.4816	1470.7969	
1477.5805	1484.8561	1495.1866	
1499.4010	1507.1504	1516.1215	
1665.3072	1832.8018	3048.7334	
3051.9178	3055.0093	3059.7121	
3063.8449	3072.8656	3080.2812	
3114.7058	3118.0246	3125.0514	
3127.7764	3130.4904	3141.2093	
3153.6757	3156.2669	3181.6045	

Rotational constants (GHz):			1.5712200 0.3657600 0.3249600
Vibrational harmonic frequencies (cm-1):			
36.2759	40.7804	44.2004	
93.4759	132.112		

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.15915685
Electronic state : 1-A
Cartesian coordinates (Angs):
C      0.663108      -0.483648      -0.284151
H      1.032899      -0.600886      -1.304426
C      1.713913      -0.970059      0.692153
C      3.016237      -0.273091      0.573950
H      1.378634      -0.852147      1.728334
H      1.903674      -2.043255      0.571581
H      3.874930      -0.485447      1.207716
C     -0.778978      -1.067067      -0.203357
C      0.083000      0.934728      -0.118312
C     -1.107053      -2.184063      -1.174219
C     -1.175984      -1.456766      1.215744
H     -0.997248      -0.651838      1.931935
H     -2.235508      -1.700488      1.254112
H     -0.609048      -2.331562      1.540507
H     -2.177972      -2.390422      -1.163754
H     -0.582415      -3.102533      -0.900895
H     -0.818165      -1.917957      -2.191922
H      0.534928      1.734617      -0.698083
H      0.053179      1.229312      0.932203
C     -1.268883      0.356537      -0.587441
H     -1.336441      0.435133      -1.677518
C     -2.572491      0.880415      -0.042756
C     -2.646484      2.361584      0.225739
H     -2.247804      2.920759      -0.621903
H     -2.021026      2.604031      1.086943
H     -3.672569      2.653268      0.428103
O     -3.511023      0.144856      0.145132
O      3.170289      0.610892      -0.281272
O      4.385940      1.232751      -0.352241
Rotational constants (GHz):      1.3591000      0.4294700      0.3645600
Vibrational harmonic frequencies (cm-1):
36.5094      44.8776      86.6247
88.1902      133.5848      144.3871
158.1500      187.1734      225.2614
253.0740      258.0822      283.0472
313.7556      326.1514      336.0399
361.7448      408.3667      464.8837
505.0290      516.3013      593.8224
617.4284      675.2750      736.1319
799.9202      816.9502      901.9265
922.3133      943.2726      956.7094
965.6444      980.2772      989.6109
992.8766      1013.9867      1031.0478
1048.2312      1091.4648      1131.0421
1153.6594      1177.9765      1200.7467
1214.5325      1237.6458      1252.6618
1264.0989      1290.3499      1314.3627
1336.1715      1357.0746      1382.0573
1394.1446      1405.2173      1419.0931
1428.9830      1448.2345      1464.5780
1476.7688      1484.6476      1495.6929
1500.1345      1507.0537      1516.2618
1664.0312      1830.4156      3033.8086
3045.9391      3049.5884      3053.0538
3061.8746      3064.8618      3076.8420
3087.3074      3112.6913      3114.7195
3126.1032      3128.4666      3153.0356
3154.2298      3162.2659      3181.5293
Zero-point correction (Hartree): 0.246411

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ApineneCI.J.a.mtm
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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.15653253
Electronic state : 1-A
Cartesian coordinates (Angs):
C      0.335620      1.090530      1.000598
H      0.080862      2.031760      1.490639
C      1.863288      1.007352      0.955957
C      2.389550      -0.299248      0.503009
H      2.273436      1.789746      0.316506
H      2.244985      1.173011      1.969271
H      2.130892      -1.250436      0.963325
C     -0.518256      0.990050      -0.295329
C     -0.518366      -0.031306      1.628379
C     -0.900414      2.298836      -0.955939
C      0.043618      0.018460      -1.326888
H      0.317835      -0.950036      -0.899097
H     -0.701406      -0.164317      -2.101604
H      0.933013      0.429404      -1.806084
H     -1.662265      2.126333      -1.717031
H     -0.033757      2.755795      -1.438815
H     -1.300531      3.005055      -0.227298
H     -0.763882      0.052839      2.684524
H     -0.105864      -1.022478      1.442404
C     -1.609892      0.321046      0.600164
H     -2.272203      1.097728      0.987440
C     -2.479828      -0.722968      -0.058512
C     -2.401778      -2.143811      0.433669
H     -2.475444      -2.180138      1.521323
H     -1.429871      -2.563894      0.163813
H     -3.187641      -2.735825      -0.025191
O     -3.194689      -0.403275      -0.977175
O      3.177103      -0.354340      -0.452690
O      3.608910      -1.588409      -0.849482
Rotational constants (GHz):      1.1884800      0.4855900      0.4415500
Vibrational harmonic frequencies (cm-1):
27.1337      46.3318      54.9398
95.7797      141.0445      170.6812

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173.9502	196.8515	230.8720
252.6327	279.5571	289.9012
320.7030	333.6539	360.2491
368.5742	427.3505	473.3898
494.3819	545.0418	594.2687
613.5095	625.1285	711.9186
752.6305	846.6227	889.2991
925.0214	925.9501	952.5917
960.5819	984.3798	997.7952
1006.6125	1018.4184	1039.8833
1049.2693	1125.1353	1134.4155
1155.9667	1177.0617	1195.1610
1220.8554	1249.2452	1254.5414
1264.2705	1296.5553	1305.3334
1330.0134	1354.7238	1374.7990
1389.1377	1405.1798	1414.6600
1424.1863	1461.7871	1463.4169
1474.8456	1483.1493	1495.3122
1502.8896	1507.2963	1517.1646
1667.3488	1829.1112	3041.1180
3045.7220	3048.4120	3060.2378
3079.8856	3083.3069	3094.7661
3113.5428	3116.1411	3117.1895
3122.3998	3129.5510	3134.0876
3146.7576	3164.7159	3181.9626

Zero-point correction (Hartree): 0.246794

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.15723649

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.450060 | -1.150647 | 0.918240  |
| H | -0.199440 | -1.936635 | 1.632939  |
| C | -1.936342 | -1.336599 | 0.564897  |
| C | -2.481998 | -0.287765 | -0.331549 |
| H | -2.082177 | -2.307893 | 0.091886  |
| H | -2.510837 | -1.321963 | 1.493315  |
| H | -2.680207 | -0.416977 | -1.392298 |
| C | 0.654739  | -1.128842 | -0.175524 |
| C | 0.067137  | 0.197992  | 1.452162  |
| C | 1.365680  | -2.440397 | -0.442665 |
| C | 0.208847  | -0.489895 | -1.485480 |
| H | -0.280877 | 0.477905  | -1.342316 |
| H | 1.072802  | -0.327399 | -2.129632 |
| H | -0.479849 | -1.150638 | -2.016767 |
| H | 2.245745  | -2.270222 | -1.063864 |
| H | 0.708455  | -3.138951 | -0.966107 |
| H | 1.690034  | -2.908216 | 0.487681  |
| H | 0.082775  | 0.335819  | 2.530697  |
| H | -0.448196 | 1.042722  | 0.998182  |
| C | 1.398838  | -0.107472 | 0.740858  |
| H | 2.080843  | -0.649803 | 1.399385  |
| C | 2.204949  | 0.968479  | 0.051340  |
| C | 1.862809  | 2.406852  | 0.330112  |
| H | 1.752510  | 2.576024  | 1.402002  |
| H | 0.898414  | 2.641040  | -0.127663 |
| H | 2.626686  | 3.055901  | -0.086842 |
| O | 3.082493  | 0.653110  | -0.716231 |
| O | -2.702465 | 0.842989  | 0.128926  |
| O | -3.110563 | 1.817532  | -0.743314 |

Rotational constants (GHz): 1.0817200 0.5835700 0.4674200

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| 12.4112   | 40.2569   | 54.4298   |
| 108.8215  | 145.1337  | 165.2109  |
| 178.3262  | 184.3110  | 238.1585  |
| 258.8985  | 277.9188  | 307.6604  |
| 324.9338  | 337.7477  | 365.8364  |
| 378.8321  | 421.8832  | 470.8811  |
| 495.7460  | 535.6113  | 595.2885  |
| 611.0880  | 653.9550  | 719.9342  |
| 752.5036  | 831.5152  | 891.3413  |
| 924.0669  | 927.0199  | 964.9618  |
| 980.4936  | 984.8203  | 995.6100  |
| 1003.4384 | 1016.0394 | 1039.6285 |
| 1067.9247 | 1071.2021 | 1140.6392 |
| 1149.8843 | 1176.2707 | 1197.6624 |
| 1223.9643 | 1248.8222 | 1251.0278 |
| 1265.6967 | 1297.1282 | 1300.2682 |
| 1333.2970 | 1351.9414 | 1368.5921 |
| 1392.6258 | 1402.6993 | 1412.2477 |
| 1420.9654 | 1464.3851 | 1475.0981 |
| 1476.3753 | 1486.0674 | 1496.7997 |
| 1505.4506 | 1510.6382 | 1521.4358 |
| 1654.3890 | 1826.3897 | 3038.4394 |
| 3046.4711 | 3059.6632 | 3067.9393 |
| 3076.8537 | 3079.7097 | 3102.5646 |
| 3104.2804 | 3114.7034 | 3121.6579 |
| 3123.4021 | 3130.0179 | 3132.3141 |
| 3156.9495 | 3174.0518 | 3182.2183 |

Zero-point correction (Hartree): 0.246944

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.16067715

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-0.494312	-0.629628	-0.589949
H	-0.895816	-0.323499	-1.558067
C	-1.633381	-1.203708	0.256283
C	-2.693942	-0.190886	0.458939
H	-2.061526	-2.073768	-0.240882

H	-1.247766	-1.512442	1.229935
H	-2.598442	0.667095	1.121819
C	0.397023	0.520542	-0.037980
C	0.766635	-1.487274	-0.792128
C	0.054754	1.916604	-0.521440
C	0.546468	0.485989	1.477540
H	0.824423	-0.502512	1.843312
H	1.323746	1.182233	1.798094
H	-0.381197	0.790539	1.965671
H	0.817488	2.637028	-0.219451
H	-0.896152	2.251445	-0.100022
H	-0.032054	1.946081	-1.607877
H	0.819821	-2.100325	-1.687705
H	0.993524	-2.100121	0.079641
C	1.597920	-0.199116	-0.758672
H	1.731983	0.237243	-1.749910
C	2.906986	-0.205765	-0.012961
C	3.759961	1.028230	-0.159363
H	3.158207	1.921221	0.020305
H	4.127044	1.094154	-1.185115
H	4.598120	0.991868	0.529973
O	3.229917	-1.128661	0.693668
O	-3.748213	-0.262929	-0.190808
O	-4.672964	0.727070	-0.023026
Rotational constants (GHz): 1.8792400 0.3788900 0.3533000			
Vibrational harmonic frequencies (cm-1):			
21.3736	53.8307	61.5878	
81.7735	116.1497	142.3390	
158.5222	210.8046	227.6872	
250.9384	282.5176	287.7676	
321.0878	324.3201	350.1430	
376.7883	405.6813	429.0364	
499.8319	570.2504	589.2507	
608.4029	624.9506	721.1381	
779.1349	865.1645	906.7038	
933.6091	954.9719	962.3934	
965.6091	975.0173	987.4081	
1002.7479	1010.9413	1039.4111	
1087.6343	1098.0766	1120.2949	
1152.2826	1175.1176	1194.1185	
1207.1693	1215.2502	1257.8648	
1266.2927	1281.2619	1299.1792	
1328.6141	1367.0054	1380.5011	
1387.8409	1407.0380	1414.4084	
1429.0488	1463.5330	1474.1512	
1476.6775	1486.5541	1494.2516	
1501.0975	1508.1227	1513.2247	
1660.1308	1836.1737	3046.0534	
3055.2738	3063.4113	3068.7460	
3078.0792	3085.8042	3099.1301	
3110.0179	3117.3249	3124.9539	
3127.3897	3131.3228	3136.6124	
3156.7510	3158.8905	3180.0485	
Zero-point correction (Hartree): 0.246776			
ApineneCI.J.a.pmp			
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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.16236804			
Electronic state : 1-A			
Cartesian coordinates (Angs):			
C	0.405400	0.975740	-0.701966
H	0.649967	0.932420	-1.766586
C	1.630019	1.460010	0.076125
C	2.770644	0.564630	-0.216605
H	1.881330	2.473284	-0.246872
H	1.438950	1.472728	1.148000
H	3.226577	0.475489	-1.201538
C	-0.271586	-0.365852	-0.302889
C	-0.941034	1.695283	-0.516040
C	0.132907	-1.575830	-1.122418
C	-0.175296	-0.663886	1.188878
H	-0.477395	0.186995	1.800063
H	-0.830227	-1.498256	1.447166
H	0.841492	-0.948780	1.460806
H	-0.486685	-2.442026	-0.882617
H	1.169939	-1.851027	-0.910526
H	0.041929	-1.377228	-2.191208
H	-1.197289	2.477884	-1.225245
H	-1.075582	2.068316	0.498376
C	-1.632666	0.334319	-0.670545
H	-1.882020	0.109250	-1.709305
C	-2.803847	0.018015	0.222413
C	-3.518830	-1.278898	-0.058494
H	-2.796476	-2.093402	-0.137843
H	-4.028037	-1.210003	-1.021423
H	-4.240541	-1.488675	0.725191
O	-3.123077	0.743025	1.132066
O	3.205669	-0.197860	0.659711
O	4.191133	-1.078685	0.311074
Rotational constants (GHz): 1.6441100 0.4257800 0.3929700			
Vibrational harmonic frequencies (cm-1):			
39.4032	54.0099	65.6164	
86.2537	117.5139	149.2228	
157.8387	206.8544	237.2990	
248.2923	286.4167	291.8581	
320.4095	330.5875	352.7925	
380.2595	406.4494	433.4957	
493.1755	576.6231	586.7313	
602.9610	624.8152	718.8775	
778.0226	871.6604	908.9840	
930.7224	951.4973	959.2301	
966.6756	973.9216	983.4581	

1005.5451	1026.5677	1052.2302
1058.1144	1102.7019	1116.5247
1154.7325	1177.4703	1194.7602
1206.3638	1215.1326	1252.6010
1264.3806	1275.2182	1293.4699
1329.0511	1369.3967	1379.9871
1392.3296	1408.5310	1417.0289
1429.1496	1464.2700	1472.0075
1476.6514	1486.1731	1496.7747
1501.9137	1509.5787	1515.2828
1663.2633	1836.7374	3040.6632
3056.6673	3059.1555	3063.9170
3066.5051	3082.8734	3100.6873
3106.6572	3121.7448	3122.6522
3126.2088	3138.1743	3139.7536
3153.7536	3158.5570	3180.4720

Zero-point correction (Hartree): 0.246849

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E (CCSD(T)/Aug-CC-pVTZ) (Hartree): -615.23399964

E (CCSD/Aug-CC-pVTZ) (Hartree): -615.11507060

T1 diagnostic: 0.022003

E (MP2/Aug-CC-pVTZ) (Hartree): -615.04242175

E (MP3/Aug-CC-pVTZ) (Hartree): -615.09857946

E (RHF/Aug-CC-pVTZ) (Hartree): -612.61170537

E (RM062X/Aug-CC-pVTZ) (Hartree): -616.16296639

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.528652 | -0.809613 | -0.690760 |
| H | -0.950679 | -0.539145 | -1.659742 |
| C | -1.574728 | -1.531824 | 0.136897  |
| C | -2.815638 | -0.764608 | 0.386538  |
| H | -1.859309 | -2.473809 | -0.346152 |
| H | -1.172247 | -1.824476 | 1.112452  |
| H | -3.635841 | -1.119330 | 1.007706  |
| C | 0.220069  | 0.430487  | -0.106297 |
| C | 0.822933  | -1.523742 | -0.866121 |
| C | -0.197835 | 1.792213  | -0.629346 |
| C | 0.274767  | 0.424250  | 1.414925  |
| H | 0.640843  | -0.522765 | 1.813209  |
| H | 0.942217  | 1.209203  | 1.775501  |
| H | -0.715663 | 0.624995  | 1.829079  |
| H | 0.547706  | 2.545592  | -0.365403 |
| H | -1.153482 | 2.103644  | -0.208267 |
| H | -0.295082 | 1.779881  | -1.715703 |
| H | 0.976289  | -2.096853 | -1.776964 |
| H | 1.076080  | -2.143012 | -0.005468 |
| C | 1.525040  | -0.166779 | -0.756560 |
| H | 1.685312  | 0.304703  | -1.727558 |
| C | 2.776985  | -0.075567 | 0.075458  |
| C | 3.523224  | 1.232483  | 0.012520  |
| H | 2.834950  | 2.061653  | 0.186502  |
| H | 3.935292  | 1.367135  | -0.989048 |
| H | 4.323659  | 1.245870  | 0.746133  |
| O | 3.136528  | -0.983541 | 0.784827  |
| O | -2.954057 | 0.357252  | -0.121594 |
| O | -4.099600 | 1.055405  | 0.144291  |

Rotational constants (GHz): 1.6826000 0.4460500 0.4025400

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| 38.9440   | 59.0557   | 63.0574   |
| 96.4458   | 126.5174  | 130.7494  |
| 154.5536  | 220.6120  | 236.1322  |
| 257.9406  | 277.6577  | 292.4643  |
| 309.0556  | 332.8125  | 336.4484  |
| 375.5673  | 411.0886  | 435.9563  |
| 487.8860  | 575.1252  | 589.2329  |
| 623.8553  | 683.3331  | 713.1533  |
| 778.3211  | 831.4383  | 905.6230  |
| 926.7679  | 948.3357  | 962.9669  |
| 965.4437  | 978.3868  | 984.8473  |
| 996.1498  | 1005.9816 | 1032.7613 |
| 1050.1657 | 1109.4395 | 1121.2049 |
| 1158.4559 | 1170.1569 | 1194.1761 |
| 1195.4743 | 1212.2820 | 1261.3707 |
| 1266.7490 | 1280.9426 | 1309.9142 |
| 1342.7200 | 1370.2776 | 1380.5259 |
| 1399.5350 | 1409.5522 | 1426.2178 |
| 1427.3141 | 1446.2330 | 1464.5477 |
| 1476.5894 | 1486.5339 | 1496.1278 |
| 1499.8795 | 1509.5605 | 1511.1823 |
| 1666.3466 | 1832.9665 | 3038.0705 |
| 3048.9058 | 3052.1537 | 3063.3459 |
| 3063.6846 | 3086.0309 | 3087.3668 |
| 3093.2825 | 3114.0358 | 3117.3984 |
| 3125.8740 | 3128.2751 | 3138.1881 |
| 3151.7313 | 3159.9608 | 3180.3439 |

Zero-point correction (Hartree): 0.246657

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E (RM062X/Aug-CC-pVTZ) (Hartree): -616.16015166

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-0.546240	0.606533	-0.450867
H	-0.745630	1.097805	-1.406600
C	-1.716319	0.850960	0.501958
C	-2.975027	0.386242	-0.120898
H	-1.571101	0.324143	1.443902
H	-1.805400	1.921946	0.708389
H	-3.403727	0.829149	-1.018226
C	0.890612	0.986451	0.006227

C	-0.074174	-0.838381	-0.689605
C	1.419446	2.307555	-0.516178
C	1.079786	0.880819	1.513283
H	0.740335	-0.077925	1.905182
H	2.135540	0.983770	1.771409
H	0.536335	1.678766	2.022192
H	2.475477	2.435491	-0.270643
H	0.875782	3.141097	-0.065491
H	1.310152	2.375950	-1.599065
H	-0.455156	-1.360552	-1.563158
H	-0.212599	-1.465748	0.190658
C	1.366509	-0.312863	-0.743744
H	1.676110	-0.047636	-1.756226
C	2.451249	-1.105506	-0.061184
C	3.864359	-0.638760	-0.302737
H	3.934933	0.438411	-0.139702
H	4.131544	-0.820781	-1.345215
H	4.552763	-1.166074	0.350768
O	2.197810	-2.030595	0.669616
O	-3.577949	-0.588414	0.353192
O	-4.711932	-1.009254	-0.278521
Rotational constants (GHz): 1.4836500 0.3952600 0.3496800			
Vibrational harmonic frequencies (cm-1):			
30.8038	45.8452	60.8774	
83.3955	116.2687	130.2296	
160.5350	186.8337	229.3430	
237.1722	278.5121	283.7208	
326.8760	336.3881	344.2655	
364.9678	396.7298	455.9886	
481.1875	578.2281	584.4228	
610.9927	625.4197	736.3632	
796.5311	852.1199	905.3950	
932.1006	946.3339	960.3734	
964.8956	967.0024	985.0584	
1001.4593	1018.2939	1048.3830	
1061.5693	1101.0499	1128.6416	
1157.9757	1177.6448	1194.5062	
1206.6976	1230.3728	1250.5143	
1262.3202	1274.9595	1300.4084	
1326.7532	1367.9629	1382.2576	
1391.4630	1404.9437	1415.1651	
1425.3365	1464.0444	1470.9827	
1476.3216	1486.7153	1492.9797	
1499.1907	1509.5272	1511.2859	
1663.3420	1838.0138	3045.8880	
3051.9568	3053.9361	3060.7508	
3062.7531	3084.0835	3098.2345	
3110.9103	3118.0294	3124.0743	
3125.4641	3134.1267	3137.6959	
3156.9614	3158.0864	3179.7340	
Zero-point correction (Hartree): 0.246586			
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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.16061827			
Electronic state : 1-A			
Cartesian coordinates (Angs):			
C	-0.582499	0.265766	-0.328085
H	-0.933662	0.652495	-1.286884
C	-1.709436	0.375625	0.698311
C	-2.870643	-0.429435	0.260129
H	-1.363470	-0.018278	1.657778
H	-2.024417	1.409711	0.838612
H	-2.834771	-1.507909	0.116819
C	0.796169	0.911197	-0.008146
C	0.118816	-1.090372	-0.532879
C	1.048126	2.266313	-0.639025
C	1.108716	0.936810	1.481614
H	0.973497	-0.038644	1.949304
H	2.145487	1.235954	1.647261
H	0.471232	1.661044	1.991424
H	2.082036	2.584451	-0.491539
H	0.404059	3.023300	-0.186256
H	0.846514	2.245937	-1.710418
H	-0.222849	-1.722439	-1.348511
H	0.161254	-1.677312	0.385071
C	1.438073	-0.332929	-0.727666
C	1.626483	-0.084306	-1.773438
C	2.686496	-0.888800	-0.093291
C	3.977308	-0.200946	-0.456856
H	3.869026	0.879405	-0.343157
H	4.203039	-0.388780	-1.508051
H	4.788583	-0.567432	0.164857
O	2.645570	-1.802748	0.692972
O	-3.946399	0.128409	-0.003901
O	-4.981521	-0.646483	-0.442510
Rotational constants (GHz): 1.7019200 0.3595200 0.3314000			
Vibrational harmonic frequencies (cm-1):			
38.6614	44.0424	62.2092	
84.8706	124.2766	135.1168	
154.6355	204.1850	220.2726	
243.2541	276.1896	281.6708	
319.3383	329.2396	352.9720	
356.8683	398.4700	454.5093	
487.3871	571.2600	588.1641	
608.6525	626.6551	739.0084	
798.0903	855.5826	906.7944	
931.7184	945.5560	959.8539	
965.6312	969.5976	991.3546	
1002.7462	1010.7105	1038.1053	
1070.2026	1109.9891	1137.9550	
1164.9406	1173.5448	1194.7356	

1209.2356	1222.8643	1260.4581
1264.9468	1274.6408	1303.5452
1329.2053	1365.4400	1380.8239
1391.8470	1404.9255	1414.1988
1424.8443	1464.4357	1470.4178
1476.7445	1486.3299	1493.1439
1499.3884	1509.4281	1510.9337
1665.0273	1836.3597	3047.2911
3053.9243	3058.7980	3062.8859
3073.8514	3086.5622	3091.5853
3112.8676	3118.7488	3124.5746
3125.6588	3126.3516	3135.0237
3151.7166	3160.4973	3179.0705

Zero-point correction (Hartree): 0.246720

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.16108399

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.677359 | 0.432138  | -0.247332 |
| H | -1.056185 | 0.680897  | -1.240142 |
| C | -1.698032 | 0.836953  | 0.796576  |
| C | -3.034249 | 0.227821  | 0.596475  |
| H | -1.365270 | 0.563208  | 1.803343  |
| H | -1.837893 | 1.924650  | 0.822088  |
| H | -3.872523 | 0.375618  | 1.274257  |
| C | 0.779261  | 0.960385  | -0.121403 |
| C | -0.137717 | -1.009757 | -0.245767 |
| C | 1.126726  | 2.148429  | -0.997020 |
| C | 1.201692  | 1.206591  | 1.321038  |
| H | 0.997677  | 0.348813  | 1.962292  |
| H | 2.273896  | 1.404885  | 1.375496  |
| H | 0.685165  | 2.078643  | 1.726217  |
| H | 2.195985  | 2.366608  | -0.962358 |
| H | 0.599058  | 3.042048  | -0.655485 |
| H | 0.848510  | 1.966504  | -2.035483 |
| H | -0.608744 | -1.720951 | -0.917799 |
| H | -0.095891 | -1.433645 | 0.757691  |
| C | 1.237107  | -0.454245 | -0.639060 |
| H | 1.375138  | -0.411494 | -1.720795 |
| C | 2.465691  | -1.025853 | 0.017995  |
| C | 3.789203  | -0.580712 | -0.550741 |
| H | 3.806240  | 0.506670  | -0.647360 |
| H | 3.906797  | -0.990525 | -1.555449 |
| H | 4.604899  | -0.917378 | 0.082022  |
| O | 2.393970  | -1.759969 | 0.972729  |
| O | -3.245475 | -0.492725 | -0.389623 |
| O | -4.494844 | -1.026689 | -0.539743 |

Rotational constants (GHz): 1.4892400 0.4107400 0.3720100

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| 41.8050   | 54.2883   | 75.8992   |
| 94.3052   | 122.9637  | 140.3244  |
| 150.1422  | 196.8704  | 224.9363  |
| 241.9744  | 257.8341  | 290.0635  |
| 311.2000  | 335.3928  | 349.1336  |
| 360.7134  | 401.1486  | 458.6439  |
| 481.3772  | 576.0320  | 586.2187  |
| 623.5703  | 668.1645  | 744.5614  |
| 800.4527  | 827.3408  | 905.7191  |
| 935.0215  | 948.7786  | 959.7396  |
| 962.8299  | 965.2572  | 988.1273  |
| 995.5264  | 1004.7977 | 1029.0149 |
| 1047.5699 | 1095.2543 | 1139.0989 |
| 1149.6728 | 1176.3296 | 1196.9724 |
| 1209.0222 | 1222.3194 | 1256.8353 |
| 1266.7213 | 1278.3351 | 1324.7487 |
| 1335.2781 | 1370.7676 | 1381.1521 |
| 1401.3506 | 1407.6906 | 1424.0609 |
| 1430.5257 | 1448.3938 | 1464.5088 |
| 1476.5105 | 1486.7309 | 1493.6549 |
| 1500.2685 | 1509.3723 | 1511.8102 |
| 1663.8427 | 1835.9063 | 3030.9097 |
| 3045.7118 | 3052.7013 | 3062.1733 |
| 3063.3814 | 3083.6029 | 3086.6908 |
| 3097.2706 | 3109.8970 | 3116.6632 |
| 3123.9675 | 3126.3588 | 3133.4862 |
| 3160.0739 | 3162.5044 | 3178.9542 |

Zero-point correction (Hartree): 0.246610

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.15925914

Electronic state : 1-A

Cartesian coordinates (Angs):

C	0.341989	1.212366	0.850819
H	0.088676	2.223930	1.173548
C	1.868436	1.135877	0.791789
C	2.408620	-0.208931	0.488662
H	2.267963	1.840594	0.061554
H	2.256668	1.424452	1.774912
H	2.149334	-1.110869	1.038938
C	-0.538063	0.880463	-0.388023
C	-0.479396	0.209749	1.682958
C	-0.953618	2.070405	-1.231200
C	0.026534	-0.230086	-1.265212
H	0.310917	-1.117437	-0.696414
H	-0.720027	-0.547859	-1.995897
H	0.899582	0.117294	-1.818957
H	-1.684219	1.782368	-1.989424
H	-0.089177	2.486883	-1.752963
H	-1.392232	2.856940	-0.616025

H	-0.710954	0.478627	2.710323
H	-0.080383	-0.803359	1.660916
C	-1.597860	0.338066	0.640862
H	-2.303550	1.135245	0.882131
C	-2.344109	-0.907038	0.236907
C	-3.514057	-0.706787	-0.692200
H	-3.218844	-0.079415	-1.535207
H	-4.308250	-0.176783	-0.163310
H	-3.883042	-1.665031	-1.045184
O	-1.999726	-2.001232	0.608926
O	3.213345	-0.346156	-0.444845
O	3.674717	-1.603871	-0.711721
Rotational constants (GHz):			
Vibrational harmonic frequencies (cm-1):			
45.4674	49.7398	67.2511	
95.2773	117.0538	148.3950	
180.0070	205.9816	231.9009	
247.5488	278.4353	287.1144	
316.4810	347.8159	364.1393	
368.5727	391.0314	436.6273	
539.8196	575.2658	587.3948	
615.4921	633.6294	714.1222	
767.2870	845.7955	906.8913	
927.1438	950.9760	953.6579	
961.4200	972.6621	985.2338	
1000.9202	1009.6048	1040.4907	
1054.5345	1128.3521	1134.4497	
1157.0547	1172.3147	1193.3478	
1208.1283	1220.1560	1255.5276	
1262.6288	1292.4679	1304.6008	
1332.5448	1369.3148	1377.1299	
1398.9835	1408.2046	1420.2006	
1428.0119	1459.6706	1464.6456	
1476.7862	1485.6591	1494.3762	
1503.2908	1508.9685	1513.0519	
1665.1931	1837.4566	3037.2325	
3046.7069	3052.9080	3062.5124	
3074.7302	3083.2039	3101.6699	
3112.6964	3113.1980	3116.7664	
3123.0259	3125.1723	3131.7589	
3155.9701	3167.2035	3179.3871	
Zero-point correction (Hartree): 0.246903			

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.15684792

Electronic state : 1-A

Cartesian coordinates (Angs):

|                                          |           |           |           |
|------------------------------------------|-----------|-----------|-----------|
| C                                        | 0.428907  | 1.133895  | 0.839849  |
| H                                        | 0.166803  | 1.937739  | 1.530877  |
| C                                        | 1.888442  | 1.379129  | 0.425468  |
| C                                        | 2.506728  | 0.298398  | -0.382624 |
| H                                        | 1.953842  | 2.310949  | -0.138947 |
| H                                        | 2.482063  | 1.492517  | 1.334113  |
| H                                        | 2.581667  | 0.294889  | -1.466678 |
| C                                        | -0.713496 | 1.024797  | -0.205135 |
| C                                        | -0.013870 | -0.210073 | 1.443054  |
| C                                        | -1.461655 | 2.310241  | -0.500690 |
| C                                        | -0.290872 | 0.335787  | -1.496403 |
| H                                        | 0.224386  | -0.609626 | -1.316815 |
| H                                        | -1.164091 | 0.113577  | -2.113122 |
| H                                        | 0.358413  | 0.991154  | -2.080961 |
| H                                        | -2.332641 | 2.126353  | -1.132497 |
| H                                        | -0.816243 | 3.013813  | -1.031943 |
| H                                        | -1.801566 | 2.788826  | 0.418313  |
| H                                        | 0.027560  | -0.315763 | 2.523714  |
| H                                        | 0.476680  | -1.066035 | 0.981556  |
| C                                        | -1.388203 | 0.019237  | 0.798255  |
| H                                        | -2.065949 | 0.572541  | 1.451286  |
| C                                        | -2.108681 | -1.152475 | 0.182758  |
| C                                        | -3.511763 | -0.885138 | -0.302391 |
| H                                        | -3.526315 | 0.007907  | -0.930182 |
| H                                        | -4.158906 | -0.683336 | 0.552981  |
| H                                        | -3.887975 | -1.740798 | -0.854979 |
| O                                        | -1.579059 | -2.226839 | 0.050618  |
| O                                        | 2.982968  | -0.689533 | 0.198237  |
| O                                        | 3.529721  | -1.678315 | -0.566300 |
| Rotational constants (GHz):              |           |           |           |
| Vibrational harmonic frequencies (cm-1): |           |           |           |
| 27.7943                                  | 49.8757   | 59.4325   |           |
| 92.1984                                  | 120.9757  | 144.9386  |           |
| 170.2863                                 | 189.4804  | 229.5372  |           |
| 243.7508                                 | 282.0043  | 292.8987  |           |
| 332.7437                                 | 345.0140  | 362.3529  |           |
| 372.6132                                 | 388.7147  | 434.8531  |           |
| 537.8955                                 | 569.3763  | 585.9626  |           |
| 621.5682                                 | 650.5179  | 721.2866  |           |
| 765.8855                                 | 837.8821  | 909.0787  |           |
| 930.7877                                 | 950.6729  | 964.4808  |           |
| 966.0206                                 | 978.6066  | 986.1319  |           |
| 1001.6252                                | 1004.3739 | 1041.2222 |           |
| 1070.0522                                | 1073.4980 | 1141.3156 |           |
| 1152.1407                                | 1174.7198 | 1195.1608 |           |
| 1208.3308                                | 1229.3619 | 1251.8039 |           |
| 1265.3709                                | 1297.9363 | 1301.3610 |           |
| 1336.4714                                | 1363.8749 | 1376.0479 |           |
| 1398.9470                                | 1406.2905 | 1418.3300 |           |
| 1425.6525                                | 1464.5354 | 1475.9529 |           |
| 1476.7906                                | 1487.1951 | 1493.9236 |           |
| 1505.8761                                | 1510.0752 | 1515.3263 |           |
| 1652.2286                                | 1841.4653 | 3043.9331 |           |
| 3046.7334                                | 3062.3580 | 3064.9326 |           |



|           |           |           |
|-----------|-----------|-----------|
| 3074.9505 | 3080.3043 | 3105.1529 |
| 3108.9022 | 3112.4291 | 3118.6636 |
| 3122.4588 | 3123.4511 | 3125.5681 |
| 3162.3706 | 3175.4287 | 3180.2805 |

Zero-point correction (Hartree): 0.246910

Population analysis as 298K (%)

| Compound                   | Qtot      | Erel | Erel2 | n*Q*MB    | %      |
|----------------------------|-----------|------|-------|-----------|--------|
| ApineneCI.J.a.13Hshift.pmt | 4.265e+44 | 0.00 | 0.00  | 4.265e+44 | 36.1   |
| ApineneCI.J.a.13Hshift.pmp | 4.516e+44 | 0.36 | 0.36  | 2.460e+44 | 20.8   |
| ApineneCI.J.a.13Hshift.pmm | 6.646e+44 | 0.89 | 0.89  | 1.491e+44 | 12.6   |
| ApineneCI.J.a.13Hshift.ppt | 4.307e+44 | 0.91 | 0.91  | 9.282e+43 | 7.86   |
| ApineneCI.J.a.13Hshift.ppp | 9.701e+44 | 1.47 | 1.47  | 8.078e+43 | 6.84   |
| ApineneCI.J.a.13Hshift.ppm | 8.281e+44 | 1.45 | 1.45  | 7.103e+43 | 6.01   |
| ApineneCI.J.a.13Hshift.mpt | 6.338e+44 | 2.03 | 2.03  | 2.060e+43 | 1.74   |
| ApineneCI.J.a.13Hshift.mmt | 5.714e+44 | 2.06 | 2.06  | 1.750e+43 | 1.48   |
| ApineneCI.J.a.13Hshift.mpm | 1.043e+45 | 2.43 | 2.43  | 1.712e+43 | 1.45   |
| ApineneCI.J.a.13Hshift.ptm | 3.374e+44 | 1.84 | 1.84  | 1.521e+43 | 1.29   |
| ApineneCI.J.a.13Hshift.mmp | 7.161e+44 | 2.32 | 2.32  | 1.418e+43 | 1.2    |
| ApineneCI.J.a.13Hshift.mpp | 1.307e+45 | 2.76 | 2.76  | 1.229e+43 | 1.04   |
| ApineneCI.J.a.13Hshift.mmm | 1.186e+45 | 2.78 | 2.78  | 1.091e+43 | 0.923  |
| ApineneCI.J.a.13Hshift.mtm | 5.776e+44 | 2.99 | 2.99  | 3.726e+42 | 0.315  |
| ApineneCI.J.a.13Hshift.ptp | 1.243e+45 | 3.71 | 3.71  | 2.358e+42 | 0.2    |
| ApineneCI.J.a.13Hshift.ptt | 4.322e+44 | 3.52 | 3.52  | 1.141e+42 | 0.0966 |
| Total                      |           |      |       | 1.181e+45 | 100    |

ApineneCI.J.a.13Hshift.mmm

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.10811135

Electronic state : 1-A

Cartesian coordinates (Angs):

C	0.459872	0.768178	-0.393548
H	0.844466	0.744064	-1.415135
C	1.572276	1.248102	0.546915
C	2.686576	0.273691	0.479107
H	1.907918	2.244110	0.251846
H	1.196889	1.277168	1.569831
H	3.382828	-0.864573	0.652907
C	-0.292039	-0.566144	-0.111907
C	-0.885939	1.516801	-0.367529
C	0.178895	-1.779544	-0.888662
C	-0.385895	-0.881687	1.376065
H	-0.774033	-0.040998	1.955367
H	-1.052598	-1.726501	1.535991
H	0.600770	-1.137764	1.766031
H	-0.525674	-2.602680	-0.763997
H	1.157766	-2.110071	-0.533730
H	0.263028	-1.556865	-1.953353
H	-1.031172	2.322212	-1.083365
H	-1.113457	1.883005	0.634120
C	-1.560806	0.157188	-0.645442
H	-1.639244	0.002932	-1.726478
C	-2.913540	-0.173426	-0.067752
C	-3.900397	0.960688	0.045349
H	-3.924940	1.536859	-0.880717
H	-3.577980	1.641619	0.835393
H	-4.887065	0.573697	0.281216
O	-3.188632	-1.299686	0.266036
O	3.661370	0.541457	-0.262851
O	4.454571	-0.657932	-0.123372

Rotational constants (GHz): 1.8645400 0.3908700 0.3573900

Vibrational harmonic frequencies (cm-1):

11723.7450	26.5985	29.4372
55.4831	88.2067	121.4657
129.8761	160.6051	197.8876
232.2299	263.5228	270.8129
313.1884	322.1352	324.7718
376.3675	398.1692	406.2220
445.0507	512.1100	534.5256
605.4686	619.6132	710.6780
734.1947	767.5545	864.5166
896.7442	919.4617	947.2896
960.8166	971.6820	989.9388
1014.8494	1025.8054	1035.7816
1071.2572	1107.7623	1115.4814
1152.0187	1171.0579	1185.4992
1200.0078	1228.6046	1238.9496
1249.6874	1268.1013	1284.8306
1299.1458	1326.6983	1349.9899
1384.8939	1395.0255	1409.8446
1421.4545	1463.6980	1474.1627
1476.5229	1487.6427	1495.1646
1499.8522	1510.1109	1516.1318
1594.0563	1832.9913	2144.1115
3047.9372	3052.8172	3055.4642
3064.2339	3070.1952	3074.9260
3086.2014	3116.5232	3118.3915
3125.7516	3129.3345	3132.2353
3146.5813	3152.2615	3180.7418

Zero-point correction (Hartree): 0.241899

ApineneCI.J.a.13Hshift.mmp

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.10876817

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |          |           |
|---|-----------|----------|-----------|
| C | -0.375315 | 0.933497 | 0.597599  |
| H | -0.630021 | 0.964330 | 1.658875  |
| C | -1.561432 | 1.452978 | -0.215508 |

|                                                |           |           |           |
|------------------------------------------------|-----------|-----------|-----------|
| C                                              | -2.755505 | 0.646869  | 0.128936  |
| H                                              | -1.766396 | 2.484179  | 0.083503  |
| H                                              | -1.359383 | 1.425365  | -1.287283 |
| H                                              | -3.714483 | 0.069105  | 0.877942  |
| C                                              | 0.230753  | -0.464255 | 0.277944  |
| C                                              | 1.010846  | 1.568662  | 0.385112  |
| C                                              | -0.255010 | -1.614056 | 1.137408  |
| C                                              | 0.139585  | -0.822911 | -1.201264 |
| H                                              | 0.509379  | -0.022021 | -1.845479 |
| H                                              | 0.735867  | -1.710742 | -1.402523 |
| H                                              | -0.893798 | -1.032460 | -1.481016 |
| H                                              | 0.349057  | -2.503714 | 0.955947  |
| H                                              | -1.295404 | -1.856689 | 0.904884  |
| H                                              | -0.193070 | -1.365826 | 2.198084  |
| H                                              | 1.301525  | 2.381988  | 1.045915  |
| H                                              | 1.149138  | 1.882504  | -0.649847 |
| C                                              | 1.604997  | 0.167326  | 0.641557  |
| H                                              | 1.791020  | 0.038637  | 1.712596  |
| C                                              | 2.850900  | -0.298683 | -0.068671 |
| C                                              | 3.880196  | 0.749554  | -0.406453 |
| H                                              | 4.054596  | 1.402747  | 0.449712  |
| H                                              | 3.500906  | 1.378064  | -1.214629 |
| H                                              | 4.804762  | 0.275221  | -0.721285 |
| O                                              | 3.011809  | -1.464650 | -0.333725 |
| O                                              | -3.292212 | -0.048012 | -0.766360 |
| O                                              | -4.340071 | -0.702908 | -0.018087 |
| Rotational constants (GHz):                    |           |           | 1.7699400 |
| Vibrational harmonic frequencies (cm-1):       |           |           | 0.4106600 |
|                                                |           |           | 0.3752900 |
| 11732.8623                                     | 29.8298   | 39.6369   |           |
| 55.7694                                        | 82.9515   | 133.7643  |           |
| 154.2033                                       | 159.2102  | 186.8983  |           |
| 234.2300                                       | 256.4931  | 273.7114  |           |
| 315.7712                                       | 319.3347  | 322.2208  |           |
| 383.6131                                       | 394.4981  | 409.7752  |           |
| 445.3821                                       | 510.2948  | 528.0355  |           |
| 608.0283                                       | 619.7506  | 713.5499  |           |
| 727.0317                                       | 767.7302  | 865.3057  |           |
| 894.8381                                       | 918.8089  | 943.5735  |           |
| 959.9334                                       | 970.7089  | 988.7301  |           |
| 1011.3801                                      | 1025.1482 | 1036.2664 |           |
| 1077.1200                                      | 1104.7328 | 1111.3712 |           |
| 1140.9748                                      | 1174.9146 | 1184.7512 |           |
| 1198.9777                                      | 1236.0505 | 1243.5815 |           |
| 1245.7703                                      | 1264.2828 | 1279.5879 |           |
| 1297.0718                                      | 1324.5954 | 1351.8004 |           |
| 1390.5291                                      | 1400.0905 | 1412.8978 |           |
| 1423.6643                                      | 1461.3194 | 1464.8853 |           |
| 1478.0052                                      | 1485.8241 | 1496.4004 |           |
| 1500.0279                                      | 1510.1229 | 1516.8247 |           |
| 1592.9476                                      | 1832.8592 | 2141.7674 |           |
| 3043.5314                                      | 3053.6105 | 3056.0659 |           |
| 3060.0674                                      | 3063.2712 | 3074.7911 |           |
| 3086.7744                                      | 3111.4986 | 3119.0826 |           |
| 3121.8147                                      | 3124.7424 | 3129.7230 |           |
| 3144.6296                                      | 3151.7103 | 3180.3077 |           |
| Zero-point correction (Hartree):               |           |           | 0.241832  |
| ApineneCI.J.a.13Hshift.mmt                     |           |           |           |
| ~~~~~                                          |           |           |           |
| E(RM062X/Aug-CC-pVT2) (Hartree): -616.10884470 |           |           |           |
| Electronic state : 1-A                         |           |           |           |
| Cartesian coordinates (Angs):                  |           |           |           |
| C                                              | 0.466855  | 0.849342  | -0.491443 |
| H                                              | 0.842177  | 0.798104  | -1.514906 |
| C                                              | 1.527225  | 1.443401  | 0.417275  |
| C                                              | 2.832174  | 0.745503  | 0.463791  |
| H                                              | 1.760981  | 2.475449  | 0.127653  |
| H                                              | 1.180525  | 1.521949  | 1.451852  |
| H                                              | 4.089054  | 0.434823  | 0.836400  |
| C                                              | -0.204173 | -0.517397 | -0.132765 |
| C                                              | -0.922260 | 1.517094  | -0.471050 |
| C                                              | 0.266940  | -1.745367 | -0.888538 |
| C                                              | -0.212823 | -0.782233 | 1.367283  |
| H                                              | -0.622983 | 0.055184  | 1.936508  |
| H                                              | -0.817820 | -1.658655 | 1.589607  |
| H                                              | 0.804160  | -0.968917 | 1.720645  |
| H                                              | -0.454839 | -2.552688 | -0.755601 |
| H                                              | 1.236910  | -2.087009 | -0.527710 |
| H                                              | 0.357491  | -1.537746 | -1.955969 |
| H                                              | -1.138374 | 2.267281  | -1.228294 |
| H                                              | -1.141624 | 1.933925  | 0.513398  |
| C                                              | -1.531052 | 0.111756  | -0.641770 |
| H                                              | -1.646927 | -0.108749 | -1.708039 |
| C                                              | -2.840398 | -0.250415 | 0.011001  |
| C                                              | -3.887058 | 0.833387  | 0.078251  |
| H                                              | -3.974824 | 1.337402  | -0.885286 |
| H                                              | -3.579847 | 1.587580  | 0.805202  |
| H                                              | -4.841539 | 0.410674  | 0.377003  |
| O                                              | -3.040609 | -1.361309 | 0.437361  |
| O                                              | 3.032314  | -0.199732 | -0.336100 |
| O                                              | 4.380157  | -0.581338 | 0.016905  |
| Rotational constants (GHz):                    |           |           | 1.8220500 |
| Vibrational harmonic frequencies (cm-1):       |           |           | 0.4183500 |
|                                                |           |           | 0.3799700 |
| 11725.0064                                     | 31.7438   | 44.1133   |           |
| 64.3438                                        | 88.8122   | 122.5586  |           |
| 136.2126                                       | 161.4152  | 212.1149  |           |
| 234.0157                                       | 254.0952  | 266.8871  |           |
| 299.7521                                       | 313.6749  | 327.6195  |           |
| 341.8579                                       | 394.7511  | 401.9816  |           |
| 471.4539                                       | 509.7725  | 535.0710  |           |
| 608.4466                                       | 620.7531  | 713.8826  |           |
| 755.9929                                       | 765.1188  | 829.9638  |           |

|           |           |           |
|-----------|-----------|-----------|
| 900.4747  | 909.3036  | 924.8220  |
| 965.4815  | 967.5462  | 981.4064  |
| 1011.1156 | 1022.5946 | 1036.7207 |
| 1090.7205 | 1101.3442 | 1112.9816 |
| 1132.1713 | 1165.2969 | 1179.5608 |
| 1198.0873 | 1208.3910 | 1238.7357 |
| 1253.2663 | 1271.5179 | 1290.3134 |
| 1308.9464 | 1340.5242 | 1361.2727 |
| 1392.2941 | 1403.5879 | 1413.7325 |
| 1423.1756 | 1427.0156 | 1465.0130 |
| 1477.0414 | 1484.6597 | 1495.7283 |
| 1498.4941 | 1507.1608 | 1514.7519 |
| 1587.8038 | 1832.1119 | 2140.6084 |
| 3038.4664 | 3046.1411 | 3050.6205 |
| 3055.5449 | 3064.6106 | 3073.0715 |
| 3076.8439 | 3089.8660 | 3107.6276 |
| 3124.8967 | 3126.1822 | 3136.6840 |
| 3139.5946 | 3151.6091 | 3180.8638 |

Zero-point correction (Hartree): 0.241497

ApineneCI.J.a.13Hshift.mpm

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.10849491

Electronic state : 1-A

Cartesian coordinates (Angs):

C	0.579376	-0.606883	-0.452339
H	0.823704	-0.894665	-1.476601
C	1.731857	-1.002224	0.477647
C	2.950185	-0.336177	-0.033997
H	1.522906	-0.695672	1.503381
H	1.877752	-2.082933	0.439025
H	3.978645	-0.030031	-0.846666
C	-0.863131	-1.098018	-0.124859
C	0.078518	0.848894	-0.427736
C	-1.340651	-2.320087	-0.882981
C	-1.102313	-1.264594	1.370161
H	-0.815282	-0.376652	1.936990
H	-2.157269	-1.451068	1.560368
H	-0.526697	-2.109958	1.751858
H	-2.409422	-2.467579	-0.723284
H	-0.819458	-3.216676	-0.539953
H	-1.164846	-2.213001	-1.954274
H	0.484396	1.540341	-1.162099
H	0.188747	1.284957	0.566153
C	-1.339580	0.283945	-0.654089
H	-1.536734	0.212276	-1.728582
C	-2.549653	0.942878	-0.041761
C	-2.526038	2.445944	0.061341
H	-2.191547	2.885797	-0.879288
H	-1.804520	2.743752	0.824535
H	-3.510894	2.816738	0.328576
O	-3.493671	0.286772	0.325497
O	3.336318	0.707585	0.545643
O	4.450991	1.092180	-0.289699

Rotational constants (GHz): 1.3424300 0.4236000 0.3575900

Vibrational harmonic frequencies (cm-1):

11728.1757	33.5171	36.6838
54.0833	86.9213	115.6656
137.3997	157.5323	172.1337
227.3629	251.2995	275.5658
310.4260	322.5781	327.3013
356.3901	394.1552	412.7123
474.0764	506.6919	516.4240
598.6568	630.1931	719.0892
741.9810	788.8577	858.2627
896.1055	910.5814	928.8408
967.1809	973.0377	982.5934
1009.9837	1022.7621	1037.6829
1070.7618	1095.7799	1125.6839
1160.2707	1168.4478	1187.3874
1198.2681	1227.5354	1241.7237
1253.2174	1256.4203	1281.2036
1299.5764	1320.6337	1351.3042
1388.0046	1396.6414	1409.1102
1421.3061	1464.6700	1472.0170
1476.2395	1484.6497	1494.4712
1498.7901	1507.2969	1515.5300
1588.9658	1831.7270	2141.6821
3047.2482	3052.1499	3054.9855
3064.7220	3069.3901	3075.8067
3084.6094	3115.0156	3117.1071
3125.9985	3128.8650	3129.9905
3146.2829	3151.5587	3181.9769

Zero-point correction (Hartree): 0.241736

ApineneCI.J.a.13Hshift.mpp

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.10790265

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.581764 | 0.300393  | -0.341709 |
| H | -0.924941 | 0.477355  | -1.362979 |
| C | -1.723511 | 0.589445  | 0.633567  |
| C | -2.838312 | -0.342013 | 0.349816  |
| H | -1.383181 | 0.386903  | 1.651928  |
| H | -2.051467 | 1.628890  | 0.566109  |
| H | -3.503379 | -1.500043 | 0.183046  |
| C | 0.783850  | 1.026159  | -0.144510 |
| C | 0.144173  | -1.056043 | -0.269899 |
| C | 1.019270  | 2.254863  | -0.999814 |
| C | 1.082135  | 1.323459  | 1.319167  |
| H | 0.970130  | 0.441184  | 1.952923  |

|                                                |           |           |           |
|------------------------------------------------|-----------|-----------|-----------|
| H                                              | 2.105320  | 1.677276  | 1.426754  |
| H                                              | 0.407441  | 2.096369  | 1.691996  |
| H                                              | 2.060357  | 2.571184  | -0.925074 |
| H                                              | 0.387957  | 3.082908  | -0.670282 |
| H                                              | 0.795878  | 2.053255  | -2.048372 |
| H                                              | -0.190433 | -1.849037 | -0.933680 |
| H                                              | 0.166108  | -1.436253 | 0.752341  |
| C                                              | 1.439539  | -0.297666 | -0.627893 |
| H                                              | 1.555296  | -0.268859 | -1.716274 |
| C                                              | 2.773193  | -0.724483 | -0.069506 |
| C                                              | 2.995762  | -2.205809 | 0.097224  |
| H                                              | 2.683928  | -2.739759 | -0.801567 |
| H                                              | 2.375272  | -2.573971 | 0.916475  |
| H                                              | 4.040660  | -2.403446 | 0.316354  |
| O                                              | 3.620935  | 0.088546  | 0.207426  |
| O                                              | -3.929602 | 0.130718  | -0.046211 |
| O                                              | -4.698951 | -1.075988 | -0.246008 |
| Rotational constants (GHz):                    |           |           |           |
|                                                | 1.5231700 | 0.3770400 | 0.3313900 |
| Vibrational harmonic frequencies (cm-1):       |           |           |           |
| i1726.5141                                     | 32.9375   |           | 37.4838   |
| 41.0701                                        | 91.1581   |           | 115.9517  |
| 138.6745                                       | 155.9771  |           | 193.5358  |
| 222.9543                                       | 252.1890  |           | 272.3710  |
| 300.6010                                       | 314.6253  |           | 323.1604  |
| 358.6138                                       | 365.1885  |           | 410.0041  |
| 488.4326                                       | 504.4123  |           | 519.3142  |
| 599.9239                                       | 630.8746  |           | 716.4320  |
| 742.6015                                       | 790.7511  |           | 857.0571  |
| 897.8495                                       | 911.5248  |           | 928.6382  |
| 966.4957                                       | 970.2273  |           | 981.6883  |
| 1007.3951                                      | 1019.6791 |           | 1040.3401 |
| 1058.5450                                      | 1109.2209 |           | 1126.5517 |
| 1150.9830                                      | 1180.2920 |           | 1196.1847 |
| 1199.0832                                      | 1230.4240 |           | 1240.5532 |
| 1254.0430                                      | 1262.9078 |           | 1280.8528 |
| 1302.1936                                      | 1323.8669 |           | 1351.7431 |
| 1387.2411                                      | 1396.1627 |           | 1410.3751 |
| 1419.9806                                      | 1464.2528 |           | 1465.0316 |
| 1477.5652                                      | 1484.5913 |           | 1494.3143 |
| 1499.1939                                      | 1506.6367 |           | 1514.9965 |
| 1596.0049                                      | 1831.9721 |           | 2146.4640 |
| 3047.8622                                      | 3051.8320 |           | 3054.4572 |
| 3057.1822                                      | 3064.2244 |           | 3073.2513 |
| 3085.1158                                      | 3113.7921 |           | 3115.5705 |
| 3117.3401                                      | 3125.4199 |           | 3129.2809 |
| 3148.2469                                      | 3152.6616 |           | 3181.6927 |
| Zero-point correction (Hartree): 0.241669      |           |           |           |
| ApineneCI.J.a.13Hshift.mpt                     |           |           |           |
| ~~~~~                                          |           |           |           |
| E(RM062X/Aug-CC-pVT2) (Hartree): -616.10883712 |           |           |           |
| Electronic state : 1-A                         |           |           |           |
| Cartesian coordinates (Angs):                  |           |           |           |
| C                                              | -0.641285 | 0.476986  | -0.311740 |
| H                                              | -0.986615 | 0.632706  | -1.335750 |
| C                                              | -1.723148 | 0.912129  | 0.656775  |
| C                                              | -3.029696 | 0.228248  | 0.510827  |
| H                                              | -1.424123 | 0.758880  | 1.699658  |
| H                                              | -1.932484 | 1.985498  | 0.585581  |
| H                                              | -4.316668 | -0.106055 | 0.731977  |
| C                                              | 0.793682  | 1.069375  | -0.173674 |
| C                                              | -0.049756 | -0.941621 | -0.188926 |
| C                                              | 1.134215  | 2.227385  | -1.090446 |
| C                                              | 1.151877  | 1.404437  | 1.269408  |
| H                                              | 0.959763  | 0.570420  | 1.947960  |
| H                                              | 2.208513  | 1.652502  | 1.344628  |
| H                                              | 0.570590  | 2.261700  | 1.614330  |
| H                                              | 2.202135  | 2.444172  | -1.043952 |
| H                                              | 0.592226  | 3.128558  | -0.794528 |
| H                                              | 0.874559  | 1.999287  | -2.125160 |
| H                                              | -0.478183 | -1.722679 | -0.810997 |
| H                                              | -0.042756 | -1.278243 | 0.849141  |
| C                                              | 1.306931  | -0.333316 | -0.601704 |
| H                                              | 1.402353  | -0.367146 | -1.691996 |
| C                                              | 2.602793  | -0.864737 | -0.045660 |
| C                                              | 2.681731  | -2.352114 | 0.185172  |
| H                                              | 2.298355  | -2.891609 | -0.682026 |
| H                                              | 2.045883  | -2.619757 | 1.031209  |
| H                                              | 3.706539  | -2.643097 | 0.394944  |
| O                                              | 3.532470  | -0.128890 | 0.180959  |
| O                                              | -3.144153 | -0.657345 | -0.370669 |
| O                                              | -4.518835 | -1.059485 | -0.182192 |
| Rotational constants (GHz):                    |           |           |           |
|                                                | 1.4008600 | 0.4200000 | 0.3589100 |
| Vibrational harmonic frequencies (cm-1):       |           |           |           |
| i1723.0036                                     | 33.8248   |           | 42.2624   |
| 84.9842                                        | 88.7172   |           | 120.2499  |
| 133.7075                                       | 159.0523  |           | 182.8092  |
| 225.7313                                       | 253.4717  |           | 258.2665  |
| 281.6542                                       | 314.3963  |           | 324.7195  |
| 344.1526                                       | 373.8429  |           | 408.4340  |
| 501.3534                                       | 504.9963  |           | 518.6365  |
| 601.7324                                       | 632.2775  |           | 724.9518  |
| 753.4810                                       | 796.3412  |           | 815.5642  |
| 900.7446                                       | 919.0147  |           | 924.6493  |
| 956.2578                                       | 966.3559  |           | 982.6328  |
| 1009.1289                                      | 1024.5430 |           | 1039.0238 |
| 1053.5206                                      | 1106.8718 |           | 1121.0344 |
| 1150.4326                                      | 1163.0386 |           | 1180.5207 |
| 1201.3016                                      | 1221.2274 |           | 1238.0947 |
| 1253.7263                                      | 1263.8271 |           | 1290.3189 |
| 1316.1122                                      | 1343.5940 |           | 1359.3363 |
| 1392.3346                                      | 1403.8580 |           | 1413.7341 |

|           |           |           |
|-----------|-----------|-----------|
| 1419.9422 | 1428.1655 | 1463.8926 |
| 1476.6792 | 1484.9393 | 1495.7280 |
| 1499.1028 | 1507.4903 | 1516.1776 |
| 1583.7987 | 1830.2986 | 2139.1110 |
| 3043.1132 | 3046.4613 | 3050.3547 |
| 3053.4993 | 3064.6244 | 3066.2692 |
| 3077.6428 | 3085.4986 | 3112.9693 |
| 3115.0310 | 3125.9631 | 3128.9391 |
| 3151.8660 | 3153.2739 | 3181.1839 |

Zero-point correction (Hartree): 0.241433

ApineneCI.J.a.13Hshift.mtm

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.10758870

Electronic state : 1-A

Cartesian coordinates (Angs):

C	0.342478	0.985099	1.077770
H	0.103077	1.846134	1.703987
C	1.862063	0.899487	0.970869
C	2.368615	-0.350654	0.356534
H	2.275945	1.771923	0.459253
H	2.278829	0.886427	1.985956
H	2.516378	-1.662261	0.103889
C	-0.535302	1.065352	-0.205495
C	-0.484724	-0.226764	1.551411
C	-0.944616	2.454374	-0.652874
C	0.047366	0.276830	-1.371460
H	0.318728	-0.745271	-1.092917
H	-0.680494	0.212560	-2.178704
H	0.942434	0.768532	-1.757437
H	-1.700879	2.390046	-1.435943
H	-0.086987	3.000129	-1.052763
H	-1.358250	3.029493	0.176896
H	-0.720370	-0.292624	2.611040
H	-0.041555	-1.166929	1.226435
C	-1.593205	0.246662	0.588975
H	-2.269271	0.934794	1.105384
C	-2.464163	-0.732516	-0.158384
C	-2.691919	-2.081951	0.471305
H	-2.915470	-1.977229	1.533768
H	-1.774650	-2.669650	0.394951
H	-3.495322	-2.601187	-0.042318
O	-2.957487	-0.426126	-1.216458
O	3.323837	-0.273347	-0.451859
O	3.529687	-1.668077	-0.770855

Rotational constants (GHz): 1.1686400 0.4836500 0.4355800

Vibrational harmonic frequencies (cm-1):

i1727.3216	22.0245	51.0077
62.1282	107.1060	140.2321
151.0636	159.8150	194.9247
231.8084	263.3213	274.7119
296.9727	328.5967	335.3154
347.3233	368.5234	414.2535
470.1507	506.4347	583.9676
614.3187	625.3240	687.7630
721.4469	765.1060	842.1404
895.1257	911.8725	927.1243
956.0433	964.3137	986.4161
1005.9084	1012.7776	1038.9701
1047.9737	1112.1358	1130.0880
1151.5198	1179.1559	1196.0343
1200.1038	1219.1727	1242.5490
1255.0978	1265.6650	1293.9606
1312.0778	1331.0612	1354.6927
1391.1096	1398.4901	1410.3304
1421.2722	1436.1086	1464.2970
1475.8933	1485.1476	1496.4845
1503.3361	1508.4542	1517.3613
1594.8939	1830.5876	2146.3832
3027.9814	3045.1541	3047.7148
3057.2870	3063.7502	3078.3927
3088.8038	3097.8888	3110.2619
3114.8583	3125.6233	3128.9463
3143.5531	3151.6829	3181.2000

Zero-point correction (Hartree): 0.241711

ApineneCI.J.a.13Hshift.pmm

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.11125990

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.499354 | -0.728021 | -0.577468 |
| H | -0.909576 | -0.471057 | -1.556050 |
| C | -1.620946 | -1.319035 | 0.288134  |
| C | -2.659638 | -0.277844 | 0.462430  |
| H | -2.033573 | -2.205171 | -0.197716 |
| H | -1.223768 | -1.590107 | 1.265817  |
| H | -3.268170 | 0.838521  | 0.904667  |
| C | 0.336930  | 0.474433  | -0.057929 |
| C | 0.797020  | -1.538824 | -0.746332 |
| C | -0.070937 | 1.836279  | -0.584800 |
| C | 0.469621  | 0.492696  | 1.459130  |
| H | 0.799288  | -0.467592 | 1.856407  |
| H | 1.202153  | 1.241305  | 1.767090  |
| H | -0.485585 | 0.754266  | 1.917116  |
| H | 0.647874  | 2.604813  | -0.293631 |
| H | -1.044491 | 2.124768  | -0.180955 |
| H | -0.144998 | 1.831835  | -1.672787 |
| H | 0.880052  | -2.176782 | -1.622104 |
| H | 1.044483  | -2.113587 | 0.145225  |
| C | 1.572092  | -0.215322 | -0.749715 |
| H | 1.695032  | 0.194827  | -1.753639 |

|                                                           |           |           |           |
|-----------------------------------------------------------|-----------|-----------|-----------|
| C                                                         | 2.874629  | -0.142023 | 0.002569  |
| C                                                         | 3.659376  | 1.135136  | -0.156844 |
| H                                                         | 3.008089  | 1.995557  | 0.007718  |
| H                                                         | 4.028302  | 1.207132  | -1.181519 |
| H                                                         | 4.494265  | 1.154275  | 0.537172  |
| O                                                         | 3.244657  | -1.036535 | 0.722577  |
| O                                                         | -3.638939 | -0.280046 | -0.321382 |
| O                                                         | -4.335984 | 0.913101  | 0.101574  |
| Rotational constants (GHz): 1.8133700 0.4011100 0.3702100 |           |           |           |
| Vibrational harmonic frequencies (cm-1):                  |           |           |           |
| i1726.6396                                                | 27.9570   |           | 53.0452   |
| 60.7313                                                   | 87.8494   |           | 115.7338  |
| 120.1613                                                  | 153.2635  |           | 207.9713  |
| 231.6090                                                  | 253.4818  |           | 284.3360  |
| 299.2252                                                  | 326.4208  |           | 331.3711  |
| 375.4066                                                  | 391.6849  |           | 411.3491  |
| 435.7595                                                  | 506.2743  |           | 575.4034  |
| 600.5864                                                  | 624.1874  |           | 707.4503  |
| 735.2038                                                  | 779.5038  |           | 867.5350  |
| 907.2338                                                  | 922.9765  |           | 956.4499  |
| 958.5032                                                  | 969.0592  |           | 977.6377  |
| 1003.8956                                                 | 1024.8950 |           | 1035.2638 |
| 1071.6738                                                 | 1105.0802 |           | 1119.8159 |
| 1155.2317                                                 | 1169.2324 |           | 1181.3157 |
| 1194.1957                                                 | 1209.7636 |           | 1227.1523 |
| 1253.0298                                                 | 1263.3070 |           | 1280.5193 |
| 1294.3189                                                 | 1328.7839 |           | 1365.2217 |
| 1384.6855                                                 | 1405.0795 |           | 1413.3556 |
| 1425.8085                                                 | 1464.3511 |           | 1475.6801 |
| 1476.1250                                                 | 1487.4633 |           | 1494.2608 |
| 1499.7025                                                 | 1510.8722 |           | 1513.1385 |
| 1591.4992                                                 | 1835.8226 |           | 2139.3805 |
| 3045.1173                                                 | 3054.7890 |           | 3062.9180 |
| 3071.1024                                                 | 3074.7964 |           | 3085.3982 |
| 3100.4396                                                 | 3110.8115 |           | 3120.1270 |
| 3124.1636                                                 | 3125.5661 |           | 3133.8401 |
| 3136.7200                                                 | 3159.2126 |           | 3179.7359 |
| Zero-point correction (Hartree): 0.242033                 |           |           |           |
| ApineneCI.J.a.13Hshift.pmp                                |           |           |           |
| ~~~~~                                                     |           |           |           |
| E(RM062X/Aug-CC-pVTZ) (Hartree): -616.11202352            |           |           |           |
| Electronic state : 1-A                                    |           |           |           |
| Cartesian coordinates (Angs):                             |           |           |           |
| C                                                         | 0.425080  | 0.909834  | -0.727047 |
| H                                                         | 0.702610  | 0.785200  | -1.775671 |
| C                                                         | 1.632112  | 1.449295  | 0.045303  |
| C                                                         | 2.767550  | 0.527381  | -0.182431 |
| H                                                         | 1.901990  | 2.423057  | -0.369268 |
| H                                                         | 1.410982  | 1.559257  | 1.107781  |
| H                                                         | 3.698255  | -0.190606 | -0.843228 |
| C                                                         | -0.274856 | -0.392283 | -0.247367 |
| C                                                         | -0.918451 | 1.651512  | -0.629725 |
| C                                                         | 0.141315  | -1.661742 | -0.964161 |
| C                                                         | -0.221612 | -0.577639 | 1.264418  |
| H                                                         | -0.534271 | 0.318472  | 1.801017  |
| H                                                         | -0.887592 | -1.387827 | 1.567668  |
| H                                                         | 0.786398  | -0.843826 | 1.583938  |
| H                                                         | -0.484100 | -2.507086 | -0.670611 |
| H                                                         | 1.174671  | -1.917907 | -0.714771 |
| H                                                         | 0.072364  | -1.543902 | -2.046279 |
| H                                                         | -1.147052 | 2.381554  | -1.401737 |
| H                                                         | -1.077095 | 2.099540  | 0.350185  |
| C                                                         | -1.619130 | 0.288369  | -0.703448 |
| H                                                         | -1.841034 | -0.010842 | -1.729575 |
| C                                                         | -2.816624 | 0.045151  | 0.176623  |
| C                                                         | -3.538614 | -1.261144 | -0.035580 |
| H                                                         | -2.823378 | -2.085647 | -0.044007 |
| H                                                         | -4.023870 | -1.250974 | -1.013199 |
| H                                                         | -4.281238 | -1.412251 | 0.742081  |
| O                                                         | -3.151853 | 0.832427  | 1.026985  |
| O                                                         | 3.190598  | -0.157114 | 0.780416  |
| O                                                         | 4.197723  | -0.961390 | 0.127120  |
| Rotational constants (GHz): 1.6864300 0.4241000 0.3920800 |           |           |           |
| Vibrational harmonic frequencies (cm-1):                  |           |           |           |
| i1722.1174                                                | 39.9129   |           | 54.2119   |
| 63.6912                                                   | 78.2845   |           | 118.6796  |
| 139.3297                                                  | 152.4925  |           | 195.5767  |
| 232.7551                                                  | 245.1110  |           | 286.4929  |
| 300.7946                                                  | 319.2987  |           | 332.7642  |
| 380.2494                                                  | 387.9421  |           | 418.6383  |
| 434.8939                                                  | 497.1535  |           | 577.7231  |
| 601.0397                                                  | 624.3179  |           | 712.1590  |
| 727.6754                                                  | 781.2068  |           | 870.0355  |
| 907.6362                                                  | 923.5176  |           | 950.9470  |
| 958.7428                                                  | 968.4682  |           | 975.1624  |
| 1002.9198                                                 | 1019.9487 |           | 1035.8021 |
| 1077.3049                                                 | 1105.4757 |           | 1110.4957 |
| 1144.8886                                                 | 1172.9804 |           | 1181.7499 |
| 1194.1346                                                 | 1209.6897 |           | 1240.1729 |
| 1249.9847                                                 | 1262.3293 |           | 1273.3520 |
| 1292.2576                                                 | 1328.4693 |           | 1368.1861 |
| 1390.0273                                                 | 1406.6609 |           | 1415.5316 |
| 1427.2867                                                 | 1464.6629 |           | 1465.4745 |
| 1476.0535                                                 | 1485.0731 |           | 1494.6116 |
| 1501.1392                                                 | 1509.0687 |           | 1513.5669 |
| 1587.8952                                                 | 1835.3962 |           | 2142.6967 |
| 3041.4622                                                 | 3057.4733 |           | 3063.4486 |
| 3066.3316                                                 | 3073.2568 |           | 3082.5635 |
| 3100.3609                                                 | 3106.9253 |           | 3121.4824 |
| 3122.9982                                                 | 3125.8495 |           | 3126.1299 |
| 3139.7722                                                 | 3158.0363 |           | 3179.5726 |

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Zero-point correction (Hartree): 0.241959

ApineneCI.J.a.13Hshift.pmt
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E(RM062X/Aug-CC-pVT2) (Hartree): -616.11224556
Electronic state : 1-A
Cartesian coordinates (Angs):
 C -0.508710 -0.782838 -0.698844
 H -0.909614 -0.525319 -1.680531
 C -1.585207 -1.456938 0.132755
 C -2.831699 -0.694541 0.365896
 H -1.900002 -2.401255 -0.327875
 H -1.213465 -1.749950 1.119504
 H -4.052795 -0.374338 0.841412
 C 0.261846 0.450643 -0.130587
 C 0.828718 -1.532747 -0.838162
 C -0.117107 1.808673 -0.690564
 C 0.289888 0.477665 1.390993
 H 0.627962 -0.468074 1.815858
 H 0.966945 1.256535 1.746962
 H -0.703935 0.705032 1.783047
 H 0.632217 2.556286 -0.421279
 H -1.077800 2.141176 -0.298116
 H -0.187618 1.777321 -1.778580
 H 0.982339 -2.129115 -1.733888
 H 1.052180 -2.139323 0.039566
 C 1.561978 -0.191168 -0.746210
 H 1.749103 0.254749 -1.724514
 C 2.802298 -0.109940 0.104038
 C 3.577854 1.180443 0.026384
 H 2.904953 2.028083 0.168545
 H 4.011645 1.283092 -0.969813
 H 4.364612 1.193321 0.774673
 O 3.131263 -1.010379 0.837213
 O -2.971228 0.411914 -0.209933
 O -4.275771 0.810497 0.266574
Rotational constants (GHz): 1.7381200 0.4307400 0.3940200
Vibrational harmonic frequencies (cm-1):
 i1730.5757 39.1406 57.8299
 65.3918 85.3340 114.6221
 124.1859 154.0870 222.1614
 231.5177 247.0370 277.1093
 289.8976 310.1543 332.9245
 346.1791 375.7930 429.2111
 438.7974 514.4313 577.5869
 603.8298 623.4893 712.0330
 755.3710 777.1221 833.3472
 903.7517 912.9497 939.5343
 961.9962 966.0777 977.7652
 1000.8029 1010.8533 1040.7881
 1094.2379 1099.0572 1111.7438
 1134.5715 1170.5683 1175.8785
 1194.4371 1204.9959 1213.8227
 1261.0147 1265.7954 1280.8453
 1312.2696 1350.8859 1371.2386
 1395.3436 1406.3566 1414.7635
 1424.5615 1427.0169 1463.5096
 1476.5968 1486.3138 1494.3846
 1499.5301 1509.1499 1510.6384
 1583.1963 1833.8926 2134.0056
 3041.6909 3048.5666 3052.7395
 3063.4729 3071.5464 3085.1879
 3086.6451 3093.6915 3113.3045
 3117.7851 3125.6142 3129.2907
 3137.9892 3152.5726 3179.9172
Zero-point correction (Hartree): 0.241608

ApineneCI.J.a.13Hshift.ppm
~~~~~
E(RM062X/Aug-CC-pVT2) (Hartree): -616.11020380
Electronic state : 1-A
Cartesian coordinates (Angs):
  C   -0.585464    0.575619   -0.399364
  H   -0.833139    1.019221   -1.365666
  C   -1.719280    0.857374    0.591982
  C   -2.974560    0.361228   -0.015785
  H   -1.529246    0.369202    1.548745
  H   -1.813930    1.935136    0.741148
  H   -4.011154    0.259492   -0.867188
  C    0.863935    0.990081   -0.018562
  C   -0.108525   -0.874123   -0.589432
  C    1.353172    2.291444   -0.622446
  C    1.118311    0.955484    1.481833
  H    0.809359    0.011596    1.930687
  H    2.182409    1.083854    1.689728
  H    0.584601    1.768947    1.976321
  H    2.416685    2.442724   -0.427459
  H    0.817061    3.138225   -0.187752
  H    1.197696    2.308680   -1.701608
  H   -0.521501   -1.439437   -1.420561
  H   -0.201636   -1.460798    0.324248
  C    1.322266   -0.337791   -0.729405
  H    1.584854   -0.115314   -1.765151
  C    2.444829   -1.086792   -0.059568
  C    3.840228   -0.614910   -0.381583
  H    3.903099    0.469083   -0.268318
  H    4.065448   -0.839124   -1.425741
  H    4.562627   -1.105210    0.264030
  O    2.235559   -1.981334    0.721741
  O   -3.461088   -0.709647    0.418620
  O   -4.592309   -0.878015   -0.464295
Rotational constants (GHz):    1.4868600    0.4035000    0.3582100

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Vibrational harmonic frequencies (cm-1):
11732.1024      33.3513      46.7473
  60.9884      81.1006      121.0129
 123.7652     150.2615      181.0763
 226.2122     234.7298      284.3167
 298.7059     329.8656      342.9315
 353.3409     390.1945      404.6862
 461.3979     487.5010      582.9284
 594.2847     624.1291      721.0913
 745.7436     799.8162      860.0038
 900.5887     924.7381      933.8220
 959.6814     965.1425      981.8314
1000.6758    1015.0947     1040.5420
1072.3862    1094.5620     1130.3851
1159.2811    1171.3646     1192.3437
1193.6907    1208.0034     1231.9633
1251.9721    1262.6016     1272.9120
1297.8954    1328.3133     1367.2369
1387.2452    1404.2025     1413.6361
1424.3313    1464.8101     1470.8563
1476.4779    1486.6016     1492.0764
1500.4515    1508.8253     1511.1957
1594.3224    1837.2371     2141.4122
3045.9331    3053.9001     3062.8235
3064.3727    3075.7609     3084.6354
3098.1603    3110.5903     3117.6480
3124.3298    3125.1922     3125.9811
3137.2872    3157.7291     3179.5701
Zero-point correction (Hartree): 0.241884

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ApineneCI.J.a.13Hshift.ppp
~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -616.11012382
Electronic state : 1-A
Cartesian coordinates (Angs):
C -0.591348 0.281167 -0.324998
H -0.938321 0.650326 -1.292236
C -1.709557 0.441661 0.706362
C -2.879460 -0.350885 0.264546
H -1.377061 0.024922 1.660155
H -1.978694 1.490983 0.846655
H -3.616919 -1.410492 -0.118017
C 0.797666 0.913945 -0.024720
C 0.086266 -1.089109 -0.496438
C 1.068488 2.249713 -0.688211
C 1.114457 0.969148 1.463051
H 0.965270 0.006516 1.952470
H 2.156126 1.255963 1.619836
H 0.488940 1.714276 1.957439
H 2.107702 2.555357 -0.551724
H 0.437689 3.027126 -0.251493
H 0.862904 2.206941 -1.758230
H -0.272586 -1.735453 -1.292412
H 0.117545 -1.652242 0.435895
C 1.416852 -0.357924 -0.715658
H 1.604207 -0.137195 -1.768002
C 2.661316 -0.913257 -0.073815
C 3.958976 -0.251477 -0.462605
H 3.865641 0.832629 -0.374137
H 4.175254 -0.467433 -1.510364
H 4.769511 -0.613572 0.162699
O 2.615021 -1.805384 0.736791
O -3.942468 0.255691 -0.007457
O -4.786197 -0.838626 -0.429785
Rotational constants (GHz): 1.6642700 0.3676500 0.3369800

```

```

Vibrational harmonic frequencies (cm-1):
11731.3406 33.0756 42.3021
 59.1921 82.5536 112.3718
 124.4734 149.1091 201.3949
 220.7132 242.1071 283.2743
 289.9901 321.6075 339.8170
 355.2858 371.7302 402.7585
 459.3683 500.3902 583.2537
 595.8190 624.4263 719.5932
 745.7143 801.0493 858.9453
 902.1091 924.9463 932.9692
 959.4110 965.4108 981.4361
1001.2953 1015.5228 1037.4733
1060.9670 1114.8384 1125.4313
1156.5875 1177.0989 1192.5704
1203.3941 1208.9705 1233.1364
1259.7777 1263.5454 1272.3569
1302.9099 1329.5191 1367.2157
1387.2774 1404.0776 1413.8475
1424.1811 1461.9468 1464.4412
1476.8695 1486.2382 1492.6422
1499.2075 1509.1062 1510.2289
1594.9506 1836.5734 2140.7752
3046.8370 3053.1315 3055.2865
3062.7805 3071.1996 3085.4949
3098.7652 3111.7964 3112.8681
3118.2834 3124.5974 3126.2501
3135.3642 3159.1669 3178.6899
Zero-point correction (Hartree): 0.241832

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ApineneCI.J.a.13Hshift.ppt
~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -616.11084612
Electronic state : 1-A
Cartesian coordinates (Angs):
C      -0.654790      0.435445     -0.271013
H      -1.007861      0.738914     -1.258527

```



|                                                           |           |           |           |
|-----------------------------------------------------------|-----------|-----------|-----------|
| C                                                         | -1.708227 | 0.775484  | 0.765207  |
| C                                                         | -3.048917 | 0.188722  | 0.529622  |
| H                                                         | -1.412703 | 0.452349  | 1.769189  |
| H                                                         | -1.867725 | 1.856380  | 0.856274  |
| H                                                         | -4.349916 | -0.110593 | 0.711827  |
| C                                                         | 0.795904  | 0.962242  | -0.078494 |
| C                                                         | -0.105184 | -1.001722 | -0.337152 |
| C                                                         | 1.158540  | 2.200629  | -0.874353 |
| C                                                         | 1.178465  | 1.126292  | 1.386537  |
| H                                                         | 0.959550  | 0.232949  | 1.971902  |
| H                                                         | 2.248114  | 1.323266  | 1.481628  |
| H                                                         | 0.647577  | 1.972150  | 1.826777  |
| H                                                         | 2.224861  | 2.422773  | -0.798213 |
| H                                                         | 0.615306  | 3.069740  | -0.496038 |
| H                                                         | 0.909466  | 2.077722  | -1.928825 |
| H                                                         | -0.553556 | -1.677339 | -1.059712 |
| H                                                         | -0.086042 | -1.481781 | 0.641285  |
| C                                                         | 1.275170  | -0.418197 | -0.663863 |
| H                                                         | 1.439536  | -0.312889 | -1.737718 |
| C                                                         | 2.490973  | -1.020745 | -0.010941 |
| C                                                         | 3.824929  | -0.526938 | -0.511343 |
| H                                                         | 3.832850  | 0.564508  | -0.535678 |
| H                                                         | 3.975135  | -0.868705 | -1.536943 |
| H                                                         | 4.626230  | -0.897159 | 0.121102  |
| O                                                         | 2.401167  | -1.817287 | 0.890743  |
| O                                                         | -3.218898 | -0.519757 | -0.491509 |
| O                                                         | -4.612520 | -0.874150 | -0.353430 |
| Rotational constants (GHz): 1.5352300 0.4038100 0.3655800 |           |           |           |
| Vibrational harmonic frequencies (cm-1):                  |           |           |           |
| i1722.9453                                                | 39.8976   |           | 56.9510   |
| 77.9367                                                   | 93.0345   |           | 120.4636  |
| 126.9951                                                  | 150.9752  |           | 194.6838  |
| 224.2989                                                  | 242.6627  |           | 257.6374  |
| 289.6021                                                  | 312.1104  |           | 331.0116  |
| 347.8710                                                  | 371.3256  |           | 413.5556  |
| 463.6631                                                  | 504.1981  |           | 585.1505  |
| 598.0676                                                  | 624.3435  |           | 725.9942  |
| 759.3545                                                  | 797.2934  |           | 826.3752  |
| 907.5716                                                  | 918.3521  |           | 934.7238  |
| 957.4301                                                  | 965.2354  |           | 976.9532  |
| 1002.5256                                                 | 1020.7218 | 1028.1316 |           |
| 1062.7905                                                 | 1109.9245 | 1122.8291 |           |
| 1148.3364                                                 | 1166.7714 | 1177.5322 |           |
| 1196.5458                                                 | 1209.7935 | 1226.8586 |           |
| 1256.6321                                                 | 1265.5895 | 1277.1251 |           |
| 1325.1781                                                 | 1343.5115 | 1373.6180 |           |
| 1398.4713                                                 | 1406.1153 | 1415.3765 |           |
| 1423.8247                                                 | 1429.0916 | 1464.7468 |           |
| 1477.0093                                                 | 1486.7516 | 1493.7093 |           |
| 1500.2872                                                 | 1509.2894 | 1510.7766 |           |
| 1586.2790                                                 | 1835.5618 | 2139.2716 |           |
| 3041.4890                                                 | 3045.9151 | 3053.4969 |           |
| 3062.7435                                                 | 3067.3984 | 3082.1239 |           |
| 3084.9054                                                 | 3097.9150 | 3110.2328 |           |
| 3117.4875                                                 | 3124.4378 | 3126.2314 |           |
| 3133.9102                                                 | 3161.5766 | 3178.6416 |           |
| Zero-point correction (Hartree): 0.241657                 |           |           |           |
| ApineneCI.J.a.13Hshift.ptm                                |           |           |           |
| ~~~~~                                                     |           |           |           |
| E (RM062X/Aug-CC-pVT2) (Hartree): -616.10942999           |           |           |           |
| Electronic state : 1-A                                    |           |           |           |
| Cartesian coordinates (Angs):                             |           |           |           |
| C                                                         | 0.341221  | 1.179329  | 0.899021  |
| H                                                         | 0.088451  | 2.151207  | 1.326582  |
| C                                                         | 1.857442  | 1.135217  | 0.732525  |
| C                                                         | 2.400482  | -0.189555 | 0.346440  |
| H                                                         | 2.208680  | 1.906802  | 0.042649  |
| H                                                         | 2.311526  | 1.338243  | 1.710520  |
| H                                                         | 2.608083  | -1.518619 | 0.337300  |
| C                                                         | -0.593703 | 0.936377  | -0.319538 |
| C                                                         | -0.403119 | 0.074508  | 1.670704  |
| C                                                         | -1.095178 | 2.183702  | -1.020945 |
| C                                                         | -0.023293 | -0.057707 | -1.322205 |
| H                                                         | 0.315482  | -0.980643 | -0.847968 |
| H                                                         | -0.780112 | -0.333699 | -2.059259 |
| H                                                         | 0.815862  | 0.381906  | -1.864493 |
| H                                                         | -1.851628 | 1.940758  | -1.769708 |
| H                                                         | -0.273929 | 2.685609  | -1.537581 |
| H                                                         | -1.531540 | 2.887343  | -0.311012 |
| H                                                         | -0.594072 | 0.241281  | 2.727634  |
| H                                                         | 0.046128  | -0.907489 | 1.535752  |
| C                                                         | -1.577482 | 0.252204  | 0.699318  |
| H                                                         | -2.300865 | 0.991941  | 1.048051  |
| C                                                         | -2.296618 | -0.975991 | 0.205829  |
| C                                                         | -3.516332 | -0.731040 | -0.646667 |
| H                                                         | -3.283900 | -0.012209 | -1.434497 |
| H                                                         | -4.302882 | -0.288063 | -0.033111 |
| H                                                         | -3.867794 | -1.663640 | -1.077731 |
| O                                                         | -1.897559 | -2.087833 | 0.447898  |
| O                                                         | 3.304982  | -0.225537 | -0.521626 |
| O                                                         | 3.571575  | -1.644504 | -0.583774 |
| Rotational constants (GHz): 1.2224000 0.4916500 0.4375000 |           |           |           |
| Vibrational harmonic frequencies (cm-1):                  |           |           |           |
| i1727.4858                                                | 45.2411   |           | 50.8917   |
| 67.8422                                                   | 104.8030  |           | 113.6034  |
| 145.9743                                                  | 155.2236  |           | 205.0581  |
| 229.3497                                                  | 246.5903  |           | 279.2479  |
| 287.4863                                                  | 326.7437  |           | 336.3434  |
| 353.7717                                                  | 371.1812  |           | 394.2997  |
| 434.0548                                                  | 567.2095  |           | 581.8217  |
| 615.3728                                                  | 627.0255  |           | 685.5240  |

|           |           |           |
|-----------|-----------|-----------|
| 722.1761  | 778.2534  | 842.3121  |
| 905.3485  | 921.6489  | 936.2431  |
| 956.1512  | 962.5321  | 973.3124  |
| 999.4032  | 1010.3836 | 1022.6478 |
| 1055.1860 | 1112.0230 | 1138.7389 |
| 1150.1036 | 1177.0082 | 1194.6279 |
| 1197.4966 | 1209.1151 | 1221.6256 |
| 1260.4296 | 1263.1057 | 1286.0998 |
| 1309.9733 | 1338.1732 | 1369.7975 |
| 1392.4819 | 1403.6449 | 1415.1094 |
| 1423.9128 | 1435.2357 | 1464.0004 |
| 1476.4951 | 1485.5019 | 1493.1486 |
| 1503.3277 | 1508.0774 | 1510.1208 |
| 1592.6870 | 1838.1109 | 2143.8737 |
| 3028.4169 | 3045.7299 | 3049.7565 |
| 3062.6828 | 3076.1678 | 3079.6169 |
| 3086.9139 | 3105.8964 | 3111.3849 |
| 3115.8325 | 3122.4930 | 3124.8214 |
| 3125.3693 | 3162.3656 | 3179.9549 |

Zero-point correction (Hartree): 0.241717

ApineneCI.J.a.13Hshift.ptp

~~~~~  
E(RM062X/Aug-CC-pVT2) (Hartree): -616.10642369

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-0.390256	1.066165	-0.807065
H	-0.166611	1.873669	-1.506267
C	-1.839612	1.258891	-0.352556
C	-2.448346	0.041300	0.242770
H	-1.870810	2.028482	0.427623
H	-2.461172	1.603927	-1.180966
H	-2.638916	-1.028485	1.036481
C	0.782548	1.003360	0.210719
C	0.086524	-0.267114	-1.413474
C	1.494124	2.319519	0.459091
C	0.423644	0.328041	1.527857
H	-0.015889	-0.656715	1.381776
H	1.317978	0.207914	2.142904
H	-0.284023	0.937987	2.092289
H	2.391482	2.177386	1.064228
H	0.841259	3.007811	1.001384
H	1.785602	2.795214	-0.478011
H	0.028340	-0.385946	-2.492166
H	-0.367958	-1.133058	-0.931768
C	1.464733	0.005694	-0.796777
H	2.115935	0.568297	-1.468853
C	2.225803	-1.141724	-0.185874
C	3.623724	-0.830786	0.287078
H	3.616163	0.065152	0.910618
H	4.257694	-0.614115	-0.574532
H	4.029784	-1.672264	0.840334
O	1.731352	-2.232900	-0.049417
O	-3.551564	-0.335417	-0.217308
O	-3.819310	-1.491099	0.604764

Rotational constants (GHz): 1.2584000 0.4738400 0.4050000

Vibrational harmonic frequencies (cm-1):

i1726.2386	19.5474	52.2131
60.6153	72.7161	119.5906
134.5623	151.4274	189.2537
229.7401	241.1033	279.7674
285.8176	313.8819	332.3062
353.2693	370.7506	397.9412
438.7381	568.3308	583.6099
608.9988	626.0370	690.5377
725.3142	780.2657	846.6051
906.5964	919.8772	949.0213
959.5180	969.1969	972.6946
998.9292	1011.9749	1024.5453
1056.5001	1106.3087	1134.7974
1163.7272	1173.5675	1185.2815
1196.2359	1210.3425	1238.2347
1244.4193	1264.4065	1293.3215
1318.2242	1331.4821	1371.2315
1394.1802	1405.4126	1416.0882
1427.6572	1450.2442	1465.1484
1476.6285	1484.1599	1491.5397
1501.0261	1506.1250	1510.5306
1596.7296	1838.7522	2148.6190
3035.1854	3044.9442	3055.4957
3063.1971	3075.6965	3078.6671
3094.5053	3097.9147	3109.5386
3115.0542	3123.6765	3125.8167
3152.9251	3155.7675	3180.0069

Zero-point correction (Hartree): 0.241701

ApineneCI.J.a.13Hshift.ptt

~~~~~  
E(RM062X/Aug-CC-pVT2) (Hartree): -616.10690176

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.449447  | 1.167816  | 0.849777  |
| H | 0.173802  | 2.029395  | 1.461381  |
| C | 1.934789  | 1.353693  | 0.498057  |
| C | 2.546075  | 0.247321  | -0.284169 |
| H | 2.058124  | 2.277343  | -0.066927 |
| H | 2.496838  | 1.447849  | 1.431873  |
| H | 3.075592  | -0.440988 | -1.316109 |
| C | -0.629478 | 1.013829  | -0.255557 |
| C | -0.079462 | -0.108856 | 1.524809  |
| C | -1.305592 | 2.296516  | -0.699161 |
| C | -0.150409 | 0.208179  | -1.456144 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| H | 0.308462  | -0.739453 | -1.168182 |
| H | -0.987787 | -0.025727 | -2.117024 |
| H | 0.574271  | 0.783841  | -2.035026 |
| H | -2.143368 | 2.093049  | -1.368713 |
| H | -0.600456 | 2.929676  | -1.242652 |
| H | -1.681070 | 2.860939  | 0.155192  |
| H | -0.106467 | -0.127678 | 2.611136  |
| H | 0.401042  | -1.015408 | 1.161965  |
| C | -1.402411 | 0.116746  | 0.779284  |
| H | -2.095931 | 0.743937  | 1.343160  |
| C | -2.130966 | -1.076276 | 0.217478  |
| C | -3.474598 | -0.795767 | -0.408460 |
| H | -3.390849 | 0.027551  | -1.120243 |
| H | -4.175909 | -0.478158 | 0.365146  |
| H | -3.851276 | -1.685536 | -0.903943 |
| O | -1.651822 | -2.182040 | 0.236077  |
| O | 2.757718  | -0.840471 | 0.305800  |
| O | 3.319181  | -1.629967 | -0.765192 |

Rotational constants (GHz): 1.1722300 0.5501200 0.4602500  
 Vibrational harmonic frequencies (cm-1):  
 11727.0977 42.3056 53.8109  
 62.3682 98.9459 110.6726  
 120.1966 145.3765 193.0289  
 224.7549 240.7294 283.7370  
 303.4214 338.9380 349.8760  
 361.4491 381.5427 399.3870  
 435.8532 567.7648 576.6390  
 601.4115 626.0354 692.5327  
 731.6339 775.5436 843.1593  
 903.9663 923.1398 942.3799  
 960.7440 967.0226 974.0273  
 999.4755 1010.7748 1045.0902  
 1065.7945 1110.5730 1122.3092  
 1149.2373 1172.2145 1182.6562  
 1195.6933 1208.4000 1217.9290  
 1245.3797 1261.9541 1285.7661  
 1299.2377 1337.2744 1370.4129  
 1392.8625 1404.7181 1414.2759  
 1425.6526 1464.6707 1473.7493  
 1476.9759 1485.6104 1492.6784  
 1504.6182 1507.2585 1514.0581  
 1585.6407 1840.1952 2140.4791  
 3045.2814 3048.5295 3054.3112  
 3063.1923 3070.1078 3078.4238  
 3108.0743 3110.1759 3113.8662  
 3119.7062 3123.1769 3125.6616  
 3126.1671 3164.9450 3179.8073  
 Zero-point correction (Hartree): 0.241867

Population analysis as 298K (%)

Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)

| Compound                     | Qtot      | Erel | Erel2 | n*Q*MB    | %      |
|------------------------------|-----------|------|-------|-----------|--------|
| ApineneCI.J.a.ringclose.pmtp | 1.850e+44 | 0.00 | 0.00  | 1.850e+44 | 41.9   |
| ApineneCI.J.a.ringclose.pmpm | 1.645e+44 | 0.30 | 0.30  | 9.931e+43 | 22.5   |
| ApineneCI.J.a.ringclose.pmtm | 3.562e+44 | 1.38 | 1.38  | 3.479e+43 | 7.88   |
| ApineneCI.J.a.ringclose.pppm | 5.238e+44 | 1.81 | 1.81  | 2.447e+43 | 5.55   |
| ApineneCI.J.a.ringclose.pmpm | 7.395e+44 | 2.07 | 2.07  | 2.237e+43 | 5.07   |
| ApineneCI.J.a.ringclose.pppm | 3.538e+44 | 1.95 | 1.95  | 1.305e+43 | 2.96   |
| ApineneCI.J.a.ringclose.pptp | 4.627e+44 | 2.17 | 2.17  | 1.191e+43 | 2.7    |
| ApineneCI.J.a.ringclose.pppp | 8.128e+44 | 2.82 | 2.82  | 7.000e+42 | 1.59   |
| ApineneCI.J.a.ringclose.pppm | 6.601e+44 | 2.69 | 2.69  | 6.992e+42 | 1.58   |
| ApineneCI.J.a.ringclose.mmtp | 4.708e+44 | 2.54 | 2.54  | 6.423e+42 | 1.46   |
| ApineneCI.J.a.ringclose.mmpm | 4.176e+44 | 2.47 | 2.47  | 6.410e+42 | 1.45   |
| ApineneCI.J.a.ringclose.pptm | 5.602e+44 | 2.65 | 2.65  | 6.396e+42 | 1.45   |
| ApineneCI.J.a.ringclose.mppm | 5.627e+44 | 3.22 | 3.22  | 2.461e+42 | 0.558  |
| ApineneCI.J.a.ringclose.mptm | 6.539e+44 | 3.34 | 3.34  | 2.329e+42 | 0.528  |
| ApineneCI.J.a.ringclose.mttm | 7.332e+43 | 2.17 | 2.17  | 1.891e+42 | 0.429  |
| ApineneCI.J.a.ringclose.mmpm | 2.660e+44 | 2.93 | 2.93  | 1.884e+42 | 0.427  |
| ApineneCI.J.a.ringclose.mmtm | 4.937e+44 | 3.40 | 3.40  | 1.588e+42 | 0.36   |
| ApineneCI.J.a.ringclose.mmpm | 7.699e+44 | 3.71 | 3.71  | 1.464e+42 | 0.332  |
| ApineneCI.J.a.ringclose.mptp | 5.729e+44 | 3.54 | 3.54  | 1.459e+42 | 0.331  |
| ApineneCI.J.a.ringclose.mppm | 1.074e+45 | 4.06 | 4.06  | 1.131e+42 | 0.256  |
| ApineneCI.J.a.ringclose.ptmm | 3.017e+44 | 3.41 | 3.41  | 9.564e+41 | 0.217  |
| ApineneCI.J.a.ringclose.mppp | 9.531e+44 | 4.10 | 4.10  | 9.413e+41 | 0.213  |
| ApineneCI.J.a.ringclose.pttm | 1.705e+44 | 3.62 | 3.62  | 3.786e+41 | 0.0858 |
| ApineneCI.J.a.ringclose.ptmp | 2.227e+44 | 4.07 | 4.07  | 2.299e+41 | 0.0521 |
| ApineneCI.J.a.ringclose.mtmm | 8.959e+43 | 3.77 | 3.77  | 1.551e+41 | 0.0351 |
| ApineneCI.J.a.ringclose.mtmm | 4.422e+44 | 4.81 | 4.81  | 1.308e+41 | 0.0296 |
| ApineneCI.J.a.ringclose.pttp | 3.284e+44 | 5.07 | 5.07  | 6.336e+40 | 0.0144 |
| ApineneCI.J.a.ringclose.mtpp | 3.397e+44 | 5.29 | 5.29  | 4.477e+40 | 0.0101 |
| Total                        |           |      |       | 4.412e+44 | 100    |

ApineneCI.J.a.ringclose.mmpm

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.13070592

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-0.457396	0.891355	0.813186
H	-0.724257	0.803724	1.868383
C	-1.632326	1.515707	0.042361
C	-2.807133	0.628834	0.120391
H	-1.884165	2.464799	0.525233
H	-1.372759	1.690479	-0.999883
H	-3.271137	0.404090	1.078771
C	0.171058	-0.452001	0.342857
C	0.917225	1.571173	0.669127
C	-0.241039	-1.696049	1.102457
C	0.038432	-0.677022	-1.157914
H	0.320765	0.203204	-1.740478
H	0.682726	-1.501960	-1.463504

H	-0.991242	-0.942769	-1.405006
H	0.416878	-2.525531	0.839246
H	-1.267385	-1.967922	0.848293
H	-0.170916	-1.537055	2.179959
H	1.201658	2.301707	1.423142
H	1.029299	2.018743	-0.318618
C	1.551471	0.170934	0.739359
H	1.776828	-0.107131	1.770206
C	2.737671	-0.229917	-0.103666
C	3.385704	0.808426	-0.982548
H	3.607234	1.710924	-0.411202
H	2.692105	1.094117	-1.776438
H	4.290873	0.402079	-1.423243
O	3.125602	-1.372642	-0.078926
O	-3.321077	0.126225	-0.918143
O	-3.344338	-1.216102	-0.316496
Rotational constants (GHz):			
	1.5547100	0.4671100	0.4249200
Vibrational harmonic frequencies (cm-1):			
i567.1200	27.7512		51.9114
72.1868	87.4806		148.2341
164.6813	188.4201		200.8052
241.4003	260.5306		278.8086
323.0771	341.7621		343.6182
393.3109	438.4804		452.0431
494.6758	503.9243		542.0059
606.0163	621.8760		715.7329
768.6615	835.5073		878.9359
901.2635	919.5101		928.3193
969.9697	970.6988		997.4165
1010.4490	1014.2150		1042.8478
1058.7260	1084.1037		1110.2843
1148.9632	1176.4542		1198.5186
1210.6737	1242.1271		1255.7068
1261.8315	1276.3741		1293.8909
1323.4896	1350.5774		1376.8633
1387.8309	1391.8569		1408.1125
1421.9209	1461.5133		1465.7659
1475.5904	1486.6839		1497.4075
1500.0195	1511.7768		1520.0671
1600.0391	1828.7485		3046.0313
3048.4497	3054.8723		3062.4656
3072.8002	3085.8558		3089.6475
3117.4290	3121.5415		3124.2374
3127.7064	3132.4653		3141.5701
3144.1576	3156.0264		3181.9130
Zero-point correction (Hartree): 0.245517			
ApineneCI.J.a.ringclose.mmp			
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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.12864332			
Electronic state : 1-A			
Cartesian coordinates (Angs):			
C	0.407840	-0.699706	0.672307
H	0.644216	-0.662100	1.738613
C	1.649450	-1.090905	-0.110553
C	2.773058	-0.157693	0.106143
H	2.016751	-2.067251	0.235291
H	1.471235	-1.186738	-1.182287
H	2.932679	0.309748	1.076099
C	-0.363578	0.599911	0.288546
C	-0.885115	-1.509441	0.461768
C	-0.069049	1.830509	1.123394
C	-0.255155	0.921712	-1.197239
H	-0.507593	0.065877	-1.826857
H	-0.934033	1.732338	-1.453617
H	0.761788	1.233448	-1.446511
H	-0.793096	2.616059	0.904101
H	0.927382	2.221625	0.902759
H	-0.118530	1.605206	2.189878
H	-1.093489	-2.323223	1.152182
H	-0.951896	-1.884122	-0.560226
C	-1.658675	-0.185596	0.635274
H	-1.899207	-0.039220	1.693285
C	-2.927700	0.086256	-0.132358
C	-3.829355	-1.091722	-0.398570
H	-3.960087	-1.682960	0.508922
H	-3.361550	-1.743895	-1.138629
H	-4.788983	-0.748976	-0.773408
O	-3.205416	1.203466	-0.493444
O	3.546600	0.155473	-0.839798
O	4.734326	-0.067160	-0.005742
Rotational constants (GHz):			
	1.8601100	0.3774200	0.3532400
Vibrational harmonic frequencies (cm-1):			
i560.3157	31.8934		38.8107
53.3190	71.2723		125.1492
141.9678	161.7812		214.9518
237.7886	268.5322		274.3527
311.5974	321.9471		328.9918
386.3147	404.2896		442.9226
467.4546	519.9075		539.2265
612.5009	622.4340		716.7905
760.5294	803.8600		833.8833
889.0680	915.6799		942.5535
962.9902	971.7254		991.4041
1020.0449	1026.3439		1036.1802
1069.7912	1107.3386		1113.4156
1155.4777	1174.2245		1189.6417
1201.9227	1238.6418		1249.3773
1261.2910	1282.1621		1295.8099
1323.3876	1355.1362		1382.6464
1392.5315	1404.6429		1416.2318
1424.4674	1436.0522		1464.0889

1477.0850	1483.1260	1496.6843
1500.5423	1506.6771	1515.7265
1605.9581	1833.5091	3021.1749
3044.0783	3049.7691	3052.7439
3064.0574	3064.7596	3084.7896
3110.9387	3112.6743	3116.3269
3125.7861	3128.9181	3145.3419
3149.9460	3151.5331	3180.1799

Zero-point correction (Hartree): 0.244696

ApineneCI.J.a.ringclose.mmtm

E(RM062X/Aug-CC-pVTZ) (Hartree): -616.12926473

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-0.536466	-0.727484	-0.392315
H	-0.954950	-0.655133	-1.396553
C	-1.601089	-1.220649	0.568608
C	-2.817185	-0.385943	0.631379
H	-1.967256	-2.208593	0.250827
H	-1.221633	-1.363714	1.582649
H	-3.506474	-0.456272	1.468919
C	0.247649	0.586496	-0.076762
C	0.797273	-1.497404	-0.425466
C	-0.183903	1.837531	-0.816973
C	0.346949	0.855164	1.419419
H	0.721132	-0.007632	1.975045
H	1.022329	1.686587	1.608520
H	-0.636676	1.116198	1.818816
H	0.575710	2.612445	-0.703838
H	-1.128244	2.219643	-0.428018
H	-0.317511	1.636765	-1.880846
H	0.920822	-2.268865	-1.181919
H	1.035258	-1.918029	0.552961
C	1.497715	-0.140697	-0.644157
H	1.573608	0.059453	-1.717996
C	2.863244	0.123604	-0.064267
C	3.840884	-1.024461	-0.092968
H	3.844064	-1.494859	-1.077293
H	3.525965	-1.786182	0.622676
H	4.835321	-0.673336	0.165388
O	3.158722	1.206600	0.378087
O	-3.076150	0.449806	-0.278552
O	-4.464058	-0.023332	-0.386827

Rotational constants (GHz): 1.8741400 0.4100900 0.3782800

Vibrational harmonic frequencies (cm-1):

i560.4417	36.3749	45.0768
54.0995	75.8819	127.2897
139.0675	165.3481	213.0604
243.0834	267.0199	282.0505
313.0159	327.4854	343.2903
359.0174	402.5402	406.8723
498.5033	519.3392	583.6226
619.8441	669.3220	715.5247
754.0907	805.6791	835.9633
875.8166	908.0916	932.9089
966.0276	970.8821	990.3215
1009.7307	1020.5574	1033.8481
1038.9946	1108.0069	1112.0417
1147.2026	1165.0577	1189.7987
1202.4994	1237.4019	1253.5996
1263.6387	1291.5901	1306.5524
1334.3408	1362.5917	1375.2491
1394.0697	1406.4760	1418.4260
1425.2587	1430.4366	1465.1618
1477.6001	1483.4995	1495.7009
1499.6364	1506.2846	1514.6613
1594.3644	1833.4743	3009.2677
3044.0417	3051.3339	3055.7041
3064.7965	3075.6173	3088.8106
3101.8843	3105.2698	3126.1106
3126.7797	3133.7427	3140.9790
3153.4092	3160.7066	3181.1437

Zero-point correction (Hartree): 0.244821

ApineneCI.J.a.ringclose.mmtm

E(RM062X/Aug-CC-pVTZ) (Hartree): -616.13071237

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-0.485116	0.979091	0.532619
H	-0.818452	1.015801	1.570506
C	-1.558785	1.542186	-0.376751
C	-2.827644	0.784542	-0.380992
H	-1.814878	2.577643	-0.113405
H	-1.224395	1.595628	-1.417604
H	-3.588949	0.974409	-1.133967
C	0.101913	-0.441487	0.240018
C	0.929286	1.575247	0.403123
C	-0.393009	-1.589254	1.099302
C	0.012258	-0.810846	-1.235202
H	0.414563	-0.031424	-1.887708
H	0.577258	-1.721258	-1.424805
H	-1.031600	-0.994305	-1.504698
H	0.287830	-2.435754	0.996039
H	-1.390646	-1.903638	0.792075
H	-0.427590	-1.303600	2.152308
H	1.217569	2.361656	1.097110
H	1.119434	1.915756	-0.616138
C	1.481509	0.155784	0.638405
H	1.644428	-0.002079	1.709600
C	2.735599	-0.311433	-0.055046

C	3.810203	0.721838	-0.287148
H	3.970262	1.314195	0.614850
H	3.484891	1.411708	-1.068148
H	4.731593	0.236698	-0.594893
O	2.874110	-1.462886	-0.387224
O	-3.087532	-0.057346	0.520307
O	-3.535154	-1.060449	-0.463220
Rotational constants (GHz): 1.6731400 0.4687700 0.4174100			
Vibrational harmonic frequencies (cm-1):			
1558.2460	20.5774	50.1622	
70.9055	78.0288	133.4099	
149.0666	163.9480	216.6889	
253.0385	274.5498	283.2172	
317.5749	339.5253	347.5994	
377.7323	405.8837	408.6293	
495.0162	515.5780	584.6929	
619.4861	664.2713	717.2422	
769.2312	790.1248	840.5778	
894.5281	915.7436	934.8583	
948.4721	970.6319	977.4729	
1001.1818	1027.0895	1028.1430	
1040.4366	1109.1611	1111.8867	
1138.4505	1169.1828	1189.8782	
1202.4810	1237.7334	1254.8444	
1268.5703	1288.8791	1305.9245	
1338.5478	1358.6724	1375.7880	
1390.0039	1404.8344	1414.0160	
1424.5308	1428.1882	1464.4661	
1477.6753	1483.4853	1497.9635	
1501.6797	1508.0395	1519.3371	
1604.7424	1833.1435	3022.7568	
3037.6969	3049.1031	3051.7157	
3064.3707	3069.2244	3075.9747	
3092.1945	3102.0877	3120.2988	
3126.3005	3138.8022	3139.3301	
3149.0909	3155.0522	3179.5750	
Zero-point correction (Hartree): 0.244905			

ApineneCI.J.a.ringclose.mpm

E(RM062X/Aug-CC-pVTZ) (Hartree): -616.12789507

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-0.538037	0.294761	-0.514551
H	-0.783261	0.578260	-1.541312
C	-1.775954	0.422178	0.354248
C	-2.934011	-0.317747	-0.185183
H	-1.613539	0.110191	1.387322
H	-2.106746	1.470645	0.396845
H	-3.067723	-0.450127	-1.257147
C	0.770910	1.029426	-0.100504
C	0.233338	-1.040807	-0.521846
C	1.040769	2.355409	-0.782736
C	0.908986	1.165104	1.411293
H	0.764156	0.214089	1.928144
H	1.902168	1.530400	1.663884
H	0.172379	1.873048	1.795457
H	2.052625	2.694891	-0.558670
H	0.341912	3.119300	-0.434467
H	0.938959	2.269630	-1.865551
H	0.000858	-1.762449	-1.301835
H	0.170644	-1.535027	0.448646
C	1.526301	-0.209897	-0.657149
H	1.749694	-0.052010	-1.717248
C	2.814175	-0.655172	-0.011584
C	3.072739	-2.138812	0.041766
H	2.865500	-2.595612	-0.927048
H	2.392492	-2.597964	0.761691
H	4.098944	-2.327609	0.341888
O	3.600998	0.151367	0.420129
O	-3.775154	-0.850515	0.588944
O	-4.900139	-0.296642	-0.174463
Rotational constants (GHz): 1.5677200 0.3684500 0.3295100			
Vibrational harmonic frequencies (cm-1):			
1564.4011	33.3847	35.6045	
52.6338	80.4754	110.2560	
135.9287	163.9781	188.7830	
229.1148	262.2809	273.3198	
309.5514	319.9002	328.1943	
365.1534	406.5992	424.9744	
498.5839	514.4854	531.0128	
603.2303	635.6068	728.1205	
767.2324	810.0740	836.2330	
888.3843	905.3457	927.9771	
966.4935	970.5881	982.7909	
1009.6121	1026.2021	1042.7513	
1072.0625	1098.9652	1130.5746	
1149.8378	1178.2777	1200.9188	
1211.4285	1230.9795	1245.5370	
1257.4618	1285.9485	1300.4363	
1318.9479	1355.1584	1381.2936	
1393.3394	1403.8667	1417.5637	
1423.7993	1429.0586	1464.2828	
1477.1093	1484.0675	1495.8161	
1499.1776	1507.1601	1516.2447	
1605.2957	1833.1414	3009.2746	
3047.4624	3051.7354	3054.7423	
3061.0268	3064.3653	3081.8409	
3108.2612	3114.9378	3116.9387	
3125.5605	3130.2940	3141.0170	
3150.3721	3153.0576	3181.9894	
Zero-point correction (Hartree): 0.244505			

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ApineneCI.J.a.ringclose.mppm
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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.13118855
Electronic state : 1-A
Cartesian coordinates (Angs):
C      0.709430      -0.619172      -0.394792
H      1.003792      -0.829470      -1.424637
C      1.822469      -1.091521      0.564664
C      3.017862      -0.331673      0.176000
H      1.547385      -0.838220      1.588672
H      1.984848      -2.163871      0.460691
H      3.737056      -0.708808      -0.546744
C     -0.746509      -1.128486      -0.169851
C      0.216530      0.832233      -0.284141
C     -1.191010      -2.289428      -1.036271
C     -1.050854      -1.402030      1.296805
H     -0.789629      -0.557894      1.938002
H     -2.112952      -1.597717      1.427557
H     -0.493074      -2.275527      1.640730
H     -2.267089      -2.438943      -0.939840
H     -0.692240      -3.213119      -0.733879
H     -0.962665      -2.106782      -2.087216
H      0.679214      1.565450      -0.937831
H      0.279496      1.190191      0.744248
C     -1.190596      0.292338      -0.619309
H     -1.334912      0.301062      -1.704663
C     -2.424601      0.917486      -0.020606
C     -2.410012      2.415450      0.140143
H     -2.055839      2.890637      -0.775734
H     -1.705461      2.686908      0.928432
H     -3.402134      2.772925      0.398550
O     -3.377441      0.244635      0.290435
O      3.212263      0.823010      0.654343
O      3.423671      1.401355      -0.681301
Rotational constants (GHz):      1.2519900      0.4925600      0.4020900
Vibrational harmonic frequencies (cm-1):
i546.1409      37.2574      48.2194
66.1116      97.0369      119.2029
131.6821      158.8925      176.1406
229.0074      255.8868      278.4496
314.7079      321.3932      348.9063
393.3284      411.5831      481.9719
515.0895      519.6066      536.6192
601.9476      633.3374      730.4596
773.7835      830.7228      887.3419
896.5988      925.3843      938.0666
965.9411      972.0277      984.0589
1010.2423      1014.5986      1033.1865
1038.5857      1084.9476      1120.7704
1143.9243      1175.2329      1195.2675
1202.2561      1235.8489      1244.0299
1255.8642      1272.5566      1293.5156
1317.3908      1350.9750      1374.2283
1386.7185      1396.7575      1409.4418
1421.0256      1463.7350      1475.8648
1477.8281      1484.6074      1495.5017
1501.1801      1507.1354      1516.0005
1591.5718      1830.6317      3046.8885
3051.2789      3054.3733      3065.7534
3075.3875      3081.1645      3090.9189
3114.3415      3116.2556      3127.0121
3129.6558      3142.1506      3153.7076
3162.0728      3165.8662      3181.9614
Zero-point correction (Hartree): 0.245270

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ApineneCI.J.a.ringclose.mppm
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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.12992856
Electronic state : 1-A
Cartesian coordinates (Angs):
C     -0.730989      0.295179      -0.157417
H     -1.186401      0.323102      -1.148457
C     -1.791447      0.723365      0.876920
C     -2.891726      -0.236583      0.709923
H     -1.381112      0.677736      1.884239
H     -2.140692      1.730394      0.642976
H     -2.941070      -1.162330      1.277955
C      0.636687      1.038843      -0.191371
C      0.007715      -1.041933      0.025737
C      0.768719      2.145090      -1.218307
C      1.074643      1.523762      1.184219
H      1.034682      0.732279      1.935451
H      2.098978      1.887663      1.144083
H      0.430115      2.339886      1.516918
H      1.808003      2.468171      -1.290481
H      0.163592      3.009598      -0.936577
H      0.442899      1.808661      -2.203221
H     -0.397712      -1.908782      -0.489500
H      0.147664      -1.280892      1.081514
C      1.250409      -0.340406      -0.563775
H      1.247431      -0.456904      -1.652350
C      2.638175      -0.700619      -0.099324
C      2.897287      -2.158697      0.181776
H      2.509344      -2.775832      -0.629807
H      2.362787      -2.452539      1.087097
H      3.961104      -2.328773      0.316985
O      3.496543      0.139653      0.017136
O     -3.786312      -0.030571      -0.157586
O     -3.624786      -1.371512      -0.737939
Rotational constants (GHz):      1.4030600      0.4371500      0.3791600
Vibrational harmonic frequencies (cm-1):

```

i540.6682	35.6835	43.9292
66.1832	85.1470	112.5899
136.8364	154.7729	188.8976
222.6701	253.2410	274.8902
310.5057	320.5343	350.5389
385.9239	405.3465	469.6666
512.6595	520.5910	540.3611
603.0382	632.8768	732.2996
768.6131	827.4841	885.8873
904.2266	928.2223	931.1525
966.9176	974.3597	984.4222
1004.1869	1024.7365	1032.0579
1044.1598	1079.5087	1130.2105
1138.4945	1178.3831	1194.9195
1211.3742	1225.1683	1240.1181
1253.6327	1280.0001	1295.5255
1320.6949	1352.8584	1377.6004
1387.3209	1396.4469	1409.3974
1420.1687	1465.1310	1477.6160
1478.4412	1485.4002	1494.2647
1499.0893	1507.5150	1515.2986
1597.9793	1831.1746	3048.2594
3051.7165	3055.6702	3064.4640
3075.4901	3077.3589	3092.0928
3113.5974	3117.6563	3125.8814
3130.0974	3145.2535	3151.1758
3154.7162	3164.7497	3180.7738

Zero-point correction (Hartree): 0.245195

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.12789033

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.524114 | 0.409994  | -0.574046 |
| H | -0.710254 | 0.742918  | -1.597608 |
| C | -1.785162 | 0.576142  | 0.253636  |
| C | -2.904010 | -0.256384 | -0.227815 |
| H | -1.613057 | 0.237552  | 1.285324  |
| H | -2.126560 | 1.611188  | 0.329102  |
| H | -2.725609 | -1.186180 | -0.764244 |
| C | 0.807698  | 1.053757  | -0.083364 |
| C | 0.173603  | -0.966959 | -0.602914 |
| C | 1.180412  | 2.384280  | -0.706108 |
| C | 0.895224  | 1.127502  | 1.435951  |
| H | 0.678098  | 0.168740  | 1.912047  |
| H | 1.897971  | 1.423752  | 1.736888  |
| H | 0.187491  | 1.863898  | 1.820732  |
| H | 2.203723  | 2.650565  | -0.439230 |
| H | 0.519150  | 3.177554  | -0.350780 |
| H | 1.109136  | 2.343603  | -1.793993 |
| H | -0.062395 | -1.645388 | -1.419468 |
| H | 0.044225  | -1.493945 | 0.343752  |
| C | 1.514369  | -0.205954 | -0.656696 |
| H | 1.788682  | -0.023874 | -1.700777 |
| C | 2.749288  | -0.745237 | 0.020407  |
| C | 2.917735  | -2.242420 | 0.041987  |
| H | 2.712544  | -2.662807 | -0.943569 |
| H | 2.190702  | -2.677071 | 0.730798  |
| H | 3.921493  | -2.499547 | 0.366321  |
| O | 3.565729  | 0.001664  | 0.501638  |
| O | -4.098812 | 0.109675  | -0.056274 |
| O | -4.487616 | -1.216249 | 0.439446  |

Rotational constants (GHz): 1.4743500 0.3810800 0.3340600

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i564.5946 | 34.6924   | 35.6571   |
| 55.5890   | 85.7303   | 101.0669  |
| 139.5169  | 162.3081  | 200.3575  |
| 227.7865  | 260.9663  | 275.5786  |
| 313.2271  | 323.9821  | 327.4659  |
| 371.6466  | 404.8806  | 420.8541  |
| 498.9522  | 516.8481  | 522.0770  |
| 602.8328  | 635.5911  | 732.9496  |
| 774.4807  | 805.0320  | 838.8830  |
| 885.5414  | 905.6581  | 925.4688  |
| 967.0465  | 971.4281  | 982.2580  |
| 1007.8623 | 1027.1314 | 1041.2657 |
| 1074.5123 | 1109.0133 | 1132.7590 |
| 1148.3031 | 1173.4716 | 1194.4838 |
| 1204.5611 | 1237.3199 | 1255.7634 |
| 1262.2012 | 1284.2412 | 1305.8533 |
| 1322.8874 | 1352.0237 | 1379.3283 |
| 1392.4086 | 1401.0863 | 1415.0191 |
| 1421.1964 | 1426.9176 | 1464.6057 |
| 1477.3282 | 1484.6213 | 1495.5288 |
| 1499.8831 | 1507.2207 | 1515.8927 |
| 1605.0861 | 1832.3933 | 3017.7412 |
| 3047.7267 | 3051.9217 | 3054.7650 |
| 3063.8082 | 3067.8541 | 3080.4510 |
| 3095.0761 | 3115.0316 | 3117.0963 |
| 3125.0881 | 3129.2903 | 3141.5233 |
| 3149.5388 | 3152.6719 | 3181.5822 |

Zero-point correction (Hartree): 0.244561

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.12922102

Electronic state : 1-A

Cartesian coordinates (Angs):

C	0.665275	-0.590454	-0.398285
H	0.942351	-0.830059	-1.426725
C	1.783422	-0.998987	0.536711

C	3.071575	-0.324410	0.276558
H	1.541405	-0.753675	1.579880
H	1.966768	-2.079570	0.541668
H	3.960676	-0.582779	0.846518
C	-0.780588	-1.107453	-0.133341
C	0.142276	0.858381	-0.337705
C	-1.227844	-2.305009	-0.948026
C	-1.058501	-1.332640	1.348292
H	-0.790663	-0.465646	1.956184
H	-2.117398	-1.527435	1.504482
H	-0.492353	-2.191612	1.714156
H	-2.299763	-2.464855	-0.825456
H	-0.710805	-3.211125	-0.623615
H	-1.021793	-2.157594	-2.009137
H	0.566327	1.573960	-1.035727
H	0.222299	1.264400	0.671820
C	-1.262533	0.286826	-0.621635
H	-1.428985	0.254531	-1.703504
C	-2.495774	0.911297	-0.021926
C	-2.499490	2.412789	0.104857
H	-2.161037	2.872114	-0.824996
H	-1.791258	2.711278	0.880051
H	-3.493630	2.763085	0.365371
O	-3.436116	0.234127	0.317061
O	3.183803	0.539200	-0.635196
O	3.887432	1.472041	0.262638
Rotational constants (GHz):			
Vibrational harmonic frequencies (cm-1):			
1561.8725	36.3063	42.0816	
47.7389	97.1965	120.0956	
138.1338	167.8670	182.3424	
227.3546	259.6698	275.5442	
318.1320	323.1362	346.9372	
353.9742	405.2589	409.2430	
506.5748	515.9329	578.4202	
611.0845	663.9643	733.8234	
777.7211	813.4661	843.3471	
878.1994	906.8170	923.5262	
962.3235	966.6542	981.8926	
998.2836	1013.6005	1027.5122	
1047.2672	1082.5171	1125.7006	
1148.5384	1174.7155	1197.7093	
1206.6714	1237.2706	1252.0454	
1263.9074	1288.2386	1312.8635	
1344.9099	1360.0561	1376.2558	
1394.2695	1403.2218	1412.2696	
1419.6130	1430.5977	1464.4159	
1476.2159	1484.7899	1496.5296	
1499.0117	1507.4478	1516.7300	
1602.5146	1830.3755	3024.4980	
3045.7821	3048.8833	3052.4229	
3055.4095	3065.2327	3076.4795	
3087.1386	3112.1402	3114.2536	
3126.4496	3128.6905	3152.5014	
3159.4128	3160.5766	3181.7171	
Zero-point correction (Hartree): 0.244681			
ApineneCI.J.a.ringclose.mptp			
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E(RM062X/Aug-CC-pVT2) (Hartree): -616.12891702			
Electronic state : 1-A			
Cartesian coordinates (Angs):			
C	-0.689247	0.311760	-0.224970
H	-1.100175	0.399980	-1.231759
C	-1.762956	0.662708	0.781485
C	-2.986891	-0.159121	0.673477
H	-1.412608	0.598654	1.816763
H	-2.102237	1.701765	0.662493
H	-3.773801	-0.085759	1.419844
C	0.684404	1.043479	-0.172358
C	0.041352	-1.039107	-0.095777
C	0.865026	2.202402	-1.132389
C	1.077425	1.452878	1.242332
H	0.999497	0.624931	1.950486
H	2.107339	1.802820	1.258595
H	0.433015	2.261062	1.594040
H	1.907595	2.522495	-1.145488
H	0.252408	3.054993	-0.830482
H	0.578196	1.921176	-2.146485
H	-0.341640	-1.874512	-0.675895
H	0.135441	-1.341827	0.948722
C	1.310315	-0.315036	-0.593826
H	1.352300	-0.371007	-1.686528
C	2.676859	-0.707365	-0.094885
C	2.914877	-2.177477	0.138762
H	2.548792	-2.760348	-0.707573
H	2.348534	-2.499921	1.014531
H	3.972206	-2.362583	0.302237
O	3.537483	0.119491	0.085467
O	-3.129107	-0.999202	-0.256458
O	-4.494857	-0.525619	-0.538335
Rotational constants (GHz):			
Vibrational harmonic frequencies (cm-1):			
1561.6942	34.9450	41.9898	
65.2814	103.5931	108.4655	
133.0674	160.8611	189.9955	
223.1797	255.7739	274.7381	
310.7727	320.8450	344.7473	
352.7424	406.5110	410.4974	
506.8882	515.9110	574.8352	
612.3204	661.1704	733.2395	
768.8132	818.7328	844.1489	

884.8001	904.0531	928.9351
961.6714	967.3089	983.0680
1000.6765	1012.8562	1032.0027
1044.2952	1083.4636	1123.2191
1152.0149	1178.2199	1200.6073
1211.1427	1235.0005	1250.3619
1259.9040	1290.7050	1315.3392
1336.0885	1359.6074	1376.0468
1393.5077	1404.4477	1414.9962
1418.5997	1436.5556	1463.8708
1477.3176	1485.0512	1494.8895
1500.7111	1507.6665	1514.9202
1599.7421	1831.4976	3017.9508
3047.1211	3049.7121	3052.9175
3065.0933	3067.6392	3074.7339
3092.1846	3112.0175	3115.6137
3126.5799	3130.2026	3149.3780
3153.4317	3163.8239	3180.6700

Zero-point correction (Hartree): 0.244694

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.12697563

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.386875  | 0.638321  | 1.142377  |
| H | 0.202927  | 1.290241  | 1.997950  |
| C | 1.887574  | 0.613730  | 0.896073  |
| C | 2.401912  | -0.391465 | -0.053660 |
| H | 2.270843  | 1.592613  | 0.599453  |
| H | 2.410858  | 0.360298  | 1.830600  |
| H | 1.949393  | -1.373186 | -0.157910 |
| C | -0.585423 | 1.064552  | 0.003142  |
| C | -0.432255 | -0.656136 | 1.335749  |
| C | -0.983320 | 2.526631  | -0.027959 |
| C | -0.108672 | 0.609666  | -1.370614 |
| H | 0.114443  | -0.459640 | -1.404008 |
| H | -0.878268 | 0.798851  | -2.116502 |
| H | 0.791347  | 1.155335  | -1.663000 |
| H | -1.796339 | 2.681215  | -0.738084 |
| H | -0.141203 | 3.150278  | -0.336196 |
| H | -1.316233 | 2.864991  | 0.954345  |
| H | -0.581558 | -1.009811 | 2.352933  |
| H | -0.063096 | -1.482010 | 0.728853  |
| C | -1.599976 | 0.074513  | 0.637712  |
| H | -2.200535 | 0.600966  | 1.386491  |
| C | -2.570943 | -0.668157 | -0.245319 |
| C | -2.921694 | -2.077082 | 0.158108  |
| H | -3.139123 | -2.124584 | 1.226070  |
| H | -2.063494 | -2.727715 | -0.021344 |
| H | -3.769208 | -2.430267 | -0.421373 |
| O | -3.050991 | -0.138287 | -1.217200 |
| O | 3.408395  | -0.130463 | -0.768833 |
| O | 4.063192  | -1.393126 | -0.397958 |

Rotational constants (GHz): 1.2814500 0.4443800 0.4032000

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i551.3966 | 32.5846   | 56.0346   |
| 58.3890   | 86.5106   | 131.7294  |
| 151.1936  | 169.2717  | 191.0800  |
| 232.0537  | 263.7830  | 275.4524  |
| 313.7837  | 321.7989  | 325.4290  |
| 366.9130  | 408.6132  | 415.3989  |
| 473.4017  | 516.5535  | 587.5164  |
| 618.1228  | 647.0592  | 717.0954  |
| 747.2564  | 796.6081  | 835.7799  |
| 889.2167  | 899.5883  | 926.2986  |
| 962.6262  | 970.6819  | 989.2666  |
| 1007.4531 | 1020.4754 | 1041.0259 |
| 1041.9657 | 1117.7817 | 1126.2567 |
| 1142.9621 | 1178.5962 | 1193.3543 |
| 1210.1743 | 1239.4122 | 1248.1415 |
| 1262.2228 | 1295.3423 | 1316.9871 |
| 1326.4305 | 1359.1674 | 1385.6354 |
| 1394.2730 | 1404.0752 | 1413.7725 |
| 1419.8425 | 1424.2045 | 1464.2382 |
| 1477.5677 | 1483.5647 | 1495.3474 |
| 1502.5717 | 1506.1389 | 1515.5282 |
| 1602.5930 | 1832.5318 | 3007.0210 |
| 3046.7734 | 3049.0768 | 3052.7819 |
| 3064.0195 | 3078.5194 | 3094.7287 |
| 3095.8594 | 3109.5892 | 3116.0009 |
| 3125.5301 | 3130.3044 | 3146.3304 |
| 3149.2558 | 3173.8071 | 3181.4210 |

Zero-point correction (Hartree): 0.244784

ApineneCI.J.a.ringclose.mtmm

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.13006980

Electronic state : 1-A

Cartesian coordinates (Angs):

C	0.576743	1.168491	0.877002
H	0.399425	2.044729	1.500320
C	2.075203	1.179022	0.476107
C	2.594412	-0.191867	0.317431
H	2.211252	1.739301	-0.448761
H	2.648769	1.647912	1.277925
H	2.826807	-0.792879	1.193484
C	-0.514529	1.128488	-0.229028
C	-0.066945	-0.072797	1.533740
C	-1.120361	2.463410	-0.612497
C	-0.099430	0.350774	-1.470826
H	0.357092	-0.612001	-1.236755

H	-0.973261	0.176286	-2.100119
H	0.619739	0.924297	-2.058362
H	-2.006207	2.307550	-1.229746
H	-0.407512	3.060570	-1.186300
H	-1.416288	3.033105	0.269340
H	-0.116668	-0.098500	2.620068
H	0.378171	-0.998299	1.169570
C	-1.357575	0.259872	0.765090
H	-2.017182	0.911976	1.338665
C	-2.212663	-0.811594	0.128745
C	-1.762329	-2.244303	0.221760
H	-1.639557	-2.528806	1.268561
H	-0.784630	-2.361079	-0.252291
H	-2.490488	-2.888552	-0.261159
O	-3.213803	-0.489767	-0.465953
O	2.826590	-0.699053	-0.817645
O	2.104136	-1.929005	-0.455099
Rotational constants (GHz):		1.1234700	0.6262600 0.5051900
Vibrational harmonic frequencies (cm-1):			
i550.7924	45.1276	56.0530	
83.7705	116.9711	145.7739	
173.3680	201.9704	215.5389	
235.1364	257.3524	285.2131	
327.8919	346.5546	365.5736	
391.8009	446.5130	451.9477	
485.3483	509.1694	588.0469	
609.5840	624.0201	720.5092	
760.8419	837.2973	878.6087	
902.7023	915.6883	933.6661	
968.1442	969.7291	998.9550	
1003.5027	1019.5262	1026.7828	
1053.5121	1097.8916	1130.3757	
1152.4414	1177.0112	1199.6131	
1219.0950	1244.0629	1257.0573	
1261.3266	1288.1709	1291.8078	
1327.1611	1360.3280	1379.0812	
1393.9098	1395.6872	1407.8593	
1429.1124	1467.2234	1472.5577	
1476.5256	1487.8219	1495.3872	
1503.7516	1516.1534	1525.5675	
1598.9199	1824.5349	3044.9947	
3054.1939	3057.6824	3067.0537	
3090.7849	3092.8373	3094.1884	
3114.0029	3116.1969	3121.9546	
3128.5842	3130.7040	3138.2012	
3150.0693	3158.9184	3181.2376	
Zero-point correction (Hartree): 0.246211			
ApineneCI.J.a.ringclose.mttm			
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E(RM062X/Aug-CC-pVT2) (Hartree): -616.13252420			
Electronic state : 1-A			
Cartesian coordinates (Angs):			
C	0.607508	1.146053	0.838569
H	0.480063	1.949400	1.565273
C	2.051767	1.259721	0.303783
C	2.508592	0.071358	-0.444119
H	2.149218	2.151309	-0.315658
H	2.717828	1.341469	1.168243
H	2.624225	0.063093	-1.524288
C	-0.595931	1.173724	-0.143612
C	0.097075	-0.183991	1.424359
C	-1.301719	2.506498	-0.295181
C	-0.279212	0.576799	-1.507668
H	0.195208	-0.404017	-1.430698
H	-1.196171	0.465110	-2.086713
H	0.385758	1.240683	-2.066566
H	-2.243761	2.372778	-0.828452
H	-0.686082	3.209425	-0.862006
H	-1.520873	2.949735	0.677016
H	0.152554	-0.302359	2.503796
H	0.559791	-1.044021	0.944902
C	-1.279054	0.139911	0.811779
H	-1.925759	0.669914	1.512587
C	-2.114550	-0.922704	0.134140
C	-1.628005	-2.345059	0.166099
H	-1.448214	-2.656371	1.196777
H	-0.666945	-2.418795	-0.349830
H	-2.358298	-2.994743	-0.306195
O	-3.127723	-0.599500	-0.439797
O	2.860608	-0.965513	0.193699
O	2.064944	-1.825797	-0.694786
Rotational constants (GHz):		1.1064000	0.6540500 0.5054000
Vibrational harmonic frequencies (cm-1):			
i557.5994	46.1895	56.6682	
89.3691	144.9471	147.4893	
171.5298	185.4685	214.4973	
233.2451	255.1473	289.6013	
326.2503	341.3604	363.6292	
400.6035	439.9253	460.0060	
489.6315	499.0007	597.0887	
613.9837	647.8216	718.8256	
759.3567	844.3286	873.9274	
886.9327	914.2451	945.4908	
965.9943	974.1615	994.3095	
1003.4660	1017.0324	1031.1447	
1053.9265	1059.1490	1133.5506	
1151.4070	1172.4190	1199.8678	
1214.9288	1245.5405	1254.4933	
1261.0259	1289.6500	1298.8820	
1333.7578	1359.6602	1373.7621	
1394.6232	1396.0833	1406.9214	

1421.1013	1466.1020	1467.2840
1476.2781	1488.0035	1496.9285
1507.4212	1514.0116	1526.3541
1589.4670	1823.1985	3040.9099
3045.1095	3050.3869	3055.7469
3083.9280	3088.5325	3106.5998
3109.4201	3113.4439	3115.7882
3121.8947	3129.0430	3131.3050
3167.3865	3173.1088	3181.5126

Zero-point correction (Hartree): 0.246116

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.12667166

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.487748  | 0.843240  | 1.013826  |
| H | 0.303524  | 1.465807  | 1.890948  |
| C | 1.961242  | 1.046679  | 0.629867  |
| C | 2.502049  | 0.095039  | -0.366113 |
| H | 2.104111  | 2.065583  | 0.269749  |
| H | 2.581835  | 0.911873  | 1.521955  |
| H | 2.907553  | 0.422177  | -1.319435 |
| C | -0.625376 | 1.140679  | -0.029716 |
| C | -0.129896 | -0.548272 | 1.257927  |
| C | -1.210050 | 2.538855  | -0.010728 |
| C | -0.213588 | 0.749659  | -1.443626 |
| H | 0.159534  | -0.275719 | -1.500557 |
| H | -1.063053 | 0.825146  | -2.119691 |
| H | 0.567955  | 1.422501  | -1.806548 |
| H | -2.093532 | 2.586614  | -0.648188 |
| H | -0.485385 | 3.267814  | -0.381200 |
| H | -1.499712 | 2.830617  | 0.999745  |
| H | -0.136362 | -0.921392 | 2.278917  |
| H | 0.295773  | -1.308978 | 0.607384  |
| C | -1.441558 | 0.025277  | 0.679586  |
| H | -2.040007 | 0.467296  | 1.482609  |
| C | -2.378203 | -0.836559 | -0.129446 |
| C | -2.497389 | -2.281885 | 0.277343  |
| H | -2.609923 | -2.364759 | 1.359247  |
| H | -1.576755 | -2.805791 | 0.012777  |
| H | -3.337006 | -2.744777 | -0.232181 |
| O | -3.008309 | -0.370576 | -1.047434 |
| O | 2.500934  | -1.146172 | -0.129959 |
| O | 3.906321  | -1.293287 | -0.533740 |

Rotational constants (GHz): 1.1861800 0.5168700 0.4348000

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| 1540.4483 | 34.4924   | 58.4784   |
| 68.9180   | 78.2155   | 135.1956  |
| 153.1686  | 168.0646  | 177.5085  |
| 227.6713  | 255.1113  | 273.2912  |
| 315.3194  | 327.5844  | 344.7445  |
| 395.0332  | 408.9134  | 426.4651  |
| 491.9462  | 516.4872  | 591.1706  |
| 620.5002  | 710.5995  | 726.2096  |
| 737.8577  | 827.2172  | 840.1721  |
| 875.1505  | 899.6155  | 927.4839  |
| 963.3266  | 970.5049  | 981.9368  |
| 999.8506  | 1014.0492 | 1038.3840 |
| 1055.8270 | 1066.8023 | 1133.9998 |
| 1142.6641 | 1174.8984 | 1194.2433 |
| 1210.5909 | 1238.9373 | 1247.0134 |
| 1262.4742 | 1292.7905 | 1305.8526 |
| 1331.8566 | 1360.6085 | 1377.6860 |
| 1394.7256 | 1400.6239 | 1411.7943 |
| 1420.2536 | 1464.7290 | 1472.0439 |
| 1476.7679 | 1484.1055 | 1495.8116 |
| 1502.7875 | 1507.5937 | 1518.4392 |
| 1590.7631 | 1831.0341 | 3043.5018 |
| 3046.8901 | 3049.2586 | 3052.3602 |
| 3064.2467 | 3080.0352 | 3105.5033 |
| 3110.3871 | 3113.8168 | 3118.5634 |
| 3125.8720 | 3130.2498 | 3146.6556 |
| 3164.0691 | 3168.0832 | 3181.3741 |

Zero-point correction (Hartree): 0.245243

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.13496293

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-0.498611	0.922124	0.777662
H	-0.781354	0.831740	1.828629
C	-1.693213	1.474669	-0.021206
C	-2.835455	0.554579	0.104316
H	-1.968638	2.436134	0.421467
H	-1.434743	1.608900	-1.069523
H	-3.316189	0.393702	1.067290
C	0.206665	-0.390633	0.330961
C	0.835328	1.676367	0.642224
C	-0.141495	-1.628570	1.133750
C	0.072568	-0.659895	-1.161859
H	0.330478	0.211454	-1.765232
H	0.740568	-1.470621	-1.459172
H	-0.947756	-0.971388	-1.392328
H	0.512880	-2.461300	0.867430
H	-1.170261	-1.927310	0.922573
H	-0.037648	-1.444711	2.204452
H	1.075004	2.414987	1.402903
H	0.958004	2.120564	-0.344965
C	1.559719	0.327188	0.700526
H	1.849291	0.046770	1.714756

C	2.706526	0.093088	-0.246746
C	3.462069	-1.197933	-0.061174
H	2.762473	-2.032329	0.012776
H	4.013583	-1.160032	0.880037
H	4.151930	-1.353139	-0.885258
O	2.977391	0.874740	-1.125013
O	-3.299264	-0.062235	-0.896326
O	-3.275908	-1.346172	-0.178231

Rotational constants (GHz): 1.5503000 0.4717900 0.4305400

Vibrational harmonic frequencies (cm-1):

i561.4233	48.6792	66.2929
68.3392	93.4378	119.7280
154.4797	168.2177	206.9924
244.7936	255.5583	282.6470
316.0066	334.1357	349.7225
378.7300	430.9389	444.5308
471.0550	535.0344	580.5200
605.7825	624.1751	721.0391
781.2150	837.4593	898.6854
905.7322	924.7349	945.3331
965.0743	969.6872	976.0399
1002.9072	1013.4130	1045.4095
1057.0519	1084.8713	1107.7083
1150.2029	1175.4828	1196.7946
1204.4708	1213.7827	1244.4960
1261.3827	1272.5788	1289.2572
1322.8351	1365.9884	1379.5722
1387.7829	1403.9380	1412.1019
1426.2575	1463.2446	1464.6203
1476.5941	1484.2904	1497.5293
1500.2941	1509.8672	1517.2359
1599.4571	1835.1560	3043.4942
3053.6933	3059.3163	3063.2049
3069.8979	3084.7635	3096.8019
3113.8413	3119.5298	3123.9407
3125.5597	3136.6054	3143.7138
3154.8181	3156.6125	3179.7648

Zero-point correction (Hartree): 0.245579

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.13135263

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.437374 | -0.617926 | -0.837537 |
| H | -0.687138 | -0.363262 | -1.870528 |
| C | -1.693995 | -1.071411 | -0.109811 |
| C | -2.755765 | -0.046542 | -0.142285 |
| H | -2.115430 | -1.947769 | -0.620744 |
| H | -1.508111 | -1.366093 | 0.923052  |
| H | -2.930841 | 0.542601  | -1.040858 |
| C | 0.413775  | 0.536902  | -0.234028 |
| C | 0.804234  | -1.525482 | -0.807281 |
| C | 0.196744  | 1.907057  | -0.846073 |
| C | 0.325900  | 0.600043  | 1.285263  |
| H | 0.515362  | -0.367710 | 1.750000  |
| H | 1.062532  | 1.302396  | 1.679776  |
| H | -0.660410 | 0.948704  | 1.598872  |
| H | 0.934659  | 2.624616  | -0.482095 |
| H | -0.790035 | 2.293985  | -0.579103 |
| H | 0.265167  | 1.869221  | -1.933931 |
| H | 0.961547  | -2.193781 | -1.649703 |
| H | 0.878560  | -2.091610 | 0.120463  |
| C | 1.675407  | -0.265716 | -0.723242 |
| H | 1.974831  | 0.102026  | -1.706403 |
| C | 2.858253  | -0.270075 | 0.209898  |
| C | 3.760392  | 0.935657  | 0.142191  |
| H | 3.166165  | 1.849659  | 0.198602  |
| H | 4.274427  | 0.949372  | -0.820513 |
| H | 4.487887  | 0.908094  | 0.947781  |
| O | 3.045529  | -1.168156 | 0.992993  |
| O | -3.443703 | 0.215565  | 0.882420  |
| O | -4.691150 | 0.183154  | 0.107434  |

Rotational constants (GHz): 1.8121800 0.3853300 0.3672200

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i562.8824 | 30.0687   | 45.7975   |
| 59.9474   | 66.1247   | 119.6379  |
| 136.4231  | 150.7221  | 215.6648  |
| 236.9364  | 256.7876  | 283.0025  |
| 292.4610  | 327.5436  | 348.4530  |
| 377.7729  | 416.2369  | 432.0186  |
| 456.5707  | 525.0008  | 577.9219  |
| 609.5596  | 624.2666  | 715.2064  |
| 770.1698  | 811.1386  | 832.6883  |
| 907.9734  | 911.3650  | 954.7668  |
| 960.1410  | 970.8791  | 976.2098  |
| 1002.0783 | 1026.2929 | 1041.3589 |
| 1067.4037 | 1110.2869 | 1111.7237 |
| 1157.6967 | 1172.6241 | 1190.1975 |
| 1195.4773 | 1211.8295 | 1250.4569 |
| 1262.0459 | 1275.5012 | 1290.3501 |
| 1329.4194 | 1369.9269 | 1380.0846 |
| 1394.9370 | 1407.0575 | 1420.5337 |
| 1426.7462 | 1438.0776 | 1465.0766 |
| 1476.0186 | 1484.3454 | 1493.6692 |
| 1500.4498 | 1508.4372 | 1511.3377 |
| 1605.1002 | 1837.0930 | 3024.3221 |
| 3042.4472 | 3052.0836 | 3062.5575 |
| 3063.1555 | 3083.4768 | 3098.7162 |
| 3106.8361 | 3116.0645 | 3121.6054 |
| 3123.1933 | 3125.3146 | 3134.3409 |
| 3147.3835 | 3156.8783 | 3180.7460 |

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Zero-point correction (Hartree): 0.244794

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.13259480
Electronic state : 1-A
Cartesian coordinates (Angs):
 C -0.577734 -0.627372 -0.647576
 H -1.024475 -0.257762 -1.570925
 C -1.642038 -1.306808 0.191844
 C -2.794826 -0.462822 0.559620
 H -2.081593 -2.146706 -0.366569
 H -1.238241 -1.755562 1.103244
 H -3.491100 -0.771543 1.335294
 C 0.296944 0.503142 -0.023129
 C 0.700337 -1.433237 -0.939947
 C -0.047246 1.923402 -0.428535
 C 0.422428 0.382747 1.489066
 H 0.724806 -0.617176 1.801976
 H 1.168294 1.083642 1.868673
 H -0.528262 0.629629 1.968017
 H 0.741094 2.613938 -0.121110
 H -0.978350 2.246414 0.037413
 H -0.167762 2.002920 -1.509396
 H 0.761814 -1.952839 -1.892633
 H 0.943670 -2.127371 -0.135548
 C 1.515633 -0.145532 -0.781319
 H 1.664527 0.377849 -1.727112
 C 2.809351 -0.206394 -0.013034
 C 3.657625 1.039284 -0.041367
 H 3.047027 1.911378 0.199897
 H 4.042804 1.191378 -1.051172
 H 4.483075 0.949913 0.658438
 O 3.125387 -1.181248 0.624492
 O -2.984607 0.656489 0.006989
 O -4.404552 0.352687 -0.230510
Rotational constants (GHz): 1.8252000 0.4230900 0.3913000
Vibrational harmonic frequencies (cm-1):
 i559.3172 38.5451 55.2426
 61.3388 77.1684 129.4088
 134.3447 156.4866 222.4574
 238.6594 262.6548 278.5751
 313.4344 327.5360 341.7863
 358.3313 380.0555 434.4579
 462.5380 564.0405 583.8875
 623.1345 667.8108 713.0934
 763.0120 814.2488 837.2853
 881.8491 906.7950 951.6633
 962.0745 968.8816 978.6781
 1000.6472 1010.0362 1029.6034
 1044.5774 1107.6009 1116.3502
 1151.6697 1165.4351 1189.5106
 1195.4112 1212.3520 1260.6463
 1261.7810 1279.0117 1307.3984
 1345.1048 1372.6387 1375.1456
 1398.5179 1407.1260 1416.5738
 1425.2789 1430.7813 1465.2072
 1476.6290 1485.4896 1492.1873
 1499.4720 1508.1308 1509.2823
 1595.1087 1833.3914 3011.1703
 3047.0551 3053.3835 3063.5997
 3080.4491 3086.7180 3092.7818
 3098.6310 3110.6773 3120.3287
 3125.8494 3130.5902 3136.5008
 3153.3550 3162.7900 3180.3085
Zero-point correction (Hartree): 0.244930

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E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -615.20966989
E(CCSD/Aug-CC-pVTZ) (Hartree): -615.08915414
  T1 diagnostic: 0.023972
E(MP2/Aug-CC-pVTZ) (Hartree): -615.01389868
E(MP3/Aug-CC-pVTZ) (Hartree): -615.07038642
E(RHF/Aug-CC-pVTZ) (Hartree): -612.58509518
E(RM062X/Aug-CC-pVTZ) (Hartree): -616.13507409
Electronic state : 1-A
Cartesian coordinates (Angs):
  C    0.548434    0.931073   -0.695885
  H    0.917872    0.799511   -1.713427
  C    1.642885    1.512259    0.177851
  C    2.831299    0.649697    0.337039
  H    2.004967    2.473050   -0.213635
  H    1.281822    1.743585    1.184614
  H    3.572735    0.852115    1.106395
  C   -0.163262   -0.382993   -0.242609
  C   -0.810268    1.652703   -0.693873
  C    0.233753   -1.655832   -0.966033
  C   -0.112991   -0.588490    1.265236
  H   -0.441769    0.293365    1.817160
  H   -0.762794   -1.415956    1.556790
  H    0.904149   -0.851915    1.567753
  H   -0.491436   -2.448039   -0.766099
  H    1.211664   -2.000039   -0.627950
  H    0.272209   -1.497774   -2.044932
  H   -1.018300    2.341842   -1.508464
  H   -1.011708    2.148538    0.255816
  C   -1.505030    0.287614   -0.724822
  H   -1.727782   -0.051027   -1.738139
  C   -2.700757    0.076575    0.165020
  C   -3.434957   -1.228341   -0.009253
  H   -2.727207   -2.058899    0.011984

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|                                           |           |           |                               |
|-------------------------------------------|-----------|-----------|-------------------------------|
| H                                         | -3.915233 | -1.244921 | -0.989195                     |
| H                                         | -4.181993 | -1.347781 | 0.769738                      |
| O                                         | -3.026208 | 0.887315  | 0.997994                      |
| O                                         | 3.049366  | -0.310707 | -0.451213                     |
| O                                         | 3.344113  | -1.234264 | 0.660164                      |
| Rotational constants (GHz):               |           |           | 1.5871200 0.4841900 0.4372800 |
| Vibrational harmonic frequencies (cm-1):  |           |           |                               |
| i555.0437                                 | 43.8578   | 63.4722   |                               |
| 71.9692                                   | 80.5031   | 125.8842  |                               |
| 145.8302                                  | 159.2510  | 225.8395  |                               |
| 256.7266                                  | 277.1998  | 285.4244  |                               |
| 318.5098                                  | 342.5045  | 345.0623  |                               |
| 376.9054                                  | 389.5642  | 435.7411  |                               |
| 458.7871                                  | 567.8273  | 582.9932  |                               |
| 622.5880                                  | 666.5383  | 716.0194  |                               |
| 775.8814                                  | 797.6445  | 844.3737  |                               |
| 905.7728                                  | 921.7888  | 935.6009  |                               |
| 957.0821                                  | 969.1257  | 978.4977  |                               |
| 983.5754                                  | 1009.1528 | 1027.7117 |                               |
| 1049.6625                                 | 1108.3675 | 1114.5637 |                               |
| 1141.7580                                 | 1169.4624 | 1189.8025 |                               |
| 1196.9489                                 | 1210.8564 | 1262.5343 |                               |
| 1265.0456                                 | 1278.5333 | 1310.9440 |                               |
| 1346.3571                                 | 1372.3720 | 1376.5409 |                               |
| 1398.0578                                 | 1407.1823 | 1416.0114 |                               |
| 1426.7393                                 | 1429.9760 | 1465.6939 |                               |
| 1476.8139                                 | 1483.7199 | 1498.9789 |                               |
| 1501.0349                                 | 1508.5814 | 1518.0767 |                               |
| 1601.5158                                 | 1832.0078 | 3022.6069 |                               |
| 3041.1052                                 | 3047.9044 | 3063.9922 |                               |
| 3071.4695                                 | 3084.7566 | 3090.6621 |                               |
| 3095.0757                                 | 3109.1137 | 3113.5661 |                               |
| 3124.0053                                 | 3126.8425 | 3136.4429 |                               |
| 3151.0705                                 | 3155.3633 | 3179.0699 |                               |
| Zero-point correction (Hartree): 0.245214 |           |           |                               |

ApineneCI.J.a.ringclose.ppm

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.13024448

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-0.544135	0.330871	-0.488280
H	-0.795332	0.841205	-1.421726
C	-1.761602	0.315240	0.416542
C	-2.964173	-0.234717	-0.240396
H	-1.600496	-0.226716	1.350674
H	-2.047508	1.338958	0.701925
H	-3.095684	-0.177934	-1.319227
C	0.793374	0.915496	0.045003
C	0.178457	-0.994659	-0.794926
C	1.103632	2.338789	-0.374504
C	0.953169	0.744567	1.550053
H	0.767217	-0.280480	1.871093
H	1.968269	1.003968	1.856706
H	0.268508	1.406540	2.082781
H	2.113323	2.627936	-0.076557
H	0.410026	3.036016	0.101082
H	1.018573	2.459272	-1.455002
H	-0.080583	-1.515023	-1.713636
H	0.128026	-1.693305	0.039948
C	1.508711	-0.231831	-0.760433
H	1.799089	0.147408	-1.741872
C	2.690868	-0.875145	-0.083388
C	4.006716	-0.152430	-0.219661
H	3.879671	0.903802	0.025238
H	4.339367	-0.200371	-1.258092
H	4.753433	-0.603430	0.426892
O	2.578594	-1.886095	0.564781
O	-3.856709	-0.812757	0.437182
O	-4.923885	-0.051764	-0.223247

Rotational constants (GHz):			1.7030600 0.3628100 0.3337400
Vibrational harmonic frequencies (cm-1):			
i561.4358	36.6093	52.4665	

57.6681	81.0610	112.1846	
119.7573	154.2564	199.9880	
230.9689	255.3127	286.5170	
293.8583	323.9460	347.0932	
365.0692	403.8305	412.3986	
462.6803	527.1467	586.9663	
600.8905	624.0066	732.6743	
764.6510	819.1823	839.2755	
894.9636	918.2530	933.1467	
959.5357	965.6450	981.1704	
1002.5228	1020.1945	1043.1062	
1075.6323	1102.5458	1131.7496	
1152.3872	1176.0955	1197.0769	
1206.8982	1216.2291	1239.6354	
1263.8894	1276.6848	1300.0352	
1326.1455	1370.3220	1381.8879	
1397.1388	1408.1582	1423.0943	
1425.3851	1427.9790	1464.0351	
1476.3117	1486.4045	1494.1739	
1499.9543	1509.1765	1511.2692	
1605.1008	1836.9048	3006.4163	
3046.2951	3053.9491	3060.4931	
3062.5910	3084.1147	3094.6168	
3101.4822	3111.3786	3118.5475	
3124.0636	3126.0935	3135.4440	
3150.6359	3152.7574	3180.0482	

Zero-point correction (Hartree): 0.244676

ApineneCI.J.a.ringclose.pmp

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.13207372
Electronic state : 1-A
Cartesian coordinates (Angs):
C      -0.721409      0.583512      -0.335619
H      -1.024587      0.916893      -1.329892
C      -1.800142      0.988465      0.691929
C      -3.042618      0.370516      0.208447
H      -1.540959      0.574904      1.666881
H      -1.896604      2.072752      0.742569
H      -3.741733      0.900793      -0.433456
C       0.749470      1.019894      -0.084779
C      -0.274102      -0.884019      -0.385651
C       1.214551      2.237521      -0.858346
C       1.086729      1.148510      1.393223
H       0.796237      0.263929      1.959808
H       2.161884      1.282375      1.527455
H       0.589266      2.020472      1.822004
H       2.289938      2.389098      -0.746283
H       0.717066      3.137464      -0.489272
H       0.992651      2.137527      -1.921232
H      -0.759482      -1.524077      -1.115679
H      -0.319677      -1.359896      0.593375
C       1.151168      -0.387708      -0.667564
H       1.354251      -0.286157      -1.734974
C       2.307440      -1.067665      0.018720
C       3.683166      -0.681019      -0.463085
H       3.772643      0.406544      -0.499619
H       3.825489      -1.045959      -1.481749
H       4.443436      -1.101217      0.188462
O       2.142736      -1.838824      0.931178
O      -3.302804      -0.832268      0.496759
O      -3.563098      -1.173093      -0.909443
Rotational constants (GHz):      1.3690900      0.4675500      0.4089100
Vibrational harmonic frequencies (cm-1):
i546.8501      45.4903      52.2436
65.5901      88.6425      123.8074
127.1431      150.1389      186.0364
224.3793      237.0296      285.2014
313.3164      331.5178      348.8230
377.5768      422.1187      471.6425
489.6041      529.9286      585.0192
601.4528      624.6158      733.1799
784.0736      828.5196      884.3269
916.2107      928.8025      936.9781
959.1128      964.9756      980.0122
1001.3172      1014.8557      1025.5022
1048.2402      1082.5118      1120.7032
1151.9732      1171.5472      1191.0822
1200.1261      1208.8755      1240.8827
1260.7110      1269.1226      1288.6786
1324.4761      1364.0854      1376.8620
1385.5578      1403.0397      1412.8247
1423.9039      1464.2306      1475.8797
1476.8385      1485.8527      1492.2452
1499.5597      1507.8715      1510.1893
1593.9479      1837.2156      3045.7083
3052.3017      3062.2427      3075.0451
3080.5809      3086.8715      3106.4540
3109.8716      3116.1877      3124.0291
3126.4636      3135.7474      3141.1172
3162.0633      3173.9590      3179.7282
Zero-point correction (Hartree): 0.245328

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ApineneCI.J.a.ringclose.pppm
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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.13227980
Electronic state : 1-A
Cartesian coordinates (Angs):
C      -0.736242      0.235308      -0.137994
H      -1.199707      0.452813      -1.101451
C      -1.764065      0.530286      0.974049
C      -2.929685      -0.300324      0.639591
H      -1.355198      0.259309      1.946130
H      -2.045183      1.584319      0.946004
H      -3.027331      -1.324875      0.989690
C       0.656339      0.921041      -0.066224
C      -0.049295      -1.138428      -0.184146
C       0.822283      2.154968      -0.930412
C       1.116778      1.185278      1.359942
H       1.041776      0.298072      1.988910
H       2.160596      1.504834      1.370446
H       0.522767      1.984132      1.807554
H       1.861143      2.490722      -0.943281
H       0.216796      2.976745      -0.541567
H       0.511587      1.961179      -1.957221
H      -0.479972      -1.886023      -0.844272
H       0.096861      -1.566205      0.807945
C       1.233207      -0.429045      -0.637901
H       1.306412      -0.354527      -1.723977
C       2.549596      -0.874139      -0.056366
C       3.784482      -0.270329      -0.675053
H       3.675757      0.814017      -0.740685
H       3.895134      -0.640646      -1.695732
H       4.663757      -0.527997      -0.092366
O       2.607284      -1.633523      0.879289
O      -3.828272      0.151268      -0.124870
O      -3.772210      -1.031941      -0.995549
Rotational constants (GHz):      1.5312800      0.4176100      0.3870200
Vibrational harmonic frequencies (cm-1):
i542.0092      38.5880      52.8352
62.7234      86.1513      105.4555

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119.7711	147.3812	197.3890
219.3938	239.2322	285.4503
311.8691	327.1689	351.3863
375.1998	421.0186	452.2923
492.3244	533.4659	586.3966
601.8347	625.5263	734.5974
779.3838	828.3306	891.3986
911.8949	929.9697	942.8173
959.6267	965.6527	981.2557
1001.3178	1014.9818	1025.8857
1056.2166	1074.3953	1133.1333
1146.9885	1172.0519	1192.1302
1208.4827	1216.6704	1228.7921
1261.2259	1272.2695	1289.9204
1328.3375	1363.8934	1377.4401
1386.6820	1403.8441	1412.5081
1424.2824	1464.3783	1475.8011
1476.3901	1486.0247	1492.1929
1499.2564	1508.6447	1510.6803
1597.8200	1835.8646	3047.1457
3053.3529	3062.9412	3075.9718
3087.5358	3089.0837	3096.6123
3111.2069	3117.7520	3124.7370
3128.7658	3134.2607	3144.7177
3160.9085	3167.5044	3180.2886

Zero-point correction (Hartree): 0.245311

ApineneCI.J.a.ringclose.pppp

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.13010011

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.531501 | 0.441777  | -0.530579 |
| H | -0.725316 | 0.963336  | -1.470485 |
| C | -1.768889 | 0.508505  | 0.349014  |
| C | -2.927561 | -0.180924 | -0.250724 |
| H | -1.588842 | -0.022269 | 1.294580  |
| H | -2.063621 | 1.525757  | 0.614681  |
| H | -2.793626 | -1.055493 | -0.883962 |
| C | 0.828697  | 0.942207  | 0.034336  |
| C | 0.114035  | -0.928513 | -0.817716 |
| C | 1.239202  | 2.341133  | -0.381297 |
| C | 0.943761  | 0.765147  | 1.542125  |
| H | 0.687402  | -0.245752 | 1.860208  |
| H | 1.966671  | 0.959182  | 1.870408  |
| H | 0.291780  | 1.470590  | 2.059741  |
| H | 2.261450  | 2.562485  | -0.068567 |
| H | 0.586296  | 3.083796  | 0.082487  |
| H | 1.179290  | 2.464270  | -1.463181 |
| H | -0.151677 | -1.433795 | -1.742654 |
| H | -0.000299 | -1.622031 | 0.015556  |
| C | 1.488032  | -0.250022 | -0.752597 |
| H | 1.823635  | 0.106767  | -1.727996 |
| C | 2.611696  | -0.964752 | -0.047987 |
| C | 3.973455  | -0.327462 | -0.156615 |
| H | 3.908241  | 0.736198  | 0.080204  |
| H | 4.326111  | -0.402882 | -1.186796 |
| H | 4.675054  | -0.820918 | 0.509176  |
| O | 2.420877  | -1.964429 | 0.599122  |
| O | -4.098372 | 0.255384  | -0.076261 |
| O | -4.598519 | -1.084932 | 0.255744  |

Rotational constants (GHz): 1.6087000 0.3745900 0.3380100

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i568.7068 | 34.4165   | 48.9064   |
| 54.0096   | 89.1562   | 90.3057   |
| 125.8244  | 153.9328  | 205.4196  |
| 226.8559  | 253.1857  | 283.9072  |
| 304.9058  | 325.9953  | 347.3693  |
| 369.3656  | 407.5099  | 421.8988  |
| 467.6366  | 515.0103  | 587.9751  |
| 601.8527  | 624.1345  | 739.1226  |
| 779.8776  | 810.3677  | 839.2680  |
| 891.0965  | 917.0972  | 931.5812  |
| 959.5748  | 965.0728  | 982.5668  |
| 1002.1100 | 1015.0260 | 1038.8424 |
| 1076.1279 | 1111.0470 | 1140.3947 |
| 1145.7735 | 1171.5120 | 1195.6105 |
| 1200.6324 | 1210.5807 | 1254.8342 |
| 1264.7191 | 1272.1178 | 1307.8856 |
| 1327.3153 | 1367.7635 | 1380.4422 |
| 1393.4792 | 1405.3824 | 1417.2270 |
| 1425.0964 | 1432.0312 | 1464.7594 |
| 1477.5150 | 1486.2468 | 1493.3161 |
| 1499.4879 | 1509.1715 | 1510.8605 |
| 1605.6779 | 1837.4139 | 3018.0945 |
| 3047.1489 | 3054.1973 | 3062.6648 |
| 3066.5602 | 3084.2981 | 3093.1239 |
| 3100.0504 | 3112.8190 | 3119.3867 |
| 3124.3523 | 3126.1491 | 3133.2166 |
| 3151.9630 | 3153.8113 | 3179.3003 |

Zero-point correction (Hartree): 0.244727

ApineneCI.J.a.ringclose.pptm

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.13041820

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-0.678674	0.541637	-0.332054
H	-0.972027	0.910735	-1.316633
C	-1.763570	0.868481	0.672327
C	-3.095912	0.335110	0.318136
H	-1.535034	0.447633	1.660501

H	-1.879260	1.945058	0.846216
H	-3.963254	0.552546	0.936531
C	0.780918	0.992287	-0.044073
C	-0.188510	-0.913256	-0.448547
C	1.235096	2.253198	-0.753087
C	1.097665	1.060652	1.443985
H	0.810153	0.149015	1.968371
H	2.169418	1.199191	1.599225
H	0.586153	1.907603	1.904964
H	2.305513	2.420109	-0.617249
H	0.714396	3.126101	-0.352246
H	1.031155	2.198017	-1.822872
H	-0.635027	-1.529378	-1.222738
H	-0.240230	-1.442365	0.502725
C	1.229561	-0.375899	-0.681076
H	1.448290	-0.221798	-1.739243
C	2.388627	-1.061996	-0.007327
C	3.763683	-0.617593	-0.438520
H	3.826280	0.472242	-0.417935
H	3.936105	-0.926156	-1.471110
H	4.520912	-1.052167	0.207128
O	2.225436	-1.884383	0.859970
O	-3.271476	-0.337858	-0.733350
O	-4.046066	-1.359274	-0.007147
Rotational constants (GHz): 1.4319200 0.4382400 0.3855400			
Vibrational harmonic frequencies (cm-1):			
i566.6602	36.7592	46.5712	
57.7905	86.2866	126.0577	
129.2471	155.0382	193.6326	
224.9641	241.7799	284.5065	
315.1254	330.0115	348.1844	
353.7397	382.8328	431.3242	
471.7641	557.8667	586.5062	
621.4457	649.5224	741.1575	
780.7540	817.6912	844.7849	
885.0486	911.0574	933.6177	
958.5370	964.8021	977.5645	
995.6387	1003.5473	1026.6904	
1046.2087	1085.1820	1132.9159	
1144.5367	1173.0526	1196.6307	
1205.1366	1211.3868	1252.7321	
1265.0904	1276.6573	1322.4177	
1344.0309	1372.4336	1375.6403	
1398.0455	1406.1022	1413.8825	
1423.7756	1432.7592	1464.2919	
1476.4397	1486.3314	1493.0778	
1498.5873	1508.3861	1510.5652	
1602.8072	1836.3000	3025.8295	
3044.8354	3051.9117	3052.7016	
3062.0093	3079.0275	3083.9562	
3102.1208	3108.9280	3115.8079	
3123.5478	3125.3838	3132.6267	
3161.8269	3168.2355	3179.4873	
Zero-point correction (Hartree): 0.244779			
ApineneCI.J.a.ringclose.pptp			
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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.13128260			
Electronic state : 1-A			
Cartesian coordinates (Angs):			
C	-0.696227	0.271670	-0.196797
H	-1.114487	0.577771	-1.156534
C	-1.743490	0.455796	0.880705
C	-3.013190	-0.252677	0.613780
H	-1.391755	0.152318	1.871186
H	-2.030589	1.512439	0.988489
H	-3.774166	-0.342180	1.384725
C	0.700631	0.930093	-0.021682
C	-0.014195	-1.100789	-0.342185
C	0.914590	2.229155	-0.773441
C	1.114612	1.071801	1.437142
H	1.002656	0.138750	1.990044
H	2.162720	1.368758	1.509583
H	0.519559	1.843907	1.928256
H	1.956489	2.551161	-0.719036
H	0.302792	3.024943	-0.342262
H	0.642648	2.124980	-1.824125
H	-0.420669	-1.784268	-1.082344
H	0.086186	-1.617751	0.612413
C	1.291917	-0.371594	-0.681751
H	1.410467	-0.206028	-1.753883
C	2.579805	-0.879836	-0.089744
C	3.843999	-0.241677	-0.606984
H	3.747025	0.845597	-0.589152
H	3.993386	-0.529941	-1.649029
H	4.696591	-0.555694	-0.012370
O	2.594495	-1.716138	0.779891
O	-3.230411	-0.803629	-0.499636
O	-4.571530	-0.202285	-0.589032
Rotational constants (GHz): 1.6108700 0.4008500 0.3711100			
Vibrational harmonic frequencies (cm-1):			
i561.0056	36.1778	53.3683	
63.0813	94.7634	115.8494	
127.1280	152.4059	199.2614	
224.2409	248.5609	284.5699	
317.2696	329.2413	343.7412	
352.4443	381.5875	433.6242	
471.0464	555.6963	586.8722	
623.0772	648.3663	740.5186	
766.6441	823.6534	850.6251	
883.0687	910.7761	935.2527	
957.4658	964.5144	979.5684	

1001.0586	1009.9083	1025.8391
1043.4382	1087.1553	1130.1558
1148.9517	1175.2599	1196.2475
1207.8280	1216.8212	1245.6348
1262.5878	1278.6875	1326.0666
1333.3948	1372.7221	1377.4333
1399.3072	1407.6054	1416.5703
1424.2238	1435.9936	1464.6789
1476.3234	1486.7872	1493.4937
1500.7318	1509.5088	1511.3956
1599.3206	1835.5234	3010.7378
3045.3925	3051.6402	3062.4672
3074.4239	3086.2025	3090.6796
3097.4741	3109.7112	3115.8492
3124.0556	3126.3416	3132.1013
3159.6327	3166.6448	3179.8335

Zero-point correction (Hartree): 0.244876

ApineneCI.J.a.ringclose.ptmm

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.12942888

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.379809  | 0.902835  | 1.005182  |
| H | 0.189577  | 1.751198  | 1.664623  |
| C | 1.867995  | 0.894576  | 0.687790  |
| C | 2.407458  | -0.298057 | 0.005037  |
| H | 2.175746  | 1.779903  | 0.127131  |
| H | 2.440316  | 0.921600  | 1.627366  |
| H | 2.037384  | -1.298483 | 0.210759  |
| C | -0.657382 | 0.959835  | -0.151597 |
| C | -0.343292 | -0.335905 | 1.570566  |
| C | -1.167097 | 2.341553  | -0.511337 |
| C | -0.197615 | 0.210039  | -1.394358 |
| H | 0.117159  | -0.810803 | -1.172138 |
| H | -1.008839 | 0.140392  | -2.121750 |
| H | 0.629033  | 0.735643  | -1.876747 |
| H | -1.989624 | 2.286708  | -1.226986 |
| H | -0.372265 | 2.932695  | -0.971778 |
| H | -1.518801 | 2.874383  | 0.372759  |
| H | -0.443987 | -0.406328 | 2.650244  |
| H | 0.038916  | -1.280229 | 1.187595  |
| C | -1.582790 | 0.078982  | 0.766028  |
| H | -2.249927 | 0.731269  | 1.332261  |
| C | -2.375452 | -0.994526 | 0.066596  |
| C | -3.667471 | -0.554942 | -0.573099 |
| H | -3.496501 | 0.331101  | -1.187529 |
| H | -4.378021 | -0.270150 | 0.204865  |
| H | -4.082441 | -1.357760 | -1.174981 |
| O | -1.973790 | -2.129091 | -0.012340 |
| O | 3.335629  | -0.172925 | -0.841345 |
| O | 4.129073  | -1.233918 | -0.205134 |

Rotational constants (GHz): 1.3433600 0.4542700 0.4098000

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i552.0063 | 47.9816   | 49.7380   |
| 67.9933   | 93.2924   | 117.5260  |
| 144.6181  | 160.2885  | 200.3456  |
| 235.7391  | 249.5880  | 282.3849  |
| 301.6414  | 331.9568  | 351.7244  |
| 372.2610  | 401.6160  | 416.9650  |
| 440.0326  | 570.1312  | 586.4889  |
| 621.3215  | 646.0300  | 714.7905  |
| 755.2154  | 804.6162  | 835.5593  |
| 887.2234  | 914.2979  | 947.0990  |
| 960.7918  | 969.2610  | 972.3863  |
| 999.5678  | 1011.8771 | 1035.3142 |
| 1050.8263 | 1120.2242 | 1126.6877 |
| 1151.3384 | 1170.9599 | 1193.5119 |
| 1202.6725 | 1212.6956 | 1251.8650 |
| 1262.0520 | 1284.8929 | 1314.6271 |
| 1336.7441 | 1370.7419 | 1384.9618 |
| 1396.8390 | 1406.7943 | 1418.2332 |
| 1422.5772 | 1427.1314 | 1464.5086 |
| 1476.4874 | 1486.3602 | 1493.3250 |
| 1502.1908 | 1507.9837 | 1513.1573 |
| 1602.0480 | 1836.8241 | 3006.6242 |
| 3046.4566 | 3051.0492 | 3062.5439 |
| 3078.1869 | 3084.4139 | 3096.3739 |
| 3108.2188 | 3111.8240 | 3115.9418 |
| 3124.0000 | 3125.4308 | 3127.0846 |
| 3160.9258 | 3176.8026 | 3179.3949 |

Zero-point correction (Hartree): 0.244999

ApineneCI.J.a.ringclose.ptmp

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.12891176

Electronic state : 1-A

Cartesian coordinates (Angs):

C	0.553527	1.124654	0.890521
H	0.334082	2.031501	1.455596
C	2.060549	1.146214	0.560370
C	2.634701	-0.200884	0.367236
H	2.245327	1.756430	-0.324052
H	2.588938	1.580038	1.414033
H	2.766520	-0.864381	1.218305
C	-0.487179	1.017327	-0.256965
C	-0.114814	-0.079492	1.584715
C	-1.027336	2.339383	-0.766450
C	-0.019500	0.134916	-1.406362
H	0.385110	-0.822076	-1.072886
H	-0.847129	-0.066139	-2.089423
H	0.759212	0.640485	-1.980843

H	-1.844829	2.185987	-1.473366
H	-0.244316	2.892176	-1.290998
H	-1.394971	2.961226	0.051057
H	-0.190246	-0.065113	2.668953
H	0.294822	-1.036191	1.259788
C	-1.377352	0.232189	0.771442
H	-2.037006	0.937117	1.283132
C	-2.190253	-0.919308	0.238110
C	-3.426838	-0.549058	-0.543191
H	-3.182268	0.189161	-1.308484
H	-4.152320	-0.085868	0.128145
H	-3.861017	-1.434157	-0.998425
O	-1.861854	-2.065103	0.413173
O	3.068550	-0.587480	-0.754953
O	2.386688	-1.881897	-0.605356
Rotational constants (GHz): 1.1768000 0.5722900 0.4872100			
Vibrational harmonic frequencies (cm-1):			
i573.1873	39.8208		58.3751
69.5980	103.7361		114.4092
142.6099	179.0012		209.8384
219.6204	245.0984		284.0588
313.4122	324.6773		353.5627
382.8683	427.6126		441.0598
446.4432	570.8402		585.9142
614.9034	627.8104		724.2603
765.9729	833.7262		890.4696
906.2537	930.4516		942.5929
960.0404	968.0099		974.5905
1001.2041	1008.2439		1022.1583
1053.6553	1110.0624		1134.5327
1148.3170	1176.9485		1195.2262
1206.5371	1220.5464		1248.5115
1260.6815	1283.5829		1289.4602
1330.2590	1369.0361		1379.2266
1392.2217	1406.0495		1413.2500
1434.9564	1465.1826		1468.1656
1478.5299	1486.5162		1493.7421
1504.9727	1509.2208		1517.9563
1601.3017	1842.6238		3044.2670
3050.0280	3051.9073		3063.8969
3071.6882	3080.3924		3092.7191
3109.9817	3115.3110		3121.0095
3122.8638	3127.2854		3131.0051
3153.9647	3159.9525		3179.1358
Zero-point correction (Hartree): 0.245541			
ApineneCI.J.a.ringclose.pttm			
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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.12960300			
Electronic state : 1-A			
Cartesian coordinates (Angs):			
C	-0.622068	1.066635	-0.832979
H	-0.441042	1.852247	-1.569015
C	-2.067977	1.260658	-0.334753
C	-2.615484	0.108820	0.410888
H	-2.130771	2.163067	0.274375
H	-2.706910	1.374196	-1.215702
H	-2.752432	0.115327	1.488558
C	0.562982	1.071069	0.167490
C	-0.130261	-0.281994	-1.390278
C	1.236160	2.412619	0.382467
C	0.217584	0.408955	1.494494
H	-0.259629	-0.563724	1.359400
H	1.117535	0.259764	2.094437
H	-0.450205	1.052656	2.073185
H	2.136448	2.312804	0.991539
H	0.563802	3.096636	0.906210
H	1.515778	2.871623	-0.566600
H	-0.212719	-0.442108	-2.461809
H	-0.549549	-1.136269	-0.859660
C	1.254159	0.067745	-0.823752
H	1.861091	0.635777	-1.532667
C	2.088983	-1.024835	-0.206693
C	3.459894	-0.613951	0.274506
H	3.385736	0.269570	0.910928
H	4.077881	-0.339269	-0.582150
H	3.926243	-1.430623	0.817420
O	1.678353	-2.149850	-0.080650
O	-3.022628	-0.902880	-0.229377
O	-2.328861	-1.815520	0.687927
Rotational constants (GHz): 1.1847900 0.6005400 0.4839400			
Vibrational harmonic frequencies (cm-1):			
i570.4617	45.8252		61.3613
77.9964	103.1225		125.1225
143.2614	158.6914		195.9701
222.0300	239.4751		285.9933
314.1168	340.7078		354.1334
383.1775	434.0453		438.0569
455.5825	572.9105		584.1759
623.7335	648.7894		722.6977
764.2406	836.2796		870.9776
912.5196	921.0778		950.8217
961.2885	973.2185		974.1773
994.7059	1006.8237		1032.4578
1051.8159	1061.5584		1135.8408
1148.0885	1172.4262		1195.1879
1203.9893	1216.3772		1247.8491
1261.8373	1285.2171		1296.9217
1336.8491	1369.0471		1377.1755
1393.2625	1404.5756		1413.9971
1427.3753	1464.3475		1466.9436
1477.7091	1489.1238		1492.8935

1507.8457	1515.6899	1517.5481
1596.2503	1844.4785	3039.1768
3045.3199	3050.5371	3063.3541
3071.8140	3073.3969	3101.2802
3104.8575	3109.9567	3117.0817
3123.4787	3123.9753	3126.5203
3163.4207	3170.7126	3179.2038

Zero-point correction (Hartree): 0.245509

ApineneCI.J.a.ringclose.pttp

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E(RM062X/Aug-CC-pVTZ) (Hartree): -616.12704518

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.470537  | 0.988015  | 0.886190  |
| H | 0.271632  | 1.747532  | 1.644183  |
| C | 1.910996  | 1.219552  | 0.401792  |
| C | 2.489815  | 0.127644  | -0.414061 |
| H | 1.960569  | 2.153973  | -0.157961 |
| H | 2.564537  | 1.310447  | 1.274638  |
| H | 2.789895  | 0.272565  | -1.448240 |
| C | -0.694400 | 1.020420  | -0.137736 |
| C | -0.036785 | -0.373681 | 1.396313  |
| C | -1.374737 | 2.362523  | -0.323123 |
| C | -0.311027 | 0.412970  | -1.480393 |
| H | 0.143378  | -0.573363 | -1.373482 |
| H | -1.190744 | 0.294744  | -2.116004 |
| H | 0.383693  | 1.070859  | -2.008124 |
| H | -2.261585 | 2.275035  | -0.953535 |
| H | -0.697974 | 3.069372  | -0.809180 |
| H | -1.677316 | 2.786433  | 0.634932  |
| H | 0.017267  | -0.558999 | 2.465436  |
| H | 0.393803  | -1.219634 | 0.865472  |
| C | -1.407024 | -0.022563 | 0.798912  |
| H | -2.046340 | 0.512611  | 1.503477  |
| C | -2.193962 | -1.102684 | 0.102804  |
| C | -3.596214 | -0.735604 | -0.313746 |
| H | -3.587854 | 0.211133  | -0.857418 |
| H | -4.211419 | -0.586216 | 0.575250  |
| H | -4.023584 | -1.520917 | -0.929915 |
| O | -1.713586 | -2.180156 | -0.145178 |
| O | 2.643393  | -1.023171 | 0.080821  |
| O | 4.023798  | -1.124815 | -0.412048 |

Rotational constants (GHz): 1.2906000 0.5099400 0.4322400

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i544.1715 | 43.4223   | 58.1247   |
| 66.2203   | 78.5623   | 114.9799  |
| 141.9185  | 155.3944  | 190.7074  |
| 227.4645  | 242.2670  | 283.8335  |
| 314.9220  | 336.0840  | 349.6886  |
| 380.1828  | 415.9802  | 432.8766  |
| 458.9631  | 571.0919  | 586.3910  |
| 623.8057  | 708.3723  | 719.6082  |
| 754.1494  | 823.9422  | 841.8583  |
| 875.1457  | 914.3058  | 942.6362  |
| 959.2345  | 966.7743  | 974.0116  |
| 993.8345  | 1003.0585 | 1036.0421 |
| 1055.7694 | 1066.4678 | 1138.6116 |
| 1144.9416 | 1169.5223 | 1194.5227 |
| 1202.8109 | 1213.7001 | 1246.1262 |
| 1262.3333 | 1285.0039 | 1301.1898 |
| 1339.9190 | 1368.7549 | 1376.8074 |
| 1395.2742 | 1404.2027 | 1415.4483 |
| 1423.0511 | 1463.9166 | 1474.1160 |
| 1476.6834 | 1486.4229 | 1492.7647 |
| 1504.3526 | 1508.4445 | 1513.6934 |
| 1594.7706 | 1839.9038 | 3044.4777 |
| 3047.2542 | 3053.3161 | 3062.3337 |
| 3076.5117 | 3082.1485 | 3108.6690 |
| 3112.0471 | 3113.9694 | 3115.4674 |
| 3123.8299 | 3125.8243 | 3126.6981 |
| 3166.4515 | 3171.6091 | 3179.3934 |

Zero-point correction (Hartree): 0.245257

#####  
E-FCHOO  
#####

Population analysis as 298K (%)

Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)

| Compound | Qtot      | Erel | Erel2 | n*Q*MB    | %   |
|----------|-----------|------|-------|-----------|-----|
| E_CFHO2  | 2.110e+37 | 0.00 | 0.00  | 2.110e+37 | 100 |
| Total    |           |      |       | 2.110e+37 | 100 |

E\_CFHO2

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E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -288.47192124

E(CCSD/Aug-CC-pVTZ) (Hartree): -288.43187675

T1 diagnostic: 0.029268

E(MP2/Aug-CC-pVTZ) (Hartree): -288.42437018

E(MP3/Aug-CC-pVTZ) (Hartree): -288.41933989

E(RHF/Aug-CC-pVTZ) (Hartree): -287.54142622

E(UM062X/Aug-CC-pVTZ) (Hartree): -288.83057803

Point group : CS

Electronic state : 1-A'

Cartesian coordinates (Angs):

C	0.000000	-0.566311	0.000000
O	-0.054169	0.650567	0.000000
O	1.190322	1.298674	0.000000
H	0.930408	-1.121745	0.000000

F -1.113292 -1.230480 0.000000
 Rotational constants (GHz): 70.6849200 4.6993800 4.4064200
 Vibrational harmonic frequencies (cm-1):
 282.5625 (A') 339.6139 (A') 591.2427 (A')
 894.4767 (A') 981.6971 (A'') 1246.6885 (A')
 1354.9879 (A') 1719.2672 (A') 3234.5527 (A')
 Zero-point correction (Hartree): 0.024251

Population analysis as 298K (%)
 Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)

Compound	Qtot	Erel	Erel2	n*Q*MB	%
TS_E_CFHO2.ringclose	1.670e+37	0.00	0.00	3.340e+37	100
Total				3.340e+37	100

TS_E_CFHO2.ringclose
 ~~~~~  
 E (CCSD(T)/Aug-CC-pVTZ) (Hartree): -288.45859163  
 E (CCSD/Aug-CC-pVTZ) (Hartree): -288.41702051  
 T1 diagnostic: 0.031956  
 E (MP2/Aug-CC-pVTZ) (Hartree): -288.40846774  
 E (MP3/Aug-CC-pVTZ) (Hartree): -288.40237532  
 E (PMP2/Aug-CC-pVTZ) (Hartree): -288.40846774  
 E (PMP3/Aug-CC-pVTZ) (Hartree): -288.40237532  
 E (PUHF/Aug-CC-pVTZ) (Hartree): -287.52511090  
 E (UHF/Aug-CC-pVTZ) (Hartree): -287.52511090  
 E (UM062X/Aug-CC-pVTZ) (Hartree): -288.81300746  
 Electronic state : 1-A  
 Cartesian coordinates (Angs):  
 C -0.353240 0.225253 -0.264599  
 O 0.478397 -0.672622 -0.128722  
 H -0.196453 1.155323 -0.795323  
 F -1.549132 0.042518 0.197918  
 O 1.553863 0.311435 0.203928  
 Rotational constants (GHz): 36.3801300 5.4692600 5.0410300  
 Vibrational harmonic frequencies (cm-1):  
 i431.1145 487.2622 604.4657  
 820.7082 914.9922 1227.4402  
 1337.2751 1681.2672 3253.4284  
 Zero-point correction (Hartree): 0.023526

Population analysis as 298K (%)  
 Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)  

| Compound            | Qtot      | Erel | Erel2 | n*Q*MB    | %   |
|---------------------|-----------|------|-------|-----------|-----|
| TS_E_CFHO2.13Hshift | 1.909e+37 | 0.00 | 0.00  | 1.909e+37 | 100 |
| Total               |           |      |       | 1.909e+37 | 100 |

TS\_E\_CFHO2.13Hshift  
 ~~~~~  
 E (CCSD(T)/Aug-CC-pVTZ) (Hartree): -288.43447994
 E (CCSD/Aug-CC-pVTZ) (Hartree): -288.39177780
 T1 diagnostic: 0.022814
 E (MP2/Aug-CC-pVTZ) (Hartree): -288.38991249
 E (MP3/Aug-CC-pVTZ) (Hartree): -288.38067095
 E (RHF/Aug-CC-pVTZ) (Hartree): -287.48733253
 E (UM062X/Aug-CC-pVTZ) (Hartree): -288.79040195
 Point group : CS
 Electronic state : 1-A'
 Cartesian coordinates (Angs):
 C 0.000000 0.514666 0.000000
 O -0.192567 -0.717337 0.000000
 O 1.210865 -1.129019 0.000000
 H 1.259538 0.269723 0.000000
 F -1.045103 1.268125 0.000000
 Rotational constants (GHz): 55.0547300 5.0771700 4.6484900
 Vibrational harmonic frequencies (cm-1):
 i1707.8112 (A') 280.6597 (A'') 497.0373 (A')
 713.2039 (A') 907.1683 (A') 1131.0136 (A'')
 1356.9297 (A') 1630.1099 (A') 2254.5581 (A')
 Zero-point correction (Hartree): 0.019981

 Z-FCHOO
 #####

Population analysis as 298K (%)
 Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)

Compound	Qtot	Erel	Erel2	n*Q*MB	%
Z_CFHO2	2.251e+37	0.00	0.00	2.251e+37	100
Total				2.251e+37	100

Z_CFHO2
 ~~~~~  
 E (CCSD(T)/Aug-CC-pVTZ) (Hartree): -288.47350043  
 E (CCSD/Aug-CC-pVTZ) (Hartree): -288.43227580  
 T1 diagnostic: 0.031641  
 E (MP2/Aug-CC-pVTZ) (Hartree): -288.42595128  
 E (MP3/Aug-CC-pVTZ) (Hartree): -288.41889074  
 E (RHF/Aug-CC-pVTZ) (Hartree): -287.53708497  
 E (UM062X/Aug-CC-pVTZ) (Hartree): -288.83137504  
 Point group : CS  
 Electronic state : 1-A'  
 Cartesian coordinates (Angs):  
 C 0.000000 0.812294 0.000000  
 O -0.875840 -0.045242 -0.000000  
 O -0.497141 -1.368974 -0.000000  
 F 1.249766 0.508808 0.000000

H -0.264045 1.860686 -0.000000  
 Rotational constants (GHz): 21.9910200 7.2972300 5.4791100  
 Vibrational harmonic frequencies (cm-1):  
 306.4741 ( A') 491.6719 ( A'') 783.3772 ( A')  
 852.3034 ( A') 882.2609 ( A'') 1255.7522 ( A')  
 1371.8806 ( A') 1707.0178 ( A') 3255.3534 ( A')  
 Zero-point correction (Hartree): 0.024846

Population analysis as 298K (%)  
 Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)  
 Compound Qtot Erel Erel2 n\*Q\*MB %  
 -----  
 TS.Z\_CFHO2.ringclose 1.957e+37 0.00 0.00 3.914e+37 100  
 Total 3.914e+37 100

TS.Z\_CFHO2.ringclose  
 ~~~~~  
 E(CCSDT/Aug-CC-pVTZ) (Hartree): -288.44457176
 E(CCSDT/Aug-CC-pVTZ) (Hartree): -288.40344390
 T1 diagnostic: 0.032514
 E(MP2/Aug-CC-pVTZ) (Hartree): -288.39328918
 E(MP3/Aug-CC-pVTZ) (Hartree): -288.38898356
 E(RHF/Aug-CC-pVTZ) (Hartree): -287.51538202
 E(UM062X/Aug-CC-pVTZ) (Hartree): -288.80034767
 Electronic state : 1-A
 Cartesian coordinates (Angs):
 C 0.446396 0.500811 0.199934
 O -0.679587 0.687610 -0.251936
 H 0.940228 1.241921 0.827813
 F 1.236251 -0.468208 -0.124892
 O -1.163521 -0.691724 0.139012
 Rotational constants (GHz): 19.0107500 7.8763900 5.9233600
 Vibrational harmonic frequencies (cm-1):
 i670.9602 363.9816 590.7311
 766.7156 1026.8504 1238.0982
 1392.7940 1698.6943 3170.3401
 Zero-point correction (Hartree): 0.023347

Population analysis as 298K (%)
 Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)
 Compound Qtot Erel Erel2 n*Q*MB %

 TS.Z_CFHO2.CFHO+O1D 5.420e+37 0.00 0.00 5.420e+37 100
 Total 5.420e+37 100

TS.Z_CFHO2.CFHO+O1D
 ~~~~~  
 E(CCSDT/Aug-CC-pVTZ) (Hartree): -288.44704714  
 E(CCSDT/Aug-CC-pVTZ) (Hartree): -288.40853100  
 T1 diagnostic: 0.024742  
 E(MP2/Aug-CC-pVTZ) (Hartree): -288.38754469  
 E(MP3/Aug-CC-pVTZ) (Hartree): -288.39250294  
 E(RHF/Aug-CC-pVTZ) (Hartree): -287.53743678  
 E(UM062X/Aug-CC-pVTZ) (Hartree): -288.80507625  
 Electronic state : 1-A  
 Cartesian coordinates (Angs):  
 C -0.741746 0.481767 0.000043  
 O 0.388773 0.857065 -0.000057  
 H -1.604552 1.149333 0.000184  
 F -1.087208 -0.774139 -0.000026  
 O 1.591215 -0.491151 0.000032  
 Rotational constants (GHz): 16.3621300 6.7626400 4.7849600  
 Vibrational harmonic frequencies (cm-1):  
 i603.5998 190.9109 201.8594  
 703.0255 1051.7193 1220.8660  
 1384.0099 1828.6524 3153.9944  
 Zero-point correction (Hartree): 0.022178

#####  
 Z-(iC3H6D)(iC3H7)COO  
 #####

Population analysis as 298K (%)  
 Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)  
 Compound Qtot Erel Erel2 n\*Q\*MB %  
 -----  
 iC3H7\_iC3H7\_COO.tm 5.111e+41 0.00 0.00 5.111e+41 21.7  
 iC3H7\_iC3H7\_COO.pp 5.112e+41 0.00 0.00 5.107e+41 21.7  
 iC3H7\_iC3H7\_COO.tp 1.221e+42 0.75 0.75 3.445e+41 14.6  
 iC3H7\_iC3H7\_COO.pm 1.219e+42 0.75 0.75 3.444e+41 14.6  
 iC3H7\_iC3H7\_COO.mmp 1.116e+42 0.93 0.93 2.339e+41 9.92  
 iC3H7\_iC3H7\_COO.mmm 1.112e+42 0.93 0.93 2.326e+41 9.86  
 iC3H7\_iC3H7\_COO.mc 1.101e+42 1.13 1.13 1.646e+41 6.98  
 iC3H7\_iC3H7\_COO.pc 4.792e+41 2.42 2.42 8.009e+39 0.34  
 iC3H7\_iC3H7\_COO.tc 4.792e+41 2.42 2.42 8.000e+39 0.339  
 Total 2.358e+42 100

iC3H7\_iC3H7\_COO.mc  
 ~~~~~  
 E(RM062X/Aug-CC-pVTZ) (Hartree): -425.45202119
 Electronic state : 1-A
 Cartesian coordinates (Angs):
 C 0.081068 0.389381 -0.000678
 O -0.465582 1.513838 -0.003149
 O -1.834763 1.614092 -0.003319
 C -0.680236 -0.895278 0.002021
 C 1.580250 0.426323 -0.000874
 C -1.522239 -1.037743 1.276828
 C -1.520722 -1.043107 -1.273229

```

H      0.070377      -1.687454      0.004171
H      -2.277568      -0.258549      1.315476
H      -0.899090      -0.974441      2.169409
H      -2.003966      -2.015187      1.268571
H      -0.896247      -0.985332      -2.165250
H      -2.274921      -0.263048      -1.316781
H      -2.003997      -2.019744      -1.260670
H      1.863461      1.478873      -0.003401
C      2.128439      -0.237408      1.265502
C      2.128459      -0.243491      -1.264017
H      1.860449      -1.293764      1.305855
H      1.751127      0.248926      2.164109
H      3.215664      -0.169079      1.269463
H      1.751219      0.238529      -2.164975
H      1.860452      -1.300020      -1.299310
H      3.215687      -0.175212      -1.268252
Rotational constants (GHz):  2.0216400      1.1897800      1.1098700
Vibrational harmonic frequencies (cm-1):
  69.2419      80.7186      163.8781
 198.5495      202.5866      207.3838
 225.6481      249.7155      249.7734
 257.6859      316.7272      346.7530
 362.9784      422.6159      492.2015
 602.6376      739.3638      752.0234
 826.2689      870.4170      880.6764
 940.9604      950.2369      978.8094
 980.9803      981.2676      1060.4770
1062.0466      1121.3844      1166.8022
1191.5964      1195.5993      1214.3569
1343.5285      1346.2937      1368.3672
1383.2495      1400.1743      1407.6575
1424.3541      1481.1123      1489.0716
1494.3401      1496.7286      1506.2329
1506.5555      1513.8840      1526.3726
1639.3994      2266.4351      3064.8167
3065.4979      3066.9519      3067.2734
3097.6719      3131.4486      3132.4456
3135.5545      3140.7708      3143.5146
3144.1013      3177.2309      3178.0231
Zero-point correction (Hartree): 0.199343

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iC3H7_iC3H7_COO.mm
~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -425.45223910
Electronic state : 1-A
Cartesian coordinates (Angs):
C      -0.110702      0.150946      0.102282
O      -0.015402      1.283238      -0.414855
O      1.215297      1.767668      -0.792160
C      1.060649      -0.739971      0.361701
C      -1.501846      -0.293203      0.444569
C      1.760855      -1.145188      -0.941209
C      2.027752      -0.097020      1.364469
H      0.646408      -1.639560      0.822035
H      2.182774      -0.269474      -1.425255
H      1.067509      -1.630473      -1.628839
H      2.555879      -1.852188      -0.705361
H      1.521197      0.156160      2.296195
H      2.461105      0.803915      0.941006
H      2.817944      -0.811727      1.592864
H      -1.445161      -0.678198      1.468411
C      -2.528903      0.826962      0.372821
C      -1.884828      -1.461903      -0.476928
H      -2.614741      1.204198      -0.645340
H      -2.255773      1.661462      1.015703
H      -3.502166      0.449654      0.683336
H      -1.167379      -2.279805      -0.425504
H      -1.942691      -1.117939      -1.509990
H      -2.861927      -1.847011      -0.189361
Rotational constants (GHz):  2.1281900      1.2160500      1.0067800
Vibrational harmonic frequencies (cm-1):
  60.1925      87.9929      161.5248
 191.0876      209.1650      217.6095
 232.2737      243.5793      255.7602
 278.4332      291.1320      353.7180
 390.5070      420.0574      469.9347
 611.7219      729.0848      759.9900
 824.4583      869.0114      881.0525
 937.3632      950.2490      973.0365
 979.3412      981.6257      1059.0163
1100.9178      1133.0591      1152.5568
1169.4810      1196.7671      1213.5211
1305.8545      1316.5765      1383.1152
1389.9310      1402.7455      1418.1482
1426.1443      1480.1100      1489.1214
1493.1319      1496.1291      1503.8626
1507.5592      1515.8676      1525.2056
1644.5589      2259.2208      3040.3309
3065.6771      3066.0724      3066.8434
3074.3945      3130.4515      3131.7237
3139.7145      3145.8621      3148.0034
3153.0455      3176.3899      3176.8956
Zero-point correction (Hartree): 0.199244

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iC3H7_iC3H7_COO.mp
~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -425.45223915
Electronic state : 1-A
Cartesian coordinates (Angs):
C      0.110728      0.150729      0.101904
O      0.015460      1.283192      -0.414909
O      -1.215287      1.767736      -0.792019

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C      -1.060627      -0.740124      0.361343
C      1.501843      -0.293449      0.444282
C      -2.026623      -0.097251      1.365337
C      -1.762144      -1.144469      -0.941071
H      -0.646336      -1.640090      0.820933
H      -2.459019      0.804723      0.943094
H      -1.519376      0.154024      2.297196
H      -2.817631      -0.811267      1.593063
H      -1.069328      -1.628594      -1.630059
H      -2.185231      -0.268593      -1.423779
H      -2.556335      -1.852295      -0.704890
H      1.444951      -0.678767      1.468011
C      1.884980      -1.461798      -0.477540
C      2.528839      0.826813      0.373077
H      1.943367      -1.117355      -1.510418
H      1.167319      -2.279559      -0.426827
H      2.861880      -1.847257      -0.189761
H      2.255574      1.661027      1.016269
H      2.614715      1.204444      -0.644930
H      3.502088      0.449428      0.683526
Rotational constants (GHz):      2.1281300      1.2159500      1.0068300
Vibrational harmonic frequencies (cm-1):
60.1295      87.8147      161.4921
191.0590      209.2179      217.4109
232.2114      243.5997      255.7709
278.4307      291.0424      353.7434
390.5119      420.0345      469.9383
611.7032      729.1053      760.0035
824.4670      869.0158      881.0705
937.3772      950.2308      973.0187
979.3227      981.6149      1059.0279
1100.9232      1133.0496      1152.5696
1169.4753      1196.7467      1213.5207
1305.8908      1316.6062      1383.0978
1389.9245      1402.7381      1418.1474
1426.1339      1480.1057      1489.1082
1493.1313      1496.1180      1503.8503
1507.5415      1515.8554      1525.1725
1644.4885      2259.1289      3040.1621
3065.6393      3066.0405      3066.8805
3074.4212      3130.4027      3131.7623
3139.6749      3145.8555      3148.0338
3153.0776      3176.4467      3176.9497
Zero-point correction (Hartree): 0.199242

iC3H7_iC3H7_COO.pc
~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -425.45055752
Electronic state : 1-A
Cartesian coordinates (Angs):
C      -0.153776      -0.475795      -0.130580
O      -0.838529      -1.529371      -0.128580
O      -2.189658      -1.452672      -0.338159
C      -0.848777      0.823672      -0.348561
C      1.296811      -0.715327      0.181725
C      -1.544210      1.202399      0.973397
C      0.006776      1.964211      -0.883712
H      -1.642570      0.581739      -1.058573
H      -0.810148      1.483035      1.729336
H      -2.148791      0.372606      1.333083
H      -2.196308      2.057043      0.797942
H      0.451816      1.725182      -1.847976
H      0.801850      2.249295      -0.195465
H      -0.632318      2.836173      -1.020052
H      1.370054      -1.793451      0.329104
C      2.241098      -0.330879      -0.962180
C      1.692983      -0.026685      1.492039
H      2.362656      0.746646      -1.042836
H      1.890114      -0.715478      -1.919151
H      3.221971      -0.762254      -0.764776
H      1.053666      -0.342853      2.315331
H      1.636092      1.057812      1.408266
H      2.721976      -0.288722      1.736912
Rotational constants (GHz):      1.8559400      1.3267400      1.0712100
Vibrational harmonic frequencies (cm-1):
82.0888      112.1578      165.0713
211.9882      229.6279      238.0986
251.2440      254.8926      286.1348
302.2868      322.5667      358.2308
367.5294      418.3341      512.8732
636.3878      667.9166      735.2663
812.2845      848.8555      900.5756
942.0136      957.6417      978.3453
983.8459      994.7586      1054.6573
1079.3936      1126.0403      1159.5558
1187.6807      1194.0787      1243.5458
1346.5242      1355.9515      1370.1768
1390.1404      1400.4275      1421.2437
1429.0546      1484.4378      1492.6727
1493.0312      1500.4843      1503.9979
1514.8062      1518.3537      1523.6524
1602.0543      2262.4395      3063.9656
3067.6353      3072.2712      3074.5768
3088.9559      3134.7726      3136.1171
3138.9487      3140.6669      3145.9763
3154.4217      3158.1714      3164.5195
Zero-point correction (Hartree): 0.199947

iC3H7_iC3H7_COO.pm
~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -425.45271301
Electronic state : 1-A

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Cartesian coordinates (Angs):
  C    0.003729   -0.225953   -0.112438
  O    0.075608   -1.436596   -0.422682
  O   -1.061032   -2.086509   -0.844576
  C   -1.311186    0.470022   -0.164633
  C    1.286321    0.393186    0.361047
  C   -2.060186    0.049196    1.114782
  C   -1.237508    1.985194   -0.298438
  H   -1.840062    0.027174   -1.009355
  H   -1.562297    0.449829    1.999859
  H   -2.113305   -1.035454    1.179794
  H   -3.072347    0.450114    1.084754
  H   -0.807837    2.292876   -1.249950
  H   -0.663092    2.444952    0.506719
  H   -2.247811    2.389640   -0.247872
  H    1.008901    1.146452    1.102277
  C    2.217955   -0.628707    1.005742
  C    1.984705    1.099848   -0.810780
  H    2.540645   -1.369199    0.276023
  H    1.727651   -1.154114    1.823646
  H    3.099298   -0.121109    1.395212
  H    1.359384    1.862988   -1.268000
  H    2.253910    0.368748   -1.573097
  H    2.897375    1.575228   -0.453635
Rotational constants (GHz):    1.8294900    1.3555900    1.0055100
Vibrational harmonic frequencies (cm-1):
  49.9624      77.7257      168.0964
 191.4970     216.3084     227.8308
 244.3523     246.9390     262.7559
 279.8639     333.9301     345.2305
 386.4854     430.3163     530.6787
 595.6170     704.7596     733.5236
 813.2623     837.7084     904.1408
 939.2364     951.5732     961.2667
 979.9757     986.0524    1059.6258
1108.8531     1135.8455    1141.3513
1173.0373     1197.6657    1221.9466
1305.0056     1319.9163    1385.7324
1394.0841     1415.6900    1423.0765
1427.2028     1486.0487    1489.4763
1492.4344     1500.3782    1506.1153
1508.2578     1515.9634    1521.8375
1622.0897     2277.0510    3057.7300
3064.2256     3070.6065    3072.4929
3074.0257     3130.2106    3133.2601
3141.1635     3145.0335    3147.7909
3152.5210     3160.1829    3164.4621
Zero-point correction (Hartree): 0.199434

iC3H7_iC3H7_COO.pp
~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -425.45411290
Electronic state : 1-A
Cartesian coordinates (Angs):
  C   -0.055947    0.295230   -0.216896
  O   -0.202397    1.525738   -0.034610
  O    0.912433    2.325948    0.028890
  C    1.314961   -0.266437   -0.369634
  C   -1.319278   -0.512737   -0.221220
  C    1.997218   -0.304358    1.009635
  C    1.355948   -1.619868   -1.067514
  H    1.844836    0.487592   -0.957630
  H    1.541581   -1.061254    1.648302
  H    1.932320    0.670082    1.487782
  H    3.047824   -0.560144    0.878522
  H    0.907215   -1.580719   -2.059892
  H    0.848697   -2.394490   -0.491534
  H    2.394483   -1.926806   -1.184237
  H   -1.236401   -1.218043   -1.051581
  C   -1.397274   -1.322909    1.083193
  C   -2.566554    0.342983   -0.403664
  H   -1.441379   -0.648306    1.938716
  H   -0.543671   -1.985376    1.212093
  H   -2.301816   -1.929607    1.077488
  H   -2.513106    0.938784   -1.312854
  H   -2.692655    1.024893    0.435860
  H   -3.442665   -0.301525   -0.458685
Rotational constants (GHz):    1.8274300    1.4002400    1.0075200
Vibrational harmonic frequencies (cm-1):
  76.5976      122.1033      180.8928
 197.2710     207.2635     241.9257
 244.2960     260.8097     281.2406
 286.8364     324.6460     345.6019
 393.8548     418.7174     522.9753
 604.4619     669.4137     746.3041
 805.4409     849.4707     900.2758
 937.2162     949.0906     969.3886
 980.9700     991.2768    1061.3766
1105.7075     1133.6076    1149.4315
1166.5556     1201.7285    1225.6938
1304.9938     1317.4302    1384.4852
1393.8868     1416.5226    1422.9894
1426.4594     1483.7744    1492.3264
1493.4541     1500.4246    1504.8795
1509.4775     1518.7256    1518.9917
1617.2289     2255.9062    3063.7688
3066.8632     3069.5291    3072.2049
3074.9929     3132.9475    3137.1723
3138.6437     3140.2591    3148.5689
3153.4389     3154.2694    3165.5693
Zero-point correction (Hartree): 0.199642

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iC3H7_iC3H7_COO.tc
~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -425.45055749
Electronic state : 1-A
Cartesian coordinates (Angs):
C      0.153829      -0.475845      -0.130428
O      0.838569      -1.529411      -0.128274
O      2.189638      -1.452481      -0.337785
C      0.848836      0.823503      -0.348709
C     -1.296653      -0.715205      0.182075
C     -0.006613      1.963725      -0.884602
C      1.543395      1.202752      0.973625
H      1.643185      0.581360      -1.057983
H     -0.801954      2.248880      -0.196704
H     -0.451295      1.724273      -1.848925
H      0.632341      2.835756      -1.021033
H      2.147465      0.372991      1.334286
H      0.808841      1.484187      1.728753
H      2.196188      2.056833      0.797983
H     -1.369832      -1.793262      0.330102
C     -1.692983      -0.025890      1.491937
C     -2.240704      -0.331564      -0.962291
H     -1.636690      1.058593      1.407560
H     -1.053440      -0.341221      2.315381
H     -2.721806      -0.288389      1.736985
H     -1.889865      -0.717510      -1.918793
H     -2.361618      0.745935      -1.044352
H     -3.221819      -0.762151      -0.764430
Rotational constants (GHz):      1.8559300      1.3268900      1.0714100
Vibrational harmonic frequencies (cm-1):
      82.0621      112.2044      164.9304
     212.0667      229.6488      238.1304
     251.2499      254.8666      286.1586
     302.3141      322.5491      358.2188
     367.4973      418.3637      512.9397
     636.4251      667.9974      735.3118
     812.0794      848.7911      900.6163
     942.0066      957.5777      978.3608
     983.9513      994.7626      1054.6444
    1079.4088      1126.0714      1159.5501
    1187.6455      1194.0702      1243.5720
    1346.5944      1356.0453      1370.2624
    1390.1162      1400.4418      1421.2504
    1429.0610      1484.3934      1492.6638
    1493.0239      1500.5108      1503.9792
    1514.8117      1518.3781      1523.6608
    1602.1814      2262.6215      3064.0129
    3067.6594      3072.2642      3074.6214
    3088.7964      3134.9209      3136.2157
    3138.9471      3140.6951      3145.9791
    3154.4436      3158.0300      3164.4626
Zero-point correction (Hartree): 0.199948

iC3H7_iC3H7_COO.tm
~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -425.45411288
Electronic state : 1-A
Cartesian coordinates (Angs):
C      0.055913      0.295225      -0.216991
O      0.202462      1.525716      -0.034604
O     -0.912325      2.326064      0.028964
C     -1.314961      -0.266362      -0.369743
C      1.319133      -0.512893      -0.221108
C     -1.355878      -1.619804      -1.067664
C     -1.997151      -0.304506      1.009589
H     -1.844838      0.487632      -0.957792
H     -0.848233      -2.394320      -0.491877
H     -0.907554      -1.580532      -2.060216
H     -2.394381      -1.927000      -1.183947
H     -1.932053      0.669722      1.488119
H     -1.541535      -1.061772      1.647836
H     -3.047808      -0.560017      0.878453
H      1.236091      -1.218631      -1.051084
C      2.566562      0.342521      -0.404121
C      1.397093      -1.322340      1.083810
H      2.693196      1.024413      0.435344
H      2.512913      0.938365      -1.313266
H      3.442470      -0.302232      -0.459503
H      0.543823      -1.985239      1.212753
H      1.440539      -0.647205      1.938930
H      2.302019      -1.928474      1.078728
Rotational constants (GHz):      1.8273600      1.4002100      1.0076100
Vibrational harmonic frequencies (cm-1):
      76.6521      122.1174      180.8496
     197.2414      207.2681      241.8594
     244.2073      260.9289      281.1793
     286.8632      324.6411      345.6188
     393.8459      418.7044      522.9835
     604.4670      669.4683      746.3170
     805.4415      849.4258      900.2172
     937.2170      949.0315      969.3332
     980.9459      991.2370      1061.3630
    1105.7156      1133.5773      1149.3858
    1166.5534      1201.6941      1225.6654
    1305.0521      1317.4341      1384.4473
    1393.8641      1416.5593      1422.9749
    1426.4441      1483.7549      1492.3129
    1493.4502      1500.4141      1504.8675
    1509.4844      1518.7246      1518.9846
    1617.2038      2255.8853      3063.7852
    3066.8842      3069.5640      3072.2331
    3074.9968      3132.9298      3137.2400

```

3138.6889 3140.3114 3148.5587
3153.4419 3154.2426 3165.6521
Zero-point correction (Hartree): 0.199641

iC3H7_iC3H7_COO.tp

~~~~~  
E(RM062X/Aug-CC-pVTZ) (Hartree): -425.45271300  
Electronic state : 1-A  
Cartesian coordinates (Angs):  
C -0.003688 -0.225936 -0.112416  
O -0.075716 -1.436561 -0.422662  
O 1.060831 -2.086546 -0.844674  
C 1.311259 0.469900 -0.164652  
C -1.286243 0.393330 0.360970  
C 1.237679 1.985104 -0.298589  
C 2.060123 0.049203 1.114882  
H 1.840202 0.026993 -1.009286  
H 0.663101 2.444927 0.506403  
H 0.808235 2.292694 -1.250231  
H 2.247993 2.389484 -0.247877  
H 2.113494 -1.035440 1.179834  
H 1.561925 0.449555 1.999909  
H 3.072147 0.450478 1.085090  
H -1.008828 1.146676 1.102121  
C -1.984864 1.099713 -0.810878  
C -2.217758 -0.628502 1.005975  
H -2.253939 0.368473 -1.573091  
H -1.359794 1.863006 -1.268156  
H -2.897624 1.574857 -0.453648  
H -1.727251 -1.153815 1.823826  
H -2.540636 -1.369081 0.276437  
H -3.098990 -0.120824 1.395606  
Rotational constants (GHz): 1.8294700 1.3555600 1.0055600  
Vibrational harmonic frequencies (cm-1):  
49.9281 77.6916 168.0777  
191.4692 216.2916 227.7673  
244.3624 246.9395 262.7820  
279.7904 333.9043 345.2245  
386.5027 430.3215 530.6779  
595.6388 704.7737 733.5299  
813.2570 837.6857 904.1475  
939.2309 951.5722 961.2642  
979.9801 986.0598 1059.6175  
1108.8658 1135.8441 1141.3474  
1173.0305 1197.6433 1221.9308  
1305.0275 1319.9404 1385.7425  
1394.0718 1415.6871 1423.0414  
1427.2045 1486.0549 1489.4778  
1492.4285 1500.3635 1506.1159  
1508.2526 1515.9527 1521.8261  
1622.1394 2277.1366 3057.7468  
3064.2583 3070.6534 3072.4981  
3074.0252 3130.2192 3133.3462  
3141.2131 3145.0767 3147.7460  
3152.5400 3160.1936 3164.5502  
Zero-point correction (Hartree): 0.199435

Population analysis as 298K (%)  
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)  
Compound Qtot Erel Erel2 n\*Q\*MB %  
-----  
TS.iC3H7\_iC3H7\_COO.ringclose.ct 8.892e+41 0.04 0.04 1.665e+42 49.4  
TS.iC3H7\_iC3H7\_COO.ringclose.pt 8.033e+41 0.00 0.00 1.607e+42 47.6  
TS.iC3H7\_iC3H7\_COO.ringclose.pp 8.351e+41 1.83 1.83 7.598e+40 2.25  
TS.iC3H7\_iC3H7\_COO.ringclose.mt 1.146e+42 3.08 3.08 1.270e+40 0.376  
TS.iC3H7\_iC3H7\_COO.ringclose.pm 7.276e+41 2.90 2.90 1.090e+40 0.323  
TS.iC3H7\_iC3H7\_COO.ringclose.cm 3.043e+41 3.69 3.69 1.192e+39 0.0353  
TS.iC3H7\_iC3H7\_COO.ringclose.cp 4.483e+41 5.29 5.29 1.174e+38 0.00348  
TS.iC3H7\_iC3H7\_COO.ringclose.mm 7.284e+41 5.92 5.92 6.676e+37 0.00198  
TS.iC3H7\_iC3H7\_COO.ringclose.mp 4.585e+41 6.17 6.17 2.740e+37 0.000812  
Total 3.373e+42 100

TS.iC3H7\_iC3H7\_COO.ringclose.cm

~~~~~  
E(RM062X/Aug-CC-pVTZ) (Hartree): -425.41478029
Electronic state : 1-A
Cartesian coordinates (Angs):
C 0.039439 0.391494 -0.459677
O 0.205969 1.503288 -1.065886
O -0.281092 2.312783 0.066071
C -1.318141 -0.020170 0.035108
C 1.293102 -0.418247 -0.368854
H -1.958583 0.823444 -0.206846
C -1.818489 -1.260794 -0.724727
C -1.364809 -0.231845 1.547845
H -1.409613 -2.186387 -0.327502
H -1.596018 -1.208092 -1.791148
H -2.901841 -1.303698 -0.617541
H -1.071721 0.681638 2.060143
H -0.712347 -1.045380 1.866329
H -2.382084 -0.492620 1.839558
H 1.861471 -0.146970 -1.262300
C 2.047866 0.191610 0.838232
C 1.200433 -1.932318 -0.251285
H 1.550535 -0.070955 1.771328
H 2.091549 1.275965 0.763070
H 3.057136 -0.217115 0.855586
H 0.726154 -2.384741 -1.119515
H 0.658751 -2.239641 0.641701
H 2.211188 -2.332395 -0.174194
Rotational constants (GHz): 1.6461600 1.5964800 1.1351300

Vibrational harmonic frequencies (cm-1):

i467.8375	94.2203	118.9073
179.6180	205.8876	222.0845
228.8520	252.0425	279.6155
300.2459	301.5875	358.5648
360.3677	398.6543	481.5442
565.9948	663.4640	699.5216
830.0435	836.1173	850.7358
904.2602	944.6910	961.6317
970.7328	989.0199	1034.3185
1056.9220	1123.5457	1157.6121
1177.1930	1194.2403	1218.1975
1285.5821	1310.6867	1377.8682
1391.9173	1397.1898	1415.5076
1427.8983	1486.1207	1489.4375
1492.2943	1493.9525	1506.5901
1511.0927	1518.5847	1521.9116
1547.7262	2310.1624	3064.6260
3066.3629	3068.9677	3071.3474
3076.4958	3130.6636	3133.7792
3141.4570	3146.8428	3157.7457
3161.1937	3163.5022	3164.5005

Zero-point correction (Hartree): 0.198183

TS.iC3H7_iC3H7_COO.ringclose.cp
 ~~~~~  
 E(RM062X/Aug-CC-pVTZ) (Hartree): -425.41213254  
 Electronic state : 1-A  
 Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.108756  | 0.544647  | 0.044016  |
| O | 0.338351  | 1.761544  | 0.340478  |
| O | 1.592898  | 1.846879  | -0.434824 |
| C | 1.105943  | -0.523052 | 0.399057  |
| C | -1.288066 | 0.306364  | -0.460724 |
| H | 1.926262  | 0.024199  | 0.855615  |
| C | 0.493787  | -1.467148 | 1.445785  |
| C | 1.670335  | -1.293561 | -0.795133 |
| H | -0.315444 | -2.074984 | 1.045091  |
| H | 0.123046  | -0.920439 | 2.312676  |
| H | 1.276079  | -2.144139 | 1.788376  |
| H | 2.024309  | -0.600674 | -1.555130 |
| H | 0.940049  | -1.971931 | -1.232108 |
| H | 2.513723  | -1.892976 | -0.453099 |
| H | -1.482841 | 1.176154  | -1.090649 |
| C | -1.531282 | -0.949240 | -1.289017 |
| C | -2.248436 | 0.394948  | 0.741890  |
| H | -1.384874 | -1.863859 | -0.718281 |
| H | -0.888421 | -0.980705 | -2.166207 |
| H | -2.565557 | -0.938616 | -1.632398 |
| H | -2.070855 | 1.297965  | 1.323054  |
| H | -2.139380 | -0.472495 | 1.391149  |
| H | -3.272314 | 0.417372  | 0.371434  |

Rotational constants (GHz): 1.7297300 1.4359300 1.1222300

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i482.3501 | 70.5800   | 114.1422  |
| 169.9229  | 217.6780  | 231.6154  |
| 232.4098  | 247.4057  | 256.8328  |
| 286.6818  | 295.8633  | 338.3820  |
| 342.7915  | 409.1087  | 488.8181  |
| 569.9488  | 650.0612  | 702.7456  |
| 823.3106  | 831.2821  | 851.3667  |
| 906.0889  | 939.1436  | 962.5221  |
| 967.0223  | 984.1195  | 1039.7132 |
| 1061.2685 | 1128.7561 | 1157.6414 |
| 1169.4509 | 1195.6694 | 1223.6275 |
| 1306.2688 | 1313.4860 | 1375.9920 |
| 1390.7633 | 1395.1002 | 1411.9031 |
| 1427.3532 | 1486.0718 | 1489.6678 |
| 1494.3020 | 1498.1373 | 1508.0807 |
| 1509.9050 | 1519.2251 | 1520.1634 |
| 1551.3987 | 2308.4148 | 3067.0270 |
| 3072.5553 | 3074.9984 | 3078.7052 |
| 3081.0085 | 3135.6085 | 3139.8281 |
| 3143.2810 | 3147.9575 | 3149.3293 |
| 3156.4352 | 3165.3642 | 3166.3704 |

Zero-point correction (Hartree): 0.198088

TS.iC3H7\_iC3H7\_COO.ringclose.ct  
 ~~~~~  
 E(RM062X/Aug-CC-pVTZ) (Hartree): -425.42003197
 Electronic state : 1-A
 Cartesian coordinates (Angs):

C	0.016857	0.171000	-0.331335
O	0.460227	1.027313	-1.160563
O	-0.292545	2.153593	-0.567759
C	-1.442869	-0.110589	-0.162922
C	1.049697	-0.625491	0.395883
H	-1.965280	0.583883	-0.814398
C	-1.704439	-1.556305	-0.615460
C	-1.897840	0.110548	1.278504
H	-1.263576	-2.284883	0.064886
H	-1.323246	-1.741183	-1.619930
H	-2.780583	-1.725413	-0.629944
H	-1.744931	1.149223	1.562951
H	-1.352302	-0.533446	1.971351
H	-2.956533	-0.131334	1.366311
H	0.566396	-1.442240	0.930017
C	2.097818	-1.175470	-0.573104
C	1.687756	0.336804	1.414595
H	2.567141	-0.361651	-1.122972
H	1.656386	-1.869396	-1.287752
H	2.866689	-1.703266	-0.010629

```

H      0.952720      0.722253      2.119359
H      2.132712      1.182850      0.893374
H      2.461079      -0.195637      1.966980
Rotational constants (GHz):      1.8392100      1.3400600      1.1529300
Vibrational harmonic frequencies (cm-1):
1463.0814      58.0508      87.6826
162.7604      196.5161      198.7180
218.3089      241.9107      248.4504
253.1848      280.0340      311.5030
364.1500      417.2806      502.2766
556.3329      704.7973      726.2483
822.4673      830.2744      842.6498
898.1571      945.3051      959.9852
966.9804      987.4307      1043.5722
1080.7327      1108.5932      1128.6876
1169.3808      1193.0664      1200.4499
1277.5722      1328.8277      1388.4269
1392.4346      1398.0958      1413.7877
1423.8133      1485.7325      1486.4381
1492.1950      1494.8312      1502.3274
1503.9456      1512.3305      1520.5668
1569.8555      2317.2177      3059.8979
3062.2878      3068.9167      3069.0191
3107.6244      3126.9607      3135.4545
3138.6015      3140.9284      3146.7144
3153.5536      3157.6775      3159.5035
Zero-point correction (Hartree): 0.197612

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TS.iC3H7_iC3H7_COO.ringclose.mm
~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -425.41096047
Electronic state : 1-A
Cartesian coordinates (Angs):
C      -0.029205      -0.217162      -0.328318
O      0.319214      -1.149139      -1.122140
O      0.962945      -2.012730      -0.111992
C      0.919504      0.657587      0.432653
C      -1.507099      0.015236      -0.288328
H      0.388561      1.008222      1.320126
C      2.280251      0.110288      0.832674
C      1.125347      1.871936      -0.511121
H      2.800687      -0.292917      -0.032425
H      2.185128      -0.688526      1.559710
H      2.868680      0.926580      1.255610
H      0.198830      2.316957      -0.862853
H      1.710031      1.556756      -1.374816
H      1.686063      2.634842      0.025860
H      -1.884752      -0.306687      -1.260648
C      -1.969956      -1.037890      0.752160
C      -2.043295      1.394433      0.066770
H      -1.641342      -0.750447      1.751521
H      -1.562096      -2.020349      0.524327
H      -3.058109      -1.075609      0.742090
H      -1.888596      2.116909      -0.731490
H      -1.596849      1.785603      0.980570
H      -3.116787      1.317046      0.236539
Rotational constants (GHz):      1.9173100      1.4447700      1.0249700
Vibrational harmonic frequencies (cm-1):
1414.0603      59.2253      67.1400
179.4094      186.8932      221.7779
229.1492      254.8589      278.1125
311.7597      324.9018      348.5601
361.3125      411.2509      497.2600
552.9721      680.2384      726.4414
801.7177      831.8937      859.2357
895.3332      918.0917      946.0137
972.9752      987.7503      1014.8487
1065.8952      1115.5547      1157.6299
1168.1378      1178.3866      1204.0777
1282.7128      1327.4448      1376.7172
1391.7396      1405.2405      1424.3021
1426.7568      1480.2961      1483.0186
1488.3164      1490.1802      1498.9004
1503.4707      1511.5336      1522.5063
1560.5756      2264.0686      3065.1243
3066.8134      3073.8253      3078.3980
3082.0712      3138.1131      3141.6262
3147.0504      3150.7606      3152.3675
3162.9569      3176.8389      3188.4651
Zero-point correction (Hartree): 0.197907

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TS.iC3H7_iC3H7_COO.ringclose.mp
~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -425.41073696
Electronic state : 1-A
Cartesian coordinates (Angs):
C      0.041514      -0.377068      0.060607
O      0.402153      -1.453599      -0.507569
O      1.457922      -1.855198      0.439887
C      0.924984      0.816573      0.242612
C      -1.431350      -0.318580      0.361265
H      0.625431      1.318296      1.163622
C      2.431799      0.626018      0.213566
C      0.511892      1.729171      -0.946728
H      2.729004      0.055438      -0.663462
H      2.777389      0.085629      1.087251
H      2.903942      1.609215      0.175342
H      -0.557568      1.912814      -1.011544
H      0.842490      1.274810      -1.880718
H      1.014443      2.687797      -0.833090
H      -1.562065      -1.227857      0.959606
C      -1.924144      0.865590      1.181910

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C      -2.239562      -0.515690      -0.931085
H      -1.824299      1.811768      0.652094
H      -1.397429      0.945218      2.131517
H      -2.981860      0.724222      1.401362
H      -1.875130      -1.371652      -1.494073
H      -2.180600      0.371940      -1.560814
H      -3.285155      -0.683347      -0.678514
Rotational constants (GHz):      2.0219100      1.3174600      1.0269700
Vibrational harmonic frequencies (cm-1):
i404.9253      60.3487      100.6789
183.6395      208.5744      226.8347
253.0002      262.3145      280.6376
295.5415      320.1522      353.4048
367.2140      403.6861      491.0098
550.2313      646.4692      740.3697
802.7290      835.3689      856.9514
888.3056      933.8278      943.2448
972.6313      983.8229      1018.9652
1077.9944      1136.5835      1151.2653
1158.2951      1173.9999      1215.7938
1293.9197      1327.2884      1371.1275
1394.1006      1402.1159      1423.9560
1429.4642      1481.3788      1483.3145
1492.3083      1496.9282      1498.8029
1510.7070      1514.9399      1517.7512
1558.3958      2276.6313      3035.2232
3068.7667      3073.3396      3073.7150
3077.1536      3140.8199      3143.8953
3145.7792      3148.3236      3149.5972
3164.2673      3169.9244      3192.4386
Zero-point correction (Hartree): 0.198087

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TS.iC3H7_iC3H7_COO.ringclose.mt
~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -425.41538459
Electronic state : 1-A
Cartesian coordinates (Angs):
C      -0.023425      -0.099519      -0.070487
O      -0.093672      -0.964161      -0.997111
O      0.589645      -2.059354      -0.283150
C      1.244780      0.444775      0.508115
C      -1.332828      0.485382      0.355868
H      1.095856      0.503685      1.590804
C      2.541495      -0.276492      0.182347
C      1.315377      1.896917      -0.033891
H      2.601590      -0.483073      -0.885145
H      2.608591      -1.225089      0.701310
H      3.380128      0.361614      0.464073
H      0.421715      2.482734      0.170927
H      1.480780      1.878959      -1.111668
H      2.162551      2.398224      0.429526
H      -1.153334      1.322019      1.029538
C      -2.157505      0.938996      -0.848622
C      -2.049933      -0.635717      1.129733
H      -2.314335      0.106253      -1.531909
H      -1.663371      1.744849      -1.390880
H      -3.128458      1.296218      -0.508468
H      -1.469985      -0.964442      1.990941
H      -2.203235      -1.495186      0.479319
H      -3.014048      -0.264703      1.475345
Rotational constants (GHz):      2.0951500      1.3074100      1.0195200
Vibrational harmonic frequencies (cm-1):
i413.9127      39.0410      77.6432
161.3171      196.1122      208.7559
225.6972      251.0299      265.2394
270.6330      310.6640      341.4357
365.1673      415.3992      471.6265
594.5217      682.5935      754.1985
797.9525      840.1048      856.6784
884.0029      924.6803      950.4457
975.2180      987.3381      1040.5264
1081.4239      1111.1823      1127.2344
1155.1929      1174.9248      1198.3559
1307.0321      1336.2025      1388.7286
1396.8577      1402.1377      1423.2435
1426.1429      1482.7009      1484.2948
1485.9891      1489.7617      1501.5666
1504.9974      1508.0016      1518.3286
1572.2593      2246.3415      3068.6157
3068.6729      3069.1943      3072.1734
3103.5673      3139.1188      3140.5628
3144.0345      3145.2813      3153.3939
3156.5641      3158.5354      3196.1769
Zero-point correction (Hartree): 0.197806

```

```

TS.iC3H7_iC3H7_COO.ringclose.pm
~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -425.41580534
Electronic state : 1-A
Cartesian coordinates (Angs):
C      -0.093874      -0.284919      -0.180682
O      -0.066767      -1.511405      0.154495
O      0.751395      -1.250871      1.354720
C      1.143663      0.522117      -0.490403
C      -1.442201      0.294199      -0.503755
H      0.815395      1.222434      -1.266701
C      1.693131      1.353716      0.674584
C      2.232612      -0.384050      -1.064165
H      2.200490      0.691233      1.369459
H      0.912366      1.878737      1.220305
H      2.397017      2.089198      0.284269
H      1.886419      -0.922759      -1.945633

```

```

H      2.536727      -1.104544      -0.308837
H      3.090500      0.224350      -1.348523
H     -1.392481      0.549936      -1.569120
C     -2.574479     -0.691556     -0.257821
C     -1.654846      1.605878      0.269223
H     -2.619573     -0.957698      0.797718
H     -2.438932     -1.609219     -0.825708
H     -3.522828     -0.239339     -0.544842
H     -0.922098      2.364264      0.001859
H     -1.598021      1.427229      1.342774
H     -2.646041      1.992078      0.037368
Rotational constants (GHz):   2.1851900   1.2592700   1.0448500
Vibrational harmonic frequencies (cm-1):
1531.7202      37.5027      113.9045
177.9101      196.5956      213.5463
240.8865      258.9100      283.7153
288.4335      299.7211      331.3701
366.1331      424.3929      477.1651
570.8121      676.9418      734.4071
817.3705      845.6260      864.9856
895.7239      935.1103      955.3587
981.2635      984.7865      1052.5409
1079.1154     1109.2069      1152.1574
1164.7891     1200.9587      1208.9654
1285.3379     1298.2448      1375.3286
1393.9219     1405.5780      1414.1015
1425.6042     1481.2154      1488.9514
1491.4865     1497.4797      1500.1534
1508.1948     1512.3286      1523.1875
1559.0420     2229.7467      3029.0674
3070.0203     3070.9465      3074.3668
3074.9086     3138.9781      3144.6132
3147.9327     3148.8224      3156.8487
3157.1939     3165.5783      3176.9446
Zero-point correction (Hartree): 0.197942

```

TS.iC3H7_iC3H7_COO.ringclose.pp

~~~~~

E(RM062X/Aug-CC-pVTZ) (Hartree): -425.41710061

Electronic state : 1-A

Cartesian coordinates (Angs):

```

C      0.077580     -0.296291      0.074593
O     -0.038756     -1.559441      0.182789
O     -1.103222     -1.658803     -0.831437
C     -1.043120      0.663442      0.332703
C      1.455591      0.199010     -0.257354
H     -0.585613      1.414649      0.987965
C     -1.474986      1.379525     -0.953443
C     -2.234366      0.056821      1.062194
H     -1.972881      0.658223     -1.597418
H     -0.632844      1.805623     -1.498620
H     -2.164700      2.185414     -0.705567
H     -1.912697     -0.565476      1.896388
H     -2.818620     -0.561394      0.388852
H     -2.855029      0.863733      1.452344
H      1.412115      0.191606     -1.358976
C      1.780957      1.616342      0.206215
C      2.536562     -0.795546      0.169104
H      1.794074      1.669048      1.295784
H      1.076196      2.356575     -0.165286
H      2.772675      1.890414     -0.149745
H      2.351086     -1.786202     -0.234755
H      2.577021     -0.870027      1.256251
H      3.505740     -0.446053     -0.182102

```

Rotational constants (GHz): 2.1164800 1.3119300 0.9924500

Vibrational harmonic frequencies (cm-1):

```

1470.3014      36.5486      113.5487
170.8991      194.1098      198.5902
228.0286      250.4804      285.8775
307.0197      312.6147      321.5853
378.0989      453.1255      468.3778
522.5689      648.0823      705.5121
811.7638      843.5010      866.5280
892.1446      933.7516      960.9330
979.9126      981.8756      1045.0706
1074.0395     1091.2234      1152.6111
1170.8344     1206.4610      1211.8641
1292.1641     1303.8362      1363.4891
1393.2693     1405.4960      1413.8277
1426.7100     1478.5938      1491.6011
1495.3511     1496.5939      1497.9135
1510.8741     1516.6710      1519.2115
1554.7699     2224.3916      2982.6888
3069.1860     3070.4286      3072.4681
3073.9667     3136.7424      3137.2200
3138.8450     3141.7954      3159.0873
3163.3511     3174.9422      3184.8019

```

Zero-point correction (Hartree): 0.197535

TS.iC3H7\_iC3H7\_COO.ringclose.pt

~~~~~

E(RM062X/Aug-CC-pVTZ) (Hartree): -425.42021290

Electronic state : 1-A

Cartesian coordinates (Angs):

```

C     -0.069534     -0.218372     -0.171642
O     -0.149250     -1.409783      0.264410
O      0.779985     -1.198120      1.389426
C      1.196733      0.444893     -0.604524
C     -1.372924      0.491916     -0.352210
H      0.925196      0.821045     -1.602710
C      1.498810      1.671764      0.265401
C      2.403078     -0.471363     -0.734902

```


H	1.728665	1.335854	1.274800
H	0.661509	2.368714	0.305188
H	2.359418	2.198703	-0.144106
H	2.128017	-1.428182	-1.176256
H	2.837067	-0.669424	0.239616
H	3.143627	0.009313	-1.374906
H	-1.195484	1.425671	-0.886388
C	-2.353619	-0.383560	-1.136570
C	-1.913965	0.796648	1.054547
H	-2.517378	-1.325001	-0.615237
H	-1.986268	-0.600214	-2.139060
H	-3.307035	0.135397	-1.224350
H	-1.231026	1.425960	1.622926
H	-2.051532	-0.133213	1.604225
H	-2.872133	1.307043	0.964971
Rotational constants (GHz): 2.2144000 1.1936200 1.1017400			
Vibrational harmonic frequencies (cm-1):			
i442.4673	52.7672		95.8805
162.9490	190.6254		199.4824
215.2855	248.1151		260.9972
278.0031	296.8897		316.6024
359.9641	431.6660		479.1370
588.3503	682.2095		735.3834
809.2504	846.2547		859.8892
889.8786	945.3086		960.1813
979.1473	987.1582		1041.2494
1081.6190	1105.1656		1128.5801
1153.4942	1196.4842		1208.1163
1312.9794	1332.1708		1386.9460
1394.9601	1396.4104		1418.6971
1423.3916	1480.6088		1486.1037
1490.3714	1493.7937		1498.7012
1503.3620	1512.2473		1519.8554
1573.9207	2191.9920		3067.7198
3069.7770	3070.0067		3073.0609
3091.1131	3138.5865		3140.4944
3142.4552	3147.8840		3153.0454
3156.4117	3157.9193		3182.8852
Zero-point correction (Hartree): 0.197731			
Population analysis as 298K (%)			
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)			
Compound	Qtot	Erel	Erel2 n*Q*MB %

TS.iC3H7_iC3H7_COO.14Hshift.m	5.931e+41	0.00	0.00 1.186e+42 71.7
TS.iC3H7_iC3H7_COO.14Hshift.p	7.205e+41	0.72	0.72 4.283e+41 25.9
TS.iC3H7_iC3H7_COO.14Hshift.c	6.808e+41	2.10	2.10 3.942e+40 2.38
Total			1.654e+42 100
TS.iC3H7_iC3H7_COO.14Hshift.c			
~~			
E(RM062X/Aug-CC-pVT2) (Hartree): -425.41917183			
Electronic state : 1-A			
Cartesian coordinates (Angs):			
C	0.049849	-0.454190	0.022989
O	0.648824	-1.608099	-0.002377
O	1.979418	-1.471270	-0.393606
C	0.875585	0.663392	-0.242137
C	-1.433180	-0.581412	0.202312
H	1.706259	-0.255447	-0.811134
C	1.896314	1.006537	0.858142
C	0.268316	1.901657	-0.864672
H	2.756213	1.516494	0.424347
H	2.251122	0.121982	1.378396
H	1.430391	1.681920	1.580031
H	-0.407182	2.434891	-0.189083
H	-0.266998	1.685267	-1.786210
H	1.074256	2.592475	-1.113944
H	-1.613459	-1.643361	0.377986
C	-1.880134	0.214480	1.429737
C	-2.220990	-0.171331	-1.046884
H	-1.686528	1.278337	1.292810
H	-1.360218	-0.115569	2.328192
H	-2.950709	0.082930	1.584933
H	-1.812799	-0.627852	-1.947781
H	-2.227566	0.908938	-1.173314
H	-3.253275	-0.500850	-0.934295
Rotational constants (GHz): 1.9799900 1.2903400 1.0614800			
Vibrational harmonic frequencies (cm-1):			
i1195.5208	50.1316		118.1610
177.8054	192.6433		207.9374
211.6676	239.5927		260.8254
298.0041	299.5174		338.7917
360.7943	378.3282		480.2365
591.0091	639.9453		744.2374
765.5871	898.5363		922.1465
941.6783	962.2697		982.0255
994.3585	1018.5384		1044.7473
1075.1086	1090.0368		1132.2299
1179.0982	1194.2987		1248.5262
1322.6887	1342.6764		1352.1406
1392.6487	1398.2655		1408.6593
1423.4217	1446.9847		1485.5672
1490.5010	1491.6037		1496.1097
1497.7027	1507.3125		1513.8383
1523.3970	1555.5014		3039.8044
3046.9967	3065.9779		3072.2069
3079.6010	3106.4599		3113.2807
3139.3368	3141.1070		3142.3793
3146.7946	3162.3109		3171.5833
Zero-point correction (Hartree): 0.196186			

```

TS.ic3H7_ic3H7_COO.14Hshift.m
~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -425.42233952
Electronic state : 1-A
Cartesian coordinates (Angs):
  C      0.072574      0.243241     -0.092160
  O      0.090017      1.528488      0.076012
  O     -1.194985      2.056179     -0.060367
  C     -1.199934     -0.343353     -0.282947
  C      1.415080     -0.403838     -0.220262
  H     -1.572552      0.920113     -0.626334
  C     -2.140951     -0.373300      0.931550
  C     -1.254562     -1.625935     -1.083875
  H     -3.177431     -0.426140      0.598871
  H     -2.026587      0.505703      1.558321
  H     -1.933085     -1.265833      1.527209
  H     -0.906437     -2.490959     -0.510780
  H     -0.673317     -1.569173     -2.003307
  H     -2.288582     -1.826642     -1.364840
  H      1.350910     -1.041875     -1.105592
  C      2.559184      0.587418     -0.389208
  C      1.625476     -1.313487      0.998690
  H      2.650943      1.223264      0.490619
  H      2.405918      1.231955     -1.252485
  H      3.495139      0.045822     -0.518912
  H      0.808938     -2.025545      1.113217
  H      1.688441     -0.713916      1.907273
  H      2.556251     -1.868590      0.890849
Rotational constants (GHz):      1.9780000      1.3408400      0.9910900
Vibrational harmonic frequencies (cm-1):
  i1192.8875      60.7492      118.6752
  172.6604      180.7195      218.1574
  225.1558      238.2094      265.4277
  275.0070      293.2252      348.8670
  354.1149      399.9385      498.7927
  560.7381      622.8672      749.5350
  769.1526      890.9083      923.6582
  936.7029      968.0202      980.7753
  992.3264      1009.2504      1046.6487
  1084.3117      1119.9519      1127.0288
  1152.3481      1205.5805      1229.1766
  1309.5557      1341.0121      1346.5657
  1392.0101      1398.1003      1420.2881
  1421.7018      1446.1839      1485.4962
  1488.6680      1493.4632      1497.4363
  1497.9296      1505.5221      1509.1251
  1516.4381      1556.2424      3036.8652
  3047.3253      3063.1700      3068.3827
  3073.1088      3104.7891      3113.1695
  3134.0816      3137.1218      3143.9733
  3145.7450      3152.3695      3174.4659
Zero-point correction (Hartree): 0.196011

```

```

TS.ic3H7_ic3H7_COO.14Hshift.p
~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -425.42129666
Electronic state : 1-A
Cartesian coordinates (Angs):
  C     -0.041338     -0.163766      0.057338
  O     -0.105179     -1.413837     -0.281172
  O      1.117123     -1.841543     -0.804509
  C      1.222335      0.454932     -0.073131
  C     -1.380357      0.474036      0.279787
  H      1.469119     -0.545236     -0.939949
  C      2.341686      0.008257      0.880226
  C      1.221125      1.950594     -0.300869
  H      3.313291      0.202332      0.426450
  H      2.277679     -1.049199      1.115566
  H      2.280278      0.586881      1.804392
  H      1.096761      2.504727      0.634046
  H      0.442243      2.269562     -0.992161
  H      2.178892      2.251125     -0.726170
  H     -1.195500      1.460287      0.706098
  C     -2.114131      0.632306     -1.057323
  C     -2.212104     -0.352027      1.264071
  H     -2.302076     -0.347447     -1.494961
  H     -1.534383      1.219044     -1.768800
  H     -3.069218      1.131350     -0.896612
  H     -1.699775     -0.473156      2.217553
  H     -2.413201     -1.340833      0.854916
  H     -3.162951      0.147605      1.444496
Rotational constants (GHz):      2.0445700      1.2484300      1.0192300
Vibrational harmonic frequencies (cm-1):
  i1200.4036      58.0743      114.9718
  168.7225      184.4774      207.3805
  215.3252      234.0911      263.9273
  265.3679      274.7243      343.7414
  358.5821      380.7156      503.1143
  559.7918      654.5367      746.7071
  772.6330      890.9228      924.9975
  942.2958      969.3656      981.0316
  989.6698      999.1864      1046.4935
  1092.0454      1115.8903      1131.2434
  1151.8547      1203.9047      1224.8605
  1337.0398      1342.4523      1354.2113
  1392.9909      1397.3816      1409.7289
  1421.0212      1444.8862      1487.6268
  1490.4434      1491.9195      1496.1065
  1502.7682      1506.5063      1508.8164
  1519.1082      1561.0004      3040.8080
  3054.1976      3066.5805      3069.9812

```

```

3092.0071          3107.5607          3117.6447
3136.9287          3142.4209          3144.0932
3145.8376          3151.8246          3179.1454
Zero-point correction (Hartree): 0.196113

```

```

#####
Z- (iC3H6D) (tC4H9)COO
#####

```

```

Population analysis as 298K (%)
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)
Compound      Qtot      Erel      Erel2      n*Q*MB      %
-----
iC3H7_tC4H9_COO.c 3.309e+42 0.00    0.00    3.309e+42 98
iC3H7_tC4H9_COO.t 1.412e+42 2.23    2.23    6.584e+40 1.95
Total          3.375e+42 100

```

```

iC3H7_tC4H9_COO.c
~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -464.76161067
Electronic state : 1-A
Cartesian coordinates (Angs):
C      -0.073733      0.228599      0.000027
O      -0.342205      1.448956     -0.000042
O      -1.648737      1.874825     -0.000014
C      -1.128546     -0.832035      0.000056
C      1.399239     -0.108251      0.000052
C      -1.978984     -0.767186      1.275459
C      -1.978713     -0.767229     -1.275574
H      -0.600916     -1.785524      0.000112
H      -2.518934      0.173630      1.320124
H      -1.358689     -0.864852      2.167047
H      -2.687223     -1.595395      1.263776
H      -1.358243     -0.865371     -2.166988
H      -2.518320      0.173767     -1.320583
H      -2.687239     -1.595190     -1.263831
C      1.704945     -0.936042      1.258206
C      1.704924     -0.936217     -1.258045
C      2.258059      1.154154     -0.000084
H      1.130993     -1.861408      1.292244
H      1.493184     -0.362714      2.161051
H      2.763567     -1.196759      1.260570
H      1.493025     -0.363024     -2.160943
H      1.131061     -1.861644     -1.291903
H      2.763574     -1.196817     -1.260447
H      2.064512      1.764637      0.880403
H      2.064472      1.764458     -0.880689
H      3.309564      0.867198     -0.000078
Rotational constants (GHz):      1.7399900      1.0231900      0.8979500
Vibrational harmonic frequencies (cm-1):
64.1182      86.4983      164.9192
196.2096      197.4301      212.3994
231.0833      250.8700      259.2349
267.1206      297.0892      303.5530
324.8214      341.3099      389.1683
407.7825      426.4766      469.7832
581.0119      742.9813      754.4442
828.4888      829.7178      871.0711
934.4274      954.1552      957.1026
971.9107      981.1337      982.2926
1034.7139      1051.1763      1072.0947
1121.8831      1168.4305      1192.6643
1237.7734      1258.7205      1268.8145
1361.2904      1383.1162      1397.6334
1404.0867      1410.7803      1435.3781
1479.7872      1482.8475      1487.8495
1488.3197      1496.7119      1505.0398
1507.1935      1508.1099      1521.7500
1529.3986      1629.4921      2279.4422
3060.9025      3062.0356      3067.0819
3067.5057      3071.1506      3130.6772
3131.6924      3134.0451      3134.8102
3139.3784      3141.1359      3144.6707
3152.2285      3180.4836      3180.6785
Zero-point correction (Hartree): 0.227342

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```

iC3H7_tC4H9_COO.t
~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -464.75874451
Electronic state : 1-A
Cartesian coordinates (Angs):
C      -0.153960      0.358978     -0.179137
O      -0.300565      1.604088     -0.254378
O      -1.552749      2.135073     -0.425091
C      -1.383709     -0.485501     -0.269145
C      1.272977     -0.082121      0.077164
C      -1.232520     -1.920558     -0.756506
C      -2.088874     -0.418462      1.099605
H      -2.017314      0.069947     -0.963900
H      -0.625382     -2.536488     -0.094778
H      -0.814166     -1.970542     -1.759968
H      -2.226052     -2.367314     -0.791557
H      -2.196748      0.616003      1.418994
H      -1.536446     -0.983912      1.850211
H      -3.082271     -0.855484      1.006558
C      2.189634      1.135786      0.216370
C      1.310978     -0.882314      1.388569
C      1.788964     -0.949723     -1.082825
H      1.864406      1.790453      1.022703
H      2.215740      1.720436     -0.701690
H      3.198808      0.787598      0.435398

```

H	0.687730	-1.773230	1.349225	
H	0.984081	-0.268103	2.228046	
H	2.337875	-1.197709	1.576069	
H	1.651402	-0.446927	-2.040585	
H	1.306459	-1.921619	-1.124222	
H	2.857440	-1.112904	-0.939313	
Rotational constants (GHz):			1.5429200	1.1651100 0.8806500
Vibrational harmonic frequencies (cm-1):				
73.5148	122.1622			163.2814
215.0164	229.8766			242.2062
243.9380	258.5259			280.2672
297.3896	316.0162			325.7386
341.2677	365.3102			386.9131
417.1636	423.9200			524.8601
597.0170	668.8439			735.6029
816.5174	832.4534			864.1455
950.5674	958.0447			960.8773
972.7611	978.6621			989.2307
1044.1506	1052.2021			1070.4017
1125.0592	1167.8411			1198.0890
1238.5639	1252.5775			1275.9193
1356.3016	1389.8571			1398.3167
1406.6230	1423.8763			1437.0708
1481.0744	1483.9377			1489.0742
1493.9098	1502.1791			1504.0337
1506.4926	1515.6801			1522.5925
1530.0532	1585.5131			2259.9462
3064.3140	3067.1230			3067.1570
3071.9593	3073.8652			3131.1374
3132.5145	3135.0534			3138.5987
3145.6314	3148.7039			3154.1015
3157.8247	3162.3019			3177.0044
Zero-point correction (Hartree): 0.228023				
Population analysis as 298K (%)				
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)				
Compound	Qtot	Erel	Erel2	n*Q*MB %

TS.iC3H7_tC4H9_COO.ringclose.p	1.834e+42	0.00	0.00	3.668e+42 99.8
TS.iC3H7_tC4H9_COO.ringclose.c	2.461e+42	4.29	4.29	3.507e+39 0.0955
TS.iC3H7_tC4H9_COO.ringclose.m	2.193e+42	4.49	4.49	2.243e+39 0.0611
Total				3.673e+42 100
TS.iC3H7_tC4H9_COO.ringclose.c				
~~				
E(RM062X/Aug-CC-pVTZ) (Hartree): -464.72113143				
Electronic state : 1-A				
Cartesian coordinates (Angs):				
C	-0.118819	0.430375	-0.229354	
O	0.084881	1.558794	-0.781809	
O	-0.791799	2.330953	0.124652	
C	-1.521946	-0.112787	-0.166852	
C	1.149115	-0.318534	0.121445	
H	-2.124913	0.692842	-0.575689	
C	-1.643878	-1.326604	-1.103600	
C	-2.047393	-0.412064	1.236884	
H	-1.104857	-2.202026	-0.748069	
H	-1.299071	-1.089809	-2.110089	
H	-2.698754	-1.593153	-1.168075	
H	-1.860519	0.432987	1.896591	
H	-1.609305	-1.311071	1.664925	
H	-3.124467	-0.566643	1.176246	
C	2.110877	0.687256	0.776878	
C	0.965385	-1.500598	1.071653	
C	1.750325	-0.798417	-1.215960	
H	1.656566	1.138194	1.659006	
H	2.372883	1.485864	0.088511	
H	3.016105	0.160293	1.078738	
H	0.281993	-2.256376	0.694267	
H	0.615434	-1.168820	2.048090	
H	1.936867	-1.975593	1.211566	
H	1.861117	0.031442	-1.912532	
H	1.136719	-1.571532	-1.677043	
H	2.737557	-1.216335	-1.015743	
Rotational constants (GHz):			1.5008700	1.1937200 0.9547000
Vibrational harmonic frequencies (cm-1):				
i460.1413	43.1848			110.7876
168.1419	185.2177			221.3110
236.2598	243.6841			255.8458
265.9082	276.9335			301.6302
327.3969	351.6712			377.0072
391.7079	418.2656			504.5348
565.5749	636.7987			709.0938
819.9831	828.3669			845.7892
863.2308	954.1026			963.6908
966.2899	967.2556			978.5953
1033.3898	1052.0120			1059.5774
1094.9788	1163.6337			1192.9133
1223.6236	1244.7838			1263.5732
1323.3579	1391.3125			1393.9911
1401.9733	1416.5042			1435.5231
1478.9473	1483.9483			1491.0751
1494.1541	1495.1277			1502.4751
1507.9268	1510.7121			1520.0020
1525.9297	1542.5081			2311.3582
3062.4937	3067.6816			3068.9257
3074.2837	3076.7970			3134.6017
3135.1306	3137.2782			3140.3914
3143.5543	3150.2941			3151.2920
3162.3048	3170.2854			3178.1928
Zero-point correction (Hartree): 0.225965				

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TS.iC3H7_tC4H9_COO.ringclose.m
~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -464.72081439
Electronic state : 1-A
Cartesian coordinates (Angs):
  C      0.149591      0.223220      0.115306
  O      0.323440      1.209830      0.896549
  O      1.120640      2.064898     -0.005981
  C      1.261488     -0.644032     -0.385839
  C     -1.301055     -0.133843     -0.114156
  H      0.935738     -1.102960     -1.318508
  C      2.654299     -0.061059     -0.554516
  C      1.311290     -1.757254      0.700301
  H      2.978862      0.431947      0.358043
  H      2.677273      0.675248     -1.350428
  H      3.342028     -0.876552     -0.786606
  H      0.340457     -2.186375      0.938573
  H      1.736025     -1.340982      1.613065
  H      1.959334     -2.556692      0.345660
  C     -1.859352      1.098935     -0.862537
  C     -1.549601     -1.375920     -0.966401
  C     -2.006213     -0.261788      1.244197
  H     -1.351622      1.244201     -1.816051
  H     -1.728893      2.001202     -0.269995
  H     -2.919714      0.930837     -1.052752
  H     -1.139058     -2.284100     -0.528601
  H     -1.145735     -1.260880     -1.971797
  H     -2.626639     -1.514867     -1.061965
  H     -1.827607      0.615941      1.861043
  H     -1.666926     -1.146884      1.783329
  H     -3.078848     -0.356459      1.074309
Rotational constants (GHz):      1.7005700      1.1213000      0.8913900
Vibrational harmonic frequencies (cm-1):
i387.5361      47.3322      93.2301
166.5449      187.3184      232.5523
239.9177      252.3230      267.6577
285.9579      299.6384      321.4127
330.8139      357.1738      373.6096
386.5683      410.2199      480.2391
567.0317      684.0649      726.7154
802.4447      822.1496      849.2999
862.7663      924.2178      954.2597
966.3556      972.1944      977.3274
1023.1761      1039.4308      1055.4160
1087.7865      1156.9922      1168.2410
1214.6190      1250.2796      1274.6682
1344.6883      1389.1380      1395.6914
1406.7185      1423.1820      1434.9516
1475.6503      1480.8803      1483.9939
1486.4880      1492.3859      1495.9162
1500.5734      1507.8643      1517.6023
1524.7556      1552.5004      2287.7428
3063.8670      3064.7293      3066.2584
3070.8236      3075.4714      3132.2435
3133.7293      3137.9439      3147.8834
3149.0141      3152.0039      3161.0437
3162.3341      3167.0330      3188.2609
Zero-point correction (Hartree): 0.225961

TS.iC3H7_tC4H9_COO.ringclose.p
~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -464.72785152
Electronic state : 1-A
Cartesian coordinates (Angs):
  C      0.100696     -0.292454     -0.201790
  O      0.244653     -1.559244     -0.229592
  O      1.176115     -1.600329      0.909748
  C      1.244662      0.660873     -0.380003
  C     -1.328736      0.171094     -0.086608
  H      0.846129      1.411077     -1.072775
  C      1.617660      1.391839      0.916580
  C      2.470470      0.017553     -1.018543
  H      2.046743      0.670227      1.607482
  H      0.762823      1.865911      1.396387
  H      2.351255      2.165026      0.690309
  H      2.201075     -0.558764     -1.902741
  H      2.956781     -0.649197     -0.313763
  H      3.163072      0.804019     -1.318296
  C     -1.675383     -0.057371      1.403510
  C     -1.559780      1.631853     -0.462782
  C     -2.222087     -0.733467     -0.947807
  H     -1.102910      0.603209      2.053196
  H     -1.465900     -1.085914      1.691551
  H     -2.736948      0.151197      1.540999
  H     -1.360114      1.809041     -1.520124
  H     -0.949187      2.315076      0.124796
  H     -2.605381      1.878163     -0.277491
  H     -2.124310     -1.776664     -0.659235
  H     -1.975104     -0.638343     -2.005574
  H     -3.259187     -0.427005     -0.811302
Rotational constants (GHz):      1.7714500      1.0737900      0.9276000
Vibrational harmonic frequencies (cm-1):
i442.5127      59.0525      112.5725
165.9609      190.0385      199.4642
229.5745      245.8950      261.7629
281.8273      290.7959      311.3788
313.5283      353.8635      366.2863
381.9128      442.4240      484.5252
560.3195      683.1789      691.1253
812.4526      822.8815      860.2725
868.9074      949.8220      955.7013

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965.6015	976.1262	979.2858
1018.4721	1050.1611	1064.9213
1084.3159	1158.3472	1194.3850
1221.6678	1256.5433	1273.6021
1343.0739	1390.1691	1395.1541
1403.4942	1413.1164	1433.3633
1475.5932	1480.7721	1488.0352
1491.9606	1495.3341	1497.8355
1504.1336	1509.7499	1517.3082
1525.8916	1545.5521	2229.9916
3064.0939	3064.9107	3067.9640
3072.6933	3074.1364	3130.4325
3134.9022	3138.6140	3139.3495
3142.9819	3152.8533	3157.2982
3166.6861	3167.5697	3181.1686

Zero-point correction (Hartree): 0.225846

Population analysis as 298K (%)

Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)

Compound	Qtot	Erel	Erel2	n*Q*MB	%
TS.iC3H7_tC4H9_COO.14Hshift	1.610e+42	0.00	0.00	3.220e+42	100
Total				3.220e+42	100

TS.iC3H7_tC4H9_COO.14Hshift

~~~~~

E(RM062X/Aug-CC-pVT2) (Hartree): -464.72753015

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.126859 | 0.315213  | -0.058063 |
| O | -0.323297 | 1.596483  | -0.168109 |
| O | -1.646274 | 1.880234  | -0.503855 |
| C | -1.295566 | -0.476429 | -0.183220 |
| C | 1.329503  | -0.064029 | 0.084712  |
| H | -1.817656 | 0.627634  | -0.802893 |
| C | -2.279466 | -0.355227 | 0.996153  |
| C | -1.220288 | -1.892046 | -0.710025 |
| H | -3.296377 | -0.555216 | 0.658835  |
| H | -2.259827 | 0.631382  | 1.449406  |
| H | -2.021047 | -1.099585 | 1.753883  |
| H | -0.720849 | -2.585097 | -0.026050 |
| H | -0.730728 | -1.952288 | -1.678972 |
| H | -2.238620 | -2.259886 | -0.840362 |
| C | 2.213927  | 1.182545  | 0.166260  |
| C | 1.463190  | -0.875579 | 1.380912  |
| C | 1.787351  | -0.915167 | -1.110541 |
| H | 1.916151  | 1.831220  | 0.988293  |
| H | 2.169702  | 1.762052  | -0.754378 |
| H | 3.244673  | 0.867915  | 0.329023  |
| H | 0.828185  | -1.760575 | 1.364475  |
| H | 1.190940  | -0.271709 | 2.247074  |
| H | 2.498133  | -1.198241 | 1.500325  |
| H | 1.544512  | -0.432385 | -2.057524 |
| H | 1.347936  | -1.908357 | -1.098364 |
| H | 2.870683  | -1.026288 | -1.054174 |

Rotational constants (GHz): 1.6589100 1.1184400 0.8729800

Vibrational harmonic frequencies (cm-1):

|            |           |           |
|------------|-----------|-----------|
| i1181.9109 | 54.4185   | 119.4571  |
| 178.6741   | 209.6302  | 217.0418  |
| 225.4291   | 257.0276  | 264.4999  |
| 282.6579   | 301.1365  | 308.0245  |
| 329.7607   | 338.1493  | 381.8950  |
| 385.3350   | 410.2128  | 490.3173  |
| 585.5423   | 610.0739  | 745.8085  |
| 767.6623   | 842.3684  | 915.1181  |
| 955.9562   | 958.2975  | 963.6070  |
| 972.7347   | 996.1961  | 1014.7281 |
| 1044.3918  | 1045.3476 | 1057.2987 |
| 1091.9184  | 1134.0326 | 1205.4702 |
| 1239.9805  | 1253.1015 | 1285.7631 |
| 1345.6184  | 1392.1029 | 1396.0426 |
| 1398.5206  | 1409.7055 | 1420.2870 |
| 1442.9761  | 1478.3229 | 1482.3360 |
| 1485.7663  | 1490.7675 | 1493.6817 |
| 1499.5782  | 1504.2155 | 1506.1519 |
| 1516.9883  | 1527.7470 | 1543.8024 |
| 3038.3488  | 3044.5150 | 3060.0601 |
| 3066.3931  | 3070.8844 | 3105.0850 |
| 3111.9081  | 3130.7740 | 3132.1356 |
| 3142.7183  | 3143.9562 | 3148.7333 |
| 3152.0070  | 3170.3720 | 3173.6073 |

Zero-point correction (Hartree): 0.224320

#####

E- (OH)CHOO

#####

Population analysis as 298K (%)

Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)

| Compound   | Qtot      | Erel | Erel2 | n*Q*MB    | %     |
|------------|-----------|------|-------|-----------|-------|
| H_OH_COO.c | 2.383e+37 | 0.00 | 0.00  | 2.383e+37 | 99.5  |
| H_OH_COO.t | 2.448e+37 | 3.14 | 3.14  | 1.213e+35 | 0.507 |
| Total      |           |      |       | 2.395e+37 | 100   |

H\_OH\_COO.c

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E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -264.48329286

E(CCSD/Aug-CC-pVTZ) (Hartree): -264.44268250

T1 diagnostic: 0.026781

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E(MP2/Aug-CC-pVTZ) (Hartree): -264.43312868
E(MP3/Aug-CC-pVTZ) (Hartree): -264.43136631
E(RHF/Aug-CC-pVTZ) (Hartree): -263.56156782
E(UM062X/Aug-CC-pVTZ) (Hartree): -264.82765914
Electronic state : 1-A
Cartesian coordinates (Angs):
  C      -0.433043      0.377152      -0.000491
  O       0.475899     -0.452644      0.000261
  O       1.783501      0.101465     -0.000062
  H      -0.218316      1.439430      0.000556
  O      -1.688173      0.008254      0.000268
  H      -1.753245     -0.958941     -0.001345
Rotational constants (GHz):   62.0657400   4.7931400   4.4495200
Vibrational harmonic frequencies (cm-1):
  253.0698      334.6241      590.6687
  620.8422      871.6852     1045.4869
  1189.7092     1335.4345     1412.9329
  1715.2340     3229.9094     3778.8489
Zero-point correction (Hartree): 0.037313

H_OH_COO.t
~~~~~
E(UM062X/Aug-CC-pVTZ) (Hartree): -264.82240958
Electronic state : 1-A
Cartesian coordinates (Angs):
  C      -0.429436      0.317917      0.000213
  O       0.509055     -0.472748      0.000455
  O       1.780626      0.153753     -0.000279
  H      -0.226247      1.385897     -0.000226
  O      -1.651744     -0.161444     -0.000584
  H      -2.300633      0.550103      0.002215
Rotational constants (GHz):   65.3240200   4.7667200   4.4425500
Vibrational harmonic frequencies (cm-1):
  257.2107      340.9268      455.8539
  604.6148      884.1237     1028.9788
  1193.4083     1304.6517     1400.8216
  1749.5863     3184.5458     3868.1809
Zero-point correction (Hartree): 0.037072

Population analysis as 298K (%)
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)
Compound      Qtot      Erel      Erel2      n*Q*MB      %
-----
TS.H_OH_COO.isomrot.c 2.567e+37 0.00   0.00   5.135e+37 93.2
TS.H_OH_COO.isomrot.t 2.836e+37 1.61   1.61   3.758e+36 6.82
Total          5.510e+37 100

TS.H_OH_COO.isomrot.c
~~~~~
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -264.42709819
E(CCSD/Aug-CC-pVTZ) (Hartree): -264.39153323
T1 diagnostic: 0.028209
E(MP2/Aug-CC-pVTZ) (Hartree): -264.36727977
E(MP3/Aug-CC-pVTZ) (Hartree): -264.37807087
E(PMP2/Aug-CC-pVTZ) (Hartree): -264.38735646
E(PMP3/Aug-CC-pVTZ) (Hartree): -264.39807702
E(PUHF/Aug-CC-pVTZ) (Hartree): -263.56291314
E(UHF/Aug-CC-pVTZ) (Hartree): -263.54271727
E(UM062X/Aug-CC-pVTZ) (Hartree): -264.77315886
Electronic state : 1-A
Cartesian coordinates (Angs):
  C       0.575639      0.616340     -0.139517
  O      -0.696573      0.421666      0.413157
  O      -1.380721     -0.492402     -0.245193
  H       0.585369      1.109425     -1.101484
  O       1.414269     -0.420189     -0.026667
  H       1.264990     -0.880064      0.808203
Rotational constants (GHz):   23.0386000   6.1933800   5.4577300
Vibrational harmonic frequencies (cm-1):
  i282.8090      327.9231      345.3056
  617.9703      838.6930     1007.5459
  1155.8814     1207.4926     1325.2057
  1383.9498     3215.5168     3834.9388
Zero-point correction (Hartree): 0.034766

TS.H_OH_COO.isomrot.t
~~~~~
E(UM062X/Aug-CC-pVTZ) (Hartree): -264.77042741
Electronic state : 1-A
Cartesian coordinates (Angs):
  C      -0.558691      0.593927      0.165517
  O       0.722049      0.465465     -0.353603
  O       1.375679     -0.531585      0.206525
  H      -0.600292      0.994729      1.172552
  O      -1.337050     -0.446778     -0.169803
  H      -2.132985     -0.455111      0.369395
Rotational constants (GHz):   23.4689000   6.2659300   5.4630000
Vibrational harmonic frequencies (cm-1):
  i288.2708      261.7303      335.3700
  625.0414      831.7627     1023.0755
  1156.3645     1230.7592     1274.1966
  1400.6245     3161.7448     3885.2497
Zero-point correction (Hartree): 0.034596

Population analysis as 298K (%)
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)
Compound      Qtot      Erel      Erel2      n*Q*MB      %
-----
TS.H_OH_COO.13Hshift.c 2.080e+37 0.00   0.00   2.080e+37 51.8
TS.H_OH_COO.13Hshift.t 2.022e+37 0.03   0.03   1.937e+37 48.2

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Total                                     4.017e+37 100

TS_H_OH_COO.13Hshift.c
~~~~~
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -264.44468974
E(CCSD/Aug-CC-pVTZ) (Hartree): -264.40118388
  T1 diagnostic: 0.021918
E(MP2/Aug-CC-pVTZ) (Hartree): -264.39721544
E(MP3/Aug-CC-pVTZ) (Hartree): -264.39109245
E(RHF/Aug-CC-pVTZ) (Hartree): -263.50441825
E(RM062X/Aug-CC-pVTZ) (Hartree): -264.78661465
Electronic state : 1-A
Cartesian coordinates (Angs):
  C      0.386125      -0.359803      0.000023
  O     -0.430061      0.608309     -0.000032
  O     -1.668578     -0.175261     -0.000047
  H     -0.663282     -1.117796      0.000014
  O      1.660601     -0.126880      0.000056
  H      1.850843      0.827263      0.000032
Rotational constants (GHz):  49.9846200      5.1930300      4.7042900
Vibrational harmonic frequencies (cm-1):
  i1697.5411      255.7580      480.0525
  663.2195      721.4573      911.6499
  1143.2980      1207.9370      1456.3296
  1583.9197      2237.4046      3707.9174
Zero-point correction (Hartree): 0.032735

TS_H_OH_COO.13Hshift.t
~~~~~
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -264.44531715
E(CCSD/Aug-CC-pVTZ) (Hartree): -264.40184485
  T1 diagnostic: 0.021786
E(MP2/Aug-CC-pVTZ) (Hartree): -264.39847977
E(MP3/Aug-CC-pVTZ) (Hartree): -264.39207005
E(RHF/Aug-CC-pVTZ) (Hartree): -263.50446781
E(RM062X/Aug-CC-pVTZ) (Hartree): -264.78685319
Electronic state : 1-A
Cartesian coordinates (Angs):
  C     -0.392439      0.297005      0.000022
  O      0.472837     -0.617721     -0.000033
  O      1.664303      0.231267     -0.000052
  H      0.595239      1.122038      0.000010
  O     -1.641626     -0.066051      0.000056
  H     -2.204721      0.715979      0.000096
Rotational constants (GHz):  51.5226600      5.1538300      4.6851700
Vibrational harmonic frequencies (cm-1):
  i1692.4492      273.8149      481.3579
  595.3085      730.8135      917.3760
  1140.9673      1200.5535      1423.7305
  1642.9211      2225.5429      3858.8939
Zero-point correction (Hartree): 0.033014

Population analysis as 298K (%)
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)
Compound      Qtot      Erel      Erel2 n*Q*MB      %
-----
TS_H_OH_COO.introt 1.994e+37 0.00  0.00  7.977e+37 100
Total          7.977e+37 100

TS_H_OH_COO.introt
~~~~~
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -264.46911554
E(CCSD/Aug-CC-pVTZ) (Hartree): -264.42708224
  T1 diagnostic: 0.032838
E(MP2/Aug-CC-pVTZ) (Hartree): -264.41752686
E(MP3/Aug-CC-pVTZ) (Hartree): -264.41456247
E(RHF/Aug-CC-pVTZ) (Hartree): -263.54012770
E(UM062X/Aug-CC-pVTZ) (Hartree): -264.81231570
Electronic state : 1-A
Cartesian coordinates (Angs):
  C     -0.427964      0.367659     -0.001430
  O      0.505018     -0.437229     -0.016941
  O      1.777362      0.096932      0.021163
  H     -0.208032      1.431356      0.025867
  O     -1.673877     -0.084922     -0.100875
  H     -2.092209     -0.235563      0.755934
Rotational constants (GHz):  65.1229000      4.7350500      4.4698900
Vibrational harmonic frequencies (cm-1):
  i528.8326      287.3537      364.7446
  612.6396      937.6099      941.7138
  1152.1127      1263.3335      1377.1924
  1662.0705      3190.6775      3817.6833
Zero-point correction (Hartree): 0.035556

Population analysis as 298K (%)
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)
Compound      Qtot      Erel      Erel2 n*Q*MB      %
-----
TS_H_OH_COO.ringclose.c 1.728e+37 0.00  0.00  3.457e+37 99.6
TS_H_OH_COO.ringclose.t 1.717e+37 3.31  3.31  1.286e+35 0.371
Total          3.470e+37 100

TS_H_OH_COO.ringclose.c
~~~~~
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -264.47207538
E(CCSD/Aug-CC-pVTZ) (Hartree): -264.42990090
  T1 diagnostic: 0.029917
E(MP2/Aug-CC-pVTZ) (Hartree): -264.41934086
E(MP3/Aug-CC-pVTZ) (Hartree): -264.41677499
E(RHF/Aug-CC-pVTZ) (Hartree): -263.54631495

```


E(RM062X/Aug-CC-pVTZ) (Hartree): -264.81247215
 Electronic state : 1-A
 Cartesian coordinates (Angs):
 C 0.358557 -0.273997 0.276453
 O -0.489491 0.643627 0.214655
 O -1.568494 -0.271403 -0.263924
 H 0.152116 -1.230938 0.737960
 O 1.565630 -0.107136 -0.173405
 H 1.635381 0.754218 -0.615283
 Rotational constants (GHz): 33.3763600 5.5826500 5.1642300
 Vibrational harmonic frequencies (cm-1):
 i373.3941 445.9297 593.8453
 709.7539 840.7808 970.3046
 1197.4058 1351.3896 1378.8466
 1658.2546 3244.8395 3764.5663
 Zero-point correction (Hartree): 0.036806

TS_H_OH_COO.ringclose.t
 ~~~~~  
 E(RM062X/Aug-CC-pVTZ) (Hartree): -264.80704583  
 Electronic state : 1-A  
 Cartesian coordinates (Angs):  
 C 0.355553 -0.188922 0.274991  
 O -0.533885 0.672339 0.131918  
 O -1.559900 -0.351751 -0.212845  
 H 0.177190 -1.099549 0.838837  
 O 1.535243 0.041061 -0.229962  
 H 2.157822 -0.660116 -0.001665  
 Rotational constants (GHz): 34.4015500 5.5712000 5.1193500  
 Vibrational harmonic frequencies (cm-1):  
 i392.9289 479.6358 581.2042  
 625.1796 846.9338 940.9843  
 1182.7489 1337.8262 1372.4769  
 1693.1918 3192.3192 3836.1039  
 Zero-point correction (Hartree): 0.036653

#####  
 E- (CH3) (OH)CHOO  
 #####

Population analysis as 298K (%)  
 Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)  

| Compound     | Qtot      | Erel | Erel2 | n*Q*MB    | %     |
|--------------|-----------|------|-------|-----------|-------|
| CH3_OH_COO.c | 2.243e+38 | 0.00 | 0.00  | 2.243e+38 | 99.9  |
| CH3_OH_COO.t | 2.306e+38 | 3.88 | 3.88  | 3.279e+35 | 0.146 |
| Total        |           |      |       | 2.246e+38 | 100   |

CH3\_OH\_COO.c  
 ~~~~~  
 E(CCS(D)T)/Aug-CC-pVTZ (Hartree): -303.74588007
 E(CCS(D)/Aug-CC-pVTZ) (Hartree): -303.69708485
 T1 diagnostic: 0.024540
 E(MP2/Aug-CC-pVTZ) (Hartree): -303.67842602
 E(MP3/Aug-CC-pVTZ) (Hartree): -303.68578993
 E(RHF/Aug-CC-pVTZ) (Hartree): -302.62786835
 E(UM062X/Aug-CC-pVTZ) (Hartree): -304.15636773
 Electronic state : 1-A
 Cartesian coordinates (Angs):
 C -0.408536 -0.029063 0.000059
 O 0.567949 -0.799116 0.000017
 O 1.830717 -0.162207 0.000009
 C -0.280984 1.433093 -0.000087
 H 0.319480 1.711571 -0.866643
 H 0.317259 1.712283 0.867776
 H -1.256873 1.905019 -0.001315
 O -1.612099 -0.566288 0.000135
 H -1.535283 -1.532172 -0.000937
 Rotational constants (GHz): 9.4174200 4.6395100 3.1672900
 Vibrational harmonic frequencies (cm-1):
 178.3538 266.9102 315.8662
 451.2075 507.7631 595.7298
 634.7364 851.3145 937.7213
 1043.2269 1061.6791 1248.4699
 1387.6178 1422.8284 1443.3043
 1538.1057 1694.6342 3080.1678
 3136.2363 3207.6151 3781.4593
 Zero-point correction (Hartree): 0.065577

CH3_OH_COO.t
 ~~~~~  
 E(UM062X/Aug-CC-pVTZ) (Hartree): -304.14999097  
 Electronic state : 1-A  
 Cartesian coordinates (Angs):  
 C 0.396487 -0.076621 -0.000121  
 O -0.605531 -0.806158 -0.000303  
 O -1.831844 -0.108925 0.000214  
 C 0.291841 1.394266 -0.000086  
 H -0.300637 1.684419 0.867989  
 H -0.304592 1.684042 -0.865544  
 H 1.267507 1.873462 -0.002137  
 O 1.552678 -0.716743 0.000278  
 H 2.285334 -0.093189 -0.000578  
 Rotational constants (GHz): 9.6071000 4.6150000 3.1768100  
 Vibrational harmonic frequencies (cm-1):  
 176.2648 271.0343 331.6183  
 438.0370 464.0998 550.0421  
 600.7169 848.8339 949.8835  
 1043.8742 1053.3943 1231.7296  
 1394.2934 1418.1181 1430.5357  
 1513.5999 1720.8722 3073.1385

```

3136.8467          3176.9009          3877.5972
Zero-point correction (Hartree): 0.065387

Population analysis as 298K (%)
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)
Compound          Qtot      Erel    Erel2  n*Q*MB    %
-----
TS.CH3_OH_COO.isomrot.t 2.647e+38 0.00    0.00   5.294e+38 100
Total                    5.294e+38 100

TS.CH3_OH_COO.isomrot.t
~~~~~
E (CCSD(T)/Aug-CC-pVTZ) (Hartree): -303.66437847
E (CCSD/Aug-CC-pVTZ) (Hartree): -303.58032606
T1 diagnostic: 0.108736
E (MP2/Aug-CC-pVTZ) (Hartree): -303.55756044
E (MP3/Aug-CC-pVTZ) (Hartree): -303.56146030
E (PMP2/Aug-CC-pVTZ) (Hartree): -303.55756044
E (PMP3/Aug-CC-pVTZ) (Hartree): -303.56146030
E (PUHF/Aug-CC-pVTZ) (Hartree): -302.49958379
E (UHF/Aug-CC-pVTZ) (Hartree): -302.49958379
E (UM062X/Aug-CC-pVTZ) (Hartree): -304.08929231
Electronic state : 1-A
Cartesian coordinates (Angs):
C -0.432611 -0.112175 -0.393445
O 0.946325 0.005844 -0.609084
O 1.596280 0.191563 0.519078
C -1.111815 1.112050 0.106199
O -0.704014 -1.315934 0.154838
H -0.850816 1.961419 -0.520549
H -0.800684 1.326927 1.134023
H -2.193168 0.983361 0.081563
H -1.597503 -1.322744 0.509786
Rotational constants (GHz): 7.6891000 4.8983000 3.6076200
Vibrational harmonic frequencies (cm-1):
1188.0550 177.4445 228.3427
282.4449 385.4192 443.4043
655.1201 837.9174 990.8879
1064.4424 1097.3325 1170.2824
1339.1145 1342.1232 1411.4330
1474.4090 1486.7905 3032.6888
3121.0092 3162.5273 3880.3011
Zero-point correction (Hartree): 0.062840

Population analysis as 298K (%)
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)
Compound Qtot Erel Erel2 n*Q*MB %

TS.CH3_OH_COO.14Hshift.c 9.911e+37 0.00 0.00 1.982e+38 96.9
TS.CH3_OH_COO.14Hshift.t 1.008e+38 2.05 2.05 6.325e+36 3.09
Total 2.045e+38 100

TS.CH3_OH_COO.14Hshift.c
~~~~~
E (CCSD(T)/Aug-CC-pVTZ) (Hartree): -303.71707300
E (CCSD/Aug-CC-pVTZ) (Hartree): -303.66493437
T1 diagnostic: 0.021910
E (MP2/Aug-CC-pVTZ) (Hartree): -303.65509313
E (MP3/Aug-CC-pVTZ) (Hartree): -303.65609770
E (RHF/Aug-CC-pVTZ) (Hartree): -302.57818516
E (RM062X/Aug-CC-pVTZ) (Hartree): -304.12816084
Electronic state : 1-A
Cartesian coordinates (Angs):
C      -0.454892       0.059830       0.076404
O       0.433171      -0.875144       0.086210
O       1.712550      -0.292883      -0.075373
C      -0.007258       1.389065      -0.017573
O      -1.700499      -0.342178      -0.029030
H       0.535868       1.729721       0.860556
H      -0.725492       2.094342      -0.408569
H       1.123842       0.862595      -0.473166
H      -1.723092      -1.298375      -0.186263
Rotational constants (GHz): 10.1523200 4.7989900 3.3213400
Vibrational harmonic frequencies (cm-1):
11545.3510     272.1697      448.7441
501.1435       538.7845      599.4001
714.6790       733.1242      910.5274
964.2083       1024.8247     1060.5734
1232.0525      1348.4535     1431.0334
1545.2003      1636.2285     1906.3943
3136.9083      3247.5078     3768.0063
Zero-point correction (Hartree): 0.061556

TS.CH3_OH_COO.14Hshift.t
~~~~~
E (RM062X/Aug-CC-pVTZ) (Hartree): -304.12490525
Electronic state : 1-A
Cartesian coordinates (Angs):
C -0.443515 -0.006246 0.063907
O 0.500768 -0.870250 0.066159
O 1.737895 -0.199225 -0.060727
C -0.081256 1.360560 -0.014122
O -1.638076 -0.548035 -0.051461
H 0.398504 1.736055 0.886516
H -0.827325 2.023483 -0.432163
H 1.084702 0.924936 -0.451166
H -2.311944 0.129723 0.066339
Rotational constants (GHz): 10.3306500 4.7462500 3.3122700
Vibrational harmonic frequencies (cm-1):
11528.9360 278.5053 456.6637

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```

489.0746 500.2676 568.2268
713.3411 730.8378 907.6172
955.3327 1032.0014 1066.0559
1213.0131 1357.3144 1435.8144
1557.6420 1625.7044 1917.5159
3130.9706 3224.0182 3865.0062
Zero-point correction (Hartree): 0.061567

Population analysis as 298K (%)
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)
Compound Qtot Erel Erel2 n*Q*MB %

TS.CH3_OH_COO.introt 1.995e+38 0.00 0.00 7.980e+38 100
Total 7.980e+38 100

TS.CH3_OH_COO.introt
~~~~~
E (CCSD(T)/Aug-CC-pVTZ) (Hartree): -303.73058051
E (CCSD(T)/Aug-CC-pVTZ) (Hartree): -303.68052814
T1 diagnostic: 0.028692
E (MP2/Aug-CC-pVTZ) (Hartree): -303.66210095
E (MP3/Aug-CC-pVTZ) (Hartree): -303.66827983
E (RHF/Aug-CC-pVTZ) (Hartree): -302.60624255
E (UM062X/Aug-CC-pVTZ) (Hartree): -304.14007351
Electronic state : 1-A
Cartesian coordinates (Angs):
C      -0.402213      -0.034495      -0.010047
O       0.574026      -0.802334      -0.009457
O       1.817767      -0.193452      0.017428
C      -0.235839      1.426546      0.004678
O      -1.606198      -0.616607      -0.101023
H       0.380619      1.700198      -0.854357
H       0.366146      1.692525      0.875599
H      -1.197314      1.926928      -0.007334
H      -2.005900      -0.772821      0.762721
Rotational constants (GHz): 9.4424500 4.5963100 3.1781700
Vibrational harmonic frequencies (cm-1):
i507.9435      174.2830      302.3428
324.4166      461.1699      508.9555
614.0392      857.0559      963.1672
993.9544      1057.1377     1174.3134
1365.0299     1404.2593     1440.4737
1494.7705     1652.8526     3066.7876
3115.6851     3203.8567     3828.8209
Zero-point correction (Hartree): 0.063796

Population analysis as 298K (%)
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)
Compound      Qtot      Erel      Erel2  n*Q*MB      %
-----
TS.CH3_OH_COO.ringclose.c 1.379e+38 0.00    0.00   2.758e+38 99.9
TS.CH3_OH_COO.ringclose.t 1.260e+38 4.35    4.35   1.614e+35 0.0585
Total              2.760e+38 100

TS.CH3_OH_COO.ringclose.c
~~~~~
E (CCSD(T)/Aug-CC-pVTZ) (Hartree): -303.72784591
E (CCSD(T)/Aug-CC-pVTZ) (Hartree): -303.67803909
T1 diagnostic: 0.026460
E (MP2/Aug-CC-pVTZ) (Hartree): -303.65766814
E (MP3/Aug-CC-pVTZ) (Hartree): -303.66528301
E (RHF/Aug-CC-pVTZ) (Hartree): -302.60897371
E (RM062X/Aug-CC-pVTZ) (Hartree): -304.13465974
Electronic state : 1-A
Cartesian coordinates (Angs):
C 0.317243 -0.069086 -0.101687
O -0.701583 -0.691063 -0.514872
O -1.632364 0.030576 0.403557
C 0.512369 1.399032 -0.085020
O 1.360184 -0.776931 0.247572
H 1.122400 -1.717031 0.223901
H 0.549833 1.739212 0.948139
H -0.326562 1.870123 -0.581825
H 1.466762 1.627367 -0.560034
Rotational constants (GHz): 8.0818500 5.1646500 3.5814300
Vibrational harmonic frequencies (cm-1):
i368.0677 209.7026 329.9205
430.8627 530.1175 555.2516
698.2903 851.4479 893.5525
1037.1094 1051.2847 1235.8235
1386.4996 1446.9380 1454.0000
1491.6553 1654.8416 3083.1708
3152.5772 3218.5669 3769.6087
Zero-point correction (Hartree): 0.064885

TS.CH3_OH_COO.ringclose.t
~~~~~
E (RM062X/Aug-CC-pVTZ) (Hartree): -304.12770116
Electronic state : 1-A
Cartesian coordinates (Angs):
C       0.293080      -0.111330      -0.103815
O      -0.738332      -0.714876      -0.494611
O      -1.625465      0.058260      0.418042
C       0.498562      1.364178      -0.109176
O       1.304278      -0.882293      0.218488
H       2.084554      -0.360540      0.442710
H       0.559268      1.727277      0.915765
H      -0.351198      1.833280      -0.589487
H       1.433676      1.594168      -0.626390
Rotational constants (GHz): 8.2364400 5.1279600 3.5873000

```

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i383.1941 | 230.8022  | 355.9179  |
| 443.2684  | 546.7995  | 558.2650  |
| 617.1134  | 852.0705  | 901.2272  |
| 1029.1316 | 1049.1601 | 1218.6536 |
| 1380.8208 | 1435.8611 | 1453.2107 |
| 1480.1015 | 1681.0118 | 3057.9817 |
| 3137.4651 | 3212.1089 | 3831.8801 |

Zero-point correction (Hartree): 0.064866

#####  
H2O  
#####

Population analysis as 298K (%)  
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)  
Compound Qtot Erel Erel2 n\*Q\*MB %  
-----  
H2O 6.347e+33 0.00 0.00 6.347e+33 100  
Total 6.347e+33 100

H2O  
~~~  
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -76.34229069
E(CCSD/Aug-CC-pVTZ) (Hartree): -76.33364955
T1 diagnostic: 0.010015
E(MP2/Aug-CC-pVTZ) (Hartree): -76.32895555
E(MP3/Aug-CC-pVTZ) (Hartree): -76.33161303
E(RHF/Aug-CC-pVTZ) (Hartree): -76.06049404
E(RM062X/Aug-CC-pVTZ) (Hartree): -76.43009226
Point group : C2v
Electronic state : 1-A1
Cartesian coordinates (Angs):
H 0.000000 0.762659 -0.465620
O 0.000000 0.000000 0.116405
H 0.000000 -0.762659 -0.465620
Rotational constants (GHz): 833.4187400 431.0632300 284.1133200
Vibrational harmonic frequencies (cm-1):
1616.6399 3870.6385 3974.4091
Zero-point correction (Hartree): 0.021555

CH2OO
#####

Population analysis as 298K (%)
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)
Compound Qtot Erel Erel2 n*Q*MB %

TS.CH2O2+H2O.u 4.071e+37 0.00 0.00 8.141e+37 80.7
TS.CH2O2+H2O.d 3.878e+37 0.82 0.82 1.952e+37 19.3
Total 1.009e+38 100

TS.CH2O2+H2O.d
~~~~~  
E(RM062X/Aug-CC-pVTZ) (Hartree): -266.01045295  
Electronic state : 1-A  
Cartesian coordinates (Angs):  
C 0.004085 1.001578 0.249797  
O -0.891794 0.365014 -0.358394  
O -0.932992 -0.954505 0.184246  
H 0.319914 1.932207 -0.208641  
H 0.175211 0.797724 1.299533  
O 1.428283 -0.320889 -0.204181  
H 0.598352 -0.931050 -0.059570  
H 2.054045 -0.525317 0.496529  
Rotational constants (GHz): 12.0772300 7.2340400 5.0629200  
Vibrational harmonic frequencies (cm-1):  
i419.4412 335.3939 399.5467  
532.1860 606.9326 643.5986  
862.5507 902.6285 1150.2228  
1201.3322 1239.5316 1425.4834  
1582.5914 1679.0477 2485.9451  
3137.0105 3261.2706 3889.5268  
Zero-point correction (Hartree): 0.057717

TS.CH2O2+H2O.u  
~~~~~  
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -265.67504366
E(CCSD/Aug-CC-pVTZ) (Hartree): -265.63180878
T1 diagnostic: 0.026589
E(MP2/Aug-CC-pVTZ) (Hartree): -265.61879107
E(MP3/Aug-CC-pVTZ) (Hartree): -265.61927797
E(RHF/Aug-CC-pVTZ) (Hartree): -264.69167418
E(RM062X/Aug-CC-pVTZ) (Hartree): -266.01181904
Electronic state : 1-A
Cartesian coordinates (Angs):
C -0.002605 1.004599 -0.244771
O 0.877984 0.366366 0.384564
O 0.946631 -0.945857 -0.169682
H -0.331487 1.933947 0.209013
H -0.158126 0.805081 -1.297301
O -1.466003 -0.348317 0.000251
H -0.618536 -0.938216 -0.083620
H -1.745108 -0.405942 0.919468
Rotational constants (GHz): 12.0164000 7.1558500 5.0275700
Vibrational harmonic frequencies (cm-1):
i404.7452 308.2814 416.9781
534.8121 578.1826 608.4529

862.3356	913.9099	1183.1497
1234.2885	1247.7595	1427.4940
1606.2367	1622.8601	2544.1395
3135.4897	3261.3212	3877.2829

Zero-point correction (Hartree): 0.057781

Z-CH3CHOO
#####

Population analysis as 298K (%)
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)

Compound	Qtot	Erel	Erel2	n*Q*MB	%
TS.CH3CHO2s+H2O.hydroxyhydroperoxide.a	3.103e+38	0.00	0.00	6.205e+38	92
TS.CH3CHO2s+H2O.hydroxyhydroperoxide.b	2.615e+38	1.35	1.35	5.392e+37	7.99
Total				6.744e+38	100

TS.CH3CHO2s+H2O.hydroxyhydroperoxide.a
~~~~~  
E (CCSD(T)/Aug-CC-pVTZ) (Hartree): -304.92757493  
E (CCSD/Aug-CC-pVTZ) (Hartree): -304.87622456  
Tl diagnostic: 0.023431  
E (MP2/Aug-CC-pVTZ) (Hartree): -304.85419572  
E (MP3/Aug-CC-pVTZ) (Hartree): -304.86406630  
E (RHF/Aug-CC-pVTZ) (Hartree): -303.74814982  
E (RM062X/Aug-CC-pVTZ) (Hartree): -305.33049413  
Electronic state : 1-A  
Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.496357  | -0.186552 | 0.639820  |
| O | -0.639891 | -0.760573 | 0.630502  |
| O | -1.224678 | -0.618714 | -0.667149 |
| H | 0.842857  | 0.027876  | 1.649339  |
| C | 1.512187  | -0.312182 | -0.434573 |
| H | 2.204578  | 0.522803  | -0.387398 |
| H | 1.046009  | -0.380709 | -1.409578 |
| H | 2.061021  | -1.235125 | -0.225615 |
| O | -0.211797 | 1.538171  | -0.074024 |
| H | -0.822398 | 0.818107  | -0.552085 |
| H | -0.772407 | 1.968372  | 0.579222  |

Rotational constants (GHz): 5.8402500 5.0030200 3.7412600  
Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| 1475.9664 | 166.0686  | 261.2886  |
| 326.9924  | 387.0260  | 474.1827  |
| 585.5751  | 632.9037  | 655.5919  |
| 862.1330  | 916.6847  | 971.5011  |
| 1098.4757 | 1174.1919 | 1293.1901 |
| 1364.6847 | 1399.6386 | 1450.6926 |
| 1483.1954 | 1593.7923 | 1621.5526 |
| 2253.3834 | 3063.5081 | 3152.4117 |
| 3159.9509 | 3220.6672 | 3877.0108 |

Zero-point correction (Hartree): 0.085309

TS.CH3CHO2s+H2O.hydroxyhydroperoxide.b  
~~~~~  
E (RM062X/Aug-CC-pVTZ) (Hartree): -305.32848973
Electronic state : 1-A
Cartesian coordinates (Angs):

C	0.476201	-0.237788	0.634597
O	-0.693155	-0.735856	0.606096
O	-1.269740	-0.506398	-0.683854
H	0.834736	-0.079709	1.649142
C	1.480816	-0.408723	-0.447817
H	2.251256	0.354419	-0.371276
H	1.009445	-0.410819	-1.423336
H	1.952555	-1.380398	-0.274751
O	-0.198106	1.549296	0.110512
H	-0.838813	0.909564	-0.435351
H	0.336722	2.029676	-0.527146

Rotational constants (GHz): 5.8213900 5.0098100 3.7345400
Vibrational harmonic frequencies (cm-1):

1482.7218	214.6418	272.5750
317.1927	393.3948	456.2468
610.3323	635.6890	667.3900
863.3081	917.6571	977.4029
1101.2588	1164.8475	1203.7659
1367.3075	1395.0989	1459.5079
1488.4202	1564.5866	1679.6249
2276.6668	3063.1104	3144.6541
3166.8272	3212.3391	3893.7209

Zero-point correction (Hartree): 0.085449

E-CH3CHOO
#####

Population analysis as 298K (%)
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)

Compound	Qtot	Erel	Erel2	n*Q*MB	%
TS.CH3CHO2a+H2O.hydroxyhydroperoxide.a	4.034e+38	0.00	0.00	8.067e+38	72.3
TS.CH3CHO2a+H2O.hydroxyhydroperoxide.b	4.527e+38	0.64	0.64	3.098e+38	27.7
Total				1.117e+39	100

TS.CH3CHO2a+H2O.hydroxyhydroperoxide.a
~~~~~  
E (CCSD(T)/Aug-CC-pVTZ) (Hartree): -304.93218161  
E (CCSD/Aug-CC-pVTZ) (Hartree): -304.88116794  
Tl diagnostic: 0.022731  
E (MP2/Aug-CC-pVTZ) (Hartree): -304.85931884

E(MP3/Aug-CC-pVTZ) (Hartree): -304.86920222  
 E(RHF/Aug-CC-pVTZ) (Hartree): -303.75429847  
 E(RM062X/Aug-CC-pVTZ) (Hartree): -305.33507017  
 Electronic state : 1-A  
 Cartesian coordinates (Angs):  
 C -0.470799 -0.222800 0.365783  
 O 0.331777 -0.919429 -0.325213  
 O 1.660463 -0.591741 0.089294  
 H -0.190666 -0.009276 1.391495  
 C -1.885963 -0.150594 -0.060405  
 H -2.453431 -0.904093 0.488621  
 H -1.980192 -0.331046 -1.127451  
 H -2.284830 0.827026 0.200906  
 O 0.441663 1.518795 -0.000030  
 H 1.241237 0.818052 0.022528  
 H 0.337234 1.778698 -0.920769  
 Rotational constants (GHz): 7.2167500 4.2516700 2.9161300  
 Vibrational harmonic frequencies (cm-1):  
 i441.5284 148.3853 253.2146  
 292.0912 395.0726 463.3525  
 553.5688 594.2571 628.2477  
 887.3643 970.7646 1009.6113  
 1143.4049 1183.3231 1280.3354  
 1361.3418 1412.9010 1458.8672  
 1479.4101 1604.4557 1613.3681  
 2209.1687 3075.4991 3148.4854  
 3178.5684 3192.5715 3873.6497  
 Zero-point correction (Hartree): 0.085229

TS.CH3CHO2a+H2O.hydroxyhydroperoxide.b  
 ~~~~~  
 E(RM062X/Aug-CC-pVTZ) (Hartree): -305.33391507
 Electronic state : 1-A
 Cartesian coordinates (Angs):
 C -0.472284 -0.212766 0.373467
 O 0.327779 -0.931771 -0.296251
 O 1.658637 -0.591183 0.100883
 H -0.190000 0.017611 1.395459
 C -1.883939 -0.146596 -0.062503
 H -2.451438 -0.910717 0.471800
 H -1.958538 -0.312343 -1.132928
 H -2.293622 0.826609 0.196764
 O 0.421159 1.473737 -0.200670
 H 1.236544 0.788351 -0.110999
 H 0.533790 2.140401 0.482423
 Rotational constants (GHz): 7.2916600 4.2681400 2.9312400
 Vibrational harmonic frequencies (cm-1):
 i463.6330 118.6171 260.1721
 295.8092 405.6916 445.0667
 554.0334 636.3040 665.2036
 889.4254 966.5288 1008.7986
 1117.9587 1168.0563 1230.4326
 1352.0610 1410.3980 1452.9350
 1478.6467 1567.0903 1671.9281
 2167.0238 3076.3590 3152.4960
 3172.9839 3194.7397 3889.8868
 Zero-point correction (Hartree): 0.085086

 (CH3)2COO
 #####

Population analysis as 298K (%)
 Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)

Compound	Qtot	Erel	Erel2	n*Q*MB	%
TS.CH3_CH3_COO+H2O.u	2.486e+39	0.00	0.00	4.972e+39	85.6
TS.CH3_CH3_COO+H2O.d	2.510e+39	1.06	1.06	8.345e+38	14.4
Total				5.807e+39	100

TS.CH3_CH3_COO+H2O.d
 ~~~~~  
 E(RM062X/Aug-CC-pVTZ) (Hartree): -344.65034022  
 Electronic state : 1-A  
 Cartesian coordinates (Angs):  
 C -0.447063 -0.213187 0.049229  
 O 0.441692 -0.929514 -0.535303  
 O 1.740905 -0.569562 -0.057783  
 C -1.757140 -0.166473 -0.656308  
 H -1.616288 -0.314169 -1.722234  
 H -2.401705 -0.950061 -0.254469  
 H -2.230434 0.794766 -0.471013  
 C -0.421098 0.013666 1.525778  
 H -0.911211 -0.852795 1.978412  
 H 0.595789 0.076482 1.893453  
 H -0.997073 0.898644 1.784220  
 O 0.497296 1.454127 -0.481315  
 H 1.318991 0.766772 -0.318338  
 H 0.554594 2.135921 0.192983  
 Rotational constants (GHz): 4.3052500 2.9705300 2.8606300  
 Vibrational harmonic frequencies (cm-1):  
 i539.3724 105.0121 212.0065  
 230.4145 300.9288 330.1594  
 389.0056 421.1392 489.3773  
 571.5965 650.8047 659.0820  
 824.9259 929.3141 941.5624  
 995.6386 1076.5721 1082.9128  
 1205.2511 1308.3201 1401.1749  
 1422.4580 1441.3819 1461.5105  
 1475.7281 1499.1630 1539.0603  
 1645.8413 2044.3655 3064.9105

3078.5101 3145.9454 3155.2716  
3193.0690 3213.1139 3894.5808  
Zero-point correction (Hartree): 0.112542

TS.CH3\_CH3\_COO+H2O.u

~~~~~  
E (CCSD(T)/Aug-CC-pVTZ) (Hartree): -344.18382290
E (CCSD/Aug-CC-pVTZ) (Hartree): -344.12433297

T1 diagnostic: 0.021018
E (MP2/Aug-CC-pVTZ) (Hartree): -344.09390530
E (MP3/Aug-CC-pVTZ) (Hartree): -344.11241682
E (RHF/Aug-CC-pVTZ) (Hartree): -342.80774480
E (RM062X/Aug-CC-pVTZ) (Hartree): -344.65202757

Electronic state : 1-A

Cartesian coordinates (Angs):

C	0.446831	-0.159025	0.153995
O	-0.444634	-0.041699	1.070709
O	-1.740295	-0.261381	0.508122
C	1.759605	0.460506	0.490188
H	1.639889	1.235225	1.241921
H	2.429164	-0.314247	0.866632
H	2.198688	0.872591	-0.415957
C	0.424478	-1.278062	-0.832126
H	0.901363	-2.129352	-0.338547
H	-0.589587	-1.542872	-1.102708
H	1.004270	-1.010985	-1.710427
O	-0.512556	1.075169	-1.091924
H	-1.319342	0.595599	-0.550023
H	-0.470055	1.976817	-0.758496

Rotational constants (GHz): 4.3119700 2.9739800 2.8508600

Vibrational harmonic frequencies (cm-1):

i527.2066	123.3678	180.2803
221.7125	305.0469	337.7015
388.7840	409.5960	514.4764
579.2620	609.1724	649.0767
819.0691	931.2559	941.5915
992.5475	1076.1169	1082.0690
1276.9216	1310.8371	1403.5481
1421.2034	1450.3144	1458.3311
1475.8663	1497.2915	1581.9670
1610.9308	2014.3403	3067.0944
3077.7544	3149.1381	3161.9524
3184.1499	3220.0477	3874.7141

Zero-point correction (Hartree): 0.112536

Z-(C2H5)CHOO
#####

Population analysis as 298K (%)

Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)

Compound	Qtot	Erel	Erel2	n*Q*MB	%
TS.C2H5_H_COO+H2O.tu	2.637e+39	0.00	0.00	5.274e+39	47.3
TS.C2H5_H_COO+H2O.mu	3.891e+39	0.27	0.27	4.893e+39	43.9
TS.C2H5_H_COO+H2O.md	3.435e+39	1.40	1.40	6.495e+38	5.83
TS.C2H5_H_COO+H2O.td	2.737e+39	1.68	1.68	3.221e+38	2.89
Total				1.114e+40	100

TS.C2H5_H_COO+H2O.md

~~~~~  
E (RM062X/Aug-CC-pVTZ) (Hartree): -344.63656181

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.008902 | 0.182078  | 0.685102  |
| O | -0.584976 | -0.950412 | 0.642956  |
| O | -1.051207 | -1.183660 | -0.690525 |
| H | 0.092241  | 0.557880  | 1.701772  |
| C | 0.972691  | 0.653544  | -0.334396 |
| C | 2.280400  | -0.110699 | -0.094562 |
| H | 0.598265  | 0.451857  | -1.332062 |
| H | 1.121835  | 1.724264  | -0.200226 |
| H | 2.123916  | -1.174610 | -0.262020 |
| H | 2.649033  | 0.031199  | 0.921521  |
| H | 3.044512  | 0.242460  | -0.783589 |
| O | -1.613840 | 1.110485  | -0.003269 |
| H | -1.651672 | 0.200297  | -0.531239 |
| H | -1.443082 | 1.805811  | -0.644317 |

Rotational constants (GHz): 5.1232600 2.6068000 2.1416400

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i458.6678 | 71.5457   | 202.4688  |
| 222.9885  | 297.8883  | 339.7929  |
| 395.1470  | 501.7647  | 608.0794  |
| 631.0630  | 663.9761  | 818.5253  |
| 885.1701  | 921.5200  | 1011.6232 |
| 1028.6721 | 1097.6127 | 1177.4100 |
| 1193.6858 | 1288.9965 | 1334.0335 |
| 1373.0822 | 1406.7034 | 1480.2086 |
| 1500.8729 | 1506.7976 | 1561.5502 |
| 1676.8479 | 2325.2426 | 3071.3525 |
| 3099.5856 | 3140.7191 | 3155.2948 |
| 3159.6235 | 3183.8570 | 3893.6531 |

Zero-point correction (Hartree): 0.114426

TS.C2H5\_H\_COO+H2O.mu

~~~~~  
E (RM062X/Aug-CC-pVTZ) (Hartree): -344.63839094

Electronic state : 1-A

Cartesian coordinates (Angs):

C	0.014096	-0.209663	0.684815
O	0.578928	0.931006	0.667583

```

O      1.010172      1.210465      -0.667821
H      -0.066153      -0.615359      1.692871
C      -0.971915      -0.672222      -0.330978
C      -2.270233      0.106897      -0.088648
H      -0.596574      -0.484188      -1.330058
H      -1.119865      -1.741632      -0.196917
H      -2.104371      1.169081      -0.258844
H      -2.640613      -0.028916      0.927876
H      -3.038507      -0.240675      -0.775864
O      1.544458      -1.146458      -0.178731
H      1.566320      -0.197043      -0.635755
H      2.299615      -1.171447      0.417306
Rotational constants (GHz):      5.0838700      2.6378600      2.1620600
Vibrational harmonic frequencies (cm-1):
i451.9340      61.2200      200.3039
224.5430      303.3830      338.2392
385.6338      528.3610      595.9565
631.9056      649.3335      811.2292
885.4416      921.0078      1012.0237
1025.9808      1096.8257      1182.7248
1280.3770      1289.7716      1336.4988
1375.9625      1406.0227      1480.2052
1501.2760      1507.9083      1587.9450
1625.0231      2303.1556      3069.8582
3116.7310      3138.7688      3143.7791
3159.2040      3193.7129      3874.9399
Zero-point correction (Hartree): 0.114467

TS.C2H5_H_COO+H2O.td
~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -344.63572239
Electronic state : 1-A
Cartesian coordinates (Angs):
C      -0.070273      -0.325341      0.660640
O      -1.299090      -0.637217      0.571741
O      -1.763505      -0.317755      -0.745996
H      0.262118      -0.228621      1.693717
C      0.959534      -0.650025      -0.368310
C      2.301877      0.007143      -0.083408
H      1.056026      -1.740468      -0.301715
H      0.574556      -0.433694      -1.359431
H      2.661718      -0.243211      0.914905
H      2.240040      1.092709      -0.148748
H      3.047641      -0.328823      -0.800186
O      -0.441116      1.545812      0.133367
H      -1.141798      1.008898      -0.453251
H      0.182557      1.955826      -0.471719
Rotational constants (GHz):      5.5960200      2.4498300      2.1026100
Vibrational harmonic frequencies (cm-1):
i483.6428      100.5099      191.0212
213.5343      295.1398      370.3705
388.3252      467.7478      609.6075
643.6647      693.6638      757.5481
873.0232      929.4584      983.2413
1061.9470      1115.9572      1178.8058
1203.4343      1267.6884      1330.0939
1371.7347      1425.9527      1470.8123
1502.7680      1507.1106      1559.0742
1685.1092      2244.6191      3041.6599
3072.1110      3133.3167      3147.2744
3153.6709      3172.0553      3892.9354
Zero-point correction (Hartree): 0.114034

TS.C2H5_H_COO+H2O.tu
~~~~~
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -344.17058463
E(CCSD/Aug-CC-pVTZ) (Hartree): -344.11129264
T1 diagnostic: 0.021592
E(MP2/Aug-CC-pVTZ) (Hartree): -344.07952349
E(MP3/Aug-CC-pVTZ) (Hartree): -344.09897598
E(RHF/Aug-CC-pVTZ) (Hartree): -342.79574479
E(RM062X/Aug-CC-pVTZ) (Hartree): -344.63839371
Electronic state : 1-A
Cartesian coordinates (Angs):
C      -0.063127      -0.320630      0.667871
O      -1.295881      -0.626532      0.589640
O      -1.758823      -0.343228      -0.735469
H      0.271643      -0.200177      1.698811
C      0.967827      -0.660001      -0.351231
C      2.295575      0.031930      -0.084896
H      1.073300      -1.748017      -0.256894
H      0.582941      -0.464136      -1.346128
H      2.658500      -0.176798      0.922561
H      2.187810      1.108151      -0.197560
H      3.049749      -0.316340      -0.787007
O      -0.337575      1.528361      -0.037490
H      -1.067300      0.959519      -0.559766
H      -0.820067      2.061204      0.602062
Rotational constants (GHz):      5.6198000      2.4656000      2.1172500
Vibrational harmonic frequencies (cm-1):
i480.3360      98.7931      197.9839
220.1821      305.3966      363.8358
381.4598      484.2858      593.5266
642.0698      665.4544      754.3018
874.6542      932.3713      982.5915
1062.3291      1115.5835      1185.9654
1270.1805      1300.7841      1332.9511
1373.8482      1417.5102      1465.1884
1502.9637      1513.8346      1591.2833
1617.2865      2203.7913      3037.8877
3070.7889      3136.1957      3138.3208
3164.8756      3177.4336      3878.4098

```


Zero-point correction (Hartree): 0.114032

E-(C2H5)CHOO
#####

Population analysis as 298K (%)
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)
Compound Qtot Erel Erel2 n*Q*MB %

TS.C2H5_H_COO+H2O.mu 3.891e+39 0.00 0.00 7.781e+39 88.3
TS.C2H5_H_COO+H2O.md 3.435e+39 1.12 1.12 1.033e+39 11.7
Total 8.814e+39 100

TS.C2H5_H_COO+H2O.md

~~~~~

E(RM062X/Aug-CC-pVTZ) (Hartree): -344.63656181

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.008902 | 0.182078  | 0.685102  |
| O | -0.584976 | -0.950412 | 0.642956  |
| O | -1.051207 | -1.183660 | -0.690525 |
| H | 0.092241  | 0.557880  | 1.701772  |
| C | 0.972691  | 0.653544  | -0.334396 |
| C | 2.280400  | -0.110699 | -0.094562 |
| H | 0.598265  | 0.451857  | -1.332062 |
| H | 1.121835  | 1.724264  | -0.200226 |
| H | 2.123916  | -1.174610 | -0.262020 |
| H | 2.649033  | 0.031199  | 0.921521  |
| H | 3.044512  | 0.242460  | -0.783589 |
| O | -1.613840 | 1.110485  | -0.003269 |
| H | -1.651672 | 0.200297  | -0.531239 |
| H | -1.443082 | 1.805811  | -0.644317 |

Rotational constants (GHz): 5.1232600 2.6068000 2.1416400

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i458.6678 | 71.5457   | 202.4688  |
| 222.9885  | 297.8883  | 339.7929  |
| 395.1470  | 501.7647  | 608.0794  |
| 631.0630  | 663.9761  | 818.5253  |
| 885.1701  | 921.5200  | 1011.6232 |
| 1028.6721 | 1097.6127 | 1177.4100 |
| 1193.6858 | 1288.9965 | 1334.0335 |
| 1373.0822 | 1406.7034 | 1480.2086 |
| 1500.8729 | 1506.7976 | 1561.5502 |
| 1676.8479 | 2325.2426 | 3071.3525 |
| 3099.5856 | 3140.7191 | 3155.2948 |
| 3159.6235 | 3183.8570 | 3893.6531 |

Zero-point correction (Hartree): 0.114426

TS.C2H5\_H\_COO+H2O.mu

~~~~~

E(RM062X/Aug-CC-pVTZ) (Hartree): -344.63839094

Electronic state : 1-A

Cartesian coordinates (Angs):

C	0.014096	-0.209663	0.684815
O	0.578928	0.931006	0.667583
O	1.010172	1.210465	-0.667821
H	-0.066153	-0.615359	1.692871
C	-0.971915	-0.672222	-0.330978
C	-2.270233	0.106897	-0.088648
H	-0.596574	-0.484188	-1.330058
H	-1.119865	-1.741632	-0.196917
H	-2.104371	1.169081	-0.258844
H	-2.640613	-0.028916	0.927876
H	-3.038507	-0.240675	-0.775864
O	1.544458	-1.146458	-0.178731
H	1.566320	-0.197043	-0.635755
H	2.299615	-1.171447	0.417306

Rotational constants (GHz): 5.0838700 2.6378600 2.1620600

Vibrational harmonic frequencies (cm-1):

i451.9340	61.2200	200.3039
224.5430	303.3830	338.2392
385.6338	528.3610	595.9565
631.9056	649.3335	811.2292
885.4416	921.0078	1012.0237
1025.9808	1096.8257	1182.7248
1280.3770	1289.7716	1336.4988
1375.9625	1406.0227	1480.2052
1501.2760	1507.9083	1587.9450
1625.0231	2303.1556	3069.8582
3116.7310	3138.7688	3143.7791
3159.2040	3193.7129	3874.9399

Zero-point correction (Hartree): 0.114467

E-(CH3)(C2H5)COO
#####

Population analysis as 298K (%)
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)
Compound Qtot Erel Erel2 n*Q*MB %

TS.CH3_C2H5_COO+H2O.cu 1.902e+40 0.00 0.00 3.804e+40 50.2
TS.CH3_C2H5_COO+H2O.pu 2.618e+40 0.91 0.91 1.125e+40 14.8
TS.CH3_C2H5_COO+H2O.cd 1.647e+40 0.69 0.69 1.033e+40 13.6
TS.CH3_C2H5_COO+H2O.mu 1.602e+40 0.69 0.69 9.966e+39 13.1
TS.CH3_C2H5_COO+H2O.pd 4.886e+40 1.91 1.91 3.867e+39 5.1
TS.CH3_C2H5_COO+H2O.md 1.655e+40 1.57 1.57 2.346e+39 3.1
Total 7.580e+40 100

```

TS.CH3_C2H5_COO+H2O.cd
~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -383.95889001
Electronic state : 1-A
Cartesian coordinates (Angs):
C      0.042149      -0.406474      -0.222587
O      0.327616      0.674643      -0.850865
O      1.669601      1.069892      -0.547896
C      0.987062      -1.563918      -0.198354
H      0.766117      -2.217787      0.641434
H      2.016601      -1.227675      -0.182559
H      0.810835      -2.125284      -1.119951
C     -1.419886      -0.679146      -0.071001
C     -2.279642      0.572769      -0.012169
H     -1.704424      -1.324582      -0.908218
H     -1.531788      -1.281290      0.831113
H     -2.216543      1.135328      -0.940381
H     -1.940468      1.215909      0.797613
H     -3.319675      0.304683      0.162283
O      0.596077      0.414229      1.505909
H      1.288458      0.866402      0.798977
H      1.106437      -0.155201      2.087173
Rotational constants (GHz):      3.3663000      2.0430700      1.8673900
Vibrational harmonic frequencies (cm-1):
i549.3459      79.1874      186.3143
193.5984      225.2596      256.9452
321.8454      341.0732      403.4976
449.9287      496.1781      587.4545
648.2060      654.5412      761.1048
815.5047      938.8812      978.4977
1013.5062      1026.5449      1104.9055
1116.9257      1199.2426      1247.2165
1289.8531      1390.9739      1416.4409
1420.2748      1448.1786      1454.8994
1490.9657      1500.7351      1510.0665
1526.3643      1630.3757      2014.8032
3054.5053      3067.2063      3083.6252
3111.3440      3146.9635      3157.8659
3164.5267      3212.3233      3896.6230
Zero-point correction (Hartree): 0.141327

```

```

TS.CH3_C2H5_COO+H2O.cu
~~~~~
E(CCS(D)/Aug-CC-pVTZ) (Hartree): -383.42697727
E(CCS(D)/Aug-CC-pVTZ) (Hartree): -383.35946766
T1 diagnostic: 0.019687
E(MP2/Aug-CC-pVTZ) (Hartree): -383.31942464
E(MP3/Aug-CC-pVTZ) (Hartree): -383.34734712
E(RHF/Aug-CC-pVTZ) (Hartree): -381.85508265
E(RM062X/Aug-CC-pVTZ) (Hartree): -383.95998775
Electronic state : 1-A
Cartesian coordinates (Angs):
C      0.039715      -0.401387      -0.208618
O      0.313305      0.686672      -0.833292
O      1.668982      1.061796      -0.571359
C      0.972672      -1.566092      -0.212392
H      0.751648      -2.222440      0.623794
H      2.005355      -1.242648      -0.187420
H      0.786916      -2.104813      -1.145454
C     -1.419649      -0.672083      -0.020404
C     -2.302531      0.564788      -0.043592
H     -1.707824      -1.376954      -0.806036
H     -1.511533      -1.215848      0.920578
H     -2.237662      1.075891      -1.000937
H     -2.001580      1.272078      0.728526
H     -3.339517      0.288133      0.134823
O      0.759839      0.281253      1.526204
H      1.388112      0.770232      0.786153
H      0.187846      0.967243      1.883575
Rotational constants (GHz):      3.3819200      2.0171900      1.8465300
Vibrational harmonic frequencies (cm-1):
i533.4146      81.5232      160.7216
183.9840      217.4595      248.2074
334.0575      339.9596      397.7387
448.3262      519.9542      585.0946
607.1887      648.9536      761.3337
806.2872      940.3751      980.8653
1016.7708      1024.5000      1104.3209
1114.1949      1246.4722      1265.8485
1298.2545      1395.4602      1420.3842
1422.0058      1451.4371      1457.7226
1489.4840      1499.0720      1506.0734
1571.6452      1606.3285      1989.3288
3060.7044      3070.0913      3080.5587
3109.9948      3148.2576      3161.6157
3165.1334      3221.6120      3877.2028
Zero-point correction (Hartree): 0.141330

```

```

TS.CH3_C2H5_COO+H2O.md
~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -383.95765872
Electronic state : 1-A
Cartesian coordinates (Angs):
C      0.024843      -0.375052      0.000588
O      1.031765      -0.717040      -0.716793
O      2.232704      -0.161331      -0.170323
C      0.071841      -0.467881      1.489967
H     -0.580409      0.267993      1.951046
H      1.091804      -0.369769      1.841815
H     -0.312156      -1.459858      1.746992
C     -1.282772      -0.487042      -0.717416
C     -2.436039      0.233163      -0.032909

```

```

H      -1.125395      -0.114617      -1.727326
H      -1.492748      -1.558239      -0.796584
H      -2.197040      1.286632      0.104985
H      -2.667762      -0.203099      0.937614
H      -3.330729      0.166520      -0.648129
O       0.533100      1.556248      -0.157105
H       1.494631      1.060970      -0.142925
H       0.472014      2.081320      0.644898
Rotational constants (GHz):   4.0537000      1.8047800      1.7440100
Vibrational harmonic frequencies (cm-1):
i517.2751      70.0651      177.6191
204.7319      263.7444      280.7089
306.5215      340.9267      406.1638
451.0554      489.7363      566.1818
640.7415      652.8445      764.5813
813.3176      931.0926      973.2962
999.2364      1037.4902      1106.9580
1110.3118      1200.2592      1267.3010
1321.9878      1362.2277      1407.7631
1414.6666      1448.5924      1461.1562
1491.8672      1508.4364      1512.1489
1531.1515      1647.0430      2048.2525
3058.3010      3061.6344      3076.9220
3134.9145      3151.3236      3154.0829
3155.5644      3212.0750      3896.1010
Zero-point correction (Hartree): 0.141499

```

TS.CH3_C2H5_COO+H2O.mu

```

~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -383.95907363
Electronic state : 1-A
Cartesian coordinates (Angs):
C       0.025215      -0.364542      -0.100913
O       1.034049      -0.494556      -0.884918
O       2.231104      -0.112607      -0.199458
C       0.066479      -0.847738      1.309228
H      -0.530869      -0.208897      1.951366
H       1.089802      -0.897269      1.660527
H      -0.376722      -1.847971      1.304106
C      -1.286707      -0.285167      -0.817916
C      -2.431157      0.239654      0.039756
H      -1.141603      0.320697      -1.710926
H      -1.502229      -1.301909      -1.160969
H      -2.175993      1.207171      0.469213
H      -2.665511      -0.443720      0.854124
H      -3.326875      0.354515      -0.566796
O       0.543413      1.511569      0.420628
H       1.494297      1.023014      0.255176
H       0.424192      2.105873      -0.326772
Rotational constants (GHz):   4.0536000      1.8080100      1.7432100
Vibrational harmonic frequencies (cm-1):
i507.5532      85.1872      159.1836
187.4199      257.0586      282.6874
309.8610      344.6953      400.7226
453.3904      515.0713      572.2095
601.5132      626.7703      771.8842
807.6693      931.8452      976.0443
998.6304      1038.8338      1108.2001
1111.8515      1255.5742      1280.7589
1325.0454      1367.7036      1413.1057
1418.6914      1445.5911      1464.6238
1492.4914      1506.4197      1516.3104
1568.2019      1613.8730      2018.7828
3058.2709      3063.0853      3078.9062
3124.0722      3152.4263      3156.0977
3165.9084      3218.7679      3873.7091
Zero-point correction (Hartree): 0.141518

```

TS.CH3_C2H5_COO+H2O.pd

```

~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -383.95725893
Electronic state : 1-A
Cartesian coordinates (Angs):
C      -0.062294      0.051296      0.095917
O       0.462113      -1.038472      -0.330276
O       1.839683      -1.097909      0.054236
C       0.167663      0.529946      1.492406
H      -0.040732      1.594178      1.568704
H       1.170735      0.292560      1.825030
H      -0.547568      -0.002785      2.124980
C      -1.323966      0.431238      -0.608797
C      -2.519649      -0.345414      -0.048798
H      -1.470590      1.503389      -0.486670
H      -1.188422      0.221551      -1.667271
H      -2.688054      -0.116180      1.002590
H      -2.360433      -1.417654      -0.148057
H      -3.420548      -0.079965      -0.597756
O       1.367629      1.125126      -0.780834
H       1.900513      0.236292      -0.484527
H       1.719168      1.856254      -0.266393
Rotational constants (GHz):   3.8298200      1.8104200      1.7094700
Vibrational harmonic frequencies (cm-1):
i501.7215      25.8539      168.7610
192.0201      228.5658      265.4942
318.0002      340.0077      395.0065
437.0898      519.8847      584.3096
648.7175      677.7441      795.7252
806.9238      934.5185      969.8404
1013.2965      1026.4466      1091.2411
1114.9608      1199.5204      1253.2220
1311.5912      1359.0945      1403.9043
1414.8659      1453.8090      1481.4975

```

1497.5978 1506.5285 1512.2965
1537.4797 1652.5112 2078.2388
3067.7838 3076.4997 3100.9625
3140.5437 3148.3183 3155.3019
3163.1828 3212.3339 3895.0486
Zero-point correction (Hartree): 0.141649

TS.CH3_C2H5_COO+H2O.pu

~~~~~  
E(RM062X/Aug-CC-pVTZ) (Hartree): -383.95892688

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.059866 | -0.007738 | 0.068264  |
| O | 0.551954  | -0.894780 | -0.630134 |
| O | 1.906769  | -1.004869 | -0.183918 |
| C | 0.078677  | 0.053618  | 1.552863  |
| H | -0.286491 | 1.008279  | 1.920759  |
| H | 1.102263  | -0.115480 | 1.860576  |
| H | -0.546642 | -0.747769 | 1.955022  |
| C | -1.314615 | 0.506130  | -0.562814 |
| C | -2.537572 | -0.293741 | -0.104379 |
| H | -1.418693 | 1.552856  | -0.278130 |
| H | -1.202653 | 0.448053  | -1.644041 |
| H | -2.701448 | -0.187548 | 0.966616  |
| H | -2.414723 | -1.351274 | -0.333247 |
| H | -3.426466 | 0.065940  | -0.618021 |
| O | 1.368443  | 1.360829  | -0.213218 |
| H | 1.918736  | 0.431608  | -0.206010 |
| H | 1.359044  | 1.656275  | -1.128974 |

Rotational constants (GHz): 3.9256300 1.7853300 1.6933300

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i501.0525 | 55.3630   | 162.4132  |
| 168.3594  | 239.7874  | 263.0257  |
| 325.6957  | 351.5800  | 397.5953  |
| 426.5779  | 533.0793  | 598.2452  |
| 622.7373  | 646.5721  | 797.1745  |
| 802.2288  | 935.5144  | 975.9199  |
| 1015.6843 | 1026.1134 | 1092.2210 |
| 1112.1108 | 1258.9405 | 1267.2781 |
| 1321.0017 | 1367.0561 | 1408.4384 |
| 1416.6890 | 1454.7646 | 1479.3606 |
| 1494.9869 | 1506.4261 | 1513.8498 |
| 1571.1996 | 1613.5026 | 2041.8619 |
| 3070.6031 | 3077.0664 | 3091.8630 |
| 3137.0037 | 3154.9950 | 3157.8045 |
| 3158.5089 | 3221.9178 | 3874.9596 |

Zero-point correction (Hartree): 0.141720

#####  
Z-(C2H5)(CH3)COO  
#####

Population analysis as 298K (%)

Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)

| Compound               | Qtot      | Erel | Erel2 | n*Q*MB    | %    |
|------------------------|-----------|------|-------|-----------|------|
| TS.C2H5_CH3_COO+H2O.mu | 1.773e+40 | 0.00 | 0.00  | 3.547e+40 | 53.5 |
| TS.C2H5_CH3_COO+H2O.tu | 1.148e+40 | 0.06 | 0.06  | 2.084e+40 | 31.5 |
| TS.C2H5_CH3_COO+H2O.md | 2.214e+40 | 1.03 | 1.03  | 7.749e+39 | 11.7 |
| TS.C2H5_CH3_COO+H2O.pd | 1.218e+40 | 1.42 | 1.42  | 2.205e+39 | 3.33 |
| Total                  |           |      |       | 6.626e+40 | 100  |

TS.C2H5\_CH3\_COO+H2O.md

~~~~~

E(RM062X/Aug-CC-pVTZ) (Hartree): -383.95822886

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-0.046196	-0.418115	-0.144672
O	-0.537878	0.322901	-1.070684
O	-0.926352	1.577087	-0.502278
C	0.015739	-1.866204	-0.485694
H	-0.686056	-2.099673	-1.280100
H	1.030553	-2.117882	-0.797047
H	-0.222069	-2.446292	0.403191
C	0.945889	0.133731	0.839556
C	2.218033	0.512346	0.074241
H	0.546085	1.018833	1.320694
H	1.148797	-0.630730	1.589355
H	1.988980	1.295187	-0.646356
H	2.643511	-0.339103	-0.456383
H	2.968168	0.885087	0.768503
O	-1.674567	-0.202729	0.951634
H	-1.589074	0.766552	0.476303
H	-1.519313	-0.080602	1.891874

Rotational constants (GHz): 2.9920500 2.2901600 1.8730500

Vibrational harmonic frequencies (cm-1):

i535.7649	78.9049	117.5079
204.7184	221.6307	260.5908
312.4315	345.0215	393.1791
421.7851	550.6189	582.1409
650.0382	677.3770	783.1333
819.5025	939.1999	988.2652
1011.4263	1033.1512	1084.4331
1103.9467	1205.4992	1257.4055
1312.3975	1360.7069	1405.4734
1416.2518	1446.6692	1476.7619
1486.9606	1501.7218	1508.4303
1532.6575	1639.3870	2055.2589
3072.9542	3080.1145	3096.7500
3141.8200	3153.4381	3158.9924
3182.8120	3191.2092	3894.0124

Zero-point correction (Hartree): 0.141603

TS.C2H5_CH3_COO+H2O.mu
~~~~~  
E (CCSD(T)/Aug-CC-pVTZ) (Hartree): -383.42731269  
E (CCSD/Aug-CC-pVTZ) (Hartree): -383.35961514  
T1 diagnostic: 0.019745  
E (MP2/Aug-CC-pVTZ) (Hartree): -383.31998376  
E (MP3/Aug-CC-pVTZ) (Hartree): -383.34744706  
E (RHF/Aug-CC-pVTZ) (Hartree): -381.85429243  
E (RM062X/Aug-CC-pVTZ) (Hartree): -383.96002967  
Electronic state : 1-A  
Cartesian coordinates (Angs):  

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.064386 | -0.426475 | -0.140583 |
| O | -0.514515 | 0.340829  | -1.068116 |
| O | -0.811201 | 1.619319  | -0.499469 |
| C | -0.088346 | -1.877673 | -0.476042 |
| H | -0.783441 | -2.079159 | -1.285951 |
| H | 0.916049  | -2.189111 | -0.767164 |
| H | -0.366227 | -2.437559 | 0.414813  |
| C | 0.955627  | 0.061663  | 0.845289  |
| C | 2.218509  | 0.444222  | 0.067709  |
| H | 0.581523  | 0.924522  | 1.382343  |
| H | 1.148772  | -0.738493 | 1.558039  |
| H | 1.993935  | 1.266054  | -0.609595 |
| H | 2.610139  | -0.391343 | -0.513054 |
| H | 2.993787  | 0.763306  | 0.761025  |
| O | -1.594572 | -0.055090 | 1.070453  |
| H | -1.464481 | 0.881199  | 0.545137  |
| H | -2.396173 | -0.450301 | 0.713221  |

Rotational constants (GHz): 2.9523700 2.3242900 1.8913000  
Vibrational harmonic frequencies (cm-1):  

|           |           |           |
|-----------|-----------|-----------|
| i519.4580 | 79.8099   | 160.6580  |
| 198.1707  | 227.5779  | 251.3543  |
| 319.6390  | 348.6425  | 396.1638  |
| 407.4205  | 577.5458  | 591.9916  |
| 628.5441  | 655.1971  | 776.7537  |
| 812.3814  | 938.0070  | 987.2345  |
| 1012.6642 | 1032.0648 | 1084.9266 |
| 1104.9075 | 1249.8554 | 1270.2310 |
| 1324.9082 | 1365.6408 | 1403.8300 |
| 1415.3995 | 1454.8496 | 1478.1660 |
| 1487.9549 | 1501.3966 | 1511.2419 |
| 1575.0920 | 1614.3738 | 2029.7452 |
| 3069.8637 | 3076.7652 | 3110.2240 |
| 3138.3329 | 3147.6146 | 3159.6624 |
| 3183.5059 | 3193.8083 | 3870.9046 |

Zero-point correction (Hartree): 0.141759

TS.C2H5\_CH3\_COO+H2O.pd  
~~~~~  
E (RM062X/Aug-CC-pVTZ) (Hartree): -383.95727585
Electronic state : 1-A
Cartesian coordinates (Angs):

C	-0.075257	-0.455257	-0.207931
O	-1.310979	-0.511973	-0.554523
O	-1.892745	0.792683	-0.475412
C	0.502506	-1.772413	0.177872
H	-0.292111	-2.472112	0.416139
H	1.108851	-2.155095	-0.644849
H	1.148317	-1.638015	1.042691
C	0.831767	0.613844	-0.743731
C	2.186092	0.696288	-0.054625
H	0.966755	0.334214	-1.795419
H	0.303246	1.560757	-0.743803
H	2.760855	-0.220985	-0.175100
H	2.080017	0.882329	1.014233
H	2.769898	1.510274	-0.479048
O	-0.569371	0.432685	1.499126
H	-1.313433	0.829021	0.802606
H	-0.018286	1.167679	1.779511

Rotational constants (GHz): 3.3319000 2.0561700 1.8566100
Vibrational harmonic frequencies (cm-1):

i574.9584	123.8397	164.4884
186.9142	245.2043	283.5775
312.7631	316.7600	411.2996
445.6970	508.1335	580.0018
652.2578	653.7623	774.0533
789.2091	941.2286	981.5552
997.7475	1044.9650	1093.7688
1100.9131	1191.5456	1265.8355
1303.3179	1354.7005	1414.7246
1422.3838	1446.1810	1468.5316
1485.8417	1503.9234	1511.4232
1524.6890	1624.1065	1988.3886
3042.3409	3073.7409	3076.6516
3136.3571	3149.2725	3152.9916
3176.7326	3192.2654	3897.1627

Zero-point correction (Hartree): 0.141272

TS.C2H5_CH3_COO+H2O.tu
~~~~~  
E (RM062X/Aug-CC-pVTZ) (Hartree): -383.95959920  
Electronic state : 1-A  
Cartesian coordinates (Angs):  

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.070233  | 0.452704  | -0.225647 |
| O | 1.309638  | 0.506414  | -0.564244 |
| O | 1.890125  | -0.796613 | -0.465054 |
| C | -0.513518 | 1.775306  | 0.136207  |
| H | 0.273691  | 2.493300  | 0.346034  |
| H | -1.131812 | 2.132023  | -0.689008 |
| H | -1.157814 | 1.653990  | 1.004751  |

```

C      -0.834936      -0.628649      -0.732769
C      -2.174315      -0.711452      -0.016757
H      -0.978915      -0.367215      -1.788398
H      -0.303565      -1.573136      -0.713685
H      -2.758370      0.201462      -0.130515
H      -2.019925      -0.898852      1.044101
H      -2.761739      -1.529832      -0.427787
O       0.474140      -0.535520      1.468997
H       1.247472      -0.884896      0.779896
H       0.914958      0.051455      2.090803
Rotational constants (GHz):      3.3245800      2.0768800      1.8588700
Vibrational harmonic frequencies (cm-1):
i561.6982      114.5920      176.2940
197.5751      252.4042      286.8870
315.8690      324.8868      399.0843
453.7240      524.1765      596.4165
615.1385      647.2541      769.8621
780.9933      940.2987      984.1867
998.1960      1043.8928      1097.7212
1105.6436      1241.0445      1273.2270
1317.5795      1356.7659      1413.0986
1417.3998      1455.5205      1467.4197
1483.6841      1509.3574      1515.1462
1573.2097      1603.0770      1942.3378
3038.6131      3075.3442      3076.5456
3140.0864      3148.3384      3158.0451
3184.0256      3185.1275      3875.9088
Zero-point correction (Hartree): 0.141420

```

```

#####
Z- (iC3H7) CHOO
#####

```

```

Population analysis as 298K (%)
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)
Compound      Qtot      Erel      Erel2      n*Q*MB      %
-----
TS.iC3H7_H_COO+H2O.pu 1.660e+40 0.00      0.00      3.319e+40 92.7
TS.iC3H7_H_COO+H2O.pd 1.594e+40 1.53      1.53      2.408e+39 6.72
TS.iC3H7_H_COO+H2O.mu 1.274e+40 3.19      3.19      1.173e+38 0.328
TS.iC3H7_H_COO+H2O.tu 1.849e+40 3.59      3.59      8.633e+37 0.241
TS.iC3H7_H_COO+H2O.td 1.640e+40 4.78      4.78      1.018e+37 0.0284
TS.iC3H7_H_COO+H2O.md 1.391e+40 4.74      4.74      9.320e+36 0.026
Total      3.583e+40 100

```

```

TS.iC3H7_H_COO+H2O.md
~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -383.94121412
Electronic state : 1-A
Cartesian coordinates (Angs):
C -0.267924 -0.447702 -0.792127
O -1.461895 -0.029592 -0.894044
O -1.830048 0.725243 0.265089
H -0.090032 -1.305935 -1.440604
C 0.966533 0.331764 -0.451384
H 1.185687 0.762801 -1.441339
C 0.869409 1.477605 0.545463
C 2.115644 -0.619005 -0.119977
H 0.621400 1.108380 1.539920
H 0.107721 2.194999 0.262212
H 1.840762 1.971100 0.598399
H 2.166393 -1.462006 -0.809198
H 2.014239 -1.015323 0.890008
H 3.060829 -0.081891 -0.170091
O -0.670422 -1.313492 0.977536
H -1.285574 -0.459348 1.007677
H -0.024477 -1.226022 1.682516
Rotational constants (GHz): 3.5338700 2.0277300 1.7919500
Vibrational harmonic frequencies (cm-1):
i449.2830 71.3733 201.3432
222.0975 251.6365 296.2542
312.0348 360.5972 374.0682
425.5228 516.2714 594.0684
636.8580 698.6519 829.6817
892.0492 942.1804 976.3113
986.9941 1014.0831 1117.7758
1166.8601 1189.0520 1224.1027
1304.7184 1366.3412 1399.0313
1413.3692 1433.5356 1481.8774
1489.0888 1503.4418 1510.2333
1558.0356 1683.8450 2309.8099
2985.2950 3069.0560 3071.9080
3134.8387 3136.5158 3141.7456
3148.7681 3190.8070 3903.4734
Zero-point correction (Hartree): 0.142467

```

```

TS.iC3H7_H_COO+H2O.mu
~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -383.94368245
Electronic state : 1-A
Cartesian coordinates (Angs):
C      -0.260523      -0.458535      -0.787851
O      -1.458781      -0.049858      -0.904005
O      -1.830143      0.736073      0.231201
H      -0.078123      -1.332043      -1.416361
C       0.973419      0.321302      -0.456148
H       1.193069      0.743023      -1.450777
C       0.880537      1.470005      0.538549
C       2.109269      -0.638546      -0.105756
H       0.642628      1.091321      1.530713
H       0.121469      2.190917      0.256824

```

```

H      1.853482      1.960943      0.583208
H      2.186574     -1.461773     -0.817308
H      1.945745     -1.053766      0.886356
H      3.055440     -0.100743     -0.110106
O     -0.561396     -1.174255      1.088207
H     -1.215305     -0.342082      1.036091
H     -1.118628     -1.956843      1.045364
Rotational constants (GHz):      3.5654500      2.0225100      1.8178000
Vibrational harmonic frequencies (cm-1):
i455.8112      72.8907      210.5031
225.7235      257.6290      297.1733
307.3903      369.0093      377.7718
445.6281      511.3516      586.6415
616.8409      690.7568      837.5457
891.4773      942.8950      977.0360
987.8734      1012.8049      1116.3813
1171.3764      1224.7820      1299.0739
1303.9556      1367.2113      1395.9866
1407.4724      1430.2289      1484.7004
1496.6071      1504.7020      1516.5503
1586.2514      1615.4751      2223.9914
2978.2839      3068.6534      3074.6414
3127.4554      3138.6105      3144.8561
3161.9071      3190.7009      3884.6246
Zero-point correction (Hartree): 0.142462

```

```

TS.iC3H7_H_COO+H2O.pd
~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -383.94630453
Electronic state : 1-A
Cartesian coordinates (Angs):
C -0.235283 0.016174 0.699171
O -1.240528 -0.761381 0.663902
O -1.724624 -0.816958 -0.684011
H -0.001511 0.350473 1.710332
C 0.888560 -0.014728 -0.291171
H 0.477280 0.043827 -1.294618
C 1.871639 1.116622 -0.023768
C 1.547100 -1.391047 -0.122550
H 2.298894 1.029003 0.977196
H 1.402177 2.097152 -0.100932
H 2.691824 1.075778 -0.738445
H 0.836951 -2.180808 -0.358434
H 1.908536 -1.531821 0.897872
H 2.400871 -1.465661 -0.794542
O -1.277082 1.513314 -0.054375
H -1.685811 0.684917 -0.567096
H -0.823434 2.055210 -0.705557
Rotational constants (GHz): 3.4687800 2.1307000 1.5671300
Vibrational harmonic frequencies (cm-1):
i468.4957 81.2202 175.3686
209.5979 235.0238 263.7852
330.9704 351.3589 370.1904
433.0328 504.0795 613.7493
641.7165 695.7415 866.4681
897.1004 933.9497 952.7064
978.0045 1037.2640 1141.2270
1179.5749 1194.4940 1212.7733
1317.8268 1342.7409 1368.7750
1395.5634 1424.7470 1489.5123
1493.2994 1505.9665 1509.8659
1558.8110 1678.4241 2279.5950
3060.0894 3061.3501 3121.8920
3129.5562 3137.7209 3144.9175
3152.5578 3159.8341 3893.2772
Zero-point correction (Hartree): 0.142444

```

```

TS.iC3H7_H_COO+H2O.pu
~~~~~
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -383.41678055
E(CCSD/Aug-CC-pVTZ) (Hartree): -383.34905186
T1 diagnostic: 0.020434
E(MP2/Aug-CC-pVTZ) (Hartree): -383.30867345
E(MP3/Aug-CC-pVTZ) (Hartree): -383.33644824
E(RHF/Aug-CC-pVTZ) (Hartree): -381.84402803
E(RM062X/Aug-CC-pVTZ) (Hartree): -383.94877497
Electronic state : 1-A
Cartesian coordinates (Angs):
C      -0.228522      0.012894      0.698386
O     -1.232631     -0.768923      0.670414
O     -1.710665     -0.844782     -0.677458
H      0.002573      0.358451      1.707540
C      0.894062     -0.006823     -0.289230
H      0.481943      0.044440     -1.291997
C      1.847081      1.151197     -0.034289
C      1.575000     -1.370609     -0.105741
H      2.262705      1.099250      0.974757
H      1.339723      2.106001     -0.155835
H      2.679020      1.108451     -0.735394
H      0.880390     -2.177390     -0.331011
H      1.943962     -1.494226      0.914401
H      2.427646     -1.436295     -0.779957
O     -1.189810      1.508836     -0.198722
H     -1.608251      0.649367     -0.654280
H     -1.870585      1.860952      0.383151
Rotational constants (GHz):      3.4609900      2.1436600      1.5748900
Vibrational harmonic frequencies (cm-1):
i465.4356      73.3366      175.1260
223.4994      238.3423      264.0299
334.2788      348.7857      361.5088
431.7299      525.8799      598.6578
650.5275      668.9395      872.2315

```

|           |           |           |
|-----------|-----------|-----------|
| 895.1883  | 934.3880  | 951.9655  |
| 978.3943  | 1035.4670 | 1141.3155 |
| 1191.0890 | 1207.6822 | 1282.8297 |
| 1330.5551 | 1335.9322 | 1371.7791 |
| 1393.6798 | 1418.6123 | 1491.3666 |
| 1495.6520 | 1503.9317 | 1515.9114 |
| 1586.6527 | 1619.1031 | 2241.0135 |
| 3057.6835 | 3059.8530 | 3125.6286 |
| 3127.1755 | 3129.3752 | 3156.5910 |
| 3157.5954 | 3160.3566 | 3876.6398 |

Zero-point correction (Hartree): 0.142477

TS.iC3H7\_H\_COO+H2O.td

~~~~~

E(RM062X/Aug-CC-pVTZ) (Hartree): -383.94140209

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-0.190746	-0.661902	0.566334
O	-0.904977	-1.182370	-0.343496
O	-1.349330	-0.174106	-1.256810
H	-0.137746	-1.300106	1.448041
C	0.972562	0.272274	0.407493
H	1.116622	0.708753	1.399401
C	2.165224	-0.663504	0.129829
C	0.915900	1.378401	-0.637151
H	2.046190	-1.136901	-0.844395
H	2.266460	-1.442532	0.885373
H	3.082885	-0.077917	0.120042
H	0.067026	2.042503	-0.494621
H	0.836869	0.961055	-1.636466
H	1.830843	1.967542	-0.561909
O	-1.639991	0.635921	1.053922
H	-1.767744	0.553147	0.017653
H	-1.364652	1.537282	1.238921

Rotational constants (GHz): 3.4411400 1.9595300 1.8481000

Vibrational harmonic frequencies (cm-1):

i429.6125	62.8627	196.7065
223.1838	261.2196	280.2277
308.1940	340.7224	394.6182
402.9507	505.0491	615.7623
627.9872	735.8867	823.0752
885.6212	938.2646	953.6543
978.9828	1047.3794	1115.3287
1151.2235	1181.7764	1216.0963
1310.9724	1389.0985	1394.1282
1407.9263	1428.6345	1484.6729
1485.7954	1503.5635	1511.3755
1564.2988	1680.1876	2382.7289
3059.7538	3066.1106	3074.2123
3138.2999	3145.0512	3146.7081
3150.2608	3178.0493	3901.4020

Zero-point correction (Hartree): 0.142727

TS.iC3H7_H_COO+H2O.tu

~~~~~

E(RM062X/Aug-CC-pVTZ) (Hartree): -383.94341293

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.195853  | -0.634600 | -0.605501 |
| O | 0.900125  | -1.204056 | 0.284917  |
| O | 1.302809  | -0.248854 | 1.269840  |
| H | 0.163295  | -1.222825 | -1.523610 |
| C | -0.975431 | 0.281223  | -0.419282 |
| H | -1.134156 | 0.721098  | -1.406032 |
| C | -2.145281 | -0.677515 | -0.122788 |
| C | -0.915365 | 1.393932  | 0.617837  |
| H | -2.003755 | -1.144366 | 0.851625  |
| H | -2.244620 | -1.461979 | -0.873568 |
| H | -3.072627 | -0.107681 | -0.102911 |
| H | -0.080986 | 2.064727  | 0.434790  |
| H | -0.818382 | 0.987846  | 1.620084  |
| H | -1.840299 | 1.968410  | 0.550131  |
| O | 1.556497  | 0.822326  | -0.940277 |
| H | 1.671649  | 0.622016  | 0.084558  |
| H | 2.325775  | 0.439185  | -1.372507 |

Rotational constants (GHz): 3.4139200 2.0169800 1.8476500

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i428.1600 | 50.6993   | 196.7700  |
| 235.7246  | 262.6569  | 289.4574  |
| 314.5799  | 334.2925  | 395.5123  |
| 404.0625  | 535.3212  | 590.2305  |
| 618.6668  | 733.3833  | 829.3813  |
| 885.2169  | 942.7092  | 949.4733  |
| 980.1730  | 1044.9959 | 1120.5483 |
| 1153.6331 | 1219.9467 | 1285.3040 |
| 1306.1118 | 1387.9370 | 1394.7601 |
| 1411.4046 | 1426.5878 | 1485.5227 |
| 1491.9687 | 1505.9432 | 1518.1315 |
| 1590.8804 | 1623.5949 | 2331.3330 |
| 3063.4134 | 3074.2626 | 3076.2546 |
| 3129.4235 | 3137.0603 | 3149.3163 |
| 3154.0541 | 3186.0736 | 3879.9829 |

Zero-point correction (Hartree): 0.142834

#####  
E-(iC3H7)CHOO  
#####

Population analysis as 298K (%)  
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)  
Compound Qtot Erel Erel2 n\*Q\*MB %



```

-----
TS.H_ic3H7_COO+H2O.pu 2.564e+40 0.00 0.00 5.128e+40 28.6
TS.H_ic3H7_COO+H2O.pd 2.118e+40 0.16 0.16 3.258e+40 18.2
TS.H_ic3H7_COO+H2O.cu 3.474e+40 0.45 0.45 3.233e+40 18
TS.H_ic3H7_COO+H2O.mu 2.713e+40 0.31 0.31 3.217e+40 18
TS.H_ic3H7_COO+H2O.md 2.573e+40 0.65 0.65 1.709e+40 9.54
TS.H_ic3H7_COO+H2O.cd 3.145e+40 0.90 0.90 1.375e+40 7.67
Total 1.792e+41 100

TS.H_ic3H7_COO+H2O.cd
~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -383.95096890
Electronic state : 1-A
Cartesian coordinates (Angs):
C 0.221036 -0.183682 0.242292
O 1.046910 -0.951938 -0.332773
O 2.341416 -0.710884 0.229855
H 0.388737 0.026364 1.296320
C -1.137927 -0.034899 -0.342309
H -1.028509 -0.047948 -1.426551
C -1.962657 -1.250259 0.105524
C -1.778751 1.271247 0.111890
H -2.045063 -1.280434 1.193216
H -1.513090 -2.180998 -0.234281
H -2.968003 -1.174622 -0.305907
H -1.216342 2.129528 -0.247918
H -1.829905 1.315133 1.201759
H -2.796220 1.334702 -0.270666
O 1.303734 1.446194 -0.197304
H 2.045379 0.702085 -0.016852
H 1.376328 2.094772 0.508275
Rotational constants (GHz): 3.9473900 1.8030900 1.3203300
Vibrational harmonic frequencies (cm-1):
i426.6464 48.8151 160.4404
201.1737 217.7188 268.1196
299.1487 346.7106 393.1224
486.9133 497.3453 538.1022
637.7919 681.8179 877.6057
936.8559 941.9714 970.8582
983.3915 1075.7720 1138.0022
1188.8786 1195.5833 1237.0336
1320.0585 1336.6568 1372.6702
1398.0241 1420.3577 1490.7042
1495.4007 1504.2357 1516.1687
1566.6055 1672.1039 2185.4333
3062.3998 3064.2609 3103.8866
3133.2654 3138.8191 3151.4564
3156.4862 3161.5032 3889.7006
Zero-point correction (Hartree): 0.142302

TS.H_ic3H7_COO+H2O.cu
~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -383.95173801
Electronic state : 1-A
Cartesian coordinates (Angs):
C 0.220559 -0.172205 0.242617
O 1.043752 -0.946575 -0.329353
O 2.335978 -0.717362 0.243272
H 0.389475 0.051255 1.293113
C -1.139348 -0.018788 -0.341364
H -1.034313 0.000302 -1.426937
C -1.949627 -1.259813 0.062114
C -1.799248 1.261246 0.158982
H -2.022102 -1.333392 1.148214
H -1.493810 -2.171585 -0.318000
H -2.958956 -1.175939 -0.337856
H -1.224186 2.142042 -0.116284
H -1.889511 1.241784 1.246232
H -2.800975 1.346072 -0.259221
O 1.324724 1.488681 -0.048155
H 2.046471 0.724008 0.093611
H 1.358255 1.714870 -0.983067
Rotational constants (GHz): 3.9225500 1.7968900 1.3162200
Vibrational harmonic frequencies (cm-1):
i402.5845 48.9083 157.1742
195.9446 206.0622 264.4662
293.8773 338.4526 394.8661
486.8766 507.3467 551.6412
591.3500 642.2035 879.8278
934.4887 942.0076 972.3354
983.1524 1090.7390 1147.4897
1192.4698 1214.8597 1286.9761
1323.7652 1335.8968 1385.3419
1399.8041 1426.2484 1491.1154
1491.3835 1504.2533 1514.6134
1596.9809 1616.5564 2223.2070
3065.3810 3068.4640 3091.3389
3136.1610 3140.4986 3157.5363
3160.7663 3162.8767 3872.0937
Zero-point correction (Hartree): 0.142358

TS.H_ic3H7_COO+H2O.md
~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -383.95135091
Electronic state : 1-A
Cartesian coordinates (Angs):
C -0.214048 0.297074 0.400525
O -0.768111 0.692282 -0.668504
O -2.160099 0.886980 -0.394730
H -0.590858 0.711698 1.331395
C 1.162806 -0.262229 0.329912
H 1.251148 -0.927606 1.191170

```

```

C 1.399716 -1.041596 -0.955703
C 2.153958 0.897581 0.503009
H 1.343510 -0.380727 -1.819461
H 0.651146 -1.822878 -1.072902
H 2.388500 -1.497274 -0.933563
H 1.974818 1.453724 1.422963
H 2.078415 1.586378 -0.337880
H 3.168356 0.503553 0.534731
O -1.493658 -1.222248 0.603696
H -2.102498 -0.444091 0.194049
H -1.802185 -1.383868 1.499342
Rotational constants (GHz): 3.9274900 1.7020700 1.5115100
Vibrational harmonic frequencies (cm-1):
i445.5209 61.7170 152.9328
196.3269 226.6019 260.9087
285.8809 355.5858 374.6282
469.4628 511.4848 625.4445
637.6006 692.9885 849.7636
937.8686 940.9159 976.4548
988.8547 1075.6162 1120.8683
1155.8131 1209.1526 1224.7015
1307.4784 1358.7399 1389.1456
1406.3721 1422.5216 1491.1149
1493.7869 1506.2183 1514.3931
1554.2121 1663.6148 2153.6623
3066.1712 3073.6548 3077.6621
3139.8276 3146.7198 3149.8186
3156.6865 3162.0721 3892.0333
Zero-point correction (Hartree): 0.142289

TS_H_iC3H7_COO+H2O.mu
~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -383.95199455
Electronic state : 1-A
Cartesian coordinates (Angs):
C      -0.217680      0.302697      0.372818
O      -0.781949      0.633527      -0.713293
O      -2.167313      0.862602      -0.433265
H      -0.582991      0.765512      1.284621
C      1.161746      -0.254599      0.328488
H      1.234995      -0.911621      1.197477
C      1.438188      -1.034798      -0.948683
C      2.143730      0.911207      0.514705
H      1.374370      -0.382837      -1.818530
H      0.722393      -1.845006      -1.083070
H      2.438092      -1.463961      -0.910581
H      1.940226      1.469472      1.427827
H      2.082520      1.595846      -0.330889
H      3.159527      0.523674      0.570881
O      -1.540844      -1.125773      0.833258
H      -2.127315      -0.389760      0.336365
H      -1.476868      -1.871210      0.228330
Rotational constants (GHz):      3.9093900      1.6640200      1.5122500
Vibrational harmonic frequencies (cm-1):
i419.0526      61.7257      156.3399
193.9372      220.7313      255.1135
284.8542      353.9973      371.3388
471.0923      525.5040      581.7610
629.6848      650.7072      855.1369
935.4945      939.5091      977.9761
988.2038      1088.0526      1128.5166
1168.3254      1213.5037      1285.1864
1309.3536      1367.7984      1392.6635
1409.3837      1426.0124      1488.0490
1494.9067      1506.6593      1513.9562
1590.7302      1611.9939      2197.5245
3067.3130      3072.5727      3080.3784
3142.2633      3144.7603      3148.1389
3151.6839      3169.3825      3878.0229
Zero-point correction (Hartree): 0.142386

TS_H_iC3H7_COO+H2O.pd
~~~~~
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -383.41975544
E(CCSD/Aug-CC-pVTZ) (Hartree): -383.35245992
T1 diagnostic: 0.019784
E(MP2/Aug-CC-pVTZ) (Hartree): -383.31207968
E(MP3/Aug-CC-pVTZ) (Hartree): -383.34006138
E(RHF/Aug-CC-pVTZ) (Hartree): -381.84890093
E(RM062X/Aug-CC-pVTZ) (Hartree): -383.95206940
Electronic state : 1-A
Cartesian coordinates (Angs):
C 0.279998 -0.018052 0.600348
O 1.142962 -0.877219 0.250791
O 2.418595 -0.225890 0.212971
H 0.596554 0.734070 1.318047
C -1.165655 -0.329279 0.429206
H -1.425603 -0.888956 1.337091
C -1.981985 0.961072 0.414346
C -1.420828 -1.195221 -0.797603
H -1.785543 1.514181 -0.502738
H -1.744406 1.599331 1.266148
H -3.043995 0.726260 0.454687
H -0.881239 -2.137514 -0.740649
H -1.091740 -0.665599 -1.691381
H -2.485672 -1.404817 -0.886310
O 0.813400 1.235762 -0.868737
H 1.740821 0.787920 -0.574683
H 0.851987 2.162782 -0.618193
Rotational constants (GHz): 3.9884600 1.7840100 1.5346500
Vibrational harmonic frequencies (cm-1):
i454.3150 63.3027 175.1734

```

|           |           |           |
|-----------|-----------|-----------|
| 190.9455  | 228.5525  | 254.8398  |
| 334.3430  | 351.1215  | 396.1403  |
| 481.4695  | 491.1393  | 577.9055  |
| 639.9795  | 688.4403  | 860.9843  |
| 933.6194  | 949.1219  | 982.7578  |
| 999.7000  | 1045.3704 | 1135.4672 |
| 1167.2463 | 1213.7278 | 1222.3527 |
| 1307.2934 | 1352.2770 | 1377.0604 |
| 1403.4490 | 1423.2469 | 1491.0686 |
| 1494.9883 | 1507.3775 | 1515.1185 |
| 1552.9335 | 1661.3887 | 2137.0498 |
| 3022.4317 | 3067.1921 | 3075.1231 |
| 3138.4104 | 3147.8731 | 3153.9067 |
| 3160.3896 | 3161.8319 | 3890.8625 |

Zero-point correction (Hartree): 0.142215

TS.H\_iC3H7\_COO+H2O.pu

~~~~~

E (CCSD(T)/Aug-CC-pVTZ) (Hartree): -383.42010753

E (CCSD/Aug-CC-pVTZ) (Hartree): -383.35283307

T1 diagnostic: 0.019901

E (MP2/Aug-CC-pVTZ) (Hartree): -383.31211592

E (MP3/Aug-CC-pVTZ) (Hartree): -383.34038684

E (RHF/Aug-CC-pVTZ) (Hartree): -381.84969730

E (RM062X/Aug-CC-pVTZ) (Hartree): -383.95236693

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.281227  | -0.013303 | 0.589395  |
| O | 1.138913  | -0.880041 | 0.243235  |
| O | 2.421482  | -0.241854 | 0.225430  |
| H | 0.597809  | 0.743115  | 1.301660  |
| C | -1.167860 | -0.317234 | 0.426695  |
| H | -1.418427 | -0.874775 | 1.338617  |
| C | -1.982054 | 0.974542  | 0.422216  |
| C | -1.446477 | -1.194699 | -0.786461 |
| H | -1.774558 | 1.550522  | -0.477866 |
| H | -1.746252 | 1.599099  | 1.283324  |
| H | -3.044566 | 0.739705  | 0.449979  |
| H | -0.878117 | -2.120965 | -0.751706 |
| H | -1.180486 | -0.665603 | -1.702787 |
| H | -2.507515 | -1.434117 | -0.833761 |
| O | 0.865720  | 1.352631  | -0.764405 |
| H | 1.768294  | 0.855694  | -0.491722 |
| H | 0.665872  | 1.065604  | -1.660879 |

Rotational constants (GHz): 3.9512900 1.7732700 1.5146300

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i428.0242 | 56.2157   | 180.3776  |
| 189.2435  | 214.4484  | 244.4910  |
| 325.3931  | 344.0776  | 406.1368  |
| 484.2008  | 497.5185  | 561.7431  |
| 586.7199  | 666.9304  | 863.0590  |
| 932.2344  | 946.2715  | 983.3912  |
| 1001.8064 | 1056.3637 | 1157.9708 |
| 1169.4048 | 1213.2228 | 1287.9842 |
| 1309.5739 | 1360.1511 | 1383.6473 |
| 1408.4917 | 1430.6848 | 1488.6051 |
| 1493.6114 | 1507.0246 | 1511.5377 |
| 1588.5934 | 1614.0124 | 2170.7105 |
| 3021.7110 | 3069.3006 | 3073.5057 |
| 3137.8008 | 3145.3012 | 3155.3076 |
| 3162.7409 | 3170.3391 | 3875.2934 |

Zero-point correction (Hartree): 0.142265

#####  
E-(CH3)(iC3H7)COO  
#####

Population analysis as 298K (%)

Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)

| Compound                | Qtot      | Erel | Erel2 | n*Q*MB    | %    |
|-------------------------|-----------|------|-------|-----------|------|
| TS.CH3_iC3H7_COO+H2O.mu | 9.152e+40 | 0.05 | 0.05  | 1.689e+41 | 26.5 |
| TS.CH3_iC3H7_COO+H2O.cu | 8.416e+40 | 0.00 | 0.00  | 1.683e+41 | 26.4 |
| TS.CH3_iC3H7_COO+H2O.pu | 9.622e+40 | 0.10 | 0.10  | 1.626e+41 | 25.5 |
| TS.CH3_iC3H7_COO+H2O.md | 9.282e+40 | 0.63 | 0.63  | 6.460e+40 | 10.1 |
| TS.CH3_iC3H7_COO+H2O.pd | 7.841e+40 | 0.78 | 0.78  | 4.196e+40 | 6.58 |
| TS.CH3_iC3H7_COO+H2O.cd | 7.897e+40 | 0.95 | 0.95  | 3.161e+40 | 4.96 |
| Total                   |           |      |       | 6.379e+41 | 100  |

TS.CH3\_iC3H7\_COO+H2O.cd

~~~~~

E (RM062X/Aug-CC-pVTZ) (Hartree): -423.26697049

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.189599  | -0.129322 | 0.147874  |
| O | 0.944458  | -1.020539 | -0.384684 |
| O | 2.318097  | -0.736185 | -0.100100 |
| C | 0.401045  | 0.311172  | 1.559028  |
| H | 0.078308  | 1.337773  | 1.704835  |
| H | 1.438311  | 0.177549  | 1.842167  |
| H | -0.232638 | -0.328302 | 2.180880  |
| C | -1.175938 | -0.063261 | -0.474483 |
| H | -1.003977 | -0.076405 | -1.550481 |
| C | -1.956791 | -1.324191 | -0.081934 |
| C | -1.932297 | 1.202704  | -0.094487 |
| H | -2.123808 | -1.358976 | 0.995687  |
| H | -1.427208 | -2.225604 | -0.382690 |
| H | -2.930385 | -1.310590 | -0.569825 |
| H | -1.349097 | 2.092897  | -0.325579 |
| H | -2.185300 | 1.210180  | 0.966498  |
| H | -2.864198 | 1.249909  | -0.655945 |

```

O 1.238262 1.328051 -0.740434
H 1.996684 0.583593 -0.540560
H 1.443066 2.094746 -0.199227
Rotational constants (GHz): 2.8684500 1.5143500 1.2982100
Vibrational harmonic frequencies (cm-1):
1500.8401 66.5429 162.4873
203.0994 225.4955 257.0907
275.0912 283.4405 317.7759
342.8735 382.8163 430.9323
481.8760 533.2367 571.8018
651.3359 667.8252 785.8579
902.1539 936.4508 957.3812
974.9147 984.1783 1036.5239
1104.2531 1138.2606 1190.8640
1202.8616 1318.0918 1328.1656
1361.8047 1395.3833 1406.4392
1421.2976 1449.8369 1486.7684
1496.1493 1500.3711 1508.0404
1515.4152 1533.0929 1647.3375
2050.6453 3061.8653 3065.0077
3066.2895 3101.4984 3133.6098
3139.7918 3148.4654 3154.5368
3157.2981 3212.3060 3895.6924
Zero-point correction (Hartree): 0.170003

```

```

TS.CH3_iC3H7_COO+H2O.cu
~~~~~
E (CCSD(T)/Aug-CC-pVTZ) (Hartree): -422.67110211
E (CCSD/Aug-CC-pVTZ) (Hartree): -422.59505972
T1 diagnostic: 0.019113
E (MP2/Aug-CC-pVTZ) (Hartree): -422.54627986
E (MP3/Aug-CC-pVTZ) (Hartree): -422.58256840
E (RHF/Aug-CC-pVTZ) (Hartree): -420.90084099
E (RM062X/Aug-CC-pVTZ) (Hartree): -423.26842864
Electronic state : 1-A
Cartesian coordinates (Angs):
C      0.189677      -0.134293      0.145080
O      0.951406      -1.010514      -0.405972
O      2.319944      -0.727534      -0.098187
C      0.390809      0.286092      1.562056
H      0.140833      1.333860      1.691583
H      1.412082      0.094075      1.867726
H      -0.297313      -0.312892      2.165330
C      -1.176696      -0.056987      -0.477213
H      -1.016956      -0.060345      -1.556424
C      -1.958656      -1.323672      -0.104945
C      -1.928919      1.204259      -0.070702
H      -2.119166      -1.376431      0.972542
H      -1.432591      -2.220803      -0.424202
H      -2.934820      -1.298282      -0.587250
H      -1.334531      2.097208      -0.258222
H      -2.190393      1.178729      0.987600
H      -2.855150      1.274476      -0.639157
O      1.273454      1.405562      -0.571480
H      2.010952      0.630265      -0.414835
H      1.161336      1.467632      -1.525219
Rotational constants (GHz):      2.8736200      1.5148500      1.2938800
Vibrational harmonic frequencies (cm-1):
1492.1620      75.1522      148.5390
175.9432      226.4803      252.4118
271.5770      279.5877      319.5830
346.2150      386.0007      429.1855
483.0153      543.2515      592.5749
613.6623      640.5636      781.1642
902.2222      938.4190      958.9280
976.0923      984.4613      1037.7370
1106.0416      1137.6296      1194.7182
1260.5069      1321.3182      1332.8042
1369.5460      1397.1219      1409.9495
1423.4674      1443.0262      1487.3188
1494.7589      1500.4127      1507.9848
1519.4135      1563.1735      1613.1366
2020.1551      3065.6650      3067.5751
3068.8806      3085.4423      3136.1687
3140.9631      3150.2559      3157.4636
3167.1102      3218.6277      3873.0824
Zero-point correction (Hartree): 0.169943

```

```

TS.CH3_iC3H7_COO+H2O.md
~~~~~
E (RM062X/Aug-CC-pVTZ) (Hartree): -423.26732241
Electronic state : 1-A
Cartesian coordinates (Angs):
C -0.172241 0.310476 0.022483
O -0.633746 -0.244980 -1.037797
O -2.064644 -0.182253 -1.032226
C -0.696801 1.630679 0.489659
H -0.393355 1.816169 1.517324
H -1.771622 1.690019 0.372200
H -0.239297 2.391820 -0.147194
C 1.236895 -0.076982 0.371429
H 1.310203 0.044097 1.454146
C 1.541502 -1.521108 -0.001896
C 2.214309 0.899101 -0.297960
H 1.535730 -1.647742 -1.083362
H 0.799101 -2.191634 0.425432
H 2.527014 -1.794851 0.372559
H 2.071021 1.924472 0.039129
H 2.097764 0.867298 -1.381542
H 3.234477 0.604002 -0.057789
O -1.328556 -0.834854 1.168891
H -1.950377 -0.676951 0.289900

```

```

H -1.747083 -0.382999 1.905966
Rotational constants (GHz): 2.7381300 1.5385600 1.3779300
Vibrational harmonic frequencies (cm-1):
i541.0546 57.7859 171.6439
180.7757 231.2332 237.9800
258.3331 313.6957 314.8194
341.0917 378.6168 417.6638
485.2634 534.7020 605.0642
647.9129 674.5769 778.4269
907.2194 938.1375 952.1950
980.5607 995.9006 1029.8554
1121.0753 1141.8437 1183.1115
1196.7664 1256.8406 1319.3709
1384.0952 1400.9277 1412.8989
1422.6688 1453.6818 1484.8596
1493.6552 1496.8211 1508.2119
1515.6955 1529.8918 1626.7151
2012.7269 3067.7163 3071.9655
3075.7115 3079.2393 3142.3433
3145.7168 3148.7518 3150.0000
3162.5043 3212.8351 3896.1321
Zero-point correction (Hartree): 0.169833

```

TS.CH3\_iC3H7\_COO+H2O.mu

```

~~~~~
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -422.67106105
E(CCSD/Aug-CC-pVTZ) (Hartree): -422.59504522
T1 diagnostic: 0.018744
E(MP2/Aug-CC-pVTZ) (Hartree): -422.54649624
E(MP3/Aug-CC-pVTZ) (Hartree): -422.58265697
E(RHF/Aug-CC-pVTZ) (Hartree): -420.90065434
E(RM062X/Aug-CC-pVTZ) (Hartree): -423.26830578
Electronic state : 1-A

```

```

Cartesian coordinates (Angs):
C      -0.175799      0.298885      0.008972
O      -0.654878      -0.310009      -1.015401
O      -2.083264      -0.212727      -1.003662
C      -0.675566      1.646797      0.414513
H      -1.755703      1.696174      0.376956
H      -0.268768      2.359244      -0.307357
H      -0.310206      1.895156      1.407017
C      1.233540      -0.084425      0.367091
H      1.291299      0.025865      1.452044
C      1.568664      -1.516518      -0.026495
C      2.211244      0.909443      -0.275225
H      1.557353      -1.631626      -1.109043
H      0.855259      -2.226600      0.389627
H      2.561344      -1.774417      0.339455
H      2.050778      1.926898      0.076014
H      2.108895      0.893849      -1.360729
H      3.231322      0.621649      -0.026058
O      -1.403227      -0.627659      1.279989
H      -1.995660      -0.552303      0.371940
H      -1.167467      -1.555816      1.369586
Rotational constants (GHz):  2.7558200      1.5219700      1.3678600
Vibrational harmonic frequencies (cm-1):
i524.8841      65.6218      163.6355
172.6786      228.3364      229.4329
251.8248      307.9409      326.8904
347.0960      383.6560      412.8337
488.5625      547.2647      600.5679
633.8637      643.3187      773.2040
904.7074      936.6167      953.4210
979.1992      1000.6073      1030.8551
1118.1732      1144.0174      1183.9343
1255.6206      1265.2611      1324.7084
1386.8778      1404.7580      1416.8249
1426.2724      1458.6753      1482.5836
1491.0434      1495.2421      1509.5130
1518.7790      1564.6852      1605.2189
1988.9002      3068.4897      3073.4665
3074.4456      3079.3390      3142.0905
3145.1305      3152.2449      3153.2345
3160.4250      3222.8340      3880.7886
Zero-point correction (Hartree): 0.169896

```

TS.CH3\_iC3H7\_COO+H2O.pd

```

~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -423.26699240

```

```

Electronic state : 1-A
Cartesian coordinates (Angs):
C 0.232706 0.194228 0.386909
O 0.998735 -0.800059 0.656977
O 2.304899 -0.574639 0.116691
C 0.710530 1.596383 0.592345
H 0.268033 2.278560 -0.126792
H 1.792723 1.630111 0.549904
H 0.369956 1.896639 1.587548
C -1.236888 -0.115186 0.486822
H -1.451109 -0.031330 1.559878
C -2.085905 0.917466 -0.251973
C -1.549726 -1.533341 0.022556
H -1.827466 0.923472 -1.310792
H -1.963398 1.922306 0.148390
H -3.137047 0.649425 -0.160808
H -0.999663 -2.274250 0.596125
H -1.277567 -1.641622 -1.026820
H -2.616040 -1.725976 0.131343
O 0.689672 0.047394 -1.559395
H 1.617329 -0.246127 -1.072751
H 0.853501 0.879937 -2.009357
Rotational constants (GHz): 2.7710900 1.5826800 1.3922700

```

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i536.9755 | 62.4337   | 177.2575  |
| 191.6224  | 206.0469  | 246.2331  |
| 257.0916  | 308.4395  | 347.7795  |
| 375.6878  | 404.6969  | 423.3425  |
| 467.6699  | 515.0645  | 589.6003  |
| 641.6839  | 649.4983  | 791.0850  |
| 902.0773  | 936.2391  | 956.6458  |
| 984.1496  | 988.5846  | 1023.3074 |
| 1101.2201 | 1159.0422 | 1190.7026 |
| 1204.8679 | 1260.0468 | 1318.0825 |
| 1368.0584 | 1401.2597 | 1406.0554 |
| 1422.4871 | 1446.4716 | 1489.9419 |
| 1493.7797 | 1501.6499 | 1510.9225 |
| 1512.5299 | 1526.9581 | 1626.4623 |
| 2008.2737 | 3025.2704 | 3064.1268 |
| 3072.4850 | 3077.4655 | 3145.5980 |
| 3147.1207 | 3149.8041 | 3158.3316 |
| 3167.8235 | 3211.6071 | 3897.4574 |

Zero-point correction (Hartree): 0.169751

TS.CH3\_iC3H7\_COO+H2O.pu

~~~~~  
 E (CCSD(T)/Aug-CC-pVTZ) (Hartree): -422.67063388  
 E (CCSD/Aug-CC-pVTZ) (Hartree): -422.59445129  
 T1 diagnostic: 0.019058  
 E (MP2/Aug-CC-pVTZ) (Hartree): -422.54568548  
 E (MP3/Aug-CC-pVTZ) (Hartree): -422.58201392  
 E (RHF/Aug-CC-pVTZ) (Hartree): -420.89941394  
 E (RM062X/Aug-CC-pVTZ) (Hartree): -423.26802852  
 Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.235492  | 0.205466  | 0.375150  |
| O | 1.004736  | -0.774935 | 0.690057  |
| O | 2.313321  | -0.555194 | 0.154101  |
| C | 0.699825  | 1.618517  | 0.514148  |
| H | 0.322585  | 2.231426  | -0.297410 |
| H | 1.782208  | 1.651579  | 0.544407  |
| H | 0.285148  | 1.992196  | 1.454398  |
| C | -1.235439 | -0.098670 | 0.486358  |
| H | -1.439293 | 0.006196  | 1.559358  |
| C | -2.082688 | 0.925865  | -0.265813 |
| C | -1.571088 | -1.525439 | 0.067363  |
| H | -1.804314 | 0.943926  | -1.319417 |
| H | -1.968648 | 1.930227  | 0.137080  |
| H | -3.133539 | 0.651372  | -0.190003 |
| H | -0.959714 | -2.255590 | 0.590265  |
| H | -1.418392 | -1.652343 | -1.005579 |
| H | -2.619884 | -1.730372 | 0.276384  |
| O | 0.757054  | 0.122344  | -1.567724 |
| H | 1.659962  | -0.182268 | -1.046477 |
| H | 0.416383  | -0.678509 | -1.977716 |

Rotational constants (GHz): 2.7735600 1.5730800 1.3821300

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i519.5129 | 56.2326   | 161.6387  |
| 188.3762  | 209.3719  | 235.5546  |
| 253.0497  | 310.3230  | 348.9109  |
| 366.7630  | 400.1371  | 426.0887  |
| 465.4116  | 533.1134  | 589.0865  |
| 599.3958  | 638.4574  | 783.3418  |
| 902.0519  | 935.6362  | 958.4366  |
| 982.5034  | 991.3041  | 1022.5995 |
| 1104.1273 | 1160.3113 | 1193.5615 |
| 1255.9359 | 1277.0804 | 1319.0141 |
| 1369.5061 | 1404.6715 | 1410.2054 |
| 1427.1161 | 1443.0840 | 1489.0440 |
| 1495.3769 | 1499.9239 | 1509.5605 |
| 1519.9504 | 1558.2450 | 1611.8917 |
| 1980.0190 | 3027.7011 | 3066.6622 |
| 3070.0044 | 3074.0777 | 3135.4188 |
| 3147.2156 | 3152.0090 | 3167.4839 |
| 3169.7006 | 3216.4084 | 3877.4480 |

Zero-point correction (Hartree): 0.169702

#####  
 Z-(iC3H7) (CH3)COO  
 #####

Population analysis as 298K (%)

Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)

| Compound                | Qtot      | Erel | Erel2 | n*Q*MB    | %      |
|-------------------------|-----------|------|-------|-----------|--------|
| TS.iC3H7_CH3_COO+H2O.pu | 5.744e+40 | 0.00 | 0.00  | 5.744e+40 | 89.1   |
| TS.iC3H7_CH3_COO+H2O.pd | 6.033e+40 | 1.28 | 1.28  | 6.951e+39 | 10.8   |
| TS.iC3H7_CH3_COO+H2O.tu | 6.779e+40 | 4.15 | 4.15  | 6.154e+37 | 0.0954 |
| TS.iC3H7_CH3_COO+H2O.mu | 5.485e+40 | 4.51 | 4.51  | 2.697e+37 | 0.0418 |
| TS.iC3H7_CH3_COO+H2O.td | 8.636e+40 | 5.44 | 5.44  | 8.810e+36 | 0.0137 |
| TS.iC3H7_CH3_COO+H2O.md | 8.003e+40 | 5.57 | 5.57  | 6.625e+36 | 0.0103 |
| Total                   |           |      |       | 6.449e+40 | 100    |

TS.iC3H7\_CH3\_COO+H2O.md

~~~~~  
 E (RM062X/Aug-CC-pVTZ) (Hartree): -423.26043700

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.295976  | 0.543726  | -0.334275 |
| O | 1.459334  | 0.110400  | -0.667155 |
| O | 1.726201  | -1.170092 | -0.097922 |
| C | 0.209874  | 2.034699  | -0.424148 |
| H | 1.187203  | 2.440030  | -0.667268 |
| H | -0.524743 | 2.335456  | -1.169953 |

```

H -0.103160 2.417634 0.545296
C -0.993324 -0.230606 -0.497695
H -1.219251 0.005585 -1.548566
C -0.959424 -1.748672 -0.373744
C -2.127955 0.359269 0.340723
H -0.729841 -2.055858 0.645673
H -0.217116 -2.193940 -1.025895
H -1.948753 -2.130801 -0.629584
H -2.242296 1.432993 0.208269
H -1.971517 0.164349 1.401461
H -3.064973 -0.114781 0.053873
O 0.691571 0.164082 1.603418
H 1.255839 -0.617534 1.091191
H 0.010885 -0.268744 2.123598
Rotational constants (GHz): 2.2958300 1.8897000 1.4717700
Vibrational harmonic frequencies (cm-1):
i541.6794 58.7377 158.2427
200.1378 217.7317 261.9932
295.7140 303.0727 309.3538
374.7504 400.6321 414.2172
444.0072 554.6401 595.3540
622.1691 647.6087 737.9680
921.5124 941.6933 960.9530
984.4100 1015.4858 1033.6649
1092.9857 1146.4868 1185.7450
1201.2537 1264.8593 1314.7250
1379.3947 1407.0318 1412.1170
1430.7955 1445.4042 1478.9474
1483.2708 1487.9595 1506.0309
1509.7231 1515.6826 1624.0884
1989.3233 2995.5533 3069.5458
3077.7408 3083.8692 3133.5274
3144.2006 3155.3050 3158.5173
3186.4089 3191.9965 3906.1182
Zero-point correction (Hartree): 0.169570

```

TS.ic3H7\_CH3\_COO+H2O.mu

~~~~~  
E(RM062X/Aug-CC-pVTZ) (Hartree): -423.26244244

Electronic state : 1-A

Cartesian coordinates (Angs):

```

C 0.287619 0.545232 -0.341550
O 1.458729 0.131071 -0.674080
O 1.735568 -1.153675 -0.121342
C 0.180532 2.036696 -0.419908
H 1.159812 2.467796 -0.605205
H -0.513895 2.325119 -1.208396
H -0.214952 2.409775 0.523169
C -0.994150 -0.240514 -0.496825
H -1.221603 -0.018236 -1.551062
C -0.950165 -1.756623 -0.345587
C -2.122061 0.350063 0.351004
H -0.724578 -2.031602 0.682824
H -0.208467 -2.212402 -0.991080
H -1.938166 -2.145624 -0.595695
H -2.290031 1.408335 0.159125
H -1.894039 0.215729 1.406640
H -3.047370 -0.176770 0.124704
O 0.570139 0.043056 1.607932
H 1.181780 -0.680376 1.065671
H 1.185377 0.665516 2.006429

```

```

Rotational constants (GHz): 2.3004700 1.9018800 1.4783000
Vibrational harmonic frequencies (cm-1):
i526.7598 74.4517 174.8756
203.0174 236.4856 269.2961
297.9794 305.5288 316.8610
383.7971 401.1340 417.9539
464.0309 551.2763 598.7739
610.4227 631.7946 725.3306
921.5406 942.2574 959.0540
988.5518 1011.6317 1033.5275
1099.2489 1150.5025 1194.3690
1257.8440 1275.9220 1310.2927
1380.1277 1402.9601 1413.3030
1428.3288 1456.1784 1482.2060
1490.6728 1495.3602 1511.2215
1519.7272 1563.4745 1601.5001
1938.4247 2989.1573 3072.1207
3079.5052 3082.4815 3142.9397
3147.3130 3152.7124 3162.1968
3182.9770 3192.8061 3879.3620
Zero-point correction (Hartree): 0.169894

```

TS.ic3H7\_CH3\_COO+H2O.pd

~~~~~  
E(RM062X/Aug-CC-pVTZ) (Hartree): -423.26755689

Electronic state : 1-A

Cartesian coordinates (Angs):

```

C 0.246311 0.179963 -0.439348
O 1.250549 -0.577394 -0.707092
O 1.718330 -1.182741 0.501872
C -0.050359 1.175425 -1.507399
H 0.819405 1.306312 -2.143162
H -0.899048 0.830806 -2.099997
H -0.319111 2.123548 -1.047763
C -0.865563 -0.306012 0.459737
H -0.415617 -0.680873 1.373538
C -1.884352 0.781579 0.773044
C -1.511276 -1.499808 -0.256412
H -2.426247 1.091078 -0.121550
H -1.418055 1.667327 1.206060
H -2.615324 0.402587 1.485592

```

```

H -0.777445 -2.287444 -0.414267
H -1.932308 -1.206567 -1.219663
H -2.321912 -1.890403 0.357241
O 1.302206 1.154232 0.917814
H 1.685548 0.138247 1.010880
H 0.842866 1.365723 1.734605
Rotational constants (GHz): 2.3807100 1.7090600 1.5150100
Vibrational harmonic frequencies (cm-1):
i560.3147 91.4906 168.5788
193.3822 233.6146 246.7556
263.2962 272.7651 318.7202
348.3803 373.9255 433.7490
468.4414 558.7538 593.7049
653.0461 671.1113 757.2476
910.1150 939.5094 953.4396
979.0441 995.7734 1039.7278
1098.4945 1141.4978 1175.6395
1206.4739 1306.0979 1334.2222
1348.3325 1395.7747 1413.7194
1424.5539 1444.3065 1479.1489
1493.3365 1495.7478 1508.6587
1511.2063 1529.0383 1624.7131
2009.6245 3061.4387 3062.7863
3081.6402 3123.3352 3129.7639
3138.9222 3154.1213 3156.5576
3158.7653 3192.6480 3894.4013
Zero-point correction (Hartree): 0.169859

```

```

TS.ic3H7_CH3_COO+H2O.pu
~~~~~
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -422.67235971
E(CCSD/Aug-CC-pVTZ) (Hartree): -422.59606895
T1 diagnostic: 0.018770
E(MP2/Aug-CC-pVTZ) (Hartree): -422.54811914
E(MP3/Aug-CC-pVTZ) (Hartree): -422.58371215
E(RHF/Aug-CC-pVTZ) (Hartree): -420.89990486
E(RM062X/Aug-CC-pVTZ) (Hartree): -423.26974625
Electronic state : 1-A
Cartesian coordinates (Angs):
C      0.241989      0.184084      -0.437694
O      1.244644      -0.570810      -0.723638
O      1.701710      -1.213898      0.469042
C     -0.048583      1.209914      -1.479588
H      0.811804      1.344065      -2.128461
H     -0.908644      0.890156      -2.069564
H     -0.309686      2.148165      -0.994717
C     -0.870059      -0.305514      0.454827
H     -0.421159      -0.692484      1.363145
C     -1.868018      0.790537      0.798512
C     -1.528070      -1.479400      -0.282887
H     -2.405851      1.139291      -0.084661
H     -1.368492      1.637440      1.266496
H     -2.606372      0.400382      1.497464
H     -0.803699      -2.271699      -0.461111
H     -1.953965      -1.164430      -1.237443
H     -2.338378      -1.874277      0.328267
O      1.206991      1.077490      1.057994
H      1.609471      0.065290      1.069803
H      1.904665      1.638122      0.704586
Rotational constants (GHz):   2.3712300   1.7135800   1.5264500
Vibrational harmonic frequencies (cm-1):
i548.9264      85.0625      183.4119
203.2687      235.9190      251.2301
260.6567      276.0110      320.0767
355.5209      371.2249      427.0628
466.6115      588.0031      603.2702
631.3816      655.2497      744.5392
912.5177      937.2139      950.1653
979.8567      996.4303      1038.5916
1100.7117      1142.6053      1191.4548
1244.9000      1316.6592      1340.6210
1352.7300      1393.2353      1414.7119
1419.0804      1452.3664      1481.1440
1494.4489      1498.4218      1507.7101
1517.6192      1567.5676      1608.7597
1968.1152      3060.2029      3063.5537
3080.4363      3127.0810      3129.3996
3149.3465      3151.5456      3155.8918
3164.2020      3185.1044      3872.2805
Zero-point correction (Hartree): 0.170009

```

```

TS.ic3H7_CH3_COO+H2O.td
~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -423.26120414
Electronic state : 1-A
Cartesian coordinates (Angs):
C 0.226910 -0.578142 0.060807
O 0.896879 -0.235021 1.096699
O 1.225884 1.155621 1.058324
C 0.344391 -2.042617 -0.223209
H 1.390688 -2.273473 -0.401347
H 0.011392 -2.597174 0.654569
H -0.255560 -2.331114 -1.081503
C -1.002936 0.132894 -0.453746
H -1.102423 -0.189016 -1.492860
C -2.173572 -0.476230 0.344711
C -1.084355 1.652964 -0.389707
H -2.065809 -0.235042 1.402367
H -2.238919 -1.557548 0.236633
H -3.106807 -0.042648 -0.010370
H 1.293858 0.765188 -1.897570
H 1.649623 0.889371 -0.300528

```



```

H -1.061807 2.000984 0.638595
O 1.616422 0.246702 -1.156680
H -0.266838 2.139014 -0.915128
H -0.2023510 1.959843 -0.852739
Rotational constants (GHz): 2.2637000 1.8595500 1.4763300
Vibrational harmonic frequencies (cm-1):
i462.2022 65.7997 133.1425
199.1632 227.3696 260.4681
292.8409 294.3364 324.8247
338.5441 373.6422 416.9622
434.6209 537.2923 606.1620
644.5517 658.2956 758.1094
907.3190 933.0210 944.1656
980.1846 1025.6224 1054.9151
1118.7847 1127.4970 1177.3534
1207.1035 1250.9524 1315.7422
1393.2526 1399.2440 1417.3875
1427.3296 1466.5765 1482.7943
1486.7056 1491.3257 1505.5194
1512.1273 1530.6831 1659.8847
2125.8659 3065.8701 3071.4445
3073.1258 3084.8297 3145.3982
3150.0311 3151.1403 3161.4914
3180.1335 3190.0465 3901.9263
Zero-point correction (Hartree): 0.170140

```

TS.iC3H7\_CH3\_COO+H2O.tu

~~~~~  
E(RM062X/Aug-CC-pVT2) (Hartree): -423.26368298  
Electronic state : 1-A

```

Cartesian coordinates (Angs):
C -0.454040 0.504507 -0.030817
O -0.858826 0.147897 1.134133
O -0.447769 -1.200372 1.370553
C -1.160000 1.706225 -0.565429
H -2.119036 1.844736 -0.074655
H -0.533802 2.584712 -0.401128
H -1.292284 1.586997 -1.638969
C 0.971443 0.288226 -0.507145
H 1.058481 0.908622 -1.402099
C 1.847543 0.896138 0.601128
C 1.470551 -1.108482 -0.866024
H 1.764185 0.282533 1.497040
H 1.557120 1.917530 0.848961
H 2.884635 0.907726 0.270260
H 0.865871 -1.561385 -1.645976
H 1.469377 -1.753575 0.007396
H 2.492793 -1.013036 -1.233836
O -1.311707 -1.074540 -0.908401
H -0.992634 -1.466412 0.034484
H -2.261267 -0.942010 -0.822050
Rotational constants (GHz): 2.2029600 1.8508900 1.6343000
Vibrational harmonic frequencies (cm-1):
i468.3420 61.8043 190.3401
205.0922 249.2258 256.9267
258.4472 281.8168 331.8789
340.2812 370.0644 430.3410
449.8838 568.4863 619.6199
625.6618 670.0172 748.6054
909.0546 938.0636 953.4901
984.4286 1018.8868 1043.7854
1118.6273 1139.6291 1187.5262
1253.1834 1286.4503 1326.3040
1390.0409 1396.9018 1411.5072
1428.9097 1460.5507 1483.8963
1488.8490 1498.9591 1505.9488
1528.2898 1571.1924 1629.2217
2133.0215 3064.8023 3065.7713
3075.3852 3078.4169 3137.1692
3146.7831 3154.2954 3156.9258
3183.0740 3188.5218 3869.0134
Zero-point correction (Hartree): 0.170556

```

#####  
Z-(tC4H9)CHOO  
#####

Population analysis as 298K (%)  
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)  
Compound Qtot Erel Erel2 n\*Q\*MB %  
-----  
TS.tC4H9\_H\_COO+H2O.u 5.817e+40 0.00 0.00 1.163e+41 94.4  
TS.tC4H9\_H\_COO+H2O.d 5.814e+40 1.67 1.67 6.958e+39 5.64  
Total 1.233e+41 100

TS.tC4H9\_H\_COO+H2O.d

~~~~~  
E(RM062X/Aug-CC-pVT2) (Hartree): -423.25161605

Electronic state : 1-A

```

Cartesian coordinates (Angs):
C -0.351844 0.077591 -0.828806
O -1.359285 0.841492 -0.722289
O -1.879584 0.793481 0.610451
C 0.871647 0.019848 0.051315
H -0.159843 -0.183548 -1.870193
C 0.674888 0.043740 1.564532
C 1.695248 -1.202781 -0.357724
C 1.624587 1.300162 -0.375544
H 0.102191 -0.813993 1.913586
H 0.155876 0.940981 1.883352
H 1.660243 0.002140 2.032603

```

```

H 1.862276 -1.235606 -1.435432
H 1.208922 -2.131885 -0.061780
H 2.667704 -1.161416 0.131712
H 1.056154 2.186634 -0.098491
H 1.812125 1.323115 -1.450224
H 2.586596 1.322576 0.136128
O -1.413138 -1.493464 -0.178742
H -1.826288 -0.711288 0.383516
H -0.997055 -2.101136 0.437214
Rotational constants (GHz): 2.6291200 1.6559400 1.4560600
Vibrational harmonic frequencies (cm-1):
i428.8663 66.3417 189.4846
211.7296 248.1868 265.5987
296.1278 313.1204 333.0800
359.2326 375.8463 407.8457
433.8854 506.4889 597.7726
637.6754 689.7629 805.7525
878.6837 917.0372 958.4967
967.9193 976.6718 1022.7358
1059.3094 1080.7330 1172.3141
1224.3354 1253.8092 1314.1032
1393.5145 1397.5476 1410.8772
1436.3011 1478.0551 1484.6543
1487.0962 1501.7530 1507.7824
1515.9220 1560.0986 1682.8969
2370.4525 3058.2761 3061.9429
3067.6505 3130.1433 3130.5548
3134.2604 3136.5203 3142.5233
3150.6779 3186.7704 3903.4543
Zero-point correction (Hartree): 0.170621

```

```

TS.tc4H9_H_COO+H2O.u
~~~~~
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -422.65813120
E(CCSD/Aug-CC-pVTZ) (Hartree): -422.58149366
T1 diagnostic: 0.019892
E(MP2/Aug-CC-pVTZ) (Hartree): -422.53294891
E(MP3/Aug-CC-pVTZ) (Hartree): -422.56845495
E(RHF/Aug-CC-pVTZ) (Hartree): -420.88482739
E(RM062X/Aug-CC-pVTZ) (Hartree): -423.25420772
Electronic state : 1-A

```

```

Cartesian coordinates (Angs):
C      0.345416      -0.080434      -0.829899
O      1.356978      -0.843115      -0.731469
O      1.871490      -0.810030      0.602119
C      -0.876054      -0.016133      0.048570
H      0.152931      0.187334      -1.870799
C      -0.676099      -0.008935      1.561948
C      -1.688507      1.208918      -0.374801
C      -1.626914      -1.302426      -0.362510
H      -0.108964      0.864294      1.875915
H      -0.159119      -0.900101      1.901127
H      -1.662528      0.038894      2.027134
H      -1.874031      1.219131      -1.450737
H      -1.167253      2.123768      -0.099666
H      -2.654227      1.190310      0.129283
H      -1.062330      -2.186100      -0.068394
H      -1.812454      -1.343099      -1.437328
H      -2.590569      -1.313188      0.146400
O      1.315267      1.505706      -0.024825
H      1.744961      0.683028      0.474467
H      1.976659      1.809300      -0.653840

```

```

Rotational constants (GHz):      2.6317500      1.6691800      1.4651300
Vibrational harmonic frequencies (cm-1):
i433.6511      62.4748      190.5012
221.1858      256.3649      269.7639
299.0199      309.0711      336.5801
345.0723      377.8225      406.7424
439.8145      521.8530      589.8569
616.3752      670.1097      812.2259
880.5212      917.0330      957.8019
968.8042      979.4509      1022.2247
1058.4827      1083.0230      1224.6992
1249.5972      1292.3897      1320.0595
1390.0652      1395.2372      1403.3318
1431.5031      1477.0164      1489.1294
1491.8956      1503.2448      1507.5848
1525.0289      1583.4528      1621.4556
2286.0509      3056.2422      3059.0274
3068.6728      3120.1826      3127.4832
3130.7233      3145.6353      3149.2260
3155.8265      3187.3741      3880.8576
Zero-point correction (Hartree): 0.170555

```

```

#####
E-(tc4H9)CHOO
#####

```

```

Population analysis as 298K (%)
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)
Compound      Qtot      Erel      Erel2      n*Q*MB      %
-----
TS.H_tc4H9_COO+H2O.u 1.171e+41 0.00      0.00      2.342e+41 62.3
TS.H_tc4H9_COO+H2O.d 8.997e+40 0.14      0.14      1.415e+41 37.7
Total      3.757e+41 100

```

```

TS.H_tc4H9_COO+H2O.d
~~~~~
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -422.66646277
E(CCSD/Aug-CC-pVTZ) (Hartree): -422.59047409
T1 diagnostic: 0.018872

```

E(MP2/Aug-CC-pVTZ) (Hartree): -422.54233129  
 E(MP3/Aug-CC-pVTZ) (Hartree): -422.57773294  
 E(RHF/Aug-CC-pVTZ) (Hartree): -420.89623100  
 E(RM062X/Aug-CC-pVTZ) (Hartree): -423.26258143  
 Electronic state : 1-A  
 Cartesian coordinates (Angs):  

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.399109  | -0.178855 | 0.428857  |
| O | 1.158868  | -0.957649 | -0.219904 |
| O | 2.506853  | -0.705486 | 0.195450  |
| C | -1.023967 | -0.027794 | 0.002176  |
| H | 0.681791  | 0.044259  | 1.455153  |
| C | -1.139830 | -0.061072 | -1.518525 |
| C | -1.773462 | -1.214220 | 0.635398  |
| C | -1.568102 | 1.285438  | 0.564167  |
| H | -0.791415 | -1.011365 | -1.918721 |
| H | -0.543816 | 0.737421  | -1.958688 |
| H | -2.182749 | 0.077004  | -1.804265 |
| H | -1.682883 | -1.210101 | 1.722549  |
| H | -1.393360 | -2.161915 | 0.256727  |
| H | -2.830815 | -1.135148 | 0.382638  |
| H | -1.078163 | 2.137184  | 0.095963  |
| H | -1.424552 | 1.344529  | 1.644732  |
| H | -2.637710 | 1.346513  | 0.364284  |
| O | 1.429761  | 1.440657  | -0.152028 |
| H | 2.186728  | 0.693196  | -0.036423 |
| H | 1.570593  | 2.097265  | 0.535468  |

 Rotational constants (GHz): 2.8806300 1.4539600 1.2515500  
 Vibrational harmonic frequencies (cm-1):  

|           |           |           |
|-----------|-----------|-----------|
| 1436.3611 | 62.4810   | 160.4817  |
| 190.5382  | 216.8292  | 270.8594  |
| 274.3200  | 296.9959  | 329.3559  |
| 344.7307  | 382.6869  | 390.7319  |
| 488.7318  | 520.4101  | 561.3812  |
| 630.9591  | 690.7152  | 802.1800  |
| 943.9080  | 950.8939  | 963.2042  |
| 968.8173  | 976.2160  | 1032.3466 |
| 1065.7525 | 1102.7781 | 1212.3761 |
| 1242.1930 | 1258.4784 | 1316.7317 |
| 1363.5435 | 1396.5162 | 1403.0317 |
| 1430.0099 | 1480.0663 | 1491.4615 |
| 1492.6567 | 1503.3561 | 1507.2065 |
| 1521.2420 | 1555.7904 | 1661.1728 |
| 2142.1759 | 3058.5625 | 3060.6566 |
| 3068.7209 | 3129.0141 | 3132.7848 |
| 3142.8140 | 3146.4444 | 3150.0616 |
| 3151.8100 | 3154.0032 | 3890.8879 |

 Zero-point correction (Hartree): 0.170138

TS\_H\_tC4H9\_COO+H2O.u

~~~~~  
 E(CCS(D)/Aug-CC-pVTZ) (Hartree): -422.66681039  
 E(CCS(D)/Aug-CC-pVTZ) (Hartree): -422.59082716  
 T1 diagnostic: 0.018957  
 E(MP2/Aug-CC-pVTZ) (Hartree): -422.54239665  
 E(MP3/Aug-CC-pVTZ) (Hartree): -422.57804923  
 E(RHF/Aug-CC-pVTZ) (Hartree): -420.89691246  
 E(RM062X/Aug-CC-pVTZ) (Hartree): -423.26286544

Electronic state : 1-A  
 Cartesian coordinates (Angs):  

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.402062  | -0.178968 | 0.416857  |
| O | 1.160794  | -0.942785 | -0.252079 |
| O | 2.506934  | -0.715134 | 0.182905  |
| C | -1.025273 | -0.023681 | 0.002842  |
| H | 0.683864  | 0.025522  | 1.446575  |
| C | -1.164448 | -0.020731 | -1.516148 |
| C | -1.755333 | -1.238982 | 0.605249  |
| C | -1.580040 | 1.263457  | 0.612572  |
| H | -0.769850 | -0.936544 | -1.951948 |
| H | -0.632868 | 0.824705  | -1.954163 |
| H | -2.217535 | 0.068399  | -1.782755 |
| H | -1.638878 | -1.275165 | 1.689004  |
| H | -1.378977 | -2.169266 | 0.182304  |
| H | -2.818692 | -1.155386 | 0.380780  |
| H | -1.079616 | 2.139095  | 0.204026  |
| H | -1.451300 | 1.272676  | 1.695610  |
| H | -2.646057 | 1.332542  | 0.396275  |
| O | 1.466973  | 1.485268  | 0.039506  |
| H | 2.201244  | 0.715272  | 0.091990  |
| H | 1.409250  | 1.732790  | -0.888590 |

 Rotational constants (GHz): 2.8640400 1.4444800 1.2441900  
 Vibrational harmonic frequencies (cm-1):  

|           |           |           |
|-----------|-----------|-----------|
| i411.3542 | 52.3095   | 161.0749  |
| 189.0407  | 202.2691  | 259.2655  |
| 272.1286  | 289.3577  | 328.6877  |
| 343.0065  | 374.0734  | 395.6870  |
| 491.9649  | 532.7919  | 556.9291  |
| 591.9728  | 652.7869  | 806.0599  |
| 941.7645  | 951.7161  | 963.6564  |
| 967.8825  | 974.9323  | 1035.6433 |
| 1065.8683 | 1128.5005 | 1235.4280 |
| 1258.1603 | 1289.3366 | 1318.4895 |
| 1376.5536 | 1398.3530 | 1406.5135 |
| 1436.3684 | 1479.7896 | 1487.3938 |
| 1488.7430 | 1504.0392 | 1505.8087 |
| 1521.2321 | 1587.0622 | 1615.5018 |
| 2180.6644 | 3061.2647 | 3064.6255 |
| 3067.5902 | 3133.5843 | 3133.8622 |
| 3136.8987 | 3147.4336 | 3153.7184 |
| 3154.5219 | 3160.4320 | 3874.0931 |

 Zero-point correction (Hartree): 0.170195

#####  
Z-CHOCHO  
#####

Population analysis as 298K (%)  
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)  
Compound Qtot Erel Erel2 n\*Q\*MB %  
-----  
TS.CHO\_H\_COO+H2O.gd 1.140e+39 0.00 0.00 2.280e+39 92.7  
TS.CHO\_H\_COO+H2O.gu 1.752e+39 1.76 1.76 1.784e+38 7.26  
Total 2.459e+39 100

TS.CHO\_H\_COO+H2O.gd  
~~~~~  
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -378.83763472  
E(CCSD/Aug-CC-pVTZ) (Hartree): -378.77379490  
Tl diagnostic: 0.027492  
E(MP2/Aug-CC-pVTZ) (Hartree): -378.76217217  
E(MP3/Aug-CC-pVTZ) (Hartree): -378.75731532  
E(RHF/Aug-CC-pVTZ) (Hartree): -377.45376696  
E(RM062X/Aug-CC-pVTZ) (Hartree): -379.33383534  
Electronic state : 1-A  
Cartesian coordinates (Angs):  
C -0.208459 -0.048820 0.849971  
O -1.386226 -0.271020 0.474067  
O -1.284932 -0.509370 -0.929011  
H -0.067643 0.305032 1.867547  
C 0.861274 -0.827545 0.111180  
O 1.914898 -0.366886 -0.228031  
H 0.588727 -1.885615 -0.008687  
O 0.123368 1.647583 -0.114553  
H -0.418932 1.273070 -0.843695  
H 1.044087 1.563253 -0.401843  
Rotational constants (GHz): 5.1282000 3.1846400 2.6049000  
Vibrational harmonic frequencies (cm-1):  
i185.4067 115.5477 229.7590  
280.4243 338.2595 426.8376  
464.2440 599.4860 649.7454  
720.4244 863.2733 887.4548  
908.1487 1046.8320 1075.5272  
1309.8593 1382.5277 1603.5909  
1643.1228 1846.0391 3048.1089  
3181.2301 3514.3136 3793.6225  
Zero-point correction (Hartree): 0.068182

TS.CHO\_H\_COO+H2O.gu  
~~~~~  
E(RM062X/Aug-CC-pVTZ) (Hartree): -379.32931314  
Electronic state : 1-A  
Cartesian coordinates (Angs):  
C 0.090734 -0.215088 0.682253  
O -1.030843 -0.791262 0.596342  
O -1.547272 -0.586394 -0.717606  
H 0.464971 -0.060853 1.692372  
C 1.144929 -0.245667 -0.403829  
O 2.287756 -0.115394 -0.077336  
H 0.801689 -0.424643 -1.427546  
O -0.520344 1.539466 -0.051698  
H -1.157865 0.864717 -0.540203  
H -1.037148 2.013982 0.607227  
Rotational constants (GHz): 5.8107200 2.6636300 2.2725400  
Vibrational harmonic frequencies (cm-1):  
i440.3113 84.2250 196.9865  
280.3668 357.5167 427.5434  
461.2224 562.5155 604.7527  
655.4419 871.0795 980.4462  
1068.4950 1126.2474 1260.3607  
1320.5340 1357.3052 1578.5724  
1601.0355 1862.6579 2369.1043  
3101.1929 3174.1740 3875.3243  
Zero-point correction (Hartree): 0.066470

#####  
E-CHOCHO  
#####

Population analysis as 298K (%)  
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)  
Compound Qtot Erel Erel2 n\*Q\*MB %  
-----  
TS.H\_CHO\_COO+H2O.td 1.851e+39 0.00 0.00 3.703e+39 64.6  
TS.H\_CHO\_COO+H2O.tu 2.025e+39 0.43 0.43 1.964e+39 34.3  
TS.H\_CHO\_COO+H2O.cu 2.865e+39 2.78 2.78 5.276e+37 0.921  
TS.H\_CHO\_COO+H2O.cd 2.383e+39 3.74 3.74 8.610e+36 0.15  
Total 5.728e+39 100

TS.H\_CHO\_COO+H2O.cd  
~~~~~  
E(RM062X/Aug-CC-pVTZ) (Hartree): -379.32297602  
Electronic state : 1-A  
Cartesian coordinates (Angs):  
C -0.079763 -0.035118 0.527321  
O 0.438733 -0.949601 -0.160436  
O 1.850540 -0.861230 0.017516  
H 0.374932 0.229184 1.477906  
C -1.508058 0.355915 0.223956  
O -2.269525 -0.378175 -0.324170  
H -1.778395 1.370198 0.558262  
O 0.974615 1.409990 -0.341945  
H 1.656634 0.610348 -0.307636  
H 1.318839 2.097620 0.236088

Rotational constants (GHz): 6.3990500 2.5126600 1.9503200  
Vibrational harmonic frequencies (cm-1):  
i442.5539 69.3271 184.3756  
250.5551 327.2186 424.8962  
460.4301 615.1639 668.4890  
748.6086 889.8593 976.8490  
1001.9864 1105.0359 1182.3049  
1341.3895 1411.5273 1581.8798  
1673.8101 1882.2891 2334.0402  
3011.2197 3165.3432 3881.7042  
Zero-point correction (Hartree): 0.066496

TS.H\_CHO\_COO+H2O.cu

~~~~~  
E(RM062X/Aug-CC-pVTZ) (Hartree): -379.32516510  
Electronic state : 1-A  
Cartesian coordinates (Angs):  
C -0.013757 -0.314805 0.573044  
O 0.665289 -0.871929 -0.326399  
O 2.018079 -0.461971 -0.177921  
H 0.433476 -0.140450 1.546532  
C -1.515646 -0.353620 0.397606  
O -2.025025 0.039739 -0.607610  
H -2.094986 -0.744452 1.248556  
O 0.512909 1.554671 0.133421  
H 1.378487 1.064084 -0.079189  
H 0.089421 1.747286 -0.711736  
Rotational constants (GHz): 6.2944800 2.5948900 2.1234700  
Vibrational harmonic frequencies (cm-1):  
i357.2761 60.8188 170.7962  
238.0629 318.5011 387.6298  
495.5496 555.5374 643.6459  
772.6492 858.5151 972.2464  
1031.3229 1118.4349 1146.9818  
1336.2452 1411.1460 1587.4849  
1617.7359 1871.5024 2832.2885  
3017.2121 3181.1329 3849.2568  
Zero-point correction (Hartree): 0.067148

TS.H\_CHO\_COO+H2O.td

~~~~~  
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -378.83246849  
E(CCSD/Aug-CC-pVTZ) (Hartree): -378.76933151  
T1 diagnostic: 0.025813  
E(MP2/Aug-CC-pVTZ) (Hartree): -378.75847806  
E(MP3/Aug-CC-pVTZ) (Hartree): -378.75369876  
E(RHF/Aug-CC-pVTZ) (Hartree): -377.45011953  
E(RM062X/Aug-CC-pVTZ) (Hartree): -379.32929493  
Electronic state : 1-A  
Cartesian coordinates (Angs):  
C 0.081214 -0.275723 -0.315706  
O -0.843824 -0.915780 0.255360  
O -2.082838 -0.404087 -0.219564  
H -0.021997 0.024239 -1.353079  
C 1.449052 -0.393356 0.297996  
O 2.402715 0.058428 -0.262428  
H 1.490111 -0.897427 1.274748  
O -0.565498 1.477903 0.283575  
H -1.463063 0.981355 0.102269  
H -0.471084 2.174601 -0.373220  
Rotational constants (GHz): 7.1929600 2.3156600 1.8822600  
Vibrational harmonic frequencies (cm-1):  
i432.9580 92.1222 189.0501  
243.2693 360.6227 424.3596  
485.0619 563.4021 604.6298  
692.3635 935.8042 996.6519  
1115.7111 1117.4006 1171.7634  
1313.9525 1384.1847 1562.2286  
1641.6070 1871.9337 2468.8365  
3039.5028 3189.7426 3881.3251  
Zero-point correction (Hartree): 0.066854

TS.H\_CHO\_COO+H2O.tu

~~~~~  
E(RM062X/Aug-CC-pVTZ) (Hartree): -379.32851497  
Electronic state : 1-A  
Cartesian coordinates (Angs):  
C 0.087585 -0.263553 -0.315656  
O -0.823505 -0.914171 0.272187  
O -2.074389 -0.435605 -0.198956  
H -0.021901 0.026334 -1.354671  
C 1.458478 -0.382761 0.293513  
O 2.416260 0.074318 -0.253774  
H 1.498126 -0.906300 1.261803  
O -0.609442 1.528250 0.084243  
H -1.488588 0.971611 -0.019297  
H -0.535409 1.763903 1.015427  
Rotational constants (GHz): 7.1290300 2.3059700 1.8667100  
Vibrational harmonic frequencies (cm-1):  
i443.0619 83.8089 186.4612  
249.4944 352.7104 445.9160  
486.6907 547.3250 597.1385  
651.4940 938.9266 1001.1175  
1117.6757 1145.2243 1241.2470  
1317.1336 1386.8875 1574.2607  
1605.0735 1874.3307 2417.1486  
3021.0087 3198.5507 3863.1563  
Zero-point correction (Hartree): 0.066757

#####  
Z-(CHO) (CH3) CHOO

```

#####

Population analysis as 298K (%)
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)
Compound Qtot Erel Erel2 n*Q*MB %

TS.CHO_CH3_COO+H2O.td 7.861e+39 0.00 0.00 1.572e+40 81.5
TS.CHO_CH3_COO+H2O.tu 1.337e+40 1.19 1.19 3.573e+39 18.5
Total 1.929e+40 100

TS.CHO_CH3_COO+H2O.td
~~~~~
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -418.09613787
E(CCSD/Aug-CC-pVTZ) (Hartree): -418.02424595
  T1 diagnostic: 0.024282
E(MP2/Aug-CC-pVTZ) (Hartree): -418.00453367
E(MP3/Aug-CC-pVTZ) (Hartree): -418.00822820
E(RHF/Aug-CC-pVTZ) (Hartree): -416.51587049
E(RM062X/Aug-CC-pVTZ) (Hartree): -418.65747143
Electronic state : 1-A
Cartesian coordinates (Angs):
  C      0.053503      0.510089      -0.242902
  O      1.295345      0.391090      -0.476260
  O      1.572234      -1.000324      -0.276407
  C     -0.541265      1.864708      -0.134191
  C     -0.784804      -0.660496      -0.731969
  O     -1.740491      -1.083474      -0.145075
  H     -0.468405      -1.017753      -1.722478
  O      0.126907      -0.114768      1.615418
  H      0.821955      -0.737174      1.237849
  H     -0.670233      -0.642855      1.751227
  H      0.149362      2.534972      0.368592
  H     -0.751764      2.239751      -1.137222
  H     -1.477480      1.797072      0.415000
Rotational constants (GHz):      3.0237400      2.6034600      2.1567500
Vibrational harmonic frequencies (cm-1):
  i294.5970      103.8666      157.3966
  229.2183      251.4364      277.5234
  331.2616      369.3934      461.0827
  573.8369      584.0362      630.9039
  709.5620      829.2173      927.7549
  935.7407      1016.9944      1042.8266
  1063.5124      1301.3115      1383.5966
  1411.5854      1457.5812      1476.2017
  1585.0022      1648.3999      1849.9201
  3026.4700      3044.2601      3076.4487
  3153.1482      3190.1872      3829.5610
Zero-point correction (Hartree): 0.095522

TS.CHO_CH3_COO+H2O.tu
~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -418.65364383
Electronic state : 1-A
Cartesian coordinates (Angs):
 C -0.098962 0.393348 -0.214506
 O 1.032979 0.549312 -0.783538
 O 1.835757 -0.609671 -0.558705
 C -0.919905 1.607433 -0.000315
 C -0.827011 -0.943324 -0.290739
 O -2.006916 -0.976004 -0.100280
 H -0.216489 -1.808910 -0.566197
 O 0.672067 -0.235620 1.524187
 H 1.412557 -0.550959 0.813991
 H 1.024540 0.518333 2.007377
 H -0.284602 2.478674 0.125414
 H -1.571354 1.744044 -0.864667
 H -1.560494 1.449940 0.864135
Rotational constants (GHz): 3.4781400 2.1999800 1.9821000
Vibrational harmonic frequencies (cm-1):
 i479.5074 75.5477 143.1264
 169.8965 276.2940 290.5011
 317.5855 390.8500 464.6243
 516.6303 573.1859 592.7612
 642.7116 805.7494 933.8112
 987.2352 1037.0036 1055.1767
 1260.4407 1325.8567 1353.6128
 1417.9388 1450.1973 1468.8668
 1575.9248 1588.2158 1863.5597
 2102.0232 3081.8863 3097.9963
 3153.7525 3194.7585 3875.1003
Zero-point correction (Hartree): 0.093594

#####

E- (CH3) (CHO) CHOO
#####

Population analysis as 298K (%)
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)
Compound Qtot Erel Erel2 n*Q*MB %

TS.CH3_CHO_COO+H2O.tu 1.070e+40 0.00 0.00 2.139e+40 57.9
TS.CH3_CHO_COO+H2O.td 9.237e+39 0.11 0.11 1.530e+40 41.4
TS.CH3_CHO_COO+H2O.cu 1.263e+40 2.77 2.77 2.350e+38 0.636
Total 3.693e+40 100

TS.CH3_CHO_COO+H2O.cu
~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -418.64548103
Electronic state : 1-A
Cartesian coordinates (Angs):
  C     -0.025366      -0.396159      -0.182342

```

```

O      0.549211      0.387865      -1.002557
O      1.883762      0.639647      -0.564831
C      0.605579      -1.614387      0.392003
C      -1.539363      -0.382905      -0.317615
O      -2.174240      0.610154      -0.130674
H      -2.005535      -1.349846      -0.571769
O      0.319090      0.742517      1.395532
H      1.167917      0.933975      0.848040
H      -0.271950      1.494243      1.265055
H      0.093231      -1.909621      1.304193
H      1.659145      -1.441822      0.574896
H      0.489510      -2.407686      -0.352456
Rotational constants (GHz):      3.7224900      2.0974700      1.9794600
Vibrational harmonic frequencies (cm-1):
i402.6662      77.1136      163.1923
174.1248      234.8686      295.8736
329.5164      359.9611      433.1891
521.3119      583.3555      656.3974
706.3384      838.0812      923.3284
960.2361      1026.3692      1058.7274
1196.4388      1272.8609      1398.0759
1406.8485      1451.1367      1484.0440
1566.5977      1618.0799      1875.6129
2665.7013      2995.9619      3061.1791
3149.7036      3214.5776      3840.8954
Zero-point correction (Hartree): 0.094634

```

TS.CH3\_CHO\_COO+H2O.td

```

~~~~~
E (CCSD(T)/Aug-CC-pVTZ) (Hartree): -418.08641023
E (CCSD/Aug-CC-pVTZ) (Hartree): -418.01508453
T1 diagnostic: 0.023334
E (MP2/Aug-CC-pVTZ) (Hartree): -417.99550968
E (MP3/Aug-CC-pVTZ) (Hartree): -417.99973899
E (RHF/Aug-CC-pVTZ) (Hartree): -416.50719021
E (RM062X/Aug-CC-pVTZ) (Hartree): -418.64931525
Electronic state : 1-A
Cartesian coordinates (Angs):
C -0.082020 0.097490 0.265425
O 0.828600 -0.529143 0.902906
O 2.107428 -0.110137 0.427436
C -0.079804 1.562738 0.025086
C -1.411441 -0.634113 0.320056
O -2.426139 -0.105704 -0.021590
H -1.347972 -1.672825 0.676845
O 0.614769 -0.507710 -1.466343
H 1.512473 -0.371641 -0.916379
H 0.582521 0.155943 -2.161224
H 0.923774 1.919041 -0.173357
H -0.452747 2.024803 0.943312
H -0.775729 1.809543 -0.771865
Rotational constants (GHz): 4.3176300 1.8763000 1.8530000
Vibrational harmonic frequencies (cm-1):
i510.2156 86.8374 187.7715
195.4967 240.3522 310.6366
315.0816 397.8426 474.7669
485.5846 626.6112 635.6613
692.6604 826.3253 936.7395
982.2432 1021.7674 1060.7713
1186.9131 1312.0074 1378.3345
1404.0395 1456.7718 1478.6450
1545.9542 1640.3555 1876.8361
2236.9313 3040.0819 3068.3718
3154.1466 3216.8709 3889.7144
Zero-point correction (Hartree): 0.094232

```

TS.CH3\_CHO\_COO+H2O.tu

```

~~~~~
E (CCSD(T)/Aug-CC-pVTZ) (Hartree): -418.08650804
E (CCSD/Aug-CC-pVTZ) (Hartree): -418.01486761
T1 diagnostic: 0.023537
E (MP2/Aug-CC-pVTZ) (Hartree): -417.99577579
E (MP3/Aug-CC-pVTZ) (Hartree): -417.99939314
E (RHF/Aug-CC-pVTZ) (Hartree): -416.50576854
E (RM062X/Aug-CC-pVTZ) (Hartree): -418.64924910
Electronic state : 1-A
Cartesian coordinates (Angs):
C      0.085821      0.121255      -0.256431
O      -0.819921      -0.474056      -0.937190
O      -2.100634      -0.099373      -0.439292
C      0.076059      1.563931      0.084663
C      1.420248      -0.592110      -0.382458
O      2.429206      -0.119964      0.045716
H      1.368854      -1.572361      -0.883211
O      -0.643764      -0.433715      1.486110
H      -1.526658      -0.329678      0.890270
H      -0.534652      -1.375900      1.653732
H      0.764101      1.746795      0.903736
H      -0.926484      1.899230      0.318915
H      0.442983      2.090320      -0.800849
Rotational constants (GHz):      4.3116100      1.8775000      1.8446900
Vibrational harmonic frequencies (cm-1):
i532.1893      80.3737      165.9320
188.2305      245.9209      306.0751
330.4519      388.8337      480.7612
506.0685      584.0690      659.3351
669.8641      825.7599      941.9486
982.4094      1023.6748      1061.5969
1262.0816      1309.9661      1381.6358
1408.7100      1452.4939      1475.3380
1568.0410      1599.8582      1878.2197
2134.8631      3017.9327      3068.6507

```

3167.3298 3224.4799 3865.0379  
Zero-point correction (Hartree): 0.093988

#####  
Z- (C (O) CH3) (CH3) COO  
#####

Population analysis as 298K (%)  
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)

| Compound                | Qtot      | Erel | Erel2 | n*Q*MB    | %       |
|-------------------------|-----------|------|-------|-----------|---------|
| TS.CH3CO_CH3_COO+H2O.td | 7.658e+40 | 0.00 | 0.00  | 1.532e+41 | 99.4    |
| TS.CH3CO_CH3_COO+H2O.tu | 8.449e+40 | 3.16 | 3.16  | 8.178e+38 | 0.531   |
| TS.CH3CO_CH3_COO+H2O.cu | 6.658e+40 | 4.05 | 4.05  | 1.424e+38 | 0.0924  |
| TS.CH3CO_CH3_COO+H2O.cd | 6.096e+40 | 6.07 | 6.07  | 4.300e+36 | 0.00279 |
| Total                   |           |      |       | 1.541e+41 | 100     |

TS.CH3CO\_CH3\_COO+H2O.cd

~~~~~  
E(RM062X/Aug-CC-pVTZ) (Hartree): -457.96838706

Electronic state : 1-A

Cartesian coordinates (Angs):

C	0.410629	0.518931	0.001507
O	1.158187	0.146169	-0.956678
O	0.834667	-1.226966	-1.228165
C	0.770484	1.780406	0.695473
C	-1.084907	0.163396	-0.086462
O	-1.696293	0.971495	-0.730076
C	-1.720502	-1.008561	0.592480
O	1.105937	-0.927961	1.159808
H	1.075464	-1.405312	0.205793
H	0.547435	-1.424282	1.762514
H	1.849448	1.897745	0.710697
H	0.303834	2.605393	0.156751
H	0.378964	1.762602	1.710394
H	-1.239822	-1.928195	0.265429
H	-1.613707	-0.916005	1.674959
H	-2.775816	-1.018859	0.336364

Rotational constants (GHz): 2.3325700 1.9133200 1.6600900

Vibrational harmonic frequencies (cm-1):

i459.9100	59.1974	145.8684
186.2039	230.3138	250.5262
265.1876	294.7162	340.7828
401.1548	446.4311	525.9203
536.8535	637.4437	655.2352
666.9964	730.8393	922.6123
977.3105	1016.2034	1040.4210
1062.9390	1158.3864	1165.2484
1324.8669	1388.5786	1403.0385
1450.8966	1473.7268	1478.0538
1484.8211	1540.7580	1664.8998
1852.0860	2192.6503	3070.0910
3083.4071	3148.1417	3157.8142
3186.8972	3193.4524	3906.4330

Zero-point correction (Hartree): 0.122377

TS.CH3CO_CH3_COO+H2O.cu

~~~~~  
E(RM062X/Aug-CC-pVTZ) (Hartree): -457.97174864

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.391231  | 0.534064  | -0.011519 |
| O | 1.154527  | 0.170093  | -0.959553 |
| O | 0.871760  | -1.209942 | -1.228801 |
| C | 0.712820  | 1.811279  | 0.674230  |
| C | -1.095604 | 0.131734  | -0.076790 |
| O | -1.726732 | 0.928629  | -0.717575 |
| C | -1.682761 | -1.056166 | 0.607461  |
| O | 0.982218  | -0.972394 | 1.198226  |
| H | 1.020727  | -1.405011 | 0.229739  |
| H | 1.893830  | -0.788370 | 1.445885  |
| H | 1.775890  | 2.023438  | 0.604552  |
| H | 0.140254  | 2.603858  | 0.192271  |
| H | 0.402080  | 1.747639  | 1.715506  |
| H | -2.753968 | -1.056042 | 0.429445  |
| H | -1.225354 | -1.960636 | 0.211005  |
| H | -1.461747 | -1.021425 | 1.672938  |

Rotational constants (GHz): 2.3134600 1.9274100 1.6615600

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i413.6549 | 56.6110   | 155.4586  |
| 183.4512  | 209.3334  | 237.9285  |
| 269.5215  | 300.0253  | 340.5454  |
| 383.1754  | 444.5040  | 525.7305  |
| 581.3938  | 619.5250  | 636.0343  |
| 641.9366  | 707.9966  | 920.2248  |
| 980.0106  | 1016.8091 | 1039.9445 |
| 1064.8710 | 1170.0494 | 1278.0443 |
| 1330.9423 | 1393.6837 | 1405.6835 |
| 1457.1848 | 1463.3975 | 1476.7049 |
| 1477.6775 | 1585.6792 | 1628.7789 |
| 1847.5756 | 2219.4338 | 3080.4562 |
| 3086.7298 | 3154.1301 | 3160.7636 |
| 3184.1908 | 3189.4374 | 3874.2593 |

Zero-point correction (Hartree): 0.122519

TS.CH3CO\_CH3\_COO+H2O.td

~~~~~  
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -457.35187153

E(CCSD/Aug-CC-pVTZ) (Hartree): -457.27237396

T1 diagnostic: 0.022592

E(MP2/Aug-CC-pVTZ) (Hartree): -457.24262832

E(MP3/Aug-CC-pVTZ) (Hartree): -457.25634947
 E(RHF/Aug-CC-pVTZ) (Hartree): -455.57893626
 E(RM062X/Aug-CC-pVTZ) (Hartree): -457.97926750
 Electronic state : 1-A
 Cartesian coordinates (Angs):
 C 0.399680 0.175653 -0.472270
 O 0.758046 -0.996027 -0.778584
 O 0.339364 -1.857640 0.284241
 C 0.896706 1.310218 -1.291246
 C -0.946581 0.326865 0.248293
 O -1.067904 1.004589 1.233741
 C -2.083931 -0.304927 -0.499088
 O 1.502452 0.282177 1.201095
 H 1.268360 -0.682119 1.274902
 H 0.920537 0.741476 1.820881
 H 1.882260 1.082543 -1.685942
 H 0.201282 1.484188 -2.114893
 H 0.930558 2.204590 -0.673284
 H -2.229977 0.230200 -1.440714
 H -1.837911 -1.341259 -0.719363
 H -2.986028 -0.231272 0.100333
 Rotational constants (GHz): 2.2784100 1.9115800 1.7523500
 Vibrational harmonic frequencies (cm-1):
 i252.8878 96.3644 113.1146
 148.1198 199.5438 225.0358
 246.1915 265.8399 294.8403
 375.7042 485.4195 526.7985
 546.9802 584.8544 636.7742
 681.3336 733.5322 905.0116
 964.8051 975.4738 1004.7817
 1051.1977 1066.9640 1156.4766
 1316.5857 1383.8020 1408.4782
 1453.3498 1458.7738 1475.1557
 1482.5556 1599.9344 1654.8919
 1850.8061 3063.8697 3073.0447
 3146.1079 3150.4074 3190.6755
 3193.3223 3242.1446 3817.2970
 Zero-point correction (Hartree): 0.123582

TS.CH3CO_CH3_COO+H2O.tu
 ~~~~~  
 E(RM062X/Aug-CC-pVTZ) (Hartree): -457.97288459  
 Electronic state : 1-A  
 Cartesian coordinates (Angs):  
 C 0.289620 0.525607 -0.287381  
 O 1.254829 -0.094370 -0.849413  
 O 1.378808 -1.412719 -0.327241  
 C 0.339982 2.005941 -0.395212  
 C -1.110974 -0.078475 -0.048122  
 O -1.969934 0.720587 0.213163  
 C -1.374967 -1.539770 -0.219029  
 O 0.799078 -0.032163 1.571819  
 H 1.185214 -0.835020 0.979729  
 H 1.545236 0.495430 1.873205  
 H 1.367130 2.338710 -0.507064  
 H -0.251094 2.316750 -1.257372  
 H -0.130360 2.438173 0.484066  
 H -2.451485 -1.680523 -0.259341  
 H -0.876684 -1.922250 -1.106930  
 H -0.952168 -2.081774 0.625542  
 Rotational constants (GHz): 2.3882000 2.0272800 1.5277600  
 Vibrational harmonic frequencies (cm-1):  
 i469.9110 36.4812 151.7868  
 166.1494 250.5466 262.7581  
 296.8724 303.3261 372.1189  
 400.3338 443.2286 534.5503  
 571.0295 606.1684 615.0754  
 619.8368 703.3746 922.4468  
 984.1020 1015.0184 1043.3092  
 1060.5607 1163.8931 1275.3930  
 1334.6991 1398.0185 1416.9409  
 1444.4217 1455.8481 1467.1866  
 1469.5737 1570.4528 1581.9099  
 1844.4178 2125.2303 3084.8537  
 3086.0527 3157.0553 3157.9290  
 3187.6841 3196.6873 3875.5193  
 Zero-point correction (Hartree): 0.122230

#####  
 E-(CH3)(C(O)CH3)COO  
 #####

Population analysis as 298K (%)  
 Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)  
 Compound Qtot Erel Erel2 n\*Q\*MB %  
 -----  
 TS.CH3\_CH3CO\_COO+H2O.td 7.222e+40 0.00 0.00 1.444e+41 70.8  
 TS.CH3\_CH3CO\_COO+H2O.tu 9.604e+40 0.70 0.70 5.854e+40 28.7  
 TS.CH3\_CH3CO\_COO+H2O.cu 1.295e+41 3.31 3.31 9.690e+38 0.475  
 Total 2.039e+41 100

TS.CH3\_CH3CO\_COO+H2O.cu  
 ~~~~~  
 E(RM062X/Aug-CC-pVTZ) (Hartree): -457.96826385
 Electronic state : 1-A
 Cartesian coordinates (Angs):
 C 0.157727 -0.273894 0.021220
 O 0.804029 -0.169035 -1.067960
 O 2.204718 -0.317594 -0.826150
 C 0.452150 -1.298646 1.061334
 C -1.264652 0.273460 -0.108613

```

O      -1.436167      1.460336      -0.131404
C      -2.356741      -0.748443      -0.211022
O       1.142500      1.175588      0.944513
H       1.893521      0.833462      0.353953
H       0.769220      1.959915      0.523644
H       1.522528      -1.427712      1.164807
H       0.009322      -2.237014      0.715705
H      -0.002631      -1.015314      2.007013
H      -3.302816      -0.251428      -0.400874
H      -2.126949      -1.453192      -1.011825
H      -2.413734      -1.317933      0.718070
Rotational constants (GHz):   2.9940300   1.5579800   1.3949100
Vibrational harmonic frequencies (cm-1):
i360.1185      41.5330      142.7876
171.8660      181.3784      212.4801
240.2973      299.0857      324.3522
402.1527      423.3041      546.4730
563.0117      603.1452      610.0490
705.3357      759.5877      904.8405
956.3599      993.1175      1047.8527
1065.8480     1136.1664      1169.7555
1320.1752     1390.1571      1399.8803
1448.3353     1463.9240      1472.4712
1485.8029     1561.8805      1606.5239
1863.7681     2870.3843      3064.5779
3067.2323     3130.8743      3153.0932
3188.4188     3214.6344      3838.1550
Zero-point correction (Hartree): 0.123115

```

TS.CH3_CH3CO_COO+H2O.td

```

~~~~~
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -457.34398669
E(CCSD/Aug-CC-pVTZ) (Hartree): -457.26442653
T1 diagnostic: 0.021900

```

```

E(MP2/Aug-CC-pVTZ) (Hartree): -457.23579794
E(MP3/Aug-CC-pVTZ) (Hartree): -457.24903423
E(RHF/Aug-CC-pVTZ) (Hartree): -455.56926451
E(RM062X/Aug-CC-pVTZ) (Hartree): -457.97274992

```

Electronic state : 1-A

Cartesian coordinates (Angs):

```

C      0.181317      -0.271019      -0.261247
O      0.775451      0.728334      -0.788179
O      2.164410      0.687349      -0.450554
C      0.695336      -1.662658      -0.328796
C     -1.327060      -0.061468      -0.090347
O     -2.020799      -1.034395      0.023533
C     -1.801457      1.353528      -0.046910
O      0.837966      0.217873      1.539901
H      1.665682      0.487986      0.923210
H      1.100932      -0.530782      2.082408
H      1.777961      -1.671993      -0.295522
H      0.353632      -2.065020      -1.286416
H      0.246994      -2.268865      0.452495
H     -2.875053      1.371178      0.108671
H     -1.280118      1.874762      0.756704
H     -1.535074      1.859142      -0.975357
Rotational constants (GHz):   2.9297000   1.6279900   1.4080200
Vibrational harmonic frequencies (cm-1):
i508.5771      56.8884      150.3098
172.2473      199.7449      211.3831
293.1814      322.2000      365.3755
415.6461      448.0292      491.1497
589.7655      597.5252      635.3207
670.1175      769.1253      918.4149
957.1924      1014.1232      1024.1901
1062.7676     1157.2339      1207.7649
1333.2960     1394.3172      1411.1690
1452.6793     1463.6264      1468.0099
1477.7188     1535.2927      1637.7791
1865.0743     2178.2118      3069.7866
3075.7136     3139.9283      3157.4545
3194.3197     3219.4071      3891.9448

```

Zero-point correction (Hartree): 0.122327

TS.CH3_CH3CO_COO+H2O.tu

```

~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -457.97136056
Electronic state : 1-A

```

Cartesian coordinates (Angs):

```

C      0.180309      -0.251066      -0.262108
O      0.751474      0.797803      -0.722607
O      2.147067      0.744934      -0.426797
C      0.699164      -1.627658      -0.449561
C     -1.328788      -0.068542      -0.064602
O     -2.005700      -1.048218      0.077289
C     -1.846050      1.336631      -0.055751
O      0.968597      -0.061610      1.544377
H      1.737918      0.333352      0.908628
H      0.613069      0.682982      2.040196
H      1.781818      -1.633052      -0.438571
H      0.334975      -1.957983      -1.426297
H      0.282797      -2.283992      0.306599
H     -2.916251      1.323667      0.122162
H     -1.335546      1.920920      0.710209
H     -1.618099      1.814638      -1.008886
Rotational constants (GHz):   2.9290900   1.6155800   1.3939700
Vibrational harmonic frequencies (cm-1):
i527.0125      51.8279      145.9913
157.6810      168.2510      206.5080
294.7596      327.9894      362.7091
418.9659      461.6485      494.8174
574.2330      593.8998      622.5411

```

648.9057	763.7224	922.1347
957.0702	1011.8474	1024.0438
1061.5666	1160.5815	1270.6045
1334.0632	1398.4790	1412.9296
1449.2467	1460.0737	1468.0000
1475.4558	1559.7337	1598.5928
1867.5522	2101.4586	3070.2424
3076.4941	3137.8697	3172.1647
3193.6853	3228.0200	3871.4001

Zero-point correction (Hartree): 0.122059

Z- (CH=CH2) CHOO
#####

Population analysis as 298K (%)
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)
Compound Qtot Erel Erel2 n*Q*MB %

TS.C2H3_H_COO+H2O.tu 1.476e+39 0.01 0.01 2.922e+39 51.5
TS.C2H3_H_COO+H2O.td 1.325e+39 0.00 0.00 2.651e+39 46.8
TS.C2H3_H_COO+H2O.cu 1.315e+39 2.18 2.18 6.616e+37 1.17
TS.C2H3_H_COO+H2O.cd 1.279e+39 2.62 2.62 3.060e+37 0.54
Total 5.670e+39 100

TS.C2H3_H_COO+H2O.cd
~~~~~  
E(RM062X/Aug-CC-pVTZ) (Hartree): -343.40391304  
Electronic state : 1-A  
Cartesian coordinates (Angs):  
C -0.106615 -0.314689 -0.841342  
O -0.751971 0.783140 -0.767596  
O -0.777120 1.227843 0.593500  
H -0.367256 -0.886100 -1.729193  
C 1.205338 -0.597151 -0.244872  
C 1.945302 0.300116 0.394034  
H 1.580289 -1.591897 -0.452869  
O -1.231192 -1.176347 0.545447  
H -1.189032 -0.170697 0.882722  
H -0.712000 -1.695288 1.166475  
H 1.557695 1.287030 0.603093  
H 2.948417 0.050197 0.712045  
Rotational constants (GHz): 4.6994900 3.1843900 2.6314000  
Vibrational harmonic frequencies (cm-1):  
i494.8425 104.7517 242.5606  
282.7108 336.1411 381.8286  
476.0808 614.6188 639.3791  
669.4357 759.1419 888.1748  
976.9784 1028.0614 1045.6649  
1063.0047 1086.0198 1216.4014  
1325.1667 1381.7010 1445.2090  
1547.5845 1667.5631 1717.0342  
2214.0563 3163.1016 3174.3388  
3195.8442 3276.3503 3887.8752  
Zero-point correction (Hartree): 0.090687

TS.C2H3\_H\_COO+H2O.cu  
~~~~~  
E(RM062X/Aug-CC-pVTZ) (Hartree): -343.40452737
Electronic state : 1-A
Cartesian coordinates (Angs):
C -0.097343 -0.332115 -0.823488
O -0.692689 0.796742 -0.783065
O -0.720216 1.267085 0.570804
H -0.364196 -0.910228 -1.706566
C 1.179218 -0.667031 -0.186041
C 1.975695 0.234793 0.370598
H 1.469108 -1.704468 -0.283850
O -1.192729 -1.141579 0.632346
H -1.119826 -0.125383 0.925550
H -2.098721 -1.263887 0.329617
H 1.658048 1.262138 0.478937
H 2.955239 -0.050043 0.729214
Rotational constants (GHz): 4.7168100 3.1936600 2.6192800
Vibrational harmonic frequencies (cm-1):
i480.5354 108.0273 229.8253
280.3288 325.6363 384.1978
493.2056 588.8569 612.8966
656.1578 761.7188 883.9028
979.7497 1019.1779 1039.2422
1062.3255 1086.5086 1284.7199
1323.2043 1377.6273 1446.3940
1581.7115 1613.9625 1719.2788
2229.1597 3150.1981 3176.4915
3212.1877 3275.6198 3866.4348
Zero-point correction (Hartree): 0.090600

TS.C2H3_H_COO+H2O.td
~~~~~  
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -342.93703308  
E(CCSD/Aug-CC-pVTZ) (Hartree): -342.87543409  
T1 diagnostic: 0.023666  
E(MP2/Aug-CC-pVTZ) (Hartree): -342.85264949  
E(MP3/Aug-CC-pVTZ) (Hartree): -342.86363647  
E(RHF/Aug-CC-pVTZ) (Hartree): -341.60175629  
E(RM062X/Aug-CC-pVTZ) (Hartree): -343.40795471  
Electronic state : 1-A  
Cartesian coordinates (Angs):  
C -0.069827 0.180395 0.661008  
O 1.075253 0.745427 0.619689  
O 1.602721 0.578127 -0.698779

```

H      -0.402077      -0.056748      1.668573
C      -1.089010      0.363831      -0.372732
C      -2.360139      0.098967      -0.099253
H      -0.745107      0.757972      -1.317919
O       0.663911      -1.539716      0.027844
H       1.250987      -0.832925      -0.515492
H       0.075650      -1.971708      -0.597859
H      -2.659163      -0.295591      0.864798
H      -3.141519      0.269141      -0.826270
Rotational constants (GHz):   5.7989900   2.5992000   2.2326500
Vibrational harmonic frequencies (cm-1):
i508.5822      112.3648      217.6811
286.2568      366.8045      414.0844
439.0023      633.0387      640.2798
699.8648      718.9477      889.6456
947.0810      1010.6785      1045.3349
1057.1560      1189.2532      1216.8892
1288.4841      1344.9863      1439.9039
1532.4938      1642.2399      1720.7134
2175.7731      3164.4350      3170.6559
3234.9885      3260.1938      3888.2951
Zero-point correction (Hartree): 0.090552

```

```

TS.C2H3_H_COO+H2O.tu
~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -343.40773933
Electronic state : 1-A
Cartesian coordinates (Angs):
C 0.092132 -0.128240 0.652709
O -1.031437 -0.742799 0.660055
O -1.578139 -0.670684 -0.660206
H 0.427743 0.174014 1.642569
C 1.111368 -0.323173 -0.374785
C 2.379176 -0.060086 -0.089593
H 0.777144 -0.722486 -1.320252
O -0.649584 1.516048 -0.169630
H -1.233163 0.735374 -0.619836
H -1.231326 1.954447 0.460244
H 2.668940 0.347823 0.871496
H 3.167876 -0.240706 -0.805954
Rotational constants (GHz): 5.8069000 2.5900500 2.2275800
Vibrational harmonic frequencies (cm-1):
i525.9477 102.2617 211.6904
283.1277 361.5215 415.7652
449.7651 586.3896 649.7315
685.3989 711.8315 889.5295
947.5296 1008.8851 1040.7337
1056.4659 1209.1343 1263.3811
1294.8395 1345.3987 1444.3803
1564.8933 1605.7169 1723.1310
2104.1481 3162.3957 3166.8693
3243.6515 3263.2010 3865.4744
Zero-point correction (Hartree): 0.090346

```

```

#####
E-(CH=CH2)CHOO
#####

```

```

Population analysis as 298K (%)
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)
Compound Qtot Erel Erel2 n*Q*MB %

TS.H_C2H3_COO+H2O.tu 1.734e+39 0.00 0.00 3.469e+39 90
TS.H_C2H3_COO+H2O.cu 2.222e+39 1.45 1.45 3.860e+38 10
Total 3.855e+39 100

```

```

TS.H_C2H3_COO+H2O.cu
~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -343.41124552
Electronic state : 1-A
Cartesian coordinates (Angs):
C       0.050993      0.005367      -0.605356
O      -0.448437      -0.950725      0.071103
O      -1.869256      -0.810886      0.032650
H      -0.487103      0.327143      -1.488784
C       1.474791      0.302980      -0.453919
C       2.227434      -0.300579      0.457485
H       1.878997      1.039413      -1.134100
O      -1.012782      1.451891      0.281665
H      -1.667952      0.611262      0.296001
H      -0.686756      1.568749      1.179578
H       1.804621      -1.032493      1.133073
H       3.282684      -0.082920      0.541625
Rotational constants (GHz):   6.0705900   2.5319500   2.0363000
Vibrational harmonic frequencies (cm-1):
i451.7535      72.7446      206.1511
242.2264      331.4284      441.9926
485.8244      584.1977      611.7432
645.1274      721.8962      943.9264
1014.0962      1028.2092      1042.3208
1088.0602      1137.0876      1271.1272
1318.5844      1384.8069      1454.3972
1576.3312      1600.1427      1718.4772
2168.8795      3177.4612      3196.4429
3223.3618      3271.6349      3874.8590
Zero-point correction (Hartree): 0.090747

```

```

TS.H_C2H3_COO+H2O.tu
~~~~~
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -342.94212160
E(CCSD/Aug-CC-pVTZ) (Hartree): -342.88082025

```

```

T1 diagnostic: 0.022937
E(MP2/Aug-CC-pVTZ) (Hartree): -342.85838118
E(MP3/Aug-CC-pVTZ) (Hartree): -342.86908608
E(RHF/Aug-CC-pVTZ) (Hartree): -341.60813333
E(RM062X/Aug-CC-pVTZ) (Hartree): -343.41313033
Electronic state : 1-A
Cartesian coordinates (Angs):
 C 0.094444 -0.263902 -0.259007
 O -0.864992 -0.936264 0.249618
 O -2.080841 -0.406768 -0.273511
 H 0.004180 0.057926 -1.290673
 C 1.407481 -0.407990 0.351714
 C 2.484540 0.071069 -0.256849
 H 1.448261 -0.907714 1.310502
 O -0.685380 1.509934 0.141514
 H -1.553434 0.880935 -0.032902
 H -0.642666 1.679111 1.087917
 H 2.405460 0.577819 -1.210649
 H 3.469109 -0.018350 0.179693
Rotational constants (GHz): 6.9771600 2.2860500 1.8710800
Vibrational harmonic frequencies (cm-1):
 1542.3783 96.4432 200.0912
 259.2821 362.0739 439.3691
 508.1032 543.0958 596.9823
 631.6717 731.2801 943.1143
 977.4397 1021.4424 1037.6216
1131.1764 1213.1167 1238.6659
1308.7301 1360.2311 1452.0118
1562.2248 1584.5636 1726.1720
2009.8807 3172.2249 3185.7227
3215.3500 3266.1503 3874.1429
Zero-point correction (Hartree): 0.090326

#####
Z-(CH=CH2)(CH3)COO
#####

Population analysis as 298K (%)
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)
Compound Qtot Erel Erel2 n*Q*MB %

TS.C2H3_CH3_COO+H2O.td 9.787e+39 0.00 0.00 1.957e+40 63.1
TS.C2H3_CH3_COO+H2O.tu 1.014e+40 0.47 0.47 9.200e+39 29.7
TS.C2H3_CH3_COO+H2O.cu 8.934e+39 1.56 1.56 1.278e+39 4.12
TS.C2H3_CH3_COO+H2O.cd 9.601e+39 1.77 1.77 9.624e+38 3.1
Total 3.101e+40 100

TS.C2H3_CH3_COO+H2O.cd
~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -382.72538129
Electronic state : 1-A
Cartesian coordinates (Angs):
  C    -0.391398    -0.342725    -0.218300
  O    -0.292834     0.663654    -1.009510
  O     0.601365     1.638864    -0.460292
  C    -1.628972    -1.150370    -0.410112
  C     0.768519    -1.021292     0.392943
  C     2.023577    -0.813441     0.022153
  H     0.510957    -1.793218     1.108131
  O    -0.808788     0.850361     1.334762
  H    -0.129498     1.454505     0.744845
  H    -0.336187     0.608113     2.135836
  H     2.269329    -0.034229    -0.685293
  H     2.821434    -1.418991     0.430121
  H    -2.444237    -0.511314    -0.733404
  H    -1.433982    -1.915648    -1.163300
  H    -1.886110    -1.645283     0.523283
Rotational constants (GHz):    2.8854600    2.5952700    2.0508800
Vibrational harmonic frequencies (cm-1):
 1526.6880      111.1107      130.4698
 209.1300      275.4989      289.4447
 319.2747      401.0246      402.8398
 488.2798      616.8954      635.5350
 662.8205      693.0464      811.5611
 931.4100     1023.3169     1026.6872
1037.1628     1040.0828     1091.3256
1213.4937     1259.3363     1341.4228
1405.4301     1446.3065     1454.7524
1481.1213     1521.3975     1642.4515
1722.2101     2025.2727     3077.3001
3153.5752     3173.5576     3192.1633
3194.9627     3274.1818     3889.4954
Zero-point correction (Hartree): 0.117702

TS.C2H3_CH3_COO+H2O.cu
~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -382.72570946
Electronic state : 1-A
Cartesian coordinates (Angs):
 C -0.349480 -0.370972 -0.214442
 O -0.296124 0.625195 -1.024281
 O 0.505509 1.671316 -0.460313
 C -1.509333 -1.282928 -0.432509
 C 0.831037 -0.939387 0.461787
 C 2.071359 -0.697179 0.067470
 H 0.606012 -1.646604 1.248751
 O -0.811314 0.777655 1.367384
 H -0.182301 1.419661 0.766162
 H -1.706357 1.118544 1.269194
 H 2.275131 0.032653 -0.703372
 H 2.902766 -1.218482 0.521481

```

```

H -2.348548 -0.739588 -0.856869
H -1.205209 -2.076895 -1.116163
H -1.787561 -1.739817 0.514658
Rotational constants (GHz): 2.8727700 2.6034500 2.0576300
Vibrational harmonic frequencies (cm-1):
1513.6007 111.6374 153.0316
202.5773 270.5696 289.4514
317.5088 391.6602 404.0991
506.1682 597.4768 617.1203
635.5911 695.7442 806.9604
927.4295 1018.5463 1024.3156
1031.1599 1034.6140 1089.9564
1256.6800 1277.2433 1341.7617
1404.9383 1452.6601 1458.5309
1482.1607 1568.3815 1599.8797
1725.0235 2023.6382 3077.5734
3150.9756 3177.2411 3185.6121
3212.7965 3274.6665 3866.7877
Zero-point correction (Hartree): 0.117695

```

```

TS.C2H3_CH3_COO+H2O.td
~~~~~
E (CCSD(T)/Aug-CC-pVTZ) (Hartree): -382.19241274
E (CCSD/Aug-CC-pVTZ) (Hartree): -382.12242138
T1 diagnostic: 0.021934
E (MP2/Aug-CC-pVTZ) (Hartree): -382.09136903
E (MP3/Aug-CC-pVTZ) (Hartree): -382.11059889
E (RHF/Aug-CC-pVTZ) (Hartree): -380.65882375
E (RM062X/Aug-CC-pVTZ) (Hartree): -382.72832207
Electronic state : 1-A
Cartesian coordinates (Angs):
C      -0.048705      0.366492      -0.244030
O      1.114550      0.370183      -0.800955
O      1.795253      -0.835901      -0.459475
C      -0.662679      1.716072      -0.106157
C      -0.882773      -0.847418      -0.328366
C      -2.177616      -0.852050      -0.042706
H      -0.360378      -1.723376      -0.685469
O      0.747561      -0.006088      1.534468
H      1.409143      -0.553259      0.862722
H      0.231969      -0.653058      2.023649
H      -2.694616      0.024751      0.324954
H      -2.767177      -1.749087      -0.170219
H      0.122502      2.458397      -0.005987
H      -1.268293      1.928951      -0.987208
H      -1.301434      1.742547      0.772801
Rotational constants (GHz):      3.4190300      2.1734000      1.9478200
Vibrational harmonic frequencies (cm-1):
1570.4944      92.0004      144.7541
204.7066      285.1968      296.3032
337.8625      413.8203      455.4229
475.8069      602.0458      646.1422
678.6076      718.6109      797.9793
943.1716      1002.4137      1006.5630
1034.0984      1054.2103      1073.7609
1181.5025      1288.7827      1338.6320
1418.8466      1444.7707      1452.0884
1485.7628      1513.6524      1600.6639
1722.9166      2003.2387      3086.1378
3162.6906      3176.2546      3193.8178
3231.0592      3261.8858      3889.9740
Zero-point correction (Hartree): 0.117818

```

```

TS.C2H3_CH3_COO+H2O.tu
~~~~~
E (RM062X/Aug-CC-pVTZ) (Hartree): -382.72744386
Electronic state : 1-A
Cartesian coordinates (Angs):
C -0.062642 0.334707 -0.258131
O 1.083373 0.299133 -0.855186
O 1.777921 -0.878281 -0.443631
C -0.678631 1.691155 -0.202076
C -0.897345 -0.878101 -0.221437
C -2.194363 -0.843615 0.045806
H -0.378660 -1.790514 -0.475045
O 0.733280 -0.000606 1.533446
H 1.391843 -0.557827 0.859577
H 1.231047 0.778135 1.804071
H -2.709274 0.068375 0.317663
H -2.788614 -1.745607 0.006586
H 0.099855 2.447987 -0.227269
H -1.341573 1.823295 -1.056886
H -1.263320 1.789322 0.709299
Rotational constants (GHz): 3.4316700 2.1663200 1.9435300
Vibrational harmonic frequencies (cm-1):
1584.6256 80.1621 169.6916
196.7673 286.4606 299.7020
337.8414 406.3674 456.7722
486.7872 596.8671 616.8745
653.6187 717.5966 791.0561
940.4262 999.2118 1009.1953
1031.0325 1052.3610 1071.7638
1217.2681 1296.3748 1342.5324
1422.2528 1449.6405 1456.6191
1488.6211 1543.9699 1598.9433
1727.2107 1942.9098 3085.1330
3159.7932 3176.6886 3185.5672
3238.5720 3263.2429 3862.3501
Zero-point correction (Hartree): 0.117686

```

#####

E- (CH3) (CH=CH2) COO  
#####

Population analysis as 298K (%)  
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)  
Compound Qtot Erel Erel2 n\*Q\*MB %  
-----  
TS.CH3\_C2H3\_COO+H2O.tu 9.009e+39 0.00 0.00 1.802e+40 54.4  
TS.CH3\_C2H3\_COO+H2O.cu 1.098e+40 0.32 0.32 1.275e+40 38.5  
TS.CH3\_C2H3\_COO+H2O.cd 9.579e+39 1.61 1.61 1.260e+39 3.8  
TS.CH3\_C2H3\_COO+H2O.td 6.985e+39 1.51 1.51 1.095e+39 3.31  
Total 3.312e+40 100

TS.CH3\_C2H3\_COO+H2O.cd

~~~~~

E(RM062X/Aug-CC-pVTZ) (Hartree): -382.72586497

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.070052 | -0.362342 | -0.222766 |
| O | 0.311837  | 0.712184  | -0.827702 |
| O | 1.682515  | 0.970075  | -0.523294 |
| C | 0.743691  | -1.613388 | -0.270539 |
| C | -1.526506 | -0.483923 | -0.065534 |
| C | -2.307191 | 0.584841  | 0.005484  |
| H | -1.921422 | -1.488382 | 0.012756  |
| O | 0.625133  | 0.322378  | 1.515049  |
| H | 1.341863  | 0.737527  | 0.785182  |
| H | 1.088614  | -0.327355 | 2.049505  |
| H | -1.884345 | 1.579446  | -0.039057 |
| H | -3.377676 | 0.489166  | 0.120893  |
| H | 1.803076  | -1.388755 | -0.289646 |
| H | 0.466283  | -2.127196 | -1.195407 |
| H | 0.488065  | -2.262669 | 0.563475  |

Rotational constants (GHz): 3.5706900 2.1267900 1.9520700

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i627.0527 | 69.7000   | 212.6077  |
| 225.7715  | 236.1363  | 316.1810  |
| 333.0239  | 413.2525  | 464.1052  |
| 504.4202  | 592.1741  | 634.2391  |
| 653.6474  | 698.1834  | 826.9062  |
| 956.4307  | 987.8377  | 1016.4963 |
| 1032.9039 | 1042.5480 | 1083.3571 |
| 1163.0327 | 1264.9376 | 1342.4710 |
| 1400.3795 | 1441.1636 | 1455.4506 |
| 1488.0090 | 1503.8543 | 1564.3628 |
| 1723.8117 | 1951.2329 | 3061.8839 |
| 3143.0340 | 3178.1930 | 3208.5824 |
| 3211.9691 | 3272.7289 | 3896.1472 |

Zero-point correction (Hartree): 0.117488

TS.CH3\_C2H3\_COO+H2O.cu

~~~~~

E(RM062X/Aug-CC-pVTZ) (Hartree): -382.72833029

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.071544 | -0.336838 | -0.226705 |
| O | 0.285259  | 0.789552  | -0.741464 |
| O | 1.674972  | 1.009537  | -0.494718 |
| C | 0.725415  | -1.580658 | -0.424236 |
| C | -1.518290 | -0.469769 | 0.022905  |
| C | -2.345256 | 0.565820  | -0.023882 |
| H | -1.869304 | -1.468235 | 0.247172  |
| O | 0.804170  | 0.046759  | 1.537642  |
| H | 1.430667  | 0.578262  | 0.829077  |
| H | 0.274606  | 0.708742  | 1.992502  |
| H | -1.979193 | 1.560106  | -0.243120 |
| H | -3.404860 | 0.440375  | 0.148855  |
| H | 0.525163  | -2.281499 | 0.380742  |
| H | 1.782897  | -1.357953 | -0.488863 |
| H | 0.382869  | -2.017912 | -1.366552 |

Rotational constants (GHz): 3.5837200 2.0934200 1.9221200

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i532.3575 | 69.6145   | 199.9121  |
| 205.0407  | 230.5022  | 313.6578  |
| 335.3793  | 395.7314  | 477.3328  |
| 503.7455  | 583.6548  | 609.3260  |
| 649.6716  | 699.5162  | 816.5732  |
| 952.7734  | 994.6747  | 1028.4922 |
| 1039.2983 | 1042.3500 | 1090.7247 |
| 1254.9572 | 1272.7077 | 1341.6828 |
| 1404.1967 | 1442.5741 | 1461.1685 |
| 1487.9161 | 1551.1583 | 1597.7568 |
| 1723.6309 | 1996.2438 | 3063.0469 |
| 3159.4849 | 3176.4222 | 3211.8635 |
| 3221.0388 | 3269.8909 | 3877.6926 |

Zero-point correction (Hartree): 0.117898

TS.CH3\_C2H3\_COO+H2O.td

~~~~~

E(RM062X/Aug-CC-pVTZ) (Hartree): -382.72641251

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.099637 | 0.003713  | 0.235964  |
| O | 0.813447  | -0.722889 | 0.787243  |
| O | 2.101281  | -0.193072 | 0.476664  |
| C | -0.064973 | 1.494676  | 0.337564  |
| C | -1.373087 | -0.716144 | 0.090683  |
| C | -2.545531 | -0.108913 | -0.018600 |
| H | -1.282596 | -1.793960 | 0.080883  |
| O | 0.789617  | -0.158891 | -1.526984 |
| H | 1.642006  | -0.144824 | -0.836091 |
| H | 0.806818  | 0.651630  | -2.042019 |

```

H -2.638589 0.968864 -0.008799
H -3.457928 -0.679503 -0.119414
H -0.608548 1.954723 -0.482997
H 0.962270 1.837678 0.365429
H -0.558822 1.764215 1.273958
Rotational constants (GHz): 4.2980400 1.8386700 1.8227900
Vibrational harmonic frequencies (cm-1):
i613.7021 95.0126 207.6082
239.1083 257.6421 322.3599
345.1134 418.9986 453.2429
498.4448 569.8888 629.2030
657.2815 713.4606 820.0292
954.0951 983.0651 1017.7114
1036.9286 1041.1644 1067.7173
1171.7663 1310.3753 1332.7684
1402.7751 1445.2520 1454.5300
1494.6944 1509.7275 1578.2811
1731.6625 1978.4208 3073.8930
3154.2837 3179.2019 3211.1323
3218.1425 3265.5464 3898.3303
Zero-point correction (Hartree): 0.117870

```

```

TS.CH3_C2H3_COO+H2O.tu
~~~~~
E(CCS(D,T)/Aug-CC-pVTZ) (Hartree): -382.19272342
E(CCS(D)/Aug-CC-pVTZ) (Hartree): -382.12283965
T1 diagnostic: 0.021603
E(MP2/Aug-CC-pVTZ) (Hartree): -382.09183276
E(MP3/Aug-CC-pVTZ) (Hartree): -382.11100863
E(RHF/Aug-CC-pVTZ) (Hartree): -380.65963772
E(RM062X/Aug-CC-pVTZ) (Hartree): -382.72875525
Electronic state : 1-A
Cartesian coordinates (Angs):
C      0.091802      0.027398      -0.266807
O     -0.843256     -0.677812     -0.816360
O     -2.115679     -0.180334     -0.414966
C      0.047233      1.519225     -0.269120
C      1.373190     -0.692493     -0.233591
C      2.529292     -0.112018      0.054603
H      1.306180     -1.750308     -0.454255
O     -0.731428     -0.080101      1.542176
H     -1.601343     -0.114161      0.870825
H     -0.610141     -0.969759      1.887766
H      2.599504      0.943040      0.281712
H      3.446608     -0.683383      0.075599
H      0.585353      1.919373      0.583936
H     -0.981977      1.856042     -0.252422
H      0.529619      1.852460     -1.190470
Rotational constants (GHz):      4.2886100      1.8576700      1.8208000
Vibrational harmonic frequencies (cm-1):
i614.1588      76.9828      189.6002
217.1492      264.1762      323.4635
349.1249      409.2213      470.4877
504.0576      583.6954      601.7435
660.6388      709.0061      812.6294
957.5592      986.6842      1019.5413
1036.5414      1041.6424      1070.2129
1199.0720      1308.9267      1339.2158
1406.1345      1448.5293      1459.9035
1493.8766      1538.2842      1588.7417
1729.4175      1916.3912      3077.3058
3169.9707      3182.0268      3207.0803
3217.3464      3269.2232      3876.8918
Zero-point correction (Hartree): 0.117810

```

```

#####
Z-(CCH3=CH2)CHOO
#####

```

```

Population analysis as 298K (%)
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)
Compound      Qtot      Erel      Erel2      n*Q*MB      %
-----
TS.CCH3CH2_H_COO+H2O.tu 1.015e+40 0.00 0.00 2.030e+40 45.7
TS.CCH3CH2_H_COO+H2O.td 1.032e+40 0.19 0.19 1.494e+40 33.6
TS.CCH3CH2_H_COO+H2O.cu 1.050e+40 0.58 0.58 7.931e+39 17.9
TS.CCH3CH2_H_COO+H2O.cd 1.055e+40 1.68 1.68 1.240e+39 2.79
Total 4.441e+40 100

```

```

TS.CCH3CH2_H_COO+H2O.cd
~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -382.71679677
Electronic state : 1-A
Cartesian coordinates (Angs):
C -0.189945 -0.252481 -0.772680
O -1.356016 0.253151 -0.872091
O -1.816319 0.669099 0.418680
H 0.036478 -0.920213 -1.603295
C 0.977356 0.311723 -0.068852
C 0.938416 1.532543 0.454148
C 2.205937 -0.549783 -0.122523
O -0.769702 -1.524225 0.644223
H -1.369520 -0.665957 0.844225
H -0.142889 -1.588539 1.370455
H 0.018168 2.097463 0.475888
H 1.836302 1.973223 0.868464
H 2.505599 -0.741159 -1.154634
H 2.027270 -1.522015 0.340378
H 3.034305 -0.069016 0.391464
Rotational constants (GHz): 3.7877600 2.1397100 1.7355200
Vibrational harmonic frequencies (cm-1):

```



```

i503.2499 80.8306 152.1050
192.5672 259.5743 323.4281
372.8095 383.7790 453.0306
528.5164 617.0470 644.8128
700.0997 722.0313 884.7940
922.3843 990.1277 1020.5175
1035.0488 1047.0814 1089.9402
1208.5894 1287.5716 1381.8172
1416.4107 1448.4110 1482.8821
1495.7860 1548.5974 1673.5358
1734.1594 2164.0840 3059.0396
3111.0130 3146.2476 3160.6334
3170.8221 3275.4888 3886.8547
Zero-point correction (Hartree): 0.118630

```

TS.CCH3CH2\_H\_COO+H2O.cu

~~~~~  
E(RM062X/Aug-CC-pVTZ) (Hartree): -382.71843980

Electronic state : 1-A

Cartesian coordinates (Angs):

```

C -0.198647 -0.201247 -0.789676
O -1.359905 0.326196 -0.828714
O -1.771685 0.679534 0.498184
H 0.000123 -0.827398 -1.660155
C 0.987804 0.303426 -0.078693
C 0.996001 1.544464 0.394351
C 2.160128 -0.629229 -0.061027
O -0.679045 -1.502178 0.659853
H -1.265946 -0.642341 0.892803
H -1.295757 -2.159386 0.321555
H 0.102454 2.151338 0.381011
H 1.904337 1.961587 0.809513
H 2.410438 -0.970993 -1.067508
H 1.924767 -1.508698 0.537871
H 3.032941 -0.137005 0.360591

```

Rotational constants (GHz): 3.7399900 2.1972900 1.7398700

Vibrational harmonic frequencies (cm-1):

```

i492.8010 76.6140 168.8583
194.7020 250.3159 322.9793
368.0589 388.0215 455.6322
530.5395 590.9088 625.6194
673.1637 716.4946 882.1032
924.7793 993.4216 1014.6613
1035.1650 1046.0080 1091.2463
1267.7778 1309.4461 1377.8531
1411.2771 1449.8945 1483.2602
1500.5505 1583.1760 1607.1061
1734.3950 2150.1398 3061.3745
3123.9912 3135.7572 3161.0545
3172.7863 3272.9483 3871.0506

```

Zero-point correction (Hartree): 0.118517

TS.CCH3CH2\_H\_COO+H2O.td

~~~~~

E(CCS(D)T)/Aug-CC-pVTZ) (Hartree): -382.18334365

E(CCS(D)/Aug-CC-pVTZ) (Hartree): -382.11322969

T1 diagnostic: 0.022623

E(MP2/Aug-CC-pVTZ) (Hartree): -382.08171393

E(MP3/Aug-CC-pVTZ) (Hartree): -382.10122926

E(RHF/Aug-CC-pVTZ) (Hartree): -380.65053884

E(RM062X/Aug-CC-pVTZ) (Hartree): -382.71953228

Electronic state : 1-A

Cartesian coordinates (Angs):

```

C -0.174906 -0.536496 -0.681276
O -1.239658 0.093584 -0.997872
O -1.645122 0.914822 0.098905
H -0.036982 -1.442122 -1.266274
C 1.048694 0.055159 -0.109489
C 2.137014 -0.708635 -0.204691
C 1.067206 1.449260 0.439441
O -0.990887 -1.250892 0.989530
H -1.442791 -0.293377 0.917414
H -0.366862 -1.228494 1.720275
H 2.098133 -1.703396 -0.630214
H 3.099181 -0.356130 0.141648
H 0.525753 1.509781 1.381162
H 0.562956 2.132071 -0.241182
H 2.097909 1.765831 0.588742

```

Rotational constants (GHz): 3.6511300 2.1521900 1.8253500

Vibrational harmonic frequencies (cm-1):

```

i482.2433 57.3073 182.3080
243.6691 270.1213 317.5390
382.5984 404.2150 453.4670
544.2791 623.8173 639.1723
724.0129 739.0265 850.5850
899.7202 989.3272 998.0588
1043.1192 1061.4442 1080.6934
1195.4521 1344.9057 1366.9266
1422.3517 1452.2773 1471.9897
1481.4257 1533.5965 1640.7202
1715.5278 2229.1877 3079.3897
3151.4761 3160.4132 3165.5064
3173.6946 3253.3764 3890.5135

```

Zero-point correction (Hartree): 0.118996

TS.CCH3CH2\_H\_COO+H2O.tu

~~~~~

E(CCS(D)T)/Aug-CC-pVTZ) (Hartree): -382.18339631

E(CCS(D)/Aug-CC-pVTZ) (Hartree): -382.11328220

T1 diagnostic: 0.022073

E(MP2/Aug-CC-pVTZ) (Hartree): -382.08216796

E(MP3/Aug-CC-pVTZ) (Hartree): -382.10130155

```

E(RHF/Aug-CC-pVTZ) (Hartree): -380.65032118
E(RM062X/Aug-CC-pVTZ) (Hartree): -382.71959777
Electronic state : 1-A
Cartesian coordinates (Angs):
 C -0.149611 -0.647498 -0.574314
 O -1.207444 -0.096610 -1.040712
 O -1.647709 0.922368 -0.140884
 H 0.004635 -1.645746 -0.978600
 C 1.064536 0.028963 -0.092366
 C 2.174414 -0.700866 -0.198341
 C 1.054174 1.441249 0.402741
 O -0.930210 -0.926191 1.247094
 H -1.415258 -0.028702 0.910657
 H -1.592191 -1.623645 1.209149
 H 2.156029 -1.719474 -0.563617
 H 3.137244 -0.294495 0.080138
 H 0.494604 1.513623 1.333327
 H 0.559804 2.096551 -0.310413
 H 2.076964 1.774261 0.569052
Rotational constants (GHz): 3.7076900 2.0804000 1.8691200
Vibrational harmonic frequencies (cm-1):
 i520.7884 57.8664 183.4190
 254.6355 265.1914 309.1570
 395.7729 402.5922 460.4899
 544.6222 583.3711 627.6387
 708.7419 741.2247 857.9250
 899.6171 984.8257 1000.8516
 1043.8530 1069.1428 1080.5320
 1270.5619 1352.9485 1369.8969
 1419.9287 1456.3650 1473.6678
 1488.0057 1564.1463 1598.1431
 1717.1205 2083.8480 3080.8215
 3154.0716 3160.1445 3163.6050
 3171.7250 3257.2689 3874.3113
Zero-point correction (Hartree): 0.118756

#####
E- (CCH3=CH2) CHOO
#####

Population analysis as 298K (%)
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)
Compound Qtot Erel Erel2 n*Q*MB %

TS.H_CCH3CH2_COO+H2O.tu 1.442e+40 0.00 0.00 2.884e+40 65
TS.H_CCH3CH2_COO+H2O.td 1.292e+40 0.42 0.42 1.271e+40 28.6
TS.H_CCH3CH2_COO+H2O.cu 1.803e+40 1.59 1.59 2.478e+39 5.58
TS.H_CCH3CH2_COO+H2O.cd 2.425e+40 2.88 2.88 3.776e+38 0.85
Total 4.441e+40 100

TS.H_CCH3CH2_COO+H2O.cd
~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -382.72282963
Electronic state : 1-A
Cartesian coordinates (Angs):
  C     0.197112    -0.011185     0.455491
  O     1.055786    -0.918051     0.210740
  O     2.351899    -0.331092     0.352652
  H     0.442064     0.699007     1.239221
  C    -1.201872    -0.206143     0.060036
  C    -1.549252    -1.305878    -0.599351
  C    -2.136911     0.898317     0.446896
  O     1.003473     1.263919    -0.852357
  H     1.855536     0.731232    -0.452268
  H     1.068221     2.170996    -0.540715
  H    -0.814643    -2.053087    -0.864936
  H    -2.578576    -1.478741    -0.883393
  H    -1.821281     1.836121    -0.013477
  H    -2.144628     1.046712     1.527859
  H    -3.150420     0.678886     0.121000
Rotational constants (GHz):      4.2824300      1.7873700      1.4764000
Vibrational harmonic frequencies (cm-1):
  i505.0946      40.5174      161.1040
  177.9594      198.8378      343.3489
  361.0874      412.4741      484.3289
  534.1700      555.5315      624.9549
  670.6998      753.9570      912.3878
  957.3662      1007.8856     1014.5282
 1035.3079      1070.8884     1105.9302
 1215.2782      1285.1188     1379.4069
 1413.2114      1451.7550     1484.0490
 1496.9680      1541.8240     1637.6817
 1740.3712      2051.4127     3061.3066
 3117.8487      3161.3846     3168.2808
 3176.7071      3269.2137     3887.7305
Zero-point correction (Hartree): 0.118380

TS.H_CCH3CH2_COO+H2O.cu
~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -382.72528842
Electronic state : 1-A
Cartesian coordinates (Angs):
 C -0.201050 -0.010339 -0.463139
 O -1.065611 -0.910010 -0.217634
 O -2.357126 -0.313602 -0.362386
 H -0.442887 0.715053 -1.233079
 C 1.198310 -0.208551 -0.062673
 C 1.541089 -1.300877 0.612817
 C 2.134905 0.887712 -0.468982
 O -0.999362 1.369542 0.755962
 H -1.841897 0.821144 0.398906

```

```

H -0.853805 1.088412 1.664992
H 0.805174 -2.046709 0.880071
H 2.569035 -1.472662 0.902590
H 1.782733 1.844158 -0.079952
H 2.181212 0.975010 -1.555620
H 3.137701 0.700487 -0.093577
Rotational constants (GHz): 4.2471300 1.7853300 1.4779700
Vibrational harmonic frequencies (cm-1):
i447.5035 57.3113 159.2676
184.9268 199.4499 326.7766
359.1670 415.8004 489.8255
536.1051 554.1379 598.1187
649.4641 751.4300 914.5277
952.4163 1010.3889 1014.3777
1038.1268 1075.8107 1137.4279
1269.6594 1287.2349 1393.4399
1415.0235 1451.1661 1483.5810
1498.6437 1580.3091 1604.7550
1736.7225 2158.8005 3062.9399
3120.9070 3162.0364 3174.4653
3177.3043 3266.3549 3871.9345
Zero-point correction (Hartree): 0.118784

```

```

TS_H_CCH3CH2_COO+H2O.td
~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -382.72678974
Electronic state : 1-A
Cartesian coordinates (Angs):
C      -0.186783      0.210739      -0.473831
O      -0.941607      -0.817300      -0.477799
O      -2.293301      -0.354299      -0.466467
H      -0.505786      1.071127      -1.053186
C      1.226137      0.023785      -0.146020
C      2.077629      0.944331      -0.588841
C      1.584518      -1.174999      0.672009
O      -1.074412      0.956716      1.131590
H      -1.892829      0.488424      0.588978
H      -1.195480      1.909188      1.095130
H      1.736610      1.792873      -1.168091
H      3.137811      0.874130      -0.385950
H      1.304025      -2.090870      0.152494
H      1.030166      -1.155369      1.610759
H      2.651039      -1.193567      0.881383
Rotational constants (GHz):      4.2476200      1.7306000      1.5938800
Vibrational harmonic frequencies (cm-1):
i548.7841      75.9278      162.8636
188.2533      197.5827      330.8328
386.5798      405.2583      504.1626
543.2260      564.6341      629.3507
690.3439      757.5785      879.2911
961.4405      996.3523      998.7048
1051.6434      1075.5494      1087.0526
1205.1941      1320.7004      1373.8336
1419.0063      1452.7207      1477.8272
1491.5862      1518.5435      1598.8873
1737.0173      2034.6612      3071.8398
3134.3804      3164.7661      3168.7242
3175.8854      3257.3210      3894.2721
Zero-point correction (Hartree): 0.118428

```

```

TS_H_CCH3CH2_COO+H2O.tu
~~~~~
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -382.19129250
E(CCSD/Aug-CC-pVTZ) (Hartree): -382.12172920
T1 diagnostic: 0.021044
E(MP2/Aug-CC-pVTZ) (Hartree): -382.09100680
E(MP3/Aug-CC-pVTZ) (Hartree): -382.10995235
E(RHF/Aug-CC-pVTZ) (Hartree): -380.66047180
E(RM062X/Aug-CC-pVTZ) (Hartree): -382.72745558
Electronic state : 1-A
Cartesian coordinates (Angs):
C -0.192383 0.174187 -0.474454
O -0.932561 -0.863413 -0.381187
O -2.290251 -0.423944 -0.415905
H -0.519787 0.977249 -1.124996
C 1.225436 0.026451 -0.145281
C 2.042771 0.995263 -0.547740
C 1.638903 -1.190418 0.622240
O -1.135978 1.196857 0.932495
H -1.921083 0.589752 0.482643
H -0.950650 0.824868 1.800290
H 1.668423 1.852848 -1.091379
H 3.103387 0.960500 -0.337529
H 1.386272 -2.095615 0.070760
H 1.106883 -1.242676 1.572969
H 2.708520 -1.175821 0.815430
Rotational constants (GHz): 4.2093000 1.7684700 1.5405500
Vibrational harmonic frequencies (cm-1):
i551.1891 70.9308 162.9906
183.5116 192.2896 322.3966
383.3169 419.2034 515.6749
546.7143 561.8323 597.3138
661.4507 753.9383 882.4230
962.4028 998.5176 1003.8076
1053.6482 1074.9206 1123.3733
1231.1063 1327.4725 1386.2048
1423.7723 1455.0773 1478.1762
1492.2965 1555.6944 1581.7863
1736.1568 1986.3261 3070.5206
3129.9039 3164.2088 3170.5304
3187.1723 3259.4365 3875.5122
Zero-point correction (Hartree): 0.118424

```

#####  
Z-(CH2-CH=CH2)CHOO  
#####

Population analysis as 298K (%)

Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)

| Compound                  | Qtot      | Erel | Erel2 | n*Q*MB    | %       |
|---------------------------|-----------|------|-------|-----------|---------|
| TS.CH2CHCH2_H_COO+H2O.mmu | 2.463e+40 | 0.19 | 0.19  | 3.585e+40 | 33.5    |
| TS.CH2CHCH2_H_COO+H2O.tpu | 1.614e+40 | 0.00 | 0.00  | 3.228e+40 | 30.1    |
| TS.CH2CHCH2_H_COO+H2O.mpu | 3.795e+40 | 0.92 | 0.92  | 1.607e+40 | 15      |
| TS.CH2CHCH2_H_COO+H2O.tmu | 2.885e+40 | 1.24 | 1.24  | 7.099e+39 | 6.62    |
| TS.CH2CHCH2_H_COO+H2O.tmd | 1.382e+40 | 1.05 | 1.05  | 4.659e+39 | 4.35    |
| TS.CH2CHCH2_H_COO+H2O.mmd | 2.198e+40 | 1.45 | 1.45  | 3.803e+39 | 3.55    |
| TS.CH2CHCH2_H_COO+H2O.tcu | 9.845e+39 | 1.32 | 1.32  | 2.130e+39 | 1.99    |
| TS.CH2CHCH2_H_COO+H2O.tcd | 6.732e+39 | 1.22 | 1.22  | 1.715e+39 | 1.6     |
| TS.CH2CHCH2_H_COO+H2O.mpd | 3.172e+40 | 2.18 | 2.18  | 1.597e+39 | 1.49    |
| TS.CH2CHCH2_H_COO+H2O.tpd | 1.864e+40 | 1.99 | 1.99  | 1.291e+39 | 1.2     |
| TS.CH2CHCH2_H_COO+H2O.ppd | 1.926e+40 | 2.74 | 2.74  | 3.775e+38 | 0.352   |
| TS.CH2CHCH2_H_COO+H2O.ppu | 1.456e+40 | 2.97 | 2.97  | 1.919e+38 | 0.179   |
| TS.CH2CHCH2_H_COO+H2O.pmu | 1.375e+40 | 3.38 | 3.38  | 9.118e+37 | 0.0851  |
| TS.CH2CHCH2_H_COO+H2O.pmd | 1.336e+40 | 4.86 | 4.86  | 7.338e+36 | 0.00685 |
| Total                     |           |      |       | 1.072e+41 | 100     |

TS.CH2CHCH2\_H\_COO+H2O.mmd

~~~~~

E(RM062X/Aug-CC-pVTZ) (Hartree): -382.71385780

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.349449 | 0.175598  | 0.650593  |
| O | -1.018000 | -0.904449 | 0.690473  |
| O | -1.590387 | -1.142463 | -0.601134 |
| H | -0.141927 | 0.580537  | 1.638535  |
| C | 0.599174  | 0.521839  | -0.455969 |
| C | 1.815996  | -0.345225 | -0.259200 |
| H | 0.134551  | 0.312148  | -1.414827 |
| H | 0.864668  | 1.574869  | -0.376023 |
| C | 3.001502  | 0.117113  | 0.103523  |
| H | 1.660085  | -1.405774 | -0.421573 |
| H | 3.847555  | -0.543755 | 0.231448  |
| H | 3.168906  | 1.174210  | 0.272476  |
| O | -1.909537 | 1.213034  | 0.028718  |
| H | -2.061522 | 0.291892  | -0.459048 |
| H | -1.732253 | 1.870940  | -0.649129 |

Rotational constants (GHz): 5.0292800 1.5214400 1.3395700

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i462.8040 | 58.1089   | 85.0079   |
| 198.5073  | 259.6932  | 325.1647  |
| 373.6705  | 452.1470  | 485.8620  |
| 589.1302  | 627.2334  | 665.0589  |
| 687.2047  | 887.2358  | 912.8034  |
| 945.7548  | 987.0182  | 1016.2187 |
| 1048.1568 | 1079.7158 | 1154.2518 |
| 1191.3340 | 1259.6183 | 1300.7770 |
| 1320.5422 | 1368.7297 | 1451.6596 |
| 1470.3716 | 1550.7337 | 1675.4143 |
| 1731.8161 | 2319.2439 | 3101.6197 |
| 3160.9912 | 3162.9828 | 3176.7373 |
| 3187.1144 | 3251.5028 | 3892.8796 |

Zero-point correction (Hartree): 0.119403

TS.CH2CHCH2\_H\_COO+H2O.mmu

~~~~~

E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -382.18021578

E(CCSD/Aug-CC-pVTZ) (Hartree): -382.11144946

T1 diagnostic: 0.021215

E(MP2/Aug-CC-pVTZ) (Hartree): -382.07777979

E(MP3/Aug-CC-pVTZ) (Hartree): -382.09915446

E(RHF/Aug-CC-pVTZ) (Hartree): -380.65224823

E(RM062X/Aug-CC-pVTZ) (Hartree): -382.71592363

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.350249 | 0.201027  | 0.648713  |
| O | -1.007595 | -0.886333 | 0.713655  |
| O | -1.553069 | -1.172242 | -0.578644 |
| H | -0.157999 | 0.635671  | 1.628184  |
| C | 0.598887  | 0.540167  | -0.456106 |
| C | 1.807703  | -0.336751 | -0.254850 |
| H | 0.133746  | 0.342318  | -1.416347 |
| H | 0.860558  | 1.592793  | -0.376909 |
| C | 2.996815  | 0.117404  | 0.107114  |
| H | 1.644957  | -1.396717 | -0.415268 |
| H | 3.838394  | -0.549214 | 0.235343  |
| H | 3.171576  | 1.173831  | 0.272544  |
| O | -1.848079 | 1.238055  | -0.150653 |
| H | -1.986636 | 0.279184  | -0.564975 |
| H | -2.553586 | 1.355213  | 0.493339  |

Rotational constants (GHz): 4.9975900 1.5357400 1.3505700

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i454.8939 | 50.7177   | 85.8764   |
| 196.2963  | 264.6759  | 319.9436  |
| 363.0455  | 449.8263  | 510.0402  |
| 590.5857  | 624.5736  | 640.1618  |
| 693.2981  | 885.3887  | 909.6215  |
| 946.4909  | 986.0184  | 1011.4568 |
| 1048.6982 | 1078.9412 | 1156.6348 |
| 1258.1657 | 1275.8702 | 1308.6804 |
| 1320.3396 | 1369.7271 | 1451.4892 |
| 1468.5473 | 1578.7148 | 1622.3649 |
| 1731.2708 | 2307.9182 | 3117.5981 |

3156.0839                    3160.8656                    3179.6885  
 3189.8131                    3250.8900                    3876.1888  
 Zero-point correction (Hartree): 0.119459

TS.CH2CHCH2\_H\_COO+H2O.mpd

~~~~~

E(RM062X/Aug-CC-pVT2) (Hartree): -382.71252078

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.372467  | -0.320770 | 0.682765  |
| O | 0.649275  | 0.920549  | 0.714039  |
| O | 1.021429  | 1.351471  | -0.601049 |
| H | 0.384842  | -0.776239 | 1.670273  |
| C | -0.476815 | -0.957081 | -0.373664 |
| C | -1.921222 | -0.649535 | -0.029702 |
| H | -0.216276 | -0.538401 | -1.340637 |
| H | -0.296765 | -2.029637 | -0.367719 |
| C | -2.416830 | 0.575167  | -0.112002 |
| H | -2.539314 | -1.473028 | 0.305895  |
| H | -3.448252 | 0.780363  | 0.139441  |
| H | -1.797667 | 1.405538  | -0.433904 |
| O | 2.139484  | -0.768767 | -0.072839 |
| H | 1.942941  | 0.157941  | -0.537455 |
| H | 2.143373  | -1.439239 | -0.761486 |

Rotational constants (GHz):    4.4898600    1.8498600    1.5265500

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i469.1749 | 42.3032   | 69.6006   |
| 193.3312  | 277.6260  | 293.1046  |
| 389.4676  | 431.9565  | 498.0350  |
| 583.9442  | 629.4529  | 659.6601  |
| 676.2365  | 889.9955  | 911.2641  |
| 939.7631  | 1014.3115 | 1029.9038 |
| 1033.2293 | 1071.5474 | 1142.7819 |
| 1189.8221 | 1248.1662 | 1306.2336 |
| 1333.5519 | 1369.7061 | 1447.8420 |
| 1475.9015 | 1547.2754 | 1675.1140 |
| 1721.5074 | 2295.7880 | 3112.9583 |
| 3154.5395 | 3165.5975 | 3179.1394 |
| 3191.7554 | 3251.7061 | 3892.3677 |

Zero-point correction (Hartree): 0.119231

TS.CH2CHCH2\_H\_COO+H2O.mpu

~~~~~

E(RM062X/Aug-CC-pVT2) (Hartree): -382.71453455

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.360775  | -0.322108 | 0.675050  |
| O | 0.653798  | 0.917033  | 0.708708  |
| O | 1.027340  | 1.344526  | -0.606012 |
| H | 0.364126  | -0.777671 | 1.663716  |
| C | -0.481442 | -0.960308 | -0.381436 |
| C | -1.926483 | -0.646033 | -0.046281 |
| H | -0.209783 | -0.557187 | -1.351421 |
| H | -0.293107 | -2.029816 | -0.368714 |
| C | -2.409644 | 0.586330  | -0.076357 |
| H | -2.562089 | -1.477548 | 0.232259  |
| H | -3.444805 | 0.787976  | 0.162492  |
| H | -1.778957 | 1.426389  | -0.346294 |
| O | 2.066771  | -0.848061 | -0.203141 |
| H | 1.879592  | 0.103899  | -0.620508 |
| H | 2.802515  | -0.731311 | 0.406165  |

Rotational constants (GHz):    4.4697200    1.8618400    1.5326900

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i461.3621 | 37.1016   | 66.4182   |
| 188.4798  | 274.2943  | 297.9201  |
| 375.1345  | 436.5658  | 513.1245  |
| 582.8314  | 625.9462  | 640.1578  |
| 673.2424  | 887.9023  | 905.4313  |
| 939.5094  | 1011.6027 | 1025.7365 |
| 1031.1158 | 1075.2222 | 1140.8005 |
| 1248.1177 | 1278.8242 | 1311.8127 |
| 1333.3414 | 1370.9110 | 1447.8167 |
| 1473.2861 | 1576.9370 | 1621.7114 |
| 1721.9169 | 2278.2346 | 3129.6036 |
| 3154.8082 | 3157.0145 | 3183.4950 |
| 3194.4638 | 3251.0208 | 3876.0670 |

Zero-point correction (Hartree): 0.119235

TS.CH2CHCH2\_H\_COO+H2O.pcd

~~~~~

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.555758  | 0.745440  | 0.019210  |
| O | -0.642930 | 0.658911  | -0.211330 |
| O | -0.925921 | -0.598270 | -0.558409 |
| H | 1.025899  | 1.721279  | 0.142590  |
| C | 1.385227  | -0.543180 | 0.050348  |
| C | 1.185548  | -1.433698 | -1.177597 |
| H | 2.403325  | -0.169461 | 0.160463  |
| H | 1.093077  | -1.186071 | 0.880885  |
| C | 0.247090  | -1.137969 | -2.063788 |
| H | 1.777723  | -2.340611 | -1.299855 |
| H | 0.098567  | -1.778350 | -2.933251 |
| H | -0.426562 | -0.288830 | -1.890166 |
| O | 0.440418  | 0.695204  | -1.976829 |
| H | -0.313098 | -0.007757 | -1.670049 |
| H | 1.138249  | 0.134786  | -2.351068 |

TS.CH2CHCH2\_H\_COO+H2O.pcu

~~~~~

Cartesian coordinates (Angs):

|   |           |          |           |
|---|-----------|----------|-----------|
| C | 0.573174  | 0.752414 | 0.008735  |
| O | -0.625623 | 0.683816 | -0.227208 |

```

O -0.926319 -0.569629 -0.572796
H 1.057706 1.721196 0.132143
C 1.382562 -0.548767 0.046609
C 1.174880 -1.438920 -1.180277
H 2.405763 -0.190508 0.160648
H 1.076728 -1.185198 0.877201
C 0.245218 -1.130820 -2.071498
H 1.753576 -2.355118 -1.297752
H 0.090886 -1.770825 -2.940221
H -0.416059 -0.271035 -1.902913
O 0.466388 0.699300 -1.987706
H -0.299297 0.008758 -1.682892
H -0.032359 1.459655 -2.325705

TS.CH2CHCH2_H_COO+H2O.pmd
~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -382.70805722
Electronic state : 1-A
Cartesian coordinates (Angs):
C      0.776133      -0.433817       0.825234
O      1.196743       0.762724       0.836584
O      0.795726       1.425016      -0.363468
H      1.338963      -1.071310       1.504962
C      -0.608134      -0.907840       0.511663
C      -1.469723      -0.145512      -0.446026
H      -0.506255      -1.953096       0.206809
H      -1.095620      -0.937835       1.494376
C      -2.674106       0.297004      -0.126474
H      -1.083726       0.006319      -1.444780
H      -3.291506       0.812836      -0.847756
H      -3.076485       0.174543       0.871773
O      1.642069      -0.790180      -0.942101
H      1.357756       0.224864      -1.036798
H      1.135551      -1.295805      -1.583089
Rotational constants (GHz):   3.9955700   1.8022000   1.6789800
Vibrational harmonic frequencies (cm-1):
i478.7513          69.8774          104.5316
244.2803          250.3881          327.3856
395.6089          430.1053          453.7196
591.5523          637.4665          647.1969
770.2200          844.8508          897.0838
915.8617          968.6933          1012.3268
1020.8553         1050.9755          1152.4015
1191.3318         1257.9307          1328.7001
1372.2206         1381.8328          1441.9815
1469.1269         1557.2160          1677.1023
1737.0494         2261.0240          3032.1452
3075.3116         3153.7944          3165.9965
3208.5061         3256.9739          3894.8545
Zero-point correction (Hartree): 0.119031

TS.CH2CHCH2_H_COO+H2O.pmu
~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -382.71038203
Electronic state : 1-A
Cartesian coordinates (Angs):
C -0.770166 0.456078 0.820149
O -1.194711 -0.740098 0.861415
O -0.788838 -1.434774 -0.316674
H -1.333326 1.110460 1.485233
C 0.606639 0.932017 0.488033
C 1.466691 0.154593 -0.457947
H 0.485176 1.961464 0.144156
H 1.096947 0.992191 1.468319
C 2.659457 -0.307440 -0.122871
H 1.088432 0.026770 -1.462408
H 3.279445 -0.829639 -0.837431
H 3.050759 -0.192840 0.880838
O -1.485414 0.790042 -1.039612
H -1.245740 -0.245373 -1.051148
H -2.445710 0.844121 -1.032783
Rotational constants (GHz): 3.9483600 1.8268700 1.7048100
Vibrational harmonic frequencies (cm-1):
i480.5550 64.2585 108.5601
240.5396 254.2908 335.9966
395.2981 423.9880 476.7087
582.4881 606.7239 620.6000
781.6501 846.9227 892.6641
912.2176 965.8426 1021.3702
1031.1296 1051.7162 1158.8813
1259.2976 1296.9937 1330.5366
1373.2840 1382.1559 1433.3888
1468.2366 1592.0821 1611.9969
1737.5908 2192.0571 3030.3114
3093.4244 3141.4311 3164.7768
3219.3653 3256.0353 3882.4269
Zero-point correction (Hartree): 0.119005

TS.CH2CHCH2_H_COO+H2O.ppd
~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -382.71231537
Electronic state : 1-A
Cartesian coordinates (Angs):
C      0.868422      -0.418720      -0.795532
O      1.782130      -0.440783       0.081647
O      1.258205       0.037826       1.322101
H      1.269823      -0.474186      -1.805330
C      -0.536454      -0.931015      -0.625320
C      -1.411882      -0.399460       0.471362
H      -1.033052      -0.801710      -1.587781
H      -0.386016      -2.010088      -0.488497
C      -2.545522       0.239705       0.222225

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H      -1.070998      -0.568551      1.482248
H      -3.174208      0.601095      1.024056
H      -2.889138      0.413815      -0.791731
O       0.541057      1.516959      -0.569475
H       0.782843      1.253098      0.397921
H      -0.397768      1.731452      -0.541485
Rotational constants (GHz):    4.0563800    1.8282600    1.7793800
Vibrational harmonic frequencies (cm-1):
i406.7544      43.5616      108.3434
234.7964      261.9529      314.5425
386.6588      409.6736      459.2048
592.0086      622.2279      704.3370
787.2827      844.1235      891.5926
913.5392      979.0311      1024.7607
1049.3234      1065.2543      1143.7538
1158.4330      1267.4384      1318.5464
1366.9477      1387.3390      1444.6311
1469.0682      1575.2510      1693.0878
1725.9190      2608.2070      3027.6183
3107.1722      3153.0834      3160.7945
3228.4874      3250.4751      3858.6821
Zero-point correction (Hartree): 0.119916

```

```

TS.CH2CHCH2_H_COO+H2O.ppu
~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -382.71135099
Electronic state : 1-A
Cartesian coordinates (Angs):
C -0.891602 0.018877 -0.891458
O -1.651726 0.647421 -0.092657
O -1.034407 0.728770 1.194329
H -1.432706 -0.359417 -1.758432
C 0.575957 0.218153 -1.103996
C 1.466440 0.576359 0.046706
H 0.939571 -0.678961 -1.605128
H 0.595245 1.021358 -1.855186
C 2.489330 -0.180093 0.408030
H 1.245675 1.499236 0.562726
H 3.137229 0.105868 1.224627
H 2.700875 -1.119299 -0.088778
O -0.664034 -1.560631 0.319968
H -0.720635 -0.769366 0.998910
H -1.504667 -2.023668 0.392446
Rotational constants (GHz): 3.8357600 1.8776700 1.8358500
Vibrational harmonic frequencies (cm-1):
i433.7246 68.0571 91.5206
243.2310 275.2296 317.9965
374.0857 414.0183 469.5576
566.9126 614.7237 629.1968
815.5525 835.0655 877.6782
897.0396 970.3709 1013.8142
1035.3065 1067.2850 1146.5694
1241.8805 1267.5765 1326.8090
1371.6631 1378.6120 1434.6677
1467.9031 1587.4828 1625.7390
1735.3919 2435.8899 3007.1662
3113.3100 3140.9290 3163.8099
3225.5297 3255.5195 3874.8704
Zero-point correction (Hartree): 0.119326

```

```

TS.CH2CHCH2_H_COO+H2O.tcd
~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -382.71451298
Electronic state : 1-A
Cartesian coordinates (Angs):
C      -0.390255      -0.237706      0.699480
O      -1.658199      -0.295632      0.722181
O      -2.159960      -0.196408      -0.615691
H       0.040095      0.000821      1.670266
C       0.449323      -0.994837      -0.272138
C       1.892258      -0.595015      -0.328130
H       0.380180      -2.035599      0.072604
H      -0.022386      -0.980481      -1.252491
C       2.450875      0.456881      0.253818
H       2.516965      -1.260146      -0.913648
H       3.510698      0.642435      0.150308
H       1.886656      1.167051      0.845062
O      -0.403579      1.502636      -0.243964
H      -1.233226      1.035821      -0.674023
H       0.281710      1.569388      -0.916470
Rotational constants (GHz):    5.0041100    1.7098100    1.5143600
Vibrational harmonic frequencies (cm-1):
i443.0794      121.4240      168.1765
180.1105      284.7775      294.6370
372.3839      456.8550      540.3065
588.2165      621.9950      640.2084
704.0917      838.8538      900.0539
960.8216      992.3001      1035.0208
1051.7747      1079.0638      1125.0396
1188.1589      1224.2613      1331.1355
1348.2324      1375.7198      1451.5960
1467.3584      1567.5994      1667.4759
1733.6773      2429.9558      3026.0868
3134.7780      3161.1032      3170.4073
3180.2619      3255.7149      3869.3325
Zero-point correction (Hartree): 0.119693

```

```

TS.CH2CHCH2_H_COO+H2O.tcu
~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -382.71383659
Electronic state : 1-A
Cartesian coordinates (Angs):

```

```

C -0.346790 -0.209750 0.672958
O -1.608092 -0.344174 0.766717
O -2.172378 -0.305874 -0.548100
H 0.121289 0.072965 1.614958
C 0.490620 -0.930033 -0.326986
C 1.951557 -0.599282 -0.277017
H 0.339824 -1.987806 -0.075859
H 0.079100 -0.807155 -1.326148
C 2.489652 0.500000 0.226597
H 2.600770 -1.348939 -0.714569
H 3.560366 0.647267 0.212319
H 1.889473 1.298353 0.642449
O -0.466697 1.459132 -0.408175
H -1.307586 0.906805 -0.735321
H -0.816129 2.180230 0.125322
Rotational constants (GHz): 5.0082300 1.6792000 1.4857200
Vibrational harmonic frequencies (cm-1):
i477.5746 101.8644 122.4182
184.9206 275.9320 301.7309
361.6900 476.1306 521.8104
579.5126 599.7345 663.2505
668.4546 827.8891 903.3035
966.2991 979.9909 1031.4077
1044.1952 1084.5441 1123.2092
1227.9908 1285.2021 1334.0732
1343.4239 1373.9390 1440.9515
1465.1154 1590.3395 1622.6639
1739.2868 2253.8165 3036.6328
3138.7285 3153.6337 3173.4637
3183.7766 3258.6223 3869.9554
Zero-point correction (Hartree): 0.119171

```

```

TS.CH2CHCH2_H_COO+H2O.tmd
~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -382.71468090
Electronic state : 1-A
Cartesian coordinates (Angs):
C      -0.638028      -0.524272      0.651120
O      -1.848245      -0.502269      0.275413
O      -1.941936      0.154228      -0.994911
H      -0.526500      -0.713042      1.717621
C       0.505633      -0.877616      -0.246427
C       1.827606      -0.408494      0.277271
H       0.485587      -1.976021      -0.265513
H       0.302963      -0.525219      -1.252780
C       2.691600      0.295077      -0.437527
H       2.070700      -0.672236      1.302382
H       3.640894      0.609041      -0.026472
H       2.480080      0.567007      -1.465127
O      -0.468112      1.449430      0.542845
H      -1.095234      1.267684      -0.259686
H       0.386977      1.723500      0.196182
Rotational constants (GHz):      4.8838900      1.5892400      1.4735900
Vibrational harmonic frequencies (cm-1):
i413.5158      82.4907      97.6110
189.8363      285.2153      341.9068
363.2492      430.2955      461.8256
619.3729      620.1681      643.9818
701.2189      848.6286      894.2468
956.0839      991.6502      1027.8464
1051.2277      1061.1079      1166.0693
1189.2264      1230.1837      1290.2921
1336.1220      1371.4574      1451.4293
1472.4372      1568.2410      1660.7501
1738.4047      2567.0865      3020.8527
3151.8826      3154.7466      3162.4756
3175.5566      3252.3627      3869.6750
Zero-point correction (Hartree): 0.119597

```

```

TS.CH2CHCH2_H_COO+H2O.tmu
~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -382.71386798
Electronic state : 1-A
Cartesian coordinates (Angs):
C -0.522766 -0.457099 0.634068
O -1.770301 -0.578405 0.422141
O -2.068299 -0.025917 -0.864536
H -0.261030 -0.564796 1.686366
C 0.536340 -0.751700 -0.380950
C 1.912577 -0.535699 0.170003
H 0.377502 -1.809299 -0.626972
H 0.361041 -0.185543 -1.289054
C 2.741335 0.394396 -0.272167
H 2.222264 -1.189264 0.980076
H 3.728001 0.519229 0.151945
H 2.453153 1.064664 -1.072431
O -0.497719 1.496729 0.276949
H -1.237545 1.154307 -0.387923
H -0.957746 1.972059 0.975829
Rotational constants (GHz): 5.0768300 1.5655900 1.4104500
Vibrational harmonic frequencies (cm-1):
i462.2760 51.1385 67.2844
188.3079 290.8419 331.4669
358.0692 425.9814 482.3084
587.3801 630.8566 658.4647
680.6490 838.0369 895.5689
966.5993 990.2032 1020.6845
1040.1446 1067.1957 1175.0265
1238.2828 1281.3204 1302.0706
1335.0841 1370.8559 1444.6886
1464.3573 1584.5713 1617.5775
1745.2261 2324.3097 3036.6665

```



3143.8167 3155.3107 3168.4827  
3179.5867 3255.4079 3876.7085  
Zero-point correction (Hartree): 0.119081

TS.CH2CHCH2\_H\_COO+H2O.tpd

~~~~~

E(RM062X/Aug-CC-pVTZ) (Hartree): -382.71262685

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.417242 | -0.303989 | 0.646843  |
| O | -1.606772 | -0.744954 | 0.581589  |
| O | -2.144537 | -0.446294 | -0.712308 |
| H | -0.058444 | -0.197919 | 1.668994  |
| C | 0.604676  | -0.495567 | -0.430177 |
| C | 1.842182  | 0.315414  | -0.198426 |
| H | 0.848790  | -1.563055 | -0.383103 |
| H | 0.144957  | -0.311923 | -1.397829 |
| C | 3.032720  | -0.201708 | 0.058480  |
| H | 1.735786  | 1.394379  | -0.244755 |
| H | 3.898113  | 0.426650  | 0.215988  |
| H | 3.182769  | -1.273307 | 0.112208  |
| O | -1.000229 | 1.525807  | 0.180487  |
| H | -1.659549 | 0.934799  | -0.400559 |
| H | -0.454131 | 2.029009  | -0.429410 |

Rotational constants (GHz): 5.4019000 1.4547900 1.3071600

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i485.2198 | 64.1240   | 97.9123   |
| 182.4155  | 270.7758  | 340.4493  |
| 368.7156  | 442.1293  | 463.7622  |
| 602.0597  | 636.3958  | 658.5431  |
| 691.9478  | 835.7132  | 894.7124  |
| 970.2404  | 991.7277  | 1022.5655 |
| 1037.3354 | 1087.2176 | 1159.4451 |
| 1194.4423 | 1245.8560 | 1292.3221 |
| 1341.4824 | 1365.8893 | 1454.7455 |
| 1470.3680 | 1549.7383 | 1677.8266 |
| 1741.0043 | 2256.0951 | 3049.5717 |
| 3148.5560 | 3162.5452 | 3163.4240 |
| 3171.6434 | 3253.7348 | 3893.1160 |

Zero-point correction (Hartree): 0.119036

TS.CH2CHCH2\_H\_COO+H2O.tpu

~~~~~

E(CCSd(T)/Aug-CC-pVTZ) (Hartree): -382.17987105

E(CCSd/Aug-CC-pVTZ) (Hartree): -382.11120676

T1 diagnostic: 0.021214

E(MP2/Aug-CC-pVTZ) (Hartree): -382.07720177

E(MP3/Aug-CC-pVTZ) (Hartree): -382.09894021

E(RHF/Aug-CC-pVTZ) (Hartree): -380.65190796

E(RM062X/Aug-CC-pVTZ) (Hartree): -382.71589749

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.407853 | -0.320712 | 0.645112  |
| O | -1.610176 | -0.730961 | 0.594727  |
| O | -2.152302 | -0.432892 | -0.695648 |
| H | -0.036123 | -0.218239 | 1.664189  |
| C | 0.603402  | -0.522171 | -0.436328 |
| C | 1.828531  | 0.313859  | -0.228023 |
| H | 0.856806  | -1.586925 | -0.370633 |
| H | 0.136183  | -0.350655 | -1.401924 |
| C | 3.016926  | -0.180463 | 0.080146  |
| H | 1.690361  | 1.382195  | -0.342117 |
| H | 3.875174  | 0.462414  | 0.218119  |
| H | 3.175085  | -1.246381 | 0.194791  |
| O | -0.864871 | 1.525939  | 0.031437  |
| H | -1.567807 | 0.923934  | -0.485086 |
| H | -1.356925 | 1.993890  | 0.713092  |

Rotational constants (GHz): 5.4179100 1.4716400 1.3221600

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i473.6499 | 74.8232   | 93.2246   |
| 190.7861  | 278.7432  | 338.0272  |
| 364.2974  | 437.5297  | 485.2220  |
| 595.4603  | 630.4610  | 654.7580  |
| 683.1540  | 833.8175  | 892.9210  |
| 969.1279  | 986.2322  | 1025.1220 |
| 1053.5971 | 1085.4794 | 1164.9849 |
| 1250.8882 | 1282.8060 | 1303.6284 |
| 1326.2133 | 1366.1916 | 1451.1956 |
| 1466.7804 | 1583.9235 | 1615.0378 |
| 1737.9081 | 2232.9820 | 3045.6313 |
| 3146.1194 | 3160.4900 | 3161.8413 |
| 3196.1748 | 3250.4595 | 3877.4616 |

Zero-point correction (Hartree): 0.119133

#####  
E-(CH2-CH=CH2)CHOO  
#####

Population analysis as 298K (%)

Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)

| Compound                  | Qtot      | Erel | Erel2 | n*Q*MB    | %    |
|---------------------------|-----------|------|-------|-----------|------|
| TS.H_CH2CHCH2_COO+H2O.cmu | 2.512e+40 | 0.00 | 0.00  | 5.023e+40 | 30.3 |
| TS.H_CH2CHCH2_COO+H2O.mtu | 3.202e+40 | 0.71 | 0.71  | 1.945e+40 | 11.7 |
| TS.H_CH2CHCH2_COO+H2O.ppu | 3.469e+40 | 0.86 | 0.86  | 1.621e+40 | 9.78 |
| TS.H_CH2CHCH2_COO+H2O.cpu | 2.716e+40 | 0.82 | 0.82  | 1.353e+40 | 8.16 |
| TS.H_CH2CHCH2_COO+H2O.mmd | 2.707e+40 | 0.84 | 0.84  | 1.301e+40 | 7.85 |
| TS.H_CH2CHCH2_COO+H2O.pmu | 4.029e+40 | 1.13 | 1.13  | 1.188e+40 | 7.17 |
| TS.H_CH2CHCH2_COO+H2O.mpu | 2.888e+40 | 0.99 | 0.99  | 1.087e+40 | 6.56 |
| TS.H_CH2CHCH2_COO+H2O.cpd | 2.312e+40 | 1.02 | 1.02  | 8.259e+39 | 4.98 |
| TS.H_CH2CHCH2_COO+H2O.mpd | 3.510e+40 | 1.32 | 1.32  | 7.620e+39 | 4.6  |

```

TS_H_CH2CHCH2_COO+H2O.ppd 3.645e+40 1.42 1.42 6.581e+39 3.97
TS_H_CH2CHCH2_COO+H2O.pmd 4.633e+40 1.73 1.73 4.974e+39 3
TS_H_CH2CHCH2_COO+H2O.cmd 2.939e+40 1.74 1.74 3.138e+39 1.89
Total 1.658e+41 100

TS_H_CH2CHCH2_COO+H2O.cmd
~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -382.71709487
Electronic state : 1-A
Cartesian coordinates (Angs):
  C 0.559172 -0.247789 0.698339
  O 1.007976 -0.880356 -0.302436
  O 2.348610 -0.436719 -0.535288
  H 1.260604 -0.018392 1.494279
  C -0.901006 -0.295836 0.978624
  C -1.754538 -0.493583 -0.236679
  H -1.038009 -1.117792 1.692257
  H -1.165277 0.622079 1.503828
  C -2.729435 0.330520 -0.578168
  H -1.533598 -1.362632 -0.844061
  H -3.329932 0.155623 -1.459675
  H -2.955262 1.212956 0.008207
  O 0.968728 1.523495 -0.112769
  H 1.775057 0.919762 -0.450592
  H 1.338756 2.177166 0.487003
Rotational constants (GHz): 4.6781400 1.5343700 1.4050800
Vibrational harmonic frequencies (cm-1):
  i442.1384 59.1036 64.2662
  183.0546 258.9402 331.2007
  402.9322 408.9659 465.5501
  556.4847 623.1480 665.4893
  739.9793 871.1571 901.8826
  960.7759 986.0252 1024.2216
  1040.8433 1102.6616 1144.1614
  1199.4492 1258.1888 1324.8177
  1349.8828 1372.9720 1434.5479
  1468.3631 1558.4998 1675.5431
  1744.8580 2225.4161 3033.4966
  3116.8705 3164.8491 3171.3609
  3196.4388 3255.1596 3889.4215
Zero-point correction (Hartree): 0.118991

TS_H_CH2CHCH2_COO+H2O.cmu
~~~~~
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -382.18466439
E(CCSD/Aug-CC-pVTZ) (Hartree): -382.11649209
T1 diagnostic: 0.021136
E(MP2/Aug-CC-pVTZ) (Hartree): -382.08181864
E(MP3/Aug-CC-pVTZ) (Hartree): -382.10416579
E(RHF/Aug-CC-pVTZ) (Hartree): -380.65977943
E(RM062X/Aug-CC-pVTZ) (Hartree): -382.72042896
Electronic state : 1-A
Cartesian coordinates (Angs):
 C 0.582946 -0.436693 0.635664
 O 1.102295 -0.767896 -0.466737
 O 2.382574 -0.135799 -0.562504
 H 1.248772 -0.278655 1.477529
 C -0.869740 -0.689141 0.848794
 C -1.689844 -0.458785 -0.385542
 H -0.956845 -1.725836 1.193291
 H -1.197353 -0.048327 1.666551
 C -2.633722 0.465102 -0.464257
 H -1.461388 -1.082768 -1.241085
 H -3.203778 0.610971 -1.371186
 H -2.871941 1.101721 0.379798
 O 0.799584 1.551224 0.348925
 H 1.640210 1.161319 -0.116271
 H 0.188846 1.798447 -0.354054
Rotational constants (GHz): 4.5846100 1.5965900 1.4431100
Vibrational harmonic frequencies (cm-1):
 i356.7306 63.4902 77.2584
 179.3445 241.9643 327.6692
 379.9513 409.9104 481.6607
 551.8226 579.7252 632.5627
 751.7104 865.8857 912.1698
 951.9948 990.9763 1028.8622
 1046.6125 1101.7246 1147.9918
 1235.9378 1257.9974 1324.2306
 1348.8648 1374.5719 1440.6436
 1468.4083 1596.9326 1620.0157
 1739.6904 2529.2882 3046.4967
 3125.1818 3160.1373 3183.8105
 3193.5921 3252.2871 3859.5031
Zero-point correction (Hartree): 0.119560

TS_H_CH2CHCH2_COO+H2O.cpd
~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -382.71800648
Electronic state : 1-A
Cartesian coordinates (Angs):
  C -0.510842 0.035679 -0.724912
  O -0.767782 -0.979455 -0.012896
  O -2.180058 -1.002239 0.213360
  H -1.243144 0.312034 -1.476702
  C 0.899916 0.491382 -0.836846
  C 1.711707 0.230220 0.394598
  H 1.335144 -0.000621 -1.712024
  H 0.859023 1.559483 -1.062846
  C 2.878572 -0.390229 0.387585
  H 1.281132 0.592543 1.320933
  H 3.438062 -0.543695 1.299490
  H 3.313282 -0.769615 -0.529367

```

```

O      -1.413688      1.268918      0.558668
H      -2.019884      0.384736      0.598713
H      -1.947506      1.965036      0.166186
Rotational constants (GHz):      4.8339600      1.5042400      1.3600400
Vibrational harmonic frequencies (cm-1):
1474.4222      66.3801      80.5192
170.0214      253.7655      341.3244
395.8490      421.0510      466.6976
564.4259      634.1758      650.2475
736.5633      862.4747      905.0346
979.3828      987.6748      1027.3516
1042.8755      1077.5733      1149.4919
1209.4725      1245.9534      1320.2639
1352.3560      1373.1903      1433.7475
1464.4928      1550.4822      1660.8531
1744.3335      2131.0106      3057.0486
3097.3700      3164.2346      3176.2575
3190.4676      3254.4791      3891.8355
Zero-point correction (Hartree): 0.118763

```

```

TS_H_CH2CHCH2_COO+H2O.cpu
~~~~~
E(RM062X/Aug-CC-pVT2) (Hartree): -382.71838003
Electronic state : 1-A
Cartesian coordinates (Angs):
C -0.501049 0.059488 -0.696683
O -0.748552 -0.968412 0.002126
O -2.167072 -1.043222 0.168413
H -1.214082 0.324800 -1.469882
C 0.898728 0.556394 -0.775671
C 1.742623 0.209370 0.411421
H 1.332606 0.154363 -1.695925
H 0.825193 1.638166 -0.913219
C 2.912161 -0.400863 0.332459
H 1.345938 0.492973 1.380276
H 3.494034 -0.618662 1.216748
H 3.326323 -0.706840 -0.620565
O -1.594986 1.304776 0.418537
H -2.127806 0.377831 0.470869
H -1.212109 1.445906 1.289935
Rotational constants (GHz): 4.8996300 1.4775700 1.3207800
Vibrational harmonic frequencies (cm-1):
1459.1715 64.4746 73.5806
164.7642 247.0193 333.9265
399.6271 426.8523 488.9375
560.1759 588.8555 613.0242
745.0205 864.8440 904.6269
978.5961 987.2969 1023.9639
1034.7108 1098.4984 1165.5269
1236.2511 1285.4471 1325.9955
1360.5388 1381.4888 1434.8670
1467.5640 1591.6959 1607.1215
1745.9292 2139.5147 3059.3661
3097.0261 3165.3579 3178.1265
3184.0297 3256.4015 3876.2155
Zero-point correction (Hartree): 0.118823

```

```

TS_H_CH2CHCH2_COO+H2O.mmd
~~~~~
E(RM062X/Aug-CC-pVT2) (Hartree): -382.71863044
Electronic state : 1-A
Cartesian coordinates (Angs):
C      0.417173      -0.413609      0.235998
O      1.514950      -0.858336      -0.207516
O      2.571122      -0.123922      0.421006
H      0.385718      -0.089887      1.271852
C      -0.838147      -0.785161      -0.472901
C      -1.913684      0.244079      -0.275434
H      -0.604629      -0.931059      -1.526986
H      -1.159811      -1.743665      -0.054784
C      -2.996455      0.046379      0.458388
H      -1.752618      1.192136      -0.773950
H      -3.745310      0.817469      0.574513
H      -3.175435      -0.896157      0.961996
O      0.865995      1.469408      -0.278683
H      1.804471      1.070494      0.021909
H      0.617749      2.133342      0.370691
Rotational constants (GHz):      5.8212300      1.3785600      1.2078700
Vibrational harmonic frequencies (cm-1):
1434.6801      55.4742      74.8620
184.7421      274.5707      332.2403
391.7582      437.7285      453.9675
528.5555      634.7839      656.9391
691.8073      875.3935      924.2928
982.0293      990.8969      1048.0829
1063.8787      1103.5291      1159.4672
1213.6902      1264.8147      1301.5869
1327.2562      1359.8783      1446.9735
1463.1599      1560.9345      1670.2183
1738.6344      2212.0471      3059.8541
3128.6529      3162.1713      3172.7453
3196.0875      3251.4143      3886.6493
Zero-point correction (Hartree): 0.119107

```

```

TS_H_CH2CHCH2_COO+H2O.mpd
~~~~~
E(RM062X/Aug-CC-pVT2) (Hartree): -382.71786333
Electronic state : 1-A
Cartesian coordinates (Angs):
C 0.483563 -0.465948 0.271045
O 1.566829 -0.753274 -0.311304
O 2.595466 0.077879 0.239213

```

```

H 0.541267 -0.184813 1.318741
C -0.794750 -0.931395 -0.334709
C -1.986698 -0.396347 0.401247
H -0.799266 -0.630671 -1.381247
H -0.776508 -2.025706 -0.302604
C -2.827636 0.486669 -0.109924
H -2.138437 -0.765666 1.410441
H -3.675467 0.849644 0.454251
H -2.693155 0.873377 -1.112726
O 0.627417 1.478019 -0.204683
H 1.626011 1.215399 -0.021706
H 0.350984 2.089564 0.483091
Rotational constants (GHz): 5.6607400 1.4388800 1.2304400
Vibrational harmonic frequencies (cm-1):
1394.4313 56.2720 60.8896
171.4328 258.9815 336.7499
393.5173 401.7867 450.8443
527.4832 610.9815 646.5432
675.6711 871.0673 921.3752
976.3343 993.6234 1040.2361
1059.0637 1100.2172 1161.2648
1202.3497 1256.4755 1295.3989
1336.6699 1368.7328 1439.7891
1466.0886 1567.3345 1664.3691
1744.2692 2376.8562 3055.7256
3133.2550 3162.9167 3166.2674
3173.2384 3255.0931 3895.3418
Zero-point correction (Hartree): 0.119090

```

```

TS.H_CH2CHCH2_COO+H2O.mpu
~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -382.71849945
Electronic state : 1-A
Cartesian coordinates (Angs):
C      0.546135      -0.474993      0.386026
O      1.498422      -0.754598      -0.399259
O      2.609446      0.081658      -0.062542
H      0.795288      -0.188801      1.402936
C      -0.806734      -1.005185      0.061511
C      -1.897984      -0.040361      0.427479
H      -0.849137      -1.276822      -0.991735
H      -0.915586      -1.921646      0.653651
C      -2.883083      0.288643      -0.390221
H      -1.848153      0.389097      1.421901
H      -3.658982      0.976226      -0.084650
H      -2.948218      -0.121515      -1.390680
O      0.613818      1.498934      0.075330
H      1.621687      1.211417      -0.027710
H      0.279612      1.715455      -0.800710
Rotational constants (GHz):      5.7076900      1.4361200      1.2407100
Vibrational harmonic frequencies (cm-1):
1402.6300      48.0305      88.6747
160.7563      288.6308      311.4048
402.1982      435.6288      468.9210
544.6615      580.2195      623.8279
654.0814      908.3788      923.7981
960.8146      982.3303      1031.2033
1064.3043      1135.4845      1186.9270
1228.4307      1289.3784      1294.0706
1334.5256      1373.6912      1454.4475
1464.2829      1591.7619      1601.6662
1740.4972      2325.0816      3036.4716
3134.3795      3164.9662      3176.5409
3182.7186      3255.5967      3876.8816
Zero-point correction (Hartree): 0.119207

```

```

TS.H_CH2CHCH2_COO+H2O.mtu
~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -382.71872248
Electronic state : 1-A
Cartesian coordinates (Angs):
C -0.411064 -0.381620 -0.211576
O -1.478480 -0.892738 0.235540
O -2.576448 -0.262287 -0.433441
H -0.392309 -0.078015 -1.253536
C 0.859726 -0.630839 0.524328
C 1.939954 0.329958 0.121617
H 0.649892 -0.586758 1.594247
H 1.162163 -1.656339 0.291938
C 3.101892 -0.043194 -0.387727
H 1.716573 1.380972 0.262610
H 3.854094 0.683314 -0.661389
H 3.342200 -1.087750 -0.545872
O -0.986930 1.524215 0.093367
H -1.884311 1.023756 -0.164593
H -1.056485 1.721476 1.033020
Rotational constants (GHz): 5.9117700 1.3312900 1.1666500
Vibrational harmonic frequencies (cm-1):
1418.0801 55.0073 76.2924
159.6133 266.0275 316.5868
392.7558 440.4193 456.3522
533.9587 590.4496 614.5400
680.8246 872.8313 921.5642
977.6635 991.6666 1040.7219
1080.7111 1115.1491 1168.3418
1244.1983 1284.9095 1301.0819
1334.3365 1374.6861 1445.8512
1464.6889 1595.1737 1620.8498
1740.7901 2243.6073 3058.6084
3109.4828 3163.1921 3178.6022
3190.9835 3252.8265 3870.0777
Zero-point correction (Hartree): 0.118978

```

```

TS.H_CH2CHCH2_COO+H2O.pmd
~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -382.71696086
Electronic state : 1-A
Cartesian coordinates (Angs):
  C      -0.352143      0.064551      -0.243418
  O      -0.862118     -0.938996      0.338383
  O      -2.153307     -1.164656     -0.231438
  H      -0.562797     0.186926     -1.301576
  C       0.856219     0.683230      0.365918
  C       2.086340     0.294432     -0.409508
  H       0.708943     1.764528      0.333757
  H       0.924907     0.373333      1.406655
  C       3.066208     -0.438508      0.091186
  H       2.143202     0.645829     -1.434385
  H       3.935548     -0.692417     -0.499006
  H       3.031225     -0.806371      1.109121
  O      -1.926967     1.212460      0.159134
  H      -2.366851     0.248439     -0.012697
  H      -2.214787     1.787041     -0.555569
Rotational constants (GHz):      5.5298100      1.3384800      1.1520700
Vibrational harmonic frequencies (cm-1):
i475.2940      38.5716      66.2940
175.6063      257.9875      328.2523
409.9474      419.8489      482.5133
537.8031      631.7481      650.4029
711.3072      874.1785      938.7162
967.5148      993.2258      1032.6508
1045.9749     1105.7690      1177.5935
1213.5215     1230.9812      1295.7804
1332.5833     1363.7155      1454.6586
1469.8002     1553.8219      1662.0039
1739.5285     2124.0129      3080.7621
3145.3736     3164.9328      3169.0599
3176.9046     3256.8859      3889.9758
Zero-point correction (Hartree): 0.118852

```

```

TS.H_CH2CHCH2_COO+H2O.pmu
~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -382.71813534
Electronic state : 1-A
Cartesian coordinates (Angs):
 C -0.352318 0.064010 -0.247832
 O -0.855880 -0.925155 0.363681
 O -2.141446 -1.180090 -0.206966
 H -0.570828 0.166031 -1.306026
 C 0.856061 0.709275 0.334745
 C 2.084454 0.273942 -0.419822
 H 0.717139 1.788020 0.237049
 H 0.929468 0.451922 1.389844
 C 3.059444 -0.438424 0.118336
 H 2.140495 0.572585 -1.461016
 H 3.926683 -0.728102 -0.458231
 H 3.022802 -0.753568 1.153763
 O -1.953335 1.241516 -0.034477
 H -2.369733 0.264943 -0.131543
 H -2.076584 1.495181 0.885694
Rotational constants (GHz): 5.4738000 1.3400000 1.1520900
Vibrational harmonic frequencies (cm-1):
i436.9855 49.7041 63.2066
172.7766 249.1305 329.3509
399.1897 417.8823 501.9032
542.2887 591.1307 634.8080
686.5428 875.2353 940.8972
967.7485 991.2224 1034.8738
1049.4726 1134.3918 1187.5970
1235.2626 1269.9945 1301.4034
1333.3506 1380.5146 1455.5666
1471.6724 1596.2943 1610.9769
1738.3251 2181.4793 3076.2672
3141.8763 3166.4137 3176.1528
3181.3901 3257.1772 3873.6152
Zero-point correction (Hartree): 0.119073

```

```

TS.H_CH2CHCH2_COO+H2O.ppd
~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -382.71780136
Electronic state : 1-A
Cartesian coordinates (Angs):
  C      -0.325671      0.006318      -0.177489
  O      -1.013590     -0.910661      0.359287
  O      -2.249543     -1.007753     -0.354714
  H      -0.398634     0.120855     -1.254388
  C       0.870811     0.500813      0.556407
  C       2.048553     -0.378374      0.223191
  H       1.060922     1.526648      0.245217
  H       0.649423     0.485125      1.622933
  C       3.106686     0.034309     -0.454844
  H       1.983535     -1.405616      0.563484
  H       3.928484     -0.633046     -0.673892
  H       3.190768     1.056116     -0.804709
  O      -1.784287     1.352524      0.033509
  H      -2.316459     0.456711     -0.173611
  H      -1.920955     1.941941     -0.713283
Rotational constants (GHz):      5.5548300      1.3206900      1.1520200
Vibrational harmonic frequencies (cm-1):
i427.2553      47.4878      76.0221
161.3916      282.4833      292.2453
405.4937      427.9013      474.7976
547.3048      626.3525      655.0265
722.0515      866.6136      939.0309

```

```

967.0182          990.8833          1034.4302
1048.4736          1116.0209          1158.0787
1209.2440          1253.6078          1298.1002
1328.1509          1361.6036          1454.8913
1473.8312          1559.7747          1673.7596
1734.4188          2224.5679          3093.7090
3148.3657          3163.2319          3177.4033
3185.9218          3253.2741          3890.4584
Zero-point correction (Hartree): 0.119202
```

TS\_H\_CH2CHCH2\_COO+H2O.ppu

E(RM062X/Aug-CC-pVTZ) (Hartree): -382.71879796

Electronic state : 1-A

Cartesian coordinates (Angs):

```

C      -0.322878      -0.006857      -0.159691
O      -1.036228      -0.898931       0.387376
O      -2.255044      -0.999894      -0.354667
H      -0.375890       0.092762      -1.238764
C       0.873878       0.485835       0.576527
C       2.054777      -0.383580       0.226826
H       1.056119       1.514394       0.268664
H       0.667119       0.455997       1.646289
C       3.096395       0.038252      -0.470575
H       2.004377      -1.410922       0.569066
H       3.919610      -0.622315      -0.704338
H       3.163714       1.059772      -0.824624
O      -1.757643       1.390776      -0.176322
H      -2.289923       0.487649      -0.321655
H      -1.966831       1.685153       0.715745
```

Rotational constants (GHz): 5.4692500 1.3187400 1.1543900

Vibrational harmonic frequencies (cm-1):

```

i408.5386          53.6019          74.0664
161.2725          270.4577          295.5484
403.7541          421.2657          497.7450
548.6724          584.3176          629.7384
709.6754          866.2444          939.4087
968.9546          992.5977          1037.1478
1050.4368          1141.4079          1164.2502
1249.7794          1273.3337          1303.2287
1328.6272          1373.5775          1454.5894
1475.2085          1592.3719          1614.1321
1734.6423          2260.0232          3087.1488
3144.9447          3164.4082          3184.4716
3186.8466          3254.4750          3874.5762
```

Zero-point correction (Hartree): 0.119301

```
#####
Z-(CH(CH3)-CH=CH2)CHOO
#####
```

Population analysis as 298K (%)

Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)

| Compound                     | Qtot      | Erel | Erel2 | n*Q*MB    | %        |
|------------------------------|-----------|------|-------|-----------|----------|
| TS.CH3CHCHCH2_H_COO+H2O.ppdd | 6.757e+40 | 0.00 | 0.00  | 6.757e+40 | 32.6     |
| TS.CH3CHCHCH2_H_COO+H2O.tpuu | 6.481e+40 | 0.10 | 0.10  | 5.437e+40 | 26.2     |
| TS.CH3CHCHCH2_H_COO+H2O.pmdd | 1.454e+41 | 0.89 | 0.89  | 3.251e+40 | 15.7     |
| TS.CH3CHCHCH2_H_COO+H2O.tmuu | 1.185e+41 | 1.14 | 1.14  | 1.735e+40 | 8.37     |
| TS.CH3CHCHCH2_H_COO+H2O.tmd  | 9.752e+40 | 1.03 | 1.03  | 1.722e+40 | 8.31     |
| TS.CH3CHCHCH2_H_COO+H2O.tcuu | 6.188e+40 | 1.51 | 1.51  | 4.829e+39 | 2.33     |
| TS.CH3CHCHCH2_H_COO+H2O.tcu  | 4.640e+40 | 1.37 | 1.37  | 4.611e+39 | 2.23     |
| TS.CH3CHCHCH2_H_COO+H2O.ppdu | 6.240e+40 | 1.76 | 1.76  | 3.208e+39 | 1.55     |
| TS.CH3CHCHCH2_H_COO+H2O.tpud | 6.552e+40 | 2.03 | 2.03  | 2.134e+39 | 1.03     |
| TS.CH3CHCHCH2_H_COO+H2O.pmd  | 1.383e+41 | 2.63 | 2.63  | 1.638e+39 | 0.79     |
| TS.CH3CHCHCH2_H_COO+H2O.mmd  | 7.170e+40 | 2.89 | 2.89  | 5.439e+38 | 0.262    |
| TS.CH3CHCHCH2_H_COO+H2O.mmu  | 1.162e+41 | 3.46 | 3.46  | 3.354e+38 | 0.162    |
| TS.CH3CHCHCH2_H_COO+H2O.tmd  | 7.736e+40 | 3.30 | 3.30  | 2.947e+38 | 0.142    |
| TS.CH3CHCHCH2_H_COO+H2O.mmd  | 1.003e+41 | 3.80 | 3.80  | 1.644e+38 | 0.0793   |
| TS.CH3CHCHCH2_H_COO+H2O.ppud | 1.040e+41 | 4.08 | 4.08  | 1.058e+38 | 0.0511   |
| TS.CH3CHCHCH2_H_COO+H2O.pmuu | 6.825e+40 | 4.10 | 4.10  | 6.704e+37 | 0.0324   |
| TS.CH3CHCHCH2_H_COO+H2O.mcuu | 1.073e+41 | 4.40 | 4.40  | 6.383e+37 | 0.0308   |
| TS.CH3CHCHCH2_H_COO+H2O.ppuu | 5.956e+40 | 4.20 | 4.20  | 4.984e+37 | 0.024    |
| TS.CH3CHCHCH2_H_COO+H2O.tpu  | 4.556e+40 | 4.28 | 4.28  | 3.296e+37 | 0.0159   |
| TS.CH3CHCHCH2_H_COO+H2O.mmu  | 1.077e+41 | 4.82 | 4.82  | 3.133e+37 | 0.0151   |
| TS.CH3CHCHCH2_H_COO+H2O.mpuu | 7.479e+40 | 4.65 | 4.65  | 2.914e+37 | 0.0141   |
| TS.CH3CHCHCH2_H_COO+H2O.tpdd | 8.035e+40 | 4.95 | 4.95  | 1.892e+37 | 0.00913  |
| TS.CH3CHCHCH2_H_COO+H2O.mpd  | 6.480e+40 | 4.88 | 4.88  | 1.708e+37 | 0.00824  |
| TS.CH3CHCHCH2_H_COO+H2O.tmd  | 1.090e+41 | 5.24 | 5.24  | 1.572e+37 | 0.00759  |
| TS.CH3CHCHCH2_H_COO+H2O.tcd  | 5.324e+40 | 5.04 | 5.04  | 1.078e+37 | 0.0052   |
| TS.CH3CHCHCH2_H_COO+H2O.tcu  | 3.360e+40 | 4.94 | 4.94  | 8.015e+36 | 0.00387  |
| TS.CH3CHCHCH2_H_COO+H2O.mcu  | 1.043e+41 | 5.77 | 5.77  | 6.137e+36 | 0.00296  |
| TS.CH3CHCHCH2_H_COO+H2O.pmd  | 8.099e+40 | 5.89 | 5.89  | 3.868e+36 | 0.00187  |
| TS.CH3CHCHCH2_H_COO+H2O.mpu  | 6.714e+40 | 6.04 | 6.04  | 2.502e+36 | 0.00121  |
| TS.CH3CHCHCH2_H_COO+H2O.mpd  | 5.645e+40 | 6.41 | 6.41  | 1.132e+36 | 0.000546 |
| Total                        |           |      |       | 2.072e+41 | 100      |

TS.CH3CHCHCH2\_H\_COO+H2O.mcd

Cartesian coordinates (Angs):

```

C      0.587784      0.795771      0.005157
O      -0.613265      0.712278      0.220576
O      -0.907163      -0.552039      0.531766
H       1.067266       1.770475      -0.086531
C       1.405109      -0.499225      -0.050702
C       1.190716      -1.423185       1.148715
C       1.003666      -1.376465      -1.238411
H       2.434229      -0.148849      -0.130330
C       0.247095      -1.143531       2.034404
H       1.774554      -2.338069       1.249812
H       0.085137      -1.805773       2.884902
```

```

H      -0.418376      -0.284022      1.877004
O      0.454942      0.691345      1.998006
H      -0.300779      0.002491      1.665255
H      -0.054718      1.438978      2.347957
H      1.180427      -0.791273      -2.140983
H      -0.051555      -1.619285      -1.112984
H      1.631276      -2.267001      -1.203431

TS.CH3CHCHCH2_H_COO+H2O.mcd
~~~~~
Cartesian coordinates (Angs):
C 0.565338 0.790259 -0.001713
O -0.634824 0.690411 0.211704
O -0.911841 -0.577604 0.523493
H 1.031518 1.771385 -0.093412
C 1.400498 -0.493390 -0.055044
C 1.196760 -1.419207 1.144796
C 1.013202 -1.377055 -1.242686
H 2.424840 -0.128943 -0.133196
C 0.247820 -1.151823 2.028611
H 1.792965 -2.325882 1.247691
H 0.093509 -1.815525 2.879398
H -0.429164 -0.301674 1.869318
O 0.430404 0.685764 1.990991
H -0.315159 -0.013742 1.657526
H 1.128012 0.120107 2.357657
H 1.183442 -0.790236 -2.145455
H -0.038794 -1.634275 -1.118875
H 1.652948 -2.258830 -1.205852

TS.CH3CHCHCH2_H_COO+H2O.mcd
~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -422.01707789
Electronic state : 1-A
Cartesian coordinates (Angs):
C      -0.289289      -0.452395      0.700197
O      -0.757441      -1.331179      -0.087079
O      -1.423370      -0.703304      -1.187084
H      -0.103658      -0.857161      1.693510
C      0.541084      0.753347      0.362202
C      1.988185      0.289647      0.364370
C      0.255052      1.541517      -0.916044
H      0.420745      1.413561      1.225632
C      2.421629      -0.890609      -0.051026
H      2.700672      1.035092      0.699956
H      3.478375      -1.118852      -0.054833
H      1.749594      -1.658838      -0.412964
O      -2.082966      0.415500      0.897803
H      -2.111738      0.092663      -0.102237
H      -2.104943      1.375786      0.892142
H      -0.756582      1.940795      -0.930863
H      0.378737      0.907008      -1.787166
H      0.959052      2.372768      -0.970480
Rotational constants (GHz):      2.9276400      1.5178800      1.3488500
Vibrational harmonic frequencies (cm-1):
i438.4675      45.8166      84.8903
183.1506      250.3025      266.1480
297.1629      323.3438      335.8287
397.0426      421.7152      550.8012
630.2330      647.7963      681.6291
756.1787      812.9103      881.5580
923.7980      998.3608      1017.9678
1033.8052      1043.9166      1093.2820
1136.7992      1170.9063      1183.5674
1310.7940      1330.5908      1384.7648
1392.7379      1419.9247      1456.9892
1489.7342      1490.6476      1557.8808
1678.6628      1723.8064      2337.1597
3056.5043      3073.7839      3144.8545
3159.7124      3166.6290      3177.6706
3187.4191      3255.2384      3898.6779
Zero-point correction (Hartree): 0.147769

TS.CH3CHCHCH2_H_COO+H2O.mcd
~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -422.01935919
Electronic state : 1-A
Cartesian coordinates (Angs):
C -0.287500 -0.452947 0.703088
O -0.758604 -1.335061 -0.081408
O -1.404625 -0.708783 -1.192236
H -0.109326 -0.855982 1.699779
C 0.544520 0.751472 0.374706
C 1.988170 0.280353 0.363793
C 0.247067 1.565959 -0.884093
H 0.419803 1.399274 1.245260
C 2.417379 -0.897314 -0.064182
H 2.704951 1.020870 0.701406
H 3.473609 -1.127819 -0.076513
H 1.742244 -1.660574 -0.430931
O -2.028235 0.567738 0.812327
H -2.044001 0.175267 -0.167408
H -2.668035 0.055115 1.315543
H -0.760382 1.971804 -0.857466
H 0.358406 0.952507 -1.771888
H 0.956627 2.393250 -0.927132
Rotational constants (GHz): 2.9224700 1.5381900 1.3488500
Vibrational harmonic frequencies (cm-1):
i437.7179 44.3207 80.5402
181.6435 258.8678 270.1856
310.3541 323.4349 331.9719
394.1306 434.8278 576.6291

```

|           |           |           |
|-----------|-----------|-----------|
| 610.4815  | 612.5646  | 681.3859  |
| 754.2605  | 820.0320  | 881.8858  |
| 924.6089  | 994.5911  | 1022.1904 |
| 1032.7817 | 1042.7384 | 1093.0206 |
| 1139.6326 | 1175.7762 | 1292.5948 |
| 1307.8596 | 1330.8478 | 1389.5941 |
| 1393.4654 | 1417.7301 | 1457.1457 |
| 1491.0440 | 1505.3365 | 1587.3434 |
| 1619.9002 | 1722.9324 | 2275.0694 |
| 3073.6869 | 3075.8709 | 3146.5705 |
| 3155.0312 | 3166.0714 | 3176.9027 |
| 3192.7200 | 3254.2630 | 3881.0994 |

Zero-point correction (Hartree): 0.147867

TS.CH3CHCHCH2\_H\_COO+H2O.mmdd

~~~~~

E(RM062X/Aug-CC-pVTZ) (Hartree): -422.02046744

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.802444  | 0.575342  | -0.603633 |
| O | 1.659587  | 0.620943  | 0.330340  |
| O | 1.330567  | -0.355662 | 1.322388  |
| H | 1.159141  | 1.061526  | -1.512014 |
| C | -0.693150 | 0.535891  | -0.457688 |
| C | -1.307890 | -0.428226 | 0.516648  |
| C | -1.070813 | 1.985644  | -0.089596 |
| H | -1.070447 | 0.311110  | -1.456763 |
| C | -2.062160 | -1.445858 | 0.136548  |
| H | -1.129837 | -0.223858 | 1.563582  |
| H | -2.525594 | -2.101576 | 0.860393  |
| H | -2.223760 | -1.669717 | -0.911081 |
| O | 1.037382  | -1.375661 | -0.948356 |
| H | 1.145233  | -1.332465 | 0.079234  |
| H | 1.926753  | -1.506984 | -1.293043 |
| H | -0.658215 | 2.708477  | -0.794086 |
| H | -0.699525 | 2.219953  | 0.907477  |
| H | -2.154621 | 2.079829  | -0.092351 |

Rotational constants (GHz): 2.3428300 1.8041700 1.3888300

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i393.3583 | 50.4798   | 88.0393   |
| 183.7311  | 248.3177  | 255.9451  |
| 290.3486  | 319.6160  | 335.8864  |
| 375.4256  | 436.0699  | 535.5483  |
| 578.8223  | 642.9245  | 665.6542  |
| 810.6448  | 818.0226  | 886.0827  |
| 948.1882  | 971.0009  | 986.1327  |
| 1034.2451 | 1042.7578 | 1064.3895 |
| 1114.9722 | 1214.8491 | 1231.2208 |
| 1291.5955 | 1325.5763 | 1370.1705 |
| 1378.1325 | 1402.1102 | 1462.2350 |
| 1497.1303 | 1504.9486 | 1584.0357 |
| 1634.6040 | 1734.5514 | 2581.4771 |
| 3064.8555 | 3085.4322 | 3132.6673 |
| 3139.3390 | 3157.4355 | 3162.1266 |
| 3212.6152 | 3251.6508 | 3870.9079 |

Zero-point correction (Hartree): 0.148019

TS.CH3CHCHCH2\_H\_COO+H2O.mmdu

~~~~~

E(RM062X/Aug-CC-pVTZ) (Hartree): -422.02250029

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.855973  | 0.215241  | -0.779362 |
| O | 1.813039  | 0.277330  | 0.049269  |
| O | 1.382847  | -0.278354 | 1.294943  |
| H | 1.191816  | 0.352350  | -1.805560 |
| C | -0.570220 | 0.629695  | -0.491945 |
| C | -1.366151 | -0.159048 | 0.509523  |
| C | -0.466762 | 2.102146  | -0.051361 |
| H | -1.086340 | 0.574321  | -1.453113 |
| C | -2.449240 | -0.849964 | 0.183279  |
| H | -1.015417 | -0.108696 | 1.531857  |
| H | -3.025091 | -1.378118 | 0.930678  |
| H | -2.803646 | -0.901166 | -0.840498 |
| O | 0.714177  | -1.745667 | -0.653549 |
| H | 0.973491  | -1.525356 | 0.311946  |
| H | -0.203548 | -2.036069 | -0.605199 |
| H | 0.080291  | 2.701678  | -0.778808 |
| H | 0.053301  | 2.150443  | 0.904310  |
| H | -1.466964 | 2.515721  | 0.058271  |

Rotational constants (GHz): 2.4628300 1.7841800 1.3614600

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i377.2573 | 56.4458   | 107.4859  |
| 199.5205  | 241.8873  | 258.3884  |
| 283.3851  | 325.4297  | 341.5145  |
| 391.8443  | 434.0463  | 512.3572  |
| 598.4152  | 675.1403  | 714.7115  |
| 806.3506  | 810.4922  | 892.0432  |
| 955.1460  | 978.9568  | 987.8338  |
| 1033.2957 | 1061.8361 | 1073.2692 |
| 1115.8865 | 1128.8954 | 1230.4820 |
| 1305.4207 | 1317.3444 | 1363.6846 |
| 1385.6343 | 1400.7632 | 1461.6105 |
| 1496.4782 | 1504.8903 | 1571.8580 |
| 1686.9148 | 1723.8118 | 2729.4345 |
| 3068.3145 | 3072.2200 | 3143.9383 |
| 3153.2225 | 3157.2139 | 3161.4441 |
| 3214.1131 | 3246.4667 | 3850.8279 |

Zero-point correction (Hartree): 0.148606

TS.CH3CHCHCH2\_H\_COO+H2O.mmud

~~~~~



E(RM062X/Aug-CC-pVTZ) (Hartree): -422.01853210  
 Electronic state : 1-A  
 Cartesian coordinates (Angs):  

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.321887 | -0.733241 | 0.377651  |
| O | -1.072164 | -1.194178 | -0.535180 |
| O | -1.818629 | -0.130628 | -1.136408 |
| H | -0.014059 | -1.504088 | 1.082165  |
| C | 0.627602  | 0.433607  | 0.287361  |
| C | 1.851542  | -0.177182 | -0.364741 |
| C | 0.210318  | 1.701259  | -0.451299 |
| H | 0.886023  | 0.666886  | 1.323084  |
| C | 2.978384  | -0.451295 | 0.272251  |
| H | 1.750188  | -0.385894 | -1.425133 |
| H | 3.828322  | -0.875463 | -0.244282 |
| H | 3.092584  | -0.249888 | 1.330849  |
| O | -1.869964 | 0.126768  | 1.313230  |
| H | -2.145282 | 0.229196  | 0.306845  |
| H | -1.730831 | 1.008984  | 1.666493  |
| H | -0.694943 | 2.137686  | -0.035968 |
| H | 0.018564  | 1.491777  | -1.498936 |
| H | 1.019738  | 2.426220  | -0.365586 |

 Rotational constants (GHz): 3.1707600 1.2926300 1.2458400  
 Vibrational harmonic frequencies (cm-1):  

|           |           |           |
|-----------|-----------|-----------|
| i432.5227 | 52.9023   | 80.1103   |
| 192.3046  | 242.0144  | 268.4181  |
| 280.4709  | 313.7131  | 343.3585  |
| 378.4549  | 456.8513  | 501.3339  |
| 616.3153  | 631.0344  | 689.3815  |
| 769.4174  | 828.3408  | 881.0400  |
| 927.2548  | 989.7771  | 996.9601  |
| 1043.0678 | 1047.1931 | 1091.0827 |
| 1161.8974 | 1180.2534 | 1191.0274 |
| 1284.0223 | 1319.0411 | 1379.3309 |
| 1389.2851 | 1421.8619 | 1453.3428 |
| 1488.7430 | 1493.3845 | 1556.3378 |
| 1677.1513 | 1726.6076 | 2374.2727 |
| 3069.4139 | 3078.8492 | 3150.2494 |
| 3156.7291 | 3160.6529 | 3174.0595 |
| 3180.6168 | 3250.9014 | 3900.5573 |

 Zero-point correction (Hartree): 0.147715

TS.CH3CHCH2\_H\_COO+H2O.mmuu  
 ~~~~~  
 E(RM062X/Aug-CC-pVTZ) (Hartree): -422.02080177  
 Electronic state : 1-A  
 Cartesian coordinates (Angs):  

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.319580 | -0.701429 | 0.443155  |
| O | -1.045393 | -1.243746 | -0.446865 |
| O | -1.762976 | -0.236134 | -1.164984 |
| H | -0.029268 | -1.410627 | 1.218084  |
| C | 0.627278  | 0.457721  | 0.287269  |
| C | 1.838193  | -0.190321 | -0.352913 |
| C | 0.200458  | 1.699222  | -0.489102 |
| H | 0.890496  | 0.736006  | 1.309320  |
| C | 2.970759  | -0.445876 | 0.282198  |
| H | 1.723021  | -0.441941 | -1.402625 |
| H | 3.812827  | -0.895451 | -0.225854 |
| H | 3.097943  | -0.200281 | 1.329945  |
| O | -1.839899 | 0.375515  | 1.223913  |
| H | -2.082824 | 0.328641  | 0.202029  |
| H | -2.448192 | -0.222206 | 1.669102  |
| H | -0.688988 | 2.145562  | -0.053438 |
| H | -0.007007 | 1.457946  | -1.526790 |
| H | 1.015482  | 2.421376  | -0.439924 |

 Rotational constants (GHz): 3.1596300 1.3184000 1.2483200  
 Vibrational harmonic frequencies (cm-1):  

|           |           |           |
|-----------|-----------|-----------|
| i429.9411 | 45.1091   | 80.3749   |
| 192.9003  | 250.3622  | 277.7915  |
| 294.1042  | 310.1579  | 346.6125  |
| 368.5558  | 459.8362  | 531.3591  |
| 591.2407  | 618.4888  | 678.2781  |
| 776.3141  | 830.7155  | 881.6536  |
| 928.9210  | 988.1596  | 998.9852  |
| 1039.8354 | 1048.2525 | 1098.3261 |
| 1166.6802 | 1190.4750 | 1273.3008 |
| 1290.6992 | 1317.3552 | 1385.1661 |
| 1385.9552 | 1419.9548 | 1452.2409 |
| 1491.6242 | 1509.2095 | 1582.9625 |
| 1621.8071 | 1724.5682 | 2322.3597 |
| 3080.3587 | 3083.4968 | 3144.1704 |
| 3157.8623 | 3159.4057 | 3172.3392 |
| 3187.9375 | 3249.4414 | 3879.3670 |

 Zero-point correction (Hartree): 0.147819

TS.CH3CHCH2\_H\_COO+H2O.mpd  
 ~~~~~  
 E(RM062X/Aug-CC-pVTZ) (Hartree): -422.01857558  
 Electronic state : 1-A  
 Cartesian coordinates (Angs):  

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.761682 | -0.881990 | -0.136142 |
| O | -1.336950 | -0.592353 | 0.956400  |
| O | -1.211071 | 0.806401  | 1.211368  |
| H | -1.114613 | -1.830875 | -0.540975 |
| C | 0.615166  | -0.488889 | -0.588511 |
| C | 1.066556  | 0.927828  | -0.368326 |
| C | 1.534282  | -1.541107 | 0.052361  |
| H | 0.596035  | -0.665707 | -1.668201 |
| C | 2.202169  | 1.280914  | 0.210870  |
| H | 0.420280  | 1.688210  | -0.783860 |
| H | 2.475384  | 2.323678  | 0.287210  |
| H | 2.886541  | 0.565576  | 0.645905  |
| O | -1.728708 | 0.564375  | -1.178963 |

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H -1.635386 0.981801 -0.214246
H -2.654318 0.323377 -1.279524
H 1.179926 -2.552913 -0.143315
H 1.586509 -1.392231 1.130057
H 2.534531 -1.448841 -0.365017
Rotational constants (GHz): 2.6608400 1.5699700 1.3888500
Vibrational harmonic frequencies (cm-1):
i439.9999 52.8116 121.5352
188.7402 243.0809 280.8188
314.2215 331.3299 336.0833
396.6146 513.4597 537.3144
584.1600 610.1088 634.2630
795.8114 813.1331 885.8515
951.4088 966.2696 1000.3910
1026.4972 1043.9413 1065.7157
1142.3373 1174.0194 1285.8482
1306.4350 1342.1098 1371.7437
1392.7171 1402.9739 1456.4112
1498.8861 1513.1873 1591.0934
1615.3119 1735.0502 2272.5689
3054.8564 3071.6858 3135.4036
3143.5531 3159.4991 3178.7418
3217.7994 3259.8673 3883.9029
Zero-point correction (Hartree): 0.147852

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TS.CH3CHCHCH2_H_COO+H2O.mpd
~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -422.01621482
Electronic state : 1-A
Cartesian coordinates (Angs):
C      -0.760299      -0.881136      -0.076933
O      -1.326762      -0.525613      0.999372
O      -1.232945      0.892367      1.149533
H      -1.102362      -1.858671      -0.414060
C       0.612151      -0.500362      -0.560381
C       1.068564      0.918714      -0.364444
C       1.544823      -1.539537      0.082004
H       0.584036      -0.705435      -1.636115
C       2.225346      1.279785      0.166129
H       0.403126      1.687849      -0.732486
H       2.493432      2.324378      0.233858
H       2.931740      0.568505      0.571041
O      -1.886977      0.373322      -1.159238
H      -1.760415      0.913499      -0.265619
H      -1.458783      0.865887      -1.863976
H       1.185655      -2.553538      -0.090068
H       1.615597      -1.371307      1.155678
H       2.537941      -1.456562      -0.353847
Rotational constants (GHz):      2.6916700      1.5415700      1.3675400
Vibrational harmonic frequencies (cm-1):
i446.5669      62.8939      116.5005
191.7413      249.1873      279.3996
311.3902      332.2157      343.7456
400.9233      481.6440      539.8415
593.6584      636.8326      657.3060
791.3804      810.8787      887.2170
954.9665      966.7389      1001.9487
1025.4408      1033.7666      1066.3604
1138.7918      1169.5353      1178.3417
1302.0156      1348.7431      1366.2463
1394.1890      1403.7803      1457.0437
1499.9314      1514.2407      1557.7124
1676.3782      1733.4824      2333.3068
3038.9686      3073.8234      3144.7511
3152.6470      3160.0613      3181.2475
3207.4136      3262.8461      3898.7845
Zero-point correction (Hartree): 0.147922

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TS.CH3CHCHCH2_H_COO+H2O.mpd
~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -422.01682182
Electronic state : 1-A
Cartesian coordinates (Angs):
C -0.487797 -0.722418 0.476369
O -1.056377 -1.163908 -0.567307
O -1.555058 -0.083051 -1.359611
H -0.438352 -1.480866 1.257059
C 0.565012 0.350772 0.586656
C 1.865836 -0.435120 0.552438
C 0.530731 1.513809 -0.390596
H 0.465135 0.725587 1.610999
C 2.832864 -0.274322 -0.335337
H 1.983834 -1.181069 1.332219
H 3.732691 -0.871297 -0.282880
H 2.768259 0.451399 -1.134293
O -2.114913 0.337379 0.991086
H -2.146052 0.388757 -0.059841
H -1.964446 1.227986 1.317943
H -0.397706 2.071857 -0.308314
H 0.604006 1.167457 -1.416899
H 1.363540 2.180504 -0.166511
Rotational constants (GHz): 3.2747600 1.3079000 1.2820400
Vibrational harmonic frequencies (cm-1):
i453.5023 62.4555 86.4328
210.0621 254.8688 283.5707
318.1575 335.6409 344.8068
396.4476 474.5489 541.3439
597.6960 630.2206 665.9964
770.4045 822.8964 878.9300
919.9228 994.4823 1022.7246
1039.8313 1050.7485 1078.2462
1107.9003 1186.1648 1205.2913

```

|           |           |           |
|-----------|-----------|-----------|
| 1284.5649 | 1336.8035 | 1379.4633 |
| 1400.6334 | 1424.8113 | 1451.5134 |
| 1490.9199 | 1500.5651 | 1557.4667 |
| 1679.0636 | 1732.1236 | 2316.3392 |
| 3040.2225 | 3080.2704 | 3143.6026 |
| 3156.7271 | 3160.7654 | 3180.1753 |
| 3182.2775 | 3263.4010 | 3898.3193 |

Zero-point correction (Hartree): 0.147944

TS.CH3CHCHCH2\_H\_COO+H2O.mpuu

~~~~~  
E(RM062X/Aug-CC-pVTZ) (Hartree): -422.01900773

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.483801 | -0.734033 | 0.461300  |
| O | -1.059258 | -1.155868 | -0.588908 |
| O | -1.545901 | -0.058645 | -1.363440 |
| H | -0.435937 | -1.508899 | 1.227543  |
| C | 0.567419  | 0.333687  | 0.600934  |
| C | 1.866424  | -0.453251 | 0.540064  |
| C | 0.527101  | 1.531190  | -0.333177 |
| H | 0.456036  | 0.678881  | 1.633019  |
| C | 2.828288  | -0.269320 | -0.349057 |
| H | 1.991145  | -1.217874 | 1.300878  |
| H | 3.730276  | -0.864539 | -0.316560 |
| H | 2.756234  | 0.477050  | -1.128167 |
| O | -2.026309 | 0.473013  | 0.981439  |
| H | -2.062783 | 0.476174  | -0.075487 |
| H | -2.775501 | -0.055474 | 1.272192  |
| H | -0.397520 | 2.084824  | -0.203424 |
| H | 0.592086  | 1.227714  | -1.373558 |
| H | 1.365117  | 2.184507  | -0.089552 |

Rotational constants (GHz): 3.2621200 1.3233800 1.2853100

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i454.8284 | 55.7796   | 84.1141   |
| 206.4966  | 255.2230  | 291.1971  |
| 315.7494  | 338.6227  | 347.1547  |
| 394.1060  | 505.4503  | 536.5649  |
| 586.8425  | 609.3757  | 645.5587  |
| 772.9700  | 826.6861  | 880.6604  |
| 919.0584  | 992.9066  | 1023.3670 |
| 1040.1278 | 1050.3690 | 1078.4859 |
| 1110.6714 | 1209.9095 | 1272.2477 |
| 1301.7995 | 1336.7106 | 1383.6982 |
| 1397.6515 | 1422.9589 | 1451.1650 |
| 1497.0764 | 1504.4974 | 1587.6808 |
| 1619.5357 | 1730.8860 | 2245.6290 |
| 3058.5282 | 3080.7248 | 3130.0552 |
| 3156.4906 | 3160.7767 | 3179.9272 |
| 3186.7209 | 3262.4558 | 3882.6069 |

Zero-point correction (Hartree): 0.147915

TS.CH3CHCHCH2\_H\_COO+H2O.pcuu

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Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.591080  | 0.742907  | -0.014762 |
| O | -0.614822 | 0.661350  | -0.202505 |
| O | -0.914754 | -0.596352 | -0.532556 |
| H | 1.070300  | 1.716912  | 0.085419  |
| C | 1.413873  | -0.550214 | -0.004987 |
| C | 1.168393  | -1.447764 | -1.219105 |
| C | 2.845464  | -0.021107 | 0.103056  |
| H | 1.140328  | -1.168631 | 0.850003  |
| C | 0.202282  | -1.151704 | -2.074773 |
| H | 1.750492  | -2.359259 | -1.354963 |
| H | 0.020234  | -1.796385 | -2.934636 |
| H | -0.460406 | -0.297624 | -1.882982 |
| O | 0.408027  | 0.681596  | -2.005423 |
| H | -0.338068 | -0.015778 | -1.668499 |
| H | 1.089899  | 0.115451  | -2.400061 |
| H | 2.908014  | 0.540999  | 1.034916  |
| H | 3.016830  | 0.614390  | -0.765845 |
| H | 3.506110  | -0.888086 | 0.107611  |

TS.CH3CHCHCH2\_H\_COO+H2O.pcuu

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Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.604505  | 0.754158  | -0.028050 |
| O | -0.601635 | 0.686278  | -0.219699 |
| O | -0.915331 | -0.568849 | -0.546673 |
| H | 1.094899  | 1.722753  | 0.070612  |
| C | 1.411877  | -0.548598 | -0.011208 |
| C | 1.159920  | -1.447192 | -1.223238 |
| C | 2.849257  | -0.036140 | 0.100061  |
| H | 1.128107  | -1.160911 | 0.844844  |
| C | 0.200331  | -1.142540 | -2.083209 |
| H | 1.731628  | -2.365966 | -1.354107 |
| H | 0.013597  | -1.787857 | -2.941591 |
| H | -0.452822 | -0.280048 | -1.896501 |
| O | 0.427594  | 0.688372  | -2.019123 |
| H | -0.327880 | 0.001033  | -1.682515 |
| H | -0.081868 | 1.447301  | -2.344197 |
| H | 2.915290  | 0.528252  | 1.030294  |
| H | 3.031109  | 0.594415  | -0.770312 |
| H | 3.499552  | -0.910866 | 0.109731  |

TS.CH3CHCHCH2\_H\_COO+H2O.pmdd

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E(RM062X/Aug-CC-pVTZ) (Hartree): -422.02432828

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |          |          |          |
|---|----------|----------|----------|
| C | 0.431537 | 0.046235 | 0.725728 |
|---|----------|----------|----------|

```

O 0.837646 -1.161041 0.710741
O 1.173248 -1.519891 -0.636028
H 0.451634 0.482078 1.725344
C -0.534366 0.641170 -0.256492
C -1.878896 0.013277 0.077977
C -0.576314 2.157439 -0.135575
H -0.236844 0.333146 -1.254246
C -2.171937 -1.251355 -0.180847
H -2.604270 0.663139 0.556664
H -3.141708 -1.661592 0.066001
H -1.442007 -1.907589 -0.641945
O 2.042438 0.732025 -0.226184
H 1.906008 -0.230202 -0.655809
H 2.812311 0.662731 0.346954
H 0.382597 2.594706 -0.399444
H -0.833007 2.457898 0.882869
H -1.341526 2.556340 -0.799369
Rotational constants (GHz): 2.4764300 1.8537000 1.2163700
Vibrational harmonic frequencies (cm-1):
i476.9692 44.4586 73.5818
172.5397 224.8532 248.0365
272.5794 338.8636 346.1565
388.4528 477.9127 517.5200
586.3106 633.0500 647.7110
692.2394 867.4861 886.0199
937.1849 1011.0998 1017.9996
1033.1699 1048.5569 1116.2390
1172.7744 1196.3226 1274.3139
1306.4364 1315.2830 1335.1904
1368.2016 1413.3080 1443.7585
1499.7448 1509.8581 1574.7592
1614.9266 1718.8235 2200.7541
3060.0350 3129.4692 3136.9467
3152.5287 3156.6076 3168.1112
3172.6607 3250.6774 3877.8720
Zero-point correction (Hartree): 0.147241

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```

TS.CH3CHCH2_H_COO+H2O.pmd
~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -422.02160301
Electronic state : 1-A
Cartesian coordinates (Angs):
C      -0.442447      0.055702      -0.727183
O      -0.839953      -1.152819      -0.714493
O      -1.175903      -1.516495      0.632313
H      -0.467664      0.494070      -1.724401
C      0.533970      0.641102      0.255317
C      1.873084      -0.007975      -0.061141
C      0.615061      2.155471      0.117299
H      0.230524      0.342008      1.254608
C      2.137142      -1.279949      0.191785
H      2.618605      0.632100      -0.521537
H      3.103244      -1.705404      -0.043216
H      1.386352      -1.926302      0.632988
O      -2.120281      0.676165      0.100907
H      -1.980944      -0.259038      0.578469
H      -2.044951      1.354672      0.777055
H      -0.330225      2.645250      0.343521
H      0.901384      2.434818      -0.898456
H      1.371903      2.546915      0.794689
Rotational constants (GHz):      2.4730400      1.8537800      1.2134600
Vibrational harmonic frequencies (cm-1):
i479.5667      46.3339      77.2436
171.7917      210.6847      249.6909
272.3450      338.5268      341.7769
404.0441      470.0788      511.7283
591.8922      644.4858      677.6059
702.6293      863.1443      887.2553
933.7528      1010.4845      1019.0475
1031.2663      1050.9868      1112.3982
1167.5182      1181.9887      1206.5136
1284.2123      1318.0113      1337.1638
1366.4841      1422.9586      1442.4450
1498.6844      1504.7345      1543.3017
1678.9142      1719.0464      2249.6040
3064.4676      3128.4257      3143.6592
3151.9860      3153.3327      3155.4665
3169.2488      3251.7163      3892.9892
Zero-point correction (Hartree): 0.147288

```

```

TS.CH3CHCH2_H_COO+H2O.pmd
~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -422.01634270
Electronic state : 1-A
Cartesian coordinates (Angs):
C 0.784399 0.389484 -0.780594
O 1.486416 -0.660020 -0.892606
O 1.270588 -1.512703 0.234149
H 1.170443 1.205110 -1.391804
C -0.681543 0.480572 -0.471280
C -1.285524 -0.531780 0.454870
C -1.052381 1.909261 -0.058382
H -1.106124 0.312619 -1.472559
C -2.325852 -1.278961 0.126751
H -0.870771 -0.583982 1.453751
H -2.775644 -1.958942 0.835830
H -2.749716 -1.252038 -0.869959
O 1.571099 0.780191 1.023265
H 1.539471 -0.276055 1.020065
H 0.996936 1.087950 1.728608
H -0.553622 2.653116 -0.680376
H -0.782718 2.099130 0.979476

```

```

H -2.127674 2.041887 -0.149686
Rotational constants (GHz): 2.4660000 1.7118700 1.3035800
Vibrational harmonic frequencies (cm-1):
i464.7496 57.5934 102.4670
191.1601 224.9392 248.1197
305.1211 326.7395 340.9014
385.1914 444.5561 526.0634
615.5644 649.6419 664.3899
759.7722 817.8440 891.1502
965.4283 968.9571 977.6479
1019.3315 1030.9974 1101.3288
1114.7707 1182.3342 1223.3590
1284.8055 1319.5802 1347.9098
1389.5484 1418.7077 1463.7645
1490.4468 1509.4257 1550.6704
1678.6372 1735.1280 2269.3544
3000.9462 3071.0232 3140.2568
3146.4833 3159.9737 3162.2224
3195.8056 3253.1830 3903.8750
Zero-point correction (Hartree): 0.147231

```

```

TS.CH3CHCHCH2_H_COO+H2O.pmuu
~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -422.01915930
Electronic state : 1-A
Cartesian coordinates (Angs):
C          0.779118      0.417534      -0.773761
O          1.505479     -0.615070     -0.905138
O          1.285277     -1.507405      0.186825
H          1.159766      1.256645     -1.358059
C         -0.687981      0.486911     -0.473639
C         -1.280315     -0.528131      0.457386
C         -1.065009      1.911167     -0.051715
H         -1.106084      0.311500     -1.477084
C         -2.291294     -1.310581      0.120084
H         -0.887327     -0.535211      1.465827
H         -2.738405     -1.989158      0.832335
H         -2.694510     -1.313389     -0.885612
O          1.375077      0.736369      1.142608
H          1.414322     -0.321683      1.040413
H          2.286572      1.042471      1.153710
H         -0.623377      2.656757     -0.714787
H         -0.718305      2.099616      0.961364
H         -2.146422      2.019899     -0.082603
Rotational constants (GHz):  2.4466800    1.7314700    1.3257100
Vibrational harmonic frequencies (cm-1):
i470.9872      63.6693      107.4547
201.4210      224.7335      246.2689
300.5065      338.8995      340.0954
384.4930      474.9367      526.1067
580.3685      618.1821      664.6002
762.6860      825.1312      890.8536
964.2255      970.3775      975.8739
1025.5825     1040.2458     1099.6577
1116.5215     1224.3451     1282.4145
1299.8064     1322.2132     1347.6489
1387.7112     1412.8232     1464.4597
1496.5415     1509.6118     1586.2034
1607.9355     1735.8281     2173.3190
2995.0751     3068.8594     3132.3772
3144.6832     3161.1180     3172.0550
3204.7477     3252.0357     3886.0877
Zero-point correction (Hartree): 0.147194

```

```

TS.CH3CHCHCH2_H_COO+H2O.ppdd
~~~~~
E(CCS(D)/T)/Aug-CC-pVTZ) (Hartree): -421.42576154
E(CCS(D)/Aug-CC-pVTZ) (Hartree): -421.34836077
T1 diagnostic: 0.019935
E(MP2/Aug-CC-pVTZ) (Hartree): -421.30654366
E(MP3/Aug-CC-pVTZ) (Hartree): -421.33602078
E(RHF/Aug-CC-pVTZ) (Hartree): -419.69814799
E(RM062X/Aug-CC-pVTZ) (Hartree): -422.02633107
Electronic state : 1-A
Cartesian coordinates (Angs):
C 0.511974 0.005872 0.691521
O 1.240812 -1.037490 0.675407
O 1.731477 -1.224544 -0.657797
H 0.341419 0.387621 1.698643
C -0.523939 0.336705 -0.344691
C -1.514852 -0.803917 -0.248307
C -1.104664 1.716507 -0.091909
H -0.055352 0.286381 -1.324722
C -2.785572 -0.682961 0.101842
H -1.100399 -1.775854 -0.492544
H -3.434097 -1.547506 0.134783
H -3.228238 0.272445 0.351201
O 1.905833 1.165851 -0.121513
H 2.075980 0.230025 -0.588803
H 2.632046 1.293652 0.496878
H -0.325618 2.469209 -0.187764
H -1.538752 1.788155 0.907166
H -1.889649 1.932093 -0.814347
Rotational constants (GHz): 3.0952100 1.4733400 1.1312100
Vibrational harmonic frequencies (cm-1):
i471.3444 62.5599 106.8872
176.1968 253.3786 273.6803
306.3137 328.8789 352.0349
377.1389 510.4588 542.8242
600.8726 645.2643 656.0965
704.7993 858.2012 884.5724
942.5547 986.6599 1023.5595

```

|           |           |           |
|-----------|-----------|-----------|
| 1025.2891 | 1059.5045 | 1094.7132 |
| 1167.2552 | 1187.9725 | 1270.3398 |
| 1304.9909 | 1319.6996 | 1339.5925 |
| 1369.2410 | 1408.9193 | 1451.8300 |
| 1506.2508 | 1508.8174 | 1575.8136 |
| 1617.6438 | 1728.5416 | 2232.7486 |
| 3065.4016 | 3126.1319 | 3138.3379 |
| 3145.6041 | 3163.1653 | 3171.5877 |
| 3185.2385 | 3256.0160 | 3876.4190 |

Zero-point correction (Hartree): 0.147830

TS.CH3CHCHCH2\_H\_COO+H2O.ppd

~~~~~  
E(RM062X/Aug-CC-pVTZ) (Hartree): -422.02356828

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.523372  | 0.012111  | 0.694038  |
| O | 1.239605  | -1.038153 | 0.671484  |
| O | 1.729583  | -1.221204 | -0.663915 |
| H | 0.359136  | 0.391574  | 1.701912  |
| C | -0.520133 | 0.340263  | -0.340082 |
| C | -1.503876 | -0.807213 | -0.252585 |
| C | -1.122248 | 1.709963  | -0.077087 |
| H | -0.056170 | 0.290003  | -1.322992 |
| C | -2.778683 | -0.698586 | 0.085802  |
| H | -1.076112 | -1.774033 | -0.493336 |
| H | -3.417768 | -1.570227 | 0.113770  |
| H | -3.235179 | 0.250964  | 0.332589  |
| O | 1.999401  | 1.120355  | 0.014903  |
| H | 2.153916  | 0.214912  | -0.508695 |
| H | 1.767341  | 1.790287  | -0.633923 |
| H | -0.365896 | 2.491237  | -0.138859 |
| H | -1.569788 | 1.759395  | 0.916703  |
| H | -1.898778 | 1.928675  | -0.807468 |

Rotational constants (GHz): 3.1014500 1.4662100 1.1268600

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i475.3822 | 68.3462   | 107.6894  |
| 180.0248  | 247.8372  | 262.1443  |
| 312.6685  | 325.3917  | 365.3711  |
| 382.2068  | 489.8329  | 538.6205  |
| 615.1981  | 645.2828  | 685.0613  |
| 708.5329  | 854.7053  | 885.2595  |
| 938.9323  | 987.1316  | 1024.2801 |
| 1024.7523 | 1061.2227 | 1097.3613 |
| 1158.1924 | 1184.2509 | 1201.1098 |
| 1280.7816 | 1320.5536 | 1344.6093 |
| 1367.5042 | 1417.0971 | 1452.9282 |
| 1498.4895 | 1511.5384 | 1545.4752 |
| 1676.3345 | 1729.6964 | 2275.0091 |
| 3067.3769 | 3117.8034 | 3136.5258 |
| 3151.3209 | 3154.3119 | 3172.7129 |
| 3188.0051 | 3256.4138 | 3890.6395 |

Zero-point correction (Hartree): 0.147868

TS.CH3CHCHCH2\_H\_COO+H2O.ppu

~~~~~  
E(RM062X/Aug-CC-pVTZ) (Hartree): -422.02039368

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.795376  | 0.890878  | -0.064238 |
| O | 1.906188  | 0.409581  | -0.436432 |
| O | 1.819239  | -1.014657 | -0.504266 |
| H | 0.901097  | 1.910165  | 0.304898  |
| C | -0.576866 | 0.550345  | -0.608318 |
| C | -1.002025 | -0.896957 | -0.571101 |
| C | -1.585424 | 1.507640  | 0.020975  |
| H | -0.456438 | 0.817757  | -1.668349 |
| C | -2.065775 | -1.347933 | 0.078832  |
| H | -0.369018 | -1.574414 | -1.124743 |
| H | -2.319380 | -2.398560 | 0.049945  |
| H | -2.723069 | -0.704300 | 0.649494  |
| O | 0.767937  | -0.162563 | 1.609940  |
| H | 1.244086  | -0.824602 | 0.979397  |
| H | -0.093485 | -0.560476 | 1.778450  |
| H | -1.285645 | 2.543276  | -0.132723 |
| H | -1.668236 | 1.338424  | 1.095580  |
| H | -2.568545 | 1.370002  | -0.422775 |

Rotational constants (GHz): 2.7617100 1.5857100 1.3758100

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i402.0252 | 31.7002   | 105.6895  |
| 206.9842  | 249.0788  | 278.5223  |
| 295.6995  | 335.9283  | 355.1882  |
| 433.5632  | 437.7953  | 541.1875  |
| 597.6647  | 636.7193  | 718.3013  |
| 758.1618  | 812.2927  | 897.5863  |
| 965.9728  | 978.2948  | 986.3537  |
| 1021.4173 | 1055.7461 | 1079.1596 |
| 1138.6321 | 1164.7248 | 1174.0280 |
| 1297.2470 | 1329.8361 | 1335.7249 |
| 1398.6599 | 1417.1168 | 1453.8000 |
| 1504.3530 | 1511.5554 | 1567.3518 |
| 1695.1309 | 1721.8939 | 2619.7688 |
| 3006.6319 | 3069.7736 | 3136.1597 |
| 3149.4460 | 3159.5141 | 3171.5421 |
| 3228.1091 | 3255.2797 | 3852.5650 |

Zero-point correction (Hartree): 0.148395

TS.CH3CHCHCH2\_H\_COO+H2O.ppuu

~~~~~  
E(RM062X/Aug-CC-pVTZ) (Hartree): -422.01974089

Electronic state : 1-A

Cartesian coordinates (Angs):

```

C 0.819513 0.777022 -0.466166
O 1.844477 0.051851 -0.652149
O 1.657374 -1.236472 -0.061606
H 1.049994 1.837092 -0.580514
C -0.625330 0.435484 -0.701618
C -1.060660 -0.982054 -0.441349
C -1.509245 1.502929 -0.064312
H -0.667254 0.583592 -1.794521
C -2.058603 -1.319341 0.359352
H -0.511758 -1.742793 -0.976353
H -2.335502 -2.357126 0.481063
H -2.620826 -0.592725 0.929912
O 0.775342 0.443867 1.523061
H 1.130171 -0.466801 1.150387
H 1.535455 0.874752 1.925998
H -1.171301 2.503134 -0.335980
H -1.486101 1.414591 1.019122
H -2.534463 1.388079 -0.408994
Rotational constants (GHz): 2.6728300 1.6388400 1.4014700
Vibrational harmonic frequencies (cm-1):
1430.2851 56.7350 104.2009
208.7482 271.0051 287.2256
291.8708 333.5776 355.0525
424.0518 452.6253 543.7863
570.9613 620.8494 650.3049
767.2138 810.1713 885.9827
969.2582 973.6520 985.9408
1021.5748 1047.5701 1079.4744
1145.9870 1177.8952 1264.3211
1299.2175 1340.9606 1348.5848
1394.3319 1411.9179 1455.2177
1499.4509 1519.1239 1576.7928
1622.0226 1732.4169 2402.3958
2967.1429 3076.7500 3131.1918
3146.0471 3170.5210 3177.2990
3223.9115 3259.7522 3877.2183
Zero-point correction (Hartree): 0.147927

```

TS.CH3CHCHCH2\_H\_COO+H2O.tcdd

E(RM062X/Aug-CC-pVTZ) (Hartree): -422.01816268

Electronic state : 1-A

Cartesian coordinates (Angs):

```

C 0.357152 -0.434988 -0.756063
O 1.614605 -0.413349 -0.937170
O 2.253279 0.299206 0.123085
H -0.117747 -1.230165 -1.330890
C -0.539751 0.725472 -0.443893
C -1.977191 0.294300 -0.306000
C -0.174489 1.707509 0.673095
H -0.465601 1.273967 -1.397772
C -2.425568 -0.900769 0.043280
H -2.690619 1.091788 -0.485482
H -3.486949 -1.085964 0.132127
H -1.761658 -1.722074 0.276421
O 0.527560 -1.130071 1.136125
H 1.382417 -0.520427 1.027108
H 0.849323 -2.036369 1.100338
H 0.796455 2.156760 0.502165
H -0.170797 1.193133 1.630956
H -0.939297 2.483918 0.706192
Rotational constants (GHz): 3.0679900 1.4973200 1.3253200
Vibrational harmonic frequencies (cm-1):
1451.7436 72.7596 113.0865
190.9843 246.8910 265.2023
279.5790 331.8665 348.4393
405.2713 468.1765 562.3283
588.1503 644.9040 666.1368
700.3915 843.3813 897.6125
934.8980 980.8109 991.1488
1043.6851 1048.6023 1087.0484
1149.4336 1176.6178 1283.4646
1295.0789 1332.8590 1363.0214
1387.4903 1411.2237 1461.6674
1492.3919 1511.5109 1587.3899
1623.9475 1735.1099 2268.3304
2977.8856 3078.7501 3139.6518
3153.8260 3168.1159 3180.4625
3202.2360 3260.6128 3875.0196
Zero-point correction (Hartree): 0.147688

```

TS.CH3CHCHCH2\_H\_COO+H2O.tcdu

E(RM062X/Aug-CC-pVTZ) (Hartree): -422.01873163

Electronic state : 1-A

Cartesian coordinates (Angs):

```

C 0.369163 -0.403008 -0.796469
O 1.633303 -0.428700 -0.884307
O 2.236270 0.159755 0.270360
H -0.095324 -1.133183 -1.458370
C -0.503826 0.766397 -0.454182
C -1.930682 0.357816 -0.191028
C -0.029035 1.791869 0.575974
H -0.516527 1.280971 -1.430295
C -2.414510 -0.862821 -0.010407
H -2.613100 1.200393 -0.144036
H -3.470759 -1.007717 0.169439
H -1.795370 -1.750078 -0.029046
O 0.412465 -1.340634 0.987700
H 1.279690 -0.764277 1.037155
H -0.218000 -0.987179 1.621963
H 0.944435 2.189679 0.314911

```

```

H 0.043401 1.347655 1.566849
H -0.761406 2.598856 0.618088
Rotational constants (GHz): 3.0041400 1.5562400 1.3171700
Vibrational harmonic frequencies (cm-1):
i421.1247 94.7821 154.4385
192.9513 238.5580 271.7156
284.6626 330.0008 355.4151
410.0158 447.2795 573.8123
601.5228 632.3426 684.3235
708.8070 829.3925 890.9452
934.8515 998.6411 1003.0523
1050.9459 1056.2840 1083.8458
1144.5921 1178.5217 1184.2309
1288.1893 1330.7816 1369.7435
1393.1445 1420.6868 1466.8452
1491.6197 1494.3180 1565.9876
1664.6796 1729.5303 2444.3952
2967.7715 3075.1911 3142.8462
3148.5517 3164.8726 3175.8488
3198.5728 3256.3112 3883.6433
Zero-point correction (Hartree): 0.148102

```

TS.CH3CHCHCH2\_H\_COO+H2O.t cud

```

~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -422.02449826
Electronic state : 1-A
Cartesian coordinates (Angs):
C      0.416012      -0.041200      0.669770
O      1.671010      0.146699      0.721542
O      2.208360      0.070431      -0.604084
H      -0.015448      -0.280475      1.640787
C      -0.471389      0.612349      -0.342049
C      -1.868708      0.064702      -0.360474
C      -0.470161      2.110957      0.016911
H      -0.011281      0.512566      -1.323571
C      -2.326670      -1.005030      0.275176
H      -2.557321      0.644180      -0.967505
H      -3.366198      -1.289808      0.191720
H      -1.697715      -1.635909      0.890616
O      0.624527      -1.794690      -0.210924
H      1.408876      -1.262474      -0.644240
H      -0.042231      -1.946542      -0.888194
H      0.539592      2.508649      -0.058591
H      -0.847904      2.272451      1.027081
H      -1.116049      2.647173      -0.676385
Rotational constants (GHz):      2.7411900      1.6790400      1.2058400
Vibrational harmonic frequencies (cm-1):
i425.4067      88.9696      146.6147
167.5993      224.7600      244.9454
273.8428      321.9602      352.9678
406.0967      500.3265      541.6686
621.0415      633.9473      676.3218
705.7019      872.9059      893.8347
945.5680      992.5643      1028.1353
1044.6230      1055.7714      1091.8107
1107.1464      1177.7531      1204.0783
1308.5133      1319.8497      1343.7440
1369.3325      1399.6792      1468.8888
1497.8582      1501.3142      1565.2790
1664.7893      1727.8443      2456.6909
3066.7313      3114.1974      3142.0519
3153.5848      3162.0356      3162.8358
3171.2185      3251.5896      3872.8910
Zero-point correction (Hartree): 0.148176

```

TS.CH3CHCHCH2\_H\_COO+H2O.t cuu

```

~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -422.02377107
Electronic state : 1-A
Cartesian coordinates (Angs):
C 0.372862 -0.102592 0.662879
O 1.620066 0.122613 0.780466
O 2.200306 0.155170 -0.527719
H -0.087983 -0.423214 1.597008
C -0.502102 0.583359 -0.338312
C -1.930306 0.121719 -0.279695
C -0.385665 2.086840 -0.024294
H -0.099101 0.421173 -1.335839
C -2.384724 -1.009622 0.236002
H -2.637374 0.816341 -0.722083
H -3.441608 -1.236444 0.223920
H -1.728958 -1.758510 0.659876
O 0.630651 -1.739697 -0.433707
H 1.429026 -1.124233 -0.745974
H 1.028122 -2.436829 0.098149
H 0.646704 2.409581 -0.138473
H -0.724030 2.305250 0.989265
H -1.013371 2.643967 -0.717653
Rotational constants (GHz): 2.7767500 1.6577900 1.2001700
Vibrational harmonic frequencies (cm-1):
i459.1181 87.5084 103.1358
162.3021 232.0749 245.8100
271.7466 340.9003 346.1554
396.2578 513.6844 524.5607
591.0073 644.4671 666.3374
671.1666 879.6671 893.3473
945.3456 975.0797 1026.2839
1035.5864 1052.3477 1093.1009
1114.9728 1199.9602 1275.2914
1298.6581 1318.5047 1346.3499
1370.8496 1399.9209 1461.2474
1498.6073 1504.9617 1583.6687

```



|           |           |           |
|-----------|-----------|-----------|
| 1623.6232 | 1734.1939 | 2286.2838 |
| 3066.4105 | 3120.6878 | 3141.1590 |
| 3145.5238 | 3162.2867 | 3164.8537 |
| 3178.0334 | 3257.5024 | 3871.1571 |

Zero-point correction (Hartree): 0.147677

TS.CH3CHCH2\_H\_COO+H2O.tmd

~~~~~  
E(RM062X/Aug-CC-pVTZ) (Hartree): -422.02073036

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.400860  | -0.530147 | -0.706226 |
| O | 1.619944  | -0.362825 | -1.020730 |
| O | 2.281290  | 0.449809  | -0.048711 |
| H | -0.026068 | -1.408294 | -1.192597 |
| C | -0.620331 | 0.499339  | -0.311807 |
| C | -1.802840 | -0.198670 | 0.307936  |
| C | -0.184296 | 1.704558  | 0.515782  |
| H | -0.936065 | 0.848456  | -1.307343 |
| C | -2.957909 | -0.394132 | -0.307018 |
| H | -1.652509 | -0.535065 | 1.327292  |
| H | -3.782848 | -0.888351 | 0.187368  |
| H | -3.122615 | -0.059454 | -1.324770 |
| O | 0.839885  | -1.093393 | 1.194361  |
| H | 1.614483  | -0.412598 | 0.959256  |
| H | 1.235288  | -1.969948 | 1.184014  |
| H | 0.633584  | 2.237017  | 0.043385  |
| H | 0.138534  | 1.388213  | 1.505341  |
| H | -1.043636 | 2.365594  | 0.626693  |

Rotational constants (GHz): 3.3184600 1.3145400 1.2348400

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i453.6883 | 66.7756   | 80.3815   |
| 194.7847  | 252.8247  | 286.9433  |
| 290.3833  | 319.3896  | 356.0848  |
| 370.1779  | 478.6302  | 519.4644  |
| 581.5532  | 615.7656  | 689.0290  |
| 729.8578  | 844.5069  | 890.9413  |
| 941.7255  | 985.4074  | 989.1594  |
| 1023.7326 | 1052.2706 | 1099.9090 |
| 1168.4500 | 1211.6945 | 1270.1422 |
| 1298.8511 | 1323.1916 | 1344.8720 |
| 1388.7828 | 1417.5392 | 1457.7538 |
| 1491.3898 | 1503.4554 | 1581.2161 |
| 1610.9969 | 1734.3110 | 2241.7107 |
| 2992.4387 | 3080.0711 | 3133.6055 |
| 3152.1672 | 3158.7490 | 3192.0311 |
| 3192.9055 | 3248.4689 | 3884.5234 |

Zero-point correction (Hartree): 0.147486

TS.CH3CHCH2\_H\_COO+H2O.tmd

~~~~~  
E(RM062X/Aug-CC-pVTZ) (Hartree): -422.01753135

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.392675 | -0.542785 | 0.688047  |
| O | -1.608518 | -0.384219 | 1.011887  |
| O | -2.283499 | 0.430814  | 0.048166  |
| H | 0.044321  | -1.422604 | 1.159479  |
| C | 0.613842  | 0.511427  | 0.311144  |
| C | 1.814828  | -0.145612 | -0.317290 |
| C | 0.155886  | 1.731950  | -0.479916 |
| H | 0.924686  | 0.843513  | 1.313334  |
| C | 2.942397  | -0.415036 | 0.319353  |
| H | 1.726117  | -0.389090 | -1.371672 |
| H | 3.777634  | -0.881569 | -0.184107 |
| H | 3.070808  | -0.172983 | 1.367901  |
| O | -0.911324 | -1.228888 | -1.126064 |
| H | -1.663385 | -0.516937 | -0.943843 |
| H | -0.415316 | -0.936416 | -1.894427 |
| H | -0.665311 | 2.238521  | 0.014159  |
| H | -0.182768 | 1.448172  | -1.475351 |
| H | 1.004267  | 2.408076  | -0.585408 |

Rotational constants (GHz): 3.2634000 1.3213600 1.2257000

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i449.5761 | 47.2815   | 82.9061   |
| 199.7860  | 240.4818  | 273.7670  |
| 289.3692  | 312.6371  | 344.9770  |
| 379.9327  | 450.0578  | 515.8748  |
| 603.9065  | 637.6299  | 691.2352  |
| 718.6375  | 839.0624  | 891.1097  |
| 943.6988  | 988.2574  | 990.7839  |
| 1023.1733 | 1034.9731 | 1099.5349 |
| 1165.9410 | 1180.6235 | 1211.4614 |
| 1275.5307 | 1332.2165 | 1343.4787 |
| 1391.2769 | 1419.7242 | 1457.6429 |
| 1489.4148 | 1491.8466 | 1551.1602 |
| 1678.8723 | 1735.6294 | 2328.2104 |
| 2998.6612 | 3076.1257 | 3140.9776 |
| 3148.6443 | 3158.5627 | 3166.9271 |
| 3193.9792 | 3250.8512 | 3904.2238 |

Zero-point correction (Hartree): 0.147377

TS.CH3CHCH2\_H\_COO+H2O.tmd

~~~~~  
E(RM062X/Aug-CC-pVTZ) (Hartree): -422.02484849

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.652776  | 0.153542  | 0.720722  |
| O | 1.864153  | 0.330817  | 0.391697  |
| O | 2.052074  | -0.098038 | -0.962749 |
| H | 0.496499  | 0.177394  | 1.799065  |
| C | -0.509875 | 0.517151  | -0.155903 |

```

C -1.774913 -0.118808 0.334537
C -0.593371 2.054141 -0.097886
H -0.288260 0.212365 -1.174557
C -2.573559 -0.857607 -0.420048
H -2.040687 0.071968 1.371706
H -3.489878 -1.279600 -0.031417
H -2.340196 -1.051761 -1.460879
O 0.719479 -1.782290 0.318967
H 1.326802 -1.415372 -0.430153
H -0.098597 -2.092406 -0.082081
H 0.329369 2.491416 -0.474456
H -0.760425 2.402212 0.922817
H -1.426617 2.389362 -0.711891
Rotational constants (GHz): 2.7708300 1.5469000 1.1747800
Vibrational harmonic frequencies (cm-1):
i394.9662 61.9841 95.5801
171.0185 219.4656 239.8517
273.1217 313.2526 352.0345
396.4300 452.2256 516.7671
615.3697 627.2526 688.9027
712.7312 874.5869 892.7149
945.2262 990.2254 1002.9559
1030.3821 1044.8175 1082.8608
1151.4123 1185.5880 1209.8833
1274.5417 1322.4734 1333.9823
1368.4177 1397.8832 1461.8003
1496.8986 1500.7670 1566.9908
1657.0611 1737.3206 2608.2554
3064.0719 3134.3029 3141.6036
3143.3438 3157.2754 3159.8908
3161.6422 3250.4017 3871.8712
Zero-point correction (Hartree): 0.147984

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TS.CH3CHCHCH2\_H\_COO+H2O.tmuu

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~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -422.02433787
Electronic state : 1-A
Cartesian coordinates (Angs):
C       0.550059      0.011967      0.746254
O       1.787658      0.256699      0.583323
O       2.110353      0.051501     -0.796696
H       0.285985     -0.140262      1.793225
C      -0.531202      0.487693     -0.180983
C      -1.873815      0.042380      0.319308
C      -0.412102      2.021193     -0.213245
H      -0.346951      0.098743     -1.177238
C      -2.645522     -0.834238     -0.300167
H      -2.211839      0.498478      1.247127
H      -3.613212     -1.113092      0.093553
H      -2.326632     -1.305654     -1.221551
O       0.646805     -1.799572     -0.059295
H       1.355411     -1.267844     -0.620328
H       1.143014     -2.391949      0.514277
H       0.564809      2.306752     -0.597587
H      -0.543903      2.448373      0.782262
H      -1.189716      2.423462     -0.859403
Rotational constants (GHz):   2.8595200   1.5385800   1.1648100
Vibrational harmonic frequencies (cm-1):
i439.8218      61.3688      69.6255
176.2789      218.9807      252.0365
290.9122      326.7121      334.2838
386.0170      453.3413      538.5169
585.0269      646.9364      667.5498
698.6318      884.2993      893.3266
945.4228      990.5613      1004.6837
1022.0359     1040.4726      1092.9663
1169.1974     1208.1255      1269.2900
1295.5582     1323.8404      1330.8032
1368.8227     1396.5627      1459.2000
1497.1440     1503.5260      1578.9721
1618.6420     1743.1645      2371.6318
3063.5106     3134.6076      3136.0385
3139.7590     3159.8762      3164.5874
3166.7169     3253.7691      3877.4599
Zero-point correction (Hartree): 0.147650

```

TS.CH3CHCHCH2\_H\_COO+H2O.tpdd

```

~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -422.01841723
Electronic state : 1-A
Cartesian coordinates (Angs):
C 0.628659 -0.495991 -0.772771
O 1.866142 -0.216275 -0.757261
O 2.187344 0.599510 0.371133
H 0.429119 -1.376665 -1.385354
C -0.547857 0.427128 -0.624500
C -1.798248 -0.413926 -0.543900
C -0.484258 1.562094 0.385046
H -0.548291 0.872570 -1.635684
C -2.785447 -0.243350 0.317654
H -1.874719 -1.213487 -1.275723
H -3.653217 -0.887566 0.297102
H -2.764218 0.530850 1.072237
O 0.614607 -1.142419 1.146874
H 1.349972 -0.400398 1.164750
H 1.076697 -1.983662 1.207538
H 0.397918 2.170859 0.228447
H -0.457357 1.169408 1.399384
H -1.377740 2.175837 0.272162
Rotational constants (GHz): 3.4139800 1.3498400 1.2749500
Vibrational harmonic frequencies (cm-1):
i426.5777 54.3367 82.6201

```

|           |           |           |
|-----------|-----------|-----------|
| 197.2211  | 249.9646  | 282.6864  |
| 298.2269  | 350.0839  | 361.8802  |
| 427.9333  | 450.0722  | 535.3149  |
| 565.7858  | 607.3934  | 661.2999  |
| 723.7592  | 845.0395  | 888.8953  |
| 936.0130  | 983.8430  | 999.1468  |
| 1034.8525 | 1046.0283 | 1068.9311 |
| 1125.2774 | 1208.8249 | 1276.7024 |
| 1285.3707 | 1336.3674 | 1356.5336 |
| 1403.8456 | 1419.2452 | 1454.6337 |
| 1496.2867 | 1513.1613 | 1585.2019 |
| 1617.6266 | 1743.6091 | 2402.5553 |
| 2957.2826 | 3082.6007 | 3128.9116 |
| 3150.3953 | 3152.4907 | 3180.1003 |
| 3202.6505 | 3261.3466 | 3884.5404 |

Zero-point correction (Hartree): 0.147800

TS.CH3CHCHCH2\_H\_COO+H2O.tpd

~~~~~  
E(RM062X/Aug-CC-pVT2) (Hartree): -422.01989961  
Electronic state : 1-A  
Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.689530  | -0.359821 | -0.860780 |
| O | 1.905364  | -0.075095 | -0.656370 |
| O | 2.089877  | 0.483258  | 0.647700  |
| H | 0.573524  | -1.102429 | -1.650391 |
| C | -0.521660 | 0.506273  | -0.638820 |
| C | -1.736034 | -0.381806 | -0.530734 |
| C | -0.444622 | 1.615564  | 0.396226  |
| H | -0.588569 | 0.982489  | -1.632380 |
| C | -2.709347 | -0.241408 | 0.355091  |
| H | -1.790917 | -1.195576 | -1.248143 |
| H | -3.551686 | -0.918937 | 0.362383  |
| H | -2.707368 | 0.551046  | 1.091718  |
| O | 0.589383  | -1.494690 | 0.808136  |
| H | 1.246158  | -0.758061 | 1.110716  |
| H | -0.236223 | -1.373026 | 1.286785  |
| H | 0.440296  | 2.222739  | 0.242897  |
| H | -0.393450 | 1.213949  | 1.406402  |
| H | -1.335949 | 2.237211  | 0.308383  |

Rotational constants (GHz): 3.2670100 1.4270400 1.2854600  
Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i395.9081 | 72.0705   | 113.3676  |
| 208.0285  | 256.1917  | 292.4884  |
| 312.9494  | 331.1937  | 350.2210  |
| 434.2155  | 445.5864  | 525.9983  |
| 607.5174  | 620.1678  | 685.2900  |
| 728.0288  | 830.4080  | 882.8915  |
| 936.5602  | 988.5901  | 1015.7153 |
| 1038.7807 | 1042.7227 | 1072.3084 |
| 1114.6168 | 1159.3600 | 1213.2858 |
| 1276.6025 | 1335.6988 | 1361.9181 |
| 1402.6598 | 1423.3545 | 1454.0532 |
| 1489.8047 | 1502.3198 | 1568.2482 |
| 1656.5608 | 1735.7951 | 2588.5925 |
| 2963.0240 | 3077.4644 | 3140.4169 |
| 3147.0379 | 3157.0990 | 3176.6724 |
| 3192.3692 | 3258.3303 | 3875.7462 |

Zero-point correction (Hartree): 0.148223

TS.CH3CHCHCH2\_H\_COO+H2O.tpd

~~~~~  
E(RM062X/Aug-CC-pVT2) (Hartree): -422.02311449  
Electronic state : 1-A  
Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.536295 | 0.033913  | 0.698273  |
| O | -1.661956 | -0.556577 | 0.709568  |
| O | -2.193117 | -0.551453 | -0.621115 |
| H | -0.208434 | 0.339883  | 1.690933  |
| C | 0.527585  | -0.220629 | -0.334774 |
| C | 1.656513  | 0.755265  | -0.154500 |
| C | 0.922815  | -1.691077 | -0.168588 |
| H | 0.078122  | -0.101601 | -1.318831 |
| C | 2.915950  | 0.441720  | 0.105191  |
| H | 1.391842  | 1.804828  | -0.242081 |
| H | 3.667237  | 1.210817  | 0.217819  |
| H | 3.244981  | -0.583825 | 0.208415  |
| O | -1.324687 | 1.672680  | -0.057159 |
| H | -1.891281 | 0.921753  | -0.538886 |
| H | -0.822144 | 2.130792  | -0.736387 |
| H | 0.053188  | -2.319364 | -0.347386 |
| H | 1.307478  | -1.891393 | 0.832367  |
| H | 1.697684  | -1.944239 | -0.889945 |

Rotational constants (GHz): 3.3351200 1.3839000 1.1038800  
Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i471.9270 | 78.8341   | 90.2676   |
| 168.8179  | 237.1830  | 286.2186  |
| 316.8616  | 330.0227  | 350.4706  |
| 379.1932  | 494.8800  | 543.7174  |
| 618.7148  | 646.1860  | 665.0629  |
| 701.1911  | 880.4390  | 893.6699  |
| 940.0088  | 991.9051  | 1005.2062 |
| 1038.7580 | 1044.7662 | 1090.4887 |
| 1164.0730 | 1170.8617 | 1201.8900 |
| 1274.9252 | 1342.9431 | 1351.2910 |
| 1363.6256 | 1398.4973 | 1457.4727 |
| 1501.6365 | 1507.5223 | 1548.7490 |
| 1677.9254 | 1737.5484 | 2279.6218 |
| 3066.9626 | 3116.2050 | 3142.0890 |
| 3154.1754 | 3157.9291 | 3163.7736 |
| 3176.6387 | 3257.4805 | 3889.6515 |

Zero-point correction (Hartree): 0.147845

```

TS.CH3CHCHCH2_H_COO+H2O.tpuu
~~~~~
E (CCSD(T)/Aug-CC-pVTZ) (Hartree): -421.42569390
E (CCSD/Aug-CC-pVTZ) (Hartree): -421.34836297
Tl diagnostic: 0.020154
E (MP2/Aug-CC-pVTZ) (Hartree): -421.30624748
E (MP3/Aug-CC-pVTZ) (Hartree): -421.33592273
E (RHF/Aug-CC-pVTZ) (Hartree): -419.69830230
E (RM062X/Aug-CC-pVTZ) (Hartree): -422.02620528
Electronic state : 1-A
Cartesian coordinates (Angs):
C -0.524467 0.013991 0.695253
O -1.661447 -0.556154 0.713816
O -2.200710 -0.546599 -0.611897
H -0.183581 0.312141 1.687143
C 0.528973 -0.235574 -0.344607
C 1.640175 0.764409 -0.190542
C 0.944897 -1.698423 -0.158531
H 0.069499 -0.126329 -1.324313
C 2.893840 0.477363 0.123744
H 1.348379 1.794594 -0.359475
H 3.636184 1.258685 0.209954
H 3.229641 -0.537039 0.295607
O -1.207989 1.663455 -0.189542
H -1.808866 0.903801 -0.613345
H -1.775825 2.151538 0.414892
H 0.087349 -2.345133 -0.331053
H 1.331838 -1.882806 0.844815
H 1.726050 -1.945663 -0.875143
Rotational constants (GHz): 3.3161000 1.3972900 1.1124300
Vibrational harmonic frequencies (cm-1):
i459.8067 73.2915 97.4121
174.4373 238.9474 286.7400
316.1822 335.0964 343.0065
360.8604 517.9661 544.7731
594.4936 636.2096 663.2001
687.6747 880.8104 891.5185
938.9326 987.9202 1002.1333
1041.3539 1059.2664 1091.1962
1168.3118 1178.3043 1269.6066
1303.6612 1330.6688 1344.0994
1363.8811 1397.5747 1455.7472
1502.2453 1505.8692 1579.0168
1617.3402 1736.2794 2259.8030
3065.5876 3125.6955 3139.4737
3144.9063 3161.5122 3171.8804
3190.1414 3254.9245 3877.4024
Zero-point correction (Hartree): 0.147870

#####
E- (CH (CH3) -CH=CH2) CHOO
#####

Population analysis as 298K (%)
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)
Compound Qtot Erel Erel2 n*Q*MB %
-----
TS_H_CH3CHCHCH2_COO+H2O.cmuu 1.814e+41 0.17 0.17 1.369e+41 11.7
TS_H_CH3CHCHCH2_COO+H2O.mmud 1.354e+41 0.12 0.12 1.113e+41 9.47
TS_H_CH3CHCHCH2_COO+H2O.mmdd 1.831e+41 0.33 0.33 1.053e+41 8.96
TS_H_CH3CHCHCH2_COO+H2O.cpdd 1.021e+41 0.00 0.00 1.021e+41 8.69
TS_H_CH3CHCHCH2_COO+H2O.mmuu 1.739e+41 0.33 0.33 9.982e+40 8.5
TS_H_CH3CHCHCH2_COO+H2O.mmdu 1.593e+41 0.56 0.56 6.154e+40 5.24
TS_H_CH3CHCHCH2_COO+H2O.pmd 2.048e+41 0.94 0.94 4.221e+40 3.59
TS_H_CH3CHCHCH2_COO+H2O.cmdd 2.070e+41 0.94 0.94 4.212e+40 3.59
TS_H_CH3CHCHCH2_COO+H2O.ppuu 1.312e+41 0.68 0.68 4.196e+40 3.57
TS_H_CH3CHCHCH2_COO+H2O.pmuu 2.676e+41 1.16 1.16 3.766e+40 3.21
TS_H_CH3CHCHCH2_COO+H2O.cmd 1.570e+41 0.87 0.87 3.612e+40 3.08
TS_H_CH3CHCHCH2_COO+H2O.mpuu 1.051e+41 0.67 0.67 3.366e+40 2.87
TS_H_CH3CHCHCH2_COO+H2O.mcd 1.188e+41 0.80 0.80 3.088e+40 2.63
TS_H_CH3CHCHCH2_COO+H2O.mpdd 1.175e+41 0.87 0.87 2.697e+40 2.3
TS_H_CH3CHCHCH2_COO+H2O.ppdd 1.277e+41 1.00 1.00 2.377e+40 2.02
TS_H_CH3CHCHCH2_COO+H2O.pmd 2.455e+41 1.39 1.39 2.357e+40 2.01
TS_H_CH3CHCHCH2_COO+H2O.mcd 1.200e+41 0.96 0.96 2.354e+40 2
TS_H_CH3CHCHCH2_COO+H2O.mpud 9.672e+40 0.86 0.86 2.275e+40 1.94
TS_H_CH3CHCHCH2_COO+H2O.ppud 1.198e+41 0.99 0.99 2.243e+40 1.91
TS_H_CH3CHCHCH2_COO+H2O.ppd 1.260e+41 1.07 1.07 2.059e+40 1.75
TS_H_CH3CHCHCH2_COO+H2O.pcuu 1.515e+41 1.24 1.24 1.868e+40 1.59
TS_H_CH3CHCHCH2_COO+H2O.mcuu 9.492e+40 0.98 0.98 1.802e+40 1.53
TS_H_CH3CHCHCH2_COO+H2O.pmd 2.142e+41 1.50 1.50 1.716e+40 1.46
TS_H_CH3CHCHCH2_COO+H2O.cpuu 1.208e+41 1.31 1.31 1.324e+40 1.13
TS_H_CH3CHCHCH2_COO+H2O.mpd 1.068e+41 1.24 1.24 1.319e+40 1.12
TS_H_CH3CHCHCH2_COO+H2O.pcud 1.322e+41 1.55 1.55 9.589e+39 0.816
TS_H_CH3CHCHCH2_COO+H2O.cpud 1.013e+41 1.47 1.47 8.436e+39 0.718
TS_H_CH3CHCHCH2_COO+H2O.cmud 2.368e+41 2.08 2.08 7.056e+39 0.601
TS_H_CH3CHCHCH2_COO+H2O.pcd 9.594e+40 1.57 1.57 6.779e+39 0.577
TS_H_CH3CHCHCH2_COO+H2O.cpd 1.162e+41 1.73 1.73 6.288e+39 0.535
TS_H_CH3CHCHCH2_COO+H2O.ccd 8.999e+40 1.62 1.62 5.834e+39 0.497
TS_H_CH3CHCHCH2_COO+H2O.ccuu 1.014e+41 1.94 1.94 3.853e+39 0.328
TS_H_CH3CHCHCH2_COO+H2O.ccd 8.857e+40 2.62 2.62 1.056e+39 0.0899
TS_H_CH3CHCHCH2_COO+H2O.ccd 9.856e+40 3.32 3.32 3.636e+38 0.031
Total 1.175e+42 100

TS_H_CH3CHCHCH2_COO+H2O.ccdd
~~~~~
E (RM062X/Aug-CC-pVTZ) (Hartree): -422.02716274
Electronic state : 1-A
Cartesian coordinates (Angs):
C -0.416399 0.599182 0.453438
O -1.229741 -0.281824 0.851429

```

```

O -2.521490 0.032171 0.318685
H -0.799882 1.608225 0.334359
C 1.053176 0.379278 0.588715
C 1.559679 -0.952842 0.088325
C 1.800786 1.535720 -0.080509
H 1.243972 0.426130 1.669509
C 0.870236 -2.041906 -0.216427
H 2.639381 -0.975155 -0.022540
H 1.388433 -2.921540 -0.573106
H -0.202887 -2.109447 -0.104184
O -0.886915 0.442752 -1.507905
H -1.790714 0.246904 -1.037545
H -0.542107 -0.399352 -1.823053
H 1.492720 2.494018 0.335333
H 1.598791 1.541383 -1.150521
H 2.872587 1.427449 0.072821
Rotational constants (GHz): 2.6132300 1.5578400 1.3092400
Vibrational harmonic frequencies (cm-1):
i350.6704 69.4643 113.7162
154.5619 171.8051 220.7353
308.6707 319.5873 361.3725
427.6642 467.5075 504.6739
578.7257 604.2545 636.0858
733.3127 833.8441 926.0010
984.5878 1004.6565 1018.7710
1048.5471 1066.0770 1109.9686
1131.1035 1173.6079 1241.6139
1280.4902 1333.5636 1358.1086
1386.3970 1418.4052 1454.0834
1502.2291 1507.0421 1595.9211
1610.7887 1731.0700 2518.9995
3015.6140 3074.1482 3148.6139
3156.0194 3162.5617 3171.3421
3179.8383 3263.9157 3865.4417
Zero-point correction (Hartree): 0.147957

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TS\_H\_CH3CHCHCH2\_COO+H2O.ccd

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~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -422.02482442
Electronic state : 1-A
Cartesian coordinates (Angs):
C      -0.450183      0.474166      0.550147
O      -1.177567     -0.534804      0.783856
O      -2.508184     -0.217610      0.357085
H      -0.914870      1.449305      0.668202
C       1.032916      0.375658      0.644474
C       1.651657     -0.922310      0.198391
C       1.678480      1.568012     -0.072192
H       1.221444      0.496690      1.720476
C       1.119292     -1.818666     -0.615209
H       2.661944     -1.070196      0.565457
H       1.685773     -2.694241     -0.901403
H       0.121430     -1.716861     -1.016755
O      -0.996535      0.535065     -1.380419
H      -1.889988      0.228041     -0.871546
H      -1.152821      1.415796     -1.731644
H       1.271410      2.514443      0.285470
H       1.509346      1.484687     -1.143853
H       2.751650      1.569964      0.107749
Rotational constants (GHz):   2.6984200   1.5283300   1.3140100
Vibrational harmonic frequencies (cm-1):
i460.7931      72.0482      97.0129
159.0214      178.8147      241.4817
291.6106      335.3127      348.5612
433.5632      464.8739      489.9733
624.3189      639.5708      676.4730
724.1101      831.5476      940.0724
979.0253      1000.7405     1005.0694
1040.5270      1071.8118     1104.7143
1120.4878      1155.3219     1225.2358
1280.5899      1340.9378     1363.1667
1390.3988      1408.7656     1462.2005
1496.9643      1509.3864     1548.7304
1654.1408      1741.7146     2119.2825
3009.6407      3068.2008     3142.2254
3158.2221      3160.3395     3166.9169
3184.7889      3272.0072     3891.0363
Zero-point correction (Hartree): 0.147217

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TS\_H\_CH3CHCHCH2\_COO+H2O.ccd

```

~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -422.02401775
Electronic state : 1-A
Cartesian coordinates (Angs):
C -0.370860 -0.627972 -0.275936
O -0.865777 -0.414228 0.869630
O -2.289223 -0.527779 0.758586
H -0.876930 -1.363398 -0.894745
C 1.069672 -0.349181 -0.525789
C 1.621142 0.935354 0.030946
C 1.854115 -1.564294 0.010417
H 1.182134 -0.334627 -1.613760
C 0.955500 1.931648 0.589898
H 2.699198 1.012992 -0.073410
H 1.486981 2.807691 0.935809
H -0.116606 1.916639 0.718806
O -1.507154 0.776469 -1.137764
H -2.153028 0.356957 -0.401241
H -1.862630 0.543800 -1.999660
H 1.491024 -2.498076 -0.418063
H 1.763972 -1.615973 1.093914
H 2.905712 -1.455037 -0.248482

```

Rotational constants (GHz): 2.6006400 1.5523100 1.2669400  
Vibrational harmonic frequencies (cm-1):  
i426.2724 72.0265 99.2785  
147.0196 179.8509 240.3030  
275.8955 321.1488 351.5773  
418.9121 466.1328 510.5764  
614.1645 622.6147 688.7015  
744.4952 824.1355 938.3748  
977.4055 1000.0497 1020.5319  
1043.1042 1054.2193 1081.8754  
1124.9688 1171.5029 1224.9768  
1285.4912 1340.9688 1363.0253  
1402.8933 1416.5743 1464.4841  
1499.0816 1505.7810 1556.6261  
1663.7698 1742.3819 2192.0699  
3058.2820 3070.3728 3145.0609  
3156.7640 3158.7014 3161.8432  
3185.4591 3274.8522 3894.1697  
Zero-point correction (Hartree): 0.147517

TS.H\_CH3CHCHCH2\_COO+H2O.ccuu

~~~~~  
E(RM062X/Aug-CC-pVT2) (Hartree): -422.02699353

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.397947  | -0.649504 | 0.327615  |
| O | 0.893251  | -0.478996 | -0.821898 |
| O | 2.319218  | -0.525672 | -0.708559 |
| H | 0.935290  | -1.306846 | 1.004185  |
| C | -1.046806 | -0.372315 | 0.560363  |
| C | -1.558202 | 0.957152  | 0.070817  |
| C | -1.860220 | -1.530615 | -0.051941 |
| H | -1.176549 | -0.404672 | 1.644247  |
| C | -0.993675 | 1.793570  | -0.787223 |
| H | -2.529284 | 1.212010  | 0.484373  |
| H | -1.496781 | 2.713183  | -1.053055 |
| H | -0.043377 | 1.592013  | -1.261891 |
| O | 1.485112  | 0.796856  | 1.234199  |
| H | 2.137551  | 0.445295  | 0.514265  |
| H | 1.151251  | 1.645638  | 0.925413  |
| H | -1.543253 | -2.492283 | 0.350236  |
| H | -1.734380 | -1.539457 | -1.132746 |
| H | -2.915377 | -1.392116 | 0.177244  |

Rotational constants (GHz): 2.6005100 1.5447100 1.2894900

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i327.1973 | 72.9334   | 105.8826  |
| 137.9399  | 179.5233  | 247.6809  |
| 256.7247  | 319.0565  | 343.1613  |
| 410.0128  | 450.9416  | 537.5931  |
| 579.7191  | 627.1307  | 681.5392  |
| 729.2769  | 822.0033  | 929.2501  |
| 984.9071  | 1003.4314 | 1014.8090 |
| 1048.1279 | 1051.3345 | 1101.0975 |
| 1129.1274 | 1174.6207 | 1237.0949 |
| 1294.0339 | 1341.4613 | 1366.4630 |
| 1404.6431 | 1425.1387 | 1455.8239 |
| 1498.3212 | 1505.9499 | 1600.9831 |
| 1612.6262 | 1734.4773 | 2583.5120 |
| 3070.7838 | 3078.6937 | 3146.5287 |
| 3159.2589 | 3160.4136 | 3172.5668 |
| 3178.0183 | 3262.6149 | 3865.2250 |

Zero-point correction (Hartree): 0.148292

TS.H\_CH3CHCHCH2\_COO+H2O.cmdd

~~~~~  
E(RM062X/Aug-CC-pVT2) (Hartree): -422.02730021

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.595764 | 0.117784  | 0.598736  |
| O | -1.044638 | -1.042149 | 0.360267  |
| O | -2.465175 | -0.933752 | 0.217986  |
| H | -1.219319 | 0.785635  | 1.185787  |
| C | 0.875001  | 0.362069  | 0.521066  |
| C | 1.541596  | -0.480323 | -0.525809 |
| C | 1.148795  | 1.856774  | 0.323763  |
| H | 1.251611  | 0.066468  | 1.508042  |
| C | 2.528994  | -1.325419 | -0.286303 |
| H | 1.181927  | -0.340404 | -1.541037 |
| H | 2.994518  | -1.889200 | -1.082307 |
| H | 2.902233  | -1.486259 | 0.717924  |
| O | -1.535215 | 0.987009  | -0.950020 |
| H | -2.210389 | 0.222787  | -0.627184 |
| H | -1.186277 | 0.691287  | -1.796659 |
| H | 0.611778  | 2.453986  | 1.060196  |
| H | 0.827904  | 2.174506  | -0.666162 |
| H | 2.214501  | 2.047019  | 0.426822  |

Rotational constants (GHz): 2.8184300 1.3867900 1.1064200

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i444.6064 | 43.7709   | 72.4383   |
| 163.7762  | 181.4584  | 218.7999  |
| 294.9578  | 316.2436  | 352.8068  |
| 430.1212  | 471.6874  | 492.3144  |
| 580.2027  | 595.1872  | 655.4890  |
| 745.3170  | 846.6510  | 939.3222  |
| 978.2687  | 985.7602  | 991.1186  |
| 1030.5826 | 1066.2770 | 1111.0431 |
| 1148.4931 | 1213.1635 | 1275.2444 |
| 1288.2215 | 1314.2199 | 1344.4181 |
| 1374.1072 | 1417.4370 | 1462.3728 |
| 1497.7849 | 1501.7190 | 1585.1336 |
| 1612.8088 | 1743.1504 | 2138.8776 |
| 3033.0118 | 3076.2432 | 3149.6487 |

3159.6227 3165.1007 3167.8108  
3171.5011 3254.5216 3873.9178  
Zero-point correction (Hartree): 0.147015

TS.H\_CH3CHCHCH2\_COO+H2O.cmdu

~~~~~  
E(RM062X/Aug-CC-pVTZ) (Hartree): -422.02733639

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.602974 | 0.127191  | 0.614690  |
| O | -1.065503 | -1.030071 | 0.395011  |
| O | -2.479444 | -0.903625 | 0.207564  |
| H | -1.228331 | 0.812815  | 1.179821  |
| C | 0.870248  | 0.347721  | 0.535998  |
| C | 1.506185  | -0.505019 | -0.522848 |
| C | 1.164425  | 1.836519  | 0.325194  |
| H | 1.252299  | 0.050218  | 1.520113  |
| C | 2.531261  | -1.310647 | -0.305802 |
| H | 1.077979  | -0.401321 | -1.514416 |
| H | 2.975768  | -1.884092 | -1.106971 |
| H | 2.957780  | -1.429635 | 0.683166  |
| O | -1.409777 | 0.857406  | -1.069605 |
| H | -2.139797 | 0.151106  | -0.726278 |
| H | -1.800310 | 1.732218  | -0.993312 |
| H | 0.634521  | 2.451695  | 1.053485  |
| H | 0.861416  | 2.137602  | -0.675847 |
| H | 2.231600  | 2.015123  | 0.433081  |

Rotational constants (GHz): 2.8466200 1.3880400 1.1243300

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i459.5320 | 52.6329   | 74.7585   |
| 162.8630  | 184.4039  | 237.3287  |
| 301.5491  | 320.1779  | 355.2339  |
| 422.4446  | 470.4473  | 473.5269  |
| 603.6645  | 638.1217  | 668.6774  |
| 739.6317  | 845.1236  | 941.1147  |
| 974.0676  | 980.6002  | 988.9616  |
| 1041.4311 | 1053.9550 | 1110.8159 |
| 1127.0393 | 1208.4931 | 1216.0976 |
| 1284.3529 | 1306.0870 | 1337.4514 |
| 1364.0714 | 1407.7248 | 1460.9347 |
| 1497.3939 | 1508.9157 | 1547.5027 |
| 1659.7259 | 1743.0233 | 2128.8341 |
| 3034.2522 | 3068.8555 | 3143.1331 |
| 3161.4022 | 3162.2313 | 3163.2572 |
| 3180.1370 | 3252.6916 | 3891.8730 |

Zero-point correction (Hartree): 0.146935

TS.H\_CH3CHCHCH2\_COO+H2O.cmdu

~~~~~  
E(RM062X/Aug-CC-pVTZ) (Hartree): -422.02581298

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.602043 | 0.457697  | 0.332977  |
| O | -1.132110 | 0.407231  | -0.815244 |
| O | -2.537903 | 0.196772  | -0.642917 |
| H | -1.184332 | 0.917761  | 1.126481  |
| C | 0.884343  | 0.402207  | 0.442038  |
| C | 1.508513  | -0.470186 | -0.606736 |
| C | 1.403592  | 1.850443  | 0.358801  |
| H | 1.103995  | 0.000484  | 1.432781  |
| C | 2.292739  | -1.497312 | -0.330227 |
| H | 1.295373  | -0.201817 | -1.635589 |
| H | 2.741193  | -2.090578 | -1.114633 |
| H | 2.505319  | -1.786130 | 0.692154  |
| O | -1.352604 | -1.309574 | 0.868200  |
| H | -2.123694 | -0.902702 | 0.267771  |
| H | -1.691836 | -1.358727 | 1.766189  |
| H | 0.923801  | 2.490563  | 1.099108  |
| H | 1.211473  | 2.262349  | -0.631148 |
| H | 2.476779  | 1.856272  | 0.535465  |

Rotational constants (GHz): 2.7349400 1.3758700 1.1323500

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i414.0705 | 43.9165   | 63.9237   |
| 160.0890  | 179.7552  | 231.9951  |
| 273.3398  | 327.4825  | 344.1245  |
| 396.3798  | 459.3100  | 495.9131  |
| 616.8332  | 640.0735  | 691.5395  |
| 746.8772  | 836.4898  | 938.4993  |
| 972.8565  | 981.1437  | 988.7251  |
| 1039.7528 | 1055.1601 | 1083.1995 |
| 1130.8571 | 1199.9163 | 1225.3420 |
| 1288.6449 | 1321.8268 | 1349.5967 |
| 1369.3740 | 1406.2213 | 1464.5454 |
| 1498.1669 | 1505.5581 | 1558.3250 |
| 1674.7108 | 1744.8128 | 2265.8024 |
| 3067.9236 | 3087.3197 | 3141.7453 |
| 3157.7910 | 3160.0287 | 3162.7096 |
| 3183.0878 | 3253.0220 | 3890.3562 |

Zero-point correction (Hartree): 0.147341

TS.H\_CH3CHCHCH2\_COO+H2O.cmuu

~~~~~  
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -421.42983616

E(CCSD/Aug-CC-pVTZ) (Hartree): -421.35332144

T1 diagnostic: 0.020097

E(MP2/Aug-CC-pVTZ) (Hartree): -421.31008428

E(MP3/Aug-CC-pVTZ) (Hartree): -421.34067678

E(RHF/Aug-CC-pVTZ) (Hartree): -419.70812441

E(RM062X/Aug-CC-pVTZ) (Hartree): -422.02945642

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |          |          |
|---|-----------|----------|----------|
| C | -0.598372 | 0.471895 | 0.390749 |
|---|-----------|----------|----------|

```

O -1.167373 0.497024 -0.736038
O -2.554794 0.201665 -0.544864
H -1.175861 0.792877 1.252347
C 0.893877 0.454403 0.442048
C 1.469505 -0.455695 -0.604580
C 1.392230 1.901439 0.284085
H 1.158959 0.084979 1.433681
C 2.163209 -1.547298 -0.324328
H 1.286730 -0.170325 -1.635143
H 2.570032 -2.172863 -1.106725
H 2.352028 -1.847674 0.699773
O -1.256895 -1.375286 0.887471
H -2.046609 -0.995611 0.339098
H -0.792646 -1.990571 0.309314
H 0.939426 2.559058 1.025493
H 1.145219 2.277529 -0.707763
H 2.472525 1.926918 0.409538
Rotational constants (GHz): 2.6492200 1.4574700 1.1376900
Vibrational harmonic frequencies (cm-1):
i332.4550 58.7987 70.2832
158.1353 176.2724 232.8730
255.2825 312.1118 346.4520
396.2094 452.4983 512.5323
569.5081 637.7775 654.2220
758.3556 838.2212 929.9396
979.0023 988.2790 990.9188
1045.4097 1058.6207 1085.7107
1137.5163 1219.4756 1237.4377
1299.1458 1320.1310 1347.5377
1372.9245 1408.3455 1463.3239
1499.6788 1504.8190 1593.9995
1619.9047 1735.8915 2577.5258
3070.6009 3093.3116 3145.5764
3158.2129 3159.6188 3174.3527
3179.9198 3250.2283 3858.5585
Zero-point correction (Hartree): 0.147934

TS_H_CH3CHCHCH2_COO+H2O.cpdd
~~~~~
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -421.42938522
E(CCSD/Aug-CC-pVTZ) (Hartree): -421.35267391
T1 diagnostic: 0.020110
E(MP2/Aug-CC-pVTZ) (Hartree): -421.30939414
E(MP3/Aug-CC-pVTZ) (Hartree): -421.34018452
E(RHF/Aug-CC-pVTZ) (Hartree): -419.70582470
E(RM062X/Aug-CC-pVTZ) (Hartree): -422.02982271
Electronic state : 1-A
Cartesian coordinates (Angs):
C      -0.681266      0.518179      0.415789
O      -1.423848      -0.428747      0.797605
O      -2.681877      -0.308437      0.123000
H      -1.157437      1.464382      0.175812
C       0.785794      0.460859      0.709864
C       1.312123      -0.930374      0.465450
C       1.510176      1.571504      -0.039443
H       0.851518      0.659650      1.788265
C       2.301908      -1.231463      -0.359968
H       0.808465      -1.718434      1.012935
H       2.621988      -2.256361      -0.486694
H       2.830661      -0.478061      -0.928879
O      -0.909049      0.142248      -1.561677
H      -1.833547      -0.116440      -1.169348
H      -0.444241      -0.682705      -1.740213
H       1.088274      2.542047      0.217395
H       1.414477      1.433483      -1.115215
H       2.565625      1.579696      0.224365
Rotational constants (GHz):      3.0794800      1.3008200      1.2409700
Vibrational harmonic frequencies (cm-1):
i350.9042      58.5129      89.0514
176.4550      192.9917      265.8470
297.7097      320.3559      361.3251
424.1122      488.2340      513.8815
565.7404      581.7480      630.4967
751.5871      832.1746      928.4560
977.1604      990.5930      1017.9889
1026.3124      1054.1909      1107.6489
1154.6579      1181.2285      1245.2743
1301.6082      1328.1960      1340.3045
1373.6568      1415.3685      1455.5993
1503.0815      1512.1289      1588.2477
1615.7327      1734.4655      2523.1390
3016.3475      3078.2455      3149.7392
3160.2813      3172.2243      3172.9139
3189.4965      3256.8187      3858.5246
Zero-point correction (Hartree): 0.148035

TS_H_CH3CHCHCH2_COO+H2O.cpdu
~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -422.02657809
Electronic state : 1-A
Cartesian coordinates (Angs):
C -0.678558 0.223161 0.597208
O -1.328286 -0.853975 0.461315
O -2.651688 -0.516558 0.027267
H -1.228017 1.090848 0.952007
C 0.804038 0.171198 0.770364
C 1.411683 -1.014235 0.070641
C 1.420727 1.519952 0.418550
H 0.918722 0.018093 1.854177
C 2.459367 -0.962019 -0.734110
H 0.931264 -1.965086 0.266451
H 2.844008 -1.860263 -1.196156

```



```

H 2.965965 -0.035512 -0.969119
O -1.071488 0.808725 -1.273648
H -1.963679 0.311514 -0.988712
H -1.287547 1.739954 -1.374060
H 0.905198 2.326958 0.938975
H 1.354958 1.695846 -0.653458
H 2.467295 1.543768 0.714513
Rotational constants (GHz): 3.1250100 1.3024400 1.1805300
Vibrational harmonic frequencies (cm-1):
i424.5902 51.6045 80.9622
176.7243 194.1048 276.6895
297.1534 340.1073 368.4633
432.7650 471.2781 513.0527
579.0955 625.3277 656.8290
753.0632 825.4455 941.3691
975.8744 984.0401 1012.7064
1025.3212 1044.6939 1107.6644
1145.4529 1180.4153 1207.0568
1299.5045 1336.3279 1344.9339
1366.4105 1408.4761 1456.3792
1500.0844 1514.9431 1553.8823
1673.2074 1740.8811 2240.7991
2996.6625 3074.8059 3145.0542
3160.2740 3161.6408 3176.5951
3196.6404 3260.0510 3889.1990
Zero-point correction (Hartree): 0.147543

```

TS.H\_CH3CHCHCH2\_COO+H2O.cpub

```

~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -422.02695796
Electronic state : 1-A
Cartesian coordinates (Angs):
C      -0.614030      0.537762      0.208465
O      -0.975229      0.186062      -0.952730
O      -2.405999      0.202981      -0.985517
H      -1.216722      1.291070      0.707672
C      0.803222      0.321048      0.619057
C      1.340010      -0.970647      0.067639
C      1.606550      1.571029      0.246267
H      0.767125      0.243712      1.710258
C      2.485189      -1.107570      -0.578855
H      0.705832      -1.832296      0.243051
H      2.807034      -2.076986      -0.932267
H      3.138767      -0.270254      -0.785342
O      -1.724283      -0.878648      1.075779
H      -2.320744      -0.575635      0.239750
H      -2.190747      -0.610937      1.872183
H      1.145484      2.468502      0.656953
H      1.667616      1.675681      -0.835998
H      2.614802      1.494242      0.648047
Rotational constants (GHz):      3.0882900      1.2513700      1.1713000
Vibrational harmonic frequencies (cm-1):
i453.0710      60.0879      98.8791
143.9505      209.5557      274.5529
285.6683      316.2879      348.7871
439.5617      498.4670      538.8876
573.3033      634.9379      693.4960
759.0377      817.9991      939.9001
971.5872      984.2848      1010.7260
1041.0810      1056.0576      1084.9507
1146.7779      1169.4633      1215.0745
1302.2756      1334.1449      1357.5012
1367.7777      1406.1893      1456.4211
1500.2894      1512.1202      1550.0823
1661.2595      1742.0613      2148.5335
3053.4647      3073.3632      3145.5384
3157.0651      3163.5779      3172.7041
3186.9399      3256.3864      3891.1480
Zero-point correction (Hartree): 0.147516

```

TS.H\_CH3CHCHCH2\_COO+H2O.cpuu

```

~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -422.02724798
Electronic state : 1-A
Cartesian coordinates (Angs):
C -0.612737 0.529857 0.137652
O -0.973584 0.028445 -0.968611
O -2.402303 0.088150 -1.022671
H -1.198258 1.356525 0.528104
C 0.798906 0.355382 0.589029
C 1.374713 -0.957030 0.136635
C 1.593361 1.590036 0.151220
H 0.736719 0.354794 1.681990
C 2.526182 -1.116271 -0.493141
H 0.773426 -1.830340 0.367024
H 2.872860 -2.101289 -0.771744
H 3.160466 -0.280896 -0.758054
O -1.850180 -0.575840 1.251641
H -2.393773 -0.416102 0.344992
H -1.605187 -1.506200 1.258644
H 1.112002 2.503217 0.497943
H 1.672556 1.629020 -0.934340
H 2.595181 1.553387 0.574210
Rotational constants (GHz): 3.1127900 1.2149300 1.1634900
Vibrational harmonic frequencies (cm-1):
i440.6751 58.9483 87.0118
145.2089 199.3429 273.4896
284.0679 315.5052 350.3783
433.9771 511.0253 544.5913
568.2732 593.3222 650.4300
759.4901 821.2101 940.1158
976.7457 983.5505 1010.6810

```

|           |           |           |
|-----------|-----------|-----------|
| 1031.0885 | 1048.5268 | 1109.7114 |
| 1156.3405 | 1178.7396 | 1278.8059 |
| 1303.5409 | 1341.3477 | 1364.6066 |
| 1379.8168 | 1408.4727 | 1457.4754 |
| 1501.2683 | 1513.1417 | 1588.0001 |
| 1608.5744 | 1742.1113 | 2148.4854 |
| 3054.6610 | 3074.0819 | 3148.2713 |
| 3155.8703 | 3169.0090 | 3176.3124 |
| 3181.0872 | 3260.8582 | 3878.0125 |

Zero-point correction (Hartree): 0.147547

TS\_H\_CH3CHCHCH2\_COO+H2O.mcdd

~~~~~  
E(RM062X/Aug-CC-pVT2) (Hartree): -422.02814280

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.354367 | -0.203490 | 0.344918  |
| O | -0.850775 | -0.605336 | -0.750285 |
| O | -2.115841 | -1.208256 | -0.459018 |
| H | -0.544779 | -0.799829 | 1.231265  |
| C | 0.820304  | 0.711774  | 0.313524  |
| C | 2.096370  | -0.089157 | 0.438790  |
| C | 0.842369  | 1.611654  | -0.921400 |
| H | 0.722204  | 1.325838  | 1.212642  |
| C | 2.233588  | -1.373311 | 0.147900  |
| H | 2.955897  | 0.483119  | 0.770070  |
| H | 3.192940  | -1.862287 | 0.242846  |
| H | 1.407138  | -1.980098 | -0.202597 |
| O | -1.983522 | 0.795581  | 0.924702  |
| H | -2.376621 | -0.038935 | 0.393612  |
| H | -2.141461 | 1.564948  | 0.368718  |
| H | -0.058593 | 2.221822  | -0.976966 |
| H | 0.909781  | 1.010341  | -1.825382 |
| H | 1.705015  | 2.274351  | -0.879788 |

Rotational constants (GHz): 2.9068800 1.3927300 1.1584700

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i425.6903 | 63.6235   | 98.4011   |
| 133.0321  | 202.4900  | 234.7821  |
| 255.5427  | 328.2624  | 343.5295  |
| 429.3113  | 473.6346  | 542.5260  |
| 585.3252  | 647.4237  | 673.0543  |
| 705.5456  | 840.0914  | 935.0938  |
| 960.7298  | 995.1198  | 1024.1054 |
| 1040.8075 | 1069.4185 | 1122.1512 |
| 1140.5380 | 1175.6791 | 1280.2444 |
| 1311.3468 | 1325.8578 | 1358.0925 |
| 1400.8110 | 1414.6348 | 1462.9601 |
| 1495.5817 | 1502.0683 | 1589.1539 |
| 1611.7782 | 1728.2775 | 2195.2947 |
| 3070.2256 | 3074.4633 | 3146.4781 |
| 3161.4342 | 3163.5806 | 3178.3695 |
| 3182.9310 | 3252.7588 | 3873.9850 |

Zero-point correction (Hartree): 0.147627

TS\_H\_CH3CHCHCH2\_COO+H2O.mcdv

~~~~~  
E(RM062X/Aug-CC-pVTZ) (Hartree): -422.02770358

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.350338 | -0.207350 | 0.355979  |
| O | -0.836083 | -0.638514 | -0.732203 |
| O | -2.110317 | -1.221848 | -0.441043 |
| H | -0.546115 | -0.789068 | 1.251566  |
| C | 0.816851  | 0.715823  | 0.306532  |
| C | 2.102535  | -0.068264 | 0.428815  |
| C | 0.803761  | 1.607240  | -0.934678 |
| H | 0.720415  | 1.341355  | 1.198014  |
| C | 2.252348  | -1.356802 | 0.163408  |
| H | 2.960494  | 0.520886  | 0.733916  |
| H | 3.219402  | -1.831376 | 0.253514  |
| H | 1.429299  | -1.980644 | -0.164225 |
| O | -1.967941 | 0.888559  | 0.745859  |
| H | -2.373487 | 0.016000  | 0.276972  |
| H | -2.255957 | 0.878781  | 1.662742  |
| H | -0.124939 | 2.173058  | -0.980462 |
| H | 0.891941  | 1.001369  | -1.833903 |
| H | 1.642737  | 2.300188  | -0.899368 |

Rotational constants (GHz): 2.9305700 1.4054800 1.1573700

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i452.8694 | 61.7389   | 96.0223   |
| 130.1147  | 205.9670  | 238.1870  |
| 261.4671  | 327.3790  | 352.6463  |
| 423.3193  | 467.7332  | 528.7870  |
| 633.7901  | 651.2581  | 692.8732  |
| 714.4483  | 834.0192  | 937.5068  |
| 961.6612  | 991.1795  | 1025.0301 |
| 1040.0366 | 1063.0505 | 1103.4274 |
| 1137.8655 | 1165.3467 | 1217.4703 |
| 1305.5238 | 1325.9675 | 1351.1805 |
| 1393.7739 | 1410.5672 | 1462.0481 |
| 1497.8183 | 1503.8538 | 1552.5107 |
| 1662.8224 | 1727.2754 | 2150.0156 |
| 3066.5656 | 3077.4021 | 3154.3752 |
| 3163.1297 | 3164.1875 | 3171.1482 |
| 3177.3414 | 3252.9911 | 3891.3704 |

Zero-point correction (Hartree): 0.147453

TS\_H\_CH3CHCHCH2\_COO+H2O.mcdv

~~~~~  
E(RM062X/CC-pVDZ) (Hartree): -421.88137154

Electronic state : 1-A

Cartesian coordinates (Angs):

```

C 0.575193 -0.128693 0.636797
O 1.633104 -0.697069 0.185167
O 2.656635 0.309964 0.138083
H 0.713059 0.612523 1.432849
C -0.743803 -0.812841 0.441553
C -1.856528 0.163426 0.761592
C -0.815864 -1.443494 -0.948982
H -0.761502 -1.609763 1.207988
C -2.433971 0.934191 -0.126675
H -2.169274 0.221470 1.808478
H -3.230670 1.620210 0.164560
H -2.139282 0.913625 -1.179915
O 0.653745 1.322144 -0.737577
H 1.713955 1.106164 -0.523294
H 0.456891 2.164288 -0.304257
H -0.045731 -2.217559 -1.055676
H -0.629853 -0.676967 -1.713039
H -1.805640 -1.889844 -1.108777
Rotational constants (GHz): 3.3391653 1.3686358 1.1931042

```

TS\_H\_CH3CHCHCH2\_COO+H2O.mcuu

~~~~~  
E(RM062X/Aug-CC-pVT2) (Hartree): -422.02762586

Electronic state : 1-A

Cartesian coordinates (Angs):

```

C 0.446971 -0.014085 0.558472
O 1.528082 -0.663059 0.431541
O 2.604364 0.276537 0.359430
H 0.479698 0.909837 1.126608
C -0.833133 -0.761599 0.395213
C -2.054882 0.117213 0.392041
C -0.809675 -1.707306 -0.808857
H -0.875824 -1.378507 1.303881
C -2.096255 1.423064 0.179323
H -2.980814 -0.422765 0.560600
H -3.043029 1.945301 0.187729
H -1.208483 2.006315 -0.024633
O 0.817799 1.216088 -1.001915
H 1.781771 1.017057 -0.595032
H 0.768627 0.751083 -1.842496
H 0.045669 -2.377227 -0.765094
H -0.765616 -1.130768 -1.732325
H -1.722110 -2.300570 -0.828835
Rotational constants (GHz): 2.9524400 1.4265200 1.1769900

```

Vibrational harmonic frequencies (cm-1):

```

i427.2363 62.3328 108.1086
175.4218 181.9483 232.4602
278.7051 312.1581 372.5573
415.3202 487.5447 529.2880
577.8878 599.2627 644.4843
701.9597 852.4795 943.4632
969.3176 998.7540 1006.6545
1044.2653 1072.7964 1099.3456
1163.8549 1169.5645 1285.8968
1295.2833 1332.9595 1348.4031
1392.8499 1407.8140 1466.8363
1498.3149 1502.2181 1587.4730
1603.6083 1735.8563 2176.7379
3009.8911 3075.3220 3147.0769
3164.8528 3166.5668 3179.1543
3181.6708 3263.8380 3881.1428

```

Zero-point correction (Hartree): 0.147406

TS\_H\_CH3CHCHCH2\_COO+H2O.mdd

~~~~~  
E(RM062X/Aug-CC-pVT2) (Hartree): -422.02865826

Electronic state : 1-A

Cartesian coordinates (Angs):

```

C -0.417161 -0.362556 0.172650
O -1.119712 -0.384233 -0.882069
O -2.373064 -0.995551 -0.557458
H -0.514788 -1.195204 0.861509
C 0.825613 0.466351 0.189970
C 1.950465 -0.424372 -0.284130
C 0.699376 1.727020 -0.658938
H 0.999700 0.716385 1.237837
C 2.922018 -0.872845 0.493449
H 1.920769 -0.690266 -1.336244
H 3.708214 -1.503932 0.102962
H 2.966534 -0.618745 1.545601
O -1.830325 0.470275 1.317170
H -2.380158 -0.139308 0.640818
H -2.006744 1.380935 1.061693
H -0.141698 2.336632 -0.330640
H 0.541329 1.470964 -1.705110
H 1.609787 2.317030 -0.577575
Rotational constants (GHz): 3.1707700 1.1640800 1.0950900

```

Vibrational harmonic frequencies (cm-1):

```

i418.4740 53.1495 73.9414
152.3801 200.4941 220.4762
267.3339 320.6687 348.6615
405.8663 462.5684 513.0189
584.1179 620.2529 659.9836
732.2889 849.6397 935.2251
966.6457 992.2389 995.7105
1044.0754 1078.4520 1113.5092
1169.5176 1194.7775 1273.9914
1286.6613 1323.9951 1357.4201
1379.9501 1416.9672 1456.3119
1495.2219 1500.1991 1584.3825
1611.3645 1732.4708 2204.8493
3075.5098 3091.1578 3148.0568

```

3158.9822 3161.8990 3172.2556  
3180.3198 3252.6370 3878.3306  
Zero-point correction (Hartree): 0.147393

TS.H\_CH3CHCHCH2\_COO+H2O.mmd

~~~~~  
E(RM062X/Aug-CC-pVTZ) (Hartree): -422.02825640

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.414985 | -0.361441 | 0.214192  |
| O | -1.099188 | -0.485160 | -0.844743 |
| O | -2.366931 | -1.044016 | -0.483186 |
| H | -0.528751 | -1.129033 | 0.973472  |
| C | 0.823433  | 0.471633  | 0.169546  |
| C | 1.951544  | -0.436842 | -0.258938 |
| C | 0.665325  | 1.678461  | -0.750066 |
| H | 1.006201  | 0.791154  | 1.196950  |
| C | 2.946168  | -0.812220 | 0.528476  |
| H | 1.906697  | -0.778569 | -1.288345 |
| H | 3.735986  | -1.456805 | 0.168496  |
| H | 3.008497  | -0.479477 | 1.557627  |
| O | -1.840702 | 0.704748  | 1.118189  |
| H | -2.394880 | -0.000613 | 0.537551  |
| H | -1.988834 | 0.490563  | 2.043283  |
| H | -0.202712 | 2.264122  | -0.453378 |
| H | 0.526275  | 1.357250  | -1.780959 |
| H | 1.557188  | 2.299281  | -0.696047 |

Rotational constants (GHz): 3.2285200 1.1746400 1.0888400

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i440.3537 | 57.1677   | 72.8096   |
| 151.8570  | 203.5079  | 237.7253  |
| 269.1226  | 333.0622  | 343.4997  |
| 408.7493  | 462.5140  | 496.1346  |
| 629.4947  | 640.6417  | 684.9253  |
| 733.2857  | 846.1713  | 937.8416  |
| 966.7901  | 988.4039  | 997.3458  |
| 1044.3692 | 1070.6839 | 1101.2907 |
| 1155.4210 | 1195.8888 | 1218.6749 |
| 1279.8320 | 1322.3192 | 1350.9402 |
| 1373.3696 | 1412.5300 | 1455.1766 |
| 1498.3393 | 1502.8826 | 1549.1011 |
| 1664.3455 | 1729.7142 | 2165.2865 |
| 3078.3923 | 3088.0146 | 3155.9224 |
| 3160.9951 | 3161.6067 | 3171.8427 |
| 3174.8526 | 3251.6539 | 3891.7661 |

Zero-point correction (Hartree): 0.147366

TS.H\_CH3CHCHCH2\_COO+H2O.mmd

~~~~~  
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -421.42872465

E(CCSD/Aug-CC-pVTZ) (Hartree): -421.35198234

T1 diagnostic: 0.019591

E(MP2/Aug-CC-pVTZ) (Hartree): -421.30961831

E(MP3/Aug-CC-pVTZ) (Hartree): -421.33956389

E(RHF/Aug-CC-pVTZ) (Hartree): -419.70457764

E(RM062X/Aug-CC-pVTZ) (Hartree): -422.02891764

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.490273 | -0.080461 | 0.545216  |
| O | -1.562134 | 0.591677  | 0.514046  |
| O | -2.656323 | -0.332373 | 0.470056  |
| H | -0.502445 | -1.018757 | 1.091800  |
| C | 0.807651  | 0.610449  | 0.279681  |
| C | 1.819395  | -0.392290 | -0.207651 |
| C | 0.641199  | 1.781381  | -0.684642 |
| H | 1.134479  | 0.969424  | 1.263342  |
| C | 2.821239  | -0.856129 | 0.521291  |
| H | 1.683259  | -0.721822 | -1.232133 |
| H | 3.526417  | -1.570505 | 0.119493  |
| H | 2.975111  | -0.532333 | 1.543908  |
| O | -0.974747 | -1.096340 | -1.112947 |
| H | -1.911601 | -0.968469 | -0.621151 |
| H | -0.757715 | -2.032051 | -1.076716 |
| H | -0.060833 | 2.514171  | -0.294207 |
| H | 0.260083  | 1.417287  | -1.638254 |
| H | 1.603613  | 2.261641  | -0.848687 |

Rotational constants (GHz): 3.2180400 1.2527000 1.1127100

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i435.4599 | 57.7891   | 72.9437   |
| 169.1127  | 198.8295  | 238.1405  |
| 297.2552  | 333.3750  | 347.0638  |
| 433.7136  | 460.0545  | 477.2290  |
| 606.0782  | 633.9110  | 684.7401  |
| 725.3000  | 858.7864  | 943.5167  |
| 972.2776  | 986.6382  | 987.8233  |
| 1043.8442 | 1053.4918 | 1119.8151 |
| 1153.4160 | 1210.1421 | 1221.7379 |
| 1275.5714 | 1322.3577 | 1334.5560 |
| 1358.4571 | 1413.3193 | 1457.7369 |
| 1499.4389 | 1501.6554 | 1549.4611 |
| 1663.3125 | 1737.0880 | 2184.8812 |
| 3033.7673 | 3077.7040 | 3153.4841 |
| 3161.1156 | 3164.5140 | 3167.7370 |
| 3180.6804 | 3250.6736 | 3889.2980 |

Zero-point correction (Hartree): 0.147315

TS.H\_CH3CHCHCH2\_COO+H2O.mmuu

~~~~~  
E(RM062X/Aug-CC-pVTZ) (Hartree): -422.02848295

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |          |           |           |
|---|----------|-----------|-----------|
| C | 0.501875 | -0.110802 | -0.529556 |
|---|----------|-----------|-----------|

```

O 1.546278 0.603959 -0.572822
O 2.676868 -0.275248 -0.534622
H 0.533540 -1.079792 -1.017947
C -0.815015 0.544942 -0.264767
C -1.822817 -0.485443 0.166136
C -0.696540 1.698339 0.729993
H -1.124883 0.935223 -1.242014
C -2.921371 -0.774335 -0.511153
H -1.602550 -0.993562 1.098834
H -3.625543 -1.512221 -0.152884
H -3.155302 -0.281779 -1.447580
O 1.078933 -1.161028 1.086572
H 1.984388 -0.974935 0.561321
H 1.115930 -0.609287 1.874214
H 0.049424 2.420966 0.407785
H -0.408894 1.321828 1.712269
H -1.658732 2.195887 0.829058
Rotational constants (GHz): 3.3143000 1.1981700 1.0934700
Vibrational harmonic frequencies (cm-1):
i421.7897 53.1519 71.3541
161.0727 190.2234 221.8039
299.7767 316.1174 342.4630
432.5051 455.3172 486.1308
578.5474 597.2190 673.5046
719.3840 860.9096 941.0764
974.3408 982.6641 989.0427
1038.7242 1056.1314 1141.9729
1157.1217 1207.4234 1274.3348
1281.8496 1327.8269 1334.9741
1372.6885 1411.7175 1459.8960
1497.1473 1500.8248 1584.7848
1620.4363 1738.4297 2202.2605
3033.1530 3073.4899 3145.0204
3161.6286 3166.3111 3179.3393
3181.7433 3251.9078 3873.9254
Zero-point correction (Hartree): 0.147219

```

```

TS_H_CH3CHCHCH2_COO+H2O.mpdd
~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -422.02793884
Electronic state : 1-A
Cartesian coordinates (Angs):
C      0.510008      0.272480      0.359229
O      1.001160      0.647180      -0.747058
O      2.334008      1.104543      -0.496948
H      0.799889      0.823101      1.248807
C      -0.758067      -0.518357      0.357142
C      -1.876860      0.435223      0.716229
C      -0.961111      -1.289948      -0.935634
H      -0.644631      -1.213195      1.195794
C      -2.953933      0.656693      -0.018138
H      -1.756840      0.960144      1.658422
H      -3.714250      1.350038      0.312835
H      -3.119555      0.159502      -0.964388
O      2.051296      -0.900351      0.851551
H      2.505456      -0.096936      0.314234
H      2.105454      -1.672103      0.279442
H      -0.112841      -1.945791      -1.125200
H      -1.053991      -0.613483      -1.783253
H      -1.860632      -1.898811      -0.870031
Rotational constants (GHz):      3.5463100      1.1566500      1.0780900
Vibrational harmonic frequencies (cm-1):
i439.3019      53.4274      87.0092
169.5540      208.8397      270.9906
278.3960      314.0361      350.3677
434.5725      513.3658      541.9967
564.2429      592.5369      642.6696
733.7757      840.1174      934.3109
961.2755      988.5813      1034.6817
1039.2180      1051.4937      1105.0952
1137.4695      1203.8037      1268.0787
1289.7565      1332.0862      1373.1846
1382.3928      1417.0422      1453.3720
1495.9616      1506.3397      1588.5960
1607.7440      1735.1472      2163.4519
3049.7308      3078.3833      3149.5748
3158.7026      3164.9296      3176.5694
3181.2929      3261.9389      3876.4438
Zero-point correction (Hartree): 0.147540

```

```

TS_H_CH3CHCHCH2_COO+H2O.mpdu
~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -422.02730395
Electronic state : 1-A
Cartesian coordinates (Angs):
C 0.509349 0.265509 0.388368
O 0.981376 0.708230 -0.700162
O 2.325600 1.132089 -0.451614
H 0.817214 0.766672 1.301646
C -0.756981 -0.526165 0.354879
C -1.884610 0.413926 0.720915
C -0.928946 -1.272145 -0.957156
H -0.651564 -1.243614 1.175173
C -2.955869 0.640126 -0.020543
H -1.779898 0.923909 1.673468
H -3.725571 1.321364 0.314005
H -3.105791 0.157324 -0.976774
O 2.018235 -1.017156 0.620124
H 2.490031 -0.162285 0.176089
H 2.359002 -1.098858 1.514987
H -0.059452 -1.900751 -1.137830
H -1.025276 -0.578073 -1.790092

```

```

H -1.818042 -1.898506 -0.916231
Rotational constants (GHz): 3.5722900 1.1730500 1.0784700
Vibrational harmonic frequencies (cm-1):
i464.0542 54.4648 88.2618
168.5480 215.0217 273.6266
288.2599 316.5782 352.6839
438.8747 496.2646 540.1597
570.8557 633.1690 685.3088
737.3825 836.1769 936.2699
962.6569 989.4836 1031.9904
1039.0425 1051.0544 1103.6379
1109.0127 1195.1536 1217.2159
1282.9118 1331.6022 1363.7293
1375.5591 1413.9884 1452.9244
1501.6949 1505.9540 1548.0186
1659.5013 1735.3293 2128.2320
3050.6690 3080.3070 3156.6532
3160.4987 3160.5656 3166.6580
3180.6686 3262.2290 3891.7196
Zero-point correction (Hartree): 0.147490

```

```

TS_H_CH3CHCHCH2_COO+H2O.mpud
~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -422.02803809
Electronic state : 1-A
Cartesian coordinates (Angs):
C      0.626847      -0.057580      0.606177
O      1.637651      -0.708376      0.215619
O      2.744391      0.200652      0.147701
H      0.802131      0.745195      1.317225
C      -0.729184      -0.671214      0.477994
C      -1.769533      0.390292      0.726994
C      -0.880833      -1.443085      -0.824310
H      -0.777227      -1.373250      1.323332
C      -2.759760      0.699610      -0.092426
H      -1.674254      0.923034      1.668985
H      -3.471674      1.471095      0.165696
H      -2.897083      0.199477      -1.041652
O      0.797589      1.277493      -0.875945
H      1.801260      1.077998      -0.632356
H      0.602223      2.185166      -0.628673
H      -0.114674      -2.210114      -0.901942
H      -0.774274      -0.766003      -1.670459
H      -1.858696      -1.918891      -0.865737
Rotational constants (GHz):      3.5748700      1.2564400      1.1263100
Vibrational harmonic frequencies (cm-1):
i401.3314      65.7543      81.9105
174.4936      188.9276      267.1300
303.8957      335.6499      361.7422
413.1502      465.6340      528.2111
576.7173      609.3184      661.1579
721.5807      851.4667      939.4464
964.7895      989.5443      1011.0346
1042.2618      1046.4974      1095.6042
1136.3235      1196.0962      1206.1314
1283.8241      1328.9390      1354.7274
1368.8451      1410.2940      1453.4817
1501.5768      1508.9403      1556.0198
1655.0328      1741.3232      2340.2682
3002.4237      3081.7753      3152.0913
3157.6977      3160.9440      3166.8351
3179.0265      3260.6006      3897.0081
Zero-point correction (Hartree): 0.147616

```

```

TS_H_CH3CHCHCH2_COO+H2O.mpuu
~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -422.02832993
Electronic state : 1-A
Cartesian coordinates (Angs):
C 0.653092 -0.080366 0.604922
O 1.592840 -0.742068 0.074184
O 2.751339 0.098476 0.024416
H 0.914603 0.630278 1.383151
C -0.740041 -0.616462 0.528834
C -1.712015 0.534820 0.596830
C -0.941784 -1.569221 -0.638080
H -0.844801 -1.174913 1.471132
C -2.770721 0.683879 -0.180721
H -1.496966 1.281252 1.354456
H -3.425796 1.535263 -0.061936
H -3.023411 -0.026278 -0.956610
O 0.849073 1.514999 -0.584249
H 1.838239 1.159185 -0.503668
H 0.541868 1.326418 -1.476191
H -0.206116 -2.368779 -0.613395
H -0.838630 -1.040971 -1.586311
H -1.936190 -2.008615 -0.596153
Rotational constants (GHz): 3.5078600 1.2935200 1.0889800
Vibrational harmonic frequencies (cm-1):
i401.2339 51.6262 98.6009
169.7643 191.7948 259.1002
312.0117 324.8839 368.6967
446.2306 471.5069 527.5525
562.4156 583.8815 625.2620
732.6649 847.4868 939.6353
963.7660 978.7885 1023.4646
1034.2279 1048.2758 1106.0945
1148.6976 1200.5486 1269.7981
1289.1120 1329.4904 1366.6474
1372.5016 1414.6824 1455.2705
1496.6260 1508.1571 1582.6910
1594.3148 1738.6633 2306.6822

```

|           |           |           |
|-----------|-----------|-----------|
| 2999.1168 | 3076.7558 | 3147.9182 |
| 3167.7940 | 3168.3602 | 3172.5316 |
| 3180.9462 | 3260.9435 | 3880.4620 |

Zero-point correction (Hartree): 0.147617

TS\_H\_CH3CHCHCH2\_COO+H2O.pcd

~~~~~  
 E(RM062X/Aug-CC-pVT2) (Hartree): -422.02694999  
 Electronic state : 1-A  
 Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.423370 | -0.208725 | 0.227324  |
| O | -1.451909 | -0.841551 | -0.155977 |
| O | -2.605823 | -0.192490 | 0.383540  |
| H | -0.448336 | 0.245555  | 1.213380  |
| C | 0.872064  | -0.562094 | -0.416630 |
| C | 1.980542  | 0.421170  | -0.156762 |
| C | 1.266582  | -1.957539 | 0.111569  |
| H | 0.696240  | -0.646426 | -1.491894 |
| C | 1.890365  | 1.602736  | 0.432837  |
| H | 2.951674  | 0.071973  | -0.493502 |
| H | 2.776742  | 2.204864  | 0.577728  |
| H | 0.949750  | 2.018074  | 0.766726  |
| O | -1.121229 | 1.594366  | -0.363169 |
| H | -1.995788 | 1.070996  | -0.073845 |
| H | -1.132491 | 1.661062  | -1.322786 |
| H | 0.507750  | -2.695415 | -0.137658 |
| H | 1.396008  | -1.931831 | 1.193455  |
| H | 2.213043  | -2.254741 | -0.336786 |

Rotational constants (GHz): 2.7504200 1.5236300 1.0561900  
 Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i399.7364 | 63.2082   | 113.8646  |
| 161.4291  | 194.1196  | 246.3065  |
| 283.5432  | 291.3135  | 378.7204  |
| 420.9970  | 496.2023  | 530.5221  |
| 562.1815  | 585.1274  | 625.8059  |
| 688.9674  | 868.0495  | 940.7324  |
| 964.3548  | 1000.4891 | 1036.2805 |
| 1052.1479 | 1064.0897 | 1094.2790 |
| 1137.9576 | 1206.6248 | 1284.4835 |
| 1303.2044 | 1323.0882 | 1346.1674 |
| 1394.1370 | 1406.0395 | 1466.4115 |
| 1499.5836 | 1503.0971 | 1592.1147 |
| 1600.6821 | 1735.9067 | 2238.1651 |
| 3068.6213 | 3073.1963 | 3146.4122 |
| 3161.4253 | 3163.7944 | 3176.1941 |
| 3181.7916 | 3265.6713 | 3879.1398 |

Zero-point correction (Hartree): 0.147663

TS\_H\_CH3CHCHCH2\_COO+H2O.pcd

~~~~~  
 E(RM062X/CC-pVDZ) (Hartree): -421.88052339  
 Electronic state : 1-A  
 Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.522054 | -0.265661 | 0.310829  |
| O | -1.555461 | -0.711665 | -0.306768 |
| O | -2.684789 | 0.024847  | 0.186665  |
| H | -0.642180 | -0.027356 | 1.375506  |
| C | 0.822357  | -0.583419 | -0.262701 |
| C | 1.874016  | 0.304888  | 0.353883  |
| C | 1.114320  | -2.074319 | -0.037324 |
| H | 0.746750  | -0.377589 | -1.340038 |
| C | 2.250678  | 1.449430  | -0.168015 |
| H | 2.322094  | -0.047229 | 1.290027  |
| H | 3.017071  | 2.062569  | 0.308364  |
| H | 1.799295  | 1.818853  | -1.094262 |
| O | -0.927262 | 1.632289  | -0.172484 |
| H | -1.923597 | 1.174749  | -0.054818 |
| H | -0.794029 | 2.178509  | 0.614837  |
| H | 0.343573  | -2.697598 | -0.508806 |
| H | 1.142363  | -2.308118 | 1.037903  |
| H | 2.092851  | -2.326077 | -0.468047 |

Rotational constants (GHz): 2.7973200 1.4839356 1.0288810

TS\_H\_CH3CHCHCH2\_COO+H2O.pcd

~~~~~  
 E(RM062X/Aug-CC-pVT2) (Hartree): -422.02670563  
 Electronic state : 1-A  
 Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.346781  | -0.099890 | 0.164531  |
| O | 0.947948  | -0.988807 | -0.508462 |
| O | 2.201790  | -1.251795 | 0.129851  |
| H | 0.472566  | -0.116837 | 1.244082  |
| C | -0.856608 | 0.546095  | -0.425695 |
| C | -2.075973 | -0.292288 | -0.102936 |
| C | -1.024474 | 1.965685  | 0.120124  |
| H | -0.719225 | 0.582642  | -1.508351 |
| C | -2.084438 | -1.549631 | 0.311543  |
| H | -3.016464 | 0.233215  | -0.232926 |
| H | -3.019518 | -2.051563 | 0.517215  |
| H | -1.178708 | -2.127712 | 0.444907  |
| O | 1.899598  | 1.152631  | 0.050454  |
| H | 2.365647  | 0.192301  | 0.126153  |
| H | 2.096307  | 1.629173  | 0.861726  |
| H | -0.192048 | 2.595464  | -0.181215 |
| H | -1.086107 | 1.951288  | 1.209464  |
| H | -1.948864 | 2.395972  | -0.261196 |

Rotational constants (GHz): 2.7326100 1.5463300 1.0493500  
 Vibrational harmonic frequencies (cm-1):

|           |          |          |
|-----------|----------|----------|
| i442.5091 | 57.3064  | 86.5611  |
| 140.9694  | 198.2266 | 246.3123 |
| 274.0661  | 340.3889 | 370.0710 |
| 438.8800  | 468.3468 | 509.4727 |

|           |           |           |
|-----------|-----------|-----------|
| 575.3907  | 630.4948  | 655.3866  |
| 714.3348  | 860.6150  | 936.6075  |
| 959.5745  | 994.7336  | 1034.3936 |
| 1051.4892 | 1069.6218 | 1116.1425 |
| 1128.8936 | 1195.0754 | 1230.7243 |
| 1301.1956 | 1316.4318 | 1338.0424 |
| 1372.4106 | 1410.8176 | 1459.8047 |
| 1498.0849 | 1510.0097 | 1560.1886 |
| 1663.8954 | 1725.6954 | 2149.0404 |
| 3067.7799 | 3083.7147 | 3139.8540 |
| 3161.0997 | 3164.7882 | 3171.1607 |
| 3175.0268 | 3256.2832 | 3889.1174 |

Zero-point correction (Hartree): 0.147394

TS\_H\_CH3CHCHCH2\_COO+H2O.pcuu

~~~~~

E(RM062X/Aug-CC-pVTZ) (Hartree): -422.02726822

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.350492  | -0.084957 | 0.171626  |
| O | 0.945079  | -0.984251 | -0.494973 |
| O | 2.196254  | -1.250634 | 0.147424  |
| H | 0.487938  | -0.079871 | 1.249400  |
| C | -0.856856 | 0.557907  | -0.415601 |
| C | -2.068129 | -0.304344 | -0.122371 |
| C | -1.055199 | 1.959804  | 0.165857  |
| H | -0.718747 | 0.617940  | -1.497923 |
| C | -2.066197 | -1.567298 | 0.274020  |
| H | -3.012994 | 0.212533  | -0.255218 |
| H | -2.998371 | -2.081625 | 0.461498  |
| H | -1.155971 | -2.136707 | 0.412148  |
| O | 1.915761  | 1.169668  | 0.187163  |
| H | 2.362899  | 0.203620  | 0.227783  |
| H | 2.092346  | 1.505431  | -0.697559 |
| H | -0.217220 | 2.609582  | -0.070735 |
| H | -1.153677 | 1.909058  | 1.250425  |
| H | -1.967627 | 2.395098  | -0.237919 |

Rotational constants (GHz): 2.7206200 1.5462600 1.0475800

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i418.7391 | 54.5541   | 85.3956   |
| 140.5215  | 193.7791  | 228.9389  |
| 270.3577  | 333.7103  | 364.9795  |
| 443.3484  | 476.2285  | 513.2425  |
| 576.8163  | 602.4969  | 640.5403  |
| 694.9261  | 861.0932  | 933.8253  |
| 959.9740  | 995.7365  | 1033.1838 |
| 1053.5569 | 1070.1302 | 1128.7294 |
| 1137.8401 | 1209.8646 | 1278.3973 |
| 1302.7641 | 1316.2551 | 1341.6778 |
| 1385.0333 | 1419.1455 | 1460.0865 |
| 1496.5016 | 1502.9178 | 1595.0326 |
| 1615.4577 | 1726.0884 | 2182.0482 |
| 3070.8253 | 3076.0692 | 3145.1956 |
| 3165.2227 | 3169.4976 | 3170.3451 |
| 3176.3272 | 3257.6021 | 3869.3420 |

Zero-point correction (Hartree): 0.147456

TS\_H\_CH3CHCHCH2\_COO+H2O.p added

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E(RM062X/Aug-CC-pVTZ) (Hartree): -422.02780843

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.610795  | 0.322708  | 0.228979  |
| O | 1.549573  | 0.591269  | -0.576225 |
| O | 2.763558  | 0.056131  | -0.039850 |
| H | 0.840388  | 0.310038  | 1.291078  |
| C | -0.790916 | 0.552990  | -0.226106 |
| C | -1.709983 | -0.495045 | 0.334194  |
| C | -1.201476 | 1.957553  | 0.254514  |
| H | -0.804735 | 0.518246  | -1.315668 |
| C | -2.582273 | -1.170836 | -0.394286 |
| H | -1.643889 | -0.662997 | 1.404820  |
| H | -3.249245 | -1.893728 | 0.053894  |
| H | -2.659495 | -1.020683 | -1.464535 |
| O | 1.027855  | -1.631044 | 0.361299  |
| H | 1.976607  | -1.199635 | 0.219799  |
| H | 0.785361  | -2.080420 | -0.454249 |
| H | -0.523086 | 2.715678  | -0.133252 |
| H | -1.196209 | 2.006991  | 1.343784  |
| H | -2.210468 | 2.171435  | -0.091229 |

Rotational constants (GHz): 3.0031500 1.3419500 1.0099400

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i386.1997 | 40.4969   | 86.0515   |
| 149.5682  | 199.3093  | 232.7311  |
| 281.6701  | 305.8319  | 338.9556  |
| 426.1269  | 458.6662  | 515.2652  |
| 563.4834  | 598.4251  | 646.3055  |
| 707.7355  | 874.5670  | 936.3185  |
| 963.8258  | 981.1843  | 1001.1090 |
| 1036.6845 | 1057.5073 | 1137.0205 |
| 1189.0768 | 1209.2208 | 1270.6130 |
| 1297.5648 | 1312.4487 | 1332.4802 |
| 1369.5492 | 1403.8713 | 1460.8624 |
| 1499.5381 | 1501.1184 | 1590.4719 |
| 1598.8165 | 1739.1029 | 2338.2125 |
| 3068.0840 | 3101.7045 | 3143.8935 |
| 3159.1587 | 3161.1986 | 3163.9535 |
| 3171.0327 | 3253.1361 | 3875.7989 |

Zero-point correction (Hartree): 0.147511

TS\_H\_CH3CHCHCH2\_COO+H2O.p added

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E(RM062X/Aug-CC-pVTZ) (Hartree): -422.02701428  
 Electronic state : 1-A  
 Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.558102  | 0.217286  | 0.303248  |
| O | 1.578505  | 0.675840  | -0.283465 |
| O | 2.727833  | -0.015318 | 0.220206  |
| H | 0.676774  | -0.088015 | 1.339980  |
| C | -0.788498 | 0.537895  | -0.254748 |
| C | -1.840896 | -0.281004 | 0.436355  |
| C | -1.042366 | 2.044570  | -0.080089 |
| H | -0.758420 | 0.288489  | -1.315567 |
| C | -2.524694 | -1.253944 | -0.141715 |
| H | -2.035654 | -0.022553 | 1.474194  |
| H | -3.284175 | -1.805667 | 0.394863  |
| H | -2.343744 | -1.529477 | -1.173506 |
| O | 0.968616  | -1.667472 | -0.253344 |
| H | 1.921715  | -1.276749 | -0.071895 |
| H | 0.787709  | -2.335293 | 0.413420  |
| H | -0.280138 | 2.625262  | -0.594699 |
| H | -1.033505 | 2.317825  | 0.975696  |
| H | -2.020079 | 2.292957  | -0.487968 |

Rotational constants (GHz): 2.9233200 1.3939300 1.0061900  
 Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i371.5681 | 48.4503   | 59.2052   |
| 154.6540  | 184.6820  | 241.6584  |
| 270.7843  | 306.7227  | 345.2181  |
| 431.6175  | 452.1280  | 466.5136  |
| 576.7592  | 599.4164  | 669.4810  |
| 703.5533  | 874.7055  | 935.3990  |
| 959.0932  | 991.9141  | 1006.2877 |
| 1041.0251 | 1050.3944 | 1113.4239 |
| 1165.2805 | 1201.3191 | 1210.9308 |
| 1301.0452 | 1304.2322 | 1331.2630 |
| 1365.2089 | 1405.2102 | 1461.0234 |
| 1500.0482 | 1501.3749 | 1567.7131 |
| 1661.7402 | 1741.0302 | 2417.3021 |
| 3068.9875 | 3104.1374 | 3143.3196 |
| 3149.1094 | 3156.2311 | 3163.1279 |
| 3165.6189 | 3251.6809 | 3897.5648 |

Zero-point correction (Hartree): 0.147438

TS\_H\_CH3CHCHCH2\_COO+H2O.pmuu

~~~~~  
 E(RM062X/Aug-CC-pVTZ) (Hartree): -422.02651920  
 Electronic state : 1-A  
 Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.455855  | -0.130140 | 0.277323  |
| O | 0.966059  | -1.127763 | -0.312486 |
| O | 2.286936  | -1.316148 | 0.204537  |
| H | 0.714804  | 0.020175  | 1.322574  |
| C | -0.809103 | 0.443786  | -0.267683 |
| C | -1.946440 | -0.272790 | 0.421213  |
| C | -0.878364 | 1.950285  | -0.014020 |
| H | -0.836759 | 0.228480  | -1.335355 |
| C | -2.760428 | -1.121609 | -0.183127 |
| H | -2.079846 | -0.044220 | 1.474793  |
| H | -3.570680 | -1.599011 | 0.350081  |
| H | -2.641901 | -1.366857 | -1.231217 |
| O | 1.996986  | 1.049798  | -0.214660 |
| H | 2.458627  | 0.096138  | -0.043128 |
| H | 2.296340  | 1.641814  | 0.480765  |
| H | -0.094801 | 2.468778  | -0.559697 |
| H | -0.765486 | 2.164474  | 1.050518  |
| H | -1.849269 | 2.325942  | -0.330702 |

Rotational constants (GHz): 2.9839400 1.3437300 0.9858500  
 Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i456.2395 | 45.0196   | 61.6634   |
| 168.3847  | 198.2199  | 245.5183  |
| 277.9660  | 324.2717  | 351.0417  |
| 426.8641  | 478.6518  | 495.3362  |
| 551.4840  | 632.7899  | 670.9933  |
| 722.4782  | 873.6263  | 936.4148  |
| 958.1739  | 990.4471  | 1000.9176 |
| 1037.0345 | 1076.3876 | 1113.7406 |
| 1176.8818 | 1192.7117 | 1226.0122 |
| 1286.6182 | 1321.0811 | 1326.0704 |
| 1360.1353 | 1407.6110 | 1456.1546 |
| 1498.1706 | 1507.1076 | 1552.1451 |
| 1659.5121 | 1734.1676 | 2119.7156 |
| 3065.8525 | 3109.1367 | 3140.1474 |
| 3152.9654 | 3158.9623 | 3169.7230 |
| 3171.5082 | 3256.1311 | 3889.7789 |

Zero-point correction (Hartree): 0.147114

TS\_H\_CH3CHCHCH2\_COO+H2O.pmuu

~~~~~  
 E(RM062X/Aug-CC-pVTZ) (Hartree): -422.02714021  
 Electronic state : 1-A  
 Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.458556  | -0.121313 | 0.274786  |
| O | 0.969146  | -1.119354 | -0.315577 |
| O | 2.285132  | -1.313568 | 0.211521  |
| H | 0.721543  | 0.038345  | 1.317102  |
| C | -0.810822 | 0.450673  | -0.264145 |
| C | -1.939470 | -0.291326 | 0.413216  |
| C | -0.901551 | 1.950704  | 0.021972  |
| H | -0.843698 | 0.250830  | -1.335323 |
| C | -2.750111 | -1.131748 | -0.206894 |
| H | -2.067721 | -0.087599 | 1.472296  |
| H | -3.553903 | -1.627421 | 0.319289  |
| H | -2.635669 | -1.352148 | -1.260963 |
| O | 2.027387  | 1.089561  | -0.060284 |

|                                          |           |           |                               |
|------------------------------------------|-----------|-----------|-------------------------------|
| H                                        | 2.466564  | 0.123638  | 0.066180                      |
| H                                        | 2.109850  | 1.296814  | -0.996550                     |
| H                                        | -0.122174 | 2.501810  | -0.497317                     |
| H                                        | -0.792286 | 2.141387  | 1.090161                      |
| H                                        | -1.875441 | 2.319294  | -0.293764                     |
| Rotational constants (GHz):              |           |           | 2.9698100 1.3409100 0.9836800 |
| Vibrational harmonic frequencies (cm-1): |           |           |                               |
| i430.6972                                | 37.7663   | 62.6969   |                               |
| 165.9876                                 | 195.4924  | 229.6378  |                               |
| 276.5674                                 | 320.0085  | 351.9708  |                               |
| 419.1448                                 | 477.9698  | 511.3207  |                               |
| 558.8452                                 | 601.0454  | 638.1164  |                               |
| 712.6016                                 | 874.3437  | 934.7139  |                               |
| 957.9176                                 | 989.8461  | 1001.5333 |                               |
| 1037.1806                                | 1084.0351 | 1132.9534 |                               |
| 1178.6621                                | 1205.0852 | 1271.4094 |                               |
| 1295.3712                                | 1319.9609 | 1326.5152 |                               |
| 1375.9006                                | 1418.1080 | 1456.3684 |                               |
| 1498.3057                                | 1499.2394 | 1591.2750 |                               |
| 1614.2668                                | 1733.7447 | 2147.7671 |                               |
| 3073.9065                                | 3100.5649 | 3145.9462 |                               |
| 3158.7913                                | 3163.9866 | 3169.1363 |                               |
| 3170.6370                                | 3256.3585 | 3871.4964 |                               |

Zero-point correction (Hartree): 0.147203

TS\_H\_CH3CHCHCH2\_COO+H2O.pppd  
 ~~~~~  
 E(RM062X/Aug-CC-pVT2) (Hartree): -422.02791767  
 Electronic state : 1-A  
 Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.551030  | -0.170111 | -0.240679 |
| O | 1.539664  | -0.839885 | 0.178400  |
| O | 2.718889  | -0.321660 | -0.446773 |
| H | 0.582604  | 0.193031  | -1.264102 |
| C | -0.757153 | -0.319078 | 0.466154  |
| C | -1.652827 | 0.843299  | 0.124947  |
| C | -1.331324 | -1.691759 | 0.099212  |
| H | -0.539313 | -0.303921 | 1.537402  |
| C | -2.861585 | 0.748234  | -0.404429 |
| H | -1.235147 | 1.821124  | 0.335301  |
| H | -3.441479 | 1.635475  | -0.616809 |
| H | -3.318554 | -0.202943 | -0.643191 |
| O | 1.371505  | 1.624475  | 0.182718  |
| H | 2.197243  | 1.027085  | -0.102443 |
| H | 1.454300  | 1.750503  | 1.133463  |
| H | -0.641312 | -2.479669 | 0.391463  |
| H | -1.510729 | -1.765000 | -0.973587 |
| H | -2.276922 | -1.842633 | 0.616504  |

Rotational constants (GHz): 3.4436300 1.2439900 0.9755200  
 Vibrational harmonic frequencies (cm-1):

|           |           |           |  |
|-----------|-----------|-----------|--|
| i397.6451 | 54.2519   | 86.5855   |  |
| 145.0523  | 224.5253  | 277.7882  |  |
| 294.2199  | 307.7455  | 350.8899  |  |
| 429.7453  | 469.8475  | 532.2489  |  |
| 573.6059  | 594.7214  | 633.2347  |  |
| 698.9355  | 867.7247  | 937.5072  |  |
| 956.7016  | 990.6303  | 1008.6922 |  |
| 1049.0023 | 1088.2542 | 1102.6913 |  |
| 1171.7148 | 1192.2535 | 1267.8745 |  |
| 1303.8752 | 1332.4835 | 1341.3077 |  |
| 1372.0331 | 1403.6967 | 1455.8771 |  |
| 1501.7852 | 1509.1642 | 1590.8117 |  |
| 1619.9608 | 1736.4444 | 2252.2116 |  |
| 3064.3124 | 3074.0278 | 3146.8786 |  |
| 3163.6616 | 3171.3441 | 3175.5122 |  |
| 3188.8873 | 3259.6906 | 3869.8591 |  |

Zero-point correction (Hartree): 0.147717

TS\_H\_CH3CHCHCH2\_COO+H2O.pppd  
 ~~~~~  
 E(RM062X/Aug-CC-pVT2) (Hartree): -422.02779334  
 Electronic state : 1-A  
 Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.549693 | -0.212198 | 0.219599  |
| O | -1.564709 | -0.814988 | -0.234951 |
| O | -2.724708 | -0.276333 | 0.408471  |
| H | -0.566055 | 0.086817  | 1.264339  |
| C | 0.754410  | -0.393449 | -0.484227 |
| C | 1.629344  | 0.811983  | -0.257165 |
| C | 1.355324  | -1.713373 | 0.010576  |
| H | 0.527540  | -0.472121 | -1.549113 |
| C | 2.773486  | 0.814352  | 0.408103  |
| H | 1.255515  | 1.731464  | -0.691444 |
| H | 3.344686  | 1.725343  | 0.520951  |
| H | 3.187725  | -0.080151 | 0.854292  |
| O | -1.301126 | 1.588670  | -0.251518 |
| H | -2.160760 | 1.036533  | 0.037786  |
| H | -1.162476 | 2.267318  | 0.415033  |
| H | 0.693927  | -2.542630 | -0.229787 |
| H | 1.508828  | -1.696239 | 1.089975  |
| H | 2.318178  | -1.879020 | -0.469370 |

Rotational constants (GHz): 3.3929300 1.2729900 0.9905800  
 Vibrational harmonic frequencies (cm-1):

|           |           |           |  |
|-----------|-----------|-----------|--|
| i414.8855 | 49.4227   | 82.1883   |  |
| 162.5649  | 236.3619  | 281.4588  |  |
| 292.0526  | 312.3348  | 351.6036  |  |
| 418.8120  | 478.2545  | 517.7500  |  |
| 581.1071  | 627.8487  | 673.4015  |  |
| 702.7448  | 865.0959  | 937.5334  |  |
| 957.6200  | 991.8535  | 1006.0714 |  |
| 1059.5706 | 1083.4350 | 1091.6113 |  |
| 1160.7171 | 1179.4775 | 1223.1122 |  |

|           |           |           |
|-----------|-----------|-----------|
| 1294.4428 | 1330.2035 | 1344.9620 |
| 1355.7567 | 1403.6843 | 1453.4917 |
| 1501.3844 | 1508.4078 | 1560.1491 |
| 1668.4454 | 1733.3014 | 2222.8552 |
| 3070.5215 | 3087.6549 | 3143.7109 |
| 3160.7726 | 3162.7101 | 3173.4044 |
| 3194.3860 | 3256.6721 | 3888.4974 |

Zero-point correction (Hartree): 0.147715

TS\_H\_CH3CHCHCH2\_COO+H2O.ppuu

~~~~~  
E(RM062X/Aug-CC-pVTZ) (Hartree): -422.02784107

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.489399 | -0.155023 | -0.195668 |
| O | -1.210381 | -1.034624 | 0.359739  |
| O | -2.469943 | -1.067361 | -0.320617 |
| H | -0.584900 | -0.031050 | -1.271232 |
| C | 0.760968  | 0.277063  | 0.497085  |
| C | 1.763603  | -0.833891 | 0.260674  |
| C | 1.204221  | 1.644151  | -0.000459 |
| H | 0.531594  | 0.316110  | 1.563685  |
| C | 2.898282  | -0.708429 | -0.408458 |
| H | 1.485325  | -1.795525 | 0.676999  |
| H | 3.560617  | -1.553629 | -0.533577 |
| H | 3.213107  | 0.230532  | -0.843878 |
| O | -1.884120 | 1.263920  | 0.048456  |
| H | -2.459280 | 0.387259  | -0.142673 |
| H | -2.009524 | 1.852489  | -0.701028 |
| H | 0.459419  | 2.393633  | 0.254553  |
| H | 1.342202  | 1.641637  | -1.082810 |
| H | 2.150947  | 1.919836  | 0.460285  |

Rotational constants (GHz): 3.4202000 1.2537600 0.9796200

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i427.2820 | 48.1740   | 92.2499   |
| 158.8627  | 235.2245  | 272.4556  |
| 290.8022  | 319.5943  | 362.0497  |
| 431.7247  | 484.0927  | 505.1406  |
| 580.4626  | 630.5492  | 649.6803  |
| 717.3563  | 854.0261  | 936.4659  |
| 954.9932  | 987.9594  | 1026.6793 |
| 1047.9639 | 1055.0945 | 1111.4368 |
| 1169.9414 | 1181.4894 | 1219.2318 |
| 1288.9259 | 1327.6009 | 1340.4607 |
| 1369.8774 | 1409.0289 | 1452.1289 |
| 1505.1202 | 1510.0561 | 1555.8061 |
| 1669.0532 | 1730.1733 | 2184.7963 |
| 3069.7514 | 3086.7173 | 3142.1041 |
| 3162.5618 | 3166.1316 | 3174.1732 |
| 3186.0730 | 3260.0878 | 3889.5609 |

Zero-point correction (Hartree): 0.147634

TS\_H\_CH3CHCHCH2\_COO+H2O.ppuu

~~~~~  
E(RM062X/Aug-CC-pVTZ) (Hartree): -422.02841960

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.491689 | -0.142971 | -0.198299 |
| O | -1.202416 | -1.031439 | 0.357874  |
| O | -2.459617 | -1.080027 | -0.326029 |
| H | -0.597150 | -0.006509 | -1.270933 |
| C | 0.761604  | 0.298181  | 0.485780  |
| C | 1.756107  | -0.827702 | 0.282884  |
| C | 1.218273  | 1.646382  | -0.051029 |
| H | 0.539631  | 0.363357  | 1.553634  |
| C | 2.898497  | -0.725614 | -0.376598 |
| H | 1.464663  | -1.777449 | 0.716880  |
| H | 3.554260  | -1.579230 | -0.476676 |
| H | 3.225304  | 0.200720  | -0.829540 |
| O | -1.903418 | 1.288600  | -0.100460 |
| H | -2.456362 | 0.394817  | -0.249326 |
| H | -2.064343 | 1.550344  | 0.811717  |
| H | 0.465565  | 2.407221  | 0.138166  |
| H | 1.384292  | 1.598894  | -1.127595 |
| H | 2.150995  | 1.941113  | 0.426175  |

Rotational constants (GHz): 3.4010500 1.2517600 0.9772200

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i406.8513 | 45.9268   | 92.8612   |
| 157.8258  | 233.6907  | 267.9222  |
| 279.8803  | 319.9528  | 352.9576  |
| 439.2708  | 491.5305  | 517.4608  |
| 572.1887  | 589.3595  | 626.6587  |
| 705.4179  | 855.1493  | 934.0730  |
| 956.5223  | 989.3604  | 1027.1655 |
| 1048.0187 | 1060.1437 | 1130.9270 |
| 1169.6284 | 1194.0335 | 1267.4947 |
| 1300.4253 | 1326.7975 | 1344.5173 |
| 1379.6845 | 1415.6584 | 1452.0432 |
| 1500.5274 | 1509.1348 | 1587.5738 |
| 1615.6914 | 1730.4396 | 2219.2587 |
| 3071.7787 | 3077.0771 | 3145.6265 |
| 3167.6580 | 3171.2113 | 3175.2006 |
| 3187.3114 | 3261.3238 | 3871.8726 |

Zero-point correction (Hartree): 0.147708

#####  
Z- (C (CH3) 2-CH=CH2) CHOO  
#####

Population analysis as 298K (%)

Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)

| Compound                    | Qtot      | Erel | Erel2 | n*Q*MB    | %     |
|-----------------------------|-----------|------|-------|-----------|-------|
| TS.diMeCCHCH2_H_COO+H2O.mmu | 2.279e+41 | 0.00 | 0.00  | 4.558e+41 | 28.7  |
| TS.diMeCCHCH2_H_COO+H2O.ppd | 2.049e+41 | 0.18 | 0.18  | 2.998e+41 | 18.9  |
| TS.diMeCCHCH2_H_COO+H2O.tpu | 2.246e+41 | 0.29 | 0.29  | 2.741e+41 | 17.2  |
| TS.diMeCCHCH2_H_COO+H2O.ppu | 2.757e+41 | 0.72 | 0.72  | 1.638e+41 | 10.3  |
| TS.diMeCCHCH2_H_COO+H2O.mcu | 2.937e+41 | 0.94 | 0.94  | 1.192e+41 | 7.5   |
| TS.diMeCCHCH2_H_COO+H2O.mpu | 2.514e+41 | 1.36 | 1.36  | 5.060e+40 | 3.18  |
| TS.diMeCCHCH2_H_COO+H2O.tmd | 2.137e+41 | 1.30 | 1.30  | 4.748e+40 | 2.99  |
| TS.diMeCCHCH2_H_COO+H2O.tmu | 3.763e+41 | 1.66 | 1.66  | 4.525e+40 | 2.85  |
| TS.diMeCCHCH2_H_COO+H2O.pmu | 1.946e+41 | 1.36 | 1.36  | 3.910e+40 | 2.46  |
| TS.diMeCCHCH2_H_COO+H2O.tcu | 2.182e+41 | 1.60 | 1.60  | 2.912e+40 | 1.83  |
| TS.diMeCCHCH2_H_COO+H2O.mmd | 2.484e+41 | 1.72 | 1.72  | 2.733e+40 | 1.72  |
| TS.diMeCCHCH2_H_COO+H2O.tcd | 1.509e+41 | 1.72 | 1.72  | 1.664e+40 | 1.05  |
| TS.diMeCCHCH2_H_COO+H2O.tpd | 2.723e+41 | 2.32 | 2.32  | 1.086e+40 | 0.683 |
| TS.diMeCCHCH2_H_COO+H2O.mcd | 2.876e+41 | 2.71 | 2.71  | 5.875e+39 | 0.37  |
| TS.diMeCCHCH2_H_COO+H2O.mpd | 2.755e+41 | 3.13 | 3.13  | 2.783e+39 | 0.175 |
| TS.diMeCCHCH2_H_COO+H2O.pmd | 2.035e+41 | 3.26 | 3.26  | 1.643e+39 | 0.103 |
| Total                       |           |      |       | 1.589e+42 | 100   |

TS.diMeCCHCH2\_H\_COO+H2O.mcd

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E(RM062X/Aug-CC-pVTZ) (Hartree): -461.32648764

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.421195  | -0.118996 | -0.821502 |
| O | 0.969367  | -1.255945 | -0.671483 |
| O | 1.519788  | -1.369732 | 0.646555  |
| H | 0.319281  | 0.139049  | -1.875085 |
| C | -0.589875 | 0.564469  | 0.073168  |
| C | -1.882946 | -0.186405 | -0.264498 |
| C | -0.360879 | 0.521842  | 1.585851  |
| C | -0.733113 | 2.014732  | -0.395531 |
| C | -2.043221 | -1.492076 | -0.118679 |
| H | -2.701963 | 0.427413  | -0.624485 |
| H | -2.990709 | -1.963235 | -0.341093 |
| H | -1.236345 | -2.127931 | 0.228290  |
| O | 2.112594  | 0.807563  | -0.308845 |
| H | 2.144246  | -0.046317 | 0.308790  |
| H | 2.062688  | 1.576254  | 0.264224  |
| H | 0.558709  | 1.035899  | 1.863809  |
| H | -0.300977 | -0.497762 | 1.947429  |
| H | -1.197112 | 1.032569  | 2.065568  |
| H | -0.904581 | 2.075925  | -1.471159 |
| H | 0.151481  | 2.602680  | -0.156966 |
| H | -1.585677 | 2.468960  | 0.108001  |

Rotational constants (GHz): 1.9912900 1.4987600 1.1444600

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i446.3649 | 63.3759   | 86.6766   |
| 177.9997  | 229.3919  | 255.7810  |
| 270.2885  | 293.0183  | 301.5361  |
| 327.4409  | 360.0656  | 383.6815  |
| 424.7603  | 439.2030  | 539.4749  |
| 585.8731  | 641.6597  | 673.4371  |
| 695.8237  | 799.0398  | 873.1670  |
| 907.8940  | 969.1660  | 989.4047  |
| 1016.6419 | 1029.4199 | 1035.7576 |
| 1052.2785 | 1080.1527 | 1179.9571 |
| 1215.8890 | 1235.6289 | 1275.6439 |
| 1338.2211 | 1394.2859 | 1407.9457 |
| 1429.2876 | 1445.7178 | 1478.9186 |
| 1484.1227 | 1502.3702 | 1507.7288 |
| 1544.1502 | 1681.3118 | 1716.0357 |
| 2301.4444 | 3065.3171 | 3069.1404 |
| 3131.5688 | 3135.9740 | 3147.9586 |
| 3150.1987 | 3157.0753 | 3169.4337 |
| 3198.1373 | 3251.4872 | 3904.8124 |

Zero-point correction (Hartree): 0.175469

TS.diMeCCHCH2\_H\_COO+H2O.mcu

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E(RM062X/Aug-CC-pVTZ) (Hartree): -461.32934291

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.413167  | -0.121029 | -0.821230 |
| O | 0.972841  | -1.255216 | -0.677563 |
| O | 1.516523  | -1.372853 | 0.641080  |
| H | 0.310308  | 0.140143  | -1.875213 |
| C | -0.593814 | 0.565489  | 0.071317  |
| C | -1.887503 | -0.184669 | -0.261906 |
| C | -0.354117 | 0.536077  | 1.583115  |
| C | -0.720590 | 2.015455  | -0.402750 |
| C | -2.048980 | -1.491037 | -0.121127 |
| H | -2.708509 | 0.432128  | -0.612419 |
| H | -2.998716 | -1.960419 | -0.337914 |
| H | -1.241307 | -2.129232 | 0.219760  |
| O | 2.035358  | 0.883766  | -0.159036 |
| H | 2.067761  | -0.017562 | 0.398351  |
| H | 2.726760  | 0.811075  | -0.823918 |
| H | 0.567629  | 1.057165  | 1.834010  |
| H | -0.299039 | -0.479770 | 1.956648  |
| H | -1.188065 | 1.052940  | 2.060257  |
| H | -0.910634 | 2.073346  | -1.476261 |
| H | 0.186753  | 2.568927  | -0.174101 |
| H | -1.559688 | 2.483969  | 0.110438  |

Rotational constants (GHz): 1.9906300 1.5106900 1.1483800

Vibrational harmonic frequencies (cm-1):

|           |          |          |
|-----------|----------|----------|
| i448.6911 | 61.7416  | 80.0341  |
| 178.0326  | 242.7335 | 263.9974 |
| 270.8940  | 290.8662 | 311.4370 |
| 323.7096  | 356.2387 | 385.1530 |
| 428.6263  | 447.7686 | 552.3847 |

|           |           |           |
|-----------|-----------|-----------|
| 598.9562  | 621.5879  | 649.2928  |
| 691.2946  | 806.9017  | 875.9417  |
| 907.8740  | 975.1527  | 990.6781  |
| 1013.0313 | 1029.3828 | 1038.1998 |
| 1052.0736 | 1080.9373 | 1218.5489 |
| 1230.3335 | 1274.3077 | 1303.2695 |
| 1337.3184 | 1392.8795 | 1401.6594 |
| 1425.5037 | 1445.2956 | 1479.0117 |
| 1496.9606 | 1503.9028 | 1516.0935 |
| 1573.4985 | 1619.3321 | 1714.5525 |
| 2218.3982 | 3061.6321 | 3071.5305 |
| 3129.8085 | 3135.1555 | 3144.8638 |
| 3156.3783 | 3166.4886 | 3169.2693 |
| 3197.0426 | 3250.3361 | 3878.8110 |

Zero-point correction (Hartree): 0.175503

TS.diMeCCHCH2\_H\_COO+H2O.mmd  
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E(RM062X/Aug-CC-pVTZ) (Hartree): -461.32841360

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.462883  | -0.229284 | -0.791825 |
| O | 1.254519  | -1.211226 | -0.647425 |
| O | 1.977908  | -1.083370 | 0.581763  |
| H | 0.168436  | -0.097786 | -1.832632 |
| C | -0.552929 | 0.300790  | 0.200218  |
| C | -1.574910 | -0.829555 | 0.159004  |
| C | -0.117392 | 0.489914  | 1.655297  |
| C | -1.115555 | 1.606551  | -0.354541 |
| C | -2.792074 | -0.764412 | -0.357052 |
| H | -1.223371 | -1.752869 | 0.608312  |
| H | -3.451621 | -1.620466 | -0.319382 |
| H | -3.181019 | 0.132834  | -0.819610 |
| O | 1.965668  | 1.075631  | -0.594632 |
| H | 2.258803  | 0.312858  | 0.065739  |
| H | 1.821282  | 1.868840  | -0.073314 |
| H | 0.686445  | 1.219611  | 1.739820  |
| H | 0.229839  | -0.440254 | 2.090623  |
| H | -0.977048 | 0.862105  | 2.214334  |
| H | -1.424153 | 1.513290  | -1.396152 |
| H | -0.371328 | 2.399292  | -0.294328 |
| H | -1.981158 | 1.910231  | 0.232339  |

Rotational constants (GHz): 2.3420500 1.2185400 1.0784700

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i439.9472 | 59.9763   | 97.0449   |
| 193.5534  | 234.2750  | 274.1923  |
| 280.3256  | 300.0139  | 317.8810  |
| 323.8049  | 370.5117  | 375.3642  |
| 410.5945  | 481.1497  | 507.4790  |
| 599.1474  | 641.5210  | 681.1880  |
| 708.4104  | 791.3163  | 868.1034  |
| 906.7808  | 971.3814  | 980.1601  |
| 990.3915  | 1025.4615 | 1046.1371 |
| 1059.1519 | 1082.1367 | 1164.8051 |
| 1199.0441 | 1253.6394 | 1277.3714 |
| 1334.3265 | 1393.6939 | 1406.8312 |
| 1424.4460 | 1451.0820 | 1484.1284 |
| 1485.6756 | 1503.3641 | 1513.3280 |
| 1546.6314 | 1677.6450 | 1721.7337 |
| 2339.5944 | 3068.2228 | 3072.2666 |
| 3137.8993 | 3138.4228 | 3147.8608 |
| 3149.2988 | 3168.6383 | 3179.2844 |
| 3191.5620 | 3257.2696 | 3904.5875 |

Zero-point correction (Hartree): 0.175806

TS.diMeCCHCH2\_H\_COO+H2O.mmu  
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E(CCS(D)/T)/Aug-CC-pVTZ) (Hartree): -460.66701627

E(CCS(D)/Aug-CC-pVTZ) (Hartree): -460.58052747

T1 diagnostic: 0.019535

E(MP2/Aug-CC-pVTZ) (Hartree): -460.53113193

E(MP3/Aug-CC-pVTZ) (Hartree): -460.56768024

E(RHF/Aug-CC-pVTZ) (Hartree): -458.73829315

E(RM062X/Aug-CC-pVTZ) (Hartree): -461.33129957

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.457790  | -0.230369 | -0.792283 |
| O | 1.254276  | -1.211817 | -0.656067 |
| O | 1.966443  | -1.096685 | 0.578847  |
| H | 0.166385  | -0.091729 | -1.834279 |
| C | -0.556649 | 0.303563  | 0.195095  |
| C | -1.576337 | -0.828630 | 0.164061  |
| C | -0.113924 | 0.516572  | 1.645335  |
| C | -1.108259 | 1.608291  | -0.372992 |
| C | -2.794888 | -0.766108 | -0.349575 |
| H | -1.226107 | -1.747954 | 0.622960  |
| H | -3.457468 | -1.619372 | -0.301084 |
| H | -3.181612 | 0.129123  | -0.817897 |
| O | 1.898436  | 1.143580  | -0.431989 |
| H | 2.189451  | 0.326452  | 0.170308  |
| H | 2.502271  | 1.151432  | -1.180774 |
| H | 0.685477  | 1.252229  | 1.696825  |
| H | 0.231150  | -0.406349 | 2.097994  |
| H | -0.973816 | 0.896159  | 2.198934  |
| H | -1.432489 | 1.503164  | -1.409455 |
| H | -0.338833 | 2.375832  | -0.326223 |
| H | -1.964042 | 1.930482  | 0.218522  |

Rotational constants (GHz): 2.3444400 1.2294900 1.0806800

Vibrational harmonic frequencies (cm-1):

|           |          |          |
|-----------|----------|----------|
| i441.5094 | 59.6000  | 97.4264  |
| 191.5758  | 252.1398 | 282.4789 |
| 296.2447  | 299.2475 | 315.3731 |

|           |           |           |
|-----------|-----------|-----------|
| 325.0517  | 367.0313  | 378.6188  |
| 411.5836  | 503.4607  | 521.3142  |
| 596.1004  | 622.5494  | 661.5980  |
| 706.9618  | 799.6088  | 872.3592  |
| 907.6024  | 976.5248  | 981.5142  |
| 989.5713  | 1028.8724 | 1044.2212 |
| 1058.8543 | 1085.3407 | 1191.1200 |
| 1254.2089 | 1272.9035 | 1298.8549 |
| 1332.8920 | 1392.0000 | 1401.2783 |
| 1421.7021 | 1450.8324 | 1485.6920 |
| 1498.2782 | 1511.2538 | 1517.9119 |
| 1573.0288 | 1621.6593 | 1720.6033 |
| 2262.6579 | 3065.7212 | 3074.4358 |
| 3132.4765 | 3137.2352 | 3150.6787 |
| 3161.2678 | 3166.5926 | 3178.2135 |
| 3192.5678 | 3256.9984 | 3879.5007 |

Zero-point correction (Hartree): 0.175955

TS.diMeCCHCH2\_H\_COO+H2O.mpd

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E(RM062X/Aug-CC-pVTZ) (Hartree): -461.32616692

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.547920  | -0.073207 | -0.838326 |
| O | 1.142196  | -1.192412 | -0.776852 |
| O | 1.636010  | -1.429194 | 0.544875  |
| H | 0.500912  | 0.296497  | -1.863288 |
| C | -0.553218 | 0.461582  | 0.052809  |
| C | -1.773854 | -0.186246 | -0.595510 |
| C | -0.460986 | 0.154950  | 1.541056  |
| C | -0.678087 | 1.974801  | -0.173492 |
| C | -2.582013 | -1.062879 | -0.023276 |
| H | -1.977883 | 0.136368  | -1.612942 |
| H | -3.438455 | -1.449809 | -0.557968 |
| H | -2.426787 | -1.421215 | 0.984778  |
| O | 2.167136  | 0.869234  | -0.110815 |
| H | 2.205804  | -0.053756 | 0.397687  |
| H | 2.050468  | 1.556123  | 0.549448  |
| H | 0.421205  | 0.620560  | 1.975666  |
| H | -0.391049 | -0.909921 | 1.732564  |
| H | -1.345029 | 0.566916  | 2.030122  |
| H | -0.686485 | 2.225637  | -1.235089 |
| H | 0.139541  | 2.516911  | 0.298156  |
| H | -1.613547 | 2.320669  | 0.263637  |

Rotational constants (GHz): 2.1737400 1.3124200 1.0891900

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i450.6003 | 62.3807   | 77.0143   |
| 202.5233  | 222.0323  | 261.9383  |
| 294.4693  | 300.4807  | 316.0091  |
| 345.8317  | 378.6856  | 383.6231  |
| 416.2765  | 477.5284  | 520.8203  |
| 592.5942  | 639.9688  | 677.3672  |
| 706.6618  | 798.9436  | 867.2972  |
| 905.7033  | 964.4909  | 981.5879  |
| 995.1130  | 1029.6270 | 1043.8430 |
| 1063.2730 | 1073.3575 | 1171.5682 |
| 1201.1010 | 1217.5728 | 1305.8337 |
| 1342.1610 | 1400.3612 | 1408.6469 |
| 1426.6725 | 1450.1910 | 1484.8548 |
| 1486.8411 | 1506.1696 | 1511.0414 |
| 1549.2227 | 1682.9253 | 1728.0147 |
| 2292.9016 | 3066.6637 | 3072.9210 |
| 3135.0197 | 3139.0870 | 3143.2805 |
| 3151.7064 | 3152.1941 | 3181.6636 |
| 3193.1929 | 3264.8082 | 3906.7845 |

Zero-point correction (Hartree): 0.175813

TS.diMeCCHCH2\_H\_COO+H2O.mpu

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E(RM062X/Aug-CC-pVTZ) (Hartree): -461.32900666

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.543275  | -0.068396 | -0.841860 |
| O | 1.147050  | -1.185293 | -0.792199 |
| O | 1.627104  | -1.437967 | 0.529502  |
| H | 0.498660  | 0.311343  | -1.864565 |
| C | -0.556770 | 0.464184  | 0.047905  |
| C | -1.776487 | -0.189127 | -0.595546 |
| C | -0.454945 | 0.170610  | 1.538745  |
| C | -0.668182 | 1.977908  | -0.182162 |
| C | -2.580233 | -1.065680 | -0.016505 |
| H | -1.987762 | 0.131365  | -1.612372 |
| H | -3.440026 | -1.455058 | -0.544134 |
| H | -2.418051 | -1.418727 | 0.992360  |
| O | 2.074322  | 0.920638  | 0.059062  |
| H | 2.116898  | -0.046895 | 0.492716  |
| H | 2.812935  | 0.970688  | -0.554901 |
| H | 0.425639  | 0.654713  | 1.953594  |
| H | -0.382554 | -0.891953 | 1.742566  |
| H | -1.340475 | 0.582655  | 2.024888  |
| H | -0.719392 | 2.220812  | -1.245287 |
| H | 0.188221  | 2.486737  | 0.252586  |
| H | -1.581857 | 2.338307  | 0.288173  |

Rotational constants (GHz): 2.1689100 1.3243500 1.0962000

Vibrational harmonic frequencies (cm-1):

|           |          |          |
|-----------|----------|----------|
| i455.5383 | 63.3976  | 77.6863  |
| 200.6138  | 244.7927 | 263.6109 |
| 296.7832  | 301.8836 | 316.3646 |
| 344.4145  | 379.0771 | 389.4255 |
| 416.6876  | 506.0137 | 518.0026 |
| 583.9371  | 619.4769 | 648.4213 |
| 704.1990  | 805.6661 | 871.3527 |

|           |           |           |
|-----------|-----------|-----------|
| 906.4044  | 967.4758  | 985.1161  |
| 994.4338  | 1032.0989 | 1043.5718 |
| 1061.5992 | 1075.2984 | 1201.3419 |
| 1211.2375 | 1301.4521 | 1314.9948 |
| 1341.2899 | 1397.6928 | 1401.4319 |
| 1423.0826 | 1449.7450 | 1488.3751 |
| 1497.5658 | 1506.9103 | 1518.4047 |
| 1578.4897 | 1614.3896 | 1726.5184 |
| 2201.7964 | 3062.8947 | 3074.8138 |
| 3122.6123 | 3133.7354 | 3149.0121 |
| 3153.7761 | 3169.1688 | 3180.9164 |
| 3193.8649 | 3264.2069 | 3882.4081 |

Zero-point correction (Hartree): 0.175829

TS.diMeCCHCH2\_H\_COO+H2O.pmd  
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E(RM062X/Aug-CC-pVTZ) (Hartree): -461.32582074

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.785553  | 0.616563  | -0.582851 |
| O | 1.534760  | -0.268113 | -1.094220 |
| O | 1.553186  | -1.426371 | -0.254928 |
| H | 1.004007  | 1.611097  | -0.972341 |
| C | -0.631665 | 0.442680  | -0.088886 |
| C | -0.909586 | -0.757682 | 0.779323  |
| C | -1.026915 | 1.712843  | 0.679038  |
| C | -1.420539 | 0.396072  | -1.412334 |
| C | -1.889548 | -1.628197 | 0.603984  |
| H | -0.285338 | -0.850320 | 1.659335  |
| H | -2.048773 | -2.423066 | 1.318481  |
| H | -2.545052 | -1.607729 | -0.255492 |
| O | 1.841158  | 0.584468  | 1.120434  |
| H | 1.876648  | -0.425354 | 0.824402  |
| H | 1.392471  | 0.628327  | 1.967976  |
| H | -0.802448 | 2.610419  | 0.100270  |
| H | -0.507914 | 1.784010  | 1.633651  |
| H | -2.096749 | 1.687780  | 0.877525  |
| H | -1.191443 | -0.513507 | -1.964632 |
| H | -1.185648 | 1.258737  | -2.036975 |
| H | -2.486404 | 0.426057  | -1.192140 |

Rotational constants (GHz): 1.9620100 1.3581500 1.2237100

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i441.7101 | 70.2453   | 112.2628  |
| 192.9267  | 217.4223  | 238.0598  |
| 279.0803  | 315.2610  | 324.5981  |
| 335.9809  | 359.9254  | 365.0336  |
| 420.7152  | 481.8236  | 524.6647  |
| 603.3514  | 649.1388  | 664.1552  |
| 722.0560  | 793.4631  | 882.6835  |
| 921.4126  | 960.0489  | 966.3042  |
| 970.0098  | 1018.2240 | 1029.7043 |
| 1060.0100 | 1068.7502 | 1166.9362 |
| 1191.1085 | 1225.0586 | 1299.5493 |
| 1344.2105 | 1389.1030 | 1394.9320 |
| 1420.7955 | 1455.8080 | 1484.2628 |
| 1495.0245 | 1504.0797 | 1517.9340 |
| 1549.6417 | 1678.5820 | 1733.6177 |
| 2316.9288 | 3062.8899 | 3066.2589 |
| 3135.3541 | 3136.2499 | 3142.4757 |
| 3152.5067 | 3158.7606 | 3179.9400 |
| 3196.3528 | 3262.3418 | 3905.6088 |

Zero-point correction (Hartree): 0.175678

TS.diMeCCHCH2\_H\_COO+H2O.pmu  
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E(RM062X/Aug-CC-pVTZ) (Hartree): -461.32888329

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.776597 | 0.646546  | 0.563844  |
| O | -1.546636 | -0.206944 | 1.099685  |
| O | -1.560334 | -1.401344 | 0.316694  |
| H | -0.989226 | 1.658922  | 0.911856  |
| C | 0.639486  | 0.446714  | 0.083091  |
| C | 0.904982  | -0.757762 | -0.784228 |
| C | 1.044064  | 1.704568  | -0.700063 |
| C | 1.417998  | 0.398122  | 1.411959  |
| C | 1.849891  | -1.659930 | -0.579128 |
| H | 0.309753  | -0.804153 | -1.686980 |
| H | 2.011294  | -2.453460 | -1.294824 |
| H | 2.474927  | -1.666343 | 0.303234  |
| O | -1.677724 | 0.483277  | -1.252203 |
| H | -1.764438 | -0.488785 | -0.844483 |
| H | -2.552432 | 0.878825  | -1.195173 |
| H | 0.857734  | 2.609053  | -0.117177 |
| H | 0.489830  | 1.766451  | -1.634027 |
| H | 2.108157  | 1.654646  | -0.923551 |
| H | 1.175230  | -0.504900 | 1.969555  |
| H | 1.192860  | 1.268022  | 2.030579  |
| H | 2.484909  | 0.412259  | 1.194743  |

Rotational constants (GHz): 1.9481000 1.3680700 1.2451500

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i438.6564 | 66.4510   | 118.9993  |
| 186.2264  | 235.4220  | 247.4238  |
| 280.9674  | 314.3487  | 323.8282  |
| 341.4893  | 353.1295  | 363.1583  |
| 417.6102  | 515.1562  | 518.0181  |
| 586.6503  | 616.1956  | 646.6280  |
| 720.8451  | 801.7847  | 882.8200  |
| 920.6302  | 960.7801  | 965.8557  |
| 968.9684  | 1020.8570 | 1052.0928 |
| 1059.3971 | 1071.3483 | 1191.3253 |
| 1220.7250 | 1298.6957 | 1310.5440 |

|           |           |           |
|-----------|-----------|-----------|
| 1342.5394 | 1386.7648 | 1393.0124 |
| 1415.4389 | 1456.0361 | 1488.2101 |
| 1494.2344 | 1505.6840 | 1519.5894 |
| 1583.5778 | 1615.9052 | 1733.5601 |
| 2241.5585 | 3059.2726 | 3063.8150 |
| 3125.8699 | 3133.9431 | 3137.1256 |
| 3156.6025 | 3163.3038 | 3179.2817 |
| 3207.2244 | 3260.4921 | 3885.1490 |

Zero-point correction (Hartree): 0.175707

TS.diMeCCHCH2\_H\_COO+H2O.ppd

~~~~~  
E(RM062X/Aug-CC-pVTZ) (Hartree): -461.33182581

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.797178  | 0.484499  | 0.689585  |
| O | 1.903438  | 0.554246  | 0.075715  |
| O | 1.894685  | -0.354446 | -1.027480 |
| H | 0.860370  | 0.917718  | 1.687369  |
| C | -0.588717 | 0.524645  | 0.059816  |
| C | -0.928225 | -0.611281 | -0.879666 |
| C | -1.589684 | 0.648085  | 1.208214  |
| C | -0.565400 | 1.829111  | -0.765919 |
| C | -1.895217 | -1.498501 | -0.689793 |
| H | -0.319599 | -0.650250 | -1.772574 |
| H | -2.091848 | -2.259273 | -1.432661 |
| H | -2.527172 | -1.502332 | 0.189114  |
| O | 0.990520  | -1.441171 | 1.069673  |
| H | 1.448744  | -1.394392 | 0.154839  |
| H | 0.170746  | -1.921826 | 0.907713  |
| H | -1.369831 | 1.529284  | 1.811053  |
| H | -1.562762 | -0.224459 | 1.862764  |
| H | -2.599154 | 0.752266  | 0.814864  |
| H | 0.158881  | 1.741020  | -1.573966 |
| H | -0.299446 | 2.684465  | -0.143350 |
| H | -1.557681 | 1.999398  | -1.181848 |

Rotational constants (GHz): 1.9778900 1.4106800 1.2269100

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i376.6986 | 55.8790   | 113.3600  |
| 201.9614  | 235.9564  | 273.9523  |
| 286.9930  | 297.0839  | 328.8960  |
| 339.5355  | 348.3969  | 400.6175  |
| 423.3183  | 449.9499  | 523.0242  |
| 597.2366  | 645.0589  | 721.1571  |
| 729.6258  | 801.6954  | 884.2341  |
| 930.0943  | 957.6058  | 967.2513  |
| 979.5532  | 1031.4851 | 1044.7806 |
| 1066.3183 | 1079.9474 | 1133.8990 |
| 1190.2512 | 1233.8541 | 1293.3220 |
| 1332.6808 | 1391.7386 | 1394.8203 |
| 1418.3161 | 1453.5052 | 1491.7786 |
| 1493.1233 | 1508.1598 | 1518.3614 |
| 1564.9483 | 1690.0053 | 1719.6592 |
| 2723.3808 | 3059.9642 | 3063.0205 |
| 3129.4525 | 3135.4280 | 3143.3860 |
| 3151.4536 | 3156.3967 | 3170.4698 |
| 3216.4304 | 3253.1993 | 3849.8104 |

Zero-point correction (Hartree): 0.176776

TS.diMeCCHCH2\_H\_COO+H2O.ppu

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E(RM062X/Aug-CC-pVTZ) (Hartree): -461.33021904

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.757755  | 0.692299  | 0.525072  |
| O | 1.816341  | 0.722966  | -0.173863 |
| O | 1.854288  | -0.408062 | -1.047558 |
| H | 0.836700  | 1.330949  | 1.406480  |
| C | -0.661028 | 0.468909  | 0.052587  |
| C | -0.882831 | -0.676824 | -0.908402 |
| C | -1.546389 | 0.381170  | 1.294096  |
| C | -0.958806 | 1.786311  | -0.703868 |
| C | -1.617039 | -1.748268 | -0.657163 |
| H | -0.413836 | -0.556598 | -1.874839 |
| H | -1.755964 | -2.504891 | -1.416826 |
| H | -2.085449 | -1.926304 | 0.301154  |
| O | 1.079957  | -1.165158 | 1.201031  |
| H | 1.449567  | -1.224061 | 0.232928  |
| H | 1.855343  | -1.137128 | 1.770865  |
| H | -1.417513 | 1.264955  | 1.920776  |
| H | -1.305418 | -0.501077 | 1.883494  |
| H | -2.591579 | 0.331473  | 0.993826  |
| H | -0.332166 | 1.864792  | -1.590978 |
| H | -0.789060 | 2.659602  | -0.071699 |
| H | -2.005288 | 1.778738  | -1.005993 |

Rotational constants (GHz): 1.9270400 1.4194100 1.2576000

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i400.7723 | 56.6174   | 86.2749   |
| 187.5781  | 247.0068  | 264.0157  |
| 286.7078  | 300.5335  | 313.8933  |
| 333.4518  | 339.3869  | 400.9390  |
| 408.9591  | 460.2804  | 534.4629  |
| 574.6569  | 635.2332  | 655.5451  |
| 715.9144  | 807.6832  | 881.6389  |
| 917.8357  | 959.8704  | 970.1514  |
| 973.9655  | 1025.6224 | 1036.9032 |
| 1046.7480 | 1074.1328 | 1180.8188 |
| 1219.7094 | 1248.1807 | 1301.9866 |
| 1344.7329 | 1387.7469 | 1390.7075 |
| 1414.3324 | 1454.2209 | 1488.8605 |
| 1493.2220 | 1503.0121 | 1524.5790 |
| 1574.2676 | 1629.5044 | 1731.6761 |



|           |           |           |
|-----------|-----------|-----------|
| 2520.2389 | 3058.0479 | 3067.2130 |
| 3124.5808 | 3132.9681 | 3137.8565 |
| 3153.1257 | 3161.4805 | 3176.6433 |
| 3217.2028 | 3258.7971 | 3872.0311 |

Zero-point correction (Hartree): 0.176020

TS.diMeCCHCH2\_H\_COO+H2O.tcd

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E(RM062X/Aug-CC-pVTZ) (Hartree): -461.32887980

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.424515 | -0.167805 | -0.795966 |
| O | -1.662371 | 0.058302  | -0.943913 |
| O | -2.313679 | 0.150197  | 0.325604  |
| H | 0.022483  | -0.567760 | -1.705689 |
| C | 0.544154  | 0.567885  | 0.092867  |
| C | 1.871989  | -0.150408 | 0.143419  |
| C | 0.746398  | 1.891515  | -0.690310 |
| C | 0.111436  | 0.919803  | 1.520024  |
| C | 2.174733  | -1.367297 | -0.285680 |
| H | 2.653655  | 0.448435  | 0.602894  |
| H | 3.183015  | -1.744252 | -0.183653 |
| H | 1.450638  | -2.029981 | -0.741330 |
| O | -0.792228 | -1.812135 | 0.300664  |
| H | -1.572721 | -1.196421 | 0.597214  |
| H | -0.195677 | -1.921576 | 1.046585  |
| H | -0.185443 | 2.454525  | -0.712932 |
| H | 1.083124  | 1.710506  | -1.711192 |
| H | 1.505742  | 2.483863  | -0.180824 |
| H | -0.109129 | 0.033478  | 2.110758  |
| H | -0.772115 | 1.548586  | 1.513010  |
| H | 0.937486  | 1.447528  | 2.000194  |

Rotational constants (GHz): 2.0634100 1.4152500 1.1400200

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i398.6368 | 79.8332   | 149.9878  |
| 186.0390  | 227.0618  | 249.0659  |
| 262.9586  | 296.8888  | 324.3288  |
| 346.9553  | 356.1344  | 364.0175  |
| 405.7757  | 480.1495  | 549.0657  |
| 587.6682  | 632.8824  | 683.2369  |
| 707.0447  | 802.1224  | 883.5172  |
| 909.3377  | 957.4356  | 978.8266  |
| 996.8911  | 1035.4842 | 1053.5529 |
| 1069.3153 | 1072.6966 | 1161.4290 |
| 1177.1982 | 1244.6640 | 1294.2890 |
| 1350.2413 | 1393.5531 | 1394.7430 |
| 1423.3630 | 1466.6281 | 1482.1272 |
| 1485.0333 | 1501.6285 | 1507.0344 |
| 1567.6910 | 1662.8478 | 1725.9542 |
| 2514.7067 | 3062.6444 | 3069.5276 |
| 3139.1631 | 3143.4703 | 3145.6785 |
| 3151.7001 | 3153.3941 | 3173.6624 |
| 3190.0995 | 3254.6476 | 3888.1568 |

Zero-point correction (Hartree): 0.176270

TS.diMeCCHCH2\_H\_COO+H2O.tcu

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E(RM062X/Aug-CC-pVTZ) (Hartree): -461.32872664

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.404722 | -0.215251 | -0.783153 |
| O | -1.632077 | 0.052629  | -0.976296 |
| O | -2.285033 | 0.242603  | 0.280253  |
| H | 0.050771  | -0.668458 | -1.663755 |
| C | 0.558565  | 0.541460  | 0.097924  |
| C | 1.939982  | -0.060014 | -0.018229 |
| C | 0.561786  | 1.938875  | -0.569850 |
| C | 0.234851  | 0.708927  | 1.588081  |
| C | 2.256355  | -1.305655 | -0.334250 |
| H | 2.734582  | 0.637792  | 0.230399  |
| H | 3.289784  | -1.622102 | -0.360060 |
| H | 1.508138  | -2.056722 | -0.550182 |
| O | -0.818112 | -1.739443 | 0.465202  |
| H | -1.585438 | -1.052530 | 0.672779  |
| H | -1.231229 | -2.436070 | -0.055147 |
| H | -0.420431 | 2.396748  | -0.465603 |
| H | 0.824024  | 1.885757  | -1.627200 |
| H | 1.302033  | 2.559043  | -0.065495 |
| H | 0.151254  | -0.258458 | 2.075653  |
| H | -0.685209 | 1.267262  | 1.724103  |
| H | 1.062595  | 1.251369  | 2.048098  |

Rotational constants (GHz): 2.1038200 1.3923300 1.1455900

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i430.9547 | 63.6915   | 110.2357  |
| 183.1696  | 235.0437  | 256.6850  |
| 265.8846  | 307.2728  | 332.1349  |
| 339.1065  | 349.8553  | 360.9886  |
| 410.4260  | 501.8672  | 531.8511  |
| 587.0502  | 632.0681  | 663.5555  |
| 699.7576  | 812.4876  | 888.4397  |
| 909.6131  | 968.7286  | 977.0251  |
| 979.4395  | 1032.7138 | 1045.4293 |
| 1062.4573 | 1077.7953 | 1178.6563 |
| 1245.1352 | 1265.8490 | 1294.6333 |
| 1343.5193 | 1387.6238 | 1392.2128 |
| 1414.7623 | 1460.2513 | 1485.7214 |
| 1492.4833 | 1502.5887 | 1520.3164 |
| 1582.1399 | 1628.7693 | 1732.0915 |
| 2334.8203 | 3061.2561 | 3071.8457 |
| 3136.1617 | 3144.7224 | 3153.0708 |
| 3155.1001 | 3157.1771 | 3177.6579 |
| 3193.9860 | 3258.1890 | 3871.8162 |

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Zero-point correction (Hartree): 0.175937

TS.diMeCCHCH2_H_COO+H2O.tmd
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E(RM062X/Aug-CC-pVTZ) (Hartree): -461.32961588
Electronic state : 1-A
Cartesian coordinates (Angs):
C      -0.704076      0.162901      -0.817710
O      -1.917638      0.383569      -0.539407
O      -2.237798      -0.063276      0.780866
H      -0.532455      0.154536      -1.894766
C      0.526385      0.498518      -0.003893
C      1.658226      -0.341366      -0.549249
C      0.788981      1.971279      -0.418201
C      0.404724      0.432372      1.512661
C      2.521993      -1.044234      0.166386
H      1.758393      -0.334535      -1.632066
H      3.315703      -1.598393      -0.314996
H      2.477360      -1.086586      1.246643
O      -0.880816      -1.807555      -0.397697
H      -1.521011      -1.407479      0.298399
H      -0.111345      -2.153451      0.064095
H      -0.039330      2.603738      -0.101332
H      0.920815      2.073685      -1.495832
H      1.701969      2.307477      0.070414
H      0.197908      -0.576045      1.864786
H      -0.402439      1.069355      1.857283
H      1.347059      0.768973      1.947302
Rotational constants (GHz):      2.1966000      1.3055900      1.1031800
Vibrational harmonic frequencies (cm-1):
i371.4203      64.4695      108.6805
187.2325      244.5661      256.5865
277.6209      301.5998      317.6904
344.8777      358.2007      386.3824
421.0346      460.4025      520.9515
598.4662      618.2073      682.1831
710.1930      801.0235      873.3068
907.4549      952.4879      978.7672
988.4621      1031.8758      1042.2905
1050.9199      1079.8427      1135.9310
1177.3775      1225.3594      1311.7069
1344.0254      1396.8108      1403.3773
1424.0935      1454.5815      1481.6307
1489.0152      1503.5076      1510.8310
1568.3888      1652.2473      1733.2947
2673.0911      3062.3397      3073.2139
3130.8009      3139.2747      3146.0137
3146.6046      3152.6423      3176.4713
3187.5508      3258.5559      3881.8625
Zero-point correction (Hartree): 0.176345

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TS.diMeCCHCH2_H_COO+H2O.tmu
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E(RM062X/Aug-CC-pVTZ) (Hartree): -461.32883142
Electronic state : 1-A
Cartesian coordinates (Angs):
C -0.636350 0.055577 -0.834435
O -1.860279 0.355032 -0.683824
O -2.271018 0.094610 0.659694
H -0.386892 -0.070178 -1.889351
C 0.536035 0.454029 0.034881
C 1.763881 -0.154986 -0.605950
C 0.583680 1.987426 -0.193992
C 0.457437 0.178218 1.532347
C 2.658776 -0.925127 -0.011621
H 1.909062 0.101823 -1.653177
H 3.516917 -1.294594 -0.555713
H 2.569979 -1.217446 1.025619
O -0.870263 -1.813654 -0.115028
H -1.564316 -1.276666 0.441756
H -1.376414 -2.319675 -0.757871
H -0.309695 2.449742 0.223041
H 0.653552 2.241247 -1.252922
H 1.466144 2.380024 0.308842
H 0.364124 -0.885594 1.735955
H -0.390015 0.692927 1.969941
H 1.379279 0.539668 1.989767
Rotational constants (GHz): 2.2822900 1.2761200 1.0913900
Vibrational harmonic frequencies (cm-1):
i399.8703 42.8356 80.3784
186.9539 240.0592 267.8331
286.1389 304.7990 320.0147
340.6683 361.2174 391.6926
415.2254 460.2294 538.0279
577.0338 623.1435 663.1275
701.2329 810.6727 881.0682
908.6740 961.4246 978.8469
988.0133 1030.3000 1039.5308
1046.3392 1082.1775 1178.9477
1217.3087 1270.6269 1308.3817
1343.5679 1391.2765 1401.0645
1415.3532 1455.1781 1487.2735
1492.1568 1503.1209 1524.9758
1580.1154 1625.0493 1740.2513
2490.5963 3059.8251 3077.7913
3124.7899 3134.3019 3138.0203
3154.0276 3156.2353 3179.1867
3197.7369 3260.8766 3880.8457
Zero-point correction (Hartree): 0.176140

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TS.diMeCCHCH2_H_COO+H2O.tpd
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E(RM062X/Aug-CC-pVTZ) (Hartree): -461.32752691  
 Electronic state : 1-A  
 Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.513486 | -0.064414 | -0.827170 |
| O | -1.654062 | 0.471496  | -0.969564 |
| O | -2.345511 | 0.500741  | 0.283381  |
| H | -0.109430 | -0.417532 | -1.775949 |
| C | 0.548421  | 0.276449  | 0.199016  |
| C | 1.619896  | -0.786128 | 0.094561  |
| C | 1.038722  | 1.647438  | -0.305846 |
| C | 0.128922  | 0.412410  | 1.665621  |
| C | 2.841414  | -0.629563 | -0.389184 |
| H | 1.334120  | -1.760632 | 0.479659  |
| H | 3.541023  | -1.453811 | -0.400580 |
| H | 3.193097  | 0.314740  | -0.783014 |
| O | -1.332381 | -1.719373 | -0.061715 |
| H | -1.968995 | -0.977732 | 0.315459  |
| H | -0.915583 | -2.150855 | 0.687908  |
| H | 0.238872  | 2.377961  | -0.200149 |
| H | 1.349856  | 1.617951  | -1.350629 |
| H | 1.889557  | 1.961940  | 0.297485  |
| H | -0.277292 | -0.517428 | 2.060157  |
| H | -0.622697 | 1.184419  | 1.786881  |
| H | 1.019770  | 0.660912  | 2.243983  |

Rotational constants (GHz): 2.4232000 1.1890200 1.0694300  
 Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i430.1490 | 60.1895   | 86.5359   |
| 189.3767  | 229.4304  | 263.6682  |
| 292.0810  | 315.5207  | 323.3289  |
| 328.0556  | 352.9264  | 378.2465  |
| 399.8168  | 487.9149  | 513.7343  |
| 612.1839  | 638.5333  | 684.6331  |
| 704.4245  | 799.6613  | 880.1908  |
| 907.2886  | 962.8285  | 974.5318  |
| 991.3748  | 1022.3360 | 1039.0905 |
| 1057.3541 | 1085.2443 | 1158.3373 |
| 1199.4799 | 1259.6212 | 1270.2274 |
| 1343.1352 | 1389.2269 | 1393.6501 |
| 1419.2609 | 1455.6405 | 1484.6762 |
| 1487.0674 | 1503.2074 | 1511.7862 |
| 1553.2581 | 1681.8036 | 1734.1562 |
| 2377.1777 | 3064.7542 | 3072.6473 |
| 3137.5629 | 3139.3024 | 3143.6336 |
| 3155.9938 | 3158.2830 | 3176.6295 |
| 3190.1416 | 3256.6561 | 3903.1723 |

Zero-point correction (Hartree): 0.175877

TS.diMeCCHCH2\_H\_COO+H2O.tpu  
 ~~~~~  
 E(RM062X/Aug-CC-pVTZ) (Hartree): -461.33083342
 Electronic state : 1-A
 Cartesian coordinates (Angs):

C	-0.507983	-0.058207	-0.829237
O	-1.657428	0.459566	-0.979568
O	-2.348265	0.500472	0.271077
H	-0.099935	-0.416941	-1.775672
C	0.551456	0.285259	0.193761
C	1.606148	-0.795901	0.103203
C	1.055295	1.646023	-0.324940
C	0.127520	0.428448	1.658663
C	2.831073	-0.656533	-0.378291
H	1.285779	-1.754400	0.496968
H	3.521593	-1.488706	-0.378541
H	3.196935	0.280026	-0.778341
O	-1.236821	-1.694810	0.117372
H	-1.899883	-0.933962	0.414553
H	-1.712262	-2.229325	-0.525703
H	0.263856	2.387285	-0.229090
H	1.372780	1.604206	-1.367673
H	1.906573	1.956461	0.279870
H	-0.284961	-0.503149	2.038430
H	-0.612212	1.212533	1.778713
H	1.020793	0.669612	2.236497

Rotational constants (GHz): 2.4285800 1.1961400 1.0762600
 Vibrational harmonic frequencies (cm-1):

i428.5826	63.8346	94.7222
192.1021	241.6733	275.7029
297.8949	313.8175	327.5682
330.3839	345.5816	372.4125
399.1584	509.3578	520.7886
586.9063	618.5353	666.1644
712.3748	807.1923	881.6937
903.9640	965.1481	972.4982
988.0303	1023.8857	1055.5128
1061.6797	1087.8220	1188.3712
1260.0505	1268.7753	1292.5004
1332.7169	1386.9448	1392.2693
1418.1844	1454.5485	1484.9563
1495.3564	1502.0972	1519.6857
1578.3426	1618.7060	1732.0388
2309.0028	3062.7522	3074.0190
3128.8151	3136.3027	3151.0974
3154.1614	3170.2827	3183.2472
3189.1746	3253.1879	3881.5163

Zero-point correction (Hartree): 0.175955

 E- (C (CH3) 2-CH=CH2) CHOO
 #####
 Population analysis as 298K (%)

Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)

Compound	Qtot	Erel	Erel2	n*Q*MB	%
TS.H_diMeCCHCH2_COO+H2O.cmu	4.024e+41	0.00	0.00	8.048e+41	18.8
TS.H_diMeCCHCH2_COO+H2O.ppu	4.346e+41	0.16	0.16	6.583e+41	15.3
TS.H_diMeCCHCH2_COO+H2O.ppd	3.472e+41	0.24	0.24	4.665e+41	10.9
TS.H_diMeCCHCH2_COO+H2O.mmd	3.962e+41	0.44	0.44	3.748e+41	8.74
TS.H_diMeCCHCH2_COO+H2O.pcu	4.642e+41	0.71	0.71	2.780e+41	6.48
TS.H_diMeCCHCH2_COO+H2O.mmu	4.509e+41	0.72	0.72	2.672e+41	6.23
TS.H_diMeCCHCH2_COO+H2O.pcd	4.206e+41	0.73	0.73	2.434e+41	5.68
TS.H_diMeCCHCH2_COO+H2O.mpu	4.691e+41	0.87	0.87	2.171e+41	5.06
TS.H_diMeCCHCH2_COO+H2O.pmu	4.519e+41	0.92	0.92	1.919e+41	4.47
TS.H_diMeCCHCH2_COO+H2O.mpd	4.268e+41	0.94	0.94	1.755e+41	4.09
TS.H_diMeCCHCH2_COO+H2O.cpu	5.475e+41	1.15	1.15	1.580e+41	3.68
TS.H_diMeCCHCH2_COO+H2O.pmd	3.941e+41	1.00	1.00	1.467e+41	3.42
TS.H_diMeCCHCH2_COO+H2O.cpd	3.624e+41	1.12	1.12	1.087e+41	2.54
TS.H_diMeCCHCH2_COO+H2O.mcu	3.403e+41	1.18	1.18	9.296e+40	2.17
TS.H_diMeCCHCH2_COO+H2O.ccu	3.367e+41	1.52	1.52	5.154e+40	1.2
TS.H_diMeCCHCH2_COO+H2O.cmd	5.016e+41	1.85	1.85	4.419e+40	1.03
TS.H_diMeCCHCH2_COO+H2O.ccd	3.650e+41	2.58	2.58	9.393e+39	0.219
Total				4.289e+42	100

TS.H_diMeCCHCH2_COO+H2O.ccd

E(RM062X/Aug-CC-pVTZ) (Hartree): -461.33514500

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-0.461766	-0.624106	0.017664
O	-1.190783	-0.195735	0.959707
O	-2.554335	-0.474903	0.618284
H	-0.791902	-1.531872	-0.481727
C	0.991513	-0.282925	-0.028117
C	1.333589	1.138517	0.344664
C	1.650658	-1.252444	0.977989
C	1.515062	-0.581129	-1.438835
C	0.519643	2.176217	0.438697
H	2.397717	1.282354	0.512304
H	0.915821	3.151704	0.686086
H	-0.545285	2.098234	0.276481
O	-1.482072	0.411175	-1.367874
H	-2.236566	0.110948	-0.669481
H	-1.642616	-0.065190	-2.186892
H	1.430455	-2.291057	0.727615
H	1.305030	-1.050948	1.990057
H	2.731058	-1.114904	0.938520
H	1.051648	0.084420	-2.164147
H	1.316981	-1.617925	-1.717741
H	2.592985	-0.424834	-1.464392

Rotational constants (GHz): 2.0310000 1.2346600 1.1638400

Vibrational harmonic frequencies (cm-1):

i436.5351	68.0327	99.8785
152.9212	172.8298	235.7358
266.5999	291.0470	303.0876
316.7209	348.6636	374.6131
425.7177	489.9342	507.8815
587.4938	624.4510	692.1721
696.8039	801.8919	935.2245
951.9557	964.4891	975.4603
998.1663	1029.0619	1041.0856
1077.6665	1105.8883	1172.7677
1212.1004	1228.5358	1329.2624
1346.3036	1372.6714	1393.2529
1417.4831	1462.8343	1487.1477
1490.8058	1502.3272	1515.6706
1552.9852	1655.3755	1739.3371
2136.5584	3058.6197	3061.9426
3131.3556	3134.9223	3147.7082
3150.5584	3155.3360	3156.2736
3183.6304	3273.1172	3892.4939

Zero-point correction (Hartree): 0.175184

TS.H_diMeCCHCH2_COO+H2O.ccu

E(RM062X/Aug-CC-pVTZ) (Hartree): -461.33762975

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-0.456033	-0.666881	0.032482
O	-1.207530	-0.204735	0.937221
O	-2.565277	-0.489062	0.580361
H	-0.779150	-1.580976	-0.458451
C	0.988707	-0.282641	-0.013633
C	1.244813	1.205310	0.063723
C	1.660102	-0.972574	1.193952
C	1.581897	-0.833545	-1.315628
C	0.418996	2.182833	0.405599
H	2.270626	1.458616	-0.191028
H	0.772665	3.204802	0.416780
H	-0.605765	2.010252	0.703998
O	-1.423312	0.224055	-1.507307
H	-2.189236	0.033128	-0.833784
H	-1.232701	1.166871	-1.462820
H	1.525821	-2.053988	1.146158
H	1.243867	-0.601851	2.128076
H	2.728671	-0.758905	1.171630
H	1.097061	-0.386576	-2.181628
H	1.458241	-1.915722	-1.366345
H	2.647969	-0.612725	-1.353759

Rotational constants (GHz): 2.0159000 1.2361700 1.1772800

Vibrational harmonic frequencies (cm-1):

i334.9552	70.6395	119.3639
145.8424	173.0248	227.4661
252.5492	283.7054	315.0078

316.4297	343.7597	378.3741
423.2871	475.0705	538.4453
575.2277	597.5813	651.2538
709.5866	800.4108	927.0680
955.2060	968.9528	973.8514
1002.1529	1032.7889	1054.4752
1068.8087	1119.7045	1182.6155
1217.1694	1245.6344	1319.0802
1350.6976	1380.9108	1395.7424
1423.5282	1452.8737	1487.4890
1489.3918	1504.2180	1515.7443
1593.1587	1611.1410	1728.8891
2516.6960	3061.6545	3066.9800
3134.2018	3139.3924	3148.0757
3154.7677	3158.9586	3162.3890
3177.6529	3261.9238	3867.9748

Zero-point correction (Hartree): 0.175986

TS_H_diMeCCHCH2_COO+H2O.cmd

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E(RM062X/Aug-CC-pVTZ) (Hartree): -461.33669141

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.722315  | 0.421378  | -0.267360 |
| O | 1.392788  | 0.478209  | 0.804056  |
| O | 2.765295  | 0.221768  | 0.481173  |
| H | 1.205448  | 0.780276  | -1.173192 |
| C | -0.774100 | 0.401274  | -0.199683 |
| C | -1.240187 | -0.362127 | 1.014444  |
| C | -1.179847 | 1.886334  | -0.048389 |
| C | -1.315954 | -0.146430 | -1.515986 |
| C | -2.119977 | -1.348953 | 1.010890  |
| H | -0.809675 | -0.030970 | 1.952953  |
| H | -2.415191 | -1.826079 | 1.934842  |
| H | -2.570134 | -1.724111 | 0.101631  |
| O | 1.393932  | -1.413092 | -0.702119 |
| H | 2.234173  | -0.956223 | -0.247448 |
| H | 1.617636  | -1.556234 | -1.625924 |
| H | -0.788468 | 2.485568  | -0.871779 |
| H | -0.808948 | 2.296262  | 0.889577  |
| H | -2.266825 | 1.951359  | -0.056643 |
| H | -1.058267 | -1.196713 | -1.636547 |
| H | -0.909327 | 0.416817  | -2.357092 |
| H | -2.400041 | -0.043892 | -1.538753 |

Rotational constants (GHz): 2.1653200 1.1407800 1.0574500

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i404.5452 | 51.3544   | 76.6102   |
| 165.9386  | 183.3011  | 253.0236  |
| 270.5522  | 301.6819  | 313.4226  |
| 322.2150  | 363.3778  | 372.1566  |
| 445.9123  | 478.6402  | 503.4851  |
| 594.9326  | 621.8076  | 676.7885  |
| 722.4447  | 784.4587  | 933.8591  |
| 947.2580  | 964.8573  | 977.6778  |
| 983.6559  | 1027.2409 | 1049.1825 |
| 1055.5187 | 1104.7853 | 1179.0644 |
| 1209.4388 | 1251.8265 | 1306.8523 |
| 1340.9191 | 1362.6866 | 1393.9262 |
| 1415.5833 | 1457.1132 | 1489.3611 |
| 1493.4137 | 1504.3882 | 1521.0428 |
| 1554.8732 | 1674.8725 | 1739.4116 |
| 2255.3974 | 3061.0337 | 3066.9705 |
| 3135.2228 | 3137.6012 | 3148.7231 |
| 3153.7367 | 3157.7323 | 3174.4275 |
| 3185.7727 | 3258.8564 | 3889.3804 |

Zero-point correction (Hartree): 0.175569

TS\_H\_diMeCCHCH2\_COO+H2O.cmu

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E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -460.67624572

E(CCSD/Aug-CC-pVTZ) (Hartree): -460.59071124

T1 diagnostic: 0.019233

E(MP2/Aug-CC-pVTZ) (Hartree): -460.54013940

E(MP3/Aug-CC-pVTZ) (Hartree): -460.57781386

E(RHF/Aug-CC-pVTZ) (Hartree): -458.75283380

E(RM062X/Aug-CC-pVTZ) (Hartree): -461.34015211

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-0.711886	-0.451623	-0.310685
O	-1.443027	-0.512928	0.717101
O	-2.784247	-0.186535	0.334495
H	-1.158670	-0.729036	-1.261901
C	0.780485	-0.460158	-0.148268
C	1.160435	0.472265	0.977498
C	1.156430	-1.906002	0.241010
C	1.415956	-0.097957	-1.486515
C	1.947742	1.530988	0.869846
H	0.732497	0.218160	1.941579
H	2.176567	2.137752	1.735094
H	2.395303	1.827784	-0.069486
O	-1.283948	1.424912	-0.822924
H	-2.146449	1.027302	-0.408203
H	-0.902304	2.009689	-0.158889
H	0.808631	-2.613488	-0.512499
H	0.718951	-2.175984	1.200549
H	2.240924	-1.979129	0.311359
H	1.114741	0.895972	-1.812313
H	1.113401	-0.814342	-2.250379
H	2.501218	-0.133346	-1.401605

Rotational constants (GHz): 2.1206000 1.1979900 1.0555400

Vibrational harmonic frequencies (cm-1):

i334.0851	64.1268	86.4775

166.7637	180.6531	243.2106
257.0513	298.9169	302.7929
325.3730	350.0456	378.0346
448.8270	479.1697	516.6798
572.8266	598.1206	652.9639
721.1981	789.4793	929.6213
954.0700	964.4492	975.6395
989.0292	1029.1661	1053.2398
1060.6633	1107.7125	1191.8125
1243.1186	1252.3917	1298.8340
1338.8759	1366.7473	1397.4846
1420.3212	1456.3573	1490.4369
1491.0826	1506.2315	1518.9596
1585.2185	1617.6403	1731.3887
2534.6018	3063.2256	3070.9979
3137.9815	3141.4707	3154.1996
3157.8897	3163.0616	3170.5332
3180.5360	3257.2800	3856.7399

Zero-point correction (Hartree): 0.176083

TS_H_diMeCCHCH2_COO+H2O.cpd

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E(RM062X/Aug-CC-pVTZ) (Hartree): -461.33763684

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.691449  | 0.144784  | 0.495801  |
| O | 1.179379  | -1.016152 | 0.371130  |
| O | 2.606254  | -0.893265 | 0.383242  |
| H | 1.229704  | 0.845137  | 1.130108  |
| C | -0.767834 | 0.354359  | 0.235606  |
| C | -1.199988 | -0.464104 | -0.954863 |
| C | -1.481185 | -0.032702 | 1.539338  |
| C | -0.995823 | 1.844239  | -0.055892 |
| C | -2.218612 | -1.306248 | -0.986963 |
| H | -0.604301 | -0.294811 | -1.846014 |
| H | -2.473571 | -1.828586 | -1.898352 |
| H | -2.828668 | -1.514256 | -0.117882 |
| O | 1.734927  | 0.838095  | -1.071960 |
| H | 2.405909  | 0.139293  | -0.611891 |
| H | 2.111285  | 1.714519  | -0.954348 |
| H | -1.098370 | 0.554761  | 2.374430  |
| H | -1.345385 | -1.089528 | 1.762421  |
| H | -2.545696 | 0.176807  | 1.441640  |
| H | -0.527056 | 2.129564  | -0.995405 |
| H | -0.590540 | 2.463828  | 0.746397  |
| H | -2.065825 | 2.031884  | -0.128564 |

Rotational constants (GHz): 2.1851500 1.1313200 1.0552400

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i443.9937 | 63.9723   | 91.7373   |
| 157.4321  | 185.9957  | 245.6848  |
| 284.3693  | 302.4818  | 315.6616  |
| 317.7478  | 346.3410  | 381.8153  |
| 446.4121  | 492.6792  | 516.3894  |
| 581.4194  | 637.3884  | 682.2288  |
| 722.1443  | 783.7944  | 935.4168  |
| 954.5356  | 965.5958  | 974.4410  |
| 983.0799  | 1024.3981 | 1055.9807 |
| 1067.7253 | 1096.1927 | 1196.2924 |
| 1214.6964 | 1245.9650 | 1301.2271 |
| 1336.8821 | 1358.3895 | 1394.2775 |
| 1415.4147 | 1456.4768 | 1488.6364 |
| 1494.4084 | 1505.7187 | 1518.8399 |
| 1547.2307 | 1658.8560 | 1740.0718 |
| 2121.6647 | 3060.5833 | 3066.1358 |
| 3135.4200 | 3137.9775 | 3152.1624 |
| 3154.9930 | 3159.1473 | 3170.9675 |
| 3180.5941 | 3256.0340 | 3891.2131 |

Zero-point correction (Hartree): 0.175358

TS\_H\_diMeCCHCH2\_COO+H2O.cpu

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E(RM062X/Aug-CC-pVTZ) (Hartree): -461.33758022

Electronic state : 1-A

Cartesian coordinates (Angs):

C	0.688460	0.152737	0.475595
O	1.171682	-1.012496	0.364891
O	2.598513	-0.895131	0.405412
H	1.224986	0.860696	1.101969
C	-0.773005	0.368001	0.223960
C	-1.234229	-0.446885	-0.956854
C	-1.469782	-0.021987	1.536559
C	-1.000307	1.859793	-0.057176
C	-2.200487	-1.349015	-0.957173
H	-0.722016	-0.221936	-1.887956
H	-2.478338	-1.860974	-1.867707
H	-2.744018	-1.615716	-0.060740
O	1.821817	0.945533	-0.983424
H	2.452058	0.210450	-0.529440
H	1.592439	0.594780	-1.849598
H	-1.077130	0.567381	2.365276
H	-1.327123	-1.077653	1.760757
H	-2.535954	0.184666	1.450422
H	-0.511433	2.163643	-0.980276
H	-0.603768	2.469467	0.755605
H	-2.069701	2.046080	-0.142819

Rotational constants (GHz): 2.1675800 1.1311800 1.0447800

Vibrational harmonic frequencies (cm-1):

i423.4720	47.6278	84.4882
156.7744	181.9190	233.9577
280.6630	301.5846	308.0579
319.4591	341.4146	385.2591
443.2309	496.3015	530.7761

568.5792	593.1578	646.4789
716.9235	791.2651	934.1076
957.4777	968.0208	976.2056
987.0322	1024.9978	1039.5366
1064.7027	1126.6069	1199.5873
1242.5995	1286.4798	1301.3600
1338.7002	1372.4974	1396.9440
1422.2634	1457.5948	1489.2947
1489.9657	1505.6990	1517.8049
1583.2990	1614.1453	1738.8182
2141.2881	3066.1031	3068.2198
3138.6757	3141.7285	3154.6303
3156.9458	3160.3992	3160.8281
3177.8286	3258.3210	3875.8945

Zero-point correction (Hartree): 0.175338

TS_H_diMeCCHCH2_COO+H2O.mcu
 ~~~~~  
 E(RM062X/Aug-CC-pVTZ) (Hartree): -461.33763841  
 Electronic state : 1-A  
 Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.518831  | -0.091873 | 0.415846  |
| O | 1.479203  | -0.855773 | 0.096956  |
| O | 2.703880  | -0.208731 | 0.454708  |
| H | 0.638246  | 0.518618  | 1.305922  |
| C | -0.848471 | -0.454141 | -0.069559 |
| C | -1.851532 | 0.650299  | 0.154971  |
| C | -0.827768 | -0.856594 | -1.547131 |
| C | -1.261026 | -1.670010 | 0.793510  |
| C | -1.621283 | 1.907317  | 0.499435  |
| H | -2.876224 | 0.324459  | -0.002460 |
| H | -2.447726 | 2.592519  | 0.629650  |
| H | -0.624587 | 2.301095  | 0.641785  |
| O | 1.298165  | 1.525764  | -0.511119 |
| H | 2.153094  | 0.989126  | -0.170712 |
| H | 1.269855  | 1.431398  | -1.467879 |
| H | -0.137602 | -1.681412 | -1.714645 |
| H | -0.535362 | -0.013918 | -2.172442 |
| H | -1.827226 | -1.168556 | -1.849372 |
| H | -1.244147 | -1.423973 | 1.855066  |
| H | -0.593694 | -2.510703 | 0.612432  |
| H | -2.277127 | -1.958724 | 0.525864  |

Rotational constants (GHz): 2.0683300 1.2891200 1.0152500  
 Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i412.2324 | 66.5759   | 109.9068  |
| 166.3881  | 180.2015  | 228.8591  |
| 271.5386  | 284.0546  | 293.0800  |
| 315.0181  | 346.8385  | 372.4401  |
| 439.5404  | 523.9954  | 534.4114  |
| 557.3019  | 584.7040  | 645.2418  |
| 704.4492  | 802.1997  | 923.3853  |
| 952.9745  | 961.3040  | 992.5207  |
| 999.7196  | 1037.4378 | 1048.3347 |
| 1073.0112 | 1107.1417 | 1183.8541 |
| 1247.3754 | 1289.1474 | 1297.9011 |
| 1347.0214 | 1384.4051 | 1395.5700 |
| 1416.8188 | 1466.8660 | 1487.1863 |
| 1487.9780 | 1503.4705 | 1511.7620 |
| 1584.7279 | 1598.9570 | 1733.5613 |
| 2174.0652 | 3064.5516 | 3069.9674 |
| 3140.5223 | 3142.4978 | 3152.0805 |
| 3153.2159 | 3156.1138 | 3174.6846 |
| 3179.6347 | 3264.1375 | 3882.1103 |

Zero-point correction (Hartree): 0.175448

TS\_H\_diMeCCHCH2\_COO+H2O.mmd  
 ~~~~~  
 E(RM062X/Aug-CC-pVTZ) (Hartree): -461.33898142
 Electronic state : 1-A
 Cartesian coordinates (Angs):

C	0.608350	-0.068190	0.440384
O	1.608384	-0.780518	0.133680
O	2.785879	-0.113736	0.605377
H	0.650107	0.476231	1.380112
C	-0.723193	-0.384069	-0.172487
C	-1.551798	0.880443	-0.154748
C	-0.548841	-0.861204	-1.616020
C	-1.321436	-1.496193	0.702216
C	-2.620979	1.103941	0.592710
H	-1.210627	1.642830	-0.846864
H	-3.159708	2.038553	0.518584
H	-3.004780	0.374230	1.293277
O	1.373439	1.548326	-0.472542
H	2.231802	1.068243	-0.063947
H	1.246277	2.367671	0.013755
H	0.054161	-1.766256	-1.653751
H	-0.054480	-0.092743	-2.208876
H	-1.527860	-1.067979	-2.046473
H	-1.393444	-1.198270	1.748448
H	-0.703766	-2.390266	0.639696
H	-2.321901	-1.733193	0.341595

Rotational constants (GHz): 2.3779400 1.1134200 0.9754400
 Vibrational harmonic frequencies (cm-1):

i418.8937	59.5592	81.3380
160.3271	206.3187	252.0254
281.3771	297.1841	310.4407
329.9863	351.4294	376.5090
441.9873	473.9660	514.0246
594.8327	634.3056	687.8835
710.4430	790.6222	921.6169
949.1911	969.4489	984.9547
990.1505	1027.6476	1059.7937

1070.7817	1102.2668	1194.6804
1225.6682	1267.3342	1276.7657
1334.8174	1354.8745	1396.2687
1415.9225	1454.5917	1489.2244
1494.1629	1504.8364	1515.7477
1551.4065	1664.0310	1732.4482
2190.1513	3065.7567	3071.8430
3139.2430	3149.2168	3152.4430
3157.7906	3161.5394	3170.8390
3181.6556	3255.4367	3888.7197

Zero-point correction (Hartree): 0.175619

TS.H_diMeCCHCH2_COO+H2O.mmu

E(RM062X/Aug-CC-pVT2) (Hartree): -461.33849915

Electronic state : 1-A

Cartesian coordinates (Angs):

C	0.615176	-0.068391	0.435414
O	1.596382	-0.802604	0.115758
O	2.787107	-0.190313	0.626310
H	0.666483	0.456218	1.385389
C	-0.723574	-0.334680	-0.188449
C	-1.568320	0.907532	-0.022105
C	-0.575863	-0.667705	-1.675824
C	-1.289987	-1.544451	0.571160
C	-2.702687	0.992754	0.653412
H	-1.177096	1.786573	-0.523000
H	-3.246148	1.926183	0.700301
H	-3.132507	0.151077	1.179918
O	1.432846	1.626191	-0.284622
H	2.262955	1.074594	0.084801
H	1.510731	1.602352	-1.243534
H	0.089008	-1.517145	-1.819677
H	-0.176294	0.183215	-2.227824
H	-1.555194	-0.906994	-2.087681
H	-1.361192	-1.351590	1.641612
H	-0.652859	-2.412875	0.415024
H	-2.287041	-1.768150	0.193445

Rotational constants (GHz): 2.4114600 1.0899700 0.9637700

Vibrational harmonic frequencies (cm-1):

i406.0373	55.9286	83.3927
158.3571	195.8035	241.2725
283.5131	301.5199	312.0388
320.5404	352.0161	370.0969
442.7632	471.6471	524.9849
579.8985	597.0062	653.8954
709.5255	794.1824	921.8998
947.5834	966.3133	987.2131
991.2534	1026.0119	1048.2301
1072.2842	1120.2668	1199.6048
1262.9901	1277.6945	1286.6941
1341.6834	1370.3707	1395.9056
1416.6616	1456.9772	1489.6683
1492.2829	1506.0011	1516.3074
1582.0538	1619.3658	1735.7242
2200.1020	3067.3451	3069.8517
3140.8520	3142.6803	3153.2243
3157.5860	3170.9032	3172.8568
3182.9862	3258.1088	3873.8379

Zero-point correction (Hartree): 0.175578

TS.H_diMeCCHCH2_COO+H2O.mpd

E(RM062X/Aug-CC-pVT2) (Hartree): -461.33820128

Electronic state : 1-A

Cartesian coordinates (Angs):

C	0.684839	-0.174866	0.434548
O	1.657184	-0.672437	-0.202012
O	2.851287	-0.000075	0.220548
H	0.875958	0.142366	1.457041
C	-0.712979	-0.490119	-0.002131
C	-1.635568	0.477295	0.700461
C	-0.822888	-0.454359	-1.520932
C	-1.002373	-1.912248	0.529978
C	-2.486378	1.305136	0.118187
H	-1.585830	0.446118	1.786567
H	-3.127535	1.944836	0.708676
H	-2.575381	1.376132	-0.957410
O	1.116503	1.682446	-0.178875
H	2.070175	1.262360	-0.040656
H	0.988275	2.364842	0.485210
H	-0.143968	-1.180640	-1.962584
H	-0.563700	0.532464	-1.900414
H	-1.840682	-0.701512	-1.820803
H	-0.890218	-1.964134	1.613558
H	-0.325562	-2.632505	0.073339
H	-2.029247	-2.174836	0.279526

Rotational constants (GHz): 2.3157700 1.1822600 0.9686100

Vibrational harmonic frequencies (cm-1):

i383.5133	65.7286	78.1213
162.1060	178.8447	249.2204
272.5189	293.3719	306.2083
319.9039	356.5421	375.4902
442.9022	468.7498	508.7704
591.0022	606.8139	680.5198
708.0125	793.7256	919.0497
947.1342	967.5354	986.7796
992.0045	1034.5876	1044.2633
1054.5793	1103.9161	1185.8029
1207.2825	1236.0576	1308.3854
1343.1846	1363.5268	1396.9728
1414.9708	1453.2836	1490.2792

1492.7793	1505.7952	1514.7593
1555.9358	1652.2322	1740.4269
2351.5622	3062.7098	3075.5824
3137.6240	3141.4023	3150.8179
3151.4630	3153.8868	3161.1983
3177.7672	3259.8289	3896.4318

Zero-point correction (Hartree): 0.175625

TS_H_diMeCCHCH2_COO+H2O.mpu

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E(RM062X/Aug-CC-pVTZ) (Hartree): -461.33837571

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.710411 | -0.196591 | -0.409503 |
| O | -1.635231 | -0.659558 | 0.320506  |
| O | -2.867536 | -0.051719 | -0.084782 |
| H | -0.953692 | 0.037688  | -1.442451 |
| C | 0.715056  | -0.474637 | -0.038466 |
| C | 1.559788  | 0.645474  | -0.597831 |
| C | 0.870034  | -0.671767 | 1.463022  |
| C | 1.076400  | -1.778252 | -0.789103 |
| C | 2.500314  | 1.305422  | 0.056529  |
| H | 1.365219  | 0.887871  | -1.638758 |
| H | 3.077296  | 2.075219  | -0.436230 |
| H | 2.729261  | 1.109611  | 1.095522  |
| O | -1.181265 | 1.725666  | -0.112068 |
| H | -2.117655 | 1.245647  | -0.066255 |
| H | -0.951605 | 2.005066  | 0.779291  |
| H | 0.226738  | -1.478111 | 1.807992  |
| H | 0.605939  | 0.233598  | 2.009672  |
| H | 1.902263  | -0.928143 | 1.696840  |
| H | 0.960944  | -1.660971 | -1.866676 |
| H | 0.443239  | -2.599412 | -0.454911 |
| H | 2.117227  | -2.021079 | -0.581171 |

Rotational constants (GHz): 2.3183700 1.1672600 0.9611300

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i386.2907 | 48.5782   | 97.4641   |
| 156.7230  | 184.2172  | 243.2743  |
| 273.7001  | 298.9986  | 307.8924  |
| 324.6477  | 358.6471  | 370.3797  |
| 446.7661  | 477.4927  | 531.2216  |
| 561.4954  | 599.1986  | 644.9344  |
| 712.5891  | 795.9808  | 921.9689  |
| 948.8836  | 959.9558  | 979.8554  |
| 986.9036  | 1033.6309 | 1045.6938 |
| 1062.3650 | 1133.1969 | 1187.0818 |
| 1234.8493 | 1275.7976 | 1311.7026 |
| 1348.0286 | 1370.7639 | 1399.3397 |
| 1418.8161 | 1454.9674 | 1487.5019 |
| 1493.6041 | 1507.6208 | 1513.5704 |
| 1582.2430 | 1593.9480 | 1739.2041 |
| 2319.4489 | 3063.9237 | 3072.1163 |
| 3140.9447 | 3143.1870 | 3150.9763 |
| 3157.9651 | 3159.4964 | 3165.3424 |
| 3178.7645 | 3259.3641 | 3880.6835 |

Zero-point correction (Hartree): 0.175688

TS\_H\_diMeCCHCH2\_COO+H2O.pcd

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E(RM062X/Aug-CC-pVTZ) (Hartree): -461.33815986

Electronic state : 1-A

Cartesian coordinates (Angs):

C	0.459765	0.201615	-0.326822
O	1.060257	0.949819	0.500927
O	2.372806	1.207329	-0.011384
H	0.668916	0.358514	-1.381767
C	-0.820729	-0.452428	0.079612
C	-1.950604	0.519541	-0.207192
C	-1.019709	-1.705200	-0.783015
C	-0.802862	-0.821881	1.564970
C	-1.853112	1.822972	-0.418420
H	-2.929119	0.048086	-0.215416
H	-2.739020	2.415786	-0.598933
H	-0.906992	2.349249	-0.405486
O	1.925778	-1.157670	-0.280375
H	2.449939	-0.225933	-0.194325
H	2.149981	-1.533678	-1.136067
H	-0.263404	-2.450767	-0.547546
H	-0.970004	-1.464833	-1.846059
H	-2.002726	-2.128165	-0.578598
H	-0.675524	0.063294	2.183599
H	0.015749	-1.513158	1.763516
H	-1.745018	-1.301932	1.828934

Rotational constants (GHz): 2.0720000 1.3066400 1.0100800

Vibrational harmonic frequencies (cm-1):

i448.7091	66.6487	86.2771
138.8645	194.4589	228.6691
262.0642	277.4617	310.1269
337.5624	361.2608	373.9601
434.9349	482.2435	532.3362
582.3261	636.7838	689.8957
706.3367	797.5027	925.9263
943.8268	971.1424	991.1502
993.5602	1037.1569	1044.8886
1061.6263	1100.7343	1207.4353
1213.5279	1249.5582	1287.9375
1338.3406	1367.4635	1398.0272
1419.2415	1458.8166	1486.9577
1491.9234	1505.9849	1513.3663
1550.4537	1655.2440	1723.3386
2125.0197	3063.8313	3069.8549
3134.9297	3144.0960	3156.9788

3157.9422 3160.1490 3163.2193
 3172.9198 3255.0742 3889.2754
 Zero-point correction (Hartree): 0.175261

TS.H_diMeCCHCH2_COO+H2O.pcu

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 E(RM062X/Aug-CC-pVT2) (Hartree): -461.33829904

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.465087 | -0.189908 | -0.322888 |
| O | -1.068400 | -0.928453 | 0.513129  |
| O | -2.375861 | -1.198463 | -0.005837 |
| H | -0.676407 | -0.348189 | -1.376596 |
| C | 0.825382  | 0.453537  | 0.071269  |
| C | 1.937633  | -0.543761 | -0.204502 |
| C | 1.046408  | 1.686280  | -0.814508 |
| C | 0.832509  | 0.839625  | 1.552196  |
| C | 1.818340  | -1.849621 | -0.386049 |
| H | 2.922385  | -0.086435 | -0.235235 |
| H | 2.693874  | -2.458322 | -0.564328 |
| H | 0.864937  | -2.361537 | -0.353735 |
| O | -1.946014 | 1.153905  | -0.452281 |
| H | -2.453715 | 0.224794  | -0.309972 |
| H | -2.046914 | 1.638934  | 0.372874  |
| H | 0.286996  | 2.441285  | -0.624639 |
| H | 1.011727  | 1.420405  | -1.871015 |
| H | 2.027421  | 2.108887  | -0.599332 |
| H | 0.655045  | -0.028123 | 2.183001  |
| H | 0.064873  | 1.587291  | 1.756571  |
| H | 1.800873  | 1.268194  | 1.809210  |

Rotational constants (GHz): 2.0608700 1.3018500 1.0080100

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i426.4216 | 62.1591   | 87.0721   |
| 141.5464  | 192.7371  | 224.9898  |
| 256.7568  | 270.2816  | 309.8291  |
| 333.9627  | 352.7354  | 377.2529  |
| 441.1669  | 486.3401  | 539.4035  |
| 579.2967  | 601.1398  | 662.2918  |
| 700.5995  | 803.5507  | 925.2511  |
| 941.6333  | 967.1986  | 995.0696  |
| 996.8297  | 1036.7958 | 1044.8238 |
| 1064.1751 | 1127.7554 | 1209.4954 |
| 1241.7442 | 1281.1971 | 1289.5256 |
| 1340.8551 | 1379.1060 | 1402.0438 |
| 1426.6766 | 1460.3184 | 1485.5224 |
| 1488.1241 | 1504.1136 | 1510.3591 |
| 1584.1343 | 1613.4821 | 1724.3856 |
| 2154.5875 | 3064.6999 | 3069.9431 |
| 3134.0451 | 3141.1598 | 3156.9521 |
| 3161.1676 | 3162.1676 | 3169.4044 |
| 3173.4971 | 3255.5311 | 3870.8918 |

Zero-point correction (Hartree): 0.175368

TS.H\_diMeCCHCH2\_COO+H2O.pmd

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 E(RM062X/Aug-CC-pVT2) (Hartree): -461.33787047

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-0.588959	-0.185762	-0.423205
O	-1.094295	-1.136911	0.242417
O	-2.448847	-1.304290	-0.191143
H	-0.904585	-0.082035	-1.458647
C	0.720872	0.398003	0.015034
C	1.769085	-0.422836	-0.715623
C	0.805182	1.843743	-0.495080
C	0.848968	0.350044	1.531085
C	2.713575	-1.152109	-0.145696
H	1.722686	-0.364336	-1.799688
H	3.436741	-1.685156	-0.747056
H	2.803272	-1.242541	0.928275
O	-2.064375	1.066259	0.101474
H	-2.562521	0.119934	-0.000717
H	-2.383553	1.635619	-0.603909
H	0.074834	2.467663	0.015358
H	0.625864	1.894577	-1.570542
H	1.804799	2.229674	-0.300942
H	0.805250	-0.670908	1.904317
H	0.030524	0.911372	1.979310
H	1.794483	0.799180	1.833164

Rotational constants (GHz): 2.3589000 1.1448200 0.9506000

Vibrational harmonic frequencies (cm-1):

i453.9981	58.3930	81.5253
168.9458	196.1099	255.8459
275.3292	294.3895	308.7146
339.4521	350.6172	385.4694
448.1060	504.1782	507.7524
571.7375	640.2155	680.8452
716.4840	789.5100	923.1050
944.7328	971.7581	987.3527
991.2341	1030.1291	1043.1419
1068.2659	1097.0030	1207.1050
1212.9612	1231.8561	1306.1530
1343.2288	1360.8143	1398.1396
1415.6961	1451.0700	1489.2528
1494.5685	1507.3756	1516.3047
1544.4941	1654.3319	1729.6780
2111.2779	3062.6720	3074.6131
3135.2839	3149.8667	3150.8855
3156.1673	3159.7176	3161.4693
3179.6929	3261.9107	3889.5490

Zero-point correction (Hartree): 0.175388

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TS.H_diMeCCHCH2_COO+H2O.pmu
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E(RM062X/Aug-CC-pVTZ) (Hartree): -461.33803872
Electronic state : 1-A
Cartesian coordinates (Angs):
C      -0.590959      -0.183495      -0.408972
O      -1.100343      -1.119765      0.276292
O      -2.445840      -1.309237      -0.175619
H      -0.899738      -0.097077      -1.447396
C       0.722926       0.403452       0.015526
C       1.758181      -0.435366      -0.714735
C       0.815583       1.840623      -0.517081
C       0.876257       0.367932       1.529359
C       2.698172      -1.171823      -0.146669
H       1.702772      -0.384223      -1.798425
H       3.409775      -1.717544      -0.750381
H       2.796699      -1.257300       0.926962
O      -2.108574       1.095199      -0.094297
H      -2.578882       0.134179      -0.128683
H      -2.147022       1.376171       0.825273
H       0.086007       2.482705      -0.028959
H       0.631615       1.873901      -1.591264
H       1.817630       2.222753      -0.327484
H       0.807392      -0.646129       1.917153
H       0.091652       0.962428       1.997204
H       1.839194       0.792621       1.810433
Rotational constants (GHz):      2.3429500      1.1401800      0.9472400
Vibrational harmonic frequencies (cm-1):
1432.9694      53.5992      81.5660
171.7791      192.8834      244.0405
275.0549      295.2915      304.1583
332.5666      347.5398      387.4850
444.7203      503.8801      523.9058
566.7486      596.5777      646.6034
708.5977      795.0397      922.2241
942.8105      968.4041      988.0348
993.2873      1030.8687      1043.8780
1068.0635      1128.6033      1207.3397
1223.5588      1280.7570      1306.6711
1343.9180      1374.1084      1404.1620
1422.9633      1452.1501      1487.5741
1490.3783      1504.6718      1513.7439
1581.7336      1610.9695      1729.3779
2129.3081      3069.3046      3072.6313
3140.8860      3141.9953      3156.0322
3159.8604      3162.4384      3165.1212
3180.1183      3261.8145      3874.0949
Zero-point correction (Hartree): 0.175432

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TS.H_diMeCCHCH2_COO+H2O.ppd
~~~~~
E(RM062X/Aug-CC-pVTZ) (Hartree): -461.33922170
Electronic state : 1-A
Cartesian coordinates (Angs):
C      -0.550111      -0.268614      -0.340082
O      -1.277373      -1.001530      0.394149
O      -2.548732      -1.145001      -0.250633
H      -0.661140      -0.372578      -1.416184
C       0.726814       0.280141       0.222583
C       1.699646      -0.882620       0.115131
C       1.150183       1.483956      -0.612121
C       0.541004       0.669295       1.690796
C       2.766193      -0.935347      -0.666760
H       1.459328      -1.725436       0.755495
H       3.408503      -1.805092      -0.663268
H       3.044372      -0.123346      -1.325090
O      -1.920698       1.193115      -0.380436
H      -2.510316       0.298211      -0.380527
H      -2.037390       1.610414      -1.238333
H       0.442533       2.297643      -0.468224
H       1.196605       1.242705      -1.675086
H       2.136862       1.819129      -0.294871
H       0.271938      -0.194751       2.295015
H      -0.251157       1.411797       1.777851
H       1.471903       1.087762       2.071301
Rotational constants (GHz):      2.4060600      1.0945200      0.9668000
Vibrational harmonic frequencies (cm-1):
1440.1327      64.4228      88.3450
163.6641      197.8809      245.8048
281.8414      299.9229      306.8043
339.3286      362.6101      376.0305
450.3491      485.8315      505.3909
594.2135      634.0645      677.4185
715.9246      783.9486      923.4250
944.9969      973.2299      988.1268
991.8708      1029.3117      1052.6514
1073.6193      1096.7625      1198.9409
1226.9855      1260.0620      1280.5837
1336.7478      1361.0883      1399.2401
1417.4931      1451.0640      1489.7702
1494.9770      1508.2447      1515.9065
1544.3252      1659.9706      1725.0142
2133.1326      3066.5135      3072.2091
3137.6387      3150.5428      3156.5527
3158.2399      3161.8409      3166.1480
3178.7159      3258.1161      3890.1479
Zero-point correction (Hartree): 0.175528

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TS.H_diMeCCHCH2_COO+H2O.ppu
~~~~~
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -460.67508030
E(CCSD/Aug-CC-pVTZ) (Hartree): -460.58927145

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T1 diagnostic: 0.018762
E(MP2/Aug-CC-pVTZ) (Hartree): -460.53975809
E(MP3/Aug-CC-pVTZ) (Hartree): -460.57662030
E(RHF/Aug-CC-pVTZ) (Hartree): -458.74977419
E(RM062X/Aug-CC-pVTZ) (Hartree): -461.33930572
Electronic state : 1-A
Cartesian coordinates (Angs):
C -0.553769 -0.267361 -0.325309
O -1.279080 -0.977043 0.434899
O -2.542529 -1.162337 -0.214837
H -0.663770 -0.402446 -1.397475
C 0.728793 0.295874 0.212272
C 1.688931 -0.881727 0.144441
C 1.161049 1.461445 -0.670801
C 0.569044 0.733866 1.669389
C 2.748813 -0.975391 -0.642266
H 1.443830 -1.696777 0.818052
H 3.381442 -1.851597 -0.609883
H 3.029626 -0.192886 -1.334150
O -1.935643 1.166062 -0.588109
H -2.505953 0.267246 -0.507600
H -2.096602 1.654399 0.225279
H 0.451317 2.280940 -0.583463
H 1.212232 1.171639 -1.720342
H 2.145289 1.809236 -0.359185
H 0.253433 -0.095382 2.299216
H -0.171916 1.529698 1.750608
H 1.521921 1.112241 2.036960
Rotational constants (GHz): 2.3809000 1.0909400 0.9662900
Vibrational harmonic frequencies (cm-1):
i421.0174 54.8963 87.2882
164.5660 197.9928 236.8716
278.8856 291.6668 303.3916
335.6956 355.3212 375.5404
453.0392 486.1675 514.9737
575.3183 591.7911 645.5725
709.0778 789.0754 923.2138
942.6905 970.5160 992.0936
995.5858 1026.6365 1053.3821
1076.3599 1120.9161 1205.2998
1260.7810 1282.0842 1283.9789
1337.6112 1373.8452 1402.8684
1423.1159 1452.5386 1488.6788
1490.5482 1504.9527 1515.4143
1577.5145 1612.7925 1724.5202
2155.7251 3067.7244 3072.3946
3139.6091 3143.0888 3156.3975
3161.0031 3167.2811 3171.4909
3179.9368 3259.7849 3875.5832
Zero-point correction (Hartree): 0.175499

Z-nopinone oxide
#####

Population analysis as 298K (%)
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)
Compound Qtot Erel Erel2 n*Q*MB %

TS.BpineneCI+H2O.HHP.A.b.ab 9.005e+41 0.00 0.00 9.005e+41 64.3
TS.BpineneCI+H2O.HHP.A.b.aa 9.023e+41 0.41 0.41 4.524e+41 32.3
TS.BpineneCI+H2O.HHP.A.b.sb 7.072e+41 1.77 1.77 3.590e+40 2.56
TS.BpineneCI+H2O.HHP.A.b.sa 5.874e+41 2.27 2.27 1.269e+40 0.906
Total 1.401e+42 100

TS.BpineneCI+H2O.HHP.A.b.aa
~~~~~  
E(RM062X/Aug-CC-pVTZ) (Hartree): -578.06853647  
Electronic state : 1-A  
Cartesian coordinates (Angs):  
C -1.393163 -0.539345 -0.014859  
C -0.026597 -0.367645 0.748970  
C 0.940724 0.156782 -0.255511  
C -0.909446 1.824956 -0.796635  
C -1.605156 0.976015 0.261909  
C -0.665399 0.832832 1.481334  
C -2.340788 -1.412563 0.799089  
C -1.375208 -1.040676 -1.450638  
C 0.590637 1.461245 -0.911421  
O 1.697307 -0.608345 -0.962633  
H 0.362287 -1.221774 1.291638  
H -1.003066 2.879068 -0.536977  
H -1.401098 1.689778 -1.759598  
H -2.629339 1.305628 0.434307  
H -0.012703 1.676938 1.703755  
H -1.179066 0.529365 2.387046  
H -2.396343 -1.116939 1.845104  
H -2.019612 -2.454017 0.758803  
H -3.346521 -1.353034 0.379662  
H -1.006348 -2.066845 -1.480430  
H -0.743880 -0.453352 -2.114363  
H -2.388678 -1.032263 -1.856221  
H 1.206827 2.202861 -0.403335  
H 0.936536 1.423642 -1.942879  
O 2.312549 -1.577964 -0.111425  
O 2.432767 0.520040 1.010022  
H 2.614479 -0.537632 0.697826  
H 2.171913 0.509125 1.934521  
Rotational constants (GHz): 1.3657100 0.8343500 0.7542500  
Vibrational harmonic frequencies (cm-1):  
i684.2607 87.5422 139.9641

|           |           |           |
|-----------|-----------|-----------|
| 178.7248  | 191.7363  | 219.0702  |
| 258.4547  | 262.6401  | 298.1902  |
| 319.7598  | 380.7892  | 396.8655  |
| 404.1667  | 419.0320  | 450.8128  |
| 456.7633  | 548.3490  | 566.5661  |
| 607.5304  | 648.3794  | 665.3752  |
| 727.6942  | 777.1646  | 805.1684  |
| 842.4897  | 885.0768  | 904.3527  |
| 944.3816  | 958.7700  | 967.9035  |
| 973.8964  | 983.8868  | 1012.8203 |
| 1020.7604 | 1062.7708 | 1073.8449 |
| 1087.2609 | 1105.4889 | 1144.6747 |
| 1178.9008 | 1208.0247 | 1225.6908 |
| 1252.6332 | 1254.8982 | 1267.8084 |
| 1277.3197 | 1304.4846 | 1320.6347 |
| 1329.5329 | 1364.1434 | 1382.0464 |
| 1408.3964 | 1425.8390 | 1463.1335 |
| 1478.7596 | 1486.7241 | 1488.8058 |
| 1505.7968 | 1507.6532 | 1518.9002 |
| 1524.1210 | 1567.5646 | 1922.5026 |
| 3058.1692 | 3061.5921 | 3080.6762 |
| 3091.4438 | 3097.4766 | 3101.4838 |
| 3118.2991 | 3122.3453 | 3126.8573 |
| 3143.1949 | 3144.7414 | 3148.0866 |
| 3169.0379 | 3174.8724 | 3893.2974 |

Zero-point correction (Hartree): 0.241429

TS.BpineneCI+H2O.HHP.A.b.ab

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E(RM062X/Aug-CC-pVTZ) (Hartree): -578.06929709

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-1.386718	-0.537714	-0.018521
C	-0.027853	-0.356794	0.759700
C	0.939790	0.167926	-0.241501
C	-0.911016	1.827629	-0.796640
C	-1.610480	0.976245	0.257325
C	-0.678478	0.838263	1.483576
C	-2.334781	-1.417282	0.788029
C	-1.356321	-1.039802	-1.454163
C	0.597732	1.486747	-0.876660
O	1.683424	-0.597565	-0.965405
H	0.362153	-1.201862	1.313330
H	-1.022943	2.882596	-0.548169
H	-1.379049	1.677399	-1.768994
H	-2.638614	1.300014	0.417611
H	-0.023749	1.674689	1.720434
H	-1.196713	0.527586	2.383856
H	-2.398080	-1.122764	1.833712
H	-2.006630	-2.456594	0.749039
H	-3.338092	-1.363429	0.361791
H	-0.976138	-2.061949	-1.481062
H	-0.727698	-0.447216	-2.116066
H	-2.367747	-1.042334	-1.865083
H	1.170508	2.232595	-0.325425
H	0.975583	1.484408	-1.897588
O	2.273867	-1.596252	-0.130395
O	2.362711	0.429295	1.132140
H	2.541284	-0.606243	0.751783
H	3.074656	0.967962	0.773245

Rotational constants (GHz): 1.3588700 0.8408800 0.7585300

Vibrational harmonic frequencies (cm-1):

i676.0487	87.2114	138.9147
180.7548	188.3092	219.1034
251.2468	266.7491	303.7978
328.7159	379.9460	390.1420
403.7811	420.4260	456.0701
457.5555	557.6482	569.4686
609.8041	647.8132	649.8860
705.2708	777.6957	802.7560
841.9231	884.2319	904.0077
947.0011	960.4440	969.4334
974.0406	984.5606	1012.7767
1024.9857	1072.3940	1080.0763
1087.7645	1106.9463	1139.5080
1180.7427	1210.3276	1223.5016
1247.2073	1253.1556	1268.1893
1282.3990	1308.9950	1325.5937
1330.6698	1363.8154	1386.5954
1408.1137	1425.6997	1463.0848
1485.9075	1488.7124	1505.2390
1508.9179	1519.9954	1527.0258
1546.7172	1589.6484	1853.8502
3057.2798	3060.8725	3080.8823
3092.7095	3098.2353	3110.9524
3119.0088	3121.6072	3126.1462
3141.8870	3145.0207	3146.8201
3178.7546	3185.2571	3870.1798

Zero-point correction (Hartree): 0.241538

TS.BpineneCI+H2O.HHP.A.b.sa

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E(RM062X/Aug-CC-pVTZ) (Hartree): -578.06599911

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 1.359168  | -0.541064 | 0.013770  |
| C | 0.016769  | -0.380367 | -0.763729 |
| C | -1.026011 | 0.348619  | 0.010373  |
| C | 0.915435  | 1.862776  | 0.697126  |
| C | 1.612329  | 0.956180  | -0.313944 |
| C | 0.702325  | 0.789233  | -1.546679 |
| C | 2.306889  | -1.457055 | -0.755719 |

|                                                           |           |           |           |
|-----------------------------------------------------------|-----------|-----------|-----------|
| C                                                         | 1.374411  | -0.959840 | 1.476920  |
| C                                                         | -0.574812 | 1.486595  | 0.881556  |
| O                                                         | -2.225632 | 0.488988  | -0.434506 |
| H                                                         | -0.397455 | -1.216822 | -1.315308 |
| H                                                         | 0.984446  | 2.893359  | 0.349343  |
| H                                                         | 1.432121  | 1.816445  | 1.655489  |
| H                                                         | 2.647818  | 1.257365  | -0.472335 |
| H                                                         | 0.071805  | 1.632556  | -1.826062 |
| H                                                         | 1.214019  | 0.422050  | -2.429156 |
| H                                                         | 2.388631  | -1.196697 | -1.809005 |
| H                                                         | 1.966601  | -2.491853 | -0.692699 |
| H                                                         | 3.305794  | -1.405437 | -0.319605 |
| H                                                         | 1.166119  | -2.027855 | 1.575527  |
| H                                                         | 0.661441  | -0.423604 | 2.097022  |
| H                                                         | 2.374318  | -0.794058 | 1.883675  |
| H                                                         | -1.238751 | 2.323492  | 0.669145  |
| H                                                         | -0.792407 | 1.182067  | 1.904517  |
| O                                                         | -2.722622 | -0.771295 | -0.890196 |
| O                                                         | -1.627208 | -1.147310 | 1.198469  |
| H                                                         | -2.269851 | -1.265888 | 0.312383  |
| H                                                         | -1.029971 | -1.898646 | 1.228893  |
| Rotational constants (GHz): 1.3790300 0.8175100 0.7555900 |           |           |           |
| Vibrational harmonic frequencies (cm-1):                  |           |           |           |
| i581.9578                                                 | 120.7331  | 148.2547  |           |
| 191.3920                                                  | 215.0130  | 228.1641  |           |
| 255.4755                                                  | 277.0927  | 297.9087  |           |
| 320.3838                                                  | 369.0667  | 390.1631  |           |
| 408.5771                                                  | 419.2505  | 438.8957  |           |
| 480.6117                                                  | 552.4455  | 555.3090  |           |
| 613.4071                                                  | 645.1349  | 651.6960  |           |
| 719.0470                                                  | 780.3357  | 807.6596  |           |
| 848.3374                                                  | 888.2080  | 899.1514  |           |
| 933.3758                                                  | 944.5810  | 965.5138  |           |
| 979.8138                                                  | 997.0776  | 1005.5737 |           |
| 1019.5367                                                 | 1046.2680 | 1077.2573 |           |
| 1110.4163                                                 | 1139.9953 | 1155.6817 |           |
| 1171.3381                                                 | 1215.8395 | 1227.1808 |           |
| 1243.7997                                                 | 1255.6513 | 1262.4575 |           |
| 1283.1278                                                 | 1305.2009 | 1319.7915 |           |
| 1330.2301                                                 | 1367.1320 | 1380.5747 |           |
| 1406.8550                                                 | 1424.3204 | 1466.6050 |           |
| 1485.9819                                                 | 1491.7109 | 1492.3840 |           |
| 1505.4821                                                 | 1511.2203 | 1515.3177 |           |
| 1523.8179                                                 | 1592.8139 | 1954.0914 |           |
| 3051.8155                                                 | 3059.6170 | 3078.7984 |           |
| 3094.4409                                                 | 3098.9079 | 3101.4294 |           |
| 3105.1494                                                 | 3115.8969 | 3121.6933 |           |
| 3139.8076                                                 | 3146.9520 | 3169.0716 |           |
| 3171.5292                                                 | 3180.3002 | 3898.6236 |           |
| Zero-point correction (Hartree): 0.241859                 |           |           |           |
| TS.BpineneCI+H2O.HHP.A.b.sb                               |           |           |           |
| ~~~~~                                                     |           |           |           |
| E(RM062X/Aug-CC-pVTZ) (Hartree): -578.06649411            |           |           |           |
| Electronic state : 1-A                                    |           |           |           |
| Cartesian coordinates (Angs):                             |           |           |           |
| C                                                         | 1.359666  | -0.544120 | 0.027942  |
| C                                                         | 0.017376  | -0.391982 | -0.747230 |
| C                                                         | -1.018490 | 0.351839  | 0.015671  |
| C                                                         | 0.930598  | 1.874221  | 0.666703  |
| C                                                         | 1.620145  | 0.946030  | -0.329287 |
| C                                                         | 0.702184  | 0.763237  | -1.553515 |
| C                                                         | 2.293183  | -1.480894 | -0.734597 |
| C                                                         | 1.374125  | -0.950953 | 1.492639  |
| C                                                         | -0.556485 | 1.494842  | 0.878371  |
| O                                                         | -2.218711 | 0.503525  | -0.431057 |
| H                                                         | -0.396564 | -1.240297 | -1.278577 |
| H                                                         | 0.987350  | 2.896709  | 0.293476  |
| H                                                         | 1.456299  | 1.853168  | 1.620780  |
| H                                                         | 2.654996  | 1.243590  | -0.498246 |
| H                                                         | 0.075844  | 1.605927  | -1.845212 |
| H                                                         | 1.206501  | 0.377323  | -2.432153 |
| H                                                         | 2.355314  | -1.251430 | -1.796642 |
| H                                                         | 1.950533  | -2.511431 | -0.633391 |
| H                                                         | 3.299980  | -1.418449 | -0.318759 |
| H                                                         | 1.042101  | -1.982434 | 1.600681  |
| H                                                         | 0.731621  | -0.343419 | 2.123231  |
| H                                                         | 2.395616  | -0.874449 | 1.872416  |
| H                                                         | -1.226414 | 2.329490  | 0.675498  |
| H                                                         | -0.741741 | 1.202325  | 1.911088  |
| O                                                         | -2.718759 | -0.750224 | -0.898059 |
| O                                                         | -1.540022 | -1.250628 | 1.117678  |
| H                                                         | -2.215112 | -1.299199 | 0.237286  |
| H                                                         | -2.090200 | -0.982131 | 1.859857  |
| Rotational constants (GHz): 1.3754700 0.8231600 0.7561600 |           |           |           |
| Vibrational harmonic frequencies (cm-1):                  |           |           |           |
| i619.3697                                                 | 118.5016  | 138.4101  |           |
| 190.9297                                                  | 192.1805  | 220.6189  |           |
| 254.4888                                                  | 274.2734  | 288.7672  |           |
| 319.0336                                                  | 366.7399  | 387.8213  |           |
| 408.1694                                                  | 417.9554  | 439.1615  |           |
| 483.9596                                                  | 557.2714  | 567.5673  |           |
| 602.5649                                                  | 614.0641  | 644.8772  |           |
| 693.5288                                                  | 779.3649  | 801.3093  |           |
| 848.0419                                                  | 887.8229  | 897.8069  |           |
| 935.6567                                                  | 945.6468  | 968.4202  |           |
| 980.6702                                                  | 997.7788  | 1004.9465 |           |
| 1022.2433                                                 | 1045.9488 | 1075.7802 |           |
| 1111.0245                                                 | 1139.9094 | 1153.7368 |           |
| 1169.7675                                                 | 1214.5890 | 1229.3194 |           |
| 1243.1148                                                 | 1255.4502 | 1269.5304 |           |
| 1283.7702                                                 | 1312.8673 | 1323.0833 |           |

|           |           |           |
|-----------|-----------|-----------|
| 1332.3626 | 1367.7432 | 1384.5644 |
| 1407.8985 | 1424.9733 | 1461.6459 |
| 1484.0225 | 1486.9022 | 1503.3042 |
| 1506.3528 | 1514.6315 | 1520.0073 |
| 1546.5261 | 1587.9566 | 1863.9091 |
| 3059.2858 | 3063.3062 | 3079.0166 |
| 3093.1706 | 3096.6330 | 3099.7969 |
| 3116.4030 | 3124.2992 | 3133.8807 |
| 3137.7485 | 3145.2124 | 3170.5047 |
| 3178.5855 | 3184.7730 | 3873.5160 |

Zero-point correction (Hartree): 0.241548

#####  
E-nopinone oxide  
#####

Population analysis as 298K (%)  
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)  
Compound Qtot Erel Erel2 n\*Q\*MB %

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|                             |           |      |      |           |        |
|-----------------------------|-----------|------|------|-----------|--------|
| TS.BpineneCI+H2O.HHP.A.a.aa | 1.068e+42 | 0.00 | 0.00 | 1.068e+42 | 93.6   |
| TS.BpineneCI+H2O.HHP.A.a.sa | 8.097e+41 | 1.78 | 1.78 | 4.039e+40 | 3.54   |
| TS.BpineneCI+H2O.HHP.A.a.ab | 1.230e+42 | 2.16 | 2.16 | 3.207e+40 | 2.81   |
| TS.BpineneCI+H2O.HHP.A.a.sb | 6.800e+41 | 3.81 | 3.81 | 1.100e+39 | 0.0964 |
| Total                       |           |      |      | 1.141e+42 | 100    |

TS.BpineneCI+H2O.HHP.A.a.aa

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E(RM062X/Aug-CC-pVTZ) (Hartree): -578.06816713

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-1.568438	0.412006	-0.106543
C	-0.327595	-0.030556	-0.966101
C	0.881990	0.134197	-0.123740
C	-0.494110	-1.089377	1.632975
C	-1.505778	-1.020540	0.494793
C	-0.818638	-1.486917	-0.808825
C	-2.790028	0.612638	-0.994547
C	-1.423281	1.610338	0.817022
C	0.912882	-0.599424	1.198986
O	1.525032	1.239896	-0.283855
H	-0.195789	0.416808	-1.949075
H	-0.417859	-2.119753	1.978815
H	-0.850192	-0.497730	2.476287
H	-2.456394	-1.476257	0.770707
H	-0.045198	-2.247698	-0.724415
H	-1.518013	-1.761341	-1.590861
H	-2.952809	-0.213053	-1.684559
H	-2.687331	1.527933	-1.579093
H	-3.681542	0.709936	-0.372793
H	-1.319106	2.524808	0.231320
H	-0.560627	1.550126	1.477881
H	-2.317068	1.707971	1.436191
H	1.592833	-1.441032	1.114602
H	1.359022	0.083697	1.918985
O	2.840044	1.058202	0.255462
O	2.334512	-0.942889	-0.973099
H	2.869262	-0.136313	-0.447159
H	2.382073	-0.723964	-1.909021

Rotational constants (GHz): 1.5326400 0.7550700 0.7131700

Vibrational harmonic frequencies (cm-1):

i586.5726	78.5509	125.2227
181.0465	197.5963	217.2723
244.1677	272.9489	304.1416
321.3442	385.1274	392.8203
402.0681	416.6316	423.2981
479.2342	548.4723	585.5138
616.9473	647.4137	669.4376
697.0651	777.7981	804.3965
847.6114	883.4540	902.7415
929.2864	962.0900	971.5041
975.9471	984.8961	1010.7403
1026.7798	1074.3977	1082.1230
1102.8313	1132.3524	1150.3345
1196.6187	1211.2392	1226.6677
1250.5942	1257.3950	1267.2608
1284.7149	1305.8419	1328.0787
1349.3572	1363.2327	1381.6183
1410.5086	1427.4093	1471.1394
1485.5324	1489.3928	1505.6508
1506.4987	1518.5285	1523.5960
1543.2649	1601.9442	1902.8600
3058.0502	3061.5021	3078.9355
3098.2095	3110.4456	3116.3593
3119.7376	3120.6754	3124.7680
3125.2876	3146.0706	3148.7288
3166.0290	3180.0267	3870.6154

Zero-point correction (Hartree): 0.241850

TS.BpineneCI+H2O.HHP.A.a.ab

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E(RM062X/Aug-CC-pVTZ) (Hartree): -578.06465648

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -1.559015 | 0.418006  | -0.105487 |
| C | -0.323677 | -0.037850 | -0.967475 |
| C | 0.885431  | 0.113743  | -0.123105 |
| C | -0.501458 | -1.103834 | 1.626895  |
| C | -1.514859 | -1.017521 | 0.490531  |
| C | -0.836643 | -1.485299 | -0.816794 |
| C | -2.778456 | 0.638166  | -0.992142 |

|                                           |           |           |                               |
|-------------------------------------------|-----------|-----------|-------------------------------|
| C                                         | -1.401517 | 1.609446  | 0.825132                      |
| C                                         | 0.917813  | -0.654754 | 1.183641                      |
| O                                         | 1.499938  | 1.238947  | -0.237958                     |
| H                                         | -0.175199 | 0.405150  | -1.948433                     |
| H                                         | -0.449477 | -2.133052 | 1.981226                      |
| H                                         | -0.837966 | -0.497104 | 2.467121                      |
| H                                         | -2.470234 | -1.462289 | 0.768003                      |
| H                                         | -0.081325 | -2.265863 | -0.739914                     |
| H                                         | -1.539960 | -1.745536 | -1.599811                     |
| H                                         | -2.950705 | -0.180637 | -1.687990                     |
| H                                         | -2.663565 | 1.555348  | -1.571146                     |
| H                                         | -3.669173 | 0.742673  | -0.370319                     |
| H                                         | -1.281238 | 2.524891  | 0.244323                      |
| H                                         | -0.542354 | 1.535558  | 1.489134                      |
| H                                         | -2.297059 | 1.716038  | 1.440391                      |
| H                                         | 1.559375  | -1.524544 | 1.088249                      |
| H                                         | 1.399923  | -0.004787 | 1.910740                      |
| O                                         | 2.824761  | 1.069737  | 0.281519                      |
| O                                         | 2.325669  | -0.788715 | -1.143312                     |
| H                                         | 2.874189  | -0.044190 | -0.550024                     |
| H                                         | 2.596103  | -1.662030 | -0.850715                     |
| Rotational constants (GHz):               |           |           | 1.5226700 0.7561200 0.7164100 |
| Vibrational harmonic frequencies (cm-1):  |           |           |                               |
| i587.7849                                 | 66.5308   | 123.3863  |                               |
| 181.5384                                  | 196.3236  | 217.1866  |                               |
| 248.2721                                  | 273.4050  | 309.0364  |                               |
| 311.2169                                  | 385.0993  | 397.6207  |                               |
| 404.2568                                  | 420.6358  | 430.6153  |                               |
| 479.7557                                  | 532.4024  | 583.6656  |                               |
| 609.8943                                  | 651.5996  | 658.5890  |                               |
| 732.1703                                  | 781.8785  | 803.1698  |                               |
| 845.3162                                  | 883.0445  | 901.6885  |                               |
| 930.3663                                  | 959.8086  | 971.8740  |                               |
| 976.6557                                  | 986.1660  | 1009.3644 |                               |
| 1027.8322                                 | 1069.1487 | 1079.0145 |                               |
| 1099.4568                                 | 1127.5616 | 1141.4612 |                               |
| 1183.0154                                 | 1208.7996 | 1220.4426 |                               |
| 1246.5122                                 | 1253.2541 | 1264.8199 |                               |
| 1282.0605                                 | 1301.3059 | 1324.3623 |                               |
| 1333.1242                                 | 1361.7876 | 1378.8911 |                               |
| 1411.0232                                 | 1428.1726 | 1467.3584 |                               |
| 1481.5736                                 | 1486.9220 | 1489.9929 |                               |
| 1506.1766                                 | 1507.7367 | 1519.3710 |                               |
| 1523.7983                                 | 1584.5909 | 1983.4699 |                               |
| 3058.2689                                 | 3061.7742 | 3079.4894 |                               |
| 3097.3333                                 | 3104.2676 | 3116.7282 |                               |
| 3121.4027                                 | 3122.9081 | 3126.0126 |                               |
| 3144.0722                                 | 3146.2320 | 3148.6667 |                               |
| 3165.2263                                 | 3180.2376 | 3901.5691 |                               |
| Zero-point correction (Hartree): 0.241781 |           |           |                               |

TS.BpineneCI+H2O.HHP.A.a.sa

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E(RM062X/Aug-CC-pVTZ) (Hartree): -578.06542487

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-1.518891	0.424659	-0.045007
C	-0.342105	0.047781	-0.996358
C	0.948141	-0.120098	-0.283249
C	-0.484776	-1.351553	1.436420
C	-1.529394	-1.075736	0.359426
C	-0.926222	-1.403587	-1.020823
C	-2.750922	0.804745	-0.861020
C	-1.320991	1.463613	1.046026
C	0.921929	-0.816256	1.059347
O	1.968467	-0.249851	-1.060742
H	-0.214418	0.586575	-1.932781
H	-0.422231	-2.427836	1.597512
H	-0.808172	-0.909483	2.378179
H	-2.495096	-1.511251	0.615408
H	-0.208737	-2.220816	-1.077493
H	-1.662160	-1.517676	-1.808840
H	-2.971566	0.099867	-1.660279
H	-2.616201	1.790281	-1.309407
H	-3.622767	0.851953	-0.206942
H	-1.206747	2.456842	0.609073
H	-0.447423	1.285922	1.664815
H	-2.206334	1.481530	1.685482
H	1.653501	-1.618583	0.969558
H	1.307639	-0.152410	1.826013
O	3.148399	-0.072108	-0.269933
O	1.613451	1.647394	0.401075
H	2.528923	1.065435	0.227320
H	1.568654	2.294760	-0.309396
Rotational constants (GHz):			1.5400200 0.7609600 0.7107000
Vibrational harmonic frequencies (cm-1):			
i568.9444	101.7954	127.7810	
190.2346	201.8607	215.7234	
259.7164	283.3661	297.6860	
321.9486	337.0822	386.8171	
400.1063	429.7155	446.8360	
485.6396	565.0521	579.2018	
604.7993	623.6753	665.3266	
707.7626	786.6443	799.8827	
849.3027	877.5853	900.5294	
922.2448	965.0454	971.2602	
978.1313	986.8034	1010.8013	
1020.5945	1048.9065	1078.2148	
1114.8627	1145.1840	1172.5015	
1179.4019	1215.2185	1238.8188	
1247.6669	1256.7134	1266.6865	
1286.9617	1307.2487	1328.1171	

1347.3484	1367.5984	1380.9665
1409.1058	1427.3705	1465.6662
1483.5091	1488.6377	1504.6166
1507.2605	1515.6649	1522.9827
1542.5735	1602.7171	1908.4299
3057.0018	3061.1393	3079.0827
3096.4286	3103.2434	3109.7377
3115.6216	3119.4202	3123.3490
3125.4195	3144.6306	3165.3057
3179.0898	3184.3625	3872.4669

Zero-point correction (Hartree): 0.241937

TS.BpineneCI+H2O.HHP.A.a.sb

E(RM062X/Aug-CC-pVT2) (Hartree): -578.06253698

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-1.509102	0.422229	-0.043761
C	-0.335471	0.043134	-0.995493
C	0.951206	-0.120693	-0.277421
C	-0.487783	-1.371553	1.428605
C	-1.530768	-1.080375	0.353284
C	-0.926882	-1.403191	-1.028126
C	-2.734607	0.821304	-0.860563
C	-1.305850	1.459795	1.049004
C	0.918572	-0.821352	1.067409
O	1.974065	-0.263998	-1.045254
H	-0.199376	0.594584	-1.921916
H	-0.419853	-2.450603	1.566987
H	-0.816893	-0.953936	2.379781
H	-2.498321	-1.513234	0.606732
H	-0.214601	-2.224887	-1.086864
H	-1.663407	-1.511476	-1.816462
H	-2.941227	0.138007	-1.681794
H	-2.595352	1.818302	-1.281010
H	-3.615098	0.847739	-0.216960
H	-1.070299	2.430054	0.611105
H	-0.511413	1.202328	1.745493
H	-2.226736	1.561985	1.626513
H	1.656150	-1.617937	0.976156
H	1.299201	-0.175299	1.851506
O	3.148398	-0.057079	-0.250094
O	1.578825	1.700493	0.200601
H	2.510304	1.137449	0.131672
H	1.460737	1.985803	1.109402

Rotational constants (GHz): 1.5329300 0.7673500 0.7118700

Vibrational harmonic frequencies (cm-1):

1555.2971	109.6000	130.1876
192.6736	207.8249	220.1216
269.2369	291.9338	302.5957
316.9432	350.0244	387.4062
405.5706	432.5933	448.0186
490.7291	542.8828	580.9783
610.5372	647.5053	670.0719
735.5576	794.7443	800.6758
847.8020	881.2381	901.7405
922.8911	963.3610	971.1238
977.6437	985.4984	1009.6710
1022.8539	1050.6711	1077.8841
1113.5726	1145.9635	1159.8746
1172.9994	1216.2990	1226.0946
1242.3166	1253.3764	1265.1729
1284.7049	1301.8427	1326.9674
1329.4498	1367.0055	1379.4844
1406.7451	1423.1986	1464.1749
1486.6720	1492.3205	1493.9365
1504.9165	1508.6469	1522.5866
1527.8674	1599.0202	2017.9920
3059.3209	3063.4092	3078.3535
3096.2280	3103.0140	3109.9873
3117.9866	3122.0957	3126.8750
3141.4445	3146.3103	3156.4972
3162.1670	3178.6810	3904.5605

Zero-point correction (Hartree): 0.242285

E-pinonaldehyde-K-oxide
#####

Population analysis as 298K (%)

Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)

Compound	Qtot	Erel	Erel2	n*Q*MB	%
TS.ApineneCI.A.a+H2O.HHP.pmttd	8.260e+44	0.00	0.00	8.260e+44	71.9
TS.ApineneCI.A.a+H2O.HHP.pptd	9.826e+44	1.11	1.11	1.499e+44	13.1
TS.ApineneCI.A.a+H2O.HHP.mmttd	4.679e+44	1.31	1.31	5.158e+43	4.49
TS.ApineneCI.A.a+H2O.HHP.pmpd	9.769e+44	2.06	2.06	2.994e+43	2.61
TS.ApineneCI.A.a+H2O.HHP.mptd	5.773e+44	1.96	1.96	2.114e+43	1.84
TS.ApineneCI.A.a+H2O.HHP.tmtu	6.878e+44	2.27	2.27	1.489e+43	1.3
TS.ApineneCI.A.a+H2O.HHP.pmtu	5.605e+44	2.35	2.35	1.063e+43	0.926
TS.ApineneCI.A.a+H2O.HHP.pmpd	2.902e+45	3.45	3.45	8.633e+42	0.752
TS.ApineneCI.A.a+H2O.HHP.tmttd	3.887e+44	2.34	2.34	7.438e+42	0.648
TS.ApineneCI.A.a+H2O.HHP.pppd	2.236e+45	3.53	3.53	5.789e+42	0.504
TS.ApineneCI.A.a+H2O.HHP.tptu	8.010e+44	2.98	2.98	5.262e+42	0.458
TS.ApineneCI.A.a+H2O.HHP.pmmtd	1.741e+45	3.88	3.88	2.498e+42	0.218
TS.ApineneCI.A.a+H2O.HHP.tptd	4.373e+44	3.13	3.13	2.210e+42	0.192
TS.ApineneCI.A.a+H2O.HHP.mmpd	5.186e+44	3.24	3.24	2.176e+42	0.19
TS.ApineneCI.A.a+H2O.HHP.pptu	6.966e+44	3.48	3.48	1.955e+42	0.17
TS.ApineneCI.A.a+H2O.HHP.mppd	1.875e+45	4.14	4.14	1.716e+42	0.149
TS.ApineneCI.A.a+H2O.HHP.tmpu	7.676e+44	4.13	4.13	7.192e+41	0.0626
TS.ApineneCI.A.a+H2O.HHP.pttd	5.928e+44	3.99	3.99	7.077e+41	0.0616

TS.ApineneCI.A.a+H2O.HHP.mppd	1.369e+45	4.50	4.50	6.881e+41	0.0599
TS.ApineneCI.A.a+H2O.HHP.tpmu	2.501e+45	5.01	5.01	5.310e+41	0.0462
TS.ApineneCI.A.a+H2O.HHP.mttd	8.486e+43	3.03	3.03	5.088e+41	0.0443
TS.ApineneCI.A.a+H2O.HHP.ptpd	1.217e+45	4.68	4.68	4.470e+41	0.0389
TS.ApineneCI.A.a+H2O.HHP.mmmd	1.221e+45	4.72	4.72	4.210e+41	0.0367
TS.ApineneCI.A.a+H2O.HHP.pmpu	6.957e+44	4.41	4.41	4.052e+41	0.0353
TS.ApineneCI.A.a+H2O.HHP.tmpd	4.539e+44	4.28	4.28	3.305e+41	0.0288
TS.ApineneCI.A.a+H2O.HHP.ptmd	8.410e+44	4.78	4.78	2.611e+41	0.0227
TS.ApineneCI.A.a+H2O.HHP.tpmd	1.505e+45	5.13	5.13	2.605e+41	0.0227
TS.ApineneCI.A.a+H2O.HHP.tttu	5.370e+44	4.64	4.64	2.119e+41	0.0185
TS.ApineneCI.A.a+H2O.HHP.pttu	1.555e+44	3.98	3.98	1.881e+41	0.0164
TS.ApineneCI.A.a+H2O.HHP.ppmu	2.125e+45	5.57	5.57	1.758e+41	0.0153
TS.ApineneCI.A.a+H2O.HHP.tppu	1.724e+45	5.57	5.57	1.419e+41	0.0124
TS.ApineneCI.A.a+H2O.HHP.tmmu	1.490e+45	5.75	5.75	9.070e+40	0.0079
TS.ApineneCI.A.a+H2O.HHP.tttd	3.367e+44	4.95	4.95	7.877e+40	0.00686
TS.ApineneCI.A.a+H2O.HHP.tppd	1.026e+45	5.63	5.63	7.665e+40	0.00668
TS.ApineneCI.A.a+H2O.HHP.pppu	1.365e+45	5.86	5.86	6.866e+40	0.00598
TS.ApineneCI.A.a+H2O.HHP.mtmd	6.193e+44	5.58	5.58	5.035e+40	0.00439
TS.ApineneCI.A.a+H2O.HHP.tmmd	9.645e+44	5.92	5.92	4.429e+40	0.00386
TS.ApineneCI.A.a+H2O.HHP.pmmu	1.210e+45	6.12	6.12	3.907e+40	0.0034
TS.ApineneCI.A.a+H2O.HHP.ttmu	9.202e+44	6.71	6.71	1.108e+40	0.000965
TS.ApineneCI.A.a+H2O.HHP.ttmd	5.470e+44	6.76	6.76	5.981e+39	0.000521
TS.ApineneCI.A.a+H2O.HHP.ptmu	7.427e+44	6.99	6.99	5.555e+39	0.000484
Total				1.148e+45	100

TS.ApineneCI.A.a+H2O.HHP.mmmd

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E(RM062X/CC-pVDZ) (Hartree): -692.36981688

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -1.514640 | -0.614151 | -0.449069 |
| H | -1.924359 | -0.609170 | -1.472482 |
| C | -2.648212 | -0.870550 | 0.539860  |
| C | -3.746170 | 0.154684  | 0.396422  |
| H | -3.088579 | -1.862870 | 0.366853  |
| H | -2.263043 | -0.832647 | 1.572092  |
| H | -3.449949 | 1.208921  | 0.630614  |
| C | -0.559737 | 0.619865  | -0.300821 |
| C | -0.279116 | -1.541611 | -0.412613 |
| C | -0.849697 | 1.838907  | -1.162454 |
| C | -0.368258 | 1.030120  | 1.157980  |
| H | -0.263721 | 0.159153  | 1.822162  |
| H | 0.516387  | 1.673449  | 1.267937  |
| H | -1.246542 | 1.596224  | 1.505295  |
| H | 0.004844  | 2.532224  | -1.132737 |
| H | -1.739749 | 2.379030  | -0.804216 |
| H | -1.024453 | 1.552082  | -2.210383 |
| H | -0.280194 | -2.422951 | -1.065400 |
| H | -0.018673 | -1.840835 | 0.612585  |
| C | 0.555857  | -0.319737 | -0.843344 |
| H | 0.560350  | -0.256426 | -1.946080 |
| C | 1.988038  | -0.211570 | -0.438364 |
| C | 2.916522  | -1.307244 | -0.855121 |
| H | 2.941042  | -1.295891 | -1.956997 |
| H | 3.918718  | -1.123142 | -0.462832 |
| H | 2.529547  | -2.273744 | -0.515842 |
| O | -4.866404 | -0.098599 | 0.038400  |
| O | 2.392179  | 0.989290  | -0.227196 |
| O | 3.629555  | 0.973035  | 0.486898  |
| O | 2.243126  | -0.738297 | 1.524014  |
| H | 3.032211  | -0.022492 | 1.327235  |
| H | 1.641003  | -0.236627 | 2.090409  |

Rotational constants (GHz): 1.4625400 0.3535700 0.3379600

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i461.6681 | 28.9215   | 60.6953   |
| 63.9615   | 79.9854   | 132.2108  |
| 173.2034  | 175.3909  | 198.0471  |
| 213.0244  | 238.5391  | 257.6666  |
| 278.8473  | 299.0287  | 329.8038  |
| 349.4081  | 367.5835  | 369.0506  |
| 399.3522  | 437.3172  | 439.6748  |
| 504.9401  | 525.8471  | 539.5806  |
| 588.0948  | 615.3542  | 621.4875  |
| 660.4813  | 727.2057  | 780.6556  |
| 846.0725  | 894.6092  | 925.2240  |
| 942.8505  | 952.9111  | 961.2927  |
| 977.5818  | 985.2822  | 997.5620  |
| 1021.0597 | 1033.5197 | 1071.8739 |
| 1104.1448 | 1130.5059 | 1151.2835 |
| 1174.5565 | 1183.2687 | 1199.9773 |
| 1237.9644 | 1260.5711 | 1261.1647 |
| 1274.5998 | 1299.1395 | 1318.4765 |
| 1339.3226 | 1360.4826 | 1380.6941 |
| 1392.2405 | 1393.2083 | 1412.4918 |
| 1414.0858 | 1434.3884 | 1439.6872 |
| 1456.5768 | 1461.8469 | 1465.2088 |
| 1474.5017 | 1481.0211 | 1499.8529 |
| 1579.7685 | 1652.4982 | 1887.3769 |
| 2052.2526 | 2923.0723 | 3049.7603 |
| 3050.6077 | 3056.0789 | 3064.1670 |
| 3071.3587 | 3075.2415 | 3093.9967 |
| 3128.4155 | 3132.8454 | 3134.8682 |
| 3138.6271 | 3150.4825 | 3160.6658 |
| 3175.7962 | 3236.1754 | 3867.8216 |

Zero-point correction (Hartree): 0.270529

TS.ApineneCI.A.a+H2O.HHP.mmpd

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E(RM062X/CC-pVDZ) (Hartree): -692.37262017

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-1.488954	0.941022	0.418331

H	-1.845173	1.168305	1.437745
C	-2.648649	1.068660	-0.567174
C	-3.762276	0.145925	-0.137279
H	-3.013067	2.108194	-0.566047
H	-2.336929	0.797816	-1.584777
H	-4.384054	0.508644	0.719071
C	-0.658294	-0.383653	0.475737
C	-0.181946	1.724627	0.163590
C	-1.030501	-1.386021	1.556665
C	-0.589986	-1.072920	-0.886282
H	-0.411642	-0.354234	-1.700526
H	0.205941	-1.831222	-0.896335
H	-1.553491	-1.559762	-1.096558
H	-0.262796	-2.171987	1.623557
H	-1.993937	-1.866106	1.326497
H	-1.110683	-0.899257	2.540961
H	-0.071260	2.708364	0.636178
H	0.052829	1.799316	-0.907388
C	0.561923	0.528332	0.793204
H	0.617200	0.673222	1.886995
C	1.957348	0.211359	0.369165
C	2.996105	1.274481	0.537440
H	3.074038	1.469425	1.619474
H	3.958120	0.926513	0.155903
H	2.677271	2.191375	0.030799
O	-3.965093	-0.939360	-0.620203
O	2.246528	-1.039590	0.380057
O	3.446978	-1.272346	-0.358661
O	2.158301	0.330946	-1.665379
H	2.892562	-0.402235	-1.360796
H	1.482733	-0.214437	-2.091632
Rotational constants (GHz): 1.3568200 0.3897200 0.3692700			
Vibrational harmonic frequencies (cm-1):			
i459.6622	52.4596		57.4749
80.2401	81.0265		139.5978
165.2740	169.6286		194.1667
231.1904	240.9844		257.3137
291.2335	304.8321		331.4238
351.5594	378.6568		393.9951
395.5140	437.1046		451.5778
506.8669	527.8460		542.5242
589.3245	617.2444		624.0910
658.2117	723.6494		777.8991
890.9953	895.0857		918.1195
933.3399	955.5226		968.8535
973.5218	993.3156		1006.3834
1030.2631	1034.4892		1048.9050
1101.8698	1126.2657		1154.7808
1170.4369	1183.0607		1198.1355
1237.0919	1253.7678		1258.7581
1272.3251	1299.6886		1317.8677
1336.5854	1360.9468		1384.1157
1393.1604	1398.2920		1411.6520
1414.0132	1434.4231		1446.0021
1460.6502	1462.1201		1467.5569
1479.8141	1486.3128		1503.7625
1581.2157	1651.5355		1876.1362
2057.7652	2933.9106		3048.4873
3048.9074	3051.6138		3060.5545
3072.9962	3074.4279		3094.1610
3133.1300	3139.1320		3141.3095
3148.6877	3156.0525		3159.5419
3175.4554	3236.6611		3866.9047
Zero-point correction (Hartree): 0.270974			
TS.ApineneCI.A.a+H2O.HHP.mmt			
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E(RM062X/CC-pVDZ) (Hartree): -692.37534662			
Electronic state : 1-A			
Cartesian coordinates (Angs):			
C	-1.535825	-0.757585	-0.506681
H	-1.984805	-0.699185	-1.510321
C	-2.599588	-1.171337	0.491892
C	-3.788069	-0.247957	0.546176
H	-2.977470	-2.183621	0.260996
H	-2.197191	-1.248524	1.517491
H	-4.607752	-0.560585	1.238069
C	-0.671337	0.530960	-0.282431
C	-0.237288	-1.594249	-0.555705
C	-1.040466	1.773855	-1.076474
C	-0.526385	0.870086	1.198721
H	-0.352459	-0.025379	1.815084
H	0.298081	1.579355	1.359176
H	-1.457468	1.337003	1.555967
H	-0.229903	2.515529	-1.002836
H	-1.972780	2.214915	-0.701077
H	-1.187547	1.529335	-2.139780
H	-0.177216	-2.413703	-1.282893
H	0.051698	-1.963128	0.439274
C	0.512585	-0.287253	-0.876209
H	0.525766	-0.134762	-1.970140
C	1.930188	-0.121705	-0.442060
C	2.928829	-1.126370	-0.922825
H	2.964968	-1.031956	-2.020400
H	3.913468	-0.912329	-0.502391
H	2.597325	-2.136762	-0.661715
O	-3.883580	0.767591	-0.095552
O	2.260560	1.081580	-0.136188
O	3.489546	1.082190	0.592893
O	2.191855	-0.773406	1.482744
H	2.941606	-0.000904	1.347659
H	1.548767	-0.339609	2.060234

Rotational constants (GHz): 1.3882300 0.3936200 0.3721400
 Vibrational harmonic frequencies (cm-1):
 i465.7458 44.0245 58.5020
 76.2416 117.1834 146.0689
 165.9426 168.4662 197.6549
 224.9235 242.7141 254.4683
 279.4776 296.5544 330.2493
 344.0224 364.6215 384.1399
 391.2425 432.9905 449.7095
 510.8460 526.9914 585.6892
 619.4755 623.8644 642.5692
 681.5898 732.4745 754.2671
 800.0632 895.1028 916.0245
 932.1409 946.4305 955.3249
 971.6010 977.6709 996.7600
 1018.0162 1033.9901 1047.2944
 1104.8118 1119.6070 1153.3470
 1174.4459 1187.1122 1202.5872
 1236.6155 1256.8717 1264.0765
 1287.3386 1299.3763 1334.1976
 1337.1428 1361.5856 1383.4188
 1393.2527 1399.9418 1404.4156
 1412.9550 1427.2239 1436.3417
 1459.9608 1462.0310 1463.0964
 1478.1568 1480.1453 1500.2460
 1581.2357 1652.4029 1876.4249
 2028.9093 2945.3787 3046.2015
 3050.1631 3054.1020 3057.0820
 3073.7193 3074.2051 3086.0411
 3088.4097 3126.6821 3131.3974
 3150.9697 3152.9699 3171.5664
 3175.7246 3236.0248 3869.5091
 Zero-point correction (Hartree): 0.270616

TS.ApineneCI.A.a+H2O.HHP.mpm

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 E(RM062X/CC-pVDZ) (Hartree): -692.37070220

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -1.608774 | 0.393813  | -0.488909 |
| H | -1.957999 | 0.753886  | -1.471870 |
| C | -2.784655 | 0.336129  | 0.479623  |
| C | -3.868733 | -0.542657 | -0.093124 |
| H | -2.491153 | -0.081678 | 1.451974  |
| H | -3.192194 | 1.351076  | 0.627092  |
| H | -4.336589 | -0.163321 | -1.037140 |
| C | -0.317113 | 1.190051  | -0.113931 |
| C | -0.744316 | -0.871984 | -0.693477 |
| C | -0.186591 | 2.592627  | -0.683909 |
| C | -0.073024 | 1.202514  | 1.393513  |
| H | -0.278801 | 0.223840  | 1.851606  |
| H | 0.962010  | 1.496538  | 1.618503  |
| H | -0.749856 | 1.927789  | 1.870395  |
| H | 0.823058  | 2.988380  | -0.495817 |
| H | -0.913997 | 3.273883  | -0.215124 |
| H | -0.362364 | 2.599081  | -1.770325 |
| H | -0.999178 | -1.546229 | -1.520345 |
| H | -0.641899 | -1.452754 | 0.234316  |
| C | 0.458319  | 0.076901  | -0.875924 |
| H | 0.531855  | 0.366168  | -1.939499 |
| C | 1.830837  | -0.368866 | -0.495834 |
| C | 2.378245  | -1.592460 | -1.158631 |
| H | 2.451947  | -1.361026 | -2.233771 |
| H | 3.369139  | -1.824739 | -0.763240 |
| H | 1.689275  | -2.432093 | -1.019711 |
| O | -4.206165 | -1.595971 | 0.379827  |
| O | 2.586802  | 0.567963  | -0.048041 |
| O | 3.724529  | 0.010146  | 0.611861  |
| O | 1.821014  | -1.345705 | 1.303165  |
| H | 2.801672  | -0.895747 | 1.244419  |
| H | 1.380457  | -0.810914 | 1.977649  |

Rotational constants (GHz): 1.1718700 0.3875800 0.3479500  
 Vibrational harmonic frequencies (cm-1):  
 i454.2067 24.9496 46.4578  
 71.8598 91.9858 116.4581  
 159.4239 175.3991 179.7539  
 199.8325 241.4406 271.3942  
 276.3627 299.2836 322.8317  
 343.0260 359.3877 373.2113  
 417.7379 428.7492 447.9321  
 502.8087 531.3459 558.4690  
 583.0092 610.9559 618.8098  
 659.6431 744.4441 778.0153  
 854.6529 894.3153 920.2588  
 931.6035 948.8877 957.6474  
 975.3468 986.0229 1011.8320  
 1018.2000 1035.4704 1066.3056  
 1100.0325 1131.1882 1153.4464  
 1175.7016 1193.1079 1207.0842  
 1233.9648 1239.5727 1263.0629  
 1277.1124 1299.1209 1313.7994  
 1341.0481 1361.1107 1383.9093  
 1393.7957 1396.7851 1413.8952  
 1413.9793 1434.6481 1436.2231  
 1457.8648 1461.8244 1465.8252  
 1475.9055 1481.1707 1500.0915  
 1579.1859 1648.8161 1887.2095  
 2076.6514 2920.6273 3048.6940  
 3050.7526 3053.9972 3055.6166  
 3060.6431 3074.8271 3094.9422  
 3130.0398 3133.8679 3138.8243  
 3143.2602 3153.4191 3159.3811

3175.8250 3236.3126 3868.9061  
Zero-point correction (Hartree): 0.270493

TS.ApineneCI.A.a+H2O.HHP.mppd

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E(RM062X/CC-pVDZ) (Hartree): -692.37007356

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-1.591412	0.140125	-0.417029
H	-1.994495	0.355463	-1.420317
C	-2.736271	0.127964	0.589469
C	-3.757742	-0.917888	0.217867
H	-2.349530	-0.121321	1.591968
H	-3.244311	1.101948	0.636285
H	-3.358527	-1.961811	0.148644
C	-0.353051	1.065856	-0.185449
C	-0.634906	-1.074016	-0.511188
C	-0.351764	2.399609	-0.913796
C	-0.059751	1.270057	1.298971
H	-0.168035	0.338081	1.873873
H	0.955766	1.665018	1.444428
H	-0.775543	1.992213	1.720160
H	0.629874	2.887451	-0.815007
H	-1.114344	3.073751	-0.493828
H	-0.565512	2.267720	-1.985168
H	-0.858217	-1.857456	-1.246016
H	-0.448703	-1.532546	0.471111
C	0.482337	-0.066252	-0.849987
H	0.496514	0.102712	-1.941418
C	1.896338	-0.367499	-0.480130
C	2.511123	-1.616100	-1.027324
H	2.530558	-1.502136	-2.123455
H	3.529504	-1.732474	-0.651131
H	1.892144	-2.481555	-0.768835
O	-4.916101	-0.688362	-0.011365
O	2.595469	0.663455	-0.167227
O	3.790689	0.260640	0.503989
O	2.015682	-1.134134	1.415303
H	2.961842	-0.628256	1.262985
H	1.565704	-0.550725	2.041681

Rotational constants (GHz): 1.3105500 0.3570600 0.3308100

Vibrational harmonic frequencies (cm-1):

i462.8474	40.4867	44.6669
61.7966	95.1416	120.3717
163.5805	174.6770	181.3508
201.0102	235.5593	262.2150
278.7836	297.8688	325.7994
341.9206	358.7307	366.0018
421.2319	429.0779	441.5026
506.8387	517.5869	552.5664
588.5475	618.4754	625.0246
660.7293	745.5747	787.7160
851.4646	894.0660	917.5673
932.9901	946.7027	954.6839
976.5319	985.9863	1001.5046
1020.8748	1035.3588	1072.9656
1102.5690	1132.6434	1154.3221
1175.8084	1190.8801	1208.7514
1238.2151	1244.2620	1262.7447
1278.5447	1300.3824	1315.6078
1337.2571	1360.8262	1380.3291
1392.5835	1394.9803	1413.4620
1417.8626	1434.0666	1434.5073
1457.5263	1461.6550	1464.5211
1474.8453	1480.9587	1498.2800
1580.5849	1654.3540	1888.7793
2045.8578	2920.6418	3049.7084
3050.7343	3055.4426	3060.1865
3066.2020	3075.5842	3088.4856
3130.6345	3132.8757	3135.1423
3139.5466	3152.4722	3154.4426
3176.4949	3237.8821	3865.1862

Zero-point correction (Hartree): 0.270430

TS.ApineneCI.A.a+H2O.HHP.mptd

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E(RM062X/CC-pVDZ) (Hartree): -692.37417847

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -1.665481 | 0.237515  | -0.330270 |
| H | -2.105690 | 0.346591  | -1.333846 |
| C | -2.765271 | 0.371312  | 0.701959  |
| C | -3.883852 | -0.616728 | 0.476520  |
| H | -2.394760 | 0.215575  | 1.730350  |
| H | -3.210433 | 1.382914  | 0.700222  |
| H | -4.728026 | -0.564206 | 1.206210  |
| C | -0.380100 | 1.120021  | -0.246135 |
| C | -0.776276 | -1.025553 | -0.322721 |
| C | -0.341174 | 2.363482  | -1.119434 |
| C | -0.018317 | 1.472393  | 1.195541  |
| H | -0.153652 | 0.616977  | 1.874623  |
| H | 1.021176  | 1.823826  | 1.263887  |
| H | -0.677955 | 2.276699  | 1.556062  |
| H | 0.666528  | 2.806297  | -1.110438 |
| H | -1.051637 | 3.121192  | -0.752950 |
| H | -0.604147 | 2.124971  | -2.161013 |
| H | -1.084722 | -1.862723 | -0.958375 |
| H | -0.575738 | -1.386904 | 0.696771  |
| C | 0.375922  | -0.119855 | -0.805986 |
| H | 0.356641  | -0.072781 | -1.909481 |
| C | 1.788014  | -0.446429 | -0.453644 |
| C | 2.323235  | -1.777840 | -0.874438 |

|                                                           |           |           |           |
|-----------------------------------------------------------|-----------|-----------|-----------|
| H                                                         | 2.308254  | -1.787710 | -1.976488 |
| H                                                         | 3.347798  | -1.904027 | -0.518884 |
| H                                                         | 1.672206  | -2.575508 | -0.501862 |
| O                                                         | -3.894861 | -1.421891 | -0.419122 |
| O                                                         | 2.545885  | 0.578123  | -0.286898 |
| O                                                         | 3.748480  | 0.196490  | 0.384234  |
| O                                                         | 1.952064  | -0.996605 | 1.511889  |
| H                                                         | 2.912307  | -0.556583 | 1.269068  |
| H                                                         | 1.549107  | -0.323445 | 2.076962  |
| Rotational constants (GHz): 1.2095500 0.3962700 0.3590800 |           |           |           |
| Vibrational harmonic frequencies (cm-1):                  |           |           |           |
| i462.3972                                                 | 42.2877   |           | 60.3711   |
| 84.0741                                                   | 111.3872  |           | 136.3064  |
| 166.2175                                                  | 177.0444  |           | 189.6517  |
| 199.7183                                                  | 235.6551  |           | 246.8093  |
| 277.2897                                                  | 298.8657  |           | 327.2250  |
| 340.7253                                                  | 359.5264  |           | 373.5350  |
| 400.8261                                                  | 430.6722  |           | 449.3549  |
| 506.4520                                                  | 536.8058  |           | 583.7079  |
| 614.5284                                                  | 616.4856  |           | 640.4928  |
| 684.8843                                                  | 715.9537  |           | 762.2698  |
| 842.3723                                                  | 895.0367  |           | 922.5565  |
| 937.8454                                                  | 940.0747  |           | 949.5834  |
| 957.6178                                                  | 978.1146  |           | 986.2751  |
| 1019.1943                                                 | 1021.4212 |           | 1041.4736 |
| 1101.9143                                                 | 1128.2250 |           | 1159.2494 |
| 1174.6389                                                 | 1187.0441 |           | 1207.9953 |
| 1233.1829                                                 | 1244.7789 |           | 1262.1064 |
| 1291.9483                                                 | 1306.1791 |           | 1325.0491 |
| 1341.2913                                                 | 1363.1215 |           | 1385.4805 |
| 1394.0494                                                 | 1401.2117 |           | 1403.4634 |
| 1414.1734                                                 | 1427.3562 |           | 1439.0062 |
| 1458.6166                                                 | 1462.2795 |           | 1466.1512 |
| 1477.1200                                                 | 1481.8299 |           | 1500.0915 |
| 1579.6467                                                 | 1650.7637 |           | 1877.3905 |
| 2046.6211                                                 | 2947.2615 |           | 3045.7924 |
| 3047.8865                                                 | 3049.3592 |           | 3055.8591 |
| 3073.5439                                                 | 3076.3821 |           | 3088.8860 |
| 3093.3215                                                 | 3127.2181 |           | 3129.7642 |
| 3137.9745                                                 | 3150.0696 |           | 3168.8861 |
| 3177.6739                                                 | 3238.8427 |           | 3868.9604 |
| Zero-point correction (Hartree): 0.270488                 |           |           |           |

TS.ApineneCI.A.a+H2O.HHP.mtmd

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E(RM062X/CC-pVDZ) (Hartree): -692.36855450

Electronic state : 1-A

Cartesian coordinates (Angs):

C	1.543675	0.773605	0.887535
H	1.653437	1.716387	1.446709
C	2.945473	0.230982	0.617359
C	3.031100	-1.186950	0.108106
H	3.483536	0.877020	-0.092696
H	3.509243	0.240465	1.567731
H	2.510219	-1.954418	0.733850
C	0.544429	1.047503	-0.281238
C	0.448622	-0.065458	1.593578
C	0.534761	2.455336	-0.853309
C	0.669176	0.019598	-1.403447
H	0.757853	-1.007335	-1.018549
H	-0.199962	0.071437	-2.074764
H	1.579566	0.213444	-1.990397
H	-0.315090	2.582787	-1.540857
H	1.461173	2.652890	-1.414814
H	0.449602	3.209048	-0.055825
H	0.376553	-0.000841	2.686420
H	0.441682	-1.119909	1.286879
C	-0.573998	0.726230	0.750922
H	-0.838568	1.656542	1.284485
C	-1.876724	0.098553	0.381916
C	-2.773778	-0.349768	1.491765
H	-3.058494	0.556542	2.050703
H	-3.667879	-0.827725	1.086633
H	-2.231315	-1.026761	2.159915
O	3.640220	-1.514815	-0.877056
O	-2.328341	0.445907	-0.769170
O	-3.362408	-0.449941	-1.180167
O	-1.625499	-1.846105	-0.202294
H	-2.500955	-1.506633	-0.744955
H	-0.958785	-1.911099	-0.900102
Rotational constants (GHz): 1.1004400 0.4238500 0.4027700			
Vibrational harmonic frequencies (cm-1):			
i466.2512	47.5675		52.3191
80.6517	95.1994		119.8459
174.8048	180.5235		189.2028
223.6338	238.4394		256.2113
284.5210	298.4444		321.7839
349.5165	361.5835		386.1010
402.1695	432.0251		460.9151
500.9172	520.8250		581.8727
600.1141	624.3923		633.2915
656.5418	711.5300		763.2880
830.6868	895.0012		909.4123
927.8908	948.6433		958.8413
972.4387	987.8579		1002.9995
1025.9090	1034.5170		1051.9855
1111.4283	1130.4215		1145.7131
1179.4803	1189.4784		1209.3909
1231.3614	1250.0325		1262.2176
1301.9080	1312.7504		1322.1256
1338.7215	1360.3358		1380.5962
1392.3545	1397.0126		1412.8550

1419.7853	1424.8772	1435.2293
1456.8746	1461.8921	1465.1429
1475.7168	1481.7587	1500.6215
1580.6329	1654.0191	1882.8106
2040.3012	2928.5227	3039.7539
3049.0599	3052.4203	3061.5109
3071.8994	3075.4362	3098.5684
3116.9317	3131.4602	3137.1600
3138.0800	3152.6352	3161.8324
3176.2326	3236.4830	3862.7147

Zero-point correction (Hartree): 0.270630

TS.ApineneCI.A.a+H2O.HHP.mttd

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E(RM062X/CC-pVDZ) (Hartree): -692.37372010

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 1.763357  | 0.597887  | 0.753156  |
| H | 2.240093  | 1.426686  | 1.298599  |
| C | 2.891136  | -0.312831 | 0.286447  |
| C | 2.573659  | -1.676297 | -0.270203 |
| H | 3.515504  | 0.193983  | -0.472590 |
| H | 3.591295  | -0.506064 | 1.120836  |
| H | 3.478989  | -2.262823 | -0.559730 |
| C | 0.743385  | 1.220317  | -0.261912 |
| C | 0.601851  | 0.028685  | 1.601225  |
| C | 0.949675  | 2.715812  | -0.476556 |
| C | 0.654545  | 0.529557  | -1.621442 |
| H | 0.284066  | -0.496946 | -1.558329 |
| H | -0.025830 | 1.080083  | -2.283327 |
| H | 1.652010  | 0.512985  | -2.091335 |
| H | 0.096647  | 3.146244  | -1.023136 |
| H | 1.860298  | 2.898941  | -1.069475 |
| H | 1.052737  | 3.250627  | 0.480285  |
| H | 0.642665  | 0.238800  | 2.677156  |
| H | 0.422984  | -1.037987 | 1.439461  |
| C | -0.382167 | 0.896046  | 0.773865  |
| H | -0.663840 | 1.805844  | 1.330048  |
| C | -1.670033 | 0.244574  | 0.376723  |
| C | -2.659353 | -0.063232 | 1.456639  |
| H | -2.164258 | -0.581013 | 2.284999  |
| H | -3.048072 | 0.905149  | 1.811982  |
| H | -3.479111 | -0.659307 | 1.050841  |
| O | 1.480215  | -2.169703 | -0.405951 |
| O | -2.035967 | 0.458040  | -0.834628 |
| O | -3.024204 | -0.494199 | -1.233198 |
| O | -1.369399 | -1.737261 | 0.081980  |
| H | -2.119429 | -1.514192 | -0.633612 |
| H | -0.538251 | -1.939126 | -0.375944 |

Rotational constants (GHz): 0.9601600 0.5551400 0.4747200

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| 1421.3887 | 77.7596   | 105.7530  |
| 117.0299  | 135.2825  | 155.3030  |
| 164.8351  | 184.5117  | 196.7584  |
| 243.3468  | 256.3453  | 262.8200  |
| 281.3775  | 302.5408  | 315.5731  |
| 334.5507  | 349.9114  | 367.7898  |
| 408.6797  | 412.2274  | 458.3580  |
| 517.0084  | 525.9729  | 606.1888  |
| 632.5462  | 664.6814  | 673.5930  |
| 703.5138  | 747.3693  | 773.9258  |
| 779.6697  | 891.4044  | 904.1358  |
| 927.4737  | 946.0871  | 952.8775  |
| 971.0015  | 981.8136  | 993.7400  |
| 1014.6184 | 1034.6696 | 1045.3046 |
| 1087.2952 | 1126.1588 | 1146.1713 |
| 1177.3357 | 1196.9894 | 1222.4899 |
| 1239.7925 | 1250.0553 | 1265.6496 |
| 1297.1023 | 1314.4512 | 1336.1671 |
| 1353.5521 | 1369.0446 | 1385.8971 |
| 1391.2955 | 1395.3307 | 1405.2527 |
| 1410.9069 | 1427.9538 | 1433.7145 |
| 1454.8614 | 1455.8159 | 1460.6591 |
| 1473.3916 | 1476.4815 | 1480.8910 |
| 1541.0409 | 1583.5194 | 1871.1368 |
| 2294.6044 | 2952.2618 | 3035.0645 |
| 3044.1692 | 3061.8690 | 3064.0533 |
| 3066.7333 | 3071.8013 | 3073.6804 |
| 3110.8558 | 3124.8882 | 3133.2728 |
| 3151.1352 | 3174.9327 | 3198.3146 |
| 3220.9096 | 3236.4524 | 3814.8882 |

Zero-point correction (Hartree): 0.271737

TS.ApineneCI.A.a+H2O.HHP.pmmd

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E(RM062X/CC-pVDZ) (Hartree): -692.37137231

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-1.493193	-0.500077	-0.549823
H	-1.879375	-0.290439	-1.560559
C	-2.618439	-1.072723	0.308159
C	-3.808646	-0.146515	0.345955
H	-2.953573	-2.036063	-0.102158
H	-2.257029	-1.233091	1.337174
H	-3.634770	0.838096	0.850884
C	-0.668019	0.740035	-0.074708
C	-0.180825	-1.303422	-0.662490
C	-1.051710	2.081737	-0.677956
C	-0.557609	0.830899	1.444783
H	-0.244353	-0.118209	1.901424
H	0.180931	1.592912	1.737283
H	-1.525152	1.125508	1.879616

H	-0.298707	2.850784	-0.443740
H	-2.015965	2.429738	-0.275103
H	-1.144544	2.014767	-1.772036
H	-0.075368	-1.985460	-1.515311
H	0.048920	-1.839024	0.268450
C	0.578507	0.032235	-0.728029
H	0.695838	0.384780	-1.762296
C	1.897983	0.173476	-0.050008
C	2.636985	1.465910	-0.177643
H	2.015654	2.232945	0.314720
H	3.603435	1.395485	0.326288
H	2.755319	1.729130	-1.233640
O	-4.879346	-0.399367	-0.141091
O	2.090607	-0.622638	0.938559
O	3.484089	-0.712445	1.237825
O	3.272659	-0.805809	-1.211407
H	3.666459	-0.892822	-0.227079
H	2.908006	-1.686290	-1.384442
Rotational constants (GHz): 1.4590500 0.3419400 0.3268200			
Vibrational harmonic frequencies (cm-1):			
i396.5058	27.1199	52.1853	
68.5816	78.1103	121.0084	
153.1619	186.1511	195.0020	
226.6926	245.2504	251.5146	
283.3972	291.2483	316.8931	
329.7159	340.9946	370.5044	
385.1719	426.7061	459.1530	
482.6471	524.1333	552.4009	
587.2736	595.5020	640.8688	
674.3245	722.1959	776.7979	
851.6668	886.4167	918.0575	
943.6795	950.7132	963.7145	
978.8812	993.7385	1003.8275	
1010.6760	1029.0187	1071.7433	
1112.8971	1130.1855	1152.1493	
1166.5292	1179.4616	1192.3160	
1235.3595	1258.9498	1261.3473	
1275.4583	1293.1093	1324.5562	
1342.8879	1362.0626	1381.9703	
1393.8126	1401.1376	1405.5761	
1420.0040	1437.8129	1441.3846	
1452.7911	1457.8407	1462.9695	
1472.9320	1477.8138	1481.2137	
1583.6108	1649.5918	1887.0271	
2251.2274	2917.2336	3048.4816	
3060.0423	3064.6918	3068.2492	
3071.8163	3094.3101	3110.0059	
3126.4109	3133.1234	3134.9001	
3136.8689	3153.7725	3159.9571	
3174.4725	3235.5413	3837.9506	
Zero-point correction (Hartree): 0.270739			
TS.ApineneCI.A.a+H2O.HHP.pmmu			
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E(RM062X/CC-pVDZ) (Hartree): -692.36726887			
Electronic state : 1-A			
Cartesian coordinates (Angs):			
C	1.485562	-0.505590	0.570001
H	1.882411	-0.280136	1.573503
C	2.609484	-1.068423	-0.295911
C	3.785227	-0.124488	-0.355874
H	2.964551	-2.022280	0.119652
H	2.242183	-1.243735	-1.320283
H	3.589142	0.854584	-0.863007
C	0.626465	0.718337	0.096756
C	0.188087	-1.328758	0.720545
C	1.010723	2.079293	0.658449
C	0.505768	0.778760	-1.423339
H	0.264425	-0.195178	-1.867921
H	-0.281098	1.475538	-1.740992
H	1.460038	1.122920	-1.852599
H	0.242027	2.831722	0.420942
H	1.960824	2.429784	0.226231
H	1.128259	2.041787	1.751893
H	0.108514	-2.028088	1.560192
H	-0.064403	-1.855178	-0.211871
C	-0.563789	0.005393	0.817832
H	-0.563479	0.348202	1.868537
C	-1.992142	0.115929	0.394859
C	-2.589453	1.471587	0.197453
H	-2.500488	1.995712	1.163305
H	-2.028319	2.030353	-0.558440
H	-3.641820	1.379525	-0.079944
O	4.866701	-0.359900	0.115656
O	-2.698928	-0.897812	0.744134
O	-3.941598	-0.900808	0.043424
O	-2.247227	-0.331888	-1.598495
H	-3.176138	-0.636663	-1.127704
H	-1.813810	-1.177827	-1.783866
Rotational constants (GHz): 1.4859800 0.3447700 0.3282100			
Vibrational harmonic frequencies (cm-1):			
i467.5880	27.3509	59.2154	
73.3577	79.5021	148.8493	
159.5618	173.7812	201.2563	
218.3927	242.7909	259.8507	
282.5276	294.8396	311.1894	
336.0178	348.3508	369.4458	
404.5137	425.0588	443.7071	
502.0737	524.9373	538.0466	
584.7419	605.8835	626.7817	
650.0522	728.6498	779.6827	
849.4903	891.0433	920.3196	

946.1963	951.2471	962.5997
970.0297	985.7977	998.2764
1024.9434	1025.8604	1072.0126
1108.3084	1132.9309	1148.3672
1171.3966	1179.0663	1193.0866
1236.1044	1260.4022	1264.6490
1276.2809	1295.5988	1320.7885
1339.5819	1357.8309	1384.2024
1393.2437	1401.7002	1410.1802
1418.5356	1429.9219	1439.1558
1450.8579	1456.6486	1461.6037
1472.4451	1474.1151	1478.7916
1581.6635	1645.2095	1887.4477
2028.9542	2919.8242	3042.7890
3049.0711	3061.5324	3068.3489
3071.3723	3074.8893	3089.0254
3128.0606	3134.9586	3136.2966
3147.7482	3163.5193	3168.6389
3178.6853	3234.6717	3844.3217

Zero-point correction (Hartree): 0.270216

TS.ApineneCI.A.a+H2O.HHP.pmpd

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E(RM062X/CC-pVDZ) (Hartree): -692.37442079

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -1.455862 | -0.764538 | -0.672500 |
| H | -1.781861 | -0.670893 | -1.722397 |
| C | -2.601312 | -1.316964 | 0.174119  |
| C | -3.807868 | -0.426051 | 0.012734  |
| H | -2.846424 | -2.334140 | -0.169936 |
| H | -2.320499 | -1.353450 | 1.235446  |
| H | -4.408727 | -0.591330 | -0.916317 |
| C | -0.766956 | 0.572630  | -0.253585 |
| C | -0.083171 | -1.466747 | -0.628646 |
| C | -1.224877 | 1.822043  | -0.988394 |
| C | -0.781627 | 0.790859  | 1.257749  |
| H | -0.400349 | -0.080563 | 1.808867  |
| H | -0.151297 | 1.651099  | 1.530593  |
| H | -1.809231 | 0.996442  | 1.590887  |
| H | -0.566221 | 2.676185  | -0.765216 |
| H | -2.243584 | 2.096279  | -0.673188 |
| H | -1.227045 | 1.667390  | -2.078103 |
| H | 0.135623  | -2.207246 | -1.408288 |
| H | 0.121022  | -1.899900 | 0.359496  |
| C | 0.572162  | -0.080875 | -0.764579 |
| H | 0.733446  | 0.192960  | -1.816854 |
| C | 1.827426  | 0.225134  | -0.022964 |
| C | 2.448014  | 1.573935  | -0.191392 |
| H | 1.729998  | 2.302528  | 0.220909  |
| H | 3.386799  | 1.626677  | 0.364307  |
| H | 2.600675  | 1.787566  | -1.254184 |
| O | -4.105343 | 0.455198  | 0.779578  |
| O | 2.031162  | -0.489671 | 1.024448  |
| O | 3.407059  | -0.428796 | 1.403004  |
| O | 3.356488  | -0.682088 | -1.037700 |
| H | 3.692927  | -0.671356 | -0.024581 |
| H | 3.084250  | -1.601944 | -1.171328 |

Rotational constants (GHz): 1.4184500 0.3676000 0.3542300

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i405.1121 | 41.5789   | 54.9975   |
| 69.8470   | 81.8288   | 125.6274  |
| 149.1816  | 170.3676  | 201.7439  |
| 224.9296  | 248.9861  | 258.3895  |
| 267.1447  | 298.6858  | 325.6979  |
| 335.0581  | 345.5963  | 377.0524  |
| 385.1475  | 440.7929  | 460.2005  |
| 486.8842  | 532.5699  | 549.8897  |
| 590.2171  | 594.8200  | 638.2313  |
| 674.0087  | 718.9839  | 773.4140  |
| 883.2989  | 897.5422  | 917.1762  |
| 927.7166  | 956.1849  | 969.4813  |
| 985.3591  | 992.0483  | 1004.4469 |
| 1016.9476 | 1033.3367 | 1050.1984 |
| 1111.8819 | 1124.6846 | 1155.1702 |
| 1161.2477 | 1180.3574 | 1187.2537 |
| 1234.7130 | 1256.2596 | 1258.5039 |
| 1274.1780 | 1291.2702 | 1323.1531 |
| 1346.8851 | 1365.4589 | 1383.8109 |
| 1393.7174 | 1404.8310 | 1408.0096 |
| 1411.4656 | 1438.5880 | 1445.7564 |
| 1454.0946 | 1458.8206 | 1466.4650 |
| 1472.7119 | 1479.1461 | 1488.5758 |
| 1583.4596 | 1649.2488 | 1874.0434 |
| 2211.8302 | 2930.1243 | 3048.2767 |
| 3052.9959 | 3061.1184 | 3070.5237 |
| 3072.9138 | 3095.4365 | 3105.6235 |
| 3129.7317 | 3136.3456 | 3139.1693 |
| 3147.8151 | 3156.5139 | 3161.1461 |
| 3174.6539 | 3234.8462 | 3841.9780 |

Zero-point correction (Hartree): 0.270898

TS.ApineneCI.A.a+H2O.HHP.pmpu

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E(RM062X/CC-pVDZ) (Hartree): -692.37027265

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-1.447734	0.772584	0.688596
H	-1.787099	0.674047	1.734107
C	-2.592628	1.302728	-0.171848
C	-3.784260	0.389255	-0.024975
H	-2.862884	2.313819	0.171855

H	-2.305098	1.346468	-1.230888
H	-4.371979	0.514720	0.918707
C	-0.722680	-0.554757	0.282214
C	-0.085878	1.499099	0.675566
C	-1.186945	-1.818810	0.990188
C	-0.722752	-0.759941	-1.230817
H	-0.412436	0.141039	-1.776013
H	-0.034831	-1.563058	-1.527279
H	-1.740293	-1.022920	-1.555947
H	-0.514849	-2.662500	0.767107
H	-2.195956	-2.099233	0.650991
H	-1.212950	-1.680807	2.082154
H	0.106921	2.264131	1.436081
H	0.140216	1.912577	-0.318093
C	0.565699	0.119803	0.856297
H	0.612075	-0.122450	1.933828
C	1.949384	-0.147104	0.360781
C	2.423911	-1.560819	0.264115
H	2.361616	-1.981934	1.281088
H	1.767842	-2.137150	-0.396134
H	3.458196	-1.584972	-0.085931
O	-4.083071	-0.467296	-0.818383
O	2.753544	0.833060	0.567536
O	3.945922	0.668067	-0.198381
O	2.109589	0.083828	-1.676451
H	3.084830	0.359166	-1.295789
H	1.722103	0.935556	-1.925107
Rotational constants (GHz): 1.4368500 0.3710800 0.3558300			
Vibrational harmonic frequencies (cm-1):			
i456.6788	48.4086		51.3124
76.5871	85.9046		145.7227
158.0760	165.1993		199.3221
220.6227	248.7791		259.9020
274.8348	304.7487		315.9704
342.4514	354.8556		377.1235
397.3032	442.4981		443.3886
504.5912	528.4689		538.5681
583.4852	597.8251		623.5088
648.6344	723.6494		776.3113
889.6637	890.8035		914.5201
939.0506	950.9883		961.0700
977.5904	988.6103		1009.8374
1025.6897	1034.2723		1048.1828
1106.5897	1128.5703		1152.5429
1167.8903	1180.0925		1190.5294
1235.2941	1254.5673		1261.2242
1275.0368	1295.1363		1320.2005
1349.8309	1359.6372		1385.8517
1393.5736	1404.6544		1411.2428
1411.7412	1429.9957		1444.2233
1450.6346	1457.6698		1464.6200
1472.4918	1474.5185		1487.7314
1581.2726	1642.3848		1875.4150
2053.8088	2931.6229		3043.9401
3047.9181	3051.3604		3071.9717
3072.7202	3075.5949		3090.7464
3128.7337	3136.7068		3147.8665
3158.8684	3160.9469		3164.3653
3178.4266	3236.0158		3846.1900
Zero-point correction (Hartree): 0.270490			
TS.ApineneCI.A.a+H2O.HHP.pmt			
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E(RM062X/CC-pVDZ) (Hartree): -692.37753473			
Electronic state : 1-A			
Cartesian coordinates (Angs):			
C	-1.499386	-0.627159	-0.674328
H	-1.931062	-0.355890	-1.649869
C	-2.536596	-1.372984	0.143233
C	-3.814783	-0.610868	0.369992
H	-2.800522	-2.329270	-0.343010
H	-2.145433	-1.658709	1.136116
H	-4.617222	-1.168627	0.911197
C	-0.779683	0.631386	-0.087179
C	-0.126390	-1.307949	-0.858378
C	-1.238174	1.982783	-0.610221
C	-0.732096	0.620873	1.437096
H	-0.353285	-0.328242	1.842063
H	-0.077304	1.421109	1.814577
H	-1.741605	0.802890	1.836999
H	-0.542345	2.778111	-0.297954
H	-2.240529	2.217983	-0.228725
H	-1.285423	1.982718	-1.709793
H	0.041872	-1.874116	-1.783448
H	0.136991	-1.932717	0.006302
C	0.536464	0.074995	-0.754874
H	0.667613	0.543255	-1.740146
C	1.816296	0.229366	-0.009230
C	2.474772	1.570418	0.017288
H	1.780411	2.250214	0.539017
H	3.418578	1.513181	0.564052
H	2.626115	1.934768	-1.003822
O	-3.996342	0.525947	0.011991
O	2.021931	-0.643707	0.911097
O	3.407128	-0.679334	1.258805
O	3.294746	-0.553073	-1.191433
H	3.653478	-0.708483	-0.199606
H	2.987430	-1.431994	-1.458030
Rotational constants (GHz): 1.4243700 0.3763800 0.3574500			
Vibrational harmonic frequencies (cm-1):			
i400.3718	37.8131		53.1346
72.8874	104.8538		131.9557

157.8844	167.2331	203.3266
233.9410	238.8253	245.7248
275.7212	292.5118	324.1686
334.5600	343.0926	358.5019
382.1471	439.1083	456.4293
476.0888	545.6018	583.7333
589.8054	640.1155	651.2266
683.8600	732.1376	753.5339
796.4099	887.5508	912.6666
925.3136	947.2849	955.2516
976.3352	985.8482	999.6642
1007.9163	1029.8572	1049.7118
1113.6517	1118.1259	1154.7896
1163.9755	1183.2539	1195.7126
1236.1098	1257.9119	1265.5651
1280.3611	1301.5155	1339.4085
1346.1041	1366.3474	1387.0323
1396.6379	1400.1077	1402.2760
1409.1286	1426.5063	1440.2797
1453.7836	1458.6260	1461.8797
1473.9019	1478.4199	1482.6687
1581.8077	1649.1695	1875.0711
2225.1068	2950.8973	3046.6780
3052.4985	3058.6043	3070.8490
3074.9836	3088.5909	3089.2207
3108.7383	3127.3945	3133.6795
3150.0336	3153.4560	3164.4676
3176.5166	3235.3824	3842.7639

Zero-point correction (Hartree): 0.270723

TS.ApineneCI.A.a+H2O.HHP.pmtu

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E(RM062X/CC-pVDZ) (Hartree): -692.37328155

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -1.494286 | -0.639179 | -0.669999 |
| H | -1.927153 | -0.364131 | -1.644331 |
| C | -2.542946 | -1.357373 | 0.157072  |
| C | -3.808502 | -0.570565 | 0.373038  |
| H | -2.824829 | -2.313273 | -0.319936 |
| H | -2.159463 | -1.639788 | 1.153607  |
| H | -4.615986 | -1.103862 | 0.931241  |
| C | -0.735771 | 0.610536  | -0.099892 |
| C | -0.137263 | -1.347106 | -0.873922 |
| C | -1.196844 | 1.975486  | -0.588056 |
| C | -0.666434 | 0.582413  | 1.423439  |
| H | -0.350968 | -0.392342 | 1.817922  |
| H | 0.042495  | 1.325274  | 1.812899  |
| H | -1.663969 | 0.816854  | 1.827744  |
| H | -0.477805 | 2.754873  | -0.288097 |
| H | -2.181424 | 2.221853  | -0.170065 |
| H | -1.282971 | 1.992839  | -1.685435 |
| H | 0.006754  | -1.959414 | -1.771552 |
| H | 0.144744  | -1.938586 | 0.010453  |
| C | 0.520474  | 0.037652  | -0.835764 |
| H | 0.525192  | 0.468947  | -1.853308 |
| C | 1.925812  | 0.204243  | -0.360406 |
| C | 2.427539  | 1.574761  | -0.039397 |
| H | 2.337268  | 2.164827  | -0.966238 |
| H | 1.804066  | 2.037476  | 0.732246  |
| H | 3.473530  | 1.527280  | 0.271171  |
| O | -3.975636 | 0.559202  | -0.012333 |
| O | 2.707973  | -0.732396 | -0.763746 |
| O | 3.927917  | -0.713459 | -0.023494 |
| O | 2.154440  | -0.384040 | 1.598556  |
| H | 3.114453  | -0.592266 | 1.135457  |
| H | 1.767839  | -1.266229 | 1.697677  |

Rotational constants (GHz): 1.4541000 0.3786500 0.3581100

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i466.0327 | 45.4868   | 52.7163   |
| 77.8053   | 120.0458  | 146.9399  |
| 156.7533  | 163.1589  | 201.7735  |
| 232.8017  | 235.5689  | 246.4897  |
| 280.4949  | 295.6488  | 313.9703  |
| 334.0809  | 353.0334  | 368.9969  |
| 384.1195  | 440.5329  | 445.2979  |
| 507.3276  | 521.7265  | 577.8020  |
| 595.7437  | 621.1241  | 639.3039  |
| 672.3465  | 737.4687  | 752.8208  |
| 798.3687  | 891.1976  | 911.0640  |
| 931.9828  | 948.8556  | 954.3310  |
| 969.4138  | 981.0840  | 991.3563  |
| 1023.4886 | 1027.4979 | 1047.3754 |
| 1108.7624 | 1123.5621 | 1151.5859 |
| 1170.9488 | 1182.5659 | 1197.8099 |
| 1236.2172 | 1261.5182 | 1265.8562 |
| 1285.1041 | 1300.4213 | 1336.9551 |
| 1343.3545 | 1362.6945 | 1388.5913 |
| 1398.5479 | 1401.1355 | 1403.6562 |
| 1412.8917 | 1425.2609 | 1432.5226 |
| 1448.3805 | 1455.7730 | 1461.8850 |
| 1469.4711 | 1473.0538 | 1482.2935 |
| 1580.9536 | 1645.2199 | 1875.6763 |
| 2022.0755 | 2950.0432 | 3047.2597 |
| 3047.8484 | 3053.0727 | 3064.8282 |
| 3074.0418 | 3075.8285 | 3081.8619 |
| 3088.8825 | 3126.1097 | 3145.2413 |
| 3157.9935 | 3162.3865 | 3167.8500 |
| 3179.2128 | 3237.2888 | 3847.6030 |

Zero-point correction (Hartree): 0.270212

TS.ApineneCI.A.a+H2O.HHP.ppm

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E(RM062X/CC-pVDZ) (Hartree): -692.37196668
Electronic state : 1-A
Cartesian coordinates (Angs):
C -1.627796 0.366242 -0.477219
H -1.957863 0.714079 -1.470814
C -2.840515 0.163549 0.424544
C -3.785660 -0.819086 -0.221002
H -2.549421 -0.237620 1.404759
H -3.366539 1.123704 0.563374
H -4.257144 -0.466665 -1.173712
C -0.456784 1.283061 -0.007359
C -0.627849 -0.798031 -0.644573
C -0.447327 2.692109 -0.575725
C -0.301999 1.301983 1.510434
H -0.276089 0.291858 1.941646
H 0.631217 1.807790 1.801787
H -1.137934 1.854569 1.965499
H 0.483092 3.221505 -0.316897
H -1.285976 3.275815 -0.163802
H -0.543378 2.681960 -1.671662
H -0.749621 -1.458343 -1.512425
H -0.556616 -1.404860 0.268360
C 0.501141 0.246147 -0.705799
H 0.700294 0.571759 -1.736511
C 1.814771 -0.034468 -0.060439
C 2.907134 0.977129 -0.190404
H 2.550245 1.891366 0.313128
H 3.812840 0.613933 0.300328
H 3.088491 1.201406 -1.246455
O -4.010248 -1.921504 0.204480
O 1.778208 -0.871079 0.912271
O 3.085601 -1.382845 1.172944
O 2.802326 -1.360494 -1.270061
H 3.173139 -1.580871 -0.297263
H 2.183464 -2.085832 -1.441164
Rotational constants (GHz): 1.0508000 0.3975300 0.3428300
Vibrational harmonic frequencies (cm-1):
i398.2677 25.8039 45.7745
59.4039 83.9777 103.1886
158.0723 171.4132 187.5482
219.4622 226.6370 249.8318
277.1298 300.3761 318.0419
332.3060 342.1093 349.1045
400.4296 438.7744 460.1364
486.6374 539.3381 562.4270
586.4719 592.4269 641.6948
675.2989 737.9598 778.9664
854.7973 887.1085 915.4255
932.3726 948.6930 958.1115
981.1579 991.7495 1000.8098
1015.8451 1035.1737 1065.1143
1101.9092 1140.4007 1150.6554
1163.7365 1184.1019 1206.6679
1236.7079 1240.0934 1266.3866
1272.0730 1291.6457 1319.7806
1343.2562 1363.4247 1385.9567
1395.2041 1404.0506 1408.5746
1415.0603 1437.6109 1439.5026
1451.1004 1459.5020 1463.4914
1472.4479 1477.5264 1480.5374
1584.7222 1651.4931 1887.8574
2248.8947 2920.5049 3048.5235
3054.4796 3056.3258 3061.0750
3067.4017 3096.3158 3105.6897
3126.8352 3134.5222 3136.6264
3142.9942 3155.9440 3160.7955
3174.6950 3234.8255 3840.4073
Zero-point correction (Hartree): 0.270645

TS.ApineneCI.A.a+H2O.HHP.ppmu
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E(RM062X/CC-pVDZ) (Hartree): -692.36812289
Electronic state : 1-A
Cartesian coordinates (Angs):
C      -1.615491      0.373549      -0.492545
H      -1.952144      0.748103      -1.474399
C      -2.820297      0.179233      0.421023
C      -3.786982      -0.786202      -0.218764
H      -2.526843      -0.233653      1.395457
H      -3.331073      1.145384      0.574009
H      -4.256899      -0.428072      -1.169808
C      -0.411922      1.255866      -0.022315
C      -0.642960      -0.807209      -0.708140
C      -0.391483      2.685377      -0.540352
C      -0.254018      1.233646      1.495114
H      -0.306095      0.219463      1.910200
H      0.708261      1.658612      1.809886
H      -1.059880      1.830301      1.950183
H      0.550871      3.189544      -0.274150
H      -1.215214      3.266899      -0.097208
H      -0.501307      2.716814      -1.634916
H      -0.798888      -1.468964      -1.567622
H      -0.550178      -1.420018      0.200766
C      0.483767      0.233081      -0.794125
H      0.570193      0.591628      -1.836092
C      1.884133      -0.115378      -0.407964
C      2.871829      0.984425      -0.186774
H      2.927541      1.549195      -1.132012
H      2.525002      1.656591      0.604533
H      3.850596      0.563194      0.053358
O      -4.030216      -1.882595      0.212353

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|                                                           |           |           |           |
|-----------------------------------------------------------|-----------|-----------|-----------|
| O                                                         | 2.240366  | -1.282614 | -0.806716 |
| O                                                         | 3.434552  | -1.690754 | -0.141293 |
| O                                                         | 2.019839  | -0.692181 | 1.563302  |
| H                                                         | 2.801556  | -1.248647 | 1.062528  |
| H                                                         | 1.348715  | -1.369547 | 1.733183  |
| Rotational constants (GHz): 1.0685400 0.3995000 0.3436100 |           |           |           |
| Vibrational harmonic frequencies (cm-1):                  |           |           |           |
| i457.3952                                                 | 25.4777   | 46.0274   |           |
| 70.0059                                                   | 91.1505   | 122.5848  |           |
| 150.6984                                                  | 164.5360  | 178.5957  |           |
| 219.3799                                                  | 239.9314  | 251.6513  |           |
| 276.6622                                                  | 308.3267  | 317.7916  |           |
| 330.4891                                                  | 351.8543  | 360.8497  |           |
| 405.7238                                                  | 439.7199  | 445.9720  |           |
| 503.9679                                                  | 533.1976  | 558.4892  |           |
| 578.5329                                                  | 602.1624  | 625.9855  |           |
| 646.4881                                                  | 748.0635  | 777.0711  |           |
| 854.5671                                                  | 889.5240  | 919.3253  |           |
| 930.6664                                                  | 948.2322  | 957.7812  |           |
| 976.1504                                                  | 986.5585  | 1000.2332 |           |
| 1020.8526                                                 | 1033.7881 | 1065.4298 |           |
| 1104.7430                                                 | 1134.8023 | 1149.8853 |           |
| 1170.1215                                                 | 1186.1672 | 1205.6199 |           |
| 1234.2917                                                 | 1241.0391 | 1267.8071 |           |
| 1276.3631                                                 | 1294.7741 | 1317.1587 |           |
| 1346.7115                                                 | 1360.2890 | 1386.9619 |           |
| 1394.3717                                                 | 1404.0104 | 1411.6171 |           |
| 1414.6114                                                 | 1429.8555 | 1437.6600 |           |
| 1449.8046                                                 | 1456.3393 | 1462.3719 |           |
| 1472.2966                                                 | 1473.7592 | 1480.2681 |           |
| 1582.3537                                                 | 1647.1462 | 1887.0353 |           |
| 2054.7120                                                 | 2923.6906 | 3044.9652 |           |
| 3047.8497                                                 | 3053.3036 | 3055.8654 |           |
| 3069.2768                                                 | 3073.1414 | 3092.2906 |           |
| 3127.6828                                                 | 3133.7635 | 3143.4975 |           |
| 3149.0224                                                 | 3162.6330 | 3170.9811 |           |
| 3178.8350                                                 | 3235.6910 | 3844.2528 |           |

Zero-point correction (Hartree): 0.270182

TS.ApineneCI.A.a+H2O.HHP.pppd

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E(RM062X/CC-pVDZ) (Hartree): -692.37169526

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-1.598595	0.143415	-0.396064
H	-1.978792	0.384669	-1.402082
C	-2.775021	-0.041186	0.556020
C	-3.671758	-1.156295	0.079091
H	-2.399855	-0.312994	1.557200
H	-3.380282	0.873225	0.637463
H	-3.170328	-2.151620	-0.027158
C	-0.475335	1.167117	-0.044680
C	-0.526260	-0.964811	-0.505592
C	-0.579308	2.523076	-0.722282
C	-0.270146	1.319826	1.459412
H	-0.156536	0.352884	1.969084
H	0.634910	1.908926	1.672303
H	-1.126132	1.850918	1.902375
H	0.322941	3.129092	-0.544516
H	-1.440165	3.083231	-0.324408
H	-0.714016	2.416850	-1.808891
H	-0.627722	-1.702650	-1.311623
H	-0.375864	-1.484949	0.450824
C	0.526509	0.140761	-0.695689
H	0.667078	0.391822	-1.756369
C	1.876944	-0.001607	-0.082254
C	2.889607	1.070775	-0.321742
H	2.489158	1.989615	0.138687
H	3.836902	0.803026	0.151475
H	3.013747	1.237410	-1.396572
O	-4.836003	-1.024331	-0.193876
O	1.930169	-0.767606	0.946758
O	3.277670	-1.169821	1.195202
O	2.920359	-1.337774	-1.231890
H	3.334655	-1.463670	-0.259652
H	2.352932	-2.115943	-1.335015

Rotational constants (GHz): 1.1881900 0.3597300 0.3249400

Vibrational harmonic frequencies (cm-1):

i397.2369	42.2365	44.3708
53.6630	84.1038	106.8091
150.2833	172.4088	187.1847
218.5600	226.4531	248.6690
266.3777	298.7272	312.2288
331.3766	337.5954	348.4877
401.0516	431.5595	459.2467
485.2121	521.9037	559.2808
584.7900	591.3803	636.3805
675.2685	739.0176	785.7459
855.5384	885.3147	910.8271
931.2116	947.5355	956.3776
979.8983	989.7814	1006.9897
1010.3079	1030.5495	1072.2900
1105.9852	1142.7941	1147.2639
1163.6640	1182.7924	1207.0977
1238.4472	1245.0430	1267.9466
1270.5489	1294.7000	1321.2912
1343.1822	1362.8709	1381.5460
1393.4292	1403.2686	1406.7307
1418.1461	1435.6754	1438.2339
1450.9528	1458.2553	1462.2395
1471.7645	1477.0871	1479.1823
1583.2046	1649.0206	1888.0767

2247.7892	2923.1981	3049.3883
3055.3573	3060.9124	3065.4023
3069.7632	3091.8907	3107.7157
3128.2858	3133.0318	3134.6905
3137.5920	3153.4847	3157.1615
3174.8034	3236.2237	3843.9360

Zero-point correction (Hartree): 0.270505

TS.ApineneCI.A.a+H2O.HHP.pppu

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E(RM062X/CC-pVDZ) (Hartree): -692.36757557

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -1.587694 | 0.134009  | -0.409109 |
| H | -1.976043 | 0.398904  | -1.406385 |
| C | -2.756359 | -0.042160 | 0.553298  |
| C | -3.687625 | -1.124258 | 0.065651  |
| H | -2.379006 | -0.343465 | 1.545157  |
| H | -3.337304 | 0.885089  | 0.661811  |
| H | -3.209756 | -2.125751 | -0.083293 |
| C | -0.434136 | 1.131197  | -0.058415 |
| C | -0.537942 | -0.992165 | -0.561820 |
| C | -0.534759 | 2.511405  | -0.688787 |
| C | -0.220959 | 1.245297  | 1.447881  |
| H | -0.187063 | 0.267772  | 1.945800  |
| H | 0.721158  | 1.755902  | 1.687423  |
| H | -1.049097 | 1.823319  | 1.886371  |
| H | 0.377384  | 3.099788  | -0.502037 |
| H | -1.383146 | 3.067784  | -0.260744 |
| H | -0.685204 | 2.444660  | -1.776792 |
| H | -0.669596 | -1.736219 | -1.355703 |
| H | -0.361803 | -1.512758 | 0.391912  |
| C | 0.505656  | 0.112337  | -0.781302 |
| H | 0.525311  | 0.386011  | -1.851897 |
| C | 1.941323  | -0.103189 | -0.430252 |
| C | 2.854158  | 1.077906  | -0.359973 |
| H | 2.841771  | 1.541838  | -1.360033 |
| H | 2.481350  | 1.804557  | 0.369052  |
| H | 3.867643  | 0.754207  | -0.113367 |
| O | -4.855477 | -0.960842 | -0.172004 |
| O | 2.362798  | -1.277399 | -0.734811 |
| O | 3.609457  | -1.538715 | -0.091993 |
| O | 2.205352  | -0.474698 | 1.576665  |
| H | 3.002728  | -1.026145 | 1.088697  |
| H | 1.593656  | -1.174531 | 1.848135  |

Rotational constants (GHz): 1.2159400 0.3605900 0.3250200

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i466.1130 | 41.4298   | 48.9115   |
| 60.1379   | 94.8618   | 130.6364  |
| 154.9052  | 169.4436  | 182.2886  |
| 214.7922  | 241.1270  | 250.3954  |
| 269.2500  | 312.0331  | 313.0353  |
| 328.2235  | 344.2303  | 358.4069  |
| 408.3416  | 435.4148  | 442.1606  |
| 505.3978  | 519.2988  | 552.6757  |
| 583.3276  | 608.7370  | 628.6975  |
| 648.8005  | 748.8656  | 785.1250  |
| 851.8828  | 889.9133  | 913.3170  |
| 932.8904  | 946.9403  | 954.9025  |
| 973.8469  | 989.1879  | 992.6859  |
| 1026.1067 | 1030.3943 | 1073.2821 |
| 1107.0453 | 1134.3593 | 1150.8002 |
| 1172.2371 | 1184.4269 | 1207.1828 |
| 1236.8098 | 1245.3373 | 1266.8754 |
| 1277.4983 | 1297.2571 | 1317.9659 |
| 1342.9375 | 1358.8517 | 1384.0741 |
| 1392.8163 | 1403.5375 | 1411.2079 |
| 1418.4425 | 1429.8555 | 1434.9959 |
| 1448.4447 | 1455.9328 | 1461.9869 |
| 1471.7902 | 1473.2993 | 1479.2061 |
| 1582.6540 | 1644.4542 | 1888.6255 |
| 2028.7759 | 2924.3897 | 3045.5612 |
| 3048.5707 | 3055.1546 | 3063.0734 |
| 3069.6321 | 3074.0090 | 3083.2197 |
| 3128.4355 | 3133.6745 | 3135.1753 |
| 3149.5964 | 3160.1111 | 3167.2576 |
| 3176.9320 | 3235.7768 | 3845.5411 |

Zero-point correction (Hartree): 0.270104

TS.ApineneCI.A.a+H2O.HHP.pptd

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E(RM062X/CC-pVDZ) (Hartree): -692.37571642

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-1.682081	0.209002	-0.314821
H	-2.102170	0.347281	-1.323096
C	-2.816741	0.130760	0.685072
C	-3.795655	-0.968005	0.350123
H	-2.451522	-0.055358	1.710436
H	-3.386122	1.076402	0.741892
H	-4.655582	-1.079625	1.054298
C	-0.521945	1.228193	-0.106308
C	-0.649757	-0.936008	-0.355670
C	-0.609341	2.511679	-0.915482
C	-0.257560	1.527574	1.366800
H	-0.160356	0.613621	1.969233
H	0.674570	2.100074	1.490281
H	-1.078193	2.134028	1.779769
H	0.316867	3.102034	-0.832341
H	-1.436913	3.139783	-0.548659
H	-0.788182	2.299911	-1.980031
H	-0.821025	-1.735700	-1.085113

H	-0.482202	-1.372761	0.638974
C	0.429706	0.111701	-0.681762
H	0.544779	0.255145	-1.765356
C	1.793779	-0.010935	-0.095809
C	2.834595	0.989247	-0.483048
H	2.476516	1.969362	-0.125207
H	3.784882	0.744297	-0.003397
H	2.934895	1.024757	-1.572580
O	-3.684513	-1.694229	-0.604355
O	1.856896	-0.658216	1.011637
O	3.198000	-1.079961	1.263515
O	2.748177	-1.507509	-1.118016
H	3.191005	-1.541519	-0.152517
H	2.140275	-2.261667	-1.113415
Rotational constants (GHz): 1.0846000 0.4039300 0.3554100			
Vibrational harmonic frequencies (cm-1):			
i393.3594	44.9431	49.6268	
71.6151	99.6591	137.5461	
151.2330	172.0058	194.9150	
213.2957	228.3321	250.7124	
254.1341	297.5475	319.6064	
333.0407	340.3891	349.4445	
390.5972	439.0179	451.6294	
486.8274	549.0880	583.5932	
593.2844	644.4970	652.8902	
687.2268	717.0316	755.8252	
841.8163	888.7033	913.4924	
934.7310	940.6124	947.9681	
960.0913	982.2504	995.3582	
1005.9581	1020.9922	1041.6385	
1102.6423	1144.1341	1152.5785	
1164.7317	1182.8054	1206.4665	
1232.0861	1245.3302	1268.3831	
1276.5230	1314.6058	1324.2217	
1344.8680	1364.0720	1389.9050	
1399.1912	1402.5871	1403.2415	
1408.1353	1429.3644	1440.6428	
1451.8801	1458.2941	1463.3152	
1473.1913	1478.1094	1480.2371	
1582.4690	1650.8117	1877.2689	
2262.9515	2948.9371	3043.2677	
3048.0141	3059.3289	3069.6477	
3076.3073	3089.8833	3097.7426	
3108.5131	3125.2540	3132.3353	
3137.0469	3153.7788	3167.7398	
3174.8696	3235.6349	3837.6545	
Zero-point correction (Hartree): 0.270679			
TS.ApineneCI.A.a+H2O.HHP.pptu			
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E(RM062X/CC-pVDZ) (Hartree): -692.37134374			
Electronic state : 1-A			
Cartesian coordinates (Angs):			
C	-1.669397	0.195268	-0.318179
H	-2.096047	0.348793	-1.321820
C	-2.797897	0.141750	0.689995
C	-3.820361	-0.914777	0.348068
H	-2.434778	-0.069514	1.711063
H	-3.331627	1.106887	0.762905
H	-4.677142	-1.004295	1.059336
C	-0.477919	1.186262	-0.118168
C	-0.664491	-0.974079	-0.387976
C	-0.558119	2.493803	-0.891019
C	-0.205142	1.455358	1.359429
H	-0.182516	0.535833	1.958331
H	0.759507	1.956984	1.513074
H	-0.998601	2.105485	1.760359
H	0.379366	3.065487	-0.802912
H	-1.369897	3.125347	-0.496671
H	-0.753924	2.315279	-1.959019
H	-0.868989	-1.785054	-1.093927
H	-0.469626	-1.401809	0.607714
C	0.405347	0.065060	-0.756892
H	0.395318	0.222268	-1.850969
C	1.845838	-0.154225	-0.431233
C	2.790025	1.002380	-0.502760
H	2.750918	1.373008	-1.540353
H	2.463890	1.803322	0.168410
H	3.803590	0.673502	-0.263226
O	-3.746173	-1.629669	-0.618132
O	2.231461	-1.362933	-0.631323
O	3.490811	-1.591758	-0.000536
O	2.158790	-0.340545	1.595826
H	2.930157	-0.954023	1.140242
H	1.533982	-0.999044	1.933199
Rotational constants (GHz): 1.1127200 0.4032500 0.3541600			
Vibrational harmonic frequencies (cm-1):			
i464.4171	41.2755	59.5301	
81.6880	113.2154	144.5330	
152.8133	166.4680	194.8003	
203.9182	239.4056	248.0752	
264.0533	303.0744	315.4487	
328.2733	348.7688	361.1605	
393.9328	437.9425	442.1468	
505.8312	534.3635	578.3582	
599.5236	623.3245	640.7305	
675.8530	716.4369	763.5323	
840.0614	890.7581	919.0830	
938.5313	940.3067	947.1831	
956.3018	976.7247	988.2102	
1005.6734	1025.5653	1039.5052	
1106.5698	1131.5318	1155.5189	

1169.8668	1182.8270	1206.4062
1231.2184	1246.1541	1266.3579
1285.7703	1310.3029	1325.5315
1345.8710	1358.9930	1389.1758
1400.3772	1402.1054	1404.1038
1410.6295	1426.6765	1434.6807
1449.8025	1456.2223	1462.4842
1472.2993	1474.6170	1480.6671
1582.9604	1646.0565	1878.3597
2025.6420	2946.6956	3043.7961
3044.6018	3047.3950	3068.0781
3073.6708	3074.5806	3083.6905
3091.0557	3126.3588	3133.6454
3147.5209	3166.5993	3178.1937
3178.2896	3234.8575	3845.0723

Zero-point correction (Hartree): 0.270077

TS.ApineneCI.A.a+H2O.HHP.ptmd

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E(RM062X/CC-pVDZ) (Hartree): -692.36996806

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 1.519232  | 0.520530  | 1.048987  |
| H | 1.596679  | 1.326120  | 1.796198  |
| C | 2.921468  | -0.040780 | 0.826801  |
| C | 3.020664  | -1.303436 | 0.004281  |
| H | 3.576854  | 0.712011  | 0.363113  |
| H | 3.351686  | -0.291488 | 1.813483  |
| H | 2.386945  | -2.157691 | 0.348811  |
| C | 0.683538  | 1.080000  | -0.142025 |
| C | 0.323131  | -0.379186 | 1.439583  |
| C | 0.791388  | 2.576607  | -0.381580 |
| C | 0.899657  | 0.302498  | -1.437568 |
| H | 0.774664  | -0.782008 | -1.305779 |
| H | 0.178448  | 0.619832  | -2.206393 |
| H | 1.911911  | 0.485234  | -1.827595 |
| H | 0.059325  | 2.915516  | -1.131294 |
| H | 1.794204  | 2.829933  | -0.760359 |
| H | 0.621572  | 3.143531  | 0.545910  |
| H | 0.114400  | -0.511159 | 2.508891  |
| H | 0.342634  | -1.359863 | 0.948053  |
| C | -0.581401 | 0.589844  | 0.656691  |
| H | -0.949000 | 1.407545  | 1.292719  |
| C | -1.741082 | 0.065661  | -0.117810 |
| C | -2.607557 | 1.035348  | -0.853720 |
| H | -1.976183 | 1.488147  | -1.636616 |
| H | -3.447608 | 0.512269  | -1.315762 |
| H | -2.951625 | 1.822359  | -0.174964 |
| O | 3.754113  | -1.430633 | -0.941793 |
| O | -1.652374 | -1.166585 | -0.467579 |
| O | -2.941599 | -1.677084 | -0.809305 |
| O | -3.226986 | -0.340757 | 1.232142  |
| H | -3.399719 | -1.039223 | 0.445545  |
| H | -2.824645 | -0.883115 | 1.926476  |

Rotational constants (GHz): 1.0969900 0.4140000 0.3795800

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i401.7665 | 44.5544   | 56.1473   |
| 79.9760   | 91.6388   | 105.8175  |
| 151.3423  | 186.1574  | 206.4577  |
| 224.7907  | 245.5984  | 249.6788  |
| 256.6015  | 299.1612  | 321.0452  |
| 340.9033  | 354.7425  | 361.0067  |
| 389.5961  | 438.3072  | 459.0587  |
| 473.8128  | 541.9329  | 576.7390  |
| 583.8297  | 610.4318  | 633.0009  |
| 670.5800  | 707.6674  | 758.5102  |
| 829.0568  | 886.4915  | 908.4179  |
| 923.5296  | 949.3000  | 964.0069  |
| 984.1655  | 985.4107  | 1003.6800 |
| 1013.4112 | 1033.7151 | 1053.5983 |
| 1113.0171 | 1137.6058 | 1147.1168 |
| 1167.0562 | 1180.2039 | 1210.0870 |
| 1230.6223 | 1250.1872 | 1264.3159 |
| 1289.9309 | 1315.8646 | 1328.1659 |
| 1345.3036 | 1365.1289 | 1382.5783 |
| 1394.1122 | 1405.8889 | 1406.9910 |
| 1420.4411 | 1425.7942 | 1439.9536 |
| 1451.8503 | 1457.9359 | 1463.1490 |
| 1474.8506 | 1479.0986 | 1482.1403 |
| 1583.6556 | 1648.5004 | 1882.4773 |
| 2223.5541 | 2941.7838 | 3041.0687 |
| 3047.8766 | 3061.3137 | 3070.2580 |
| 3072.2917 | 3101.9974 | 3108.6153 |
| 3117.4259 | 3127.1786 | 3134.8156 |
| 3137.5509 | 3152.0341 | 3168.0085 |
| 3175.4125 | 3236.0639 | 3843.0292 |

Zero-point correction (Hartree): 0.270779

TS.ApineneCI.A.a+H2O.HHP.ptmu

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E(RM062X/CC-pVDZ) (Hartree): -692.36596766

Electronic state : 1-A

Cartesian coordinates (Angs):

C	1.517420	0.549001	1.044272
H	1.615324	1.365534	1.777275
C	2.915711	-0.005279	0.781326
C	2.994715	-1.304186	0.016966
H	3.537395	0.733718	0.253580
H	3.395504	-0.205182	1.756534
H	2.391321	-2.147201	0.438165
C	0.634051	1.086561	-0.128073
C	0.336841	-0.346020	1.493943

C	0.741307	2.577180	-0.409180
C	0.834226	0.285814	-1.411416
H	0.777067	-0.798481	-1.249746
H	0.071970	0.531313	-2.163310
H	1.825926	0.509357	-1.833525
H	-0.008526	2.896001	-1.150140
H	1.734654	2.818786	-0.818639
H	0.594815	3.169915	0.506478
H	0.169196	-0.490505	2.567343
H	0.331208	-1.325496	0.995993
C	-0.580088	0.633541	0.745273
H	-0.837970	1.475263	1.413594
C	-1.893584	0.183656	0.194540
C	-2.598277	1.050590	-0.798050
H	-2.768880	2.019892	-0.301260
H	-1.967136	1.212163	-1.677908
H	-3.554219	0.600444	-1.074867
O	3.681536	-1.473734	-0.956685
O	-2.526987	-0.603560	0.987640
O	-3.591184	-1.254275	0.295128
O	-1.683699	-1.307760	-1.204727
H	-2.641418	-1.506798	-0.736779
H	-1.117488	-2.009233	-0.851226
Rotational constants (GHz): 1.1009600 0.4188300 0.3846600			
Vibrational harmonic frequencies (cm-1):			
i464.8039	46.9232	48.7301	
80.1611	94.3095	130.4633	
152.5482	176.4035	195.3112	
229.2643	245.5672	257.8572	
262.9740	312.2964	322.6549	
329.4971	363.6638	371.5124	
388.5305	438.3839	460.5740	
498.9038	517.7034	576.2754	
595.3866	605.7431	630.2639	
648.4894	708.3760	766.1810	
829.7253	889.4596	911.0307	
925.9824	945.9623	959.3060	
977.1780	985.0485	1002.5136	
1027.7239	1032.0480	1052.0252	
1113.8335	1133.2309	1144.2291	
1176.0820	1181.2060	1208.2052	
1231.8689	1250.1499	1268.8250	
1296.7264	1315.3676	1324.7650	
1342.7674	1360.8773	1384.0446	
1393.1326	1405.3569	1411.1030	
1419.7870	1424.5557	1430.8720	
1448.4455	1455.3171	1462.4991	
1473.6797	1475.7168	1478.1262	
1580.6138	1643.5049	1883.9329	
2037.9496	2928.5630	3042.8304	
3043.9724	3048.4784	3070.2982	
3072.1403	3073.4330	3100.5707	
3117.2235	3129.2313	3133.2705	
3151.4034	3162.3900	3165.8383	
3178.5593	3236.2421	3841.7320	
Zero-point correction (Hartree): 0.270295			
TS.ApineneCI.A.a+H2O.HHP.ptpd			
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E(RM062X/CC-pVDZ) (Hartree): -692.37012493			
Electronic state : 1-A			
Cartesian coordinates (Angs):			
C	1.669092	0.474295	0.915900
H	1.812008	1.165677	1.761698
C	3.053999	-0.020022	0.489365
C	3.067396	-1.175158	-0.491380
H	3.639000	0.820466	0.084018
H	3.582429	-0.383321	1.386620
H	3.614991	-1.009737	-1.451139
C	0.732099	1.182991	-0.107298
C	0.523579	-0.500793	1.263020
C	0.801049	2.700999	-0.131334
C	0.852547	0.606960	-1.515748
H	0.744189	-0.486209	-1.533621
H	0.077938	1.023806	-2.177858
H	1.830757	0.874695	-1.947261
H	0.006600	3.128749	-0.762789
H	1.766682	3.033956	-0.544723
H	0.699681	3.121498	0.880190
H	0.407379	-0.787228	2.316054
H	0.542373	-1.400033	0.636957
C	-0.456313	0.548726	0.706846
H	-0.781041	1.257552	1.481693
C	-1.668233	0.120228	-0.046429
C	-2.625416	1.167845	-0.516244
H	-2.076497	1.791010	-1.242455
H	-3.482410	0.699782	-1.005423
H	-2.938981	1.795304	0.324232
O	2.548033	-2.238562	-0.264669
O	-1.581505	-1.023730	-0.621862
O	-2.884262	-1.515216	-0.939206
O	-3.006301	-0.587284	1.334551
H	-3.236629	-1.137002	0.452130
H	-2.514990	-1.227059	1.870982
Rotational constants (GHz): 1.0227600 0.4705400 0.4023000			
Vibrational harmonic frequencies (cm-1):			
i399.4930	35.6346	53.3120	
60.7520	104.8230	117.7818	
151.1188	179.9892	196.6088	
217.3153	230.5799	238.3459	
251.5949	296.6506	321.3121	
339.3707	350.0301	354.9447	

388.7042	442.2225	457.2362
483.2598	543.9387	585.7867
590.7891	627.0587	642.0994
671.7573	723.1111	766.5231
859.2125	887.0781	915.7040
934.4258	945.9095	952.3857
976.8867	983.9986	995.1452
1010.7446	1029.6751	1054.9986
1066.6855	1136.6245	1147.7213
1165.8711	1181.3385	1212.7086
1231.7324	1249.0805	1263.5266
1288.8248	1316.0152	1342.8943
1345.6265	1363.6256	1378.2337
1392.7438	1402.3834	1404.5694
1416.6702	1436.7112	1440.4375
1454.3098	1458.9740	1462.5850
1477.3171	1480.8856	1486.0300
1585.5174	1652.1614	1872.8148
2240.0370	2942.7513	3046.6690
3053.2142	3054.8750	3066.9389
3068.6840	3104.7666	3107.6301
3111.5922	3121.9089	3125.4823
3135.4470	3159.8627	3173.5491
3184.5234	3235.8255	3840.2986

Zero-point correction (Hartree): 0.270777

TS.ApineneCI.A.a+H2O.HHP.pttd
 ~~~~~  
 E(RM062X/CC-pVDZ) (Hartree): -692.37126002  
 Electronic state : 1-A  
 Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 1.666467  | 0.475448  | 0.914034  |
| H | 1.781113  | 1.214621  | 1.723784  |
| C | 3.064953  | -0.016182 | 0.564169  |
| C | 3.240528  | -1.292711 | -0.222746 |
| H | 3.623352  | 0.770890  | 0.024138  |
| H | 3.653151  | -0.174771 | 1.487114  |
| H | 4.310908  | -1.531476 | -0.444339 |
| C | 0.746443  | 1.140535  | -0.155102 |
| C | 0.505928  | -0.472662 | 1.296703  |
| C | 0.833160  | 2.655973  | -0.243695 |
| C | 0.861843  | 0.506341  | -1.538413 |
| H | 0.727182  | -0.581556 | -1.512890 |
| H | 0.110386  | 0.932063  | -2.221581 |
| H | 1.853451  | 0.722085  | -1.968414 |
| H | 0.044560  | 3.063436  | -0.895585 |
| H | 1.802561  | 2.959981  | -0.670725 |
| H | 0.734770  | 3.122893  | 0.747743  |
| H | 0.373779  | -0.703907 | 2.361567  |
| H | 0.517821  | -1.394018 | 0.705966  |
| C | -0.454421 | 0.561881  | 0.681778  |
| H | -0.775490 | 1.311671  | 1.419241  |
| C | -1.670076 | 0.113793  | -0.053601 |
| C | -2.587061 | 1.152076  | -0.615826 |
| H | -2.015555 | 1.686884  | -1.392969 |
| H | -3.461877 | 0.676725  | -1.064655 |
| H | -2.875576 | 1.862129  | 0.165919  |
| O | 2.369621  | -2.040845 | -0.584601 |
| O | -1.615583 | -1.074443 | -0.536192 |
| O | -2.932264 | -1.546471 | -0.825233 |
| O | -3.045267 | -0.436809 | 1.359146  |
| H | -3.282103 | -1.049223 | 0.515570  |
| H | -2.581079 | -1.046841 | 1.951335  |

Rotational constants (GHz): 1.0519100 0.4635500 0.4028400  
 Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i410.0131 | 42.0153   | 60.0052   |
| 91.7505   | 115.7844  | 123.3563  |
| 153.5170  | 178.0501  | 199.0917  |
| 218.7907  | 228.0447  | 240.5120  |
| 257.8060  | 292.0925  | 316.5908  |
| 335.7108  | 346.3168  | 351.8051  |
| 389.5929  | 439.4760  | 454.4670  |
| 483.9531  | 544.1117  | 583.2321  |
| 592.5836  | 640.6147  | 662.0733  |
| 684.0277  | 745.9352  | 763.2271  |
| 782.9504  | 888.3986  | 901.2757  |
| 928.3885  | 940.3676  | 953.0756  |
| 973.0152  | 987.7535  | 997.3514  |
| 1009.2239 | 1024.7024 | 1048.8000 |
| 1083.5573 | 1137.4963 | 1158.6937 |
| 1170.3237 | 1183.3182 | 1219.3910 |
| 1235.0909 | 1254.5929 | 1266.2460 |
| 1294.7671 | 1324.2941 | 1348.5429 |
| 1363.9590 | 1373.4439 | 1390.0788 |
| 1393.9929 | 1400.3878 | 1406.1006 |
| 1410.4967 | 1428.8603 | 1440.4874 |
| 1453.4378 | 1458.8822 | 1462.7972 |
| 1475.4364 | 1481.6336 | 1486.1870 |
| 1586.7402 | 1650.2255 | 1883.9668 |
| 2191.3764 | 2927.6119 | 3034.7504 |
| 3045.5427 | 3055.4536 | 3061.7259 |
| 3068.0994 | 3071.3468 | 3102.0911 |
| 3105.7742 | 3120.1575 | 3124.0157 |
| 3134.0896 | 3175.8356 | 3184.5918 |
| 3195.9230 | 3235.3969 | 3840.5324 |

Zero-point correction (Hartree): 0.270800

TS.ApineneCI.A.a+H2O.HHP.pttu  
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 E(RM062X/CC-pVDZ) (Hartree): -692.37186676
 Electronic state : 1-A
 Cartesian coordinates (Angs):

C	1.757314	0.397204	0.881226
H	2.264521	1.111675	1.547356
C	2.826221	-0.575381	0.399884
C	2.421804	-1.845218	-0.303722
H	3.554852	-0.068378	-0.258499
H	3.436039	-0.917801	1.257489
H	3.287505	-2.466215	-0.639431
C	0.896316	1.220793	-0.141911
C	0.476247	-0.134066	1.564804
C	1.229366	2.709596	-0.125579
C	0.929400	0.717800	-1.582549
H	0.503991	-0.281555	-1.703132
H	0.374002	1.403710	-2.239935
H	1.971597	0.715891	-1.942217
H	0.480841	3.282280	-0.695921
H	2.213787	2.889053	-0.586817
H	1.255869	3.106510	0.900801
H	0.423366	-0.023873	2.654024
H	0.233612	-1.167196	1.299227
C	-0.354278	0.867176	0.740576
H	-0.633706	1.751503	1.339423
C	-1.657609	0.372723	0.191193
C	-2.363574	1.130395	-0.886103
H	-2.488747	2.163159	-0.521517
H	-1.766280	1.143565	-1.802133
H	-3.338825	0.669360	-1.063311
O	1.297873	-2.239377	-0.500563
O	-2.298229	-0.340869	1.045359
O	-3.341015	-1.078751	0.411816
O	-1.375579	-1.239429	-1.047680
H	-2.297653	-1.461978	-0.580768
H	-0.706400	-1.828436	-0.662996

Rotational constants (GHz): 0.9528600 0.5561900 0.4549700
 Vibrational harmonic frequencies (cm-1):
 i406.7905 63.3868 90.1859
 108.0158 133.2223 142.8284
 154.2012 179.1741 203.3209
 243.6604 245.8391 247.5611
 284.5353 291.1736 308.1284
 331.2368 345.4348 361.7483
 398.6722 427.0267 444.0567
 508.8583 526.7882 595.3610
 624.1539 644.7952 672.6153
 707.8893 747.9923 772.9689
 777.9031 884.6845 899.9697
 930.1772 952.4330 954.5956
 965.5210 983.0092 994.8944
 1015.7526 1031.5309 1052.2605
 1088.1941 1135.5284 1146.4712
 1168.3563 1193.9686 1218.3409
 1243.1492 1249.9416 1272.2664
 1291.0649 1317.5440 1342.0818
 1348.8142 1366.4330 1385.9759
 1390.3167 1394.3267 1401.8295
 1410.7468 1425.7440 1433.4198
 1455.5665 1458.2994 1463.4662
 1469.3737 1478.7042 1486.0318
 1565.1985 1590.0411 1870.9430
 2309.0128 2951.3595 3034.5937
 3043.7742 3053.0769 3058.6355
 3069.7485 3073.9065 3074.8231
 3118.4528 3122.2956 3125.9376
 3130.4872 3185.0738 3194.9827
 3228.3646 3234.7829 3809.1400
 Zero-point correction (Hartree): 0.271394

TS.ApineneCI.A.a+H2O.HHP.tmmdd
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 E(RM062X/CC-pVDZ) (Hartree): -692.36791043  
 Electronic state : 1-A  
 Cartesian coordinates (Angs):  

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -1.568053 | -0.611997 | -0.468260 |
| H | -1.857611 | -0.467378 | -1.521788 |
| C | -2.820385 | -0.887016 | 0.360206  |
| C | -3.827840 | 0.227896  | 0.218882  |
| H | -3.298481 | -1.817173 | 0.021153  |
| H | -2.551869 | -0.991880 | 1.423937  |
| H | -3.527062 | 1.207217  | 0.670972  |
| C | -0.560977 | 0.518580  | -0.075214 |
| C | -0.403821 | -1.620695 | -0.402338 |
| C | -0.705765 | 1.841951  | -0.810063 |
| C | -0.503118 | 0.748204  | 1.432656  |
| H | -0.482815 | -0.191906 | 2.003190  |
| H | 0.389433  | 1.331856  | 1.694818  |
| H | -1.396920 | 1.305772  | 1.754417  |
| H | 0.126506  | 2.520281  | -0.566511 |
| H | -1.636819 | 2.350778  | -0.515010 |
| H | -0.727817 | 1.695785  | -1.899865 |
| H | -0.380472 | -2.439042 | -1.131989 |
| H | -0.299910 | -2.030560 | 0.612535  |
| C | 0.555937  | -0.432618 | -0.638305 |
| H | 0.646779  | -0.240289 | -1.716843 |
| C | 1.950320  | -0.455677 | -0.097243 |
| C | 2.268156  | -1.095395 | 1.214639  |
| H | 2.046847  | -2.169109 | 1.097954  |
| H | 3.328400  | -0.965217 | 1.440330  |
| H | 1.641896  | -0.687760 | 2.012915  |
| O | -4.880753 | 0.118374  | -0.352660 |
| O | 2.840374  | -0.375045 | -1.027424 |
| O | 4.096170  | 0.003566  | -0.474985 |
| O | 2.451679  | 1.399643  | 0.611238  |
| H | 3.396584  | 0.977984  | 0.238424  |

|                                          |           |           |           |  |
|------------------------------------------|-----------|-----------|-----------|--|
| H                                        | 2.216846  | 2.038942  | -0.077753 |  |
| Rotational constants (GHz):              | 1.5939000 | 0.3376300 | 0.3215700 |  |
| Vibrational harmonic frequencies (cm-1): |           |           |           |  |
| i522.4076                                | 26.3186   |           | 64.2567   |  |
| 66.3892                                  | 88.5381   |           | 141.8466  |  |
| 166.0408                                 | 188.6403  |           | 208.4591  |  |
| 228.9037                                 | 243.6125  |           | 260.3717  |  |
| 276.2522                                 | 301.0130  |           | 320.9718  |  |
| 353.0777                                 | 365.8545  |           | 370.0077  |  |
| 402.2854                                 | 425.6240  |           | 451.0879  |  |
| 514.1314                                 | 523.0741  |           | 564.4238  |  |
| 586.0265                                 | 609.2123  |           | 645.1097  |  |
| 657.4933                                 | 732.6374  |           | 785.4602  |  |
| 855.0645                                 | 876.0411  |           | 922.7256  |  |
| 948.2175                                 | 954.2356  |           | 960.5718  |  |
| 980.8130                                 | 991.6407  |           | 1005.1645 |  |
| 1015.2035                                | 1026.0801 |           | 1062.6003 |  |
| 1105.0930                                | 1129.6275 |           | 1150.6626 |  |
| 1175.6180                                | 1180.3581 |           | 1211.5673 |  |
| 1235.3926                                | 1261.2702 |           | 1272.8396 |  |
| 1289.0554                                | 1296.5524 |           | 1315.5250 |  |
| 1321.2928                                | 1357.8804 |           | 1382.9792 |  |
| 1390.1857                                | 1397.6986 |           | 1411.3424 |  |
| 1416.6428                                | 1425.9664 |           | 1438.7433 |  |
| 1453.1273                                | 1459.0039 |           | 1460.3669 |  |
| 1469.3302                                | 1478.3531 |           | 1496.5759 |  |
| 1582.5731                                | 1636.3419 |           | 1887.3213 |  |
| 1916.9486                                | 2920.3435 |           | 3053.6003 |  |
| 3058.8920                                | 3064.2091 |           | 3070.9686 |  |
| 3076.8384                                | 3090.4135 |           | 3102.2845 |  |
| 3130.6000                                | 3132.3954 |           | 3134.0488 |  |
| 3142.2228                                | 3159.4431 |           | 3165.4310 |  |
| 3190.8358                                | 3244.7643 |           | 3837.6988 |  |

Zero-point correction (Hartree): 0.270525

TS.ApineneCI.A.a+H2O.HHP.tmmu

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E(RM062X/CC-pVDZ) (Hartree): -692.36836046

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-1.562255	-0.589054	-0.456075
H	-1.846008	-0.490217	-1.516437
C	-2.808397	-0.883455	0.373420
C	-3.862764	0.179716	0.185816
H	-3.246171	-1.848576	0.080997
H	-2.542568	-0.927923	1.442887
H	-3.564121	1.210637	0.505403
C	-0.610658	0.598715	-0.093796
C	-0.360364	-1.552969	-0.343796
C	-0.757584	1.886366	-0.887374
C	-0.566637	0.891097	1.403782
H	-0.461261	-0.021921	2.009520
H	0.278008	1.555708	1.636758
H	-1.492255	1.394747	1.722663
H	0.117436	2.532315	-0.720366
H	-1.657846	2.441453	-0.580445
H	-0.833951	1.680466	-1.965514
H	-0.291021	-2.377095	-1.063674
H	-0.274626	-1.956539	0.675363
C	0.557976	-0.339029	-0.558582
H	0.726263	-0.165878	-1.630888
C	1.879698	-0.207254	0.128691
C	2.314877	-1.195174	1.158636
H	1.612041	-1.102133	2.003427
H	2.251815	-2.210841	0.754358
H	3.326642	-0.960366	1.495419
O	-4.950548	-0.021078	-0.286970
O	2.327094	0.998971	0.108948
O	3.730990	1.011188	0.368743
O	3.336159	-0.858976	-1.154338
H	3.817914	-0.085216	-0.588820
H	3.186790	-0.443231	-2.016048

Rotational constants (GHz):	1.5596500	0.3341800	0.3161000

Vibrational harmonic frequencies (cm-1):

i422.3084	31.6500	41.2827
62.7957	79.8606	123.8031
181.0600	195.0463	225.6208
236.0517	241.3218	255.1665
268.0356	293.4770	325.2447
331.0904	350.4527	372.2454
396.6159	440.9285	446.4979
494.6485	522.7899	534.3906
587.8979	594.3881	637.1381
673.8785	722.0311	776.2074
842.3974	883.4732	920.5739
931.5072	952.0760	966.2417
970.3737	990.8663	1011.7184
1014.0234	1027.2959	1074.0340
1110.2454	1134.6293	1151.4848
1171.2587	1180.5646	1193.3787
1239.2863	1262.5380	1272.8988
1289.5441	1296.7746	1322.2635
1334.0644	1373.5214	1383.5647
1392.5380	1397.4441	1405.9404
1413.7165	1422.6006	1437.2718
1452.5890	1458.1288	1463.7900
1474.6810	1480.1730	1484.4819
1573.7426	1648.3134	1888.0761
2164.0972	2918.9021	3052.3775
3056.7645	3062.3740	3070.3293
3072.0202	3091.3353	3100.9292
3131.6179	3132.6183	3134.8528

3143.3902 3147.4246 3158.9726
 3174.5390 3236.1016 3843.0550
 Zero-point correction (Hartree): 0.270709

TS.ApineneCI.A.a+H2O.HHP.tmpd

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 E(RM062X/CC-pVDZ) (Hartree): -692.37087833

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -1.542602 | 0.870743  | 0.559968  |
| H | -1.764489 | 0.870217  | 1.640777  |
| C | -2.830926 | 1.096433  | -0.228265 |
| C | -3.833063 | 0.033292  | 0.148770  |
| H | -3.238509 | 2.088966  | 0.021139  |
| H | -2.647290 | 1.042570  | -1.309773 |
| H | -4.358948 | 0.190890  | 1.123463  |
| C | -0.644544 | -0.367557 | 0.242190  |
| C | -0.324329 | 1.779233  | 0.301754  |
| C | -0.842498 | -1.585200 | 1.131184  |
| C | -0.718308 | -0.768110 | -1.229428 |
| H | -0.643057 | 0.097643  | -1.904179 |
| H | 0.093260  | -1.466641 | -1.473013 |
| H | -1.689615 | -1.247704 | -1.421595 |
| H | -0.091252 | -2.359577 | 0.911996  |
| H | -1.832395 | -2.030718 | 0.947313  |
| H | -0.769852 | -1.322186 | 2.197155  |
| H | -0.195687 | 2.672794  | 0.924687  |
| H | -0.263545 | 2.058619  | -0.759518 |
| C | 0.568188  | 0.556921  | 0.621306  |
| H | 0.718579  | 0.485592  | 1.708165  |
| C | 1.921595  | 0.413890  | 0.000947  |
| C | 2.192567  | 0.861302  | -1.398242 |
| H | 2.040890  | 1.953213  | -1.411489 |
| H | 3.227881  | 0.634331  | -1.660850 |
| H | 1.495689  | 0.395706  | -2.100487 |
| O | -4.039454 | -0.960658 | -0.500732 |
| O | 2.864504  | 0.384035  | 0.881050  |
| O | 4.054207  | -0.151174 | 0.311487  |
| O | 2.245735  | -1.544481 | -0.490649 |
| H | 3.236653  | -1.160663 | -0.230634 |
| H | 2.005269  | -2.070504 | 0.286481  |

Rotational constants (GHz): 1.4969100    0.3698600    0.3467200

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| 1502.7052 | 48.3898   | 61.8159   |
| 79.3588   | 86.2722   | 143.1849  |
| 165.4242  | 175.2083  | 217.4172  |
| 234.4257  | 244.7380  | 261.1241  |
| 282.8755  | 306.0235  | 325.5441  |
| 352.9706  | 369.8964  | 385.3358  |
| 400.0077  | 437.1583  | 448.6781  |
| 510.0227  | 535.5731  | 561.3605  |
| 586.7853  | 600.5380  | 642.5973  |
| 656.7724  | 727.1041  | 782.8404  |
| 872.6348  | 892.2176  | 917.7291  |
| 932.3827  | 956.9623  | 968.1384  |
| 983.6979  | 996.9601  | 1008.6462 |
| 1015.4862 | 1030.3571 | 1046.5673 |
| 1101.6156 | 1126.0157 | 1153.7316 |
| 1172.0989 | 1182.7895 | 1209.0800 |
| 1234.2269 | 1259.4853 | 1267.7743 |
| 1295.4868 | 1297.6129 | 1317.7214 |
| 1320.7513 | 1361.2530 | 1384.3040 |
| 1390.2311 | 1401.4370 | 1413.3222 |
| 1414.3925 | 1425.4932 | 1443.7097 |
| 1454.6179 | 1458.9131 | 1466.0744 |
| 1469.7992 | 1487.6169 | 1496.9410 |
| 1580.9846 | 1636.0476 | 1875.2175 |
| 1957.8181 | 2934.4276 | 3050.8482 |
| 3052.7920 | 3063.8638 | 3071.0776 |
| 3075.9313 | 3091.8579 | 3100.2644 |
| 3132.1268 | 3139.3278 | 3140.4378 |
| 3146.9040 | 3158.8650 | 3168.1073 |
| 3188.3451 | 3241.4107 | 3840.3222 |

Zero-point correction (Hartree): 0.270885

TS.ApineneCI.A.a+H2O.HHP.tmpu

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 E(RM062X/CC-pVDZ) (Hartree): -692.37118027

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-1.534988	-0.855575	-0.549345
H	-1.758566	-0.883702	-1.629278
C	-2.809770	-1.126652	0.246716
C	-3.854969	-0.107826	-0.135198
H	-3.178711	-2.137241	0.009588
H	-2.623470	-1.054582	1.326958
H	-4.363292	-0.284507	-1.115950
C	-0.705324	0.434665	-0.256402
C	-0.274220	-1.704022	-0.273763
C	-0.921693	1.622064	-1.179172
C	-0.789753	0.869692	1.205037
H	-0.629934	0.031926	1.901439
H	-0.031627	1.638174	1.415420
H	-1.786323	1.286425	1.411506
H	-0.133802	2.373314	-1.019554
H	-1.895675	2.094441	-0.977908
H	-0.894667	1.314317	-2.235736
H	-0.095643	-2.585761	-0.900906
H	-0.220408	-1.996204	0.784502
C	0.559040	-0.442883	-0.562011
H	0.779845	-0.361182	-1.635716
C	1.820828	-0.136394	0.179051

C	2.253835	-0.964015	1.342594
H	1.491082	-0.829105	2.127448
H	2.290013	-2.020893	1.058571
H	3.221993	-0.614869	1.707334
O	-4.113331	0.872020	0.516913
O	2.187711	1.089168	0.040330
O	3.569343	1.231767	0.371938
O	3.395569	-0.822356	-0.935417
H	3.786862	0.046748	-0.437354
H	3.270067	-0.516432	-1.845527
Rotational constants (GHz):		1.4675700	0.3661400 0.3418500
Vibrational harmonic frequencies (cm-1):			
i430.5663	37.7929	52.4463	
73.0615	83.4642	129.1437	
164.9250	204.1511	228.6398	
238.6539	245.0980	255.4804	
263.4633	302.6907	327.8128	
340.1529	353.8023	379.2695	
395.4528	440.4928	463.6629	
492.3761	527.7921	537.1997	
592.7051	598.1194	636.1096	
672.1990	718.1559	773.3290	
879.0944	893.1013	912.4262	
926.9277	952.3472	957.9778	
985.5174	995.5252	1008.6391	
1018.7572	1033.3406	1050.8130	
1108.7157	1129.0136	1154.9135	
1165.4346	1180.6627	1190.2998	
1237.3917	1257.0705	1267.6782	
1290.0047	1296.5223	1320.8435	
1332.9106	1374.3863	1384.7211	
1392.5875	1401.5512	1407.6213	
1414.2951	1422.7454	1443.9358	
1455.5962	1459.2876	1465.4096	
1474.8735	1484.3509	1488.5394	
1574.5472	1648.9398	1875.6045	
2134.9626	2933.2866	3049.8329	
3053.9466	3057.3600	3070.1924	
3073.0045	3092.7594	3102.1385	
3133.6206	3135.5639	3142.0707	
3144.9633	3152.8126	3158.5537	
3175.5660	3236.6720	3843.2006	
Zero-point correction (Hartree): 0.270949			
TS.ApineneCI.A.a+H2O.HHP.tmtD			
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E(RM062X/CC-pVDZ) (Hartree): -692.37367908			
Electronic state : 1-A			
Cartesian coordinates (Angs):			
C	1.596797	0.711282	-0.575093
H	1.906443	0.489223	-1.607955
C	2.809911	1.128859	0.233646
C	3.923165	0.115008	0.257024
H	3.231159	2.071956	-0.158877
H	2.549145	1.350921	1.283736
H	4.845684	0.429017	0.803261
C	0.653546	-0.438309	-0.086087
C	0.381697	1.660667	-0.578061
C	0.836631	-1.799420	-0.738127
C	0.653473	-0.570570	1.433459
H	0.586858	0.401802	1.944462
H	-0.189514	-1.191241	1.765121
H	1.594298	-1.048487	1.749485
H	0.030456	-2.486186	-0.435437
H	1.798012	-2.237800	-0.440553
H	0.827130	-1.716758	-1.835209
H	0.300586	2.409170	-1.376084
H	0.272384	2.155861	0.398060
C	-0.523800	0.414398	-0.685822
H	-0.635303	0.129158	-1.741527
C	-1.901463	0.419431	-0.105178
C	-2.210871	1.138500	1.167410
H	-2.043261	2.209896	0.968879
H	-3.257238	0.977528	1.434532
H	-1.543747	0.816006	1.971554
O	3.860776	-0.970219	-0.263339
O	-2.814223	0.233815	-0.998250
O	-4.036297	-0.156606	-0.381208
O	-2.295812	-1.396768	0.750133
H	-3.266961	-1.052761	0.377035
H	-2.036193	-2.068163	0.101814
Rotational constants (GHz):		1.5086300	0.3739200 0.3502200
Vibrational harmonic frequencies (cm-1):			
i509.3943	42.7753	63.0218	
83.4605	116.0215	142.4667	
170.1865	177.6086	218.4194	
222.8755	238.4134	259.1738	
283.3453	303.2704	322.9725	
350.8190	355.8555	379.1251	
385.7236	441.1009	447.0559	
505.1404	560.5535	578.8738	
600.6382	629.3363	659.8214	
672.4509	745.4267	753.7881	
800.2933	873.1293	915.7385	
930.4654	949.9732	957.5446	
973.5239	988.9235	992.6742	
1014.5164	1026.3819	1047.7399	
1102.6451	1117.7794	1153.3296	
1179.3520	1182.2662	1216.9913	
1233.7948	1266.4304	1275.3703	
1295.0581	1304.3731	1317.8115	
1336.0181	1363.3078	1384.4320	

1393.9131	1397.2534	1403.7718
1412.4881	1424.8076	1432.8177
1453.8589	1456.2289	1461.7081
1470.3875	1482.6799	1495.7455
1580.6107	1632.2729	1876.3298
1945.8610	2949.3641	3046.9485
3055.5966	3057.4978	3075.4094
3075.8289	3085.0488	3090.0138
3102.3416	3129.4006	3132.3704
3153.7529	3163.9466	3165.1072
3189.3623	3243.2326	3834.5682

Zero-point correction (Hartree): 0.270601

TS.ApineneCI.A.a+H2O.HHP.tmtu

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E(RM062X/CC-pVDZ) (Hartree): -692.37378940

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -1.590379 | -0.709516 | -0.551306 |
| H | -1.908014 | -0.526130 | -1.589102 |
| C | -2.784845 | -1.162200 | 0.265884  |
| C | -3.933853 | -0.188320 | 0.265397  |
| H | -3.169158 | -2.129284 | -0.105476 |
| H | -2.515033 | -1.350154 | 1.320571  |
| H | -4.843796 | -0.517668 | 0.823731  |
| C | -0.718470 | 0.503465  | -0.086511 |
| C | -0.328504 | -1.600200 | -0.526802 |
| C | -0.928446 | 1.834649  | -0.787848 |
| C | -0.725085 | 0.687493  | 1.427581  |
| H | -0.565072 | -0.257014 | 1.970914  |
| H | 0.062535  | 1.392629  | 1.730784  |
| H | -1.694647 | 1.100523  | 1.746347  |
| H | -0.089626 | 2.510036  | -0.560575 |
| H | -1.869936 | 2.298827  | -0.465970 |
| H | -0.975363 | 1.697390  | -1.878940 |
| H | -0.198351 | -2.339494 | -1.326629 |
| H | -0.221319 | -2.103261 | 0.445505  |
| C | 0.516268  | -0.318923 | -0.602583 |
| H | 0.696972  | -0.032479 | -1.648085 |
| C | 1.811491  | -0.178593 | 0.129735  |
| C | 2.267396  | -1.218355 | 1.098644  |
| H | 1.534957  | -1.226229 | 1.922974  |
| H | 2.272858  | -2.202245 | 0.618220  |
| H | 3.254349  | -0.957250 | 1.485845  |
| O | -3.908645 | 0.882620  | -0.286475 |
| O | 2.204179  | 1.044568  | 0.211608  |
| O | 3.600057  | 1.096755  | 0.509038  |
| O | 3.327589  | -0.667360 | -1.156334 |
| H | 3.758257  | 0.084672  | -0.520265 |
| H | 3.171508  | -0.192531 | -1.985687 |

Rotational constants (GHz): 1.4784900 0.3715900 0.3463300

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i431.0870 | 39.6902   | 43.7083   |
| 74.9743   | 106.9223  | 137.4046  |
| 171.2505  | 199.5798  | 230.2788  |
| 233.8792  | 240.4056  | 250.5094  |
| 267.2476  | 291.8584  | 326.6475  |
| 338.6577  | 346.8699  | 357.3655  |
| 392.6840  | 436.5928  | 460.6097  |
| 489.5523  | 523.8913  | 583.0682  |
| 587.1281  | 628.4104  | 648.5090  |
| 685.6916  | 730.9845  | 751.6229  |
| 794.6487  | 884.1359  | 909.9146  |
| 926.7433  | 937.1581  | 954.7218  |
| 970.0173  | 987.4988  | 994.1333  |
| 1013.8519 | 1027.2278 | 1049.5727 |
| 1112.6195 | 1122.6487 | 1152.4360 |
| 1167.9564 | 1184.0450 | 1196.3915 |
| 1236.4201 | 1264.8647 | 1278.6039 |
| 1290.6507 | 1301.1144 | 1331.4553 |
| 1338.3040 | 1375.8165 | 1385.5807 |
| 1392.7577 | 1399.7919 | 1402.2729 |
| 1408.0641 | 1420.9322 | 1430.7247 |
| 1453.6902 | 1458.3867 | 1460.9791 |
| 1473.1451 | 1482.2429 | 1483.1972 |
| 1573.1130 | 1647.0599 | 1876.5645 |
| 2135.7882 | 2946.0280 | 3046.3598 |
| 3051.5877 | 3058.2770 | 3074.2023 |
| 3075.3099 | 3086.1588 | 3090.5487 |
| 3102.0221 | 3126.8919 | 3136.7334 |
| 3144.9312 | 3153.2403 | 3164.9251 |
| 3175.6876 | 3236.0814 | 3845.1823 |

Zero-point correction (Hartree): 0.270595

TS.ApineneCI.A.a+H2O.HHP.tpmd

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E(RM062X/CC-pVDZ) (Hartree): -692.36906124

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-1.650315	0.315951	-0.523116
H	-1.856956	0.582303	-1.573541
C	-2.927817	0.441381	0.300807
C	-3.971112	-0.485886	-0.271062
H	-2.758045	0.153269	1.346939
H	-3.299144	1.478992	0.260482
H	-4.385456	-0.185512	-1.266434
C	-0.351709	1.058687	-0.077680
C	-0.866779	-1.012208	-0.481809
C	-0.077335	2.386378	-0.764561
C	-0.270064	1.216615	1.437801
H	-0.551437	0.298227	1.973017
H	0.748713	1.496280	1.737253

H	-0.966881	2.006552	1.758325
H	0.894072	2.801428	-0.454671
H	-0.848998	3.122656	-0.488851
H	-0.079147	2.281523	-1.859496
H	-1.080595	-1.774417	-1.240865
H	-0.928358	-1.467986	0.516850
C	0.423398	-0.177885	-0.659011
H	0.598042	0.008160	-1.728475
C	1.726740	-0.651357	-0.098324
C	1.798121	-1.389813	1.197794
H	1.250854	-2.334910	1.047096
H	2.840360	-1.606736	1.440312
H	1.315633	-0.824429	1.999670
O	-4.319179	-1.510031	0.256308
O	2.619912	-0.828553	-1.012243
O	3.917944	-0.870756	-0.429632
O	2.759695	0.941999	0.669853
H	3.536419	0.257505	0.300452
H	2.745178	1.634643	-0.007375
Rotational constants (GHz): 1.2918700 0.3637500 0.3288400			
Vibrational harmonic frequencies (cm-1):			
i519.7679	24.1644	50.6087	
70.7257	99.1081	115.7101	
161.7300	173.0620	196.6928	
225.8113	247.2762	257.4988	
280.8884	315.8657	327.3018	
331.2014	356.5571	372.0057	
391.6063	443.9870	455.3195	
515.1142	543.8223	570.0278	
579.2637	601.2720	639.7996	
655.4062	752.3409	784.1939	
863.1824	875.5605	920.7331	
931.8667	952.4638	962.2891	
984.0941	991.1790	1000.2089	
1018.3627	1026.3956	1061.6885	
1085.6727	1141.3692	1145.3522	
1180.1870	1188.1746	1217.0939	
1238.4690	1243.2192	1270.9087	
1288.3163	1295.6572	1314.8122	
1319.1817	1359.5486	1384.2781	
1390.5834	1399.3353	1412.7191	
1414.3698	1426.3370	1440.1042	
1452.7032	1458.7041	1462.4346	
1468.7428	1480.7836	1495.8463	
1582.6003	1635.1717	1884.2945	
1923.2320	2928.2137	3050.9320	
3055.7705	3060.9305	3063.4716	
3076.5440	3090.8231	3099.0955	
3128.2487	3136.2813	3140.4624	
3145.8266	3157.3561	3166.6867	
3190.6266	3244.0901	3840.6411	
Zero-point correction (Hartree): 0.270424			
TS.ApineneCI.A.a+H2O.HHP.tpmu			
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E(RM062X/CC-pVDZ) (Hartree): -692.36940832			
Electronic state : 1-A			
Cartesian coordinates (Angs):			
C	-1.658466	0.339399	-0.522073
H	-1.876883	0.585449	-1.574835
C	-2.940210	0.415045	0.302400
C	-3.936597	-0.572011	-0.252046
H	-2.752846	0.151330	1.352236
H	-3.361236	1.432714	0.247916
H	-4.374413	-0.303689	-1.246553
C	-0.400515	1.152854	-0.084102
C	-0.818357	-0.956311	-0.461685
C	-0.145166	2.465332	-0.804000
C	-0.318789	1.343171	1.427663
H	-0.507099	0.409791	1.979447
H	0.676057	1.715625	1.711539
H	-1.068527	2.078732	1.756340
H	0.860421	2.841813	-0.564275
H	-0.880397	3.225953	-0.497015
H	-0.215688	2.339957	-1.894937
H	-0.982477	-1.719719	-1.231623
H	-0.897872	-1.427549	0.528549
C	0.435899	-0.074386	-0.588810
H	0.685807	0.094267	-1.645883
C	1.710517	-0.393930	0.125667
C	1.787689	-1.524567	1.095652
H	1.118288	-1.268116	1.933742
H	1.429591	-2.446669	0.626171
H	2.810535	-1.632318	1.462171
O	-4.223923	-1.609172	0.286643
O	2.503804	0.617384	0.190742
O	3.835543	0.185372	0.470709
O	2.942940	-1.384113	-1.174793
H	3.617402	-0.827682	-0.552047
H	2.956386	-0.893233	-2.009343
Rotational constants (GHz): 1.2337100 0.3683100 0.3284700			
Vibrational harmonic frequencies (cm-1):			
i425.1659	24.8544	37.2751	
61.8024	89.0539	107.1408	
164.5415	183.0145	222.3503	
228.3857	238.7456	249.6248	
277.8322	300.7214	323.7760	
334.1972	340.1394	353.6679	
420.5472	438.1916	459.8303	
492.0661	526.3028	554.5832	
582.4210	586.2828	628.0586	
673.0101	737.3949	778.8234	

860.9236	886.1132	918.6407
925.2646	942.9764	954.8710
984.1361	992.4798	1000.1633
1019.8723	1030.1728	1061.5808
1101.3169	1137.4253	1152.7459
1164.3148	1185.2940	1204.8225
1238.4893	1244.1178	1275.7921
1290.7990	1293.5139	1317.2771
1334.4178	1375.0085	1384.2678
1392.9557	1399.7330	1407.4632
1411.1918	1422.3112	1440.7132
1452.4156	1457.7226	1463.5674
1472.3137	1480.5204	1484.6061
1572.7942	1646.3815	1883.8237
2153.2612	2925.8568	3050.0956
3057.1921	3059.3454	3062.0339
3072.5014	3092.3165	3101.2137
3131.5110	3134.6854	3141.9268
3144.2080	3148.0234	3157.0885
3174.4860	3238.4671	3845.9308

Zero-point correction (Hartree): 0.270578

TS.ApineneCI.A.a+H2O.HHP.tppd

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E(RM062X/CC-pVDZ) (Hartree): -692.36819622

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -1.630614 | 0.044218  | -0.398267 |
| H | -1.897690 | 0.177949  | -1.459346 |
| C | -2.883075 | 0.189367  | 0.457789  |
| C | -3.919492 | -0.833939 | 0.064894  |
| H | -2.630572 | 0.023052  | 1.518768  |
| H | -3.332157 | 1.187603  | 0.353279  |
| H | -3.577952 | -1.898552 | 0.127458  |
| C | -0.375759 | 0.922537  | -0.099147 |
| C | -0.739774 | -1.210526 | -0.258741 |
| C | -0.240776 | 2.188495  | -0.929258 |
| C | -0.236985 | 1.243597  | 1.386123  |
| H | -0.416574 | 0.367821  | 2.026951  |
| H | 0.768903  | 1.628543  | 1.600377  |
| H | -0.979187 | 2.008120  | 1.663030  |
| H | 0.706268  | 2.706999  | -0.714306 |
| H | -1.057691 | 2.887168  | -0.689318 |
| H | -0.283332 | 1.969715  | -2.006261 |
| H | -0.921131 | -2.066253 | -0.920764 |
| H | -0.709174 | -1.556215 | 0.785173  |
| C | 0.468906  | -0.306338 | -0.593408 |
| H | 0.574825  | -0.223349 | -1.684498 |
| C | 1.832128  | -0.617582 | -0.062120 |
| C | 2.025996  | -1.208448 | 1.295948  |
| H | 1.555512  | -2.205247 | 1.271065  |
| H | 3.093048  | -1.315104 | 1.501276  |
| H | 1.535370  | -0.602061 | 2.062206  |
| O | -5.032199 | -0.568588 | -0.306891 |
| O | 2.692310  | -0.820199 | -1.001544 |
| O | 4.015548  | -0.702766 | -0.490706 |
| O | 2.765469  | 1.121129  | 0.485617  |
| H | 3.577155  | 0.466085  | 0.143783  |
| H | 2.662024  | 1.738834  | -0.253565 |

Rotational constants (GHz): 1.4505500 0.3340200 0.3115500

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i516.0234 | 43.4504   | 47.7812   |
| 62.7604   | 102.0797  | 120.9422  |
| 161.4544  | 169.9605  | 198.0817  |
| 218.9385  | 250.7659  | 257.3234  |
| 273.2494  | 317.4659  | 323.9717  |
| 330.0275  | 355.9453  | 369.7451  |
| 392.1865  | 442.6001  | 446.5009  |
| 514.0771  | 527.8066  | 569.9155  |
| 582.6926  | 599.1234  | 641.9336  |
| 657.3146  | 754.6005  | 789.4763  |
| 851.0722  | 873.7994  | 913.2141  |
| 932.2106  | 950.9930  | 957.9779  |
| 984.0385  | 992.0648  | 1000.0094 |
| 1017.7646 | 1025.8272 | 1066.0259 |
| 1097.7924 | 1137.7474 | 1150.3612 |
| 1181.4451 | 1186.0037 | 1217.6805 |
| 1239.9382 | 1249.3180 | 1271.0361 |
| 1289.6912 | 1297.7138 | 1315.1629 |
| 1319.7590 | 1358.1867 | 1383.1624 |
| 1389.4448 | 1399.3385 | 1412.0237 |
| 1420.1003 | 1426.3388 | 1433.2162 |
| 1452.1117 | 1457.9807 | 1461.2086 |
| 1469.1910 | 1480.6603 | 1494.9749 |
| 1581.7911 | 1636.0725 | 1889.2108 |
| 1933.8415 | 2922.5316 | 3051.1402 |
| 3055.6483 | 3062.9328 | 3065.8574 |
| 3076.5462 | 3085.8270 | 3101.1086 |
| 3128.8572 | 3130.0989 | 3136.5375 |
| 3140.6434 | 3154.5164 | 3165.9079 |
| 3190.1428 | 3243.7018 | 3839.2276 |

Zero-point correction (Hartree): 0.270352

TS.ApineneCI.A.a+H2O.HHP.tppu

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E(RM062X/CC-pVDZ) (Hartree): -692.36852392

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-1.634969	0.079480	-0.398638
H	-1.909486	0.188952	-1.460405
C	-2.890265	0.182799	0.459792
C	-3.878763	-0.895907	0.092814

H	-2.624583	0.048667	1.522417
H	-3.385530	1.157035	0.339296
H	-3.486053	-1.941604	0.173005
C	-0.421908	1.019018	-0.114347
C	-0.696109	-1.140919	-0.240380
C	-0.298618	2.261297	-0.978996
C	-0.284052	1.376287	1.362705
H	-0.372734	0.497358	2.019679
H	0.692181	1.845900	1.551128
H	-1.070631	2.088732	1.653641
H	0.685917	2.730329	-0.833854
H	-1.074535	2.996533	-0.713986
H	-0.410381	2.014508	-2.045374
H	-0.832642	-1.997772	-0.911355
H	-0.684038	-1.498519	0.799973
C	0.480420	-0.193973	-0.532066
H	0.663085	-0.127033	-1.613830
C	1.809131	-0.344501	0.137806
C	2.020413	-1.357971	1.212232
H	1.375787	-1.062133	2.056842
H	1.712621	-2.347972	0.859845
H	3.065340	-1.352803	1.528906
O	-5.004970	-0.691564	-0.277021
O	2.525285	0.721183	0.055200
O	3.897846	0.415761	0.302617
O	3.048275	-1.378110	-1.122104
H	3.708143	-0.712898	-0.598887
H	2.984363	-0.979103	-2.002114
Rotational constants (GHz):			
Vibrational harmonic frequencies (cm-1):			
i424.0189	36.0548	45.6773	
48.8831	93.4968	111.4980	
165.9687	185.1975	220.2862	
229.8599	236.2078	253.4860	
270.1909	302.3553	323.8190	
333.1199	341.0970	353.9245	
421.2413	437.4193	447.9261	
493.5647	519.9560	546.7265	
585.7650	590.3171	628.5472	
674.9745	739.2057	783.8232	
851.2812	882.3963	913.3335	
925.5237	941.0792	954.6572	
980.2314	990.3202	1006.7913	
1019.8683	1027.7129	1074.6304	
1105.0861	1140.1353	1152.7786	
1167.6477	1185.8319	1206.1546	
1240.4985	1250.0961	1275.6857	
1291.1098	1296.3458	1319.0083	
1333.6270	1373.4996	1383.3720	
1392.4706	1399.8158	1407.2435	
1418.6843	1422.8161	1435.0902	
1452.5778	1457.7716	1463.2319	
1473.1553	1480.5251	1485.1195	
1573.4295	1647.7525	1888.9173	
2156.1742	2919.1111	3051.4435	
3054.2210	3058.2370	3067.9609	
3070.3427	3085.7143	3102.8314	
3131.7020	3133.0551	3134.9829	
3143.2006	3148.7319	3152.2075	
3174.7614	3237.7666	3844.0618	
Zero-point correction (Hartree): 0.270588			
TS.ApineneCI.A.a+H2O.HHP.tptd			
~~			
E(RM062X/CC-pVDZ) (Hartree): -692.37226462			
Electronic state : 1-A			
Cartesian coordinates (Angs):			
C	-1.704567	0.162000	-0.355175
H	-1.996423	0.178807	-1.416844
C	-2.925802	0.442891	0.494775
C	-4.043407	-0.537292	0.233441
H	-2.700287	0.401889	1.574999
H	-3.325838	1.457804	0.317852
H	-4.976501	-0.373544	0.825415
C	-0.403433	1.001271	-0.174639
C	-0.880898	-1.114345	-0.094749
C	-0.215647	2.157381	-1.143766
C	-0.218156	1.479781	1.263136
H	-0.435817	0.692846	2.000387
H	0.811388	1.827511	1.421587
H	-0.910404	2.313096	1.460998
H	0.764104	2.640165	-1.004711
H	-0.985308	2.926567	-0.971127
H	-0.295640	1.822570	-2.188330
H	-1.138089	-2.015189	-0.662259
H	-0.849550	-1.351839	0.979136
C	0.369334	-0.317897	-0.538536
H	0.462236	-0.360262	-1.633183
C	1.722521	-0.638714	0.010094
C	1.906686	-1.084190	1.423875
H	1.385478	-2.051509	1.513690
H	2.969695	-1.222230	1.631180
H	1.457189	-0.372258	2.121485
O	-3.964995	-1.447396	-0.551395
O	2.557780	-0.991159	-0.908277
O	3.892835	-0.886170	-0.425164
O	2.755517	1.098527	0.347840
H	3.526687	0.362286	0.073986
H	2.668180	1.627557	-0.459037
Rotational constants (GHz):			
Vibrational harmonic frequencies (cm-1):			
i524.6637	45.5005	62.5944	

89.9439	106.1541	145.6238
164.9510	176.6305	204.1511
226.6713	235.4969	259.4855
270.6596	308.6545	327.3351
333.4160	356.2965	371.2410
388.7108	437.2950	448.3375
517.2689	563.0454	581.9868
607.1970	630.8602	661.1435
675.4004	719.5803	772.2601
840.2651	876.4208	918.3751
937.0320	940.1597	951.6811
962.8148	986.7638	991.6104
1004.3791	1025.8801	1032.5958
1087.8903	1138.5459	1153.5924
1180.4671	1184.6101	1220.5519
1232.1024	1250.0236	1273.8342
1290.1548	1309.3743	1316.6018
1325.8976	1360.9900	1384.6381
1396.7599	1397.7628	1402.1027
1412.3318	1425.7007	1435.4157
1452.7476	1459.3332	1463.1481
1471.6923	1480.4123	1496.1495
1580.7034	1635.5597	1877.4596
1916.3490	2947.1628	3045.3282
3048.6394	3060.5454	3075.8320
3078.3459	3086.9566	3091.4357
3101.2856	3124.7876	3131.9139
3139.9031	3167.1925	3170.8866
3190.2017	3243.2771	3838.4151

Zero-point correction (Hartree): 0.270443

TS.ApineneCI.A.a+H2O.HHP.tptu

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E(RM062X/CC-pVDZ) (Hartree): -692.37262916

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -1.710701 | 0.186744  | -0.354553 |
| H | -2.009748 | 0.190306  | -1.414187 |
| C | -2.937460 | 0.412103  | 0.504158  |
| C | -4.009829 | -0.620243 | 0.255038  |
| H | -2.700372 | 0.384317  | 1.582616  |
| H | -3.385720 | 1.406885  | 0.328620  |
| H | -4.944528 | -0.499280 | 0.854715  |
| C | -0.453131 | 1.091793  | -0.184275 |
| C | -0.830388 | -1.054702 | -0.094035 |
| C | -0.285645 | 2.234862  | -1.170411 |
| C | -0.269470 | 1.587808  | 1.247762  |
| H | -0.391657 | 0.783729  | 1.989898  |
| H | 0.732247  | 2.022602  | 1.377385  |
| H | -1.013290 | 2.366300  | 1.476496  |
| H | 0.723530  | 2.665478  | -1.088429 |
| H | -1.018489 | 3.032464  | -0.969398 |
| H | -0.431125 | 1.889036  | -2.204717 |
| H | -1.039374 | -1.955844 | -0.680282 |
| H | -0.816502 | -1.314847 | 0.975038  |
| C | 0.385353  | -0.198637 | -0.490874 |
| H | 0.552581  | -0.245343 | -1.576342 |
| C | 1.717332  | -0.341785 | 0.172973  |
| C | 1.901137  | -1.249951 | 1.342373  |
| H | 1.286610  | -0.838607 | 2.160647  |
| H | 1.538668  | -2.253655 | 1.097192  |
| H | 2.950734  | -1.264359 | 1.642700  |
| O | -3.895512 | -1.527508 | -0.528790 |
| O | 2.479668  | 0.676419  | -0.025736 |
| O | 3.841579  | 0.335034  | 0.234793  |
| O | 2.888851  | -1.552434 | -0.989134 |
| H | 3.586055  | -0.867602 | -0.546365 |
| H | 2.820508  | -1.241623 | -1.903597 |

Rotational constants (GHz): 1.2567300 0.3753700 0.3366700

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i423.7035 | 37.2916   | 48.2596   |
| 82.0631   | 100.1801  | 137.2109  |
| 165.8087  | 195.2783  | 212.1339  |
| 230.3973  | 236.0089  | 249.2778  |
| 255.4740  | 299.0457  | 321.9958  |
| 335.2188  | 340.8218  | 353.7642  |
| 404.2368  | 437.8285  | 460.8816  |
| 488.9994  | 531.9590  | 584.2486  |
| 587.5426  | 631.6848  | 648.1440  |
| 689.1999  | 718.1108  | 756.5441  |
| 838.3857  | 884.9954  | 917.6737  |
| 929.6546  | 936.8521  | 946.4935  |
| 954.6469  | 983.1929  | 994.7928  |
| 1009.3017 | 1025.7349 | 1036.8109 |
| 1103.8272 | 1138.5580 | 1158.2861 |
| 1164.2895 | 1183.3113 | 1205.3293 |
| 1233.2659 | 1251.4143 | 1282.3571 |
| 1291.4545 | 1311.5000 | 1324.5411 |
| 1334.0360 | 1377.1629 | 1386.5994 |
| 1395.0128 | 1400.9234 | 1401.9633 |
| 1408.6320 | 1420.5618 | 1434.6604 |
| 1452.3084 | 1458.0201 | 1462.8567 |
| 1475.4313 | 1480.8030 | 1484.4360 |
| 1571.9948 | 1645.2307 | 1877.1000 |
| 2151.6657 | 2946.5248 | 3044.2617 |
| 3048.7263 | 3055.4104 | 3072.4415 |
| 3075.4159 | 3086.3849 | 3091.2772 |
| 3101.6040 | 3129.3611 | 3131.7487 |
| 3141.6313 | 3144.9138 | 3169.8580 |
| 3175.0113 | 3238.2786 | 3843.4476 |

Zero-point correction (Hartree): 0.270560

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TS.ApineneCI.A.a+H2O.HHP.ttmd
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E(RM062X/CC-pVDZ) (Hartree): -692.36660212
Electronic state : 1-A
Cartesian coordinates (Angs):
C -1.548947 0.399266 -1.106070
H -1.511080 1.103274 -1.952330
C -3.017941 0.180334 -0.751507
C -3.321203 -0.951762 0.199150
H -3.458719 1.097648 -0.332711
H -3.566390 -0.055938 -1.681282
H -2.922105 -1.952953 -0.102396
C -0.530693 0.905454 -0.039122
C -0.583158 -0.766617 -1.420690
C -0.350736 2.412619 0.039020
C -0.805072 0.332125 1.348478
H -1.001752 -0.750238 1.331232
H 0.053317 0.512191 2.009703
H -1.698921 0.811406 1.775977
H 0.438720 2.683714 0.756692
H -1.282286 2.886002 0.387448
H -0.094366 2.839654 -0.941725
H -0.496456 -1.108602 -2.459437
H -0.751441 -1.631453 -0.765094
C 0.551939 0.130452 -0.872430
H 0.907167 0.801566 -1.667570
C 1.773789 -0.469238 -0.252433
C 1.706716 -1.721559 0.558856
H 1.380300 -2.520049 -0.127760
H 2.698711 -1.959767 0.948046
H 0.977491 -1.627381 1.368090
O -3.979174 -0.835135 1.200086
O 2.853194 -0.142652 -0.878599
O 3.990061 -0.370960 -0.053111
O 2.322189 0.640542 1.377402
H 3.266702 0.262577 0.971451
H 2.322786 1.567545 1.095927
Rotational constants (GHz): 1.2940700 0.3780500 0.3691200
Vibrational harmonic frequencies (cm-1):
i507.3757 45.8738 57.8052
 81.7564 92.5396 123.8351
 167.6021 192.7808 210.4586
 215.0618 250.6816 261.0888
 266.9691 308.8572 329.0736
 348.8614 355.2755 385.5347
 390.1475 443.7397 453.9481
 491.5204 558.2054 576.9943
 597.4958 605.2736 643.0508
 654.4339 710.2571 773.9906
 831.0401 873.7803 910.0092
 926.3231 950.6877 961.8770
 984.7844 992.5193 1002.0792
 1016.7643 1027.7925 1049.5009
 1107.2203 1132.5933 1149.5111
 1178.6388 1190.7348 1220.9497
 1230.4527 1255.4522 1292.3569
 1298.3854 1313.6258 1319.8423
 1325.4057 1360.7529 1382.4726
 1390.4214 1400.3547 1411.8241
 1420.4987 1424.9530 1427.0619
 1450.9003 1458.7171 1461.3634
 1471.9692 1478.5474 1497.3595
 1582.2104 1635.8957 1883.7380
 1946.5962 2925.1609 3041.9406
 3050.8121 3062.1721 3072.6017
 3075.4037 3098.3166 3101.4067
 3118.6783 3128.7165 3136.5060
 3139.6084 3160.5846 3162.6290
 3188.8784 3241.9790 3840.6682
Zero-point correction (Hartree): 0.270571

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TS.ApineneCI.A.a+H2O.HHP.ttmu
~~~~~
E(RM062X/CC-pVDZ) (Hartree): -692.36689725
Electronic state : 1-A
Cartesian coordinates (Angs):
C      1.554159      0.352492      1.112172
H      1.523087      1.012535      1.993283
C      3.022017      0.082926      0.786689
C      3.294007     -1.002050     -0.226347
H      3.516299      1.001498      0.436116
H      3.530287     -0.236882      1.714184
H      2.861200     -2.005443      0.015119
C      0.597908      0.968919      0.046052
C      0.529306     -0.787118      1.336829
C      0.444391      2.479724      0.055656
C      0.873527      0.468293     -1.369486
H      0.975661     -0.626955     -1.420743
H      0.053990      0.763292     -2.041212
H      1.811202      0.897727     -1.752162
H      -0.400003      2.781080     -0.581877
H      1.355950      2.963394     -0.329142
H      0.259267      2.853857      1.073827
H      0.384114     -1.157694      2.358895
H      0.701896     -1.640896      0.668055
C      -0.538755      0.161311      0.763533
H      -0.959108      0.795369      1.556995
C      -1.679569     -0.333585     -0.066726
C      -1.764099     -1.761200     -0.492153
H      -0.906980     -1.943102     -1.161899
H      -1.680835     -2.418159      0.379892
H      -2.695806     -1.933360     -1.034781

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|                                                           |           |           |           |
|-----------------------------------------------------------|-----------|-----------|-----------|
| O                                                         | 3.958161  | -0.849420 | -1.218494 |
| O                                                         | -2.250192 | 0.610366  | -0.729277 |
| O                                                         | -3.555259 | 0.205264  | -1.143273 |
| O                                                         | -3.303360 | -0.570309 | 1.158571  |
| H                                                         | -3.729040 | -0.283647 | 0.214549  |
| H                                                         | -3.393342 | 0.231904  | 1.693371  |
| Rotational constants (GHz): 1.2464300 0.3786500 0.3680400 |           |           |           |
| Vibrational harmonic frequencies (cm-1):                  |           |           |           |
| i429.6797                                                 | 35.7661   |           | 46.3875   |
| 79.4669                                                   | 89.8375   |           | 109.9370  |
| 172.7426                                                  | 207.6524  |           | 224.5437  |
| 233.1985                                                  | 237.1201  |           | 252.0335  |
| 264.6607                                                  | 312.5913  |           | 328.2981  |
| 338.5270                                                  | 350.8590  |           | 364.5631  |
| 402.1080                                                  | 437.7264  |           | 467.3448  |
| 489.7476                                                  | 518.2336  |           | 577.6855  |
| 590.0858                                                  | 604.6600  |           | 636.4883  |
| 666.6842                                                  | 708.5255  |           | 760.5977  |
| 833.4137                                                  | 883.7970  |           | 906.8676  |
| 924.2639                                                  | 941.1663  |           | 952.5737  |
| 986.4126                                                  | 989.4305  |           | 1004.1154 |
| 1019.5280                                                 | 1031.9684 |           | 1053.4145 |
| 1113.0062                                                 | 1139.5876 |           | 1144.8786 |
| 1171.8354                                                 | 1182.6862 |           | 1212.2651 |
| 1232.4665                                                 | 1251.6377 |           | 1290.8874 |
| 1295.4402                                                 | 1315.0922 |           | 1326.2914 |
| 1334.2598                                                 | 1375.0490 |           | 1382.6546 |
| 1392.4669                                                 | 1401.6391 |           | 1407.3929 |
| 1419.2229                                                 | 1424.1150 |           | 1427.4338 |
| 1451.4469                                                 | 1458.1957 |           | 1463.3015 |
| 1474.4321                                                 | 1478.6628 |           | 1489.1706 |
| 1574.3947                                                 | 1646.5575 |           | 1883.0148 |
| 2140.9862                                                 | 2925.9308 |           | 3044.1805 |
| 3050.0746                                                 | 3057.5066 |           | 3073.4052 |
| 3074.1401                                                 | 3101.2400 |           | 3103.8808 |
| 3118.2688                                                 | 3131.9373 |           | 3134.8283 |
| 3141.8828                                                 | 3146.7411 |           | 3162.9160 |
| 3174.4325                                                 | 3236.6822 |           | 3842.9074 |
| Zero-point correction (Hartree): 0.270775                 |           |           |           |
| TS.ApineneCI.A.a+H2O.HHP.ttttd                            |           |           |           |
| ~~~~~                                                     |           |           |           |
| E(RM062X/CC-pVDZ) (Hartree): -692.36963695                |           |           |           |
| Electronic state : 1-A                                    |           |           |           |
| Cartesian coordinates (Angs):                             |           |           |           |
| C                                                         | -1.665351 | 0.536571  | -0.926053 |
| H                                                         | -1.664828 | 1.249785  | -1.766395 |
| C                                                         | -3.113303 | 0.377661  | -0.479138 |
| C                                                         | -3.533772 | -0.823841 | 0.332100  |
| H                                                         | -3.439316 | 1.270654  | 0.085780  |
| H                                                         | -3.783127 | 0.362021  | -1.358877 |
| H                                                         | -4.616984 | -0.809691 | 0.610386  |
| C                                                         | -0.553981 | 1.011543  | 0.061062  |
| C                                                         | -0.764800 | -0.657209 | -1.316321 |
| C                                                         | -0.308921 | 2.512262  | 0.097826  |
| C                                                         | -0.743388 | 0.474466  | 1.476510  |
| H                                                         | -0.985865 | -0.594886 | 1.490492  |
| H                                                         | 0.164780  | 0.645915  | 2.070072  |
| H                                                         | -1.581268 | 1.006971  | 1.956180  |
| H                                                         | 0.545153  | 2.758721  | 0.747393  |
| H                                                         | -1.189374 | 3.031316  | 0.509972  |
| H                                                         | -0.112863 | 2.915908  | -0.906566 |
| H                                                         | -0.758011 | -0.978446 | -2.365317 |
| H                                                         | -0.942548 | -1.515390 | -0.659952 |
| C                                                         | 0.437932  | 0.191497  | -0.839428 |
| H                                                         | 0.777729  | 0.849294  | -1.652429 |
| C                                                         | 1.663769  | -0.468572 | -0.294521 |
| C                                                         | 1.581413  | -1.702530 | 0.541920  |
| H                                                         | 1.158160  | -2.487695 | -0.105768 |
| H                                                         | 2.582372  | -1.994690 | 0.865537  |
| H                                                         | 0.914539  | -1.555338 | 1.395384  |
| O                                                         | -2.842952 | -1.754852 | 0.660673  |
| O                                                         | 2.714068  | -0.215475 | -1.001261 |
| O                                                         | 3.891477  | -0.495704 | -0.250968 |
| O                                                         | 2.391191  | 0.639025  | 1.266956  |
| H                                                         | 3.281513  | 0.194930  | 0.802391  |
| H                                                         | 2.422090  | 1.555590  | 0.954770  |
| Rotational constants (GHz): 1.2256300 0.4202800 0.3871000 |           |           |           |
| Vibrational harmonic frequencies (cm-1):                  |           |           |           |
| i514.7616                                                 | 53.3426   |           | 62.8477   |
| 100.7249                                                  | 110.3208  |           | 135.0388  |
| 155.7010                                                  | 190.7276  |           | 201.7169  |
| 220.6064                                                  | 231.9955  |           | 259.4517  |
| 268.7751                                                  | 305.7012  |           | 319.7484  |
| 334.7549                                                  | 352.9011  |           | 371.3962  |
| 391.0327                                                  | 438.3926  |           | 446.4775  |
| 510.5821                                                  | 558.3681  |           | 580.3145  |
| 601.5659                                                  | 633.8283  |           | 656.2657  |
| 675.4973                                                  | 751.7553  |           | 775.7305  |
| 784.9727                                                  | 875.6215  |           | 905.8162  |
| 935.0014                                                  | 938.7450  |           | 954.5886  |
| 969.5846                                                  | 992.2564  |           | 993.6162  |
| 1018.7188                                                 | 1022.1771 |           | 1036.6744 |
| 1084.2300                                                 | 1127.9946 |           | 1161.9781 |
| 1182.3995                                                 | 1194.2388 |           | 1232.9433 |
| 1235.2286                                                 | 1259.4463 |           | 1288.1205 |
| 1300.2397                                                 | 1317.0265 |           | 1322.6278 |
| 1358.1947                                                 | 1374.6423 |           | 1386.1271 |
| 1393.8060                                                 | 1397.1186 |           | 1405.4944 |
| 1411.3384                                                 | 1423.6232 |           | 1435.4760 |
| 1452.8531                                                 | 1459.2889 |           | 1462.3722 |
| 1476.0255                                                 | 1484.1279 |           | 1497.6125 |

|           |           |           |
|-----------|-----------|-----------|
| 1579.3398 | 1635.8325 | 1878.4887 |
| 1932.7167 | 2933.1675 | 3036.8850 |
| 3047.1276 | 3058.2477 | 3064.1907 |
| 3069.7500 | 3079.4311 | 3096.1617 |
| 3110.7146 | 3122.9039 | 3137.8386 |
| 3144.9375 | 3183.2730 | 3192.4648 |
| 3193.0520 | 3245.9941 | 3839.7281 |

Zero-point correction (Hartree): 0.270715

TS.ApineneCI.A.a+H2O.HHP.tttu

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E(RM062X/CC-pVDZ) (Hartree): -692.37024818

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-1.680297	0.521222	-0.930583
H	-1.708094	1.227032	-1.776420
C	-3.124112	0.271221	-0.513662
C	-3.470498	-0.924661	0.339775
H	-3.531847	1.158694	0.004948
H	-3.766662	0.167238	-1.407813
H	-4.557261	-0.982683	0.597665
C	-0.627445	1.080535	0.076497
C	-0.703477	-0.623903	-1.292249
C	-0.426554	2.587191	0.073222
C	-0.805498	0.572625	1.504228
H	-0.923505	-0.517205	1.549659
H	0.059291	0.864249	2.117943
H	-1.705724	1.022168	1.953853
H	0.473005	2.851735	0.648877
H	-1.289370	3.095342	0.533244
H	-0.307142	2.972487	-0.950673
H	-0.636836	-0.922495	-2.345697
H	-0.875304	-1.505138	-0.666035
C	0.430278	0.259571	-0.742277
H	0.841031	0.912391	-1.525559
C	1.585864	-0.322488	0.007126
C	1.613577	-1.767060	0.377595
H	0.761482	-1.937383	1.056451
H	1.477507	-2.384562	-0.516281
H	2.550310	-2.002032	0.887198
O	-2.717928	-1.785320	0.721090
O	2.239544	0.566487	0.671532
O	3.542372	0.080697	0.997637
O	3.129053	-0.588776	-1.310997
H	3.617006	-0.362196	-0.378442
H	3.226752	0.232137	-1.815041

Rotational constants (GHz): 1.1749700 0.4252200 0.3900300

Vibrational harmonic frequencies (cm-1):

i433.8910	38.6787	48.4803
99.5667	119.1576	128.2170
168.0608	196.6371	216.6837
231.7872	233.5935	244.9929
265.9925	291.4354	329.8226
331.0756	336.6845	353.0939
396.7894	438.6737	467.2367
487.7930	524.2779	584.9061
592.9999	637.1773	658.2067
680.9417	746.0838	767.1477
781.9792	884.9366	901.7076
928.4040	936.8830	951.1240
958.0555	990.2760	997.9149
1016.0356	1022.3621	1050.6448
1084.6552	1140.3364	1158.1355
1173.0840	1186.6724	1224.5696
1238.5384	1256.7915	1291.3907
1298.0704	1321.7048	1332.1248
1368.5386	1378.1915	1387.6000
1392.0045	1398.4164	1404.4768
1407.3323	1419.2064	1433.0306
1453.1425	1457.9067	1462.2699
1479.3362	1481.8124	1485.7570
1572.5198	1647.1060	1877.1115
2118.3528	2933.6627	3032.2738
3047.8026	3059.2612	3063.4139
3066.8780	3073.7153	3100.3563
3112.1030	3127.4027	3133.2747
3141.7398	3174.4752	3178.4247
3193.4905	3236.8694	3840.1820

Zero-point correction (Hartree): 0.270833

Z-pinonaldehyde-K-oxide
#####

Population analysis as 298K (%)

Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)

Compound	Qtot	Erel	Erel2	n*Q*MB	%
TS.ApineneCI.A.b+H2O.HHP.pmtu	4.354e+44	0.00	0.00	4.354e+44	49.8
TS.ApineneCI.A.b+H2O.HHP.tptd	7.385e+44	1.31	1.31	8.030e+43	9.19
TS.ApineneCI.A.b+H2O.HHP.mptd	5.559e+44	1.15	1.15	7.933e+43	9.08
TS.ApineneCI.A.b+H2O.HHP.tmtu	5.112e+44	1.12	1.12	7.676e+43	8.79
TS.ApineneCI.A.b+H2O.HHP.mmtu	6.738e+44	1.32	1.32	7.272e+43	8.32
TS.ApineneCI.A.b+H2O.HHP.pptu	5.055e+44	1.54	1.54	3.763e+43	4.31
TS.ApineneCI.A.b+H2O.HHP.tmtu	4.814e+44	2.05	2.05	1.513e+43	1.73
TS.ApineneCI.A.b+H2O.HHP.pmpu	5.119e+44	2.12	2.12	1.430e+43	1.64
TS.ApineneCI.A.b+H2O.HHP.mpmu	1.783e+45	2.90	2.90	1.325e+43	1.52
TS.ApineneCI.A.b+H2O.HHP.tmpu	5.638e+44	2.25	2.25	1.270e+43	1.45
TS.ApineneCI.A.b+H2O.HHP.tptu	4.624e+44	2.23	2.23	1.066e+43	1.22
TS.ApineneCI.A.b+H2O.HHP.tttu	2.208e+44	2.43	2.43	3.671e+42	0.42
TS.ApineneCI.A.b+H2O.HHP.ppmu	1.243e+45	3.55	3.55	3.091e+42	0.354

TS.ApineneCI.A.b+H2O.HHP.mppd	1.363e+45	3.63	3.63	2.988e+42	0.342
TS.ApineneCI.A.b+H2O.HHP.pppu	9.645e+44	3.42	3.42	2.975e+42	0.341
TS.ApineneCI.A.b+H2O.HHP.tppd	1.359e+45	3.64	3.64	2.916e+42	0.334
TS.ApineneCI.A.b+H2O.HHP.tpmu	1.492e+45	3.87	3.87	2.169e+42	0.248
TS.ApineneCI.A.b+H2O.HHP.tmmmd	1.145e+45	3.74	3.74	2.056e+42	0.235
TS.ApineneCI.A.b+H2O.HHP.tmpu	4.778e+44	3.26	3.26	1.937e+42	0.222
TS.ApineneCI.A.b+H2O.HHP.mmmd	1.213e+45	3.87	3.87	1.757e+42	0.201
TS.ApineneCI.A.b+H2O.HHP.tttu	1.470e+44	3.31	3.31	5.541e+41	0.0634
TS.ApineneCI.A.b+H2O.HHP.tppu	1.093e+45	4.58	4.58	4.784e+41	0.0548
TS.ApineneCI.A.b+H2O.HHP.tmmu	8.915e+44	4.84	4.84	2.518e+41	0.0288
TS.ApineneCI.A.b+H2O.HHP.ptmu	4.961e+44	4.51	4.51	2.452e+41	0.0281
TS.ApineneCI.A.b+H2O.HHP.ttmd	7.319e+44	4.74	4.74	2.439e+41	0.0279
TS.ApineneCI.A.b+H2O.HHP.pttu	3.836e+44	5.19	5.19	5.987e+40	0.00685
TS.ApineneCI.A.b+H2O.HHP.ttmu	4.955e+44	5.70	5.70	3.245e+40	0.00371
TS.ApineneCI.A.b+H2O.HHP.ptpu	7.341e+44	6.02	6.02	2.808e+40	0.00321
Total				8.736e+44	100

TS.ApineneCI.A.b+H2O.HHP.mmmd

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E(RM062X/CC-pVDZ) (Hartree): -692.37057827

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -1.421154 | 0.562690  | 0.517485  |
| H | -1.693130 | 0.347464  | 1.563425  |
| C | -2.679796 | 0.918589  | -0.269270 |
| C | -3.726958 | -0.163534 | -0.176427 |
| H | -3.124230 | 1.848703  | 0.113766  |
| H | -2.423098 | 1.063534  | -1.332334 |
| H | -3.421076 | -1.161568 | -0.580113 |
| C | -0.445484 | -0.559369 | 0.025825  |
| C | -0.256479 | 1.569333  | 0.494440  |
| C | -0.601153 | -1.904285 | 0.717706  |
| C | -0.439722 | -0.730172 | -1.490459 |
| H | -0.278685 | 0.220741  | -2.024462 |
| H | 0.360000  | -1.427130 | -1.773511 |
| H | -1.401226 | -1.145770 | -1.830725 |
| H | 0.214411  | -2.574654 | 0.420574  |
| H | -1.563369 | -2.366001 | 0.443051  |
| H | -0.585510 | -1.787251 | 1.812237  |
| H | -0.198699 | 2.309462  | 1.302659  |
| H | -0.220034 | 2.090465  | -0.473763 |
| C | 0.709031  | 0.362692  | 0.546527  |
| H | 0.927065  | 0.109661  | 1.590321  |
| C | 2.009179  | 0.497524  | -0.210514 |
| C | 2.508688  | 1.859443  | -0.567962 |
| H | 2.420612  | 2.521886  | 0.301408  |
| H | 3.547063  | 1.804079  | -0.912511 |
| H | 1.888406  | 2.267499  | -1.379447 |
| O | -4.819369 | -0.008296 | 0.304503  |
| O | 2.458125  | -0.441506 | -0.966205 |
| O | 2.288140  | -1.681247 | -0.272805 |
| O | 3.154117  | -0.073837 | 1.343005  |
| H | 2.882538  | -0.999916 | 0.872174  |
| H | 4.083955  | 0.040413  | 1.095149  |

Rotational constants (GHz): 1.3834100 0.3786300 0.3474700

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i458.3787 | 27.3058   | 35.9111   |
| 74.1912   | 89.5452   | 171.4960  |
| 182.1755  | 195.4487  | 205.4225  |
| 223.3517  | 248.1223  | 257.4268  |
| 271.0575  | 293.5503  | 316.1637  |
| 337.4342  | 352.8947  | 390.5013  |
| 397.9776  | 418.5130  | 426.1148  |
| 508.6178  | 522.0047  | 576.7608  |
| 587.1439  | 614.3754  | 624.5891  |
| 673.2408  | 732.4165  | 773.7814  |
| 839.8931  | 898.0346  | 918.3738  |
| 932.9681  | 954.8576  | 970.9702  |
| 973.8127  | 994.7122  | 1016.9382 |
| 1020.1963 | 1037.8576 | 1068.4842 |
| 1097.8349 | 1134.4129 | 1149.9012 |
| 1173.5321 | 1180.6416 | 1198.0676 |
| 1242.1600 | 1263.2286 | 1274.5082 |
| 1280.7184 | 1299.6988 | 1303.6756 |
| 1323.1336 | 1365.3941 | 1376.6109 |
| 1388.3121 | 1395.0222 | 1404.2737 |
| 1416.7457 | 1430.9647 | 1434.2470 |
| 1445.9827 | 1451.3210 | 1467.0851 |
| 1468.6166 | 1476.5756 | 1492.5636 |
| 1574.3136 | 1639.3775 | 1885.4505 |
| 2156.4730 | 2930.8267 | 3046.9215 |
| 3053.2501 | 3057.9059 | 3068.4790 |
| 3079.1776 | 3084.7754 | 3118.2962 |
| 3124.2742 | 3127.7615 | 3136.0680 |
| 3149.5277 | 3165.2761 | 3168.6093 |
| 3177.9707 | 3199.8342 | 3833.1336 |

Zero-point correction (Hartree): 0.270800

TS.ApineneCI.A.b+H2O.HHP.mmtmd

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E(RM062X/CC-pVDZ) (Hartree): -692.37458653

Electronic state : 1-A

Cartesian coordinates (Angs):

C	1.445983	0.679970	-0.601732
H	1.770904	0.402776	-1.615827
C	2.638215	1.188376	0.186082
C	3.808484	0.241411	0.231515
H	3.007911	2.140477	-0.237425
H	2.368258	1.427039	1.230283
H	4.699627	0.611517	0.796171
C	0.549362	-0.474767	-0.037050
C	0.212707	1.601086	-0.660210

C	0.770408	-1.839032	-0.670784
C	0.591926	-0.575332	1.483825
H	0.375062	0.384979	1.981463
H	-0.148130	-1.313005	1.821142
H	1.591296	-0.908775	1.805696
H	-0.004962	-2.535883	-0.328915
H	1.766961	-2.217163	-0.404425
H	0.723935	-1.767289	-1.768881
H	0.095153	2.253469	-1.535360
H	0.146484	2.213954	0.251501
C	-0.675278	0.338648	-0.582560
H	-0.913855	-0.012707	-1.592523
C	-1.952392	0.453120	0.215111
C	-2.507267	1.805171	0.527331
H	-2.482118	2.429125	-0.373993
H	-3.529402	1.715132	0.910970
H	-1.882112	2.281023	1.297129
O	3.825032	-0.843170	-0.292312
O	-2.329334	-0.466594	1.031938
O	-2.124941	-1.729703	0.392236
O	-3.125845	-0.249340	-1.263022
H	-2.787672	-1.137117	-0.755522
H	-4.049530	-0.169014	-0.981366
Rotational constants (GHz): 1.3210200 0.4236100 0.3810700			
Vibrational harmonic frequencies (cm-1):			
i468.4083	25.1859	46.4926	
87.0004	118.4364	162.4067	
179.4138	201.8131	205.5946	
215.7339	250.0621	262.9475	
272.4820	299.3258	314.9434	
330.5402	358.8998	373.4390	
399.4643	418.9979	451.8847	
493.8626	560.9122	586.1714	
609.7611	625.4181	667.2917	
679.7696	728.2714	751.0575	
799.4984	898.0445	908.0774	
931.9268	936.7781	957.4104	
972.9866	990.1275	1004.7817	
1020.5780	1038.5607	1048.4487	
1097.4803	1122.0429	1152.1264	
1171.3830	1186.1861	1201.1330	
1240.9805	1265.3122	1280.3243	
1282.8047	1299.5709	1305.8257	
1335.1570	1367.6438	1379.9892	
1389.1983	1397.4593	1402.4883	
1408.1499	1428.2528	1431.8169	
1448.4205	1451.8380	1466.4479	
1470.1432	1477.6269	1491.2114	
1573.9355	1640.7030	1879.3265	
2125.8036	2935.6426	3040.4492	
3042.7709	3060.3475	3073.1478	
3074.8980	3083.9651	3092.7596	
3115.5620	3132.4622	3140.8266	
3145.5384	3163.7766	3168.6414	
3181.9130	3201.4697	3831.2572	
Zero-point correction (Hartree): 0.270740			
TS.ApineneCI.A.b+H2O.HHP.mpm			
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E(RM062X/CC-pVDZ) (Hartree): -692.37215466			
Electronic state : 1-A			
Cartesian coordinates (Angs):			
C	-1.506554	-0.406476	0.516506
H	-1.686386	-0.722528	1.557516
C	-2.787213	-0.561726	-0.301073
C	-3.845946	0.326983	0.297968
H	-2.626864	-0.245352	-1.340898
H	-3.121462	-1.611760	-0.281334
H	-4.305170	-0.042009	1.249515
C	-0.183697	-1.077903	0.024860
C	-0.808630	0.966763	0.506046
C	0.158654	-2.387539	0.714890
C	-0.122487	-1.237684	-1.490749
H	-0.324300	-0.294703	-2.024590
H	0.875442	-1.593475	-1.778826
H	-0.869202	-1.976089	-1.821403
H	1.146680	-2.738084	0.392508
H	-0.596808	-3.150271	0.463662
H	0.165588	-2.266075	1.809134
H	-1.027025	1.666402	1.322795
H	-0.984318	1.476701	-0.452578
C	0.539982	0.209853	0.544882
H	0.847797	0.053263	1.584728
C	1.689263	0.812309	-0.227950
C	1.627982	2.247472	-0.636326
H	1.301377	2.856717	0.214899
H	2.605154	2.580133	-1.003130
H	0.889387	2.358477	-1.443792
O	-4.156807	1.397717	-0.158094
O	2.463383	0.088878	-0.958319
O	2.770159	-1.099279	-0.222195
O	2.961224	0.772288	1.326990
H	3.062018	-0.204739	0.888864
H	3.776299	1.224240	1.061552
Rotational constants (GHz): 1.1710100 0.4160000 0.3614500			
Vibrational harmonic frequencies (cm-1):			
i461.9201	27.5458	31.6849	
62.0517	89.3506	136.9112	
189.4268	197.9426	201.0781	
220.1239	244.5949	258.8356	
288.0758	294.8384	313.3541	
326.0040	351.1054	365.7810	

411.0251	419.1962	465.3300
506.1845	544.9566	570.7883
588.5791	620.3577	627.8203
680.2688	743.3435	780.3785
872.9635	897.6555	918.5816
935.0450	941.7882	958.2407
987.4508	999.7581	1006.2087
1025.5281	1035.2385	1059.5433
1081.8643	1138.5898	1145.2314
1172.1926	1186.9262	1204.3448
1242.2990	1247.9261	1274.5235
1283.0910	1295.5715	1303.7910
1318.0905	1366.4218	1377.9861
1389.5512	1396.7817	1405.1396
1412.6562	1430.2784	1440.7493
1447.1656	1449.5377	1466.7497
1469.0526	1477.4090	1491.1282
1573.7662	1640.4564	1879.2712
2148.0047	2927.0110	3047.6328
3050.1085	3057.3287	3064.5524
3082.1196	3087.3593	3120.2056
3122.2526	3136.5408	3143.2543
3151.3433	3164.7776	3169.3520
3176.8789	3200.5138	3829.3699

Zero-point correction (Hartree): 0.270833

TS.ApineneCI.A.b+H2O.HHP.mppd

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E(RM062X/CC-pVDZ) (Hartree): -692.37087206

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -1.495487 | -0.105741 | 0.393672  |
| H | -1.742215 | -0.321182 | 1.445868  |
| C | -2.757131 | -0.218478 | -0.454629 |
| C | -3.806951 | 0.756060  | 0.013932  |
| H | -2.517446 | 0.023539  | -1.504526 |
| H | -3.184180 | -1.230937 | -0.415439 |
| H | -3.478490 | 1.827146  | 0.032355  |
| C | -0.230997 | -0.940859 | 0.014052  |
| C | -0.651597 | 1.183913  | 0.322677  |
| C | -0.068258 | -2.234995 | 0.793266  |
| C | -0.114989 | -1.198802 | -1.485017 |
| H | -0.186269 | -0.274827 | -2.082378 |
| H | 0.851470  | -1.674286 | -1.697472 |
| H | -0.920025 | -1.874002 | -1.813431 |
| H | 0.885445  | -2.713510 | 0.539720  |
| H | -0.895123 | -2.922094 | 0.550034  |
| H | -0.093966 | -2.047175 | 1.877697  |
| H | -0.828782 | 1.968147  | 1.070065  |
| H | -0.707823 | 1.627847  | -0.683068 |
| C | 0.601670  | 0.293583  | 0.497766  |
| H | 0.825186  | 0.180076  | 1.564606  |
| C | 1.854647  | 0.722430  | -0.227747 |
| C | 1.989335  | 2.138664  | -0.683516 |
| H | 1.686441  | 2.814183  | 0.125397  |
| H | 3.020008  | 2.340783  | -0.994736 |
| H | 1.322171  | 2.303859  | -1.542264 |
| O | -4.917193 | 0.452196  | 0.364463  |
| O | 2.574692  | -0.114215 | -0.888032 |
| O | 2.701281  | -1.299728 | -0.096970 |
| O | 3.028670  | 0.594883  | 1.401304  |
| H | 3.035878  | -0.402692 | 1.002025  |
| H | 3.906663  | 0.935395  | 1.172688  |

Rotational constants (GHz): 1.2865800 0.3751600 0.3388300

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i459.1920 | 30.3985   | 44.7603   |
| 51.0769   | 96.8667   | 147.0737  |
| 187.2460  | 194.1092  | 203.1485  |
| 219.0198  | 244.2165  | 259.2272  |
| 275.0702  | 300.6877  | 315.5235  |
| 327.0470  | 351.8615  | 367.0961  |
| 410.9912  | 418.9971  | 441.4565  |
| 508.4881  | 529.0317  | 573.4714  |
| 587.2073  | 619.3586  | 625.2163  |
| 670.0051  | 744.9880  | 783.7447  |
| 851.6943  | 898.0467  | 912.6214  |
| 933.0054  | 937.9853  | 956.8119  |
| 983.6873  | 994.0858  | 1012.8217 |
| 1022.6923 | 1037.6020 | 1070.6809 |
| 1091.7676 | 1134.2825 | 1153.1447 |
| 1173.7563 | 1185.9399 | 1206.6065 |
| 1244.1326 | 1251.1048 | 1275.6589 |
| 1282.4784 | 1298.5763 | 1305.0231 |
| 1320.7384 | 1366.2785 | 1376.7410 |
| 1387.8861 | 1396.7762 | 1405.8410 |
| 1419.3295 | 1431.6395 | 1434.8073 |
| 1446.3728 | 1451.1778 | 1466.6893 |
| 1468.6802 | 1476.6713 | 1491.7914 |
| 1575.1685 | 1639.9980 | 1888.0244 |
| 2146.8698 | 2912.0830 | 3048.0564 |
| 3050.5701 | 3054.7127 | 3068.3106 |
| 3074.2154 | 3083.7277 | 3120.4686 |
| 3122.2363 | 3131.5213 | 3133.6215 |
| 3145.4379 | 3165.6651 | 3168.7082 |
| 3177.3957 | 3200.2776 | 3834.7269 |

Zero-point correction (Hartree): 0.270703

TS.ApineneCI.A.b+H2O.HHP.mptd

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E(RM062X/CC-pVDZ) (Hartree): -692.37483621

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-1.563874	-0.244815	0.350995
H	-1.829307	-0.358238	1.413566
C	-2.791621	-0.506541	-0.495638
C	-3.937021	0.414840	-0.158761
H	-2.582893	-0.385539	-1.573874
H	-3.153662	-1.544779	-0.384972
H	-4.877735	0.245093	-0.738031
C	-0.240479	-1.025619	0.077559
C	-0.810432	1.084613	0.168400
C	-0.004125	-2.222979	0.982773
C	-0.073906	-1.420565	-1.387479
H	-0.198840	-0.566112	-2.073036
H	0.927553	-1.843629	-1.539829
H	-0.822797	-2.181001	-1.658912
H	0.990195	-2.648067	0.798318
H	-0.767834	-2.994452	0.789557
H	-0.077259	-1.934808	2.042743
H	-1.076418	1.913607	0.834116
H	-0.874283	1.426553	-0.876245
C	0.496908	0.304176	0.450183
H	0.701082	0.312225	1.527207
C	1.734879	0.751846	-0.287204
C	1.792685	2.141285	-0.833115
H	1.431653	2.846640	-0.075130
H	2.814913	2.387154	-1.140857
H	1.132516	2.208764	-1.710142
O	-3.876528	1.288891	0.668244
O	2.514322	-0.080794	-0.883899
O	2.708542	-1.200636	-0.014088
O	2.894414	0.803970	1.357716
H	2.967718	-0.215360	1.024715
H	3.751307	1.183063	1.110749

Rotational constants (GHz): 1.1834100 0.4198700 0.3692400
 Vibrational harmonic frequencies (cm-1):
 i457.7544 33.9920 51.3815
 83.8603 113.7894 172.5074
 178.8558 190.1246 201.7082
 220.7189 242.8277 261.4625
 267.0917 290.7092 315.0037
 326.2425 358.7605 366.7055
 405.1550 418.3151 449.8537
 507.9759 557.9515 582.6940
 611.4988 623.7787 665.8880
 681.2195 720.5708 754.0671
 843.2646 898.8206 917.8606
 934.1261 939.1270 947.7018
 958.0687 986.5483 1004.1849
 1014.6598 1032.8710 1038.5529
 1085.1026 1133.2755 1158.5090
 1172.6533 1184.2190 1206.9493
 1237.7721 1252.1188 1278.0838
 1289.2863 1300.4447 1314.0474
 1328.2742 1366.5374 1382.1138
 1392.0562 1398.7906 1402.1008
 1408.5818 1429.5258 1432.8086
 1446.8251 1450.9076 1468.0003
 1470.5428 1478.7530 1494.3594
 1571.8559 1640.8592 1876.5595
 2150.6176 2940.5396 3042.2346
 3044.8480 3047.6768 3072.0287
 3076.4972 3083.3632 3088.3711
 3117.3205 3119.2386 3131.5085
 3158.6581 3165.2203 3168.0904
 3171.4692 3199.8063 3834.8845

Zero-point correction (Hartree): 0.270726

TS.ApineneCI.A.b+H2O.HHP.pmpu

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E(RM062X/CC-pVDZ) (Hartree): -692.37369492

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -1.290195 | -0.565171 | -0.850791 |
| H | -1.592456 | -0.247645 | -1.863743 |
| C | -2.453045 | -1.283168 | -0.167263 |
| C | -3.661235 | -0.382726 | -0.165487 |
| H | -2.683690 | -2.203782 | -0.726731 |
| H | -2.193767 | -1.545612 | 0.867222  |
| H | -4.218430 | -0.325495 | -1.134613 |
| C | -0.620715 | 0.649101  | -0.134013 |
| C | 0.079874  | -1.269557 | -0.908755 |
| C | -1.087438 | 2.022570  | -0.591281 |
| C | -0.664418 | 0.532825  | 1.388806  |
| H | -0.238158 | -0.418926 | 1.739362  |
| H | -0.076624 | 1.341768  | 1.849414  |
| H | -1.704150 | 0.621289  | 1.736525  |
| H | -0.488684 | 2.826682  | -0.134425 |
| H | -2.132674 | 2.183378  | -0.283208 |
| H | -1.029470 | 2.125071  | -1.685900 |
| H | 0.338908  | -1.816830 | -1.822914 |
| H | 0.248655  | -1.893899 | -0.027719 |
| C | 0.733602  | 0.115371  | -0.741601 |
| H | 0.876387  | 0.570854  | -1.732727 |
| C | 1.969456  | 0.432276  | 0.043949  |
| C | 2.603667  | 1.757971  | -0.238502 |
| H | 3.009659  | 1.738948  | -1.258291 |
| H | 1.835618  | 2.544261  | -0.195140 |
| H | 3.397202  | 1.968694  | 0.486559  |
| O | -4.005918 | 0.292610  | 0.772133  |
| O | 2.252041  | -0.019740 | 1.215028  |
| O | 2.000045  | -1.421844 | 1.281222  |
| O | 3.046331  | -0.999347 | -0.885586 |
| H | 2.675628  | -1.498585 | -0.010611 |

|                                          |           |           |           |  |
|------------------------------------------|-----------|-----------|-----------|--|
| H                                        | 3.978749  | -0.840550 | -0.675808 |  |
| Rotational constants (GHz):              | 1.2781700 | 0.4194200 | 0.3906100 |  |
| Vibrational harmonic frequencies (cm-1): |           |           |           |  |
| i439.3426                                | 46.0887   |           | 59.4359   |  |
| 75.1881                                  | 95.4381   |           | 150.0146  |  |
| 156.5933                                 | 176.1121  |           | 200.4179  |  |
| 231.6408                                 | 240.3024  |           | 257.7644  |  |
| 275.2728                                 | 300.2483  |           | 323.4093  |  |
| 340.5495                                 | 378.0062  |           | 383.6407  |  |
| 387.9899                                 | 434.2956  |           | 450.4415  |  |
| 497.8098                                 | 533.4198  |           | 569.5324  |  |
| 575.6201                                 | 613.7120  |           | 626.4608  |  |
| 653.0535                                 | 724.5370  |           | 774.5274  |  |
| 892.0983                                 | 898.1827  |           | 916.6947  |  |
| 929.3645                                 | 958.9452  |           | 978.4299  |  |
| 990.4850                                 | 1001.8703 |           | 1015.7876 |  |
| 1023.9324                                | 1033.5877 |           | 1053.4186 |  |
| 1109.3590                                | 1134.4035 |           | 1153.5178 |  |
| 1162.8517                                | 1180.9229 |           | 1189.6084 |  |
| 1234.5591                                | 1253.0402 |           | 1255.3910 |  |
| 1268.2159                                | 1291.0920 |           | 1322.0958 |  |
| 1343.3608                                | 1368.8415 |           | 1382.0276 |  |
| 1392.0136                                | 1408.0609 |           | 1413.9045 |  |
| 1427.6543                                | 1437.5760 |           | 1446.5735 |  |
| 1451.0810                                | 1455.7035 |           | 1467.9243 |  |
| 1476.9340                                | 1486.8025 |           | 1494.1124 |  |
| 1587.5238                                | 1639.9200 |           | 1873.5606 |  |
| 2158.3501                                | 2925.9214 |           | 3043.4642 |  |
| 3047.4811                                | 3056.4485 |           | 3069.8660 |  |
| 3077.9700                                | 3090.7578 |           | 3116.0161 |  |
| 3122.0883                                | 3130.8477 |           | 3134.7011 |  |
| 3147.5245                                | 3156.6251 |           | 3163.5464 |  |
| 3197.4901                                | 3202.4992 |           | 3835.1158 |  |
| Zero-point correction (Hartree):         | 0.271124  |           |           |  |

TS.ApineneCI.A.b+H2O.HHP.pmtu

E(RM062X/CC-pVDZ) (Hartree): -692.37680360

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -1.344259 | -0.489376 | -0.775648 |
| H | -1.755855 | -0.087532 | -1.714607 |
| C | -2.400559 | -1.325910 | -0.079303 |
| C | -3.686449 | -0.603743 | 0.215650  |
| H | -2.651474 | -2.214715 | -0.686158 |
| H | -2.026858 | -1.734329 | 0.876719  |
| H | -4.493418 | -1.229482 | 0.670093  |
| C | -0.629681 | 0.671860  | -0.009461 |
| C | 0.024170  | -1.163454 | -1.007719 |
| C | -1.087045 | 2.080964  | -0.352613 |
| C | -0.604636 | 0.452170  | 1.500302  |
| H | -0.182715 | -0.527577 | 1.768889  |
| H | 0.013249  | 1.218885  | 1.992302  |
| H | -1.626066 | 0.542012  | 1.902268  |
| H | -0.440890 | 2.836825  | 0.122891  |
| H | -2.116539 | 2.234662  | -0.002087 |
| H | -1.073362 | 2.248221  | -1.440720 |
| H | 0.223790  | -1.595384 | -1.995784 |
| H | 0.251189  | -1.889356 | -0.222423 |
| C | 0.694386  | 0.191676  | -0.723092 |
| H | 0.799199  | 0.748527  | -1.665654 |
| C | 1.966587  | 0.419476  | 0.034765  |
| C | 2.631315  | 1.742760  | -0.181589 |
| H | 2.995548  | 1.784183  | -1.216307 |
| H | 1.889290  | 2.544713  | -0.053060 |
| H | 3.458545  | 1.880336  | 0.523153  |
| O | -3.875350 | 0.567257  | -0.002447 |
| O | 2.273278  | -0.114270 | 1.166129  |
| O | 1.980599  | -1.510556 | 1.152495  |
| O | 2.974069  | -0.973463 | -1.015854 |
| H | 2.616937  | -1.520507 | -0.165673 |
| H | 3.915678  | -0.849750 | -0.824177 |

|                             |           |           |           |
|-----------------------------|-----------|-----------|-----------|
| Rotational constants (GHz): | 1.2811200 | 0.4309900 | 0.3935900 |
|-----------------------------|-----------|-----------|-----------|

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i437.9399 | 42.7542   | 60.4836   |
| 79.7751   | 121.4306  | 150.2938  |
| 159.8039  | 174.1918  | 204.5349  |
| 230.0866  | 241.0209  | 262.0258  |
| 277.0555  | 290.4620  | 317.5416  |
| 337.3003  | 351.9686  | 366.3477  |
| 380.2099  | 433.1083  | 450.4277  |
| 480.6958  | 557.7178  | 570.2755  |
| 608.8598  | 624.2162  | 648.8729  |
| 671.5147  | 731.3664  | 753.6364  |
| 802.8711  | 894.9617  | 915.7983  |
| 929.4624  | 941.4446  | 957.9071  |
| 985.0721  | 994.4160  | 1014.2038 |
| 1016.4295 | 1027.0058 | 1051.3467 |
| 1115.7728 | 1127.6816 | 1157.2582 |
| 1167.3062 | 1183.5755 | 1199.6252 |
| 1237.9178 | 1253.2886 | 1262.7136 |
| 1277.7280 | 1304.1851 | 1339.4694 |
| 1341.0792 | 1369.2555 | 1386.6646 |
| 1397.5343 | 1402.0272 | 1404.6447 |
| 1424.3503 | 1427.2362 | 1439.3704 |
| 1451.1707 | 1456.0035 | 1463.0064 |
| 1473.7002 | 1479.5688 | 1482.5135 |
| 1583.8079 | 1640.2589 | 1874.2246 |
| 2169.9001 | 2941.5358 | 3045.4225 |
| 3047.6153 | 3051.2944 | 3073.3228 |
| 3078.8864 | 3086.8280 | 3095.9161 |
| 3113.8885 | 3121.1726 | 3126.6949 |

3147.6447                    3162.1167                    3164.6093  
 3197.3753                    3200.3791                    3835.7571  
 Zero-point correction (Hartree): 0.270856

TS.ApineneCI.A.b+H2O.HHP.ppmu

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 E(RM062X/CC-pVDZ) (Hartree): -692.37099847

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-1.422007	0.463931	-0.499155
H	-1.693199	0.895812	-1.478259
C	-2.672469	0.319573	0.358360
C	-3.721031	-0.484672	-0.369094
H	-2.457895	-0.178770	1.313393
H	-3.098207	1.318643	0.563047
H	-4.010213	-0.077727	-1.372518
C	-0.200554	1.256358	0.057428
C	-0.514332	-0.768140	-0.698202
C	-0.089275	2.698599	-0.410515
C	-0.078598	1.158255	1.576224
H	-0.067318	0.114281	1.921425
H	0.857993	1.625305	1.917259
H	-0.912998	1.693241	2.055123
H	0.840073	3.172086	-0.055845
H	-0.927360	3.290220	-0.007616
H	-0.120601	2.770229	-1.508333
H	-0.643956	-1.367340	-1.607305
H	-0.515735	-1.412935	0.184731
C	0.690684	0.191872	-0.689728
H	0.871988	0.549247	-1.714289
C	2.043135	-0.063787	-0.095334
C	3.147022	0.829717	-0.567223
H	3.349297	0.603214	-1.622260
H	2.818656	1.877760	-0.504031
H	4.049002	0.681835	0.036405
O	-4.221356	-1.494908	0.049636
O	2.268343	-0.571476	1.064491
O	1.431326	-1.705366	1.282701
O	2.223358	-1.844852	-1.029822
H	1.803705	-2.109015	-0.082215
H	3.147943	-2.123522	-0.951321

Rotational constants (GHz): 1.0415700 0.4331200 0.3707400

Vibrational harmonic frequencies (cm-1):

1429.9479	32.1395	50.5124
69.4316	93.9282	131.8093
161.7411	172.7335	198.5544
211.3306	232.8644	256.0002
276.2643	305.2935	315.9292
334.6796	343.5407	362.5249
390.5255	440.9566	447.7401
486.0831	546.2290	562.7724
583.8032	613.9519	625.7703
651.7481	744.3311	768.2098
846.1997	894.7810	925.6636
931.6159	943.7694	956.0375
992.4622	1002.4038	1015.6524
1022.4065	1039.0938	1071.9039
1101.7288	1146.0877	1150.8034
1170.9209	1185.0980	1205.1414
1237.5268	1241.9967	1259.5662
1268.4597	1289.3598	1320.6478
1340.0122	1369.4948	1384.9002
1394.8042	1405.2995	1416.7979
1427.8472	1433.7482	1437.4337
1451.5091	1455.1663	1463.2347
1475.1790	1479.5897	1485.0889
1588.4342	1643.8937	1889.4587
2199.0822	2910.7741	3041.7152
3043.0239	3045.5828	3054.3481
3077.9170	3092.5506	3118.6559
3119.0191	3128.7394	3129.6955
3142.0017	3153.2380	3163.3990
3198.4829	3203.9035	3833.2042

Zero-point correction (Hartree): 0.270710

TS.ApineneCI.A.b+H2O.HHP.ppmu

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 E(RM062X/CC-pVDZ) (Hartree): -692.37144162

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -1.434713 | 0.255387  | -0.419412 |
| H | -1.782301 | 0.614514  | -1.402267 |
| C | -2.635351 | 0.058526  | 0.499722  |
| C | -3.586733 | -0.953751 | -0.085495 |
| H | -2.288296 | -0.326705 | 1.473394  |
| H | -3.188372 | 0.995418  | 0.660650  |
| H | -3.139805 | -1.961215 | -0.280499 |
| C | -0.261249 | 1.170664  | 0.046591  |
| C | -0.433073 | -0.906456 | -0.604090 |
| C | -0.290632 | 2.591676  | -0.493042 |
| C | -0.069045 | 1.160342  | 1.560910  |
| H | 0.043832  | 0.140033  | 1.955735  |
| H | 0.839253  | 1.717729  | 1.836477  |
| H | -0.924116 | 1.650917  | 2.050705  |
| H | 0.611018  | 3.155829  | -0.205886 |
| H | -1.157269 | 3.131889  | -0.079340 |
| H | -0.376286 | 2.604373  | -1.590082 |
| H | -0.544614 | -1.555546 | -1.480868 |
| H | -0.338826 | -1.507382 | 0.304981  |
| C | 0.686751  | 0.147305  | -0.688936 |
| H | 0.800447  | 0.468071  | -1.734933 |
| C | 2.075614  | 0.028058  | -0.137384 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 3.083653  | 0.989344  | -0.684212 |
| H | 3.264955  | 0.740277  | -1.737936 |
| H | 2.672072  | 2.008795  | -0.644800 |
| H | 4.016327  | 0.938891  | -0.112029 |
| O | -4.739280 | -0.732138 | -0.353228 |
| O | 2.382121  | -0.409683 | 1.033062  |
| O | 1.652431  | -1.599318 | 1.327089  |
| O | 2.373148  | -1.767941 | -1.006116 |
| H | 2.012470  | -2.026918 | -0.033153 |
| H | 3.320815  | -1.962903 | -0.954521 |

Rotational constants (GHz): 1.1231600 0.4044700 0.3585700  
 Vibrational harmonic frequencies (cm-1):  
 i428.7936 45.0287 49.0735  
 62.3840 93.7601 140.7759  
 160.0522 178.8309 199.2523  
 216.9544 229.9006 259.5325  
 272.5870 307.7665 315.8065  
 333.9363 345.4248 364.1969  
 391.8284 440.3597 447.0386  
 485.4945 527.9470 566.9071  
 583.7442 615.4944 626.8567  
 650.3335 744.8379 786.5662  
 858.0082 894.2955 927.4389  
 929.1332 941.0309 958.7260  
 992.7491 1003.1388 1018.2105  
 1019.7413 1028.1748 1080.2632  
 1105.6816 1141.2753 1152.8208  
 1171.4249 1183.0800 1210.4345  
 1240.4624 1246.0923 1262.1033  
 1268.0375 1294.4059 1322.4518  
 1341.8215 1368.9930 1381.0590  
 1392.7125 1405.7221 1418.0661  
 1427.8853 1436.5461 1436.8730  
 1451.3774 1454.4139 1464.1387  
 1475.2189 1478.9070 1485.2374  
 1586.5137 1643.8765 1885.6844  
 2198.7821 2929.7887 3045.3248  
 3054.8808 3057.6007 3063.8489  
 3078.0535 3093.1619 3116.5361  
 3121.0975 3130.2966 3131.3545  
 3132.9616 3151.7014 3163.4889  
 3197.2084 3204.5117 3835.6922  
 Zero-point correction (Hartree): 0.270950

TS.ApineneCI.A.b+H2O.HHP.pptu

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 E(RM062X/CC-pVDZ) (Hartree): -692.37444206

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-1.510042	0.317090	-0.334232
H	-1.901122	0.580982	-1.329346
C	-2.663109	0.233294	0.643783
C	-3.735492	-0.723478	0.185426
H	-2.328457	-0.097704	1.642464
H	-3.146701	1.214741	0.804016
H	-4.599648	-0.847294	0.883302
C	-0.287708	1.226281	-0.009043
C	-0.564009	-0.894487	-0.454189
C	-0.286685	2.587630	-0.686649
C	-0.028619	1.358630	1.490110
H	0.064443	0.377840	1.979110
H	0.910522	1.903001	1.673265
H	-0.842636	1.929751	1.962955
H	0.649690	3.137191	-0.498738
H	-1.109554	3.205473	-0.291656
H	-0.425658	2.495296	-1.774361
H	-0.755187	-1.605752	-1.264626
H	-0.455659	-1.419114	0.499197
C	0.591948	0.100018	-0.677504
H	0.674397	0.317246	-1.752723
C	1.997297	-0.018688	-0.170295
C	3.017771	0.833487	-0.857849
H	3.140407	0.466971	-1.885364
H	2.649203	1.868678	-0.910943
H	3.972915	0.802282	-0.322446
O	-3.696491	-1.328021	-0.855590
O	2.338297	-0.339352	1.028501
O	1.577342	-1.458006	1.481103
O	2.195402	-1.908224	-0.847242
H	1.861691	-2.046499	0.157528
H	3.136834	-2.132914	-0.803152

Rotational constants (GHz): 1.0435400 0.4500300 0.3933100

Vibrational harmonic frequencies (cm-1):

i424.3223	44.5821	56.9476
78.2884	120.5665	156.6431
165.2458	173.9632	200.0850
211.9483	235.6820	253.6933
257.5359	306.4770	312.1187
334.8242	363.0154	368.9250
386.6203	435.7373	445.9187
491.2326	557.8343	570.9281
614.4535	623.9105	650.4684
676.4313	715.6204	757.7849
843.8015	893.7623	927.5818
933.6971	940.1462	947.7498
959.3389	994.4235	1008.2637
1016.7977	1023.3572	1048.1942
1102.3382	1142.4326	1154.7795
1170.2344	1183.7953	1208.2624
1234.1358	1246.5868	1263.0237
1273.6594	1315.7543	1322.3899
1341.3334	1369.1606	1387.0913

1401.0568	1403.7740	1405.4652
1426.0846	1428.4837	1439.8407
1451.7635	1457.4211	1463.9056
1476.8301	1482.2698	1488.2351
1585.1831	1644.6982	1878.3076
2215.7288	2941.8863	3039.3451
3042.7229	3051.6425	3072.3485
3078.0225	3088.0248	3092.8013
3116.9179	3125.5197	3130.0554
3131.8874	3150.6287	3163.6942
3196.5703	3205.9419	3834.9486

Zero-point correction (Hartree): 0.270946

TS.ApineneCI.A.b+H2O.HHP.ptmu

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E(RM062X/CC-pVDZ) (Hartree): -692.36972644

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 1.298282  | 0.533226  | 1.112650  |
| H | 1.307103  | 1.277079  | 1.925623  |
| C | 2.738476  | 0.089263  | 0.874308  |
| C | 2.946749  | -1.064939 | -0.078984 |
| H | 3.363549  | 0.924861  | 0.524045  |
| H | 3.155775  | -0.247644 | 1.841270  |
| H | 2.304145  | -1.962429 | 0.091444  |
| C | 0.448634  | 1.128438  | -0.050819 |
| C | 0.174586  | -0.490910 | 1.389588  |
| C | 0.460307  | 2.645313  | -0.154583 |
| C | 0.749357  | 0.484368  | -1.402127 |
| H | 0.656361  | -0.611674 | -1.368081 |
| H | 0.040714  | 0.842863  | -2.164608 |
| H | 1.764569  | 0.750233  | -1.732793 |
| H | -0.230422 | 3.006927  | -0.932884 |
| H | 1.468645  | 2.993327  | -0.430762 |
| H | 0.187532  | 3.117649  | 0.801324  |
| H | -0.065451 | -0.716730 | 2.435536  |
| H | 0.289922  | -1.414995 | 0.819721  |
| C | -0.790541 | 0.469897  | 0.668514  |
| H | -1.195571 | 1.189643  | 1.395086  |
| C | -1.933721 | 0.085977  | -0.221162 |
| C | -2.942988 | 1.157452  | -0.491053 |
| H | -3.475572 | 1.377176  | 0.443400  |
| H | -2.422987 | 2.074053  | -0.806827 |
| H | -3.646273 | 0.839070  | -1.268121 |
| O | 3.777645  | -1.063885 | -0.951094 |
| O | -1.898994 | -0.813931 | -1.140412 |
| O | -1.261952 | -1.995516 | -0.657798 |
| O | -2.705259 | -1.182110 | 1.142947  |
| H | -2.085792 | -1.817906 | 0.545006  |
| H | -3.602606 | -1.406478 | 0.854477  |

Rotational constants (GHz): 1.0498900 0.4724600 0.4197900

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i431.4313 | 48.0245   | 54.8152   |
| 81.3370   | 100.8288  | 141.7524  |
| 159.2493  | 194.3376  | 204.7947  |
| 223.2072  | 237.8354  | 247.3184  |
| 270.6410  | 300.5636  | 316.3081  |
| 348.9316  | 361.9081  | 378.7200  |
| 384.9395  | 432.2394  | 458.1358  |
| 463.9458  | 562.0286  | 570.5805  |
| 594.7177  | 615.0270  | 634.1140  |
| 649.9073  | 707.0515  | 758.7382  |
| 821.3107  | 891.4135  | 916.1670  |
| 931.1661  | 952.9307  | 962.9072  |
| 986.6797  | 996.0161  | 1017.1848 |
| 1023.9677 | 1032.6757 | 1058.6428 |
| 1111.2882 | 1136.2013 | 1154.6567 |
| 1167.6100 | 1180.1401 | 1212.7869 |
| 1231.8457 | 1250.9741 | 1257.8122 |
| 1288.9260 | 1314.4455 | 1328.8450 |
| 1342.8685 | 1369.2736 | 1381.0917 |
| 1392.0895 | 1407.3257 | 1419.4948 |
| 1422.3719 | 1428.1690 | 1437.5667 |
| 1451.3699 | 1454.5465 | 1463.7239 |
| 1477.1445 | 1481.3600 | 1487.3791 |
| 1586.0582 | 1641.9349 | 1878.2896 |
| 2183.7613 | 2954.6155 | 3036.6208 |
| 3044.8342 | 3054.6899 | 3062.2586 |
| 3078.0508 | 3091.5643 | 3114.3300 |
| 3120.5693 | 3120.9733 | 3131.1072 |
| 3132.2245 | 3149.5920 | 3163.0796 |
| 3198.0822 | 3216.5079 | 3835.5467 |

Zero-point correction (Hartree): 0.270963

TS.ApineneCI.A.b+H2O.HHP.ptpu

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E(RM062X/CC-pVDZ) (Hartree): -692.36747568

Electronic state : 1-A

Cartesian coordinates (Angs):

C	1.355159	0.678577	0.866121
H	1.379137	1.318863	1.762026
C	2.799550	0.472968	0.402901
C	3.049420	-0.793945	-0.386267
H	3.107167	1.328533	-0.225930
H	3.483985	0.436431	1.261893
H	2.393612	-0.972944	-1.269934
C	0.271119	1.277541	-0.082151
C	0.427954	-0.526921	1.137112
C	0.077829	2.781856	0.031385
C	0.429516	0.859706	-1.542848
H	0.411710	-0.232420	-1.665595
H	-0.396448	1.265715	-2.147111

H	1.367928	1.264451	-1.953829
H	-0.767707	3.132647	-0.581536
H	0.978219	3.304193	-0.331245
H	-0.094345	3.089165	1.073932
H	0.379495	-0.923043	2.158123
H	0.586734	-1.340597	0.423752
C	-0.749912	0.365050	0.698628
H	-1.116692	0.925259	1.571518
C	-1.969817	-0.062092	-0.061780
C	-3.146991	0.858849	0.013690
H	-3.533562	0.845507	1.041094
H	-2.819125	1.884907	-0.210099
H	-3.925015	0.551234	-0.693332
O	3.915196	-1.581074	-0.100832
O	-1.974089	-0.797553	-1.117319
O	-1.101299	-1.913618	-0.949013
O	-2.311238	-1.625069	1.162682
H	-1.722417	-2.056786	0.384442
H	-3.204198	-1.952129	0.976938
Rotational constants (GHz):			1.0022400 0.4811100 0.4016800
Vibrational harmonic frequencies (cm-1):			
i425.4268	35.5787	60.6091	
66.6605	100.0164	145.8130	
165.0959	197.5322	200.8438	
220.4755	238.2184	238.7608	
268.9459	298.4442	313.1132	
345.0485	362.5837	367.0238	
387.7553	428.6412	459.3519	
476.9964	564.7000	574.4456	
580.3157	615.5271	629.3549	
652.7764	734.2668	766.6486	
808.4005	894.7334	922.8659	
932.3110	954.7736	967.5530	
982.8285	995.4959	1017.1579	
1023.9427	1033.2831	1062.4747	
1092.3168	1135.4818	1165.4013	
1169.3122	1185.1008	1216.1638	
1228.8389	1249.3780	1259.8518	
1288.6713	1312.0088	1324.6391	
1338.2519	1368.0687	1377.5112	
1391.4501	1405.4604	1415.3991	
1427.8115	1428.9435	1437.7510	
1452.4569	1457.1058	1463.6012	
1477.4594	1480.9942	1492.7786	
1585.9283	1645.9209	1879.1980	
2223.7371	2983.9699	3040.2734	
3042.9499	3053.6761	3069.2401	
3078.0354	3092.1957	3117.5473	
3121.4654	3124.8806	3127.3241	
3131.4553	3158.8666	3163.2695	
3198.6249	3204.0991	3834.6502	
Zero-point correction (Hartree): 0.271127			
TS.ApineneCI.A.b+H2O.HHP.pttu			
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E(RM062X/CC-pVDZ) (Hartree): -692.36839777			
Electronic state : 1-A			
Cartesian coordinates (Angs):			
C	1.438247	0.571007	0.956295
H	1.439367	1.285277	1.796991
C	2.895851	0.263717	0.640622
C	3.252221	-0.943442	-0.193650
H	3.374833	1.136128	0.158075
H	3.466496	0.130970	1.578736
H	4.350493	-1.028419	-0.395804
C	0.490851	1.173680	-0.123891
C	0.379790	-0.518040	1.247075
C	0.458060	2.693354	-0.182506
C	0.692514	0.573751	-1.513802
H	0.603912	-0.520787	-1.507038
H	-0.058215	0.974465	-2.212867
H	1.686276	0.850550	-1.902427
H	-0.296766	3.058318	-0.897092
H	1.433382	3.078324	-0.523146
H	0.246589	3.132327	0.804535
H	0.228123	-0.818861	2.290731
H	0.504545	-1.388534	0.601899
C	-0.665443	0.458078	0.671518
H	-1.003914	1.135153	1.470461
C	-1.889803	0.113392	-0.119796
C	-2.924867	1.189156	-0.228864
H	-3.376944	1.333287	0.761293
H	-2.442428	2.133489	-0.520732
H	-3.690831	0.914987	-0.962411
O	2.496728	-1.782364	-0.608113
O	-1.951970	-0.743210	-1.075874
O	-1.266757	-1.939452	-0.713528
O	-2.510190	-1.231455	1.262926
H	-1.943663	-1.824823	0.564996
H	-3.428266	-1.457921	1.052500
Rotational constants (GHz):			1.0154800 0.5273100 0.4423400
Vibrational harmonic frequencies (cm-1):			
i448.8663	43.9751	69.5986	
89.4967	122.9801	143.1697	
155.4158	186.8049	200.3569	
210.1233	225.7220	242.6023	
262.8686	297.9630	306.8267	
338.2935	352.3195	361.0389	
388.6872	432.7932	453.4375	
484.6261	560.8328	570.8758	
609.4830	626.2583	652.5336	
679.0024	750.0294	759.5212	

786.9779	892.0515	908.0118
926.7902	941.9997	955.9959
985.9010	995.4081	1001.0344
1016.4093	1024.7813	1057.0959
1082.5478	1133.2460	1166.8773
1171.4797	1181.9320	1222.1401
1232.3989	1254.3927	1260.2907
1294.2472	1323.8294	1343.0931
1368.4228	1373.0965	1389.0784
1394.7451	1401.8015	1411.9222
1426.8058	1428.2084	1440.2858
1451.8097	1453.7189	1464.8827
1476.3938	1481.9754	1491.0103
1593.4200	1640.9977	1889.0727
2122.7270	2912.5721	3032.1400
3041.4045	3047.7290	3052.9683
3065.4887	3078.1314	3085.0463
3113.8717	3117.9915	3118.6717
3128.6322	3163.3121	3172.5505
3196.3698	3236.6294	3832.9884

Zero-point correction (Hartree): 0.270722

TS.ApineneCI.A.b+H2O.HHP.tmm

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E(RM062X/CC-pVDZ) (Hartree): -692.37080042

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -1.410830 | -0.455986 | -0.600702 |
| H | -1.626618 | -0.053643 | -1.603410 |
| C | -2.707310 | -0.936268 | 0.042955  |
| C | -3.744442 | 0.157960  | 0.104265  |
| H | -3.136342 | -1.777304 | -0.520611 |
| H | -2.508206 | -1.276760 | 1.073661  |
| H | -3.421602 | 1.090464  | 0.633284  |
| C | -0.467286 | 0.555695  | 0.132319  |
| C | -0.232939 | -1.450069 | -0.701522 |
| C | -0.550493 | 2.016665  | -0.279386 |
| C | -0.520540 | 0.423539  | 1.652616  |
| H | -0.480240 | -0.623493 | 1.991731  |
| H | 0.318381  | 0.968494  | 2.110212  |
| H | -1.454272 | 0.857864  | 2.042377  |
| H | 0.334876  | 2.555954  | 0.084174  |
| H | -1.461672 | 2.487827  | 0.123049  |
| H | -0.568667 | 2.110739  | -1.375591 |
| H | -0.132021 | -2.037681 | -1.622017 |
| H | -0.227770 | -2.130752 | 0.162958  |
| C | 0.711614  | -0.250811 | -0.516992 |
| H | 0.943379  | 0.212890  | -1.478923 |
| C | 1.968687  | -0.382519 | 0.293664  |
| C | 2.250298  | -1.623434 | 1.073054  |
| H | 2.230636  | -2.483275 | 0.391921  |
| H | 3.223550  | -1.543604 | 1.569694  |
| H | 1.467845  | -1.767118 | 1.832224  |
| O | -4.843866 | 0.078680  | -0.378107 |
| O | 2.571091  | 0.666986  | 0.730338  |
| O | 2.577469  | 1.652596  | -0.309066 |
| O | 3.147703  | -0.496289 | -1.342185 |
| H | 3.049170  | 0.556119  | -1.176620 |
| H | 4.049839  | -0.691139 | -1.047576 |

Rotational constants (GHz): 1.3858700 0.3700700 0.3464600

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i442.0024 | 35.8206   | 40.4521   |
| 65.5960   | 89.3372   | 146.1846  |
| 179.8484  | 198.1013  | 206.6931  |
| 224.1847  | 243.5198  | 247.2102  |
| 265.9702  | 289.6769  | 309.5104  |
| 323.6741  | 346.1651  | 380.7786  |
| 394.3233  | 421.2144  | 445.0890  |
| 504.1521  | 526.0735  | 574.4717  |
| 593.5624  | 611.6119  | 623.7452  |
| 657.6363  | 729.5260  | 773.8424  |
| 828.6135  | 893.6597  | 919.8115  |
| 936.9859  | 951.1446  | 965.8096  |
| 971.7728  | 991.8849  | 1012.5529 |
| 1023.1101 | 1032.4708 | 1074.7488 |
| 1105.4776 | 1135.8291 | 1155.0297 |
| 1173.7265 | 1182.6367 | 1197.4870 |
| 1239.3734 | 1262.6305 | 1272.5584 |
| 1289.5432 | 1305.4214 | 1314.1277 |
| 1322.0213 | 1370.9856 | 1382.5501 |
| 1395.2167 | 1398.7192 | 1407.2000 |
| 1414.1724 | 1425.1544 | 1434.2057 |
| 1447.3365 | 1451.0901 | 1460.6524 |
| 1472.5826 | 1478.3217 | 1483.5581 |
| 1578.0633 | 1646.2933 | 1887.3209 |
| 2190.7955 | 2926.5766 | 3049.9345 |
| 3051.9467 | 3057.0789 | 3071.7693 |
| 3083.0509 | 3085.3765 | 3124.8488 |
| 3127.2099 | 3129.7381 | 3139.7449 |
| 3151.8226 | 3162.8830 | 3170.0989 |
| 3176.2597 | 3199.4929 | 3837.1901 |

Zero-point correction (Hartree): 0.270819

TS.ApineneCI.A.b+H2O.HHP.tmmu

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E(RM062X/CC-pVDZ) (Hartree): -692.36882633

Electronic state : 1-A

Cartesian coordinates (Angs):

C	1.426184	0.437058	-0.616759
H	1.629981	-0.022244	-1.597157
C	2.736799	0.915981	0.000109
C	3.740747	-0.203200	0.128024

H	3.189629	1.704993	-0.617487
H	2.548007	1.325965	1.006733
H	3.414527	-1.066595	0.761868
C	0.446522	-0.499656	0.167190
C	0.278693	1.454422	-0.769869
C	0.519055	-1.984554	-0.153888
C	0.509279	-0.275144	1.675015
H	0.515579	0.791080	1.949291
H	-0.348092	-0.763133	2.157083
H	1.432039	-0.719450	2.080687
H	-0.324879	-2.510553	0.313017
H	1.457095	-2.419606	0.226328
H	0.479061	-2.154235	-1.240137
H	0.199231	2.013473	-1.710360
H	0.273851	2.158407	0.075649
C	-0.702275	0.273579	-0.558655
H	-0.900976	-0.227498	-1.512977
C	-2.052615	0.589341	0.012873
C	-2.232743	1.602379	1.094656
H	-1.593156	1.353851	1.948873
H	-1.936592	2.591227	0.714953
H	-3.284452	1.638407	1.399239
O	4.818552	-0.211692	-0.406715
O	-3.108961	0.423126	-0.706879
O	-3.030245	-0.822247	-1.394159
O	-2.302963	-1.259966	0.874180
H	-2.658556	-1.381590	-0.149578
H	-3.121239	-1.207509	1.390383
Rotational constants (GHz): 1.3894200 0.3641700 0.3484600			
Vibrational harmonic frequencies (cm-1):			
i490.6825	33.4437	59.3808	
62.7513	95.1737	132.0403	
169.1116	190.6313	209.4527	
223.1022	241.2653	266.2056	
272.3403	293.3387	304.0881	
345.5982	358.4557	373.6857	
395.8129	427.0497	464.0909	
521.2251	538.8931	559.7557	
575.7326	609.4464	619.1417	
648.4705	725.6124	769.2013	
837.6209	905.7324	926.3834	
936.6066	955.1624	962.0130	
976.2130	993.4266	1005.5035	
1027.1121	1030.8258	1059.3859	
1099.7099	1128.1584	1153.1544	
1178.3654	1182.0493	1224.0466	
1237.9095	1270.6073	1275.6953	
1298.4402	1306.5933	1316.8065	
1326.3508	1345.8243	1378.0889	
1392.9563	1402.1441	1409.8954	
1413.5084	1431.8361	1436.9051	
1446.3596	1454.4623	1468.8904	
1471.7498	1480.3207	1493.0664	
1580.7754	1630.9956	1887.1670	
1983.7704	2924.7431	3054.1852	
3056.5147	3061.6948	3074.3991	
3084.0647	3087.1802	3124.2444	
3129.2940	3131.4362	3141.5177	
3155.1325	3163.4340	3166.1348	
3173.7261	3207.3832	3833.6401	
Zero-point correction (Hartree): 0.270591			
TS.ApineneCI.A.b+H2O.HHP.tmpd			
~~			
E(RM062X/CC-pVDZ) (Hartree): -692.37342530			
Electronic state : 1-A			
Cartesian coordinates (Angs):			
C	-1.363953	0.664002	0.791818
H	-1.506857	0.343447	1.837175
C	-2.693132	1.145569	0.215125
C	-3.709334	0.035078	0.309499
H	-3.048954	2.011561	0.796833
H	-2.589567	1.438274	-0.838832
H	-4.086752	-0.180577	1.340529
C	-0.561788	-0.451312	0.048869
C	-0.126139	1.584626	0.713299
C	-0.715275	-1.872066	0.565237
C	-0.764114	-0.407908	-1.464901
H	-0.663226	0.609061	-1.876138
H	-0.028773	-1.056921	-1.963169
H	-1.774217	-0.762555	-1.717558
H	0.073438	-2.510266	0.143933
H	-1.703803	-2.274819	0.292277
H	-0.613156	-1.901343	1.660892
H	0.098431	2.224183	1.575679
H	-0.160512	2.202406	-0.196117
C	0.720290	0.311496	0.533132
H	1.010766	-0.101511	1.502189
C	1.900009	0.296963	-0.394264
C	2.181788	1.452507	-1.295167
H	2.278949	2.361468	-0.688641
H	3.097385	1.268549	-1.867983
H	1.341370	1.588737	-1.990966
O	-4.077301	-0.629212	-0.626034
O	2.392617	-0.821823	-0.795475
O	2.438523	-1.721954	0.318004
O	3.233658	0.451721	1.114708
H	3.052521	-0.603793	1.041698
H	4.112873	0.560508	0.722694
Rotational constants (GHz): 1.3325300 0.4053600 0.3766500			
Vibrational harmonic frequencies (cm-1):			
i449.4660	40.4294	55.8315	

77.5963	92.0290	145.9873
181.7175	201.0629	213.5585
220.2881	234.5237	254.5929
265.6319	299.8619	310.4869
332.7626	347.7018	389.0424
394.3957	433.6596	454.3288
508.8603	531.2761	570.1582
596.4925	609.0718	625.3188
655.7583	725.2875	768.3262
877.9720	894.2605	913.9823
934.6930	948.3282	957.3771
988.3462	996.0568	1011.0906
1031.3385	1034.1974	1051.4736
1103.5798	1131.5640	1158.1019
1167.5057	1183.8524	1193.0279
1235.9865	1256.7994	1267.5873
1289.4959	1304.9765	1315.4398
1321.2994	1373.3226	1385.3555
1395.6112	1402.6057	1410.3480
1413.2619	1427.1190	1441.6388
1448.4333	1455.0024	1459.4387
1472.8674	1482.9173	1486.8322
1579.7968	1645.8660	1876.4158
2156.0095	2930.8438	3049.3174
3053.2655	3059.6932	3065.9839
3083.4632	3085.9375	3128.7474
3130.2737	3140.7511	3148.7478
3150.0502	3158.5012	3170.4602
3171.0064	3198.4548	3837.4217

Zero-point correction (Hartree): 0.271057

TS.ApineneCI.A.b+H2O.HHP.tmpu

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E(RM062X/CC-pVDZ) (Hartree): -692.37162428

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 1.378717  | 0.663727  | -0.793224 |
| H | 1.504174  | 0.337762  | -1.839148 |
| C | 2.726036  | 1.103550  | -0.225967 |
| C | 3.709226  | -0.035833 | -0.326106 |
| H | 3.104324  | 1.956951  | -0.812279 |
| H | 2.639820  | 1.401379  | 0.827927  |
| H | 4.066826  | -0.267961 | -1.360704 |
| C | 0.535461  | -0.416356 | -0.042492 |
| C | 0.175460  | 1.622570  | -0.709037 |
| C | 0.671479  | -1.843180 | -0.550548 |
| C | 0.753048  | -0.367232 | 1.467612  |
| H | 0.702152  | 0.656304  | 1.870768  |
| H | -0.004027 | -0.985225 | 1.968997  |
| H | 1.753178  | -0.759119 | 1.706514  |
| H | -0.071228 | -2.489191 | -0.062999 |
| H | 1.677570  | -2.231735 | -0.325677 |
| H | 0.514033  | -1.890931 | -1.638828 |
| H | -0.028327 | 2.282921  | -1.561157 |
| H | 0.221963  | 2.218671  | 0.214041  |
| C | -0.718660 | 0.364125  | -0.553566 |
| H | -0.991197 | -0.027953 | -1.540169 |
| C | -2.014672 | 0.520989  | 0.184978  |
| C | -2.125824 | 1.354979  | 1.418608  |
| H | -1.421565 | 0.991531  | 2.175266  |
| H | -1.870028 | 2.397079  | 1.178113  |
| H | -3.152362 | 1.317608  | 1.799591  |
| O | 4.071701  | -0.703935 | 0.608853  |
| O | -3.132901 | 0.399851  | -0.445656 |
| O | -3.076463 | -0.726093 | -1.316703 |
| O | -2.086995 | -1.439906 | 0.779299  |
| H | -2.544937 | -1.439162 | -0.206894 |
| H | -2.844726 | -1.512286 | 1.378752  |

Rotational constants (GHz): 1.3427100 0.3964700 0.3769800

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i481.4493 | 44.6908   | 63.1213   |
| 78.0049   | 96.3732   | 131.7950  |
| 159.1030  | 191.6530  | 213.0677  |
| 233.5214  | 244.8109  | 267.0776  |
| 274.3546  | 299.4423  | 303.4733  |
| 344.8038  | 374.0382  | 378.7123  |
| 399.9679  | 432.1532  | 472.7348  |
| 527.4907  | 533.8833  | 556.9386  |
| 572.9046  | 604.2234  | 617.5034  |
| 645.5801  | 722.7593  | 761.2719  |
| 877.5977  | 908.6921  | 919.3038  |
| 928.1382  | 955.3460  | 960.5198  |
| 986.2410  | 998.3317  | 1012.2171 |
| 1024.8596 | 1030.5227 | 1046.8927 |
| 1092.9505 | 1124.2857 | 1153.2804 |
| 1174.6544 | 1184.9976 | 1221.2135 |
| 1234.5129 | 1264.3880 | 1269.5839 |
| 1299.5088 | 1306.7793 | 1317.9210 |
| 1328.2212 | 1345.8439 | 1381.0575 |
| 1395.5729 | 1404.1241 | 1410.9101 |
| 1413.4123 | 1432.2443 | 1441.4479 |
| 1448.1264 | 1456.9637 | 1469.2068 |
| 1472.4567 | 1487.5240 | 1493.7513 |
| 1579.4348 | 1631.5836 | 1876.5988 |
| 2010.7306 | 2929.3791 | 3052.6936 |
| 3057.4455 | 3060.7469 | 3066.4691 |
| 3083.9541 | 3089.1747 | 3130.6214 |
| 3132.6854 | 3138.5939 | 3142.1752 |
| 3154.1714 | 3160.9302 | 3162.3029 |
| 3175.6677 | 3208.5993 | 3837.2890 |

Zero-point correction (Hartree): 0.270875

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TS.ApineneCI.A.b+H2O.HHP.tmtd
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E(RM062X/CC-pVDZ) (Hartree): -692.37504219
Electronic state : 1-A
Cartesian coordinates (Angs):
C -1.435413 -0.571245 -0.708489
H -1.681747 -0.119464 -1.681078
C -2.684855 -1.187899 -0.109817
C -3.827941 -0.222913 0.066683
H -3.049917 -2.020391 -0.738361
H -2.487707 -1.643600 0.877287
H -4.771544 -0.666884 0.469329
C -0.582848 0.460337 0.103432
C -0.188424 -1.474599 -0.839027
C -0.729751 1.931243 -0.248672
C -0.698498 0.259014 1.611659
H -0.607367 -0.796844 1.913054
H 0.078659 0.835656 2.135202
H -1.678792 0.621039 1.958900
H 0.118593 2.493875 0.165466
H -1.681831 2.326161 0.130784
H -0.715615 2.066573 -1.340900
H -0.015128 -1.985758 -1.794137
H -0.161462 -2.216196 -0.025999
C 0.670400 -0.236954 -0.537084
H 0.915038 0.303078 -1.454702
C 1.894745 -0.341175 0.322054
C 2.192631 -1.588427 1.086067
H 2.256903 -2.427625 0.382280
H 3.131083 -1.474639 1.639896
H 1.376468 -1.793043 1.793593
O -3.767729 0.951455 -0.194705
O 2.441581 0.718173 0.807233
O 2.464943 1.727178 -0.208981
O 3.145492 -0.371817 -1.266350
H 3.000150 0.675402 -1.074592
H 4.039637 -0.541520 -0.934431
Rotational constants (GHz): 1.3248300 0.4163500 0.3811400
Vibrational harmonic frequencies (cm-1):
i452.7574 41.9743 44.4450
89.7184 116.6511 143.6075
173.8889 198.9845 208.4948
226.8946 247.9830 251.1879
261.0257 288.1618 306.4992
333.4168 342.2994 372.3079
394.6355 433.8274 457.6413
495.8455 560.4833 592.6192
606.2662 624.8955 657.8410
673.9940 728.2712 752.4846
797.0634 892.9846 911.9162
931.0182 938.4797 953.8679
968.2566 992.6570 996.2940
1024.2338 1031.1096 1050.3885
1110.5239 1123.6343 1157.1203
1171.4576 1185.9702 1201.7635
1236.3887 1266.2309 1280.1459
1291.7920 1308.7140 1317.0412
1337.6902 1376.8285 1385.2466
1395.8573 1401.0476 1404.3304
1410.1776 1427.1149 1430.1100
1447.1831 1455.2436 1459.9483
1472.1242 1481.0047 1484.9849
1579.1452 1646.9217 1878.4387
2144.8534 2936.3164 3044.9974
3049.0311 3062.3477 3074.9183
3076.6676 3085.3932 3094.8321
3123.2627 3138.7371 3142.5666
3144.2474 3168.8773 3171.9634
3175.1673 3197.2230 3834.3338
Zero-point correction (Hartree): 0.270884

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TS.ApineneCI.A.b+H2O.HHP.tmtu
~~~~~
E(RM062X/CC-pVDZ) (Hartree): -692.37329493
Electronic state : 1-A
Cartesian coordinates (Angs):
C      1.453680      0.538391      -0.723318
H      1.684813      0.041969      -1.677754
C      2.722516      1.135559      -0.145660
C      3.843288      0.150351      0.058224
H      3.107764      1.937720      -0.801254
H      2.541298      1.627859      0.826591
H      4.797651      0.586669      0.443500
C      0.549887      -0.421224      0.122642
C      0.245439      1.480442      -0.892428
C      0.678811      -1.909567      -0.160914
C      0.670276      -0.151953      1.618620
H      0.625871      0.920215      1.867731
H      -0.130963      -0.675445      2.157285
H      1.638928      -0.534268      1.978208
H      -0.123955      -2.456173      0.353001
H      1.656490      -2.277508      0.177895
H      0.598872      -2.106388      -1.240749
H      0.100481      1.981654      -1.857860
H      0.228301      2.230945      -0.087367
C      -0.666162      0.267532      -0.581105
H      -0.885390      -0.286537      -1.500733
C      -2.000494      0.553173      0.039537
C      -2.171680      1.589821      1.101086
H      -1.488169      1.386955      1.932983
H      -1.929562      2.578282      0.684237
H      -3.210264      1.595829      1.449804

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|                                                           |           |           |           |
|-----------------------------------------------------------|-----------|-----------|-----------|
| O                                                         | 3.758198  | -1.030335 | -0.165243 |
| O                                                         | -3.082461 | 0.328150  | -0.624561 |
| O                                                         | -2.992468 | -0.933965 | -1.279808 |
| O                                                         | -2.144079 | -1.272866 | 0.968205  |
| H                                                         | -2.537008 | -1.443613 | -0.030531 |
| H                                                         | -2.942035 | -1.231176 | 1.516174  |
| Rotational constants (GHz): 1.3298500 0.4077800 0.3812400 |           |           |           |
| Vibrational harmonic frequencies (cm-1):                  |           |           |           |
| i479.8080                                                 | 40.8632   |           | 55.6466   |
| 92.5733                                                   | 115.4486  |           | 126.6036  |
| 165.0190                                                  | 178.3539  |           | 215.1926  |
| 219.2127                                                  | 247.3696  |           | 262.4371  |
| 274.5105                                                  | 294.4023  |           | 302.6914  |
| 326.5691                                                  | 371.0804  |           | 373.8097  |
| 388.6568                                                  | 432.2738  |           | 468.2474  |
| 523.3673                                                  | 552.0239  |           | 567.5143  |
| 603.7255                                                  | 616.3025  |           | 641.4169  |
| 677.0535                                                  | 721.3134  |           | 752.8436  |
| 793.3879                                                  | 906.7251  |           | 916.4829  |
| 928.7286                                                  | 940.7128  |           | 956.5681  |
| 967.2484                                                  | 990.5163  |           | 998.6672  |
| 1020.8459                                                 | 1030.3855 |           | 1046.4983 |
| 1091.8315                                                 | 1117.8539 |           | 1154.5253 |
| 1181.3207                                                 | 1185.1904 |           | 1226.6896 |
| 1236.7518                                                 | 1270.8856 |           | 1284.3024 |
| 1300.3533                                                 | 1312.3477 |           | 1323.3486 |
| 1330.6321                                                 | 1350.6943 |           | 1382.7060 |
| 1393.5421                                                 | 1401.6577 |           | 1406.6872 |
| 1410.1503                                                 | 1430.6022 |           | 1432.0348 |
| 1445.7041                                                 | 1458.9091 |           | 1466.8167 |
| 1469.3568                                                 | 1482.7161 |           | 1491.8129 |
| 1577.9190                                                 | 1633.8833 |           | 1878.5398 |
| 2012.0757                                                 | 2937.6951 |           | 3044.3274 |
| 3051.7681                                                 | 3065.5551 |           | 3073.8116 |
| 3075.5624                                                 | 3087.8953 |           | 3094.2426 |
| 3120.5127                                                 | 3138.9571 |           | 3146.7596 |
| 3150.8201                                                 | 3161.8588 |           | 3171.5853 |
| 3174.4288                                                 | 3209.4359 |           | 3835.1013 |
| Zero-point correction (Hartree): 0.270613                 |           |           |           |
| TS.ApineneCI.A.b+H2O.HHP.tpmu                             |           |           |           |
| ~~~~~                                                     |           |           |           |
| E(RM062X/CC-pVDZ) (Hartree): -692.37026488                |           |           |           |
| Electronic state : 1-A                                    |           |           |           |
| Cartesian coordinates (Angs):                             |           |           |           |
| C                                                         | -1.498505 | 0.380824  | -0.499413 |
| H                                                         | -1.603477 | 0.705722  | -1.547795 |
| C                                                         | -2.831435 | 0.537027  | 0.226691  |
| C                                                         | -3.865119 | -0.318192 | -0.460569 |
| H                                                         | -2.758600 | 0.203206  | 1.270687  |
| H                                                         | -3.150060 | 1.592373  | 0.199207  |
| H                                                         | -4.186024 | 0.037562  | -1.472024 |
| C                                                         | -0.203763 | 1.031365  | 0.083630  |
| C                                                         | -0.794342 | -0.990469 | -0.460870 |
| C                                                         | 0.199784  | 2.368248  | -0.516017 |
| C                                                         | -0.240411 | 1.119401  | 1.606014  |
| H                                                         | -0.591679 | 0.189554  | 2.078637  |
| H                                                         | 0.760782  | 1.360086  | 1.986945  |
| H                                                         | -0.932548 | 1.919253  | 1.911982  |
| H                                                         | 1.182419  | 2.674704  | -0.132048 |
| H                                                         | -0.539483 | 3.141916  | -0.252345 |
| H                                                         | 0.257537  | 2.307099  | -1.613043 |
| H                                                         | -0.979744 | -1.700787 | -1.276108 |
| H                                                         | -0.979903 | -1.488977 | 0.502145  |
| C                                                         | 0.548615  | -0.215171 | -0.484134 |
| H                                                         | 0.840370  | 0.002894  | -1.517898 |
| C                                                         | 1.743864  | -0.875916 | 0.135868  |
| C                                                         | 1.636861  | -1.673237 | 1.393238  |
| H                                                         | 1.188909  | -1.062031 | 2.184685  |
| H                                                         | 0.984595  | -2.540661 | 1.214742  |
| H                                                         | 2.628443  | -2.027863 | 1.695162  |
| O                                                         | -4.297454 | -1.345308 | -0.004809 |
| O                                                         | 2.740970  | -1.224876 | -0.603631 |
| O                                                         | 3.047584  | -0.178356 | -1.520532 |
| O                                                         | 2.668678  | 0.893087  | 0.616395  |
| H                                                         | 2.974426  | 0.692061  | -0.412348 |
| H                                                         | 3.452508  | 0.654234  | 1.133414  |
| Rotational constants (GHz): 1.1881500 0.3917600 0.3587900 |           |           |           |
| Vibrational harmonic frequencies (cm-1):                  |           |           |           |
| i496.8309                                                 | 24.8815   |           | 49.6066   |
| 68.3769                                                   | 101.0510  |           | 125.1864  |
| 139.8761                                                  | 190.4689  |           | 204.3744  |
| 223.9282                                                  | 245.8936  |           | 252.5733  |
| 284.9919                                                  | 287.9900  |           | 311.1443  |
| 325.8213                                                  | 358.6498  |           | 377.8453  |
| 388.3362                                                  | 446.0020  |           | 467.3502  |
| 537.0513                                                  | 540.4034  |           | 568.9500  |
| 573.2255                                                  | 606.3711  |           | 617.1584  |
| 650.7504                                                  | 733.4729  |           | 775.7600  |
| 863.5211                                                  | 909.3372  |           | 922.0376  |
| 931.7953                                                  | 941.7377  |           | 956.5044  |
| 986.1618                                                  | 995.1706  |           | 1001.9714 |
| 1020.0229                                                 | 1031.3045 |           | 1061.5803 |
| 1077.9209                                                 | 1141.9235 |           | 1143.0966 |
| 1182.1357                                                 | 1193.5985 |           | 1225.9649 |
| 1241.6753                                                 | 1247.3108 |           | 1277.9530 |
| 1296.1729                                                 | 1301.5832 |           | 1313.7599 |
| 1325.9604                                                 | 1344.7855 |           | 1380.1382 |
| 1393.2876                                                 | 1404.3448 |           | 1410.5428 |
| 1411.3116                                                 | 1431.5770 |           | 1439.0784 |
| 1445.7719                                                 | 1454.2348 |           | 1468.4344 |
| 1470.6562                                                 | 1480.9701 |           | 1492.1430 |

|           |           |           |
|-----------|-----------|-----------|
| 1579.9416 | 1630.1195 | 1881.5866 |
| 1973.8224 | 2924.4380 | 3050.3951 |
| 3057.9081 | 3060.0787 | 3063.3382 |
| 3085.5744 | 3088.7078 | 3126.5807 |
| 3128.3919 | 3140.3683 | 3143.8157 |
| 3155.2779 | 3160.0972 | 3164.6256 |
| 3174.9804 | 3208.2723 | 3835.1214 |

Zero-point correction (Hartree): 0.270483

TS.ApineneCI.A.b+H2O.HHP.tppd

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E(RM062X/CC-pVDZ) (Hartree): -692.37094574

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-1.489190	0.134166	-0.377964
H	-1.693081	0.408604	-1.425289
C	-2.787435	0.182285	0.419451
C	-3.802976	-0.776997	-0.147933
H	-2.592164	-0.117968	1.463647
H	-3.228478	1.189511	0.420070
H	-3.452826	-1.837911	-0.229158
C	-0.253272	0.958868	0.101231
C	-0.622197	-1.147461	-0.349151
C	-0.028854	2.301007	-0.573274
C	-0.195024	1.106280	1.619368
H	-0.368994	0.155164	2.147383
H	0.786868	1.496026	1.925124
H	-0.964102	1.816053	1.959812
H	0.968021	2.687049	-0.322150
H	-0.799093	3.022463	-0.256063
H	-0.080240	2.199086	-1.667634
H	-0.758342	-1.889509	-1.145714
H	-0.703537	-1.650017	0.626999
C	0.611719	-0.231830	-0.440486
H	0.859588	-0.020401	-1.483617
C	1.864361	-0.561030	0.320643
C	1.901341	-1.708582	1.273668
H	1.602911	-2.621853	0.744134
H	2.906370	-1.815318	1.696456
H	1.184279	-1.531871	2.088574
O	-4.908222	-0.468725	-0.509677
O	2.736112	0.354862	0.556936
O	2.886699	1.148356	-0.626112
O	2.840509	-1.199520	-1.326449
H	3.009151	-0.142077	-1.327182
H	3.692034	-1.567042	-1.046285

Rotational constants (GHz): 1.2725800 0.3686400 0.3404400

Vibrational harmonic frequencies (cm-1):

i445.6972	31.6833	49.4586
52.1209	102.4032	133.7220
175.7059	199.2996	211.0881
218.8048	230.7274	246.5335
271.8281	294.8621	308.5704
320.5826	334.6352	365.0391
403.0312	439.3035	447.4077
500.6668	528.2670	572.9296
595.8826	617.0259	627.1267
660.6091	744.0935	781.5681
847.8079	893.9647	912.8538
933.3072	937.5227	954.2560
980.3439	992.1060	1009.6779
1024.0716	1033.2522	1075.8865
1100.0389	1138.1528	1155.3348
1174.6255	1186.3191	1208.3041
1238.8931	1251.4656	1276.2890
1291.7127	1303.1088	1313.6079
1318.7960	1371.4945	1382.6437
1394.6477	1400.0612	1408.3526
1419.1738	1426.1571	1434.1347
1447.4744	1451.4031	1459.2928
1471.6298	1479.3182	1483.3930
1578.3433	1646.8090	1888.2703
2183.5440	2918.3011	3049.6828
3051.0086	3053.8836	3070.2638
3079.0999	3083.9234	3125.7018
3129.9384	3131.7961	3143.1864
3146.2207	3163.4148	3169.4686
3172.7354	3198.5695	3835.9461

Zero-point correction (Hartree): 0.270797

TS.ApineneCI.A.b+H2O.HHP.tppu

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E(RM062X/CC-pVDZ) (Hartree): -692.36904695

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -1.495699 | 0.101376  | -0.371917 |
| H | -1.680142 | 0.344281  | -1.430619 |
| C | -2.802490 | 0.201918  | 0.405725  |
| C | -3.836135 | -0.743840 | -0.151913 |
| H | -2.630261 | -0.076746 | 1.459727  |
| H | -3.217360 | 1.219809  | 0.375333  |
| H | -3.511310 | -1.814311 | -0.209473 |
| C | -0.243772 | 0.908082  | 0.097526  |
| C | -0.653226 | -1.190634 | -0.291236 |
| C | -0.010842 | 2.239056  | -0.598269 |
| C | -0.208111 | 1.085868  | 1.612090  |
| H | -0.433680 | 0.156632  | 2.157945  |
| H | 0.781669  | 1.448677  | 1.919146  |
| H | -0.961701 | 1.829909  | 1.913234  |
| H | 0.953217  | 2.665409  | -0.289173 |
| H | -0.812256 | 2.948828  | -0.337521 |
| H | -0.004027 | 2.115698  | -1.691458 |

|                                                           |           |           |           |
|-----------------------------------------------------------|-----------|-----------|-----------|
| H                                                         | -0.803181 | -1.969843 | -1.049152 |
| H                                                         | -0.726339 | -1.638528 | 0.711718  |
| C                                                         | 0.600586  | -0.291046 | -0.441858 |
| H                                                         | 0.809649  | -0.112235 | -1.502871 |
| C                                                         | 1.890503  | -0.790436 | 0.138684  |
| C                                                         | 1.938896  | -1.512432 | 1.444589  |
| H                                                         | 1.477519  | -0.899101 | 2.226659  |
| H                                                         | 1.371763  | -2.450957 | 1.359015  |
| H                                                         | 2.977754  | -1.746243 | 1.702139  |
| O                                                         | -4.930765 | -0.416077 | -0.528312 |
| O                                                         | 2.874316  | -1.084688 | -0.640435 |
| O                                                         | 3.018535  | -0.073909 | -1.633977 |
| O                                                         | 2.653488  | 1.088432  | 0.459934  |
| H                                                         | 2.919103  | 0.856874  | -0.571395 |
| H                                                         | 3.486739  | 0.964320  | 0.938544  |
| Rotational constants (GHz): 1.2843100 0.3593100 0.3410200 |           |           |           |
| Vibrational harmonic frequencies (cm-1):                  |           |           |           |
| i492.1302                                                 | 44.5628   | 50.0271   |           |
| 54.3509                                                   | 105.7712  | 121.5012  |           |
| 146.3259                                                  | 189.1577  | 200.1741  |           |
| 219.2606                                                  | 247.6303  | 254.9229  |           |
| 278.7271                                                  | 284.8225  | 313.9699  |           |
| 326.0239                                                  | 357.9894  | 377.3843  |           |
| 386.4525                                                  | 443.5774  | 453.0751  |           |
| 520.9135                                                  | 540.4809  | 569.5545  |           |
| 575.3867                                                  | 606.3714  | 616.9674  |           |
| 653.0077                                                  | 733.8044  | 781.5197  |           |
| 847.8990                                                  | 901.9955  | 921.1434  |           |
| 933.3263                                                  | 939.1134  | 956.0493  |           |
| 980.4468                                                  | 993.5937  | 999.8414  |           |
| 1026.9989                                                 | 1030.9322 | 1062.5271 |           |
| 1093.5954                                                 | 1135.6665 | 1150.1523 |           |
| 1184.0734                                                 | 1189.8703 | 1226.1641 |           |
| 1244.2587                                                 | 1252.8034 | 1278.2640 |           |
| 1297.9109                                                 | 1302.2181 | 1314.1497 |           |
| 1326.0171                                                 | 1344.0013 | 1378.2774 |           |
| 1393.0942                                                 | 1402.6975 | 1410.1492 |           |
| 1419.7237                                                 | 1431.0097 | 1434.3654 |           |
| 1445.0202                                                 | 1454.0033 | 1467.7850 |           |
| 1470.4308                                                 | 1480.8737 | 1493.0305 |           |
| 1579.6701                                                 | 1631.7682 | 1888.2841 |           |
| 1989.0205                                                 | 2918.5624 | 3052.6049 |           |
| 3053.0787                                                 | 3058.3283 | 3070.4426 |           |
| 3076.9676                                                 | 3087.1896 | 3126.0247 |           |
| 3131.0375                                                 | 3132.2150 | 3139.0777 |           |
| 3150.0165                                                 | 3160.4153 | 3164.8077 |           |
| 3173.7953                                                 | 3206.5325 | 3833.8907 |           |
| Zero-point correction (Hartree): 0.270398                 |           |           |           |
| TS.ApineneCI.A.b+H2O.HHP.tptd                             |           |           |           |
| ~~~~~                                                     |           |           |           |
| E(RM062X/CC-pVDZ) (Hartree): -692.37464270                |           |           |           |
| Electronic state : 1-A                                    |           |           |           |
| Cartesian coordinates (Angs):                             |           |           |           |
| C                                                         | -1.560277 | 0.248636  | -0.342895 |
| H                                                         | -1.787700 | 0.391903  | -1.410307 |
| C                                                         | -2.824845 | 0.457686  | 0.463594  |
| C                                                         | -3.937763 | -0.473264 | 0.050504  |
| H                                                         | -2.658093 | 0.303898  | 1.545018  |
| H                                                         | -3.203989 | 1.491710  | 0.371781  |
| H                                                         | -4.901440 | -0.345495 | 0.601988  |
| C                                                         | -0.266848 | 1.048676  | 0.002514  |
| C                                                         | -0.775880 | -1.069856 | -0.177324 |
| C                                                         | 0.014636  | 2.279905  | -0.841619 |
| C                                                         | -0.154485 | 1.382730  | 1.488226  |
| H                                                         | -0.361811 | 0.514678  | 2.134737  |
| H                                                         | 0.855349  | 1.751103  | 1.719870  |
| H                                                         | -0.874078 | 2.171798  | 1.755577  |
| H                                                         | 1.033924  | 2.642548  | -0.654360 |
| H                                                         | -0.712233 | 3.075900  | -0.610147 |
| H                                                         | -0.065075 | 2.041940  | -1.912990 |
| H                                                         | -0.997344 | -1.881226 | -0.879183 |
| H                                                         | -0.865037 | -1.450087 | 0.852138  |
| C                                                         | 0.512132  | -0.253381 | -0.397176 |
| H                                                         | 0.752479  | -0.190390 | -1.461722 |
| C                                                         | 1.755054  | -0.572081 | 0.385185  |
| C                                                         | 1.742115  | -1.630362 | 1.437292  |
| H                                                         | 1.378526  | -2.567134 | 0.997343  |
| H                                                         | 2.746356  | -1.759609 | 1.855741  |
| H                                                         | 1.051490  | -1.336904 | 2.241430  |
| O                                                         | -3.828966 | -1.311590 | -0.807444 |
| O                                                         | 2.672858  | 0.316960  | 0.539200  |
| O                                                         | 2.854922  | 0.993354  | -0.710361 |
| O                                                         | 2.694441  | -1.402424 | -1.194571 |
| H                                                         | 2.910316  | -0.357807 | -1.292317 |
| H                                                         | 3.529289  | -1.779356 | -0.878998 |
| Rotational constants (GHz): 1.1690900 0.4131800 0.3724700 |           |           |           |
| Vibrational harmonic frequencies (cm-1):                  |           |           |           |
| i446.7786                                                 | 28.2466   | 51.0767   |           |
| 86.9413                                                   | 110.0197  | 156.3811  |           |
| 178.2127                                                  | 201.3609  | 215.8396  |           |
| 225.3603                                                  | 235.2486  | 244.8927  |           |
| 252.6720                                                  | 291.7879  | 308.7788  |           |
| 321.0721                                                  | 332.3241  | 367.1829  |           |
| 398.0047                                                  | 435.4994  | 450.6857  |           |
| 503.5318                                                  | 557.4959  | 594.7007  |           |
| 604.9354                                                  | 625.7457  | 657.7609  |           |
| 677.1792                                                  | 719.9408  | 754.4446  |           |
| 839.2454                                                  | 895.8634  | 915.8013  |           |
| 935.5287                                                  | 939.0495  | 943.8103  |           |
| 953.1976                                                  | 984.9009  | 996.9074  |           |
| 1018.2507                                                 | 1029.5147 | 1037.3757 |           |

|           |           |           |
|-----------|-----------|-----------|
| 1097.5135 | 1136.7044 | 1159.4430 |
| 1172.3854 | 1184.1778 | 1207.2683 |
| 1232.9891 | 1252.6537 | 1282.8666 |
| 1297.4480 | 1312.1205 | 1313.3771 |
| 1326.2375 | 1376.5195 | 1387.3094 |
| 1394.9204 | 1401.8305 | 1402.3596 |
| 1409.2165 | 1425.9804 | 1432.4686 |
| 1446.7366 | 1451.5738 | 1461.1653 |
| 1472.4697 | 1480.0636 | 1483.5846 |
| 1576.0811 | 1646.0047 | 1878.0916 |
| 2179.1692 | 2942.3413 | 3040.5982 |
| 3047.4140 | 3052.1268 | 3073.4070 |
| 3078.4051 | 3083.0280 | 3090.5797 |
| 3124.3912 | 3126.3478 | 3143.9574 |
| 3161.5812 | 3167.0477 | 3168.2058 |
| 3171.9679 | 3198.2962 | 3835.5468 |

Zero-point correction (Hartree): 0.270789

TS.ApineneCI.A.b+H2O.HHP.tptu

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E(RM062X/CC-pVDZ) (Hartree): -692.37273704

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-1.566245	0.208411	-0.353285
H	-1.765349	0.255591	-1.434863
C	-2.845562	0.511876	0.397877
C	-3.965006	-0.435471	0.043239
H	-2.709218	0.456601	1.492753
H	-3.203249	1.538740	0.200585
H	-4.940159	-0.240161	0.553177
C	-0.259829	1.004259	-0.047757
C	-0.808734	-1.098798	-0.052080
C	0.047244	2.170955	-0.972546
C	-0.181687	1.447883	1.410385
H	-0.462908	0.649482	2.114710
H	0.836663	1.786315	1.642480
H	-0.874574	2.287367	1.578093
H	1.044533	2.577191	-0.754570
H	-0.697828	2.971613	-0.835741
H	0.021037	1.854699	-2.025897
H	-1.041477	-1.978219	-0.662565
H	-0.890870	-1.359871	1.014399
C	0.498263	-0.324607	-0.368812
H	0.698805	-0.350850	-1.446083
C	1.764001	-0.793123	0.283302
C	1.786186	-1.281643	1.693915
H	1.360040	-0.521630	2.358244
H	1.171902	-2.191044	1.767516
H	2.813694	-1.519813	1.990129
O	-3.849377	-1.353037	-0.728275
O	2.718679	-1.278616	-0.435335
O	2.912784	-0.462339	-1.587060
O	2.650625	1.060324	0.273782
H	2.884630	0.633342	-0.705974
H	3.480852	0.961538	0.763296

Rotational constants (GHz): 1.1743400 0.4028700 0.3731400

Vibrational harmonic frequencies (cm-1):

i501.5572	46.3695	59.7471
90.6148	110.7297	132.4326
174.3923	177.1262	205.8911
225.7519	233.5129	255.3144
271.8140	287.6624	302.4853
325.5743	358.1352	376.9837
389.0982	430.7936	471.6394
530.2023	554.4598	569.8406
605.5817	614.6330	651.5353
679.6624	717.7223	743.9149
841.4709	905.7969	923.1766
938.0923	939.8127	943.6722
955.4826	984.4175	995.1688
1008.1733	1027.2602	1034.5323
1080.3365	1135.5920	1154.6148
1182.4096	1186.0877	1225.3162
1240.7134	1251.7420	1287.3312
1298.0910	1307.8092	1322.4579
1328.5796	1345.9532	1384.5132
1392.7074	1401.0075	1406.7043
1409.6899	1431.1030	1432.9652
1445.2854	1454.2422	1470.3292
1471.2571	1480.0401	1493.7409
1579.7534	1628.3417	1878.0772
1956.0077	2939.6986	3042.5984
3050.0768	3056.1077	3074.6853
3080.0974	3086.8372	3091.1364
3123.5527	3128.1483	3140.2641
3159.4573	3164.3873	3166.4836
3173.7307	3206.6528	3831.4028

Zero-point correction (Hartree): 0.270347

TS.ApineneCI.A.b+H2O.HHP.ttmd

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E(RM062X/CC-pVDZ) (Hartree): -692.36939466

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -1.348288 | -0.388757 | 1.121845  |
| H | -1.193649 | -1.053427 | 1.985635  |
| C | -2.854654 | -0.257263 | 0.900805  |
| C | -3.297262 | 0.818539  | -0.058971 |
| H | -3.280214 | -1.212063 | 0.557000  |
| H | -3.327970 | -0.008781 | 1.867942  |
| H | -2.945225 | 1.852961  | 0.184967  |
| C | -0.413968 | -0.901115 | -0.017020 |

|                                                           |           |           |           |
|-----------------------------------------------------------|-----------|-----------|-----------|
| C                                                         | -0.424350 | 0.841785  | 1.299877  |
| C                                                         | -0.121438 | -2.391314 | -0.040049 |
| C                                                         | -0.840717 | -0.419790 | -1.401981 |
| H                                                         | -1.059216 | 0.659630  | -1.433242 |
| H                                                         | -0.048047 | -0.629919 | -2.135421 |
| H                                                         | -1.755709 | -0.939202 | -1.723608 |
| H                                                         | 0.714903  | -2.601261 | -0.720369 |
| H                                                         | -1.012924 | -2.951853 | -0.364809 |
| H                                                         | 0.168591  | -2.746865 | 0.960108  |
| H                                                         | -0.245502 | 1.209964  | 2.317737  |
| H                                                         | -0.733336 | 1.682810  | 0.663898  |
| C                                                         | 0.685681  | 0.001292  | 0.642164  |
| H                                                         | 1.210909  | -0.599791 | 1.388468  |
| C                                                         | 1.679748  | 0.636489  | -0.286302 |
| C                                                         | 1.529566  | 2.057541  | -0.716016 |
| H                                                         | 1.482662  | 2.696307  | 0.174635  |
| H                                                         | 2.368734  | 2.347456  | -1.357870 |
| H                                                         | 0.590439  | 2.174499  | -1.276165 |
| O                                                         | -4.010165 | 0.629460  | -1.010582 |
| O                                                         | 2.365268  | -0.093364 | -1.094011 |
| O                                                         | 2.795445  | -1.264633 | -0.390197 |
| O                                                         | 3.146394  | 0.645981  | 1.101569  |
| H                                                         | 3.220958  | -0.328233 | 0.660180  |
| H                                                         | 3.903144  | 1.123764  | 0.730578  |
| Rotational constants (GHz): 1.2089600 0.4196200 0.3937600 |           |           |           |
| Vibrational harmonic frequencies (cm-1):                  |           |           |           |
| i445.8661                                                 | 35.9862   |           | 45.8394   |
| 80.2203                                                   | 94.1247   |           | 135.9487  |
| 192.6334                                                  | 204.9791  |           | 214.8370  |
| 218.1501                                                  | 233.5780  |           | 243.5051  |
| 270.9502                                                  | 302.6776  |           | 308.1132  |
| 335.3165                                                  | 348.6250  |           | 373.9179  |
| 399.6526                                                  | 433.2183  |           | 466.8725  |
| 488.2623                                                  | 563.2559  |           | 582.4949  |
| 600.5556                                                  | 609.3934  |           | 626.7448  |
| 664.8504                                                  | 713.3091  |           | 755.1966  |
| 832.8300                                                  | 893.0827  |           | 913.0207  |
| 925.5182                                                  | 939.8886  |           | 951.8976  |
| 988.4703                                                  | 992.0393  |           | 1003.9906 |
| 1029.8522                                                 | 1033.4672 |           | 1051.7512 |
| 1110.1222                                                 | 1137.6649 |           | 1147.9775 |
| 1175.1880                                                 | 1183.7028 |           | 1215.3884 |
| 1232.5843                                                 | 1251.5603 |           | 1292.2404 |
| 1301.9543                                                 | 1314.2914 |           | 1317.0975 |
| 1325.3637                                                 | 1374.7230 |           | 1384.0818 |
| 1394.8098                                                 | 1401.9866 |           | 1408.8596 |
| 1420.0989                                                 | 1426.8002 |           | 1427.4906 |
| 1447.4154                                                 | 1451.4669 |           | 1459.0558 |
| 1474.7004                                                 | 1478.4047 |           | 1486.4828 |
| 1579.2405                                                 | 1645.4684 |           | 1883.1030 |
| 2171.9907                                                 | 2919.4098 |           | 3042.2966 |
| 3050.6353                                                 | 3054.1878 |           | 3077.5773 |
| 3083.0963                                                 | 3094.5775 |           | 3118.4171 |
| 3128.5732                                                 | 3129.7976 |           | 3143.6507 |
| 3152.7563                                                 | 3164.3113 |           | 3169.6727 |
| 3172.5853                                                 | 3197.5639 |           | 3836.9337 |
| Zero-point correction (Hartree): 0.271003                 |           |           |           |
| TS.ApineneCI.A.b+H2O.HHP.ttmu                             |           |           |           |
| ~~~~~                                                     |           |           |           |
| E(RM062X/CC-pVDZ) (Hartree): -692.36763019                |           |           |           |
| Electronic state : 1-A                                    |           |           |           |
| Cartesian coordinates (Angs):                             |           |           |           |
| C                                                         | -1.349355 | -0.513385 | 1.073890  |
| H                                                         | -1.175920 | -1.268683 | 1.855746  |
| C                                                         | -2.857928 | -0.404870 | 0.858340  |
| C                                                         | -3.336332 | 0.766659  | 0.037737  |
| H                                                         | -3.250538 | -1.323097 | 0.395963  |
| H                                                         | -3.343582 | -0.295355 | 1.844922  |
| H                                                         | -3.009069 | 1.773052  | 0.403031  |
| C                                                         | -0.390484 | -0.849725 | -0.109657 |
| C                                                         | -0.466369 | 0.712966  | 1.398609  |
| C                                                         | -0.083443 | -2.324035 | -0.315031 |
| C                                                         | -0.838637 | -0.213356 | -1.422079 |
| H                                                         | -1.108701 | 0.849093  | -1.316332 |
| H                                                         | -0.036297 | -0.300456 | -2.166868 |
| H                                                         | -1.733061 | -0.729836 | -1.802480 |
| H                                                         | 0.692605  | -2.447707 | -1.082531 |
| H                                                         | -0.990683 | -2.857209 | -0.642014 |
| H                                                         | 0.271181  | -2.786851 | 0.618074  |
| H                                                         | -0.311949 | 0.981984  | 2.451186  |
| H                                                         | -0.781777 | 1.603929  | 0.838272  |
| C                                                         | 0.685867  | -0.036225 | 0.678378  |
| H                                                         | 1.187605  | -0.716965 | 1.375869  |
| C                                                         | 1.780642  | 0.790580  | 0.071922  |
| C                                                         | 1.500071  | 2.082965  | -0.620939 |
| H                                                         | 0.762612  | 1.927316  | -1.416285 |
| H                                                         | 1.083561  | 2.797597  | 0.104074  |
| H                                                         | 2.428663  | 2.493957  | -1.032025 |
| O                                                         | -4.053865 | 0.674344  | -0.924564 |
| O                                                         | 2.977555  | 0.717770  | 0.545391  |
| O                                                         | 3.318353  | -0.645545 | 0.780702  |
| O                                                         | 2.227348  | -0.584873 | -1.383216 |
| H                                                         | 2.813389  | -0.899450 | -0.522289 |
| H                                                         | 2.882648  | -0.164337 | -1.959847 |
| Rotational constants (GHz): 1.2395600 0.4084500 0.3904400 |           |           |           |
| Vibrational harmonic frequencies (cm-1):                  |           |           |           |
| i482.1649                                                 | 44.3601   |           | 58.5551   |
| 85.5775                                                   | 91.5186   |           | 135.7621  |
| 158.8076                                                  | 195.7433  |           | 208.1768  |
| 229.0338                                                  | 249.0025  |           | 263.2898  |
| 275.1928                                                  | 298.1422  |           | 307.9632  |



|           |           |           |
|-----------|-----------|-----------|
| 329.7079  | 375.8364  | 385.5140  |
| 389.4198  | 440.1917  | 461.4984  |
| 529.2709  | 550.2803  | 569.4834  |
| 585.9642  | 608.2042  | 625.4059  |
| 650.1181  | 714.5729  | 745.0845  |
| 833.7898  | 905.3363  | 911.2953  |
| 927.1455  | 945.7083  | 955.2427  |
| 985.0619  | 994.9941  | 1001.7382 |
| 1023.4272 | 1031.8236 | 1048.1614 |
| 1101.0869 | 1129.7602 | 1146.9253 |
| 1182.8694 | 1194.0115 | 1225.4624 |
| 1229.5844 | 1265.5195 | 1300.7386 |
| 1305.9684 | 1314.0644 | 1321.1293 |
| 1329.1300 | 1348.3210 | 1378.5555 |
| 1395.8321 | 1403.2601 | 1410.2788 |
| 1419.1922 | 1426.6484 | 1432.9916 |
| 1444.9824 | 1454.2165 | 1469.3877 |
| 1471.9204 | 1478.6081 | 1496.4577 |
| 1579.9109 | 1631.2591 | 1883.1546 |
| 2007.1249 | 2920.8751 | 3041.1466 |
| 3052.2295 | 3059.5710 | 3075.5183 |
| 3086.2461 | 3094.3486 | 3117.4186 |
| 3128.1724 | 3129.9366 | 3142.4107 |
| 3157.8661 | 3163.1118 | 3166.7280 |
| 3173.6373 | 3207.1215 | 3835.8413 |

Zero-point correction (Hartree): 0.270774

TS.ApineneCI.A.b+H2O.HHP.ttttd

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E(RM062X/CC-pVDZ) (Hartree): -692.37360928

Electronic state : 1-A

Cartesian coordinates (Angs):

C	1.535432	0.710497	0.934748
H	1.650356	1.514304	1.677309
C	2.935602	0.377823	0.434125
C	3.167134	-0.879680	-0.364864
H	3.343184	1.210519	-0.168224
H	3.636574	0.297556	1.286619
H	4.230008	-1.013823	-0.684913
C	0.406085	1.139360	-0.061918
C	0.630607	-0.406608	1.511636
C	0.017294	2.608864	0.039053
C	0.631358	0.779243	-1.527481
H	0.789230	-0.294358	-1.688598
H	-0.240493	1.093784	-2.117673
H	1.514984	1.314264	-1.912334
H	-0.928683	2.769684	-0.495997
H	0.801710	3.247362	-0.399704
H	-0.121192	2.909937	1.089088
H	0.519794	-0.418289	2.602774
H	0.926003	-1.402238	1.169419
C	-0.562223	0.191592	0.734161
H	-1.211965	0.793640	1.372769
C	-1.406998	-0.730006	-0.107396
C	-1.050717	-2.170640	-0.250327
H	-1.080456	-2.641909	0.740463
H	-1.748166	-2.665433	-0.935213
H	-0.020934	-2.251549	-0.631324
O	2.348895	-1.719172	-0.652549
O	-2.089497	-0.254887	-1.093834
O	-2.681661	0.976810	-0.665123
O	-2.971595	-0.645444	1.130403
H	-3.098694	0.225342	0.499808
H	-3.631823	-1.269924	0.794131

Rotational constants (GHz): 1.0606000 0.5265100 0.4536100

Vibrational harmonic frequencies (cm-1):

i485.0825	30.8371	65.5725
118.6675	134.5466	163.9128
184.6709	209.2942	222.6537
238.6343	249.2439	265.7738
282.4672	313.7037	320.0928
329.6399	339.8915	373.8234
406.5286	432.2444	450.0139
485.8621	575.0615	600.7800
611.9379	633.6889	673.6276
681.8260	747.8882	769.1756
774.2019	892.4057	903.7725
930.1294	946.9111	954.9764
960.9234	995.7974	1006.5255
1018.3234	1035.0944	1055.3928
1086.2836	1133.4549	1151.0305
1168.9834	1198.3357	1223.5450
1249.6780	1258.4130	1289.2852
1299.3091	1312.7925	1317.8541
1359.1054	1374.7207	1382.7666
1387.8319	1396.2769	1404.0450
1409.1033	1430.3878	1435.7838
1445.3063	1452.0779	1465.9691
1474.7581	1479.3226	1489.6983
1573.2828	1643.6872	1869.6712
2074.6153	2940.2125	3031.7512
3042.5977	3057.4292	3067.7449
3075.8810	3080.1524	3115.0675
3118.9196	3137.8189	3157.8724
3163.4352	3172.8618	3173.6046
3194.7022	3198.7219	3834.5143

Zero-point correction (Hartree): 0.271528

TS.ApineneCI.A.b+H2O.HHP.tttu

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E(RM062X/CC-pVDZ) (Hartree): -692.37145667

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -1.499495 | -0.771687 | 0.902447  |
| H | -1.525682 | -1.623358 | 1.598967  |
| C | -2.945489 | -0.468711 | 0.526691  |
| C | -3.298823 | 0.852999  | -0.108367 |
| H | -3.345042 | -1.251145 | -0.145283 |
| H | -3.593828 | -0.530106 | 1.420561  |
| H | -4.394823 | 0.977202  | -0.291153 |
| C | -0.423661 | -1.088157 | -0.190720 |
| C | -0.591239 | 0.335507  | 1.488756  |
| C | -0.023227 | -2.556650 | -0.267969 |
| C | -0.750862 | -0.590581 | -1.594798 |
| H | -1.066294 | 0.457217  | -1.621592 |
| H | 0.132720  | -0.718962 | -2.235906 |
| H | -1.567317 | -1.198519 | -2.017848 |
| H | 0.873742  | -2.660396 | -0.895514 |
| H | -0.836551 | -3.158555 | -0.705107 |
| H | 0.204060  | -2.959742 | 0.730588  |
| H | -0.434777 | 0.320722  | 2.574050  |
| H | -0.898252 | 1.339674  | 1.180416  |
| C | 0.582118  | -0.236086 | 0.645088  |
| H | 1.222134  | -0.885874 | 1.248980  |
| C | 1.483281  | 0.794002  | 0.038082  |
| C | 0.967864  | 1.912819  | -0.811386 |
| H | 1.033146  | 1.597215  | -1.861364 |
| H | -0.082797 | 2.141499  | -0.594418 |
| H | 1.603957  | 2.793951  | -0.664845 |
| O | -2.541864 | 1.745276  | -0.404529 |
| O | 2.610837  | 1.088130  | 0.601085  |
| O | 3.283185  | -0.096114 | 1.011902  |
| O | 2.368549  | -0.609640 | -1.147762 |
| H | 2.962936  | -0.623482 | -0.204109 |
| H | 2.944214  | -0.139275 | -1.768939 |

Rotational constants (GHz): 1.0990100 0.4898500 0.4355700

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i599.2729 | 47.7599   | 74.2893   |
| 119.4238  | 139.6869  | 161.4259  |
| 176.7415  | 207.3549  | 215.3778  |
| 246.8140  | 252.6421  | 258.0728  |
| 280.8913  | 300.4102  | 309.2013  |
| 319.0896  | 352.5952  | 375.4218  |
| 395.2505  | 431.0784  | 475.6153  |
| 521.0011  | 562.3977  | 578.0919  |
| 606.7252  | 619.2760  | 654.2249  |
| 672.8296  | 738.1937  | 762.5595  |
| 775.1325  | 899.0711  | 926.7963  |
| 929.9345  | 944.4631  | 953.2932  |
| 968.4408  | 993.8331  | 998.3215  |
| 1015.1794 | 1023.0200 | 1041.8399 |
| 1082.7948 | 1115.6957 | 1152.1249 |
| 1185.2159 | 1197.9445 | 1212.6841 |
| 1235.2854 | 1245.9067 | 1277.0989 |
| 1300.9227 | 1313.9581 | 1327.0476 |
| 1334.8936 | 1363.1138 | 1383.8218 |
| 1387.9518 | 1393.1128 | 1402.5160 |
| 1403.4862 | 1431.2327 | 1437.1013 |
| 1449.9159 | 1456.3020 | 1468.9935 |
| 1473.1207 | 1484.2957 | 1500.3544 |
| 1569.3497 | 1615.9354 | 1855.3198 |
| 1869.1347 | 2938.8557 | 3033.8538 |
| 3045.4742 | 3061.0398 | 3065.5549 |
| 3078.6970 | 3086.1561 | 3115.6551 |
| 3123.9643 | 3139.6451 | 3151.1833 |
| 3164.6196 | 3172.8689 | 3191.4780 |
| 3197.6771 | 3204.9238 | 3835.0490 |

Zero-point correction (Hartree): 0.270776

#####  
E-pinonaldehyde-A-oxide  
#####

Population analysis as 298K (%)

Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)

| Compound                       | Qtot      | Erel | Erel2 | n*Q*MB    | %     |
|--------------------------------|-----------|------|-------|-----------|-------|
| TS.ApineneCI.J.a+H2O.HHP.pmttd | 1.804e+45 | 0.00 | 0.00  | 1.804e+45 | 27.5  |
| TS.ApineneCI.J.a+H2O.HHP.pptd  | 1.911e+45 | 0.63 | 0.63  | 6.547e+44 | 9.97  |
| TS.ApineneCI.J.a+H2O.HHP.pmmu  | 1.621e+45 | 0.57 | 0.57  | 6.172e+44 | 9.4   |
| TS.ApineneCI.J.a+H2O.HHP.pmpu  | 3.093e+45 | 0.98 | 0.98  | 5.885e+44 | 8.97  |
| TS.ApineneCI.J.a+H2O.HHP.pmmmd | 1.698e+45 | 0.64 | 0.64  | 5.750e+44 | 8.76  |
| TS.ApineneCI.J.a+H2O.HHP.ppmu  | 2.105e+45 | 0.99 | 0.99  | 3.941e+44 | 6     |
| TS.ApineneCI.J.a+H2O.HHP.pppd  | 2.772e+45 | 1.24 | 1.24  | 3.440e+44 | 5.24  |
| TS.ApineneCI.J.a+H2O.HHP.pmtu  | 1.399e+45 | 0.83 | 0.83  | 3.417e+44 | 5.2   |
| TS.ApineneCI.J.a+H2O.HHP.pptu  | 3.074e+45 | 1.34 | 1.34  | 3.180e+44 | 4.84  |
| TS.ApineneCI.J.a+H2O.HHP.pmpd  | 5.077e+44 | 0.44 | 0.44  | 2.433e+44 | 3.71  |
| TS.ApineneCI.J.a+H2O.HHP.ppmmd | 6.320e+45 | 2.34 | 2.34  | 1.207e+44 | 1.84  |
| TS.ApineneCI.J.a+H2O.HHP.pppu  | 5.598e+45 | 2.44 | 2.44  | 9.044e+43 | 1.38  |
| TS.ApineneCI.J.a+H2O.HHP.mmttd | 3.060e+45 | 2.14 | 2.14  | 8.262e+43 | 1.26  |
| TS.ApineneCI.J.a+H2O.HHP.mptd  | 2.274e+45 | 2.15 | 2.15  | 6.051e+43 | 0.922 |
| TS.ApineneCI.J.a+H2O.HHP.mpmu  | 2.800e+45 | 2.39 | 2.39  | 4.952e+43 | 0.754 |
| TS.ApineneCI.J.a+H2O.HHP.mptu  | 3.204e+45 | 2.56 | 2.56  | 4.263e+43 | 0.649 |
| TS.ApineneCI.J.a+H2O.HHP.mppd  | 3.109e+45 | 2.56 | 2.56  | 4.093e+43 | 0.624 |
| TS.ApineneCI.J.a+H2O.HHP.mmtu  | 8.900e+44 | 1.97 | 1.97  | 3.175e+43 | 0.484 |
| TS.ApineneCI.J.a+H2O.HHP.mmpd  | 2.570e+45 | 2.69 | 2.69  | 2.726e+43 | 0.415 |
| TS.ApineneCI.J.a+H2O.HHP.tmtu  | 2.672e+45 | 2.77 | 2.77  | 2.469e+43 | 0.376 |
| TS.ApineneCI.J.a+H2O.HHP.mmpu  | 3.822e+45 | 2.99 | 2.99  | 2.447e+43 | 0.373 |
| TS.ApineneCI.J.a+H2O.HHP.mmmu  | 1.795e+45 | 2.57 | 2.57  | 2.346e+43 | 0.357 |
| TS.ApineneCI.J.a+H2O.HHP.ppmmd | 6.062e+45 | 3.38 | 3.38  | 2.022e+43 | 0.308 |
| TS.ApineneCI.J.a+H2O.HHP.tmpd  | 6.651e+44 | 2.36 | 2.36  | 1.228e+43 | 0.187 |
| TS.ApineneCI.J.a+H2O.HHP.mppu  | 6.864e+45 | 3.84 | 3.84  | 1.046e+43 | 0.159 |
| TS.ApineneCI.J.a+H2O.HHP.ptpd  | 1.631e+44 | 1.74 | 1.74  | 8.696e+42 | 0.132 |

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TS.ApineneCI.J.a+H2O.HHP.ptmd 2.053e+45 3.32 3.32 7.544e+42 0.115
TS.ApineneCI.J.a+H2O.HHP.ptpu 1.550e+45 3.90 3.90 2.124e+42 0.0324
TS.ApineneCI.J.a+H2O.HHP.pttu 1.753e+45 4.26 4.26 1.322e+42 0.0201
TS.ApineneCI.J.a+H2O.HHP.mtpu 2.885e+45 4.85 4.85 7.970e+41 0.0121
TS.ApineneCI.J.a+H2O.HHP.mttu 2.959e+45 5.01 5.01 6.239e+41 0.0095
TS.ApineneCI.J.a+H2O.HHP.mtmd 2.344e+45 5.02 5.02 4.842e+41 0.00738
TS.ApineneCI.J.a+H2O.HHP.ttpd 1.122e+45 4.86 4.86 3.075e+41 0.00468
TS.ApineneCI.J.a+H2O.HHP.mtttd 1.557e+45 5.48 5.48 1.487e+41 0.00227
TS.ApineneCI.J.a+H2O.HHP.pttd 1.107e+45 5.30 5.30 1.431e+41 0.00218
Total 6.565e+45 100

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TS.ApineneCI.J.a+H2O.HHP.mmmu

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E(RM062X/CC-pVDZ) (Hartree): -692.37279103

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-0.149699	-0.685528	-0.467411
H	-0.516148	-0.495705	-1.485872
C	-1.281441	-1.263718	0.374916
C	-2.432498	-0.330411	0.495189
H	-1.639007	-2.220507	-0.031057
H	-0.921934	-1.446859	1.402507
H	-2.296449	0.682414	0.886906
C	0.632697	0.581467	0.009747
C	1.181279	-1.462391	-0.532476
C	0.222093	1.914636	-0.593147
C	0.725685	0.678046	1.532340
H	1.070601	-0.261556	1.992880
H	1.438930	1.462502	1.814293
H	-0.254224	0.929672	1.967581
H	0.993732	2.669294	-0.378042
H	-0.738582	2.263459	-0.186094
H	0.100514	1.834568	-1.683526
H	1.322156	-2.171040	-1.358390
H	1.393701	-1.973130	0.419323
C	1.890189	-0.091306	-0.612718
H	1.974661	0.211494	-1.671658
C	3.254567	0.122171	0.002796
C	4.258435	-0.993484	-0.178782
H	4.301194	-1.299152	-1.235108
H	3.938127	-1.874853	0.398047
H	5.245100	-0.666209	0.166578
O	3.527658	1.146638	0.586841
O	-3.607529	-0.803828	0.505566
O	-4.521214	0.281782	0.353992
O	-2.731088	0.713939	-1.257531
H	-3.665769	0.748155	-0.738419
H	-2.897060	0.082304	-1.973625

Rotational constants (GHz): 1.6058100 0.3196200 0.3034100

Vibrational harmonic frequencies (cm-1):

i399.9021	39.7127	51.9585
55.9677	67.9194	119.7426
128.1943	163.7730	200.7940
217.7959	250.2172	265.3417
293.6627	307.3597	314.5529
328.1695	365.3613	386.1624
398.2084	444.1643	458.6932
510.9101	535.2000	564.9337
599.2753	605.3888	622.2477
624.4544	725.4430	774.0619
863.3689	905.1588	917.8757
931.7889	951.7179	960.8672
977.0742	996.3352	1014.9672
1028.2706	1073.3936	1087.6356
1108.5780	1126.0428	1151.5733
1172.4927	1189.2694	1204.5425
1231.3209	1239.7155	1261.8044
1270.3787	1293.3466	1305.2082
1325.7599	1346.5569	1379.6709
1384.0837	1385.2066	1401.6856
1406.0726	1431.7951	1435.3368
1446.0427	1446.6157	1461.3165
1472.2418	1473.6247	1486.7593
1621.9910	1640.0212	1860.4712
2190.4904	3050.9292	3053.6268
3056.6137	3059.6757	3065.5864
3074.3731	3105.5035	3122.9664
3130.1049	3140.0740	3140.4473
3144.1542	3144.5515	3170.6104
3193.1126	3194.9196	3837.1950

Zero-point correction (Hartree): 0.271017

TS.ApineneCI.J.a+H2O.HHP.mmpd

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E(RM062X/CC-pVDZ) (Hartree): -692.37234132

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.067400  | -0.859043 | 0.511649  |
| H | 0.300248  | -0.960961 | 1.585019  |
| C | 1.294160  | -1.241299 | -0.299888 |
| C | 2.541769  | -0.600266 | 0.203736  |
| H | 1.465966  | -2.330392 | -0.230598 |
| H | 1.178738  | -1.014956 | -1.370272 |
| H | 2.583154  | -0.147436 | 1.200423  |
| C | -0.660974 | 0.508950  | 0.300814  |
| C | -1.263248 | -1.586121 | 0.229176  |
| C | -0.297142 | 1.632615  | 1.256578  |
| C | -0.585803 | 0.991936  | -1.145621 |
| H | -0.863171 | 0.206817  | -1.867605 |
| H | -1.271848 | 1.835029  | -1.294513 |
| H | 0.437888  | 1.324735  | -1.364395 |
| H | -1.017820 | 2.457911  | 1.153462  |

|                                            |           |           |           |
|--------------------------------------------|-----------|-----------|-----------|
| H                                          | 0.710788  | 2.012915  | 1.030432  |
| H                                          | -0.321300 | 1.286535  | 2.301953  |
| H                                          | -1.490650 | -2.485331 | 0.815980  |
| H                                          | -1.368867 | -1.819403 | -0.841366 |
| C                                          | -1.977482 | -0.265513 | 0.595776  |
| H                                          | -2.173753 | -0.249227 | 1.682927  |
| C                                          | -3.268860 | 0.139179  | -0.078094 |
| C                                          | -4.281871 | -0.958897 | -0.310508 |
| H                                          | -4.433472 | -1.539277 | 0.612123  |
| H                                          | -3.899446 | -1.657675 | -1.070566 |
| H                                          | -5.228361 | -0.526056 | -0.652121 |
| O                                          | -3.482171 | 1.289266  | -0.389233 |
| O                                          | 3.642959  | -0.897315 | -0.343761 |
| O                                          | 4.631347  | 0.021280  | 0.118574  |
| O                                          | 2.665589  | 1.398155  | -0.360199 |
| H                                          | 3.665926  | 1.089183  | -0.147976 |
| H                                          | 2.656494  | 1.457258  | -1.327659 |
| Rotational constants (GHz):                |           |           |           |
|                                            | 1.5986400 | 0.3210500 | 0.2927500 |
| Vibrational harmonic frequencies (cm-1):   |           |           |           |
| i394.6185                                  | 23.8609   |           | 40.5000   |
| 68.7177                                    | 81.7415   |           | 127.5991  |
| 138.2950                                   | 159.3227  |           | 185.4162  |
| 231.1538                                   | 248.1584  |           | 266.5322  |
| 290.1146                                   | 302.6415  |           | 314.4380  |
| 326.0453                                   | 357.1237  |           | 384.8744  |
| 396.8771                                   | 442.2491  |           | 457.4259  |
| 499.2835                                   | 526.5568  |           | 570.9444  |
| 591.7294                                   | 608.7083  |           | 616.1858  |
| 624.0120                                   | 720.5239  |           | 771.8678  |
| 846.7034                                   | 905.6809  |           | 917.4347  |
| 920.5845                                   | 958.4757  |           | 962.2679  |
| 974.9499                                   | 999.9222  |           | 1018.4307 |
| 1028.8167                                  | 1073.6726 |           | 1083.2807 |
| 1110.2355                                  | 1122.3133 |           | 1161.3971 |
| 1169.2850                                  | 1185.1707 |           | 1194.1072 |
| 1230.3913                                  | 1244.6766 |           | 1260.1724 |
| 1267.9751                                  | 1294.5814 |           | 1314.9859 |
| 1325.9415                                  | 1344.9239 |           | 1373.3655 |
| 1379.3744                                  | 1387.6047 |           | 1394.6965 |
| 1410.8325                                  | 1420.2548 |           | 1432.0390 |
| 1447.0770                                  | 1452.8365 |           | 1469.1438 |
| 1473.4736                                  | 1482.5537 |           | 1488.5478 |
| 1623.5938                                  | 1645.4768 |           | 1860.9581 |
| 2201.6280                                  | 3045.2316 |           | 3047.4660 |
| 3053.7582                                  | 3056.2303 |           | 3063.1787 |
| 3064.5132                                  | 3077.7478 |           | 3120.4322 |
| 3129.7142                                  | 3139.0950 |           | 3142.1548 |
| 3145.9811                                  | 3147.7216 |           | 3178.2134 |
| 3180.8601                                  | 3191.8868 |           | 3834.7409 |
| Zero-point correction (Hartree): 0.270764  |           |           |           |
| TS.ApineneCI.J.a+H2O.HHP.mmpu              |           |           |           |
| ~~~~~                                      |           |           |           |
| E(RM062X/CC-pVDZ) (Hartree): -692.37247790 |           |           |           |
| Electronic state : 1-A                     |           |           |           |
| Cartesian coordinates (Angs):              |           |           |           |
| C                                          | 0.041929  | -0.789443 | 0.615639  |
| H                                          | 0.260481  | -0.814135 | 1.696194  |
| C                                          | 1.298243  | -1.179139 | -0.163487 |
| C                                          | 2.427869  | -0.297058 | 0.225264  |
| H                                          | 1.591876  | -2.208639 | 0.090517  |
| H                                          | 1.136221  | -1.112020 | -1.247747 |
| H                                          | 2.810878  | -0.297191 | 1.250597  |
| C                                          | -0.700610 | 0.546332  | 0.293338  |
| C                                          | -1.267738 | -1.561926 | 0.353480  |
| C                                          | -0.381199 | 1.734451  | 1.185140  |
| C                                          | -0.592516 | 0.934795  | -1.180767 |
| H                                          | -0.861048 | 0.102342  | -1.851195 |
| H                                          | -1.277343 | 1.764312  | -1.397414 |
| H                                          | 0.434579  | 1.249497  | -1.417072 |
| H                                          | -1.106028 | 2.542419  | 1.005427  |
| H                                          | 0.627369  | 2.124298  | 0.973969  |
| H                                          | -0.431030 | 1.458323  | 2.249854  |
| H                                          | -1.494362 | -2.419188 | 0.999804  |
| H                                          | -1.340656 | -1.874021 | -0.699243 |
| C                                          | -2.011979 | -0.230465 | 0.606663  |
| H                                          | -2.240765 | -0.141394 | 1.683730  |
| C                                          | -3.287851 | 0.110135  | -0.130469 |
| C                                          | -4.266713 | -1.020825 | -0.349270 |
| H                                          | -4.432856 | -1.569178 | 0.590296  |
| H                                          | -3.844208 | -1.738156 | -1.069855 |
| H                                          | -5.212053 | -0.625391 | -0.736374 |
| O                                          | -3.513896 | 1.240243  | -0.499577 |
| O                                          | 2.701898  | 0.709103  | -0.492301 |
| O                                          | 3.954086  | 1.239590  | -0.066590 |
| O                                          | 4.241704  | -1.225210 | -0.147703 |
| H                                          | 4.467798  | -0.203488 | -0.111478 |
| H                                          | 4.284198  | -1.429338 | -1.093831 |
| Rotational constants (GHz):                |           |           |           |
|                                            | 1.5525600 | 0.3196700 | 0.2907200 |
| Vibrational harmonic frequencies (cm-1):   |           |           |           |
| i335.8785                                  | 31.0313   |           | 40.2090   |
| 47.1036                                    | 67.6357   |           | 116.1660  |
| 135.3675                                   | 158.2288  |           | 184.3490  |
| 219.7256                                   | 233.9022  |           | 266.3243  |
| 284.3280                                   | 303.2687  |           | 316.3748  |
| 330.6024                                   | 366.7435  |           | 399.8086  |
| 404.7833                                   | 417.0811  |           | 470.5921  |
| 508.6576                                   | 527.8611  |           | 556.6422  |
| 594.2650                                   | 601.5059  |           | 617.7322  |
| 645.5472                                   | 723.4436  |           | 771.3132  |
| 856.5966                                   | 897.3051  |           | 915.5438  |
| 944.6096                                   | 955.1968  |           | 963.0471  |

|           |           |           |
|-----------|-----------|-----------|
| 977.8529  | 1003.8181 | 1016.4302 |
| 1029.4281 | 1053.6894 | 1075.2867 |
| 1107.0026 | 1122.8559 | 1151.3947 |
| 1170.0197 | 1191.0444 | 1204.5520 |
| 1231.2014 | 1237.9373 | 1258.4601 |
| 1266.6155 | 1295.6252 | 1300.9772 |
| 1316.2496 | 1343.2548 | 1361.2654 |
| 1380.8601 | 1385.0060 | 1398.4948 |
| 1407.3381 | 1432.3068 | 1444.8247 |
| 1446.3168 | 1456.2475 | 1467.1805 |
| 1472.2084 | 1482.5682 | 1488.5257 |
| 1618.4192 | 1651.9022 | 1861.7462 |
| 2456.2198 | 3047.1327 | 3049.4027 |
| 3055.9068 | 3059.0958 | 3064.0616 |
| 3079.2889 | 3086.2435 | 3129.1219 |
| 3134.6323 | 3138.6400 | 3140.2937 |
| 3146.2874 | 3149.9666 | 3171.5308 |
| 3193.1116 | 3196.1077 | 3842.0828 |

Zero-point correction (Hartree): 0.271377

TS.ApineneCI.J.a+H2O.HHP.mmtD

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E(RM062X/CC-pVDZ) (Hartree): -692.37340387

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-0.214426	-0.792344	-0.221568
H	-0.661015	-0.898982	-1.223399
C	-1.249832	-1.155179	0.830498
C	-2.524638	-0.398852	0.752214
H	-1.520304	-2.220414	0.758616
H	-0.852973	-1.008436	1.850621
H	-3.381376	-0.665689	1.377655
C	0.575348	0.560522	-0.163703
C	1.125153	-1.557296	-0.157876
C	0.152636	1.662555	-1.121907
C	0.694396	1.098197	1.259946
H	1.076880	0.340460	1.963272
H	1.388263	1.947579	1.286238
H	-0.292370	1.435920	1.613201
H	0.949504	2.420074	-1.174027
H	-0.777903	2.145689	-0.794954
H	-0.005087	1.262882	-2.136077
H	1.235484	-2.453178	-0.782153
H	1.382021	-1.813170	0.881996
C	1.820799	-0.257072	-0.613235
H	1.883915	-0.243215	-1.716039
C	3.196456	0.112014	-0.105861
C	4.198464	-1.014371	0.012226
H	4.213709	-1.610477	-0.912688
H	3.897134	-1.691659	0.826268
H	5.193020	-0.606694	0.223484
O	3.480127	1.256998	0.165102
O	-2.524897	0.755130	0.232266
O	-3.876281	1.145432	-0.004369
O	-3.712270	-1.216308	-0.728165
H	-4.068416	-0.234698	-0.611831
H	-3.240043	-1.185043	-1.573244

Rotational constants (GHz): 1.5029600 0.3457900 0.3146800

Vibrational harmonic frequencies (cm-1):

1360.8043	31.8975	40.0042
55.7997	69.4903	107.8841
127.3068	156.5575	212.3053
224.5783	235.9735	257.7354
298.1701	303.7303	314.9444
326.2995	362.5242	394.1055
401.5509	414.3501	454.6008
506.1774	522.1059	554.1752
587.3117	594.9125	616.8947
693.9530	716.5857	765.6129
845.4619	903.5916	913.1277
928.9514	956.2438	961.2623
978.4175	994.1166	1009.5814
1023.4800	1031.5907	1072.8968
1111.4480	1118.7576	1157.0170
1162.9159	1177.9853	1194.5573
1232.0168	1238.4737	1264.5420
1288.8434	1296.2141	1307.7881
1328.9505	1343.2872	1360.8810
1380.5954	1391.6502	1396.2753
1410.2470	1418.7776	1431.6108
1446.4223	1453.6864	1464.5525
1468.5693	1479.6857	1484.1594
1614.4857	1648.9753	1860.9541
2409.2814	3047.4726	3050.3560
3054.1003	3057.8419	3064.2834
3065.7176	3072.4016	3109.6256
3124.8707	3130.2090	3138.7818
3141.7380	3162.9322	3169.1902
3191.4746	3194.3933	3845.8764

Zero-point correction (Hartree): 0.270945

TS.ApineneCI.J.a+H2O.HHP.mmtu

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E(RM062X/CC-pVDZ) (Hartree): -692.37395382

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |          |          |           |
|---|----------|----------|-----------|
| C | 0.152822 | 1.008837 | -0.230319 |
| H | 0.494260 | 1.204764 | -1.257597 |
| C | 1.258113 | 1.388395 | 0.738991  |
| C | 2.592720 | 0.828490 | 0.387798  |
| H | 1.388766 | 2.485547 | 0.767181  |
| H | 1.038466 | 1.083640 | 1.773567  |

|                                            |           |           |                     |
|--------------------------------------------|-----------|-----------|---------------------|
| H                                          | 3.467263  | 1.038074  | 1.010167            |
| C                                          | -0.476433 | -0.419577 | -0.192314           |
| C                                          | -1.255302 | 1.612652  | -0.049610           |
| C                                          | 0.086649  | -1.434311 | -1.173439           |
| C                                          | -0.543913 | -0.991093 | 1.224266            |
| H                                          | -1.031386 | -0.297166 | 1.927738            |
| H                                          | -1.125943 | -1.921059 | 1.228214            |
| H                                          | 0.463740  | -1.192567 | 1.616297            |
| H                                          | -0.536526 | -2.340793 | -1.184401           |
| H                                          | 1.119409  | -1.714395 | -0.911397           |
| H                                          | 0.120362  | -1.020642 | -2.192440           |
| H                                          | -1.490900 | 2.533862  | -0.597391           |
| H                                          | -1.502111 | 1.752716  | 1.013787            |
| C                                          | -1.809929 | 0.274375  | -0.592619           |
| H                                          | -1.874531 | 0.332262  | -1.693801           |
| C                                          | -3.130737 | -0.282593 | -0.112736           |
| C                                          | -4.259750 | 0.708356  | 0.055456            |
| H                                          | -4.352615 | 1.336443  | -0.843382           |
| H                                          | -4.034888 | 1.382412  | 0.896526            |
| H                                          | -5.196955 | 0.176045  | 0.250811            |
| O                                          | -3.273072 | -1.465741 | 0.099794            |
| O                                          | 2.802853  | 0.473449  | -0.812344           |
| O                                          | 4.027336  | -0.255854 | -0.855839           |
| O                                          | 2.889527  | -1.044559 | 1.153679            |
| H                                          | 3.565115  | -0.971347 | 0.326051            |
| H                                          | 2.229883  | -1.687333 | 0.854906            |
| Rotational constants (GHz):                |           |           | 0.3563900 0.3330200 |
| Vibrational harmonic frequencies (cm-1):   |           |           |                     |
| 1422.1085                                  | 40.3052   | 53.2669   |                     |
| 83.9397                                    | 85.8014   | 118.7946  |                     |
| 137.3510                                   | 162.8443  | 193.9896  |                     |
| 227.2783                                   | 240.9705  | 271.7992  |                     |
| 289.1730                                   | 303.3920  | 319.3298  |                     |
| 330.0379                                   | 363.0141  | 398.4728  |                     |
| 400.5184                                   | 450.2623  | 473.2731  |                     |
| 504.4135                                   | 521.6442  | 584.4316  |                     |
| 595.5321                                   | 614.0257  | 630.1214  |                     |
| 686.2491                                   | 721.9765  | 771.4724  |                     |
| 851.7960                                   | 902.0810  | 918.1408  |                     |
| 936.0130                                   | 952.3314  | 960.5993  |                     |
| 972.8115                                   | 991.5652  | 1008.2639 |                     |
| 1020.5379                                  | 1029.3927 | 1093.9452 |                     |
| 1110.0207                                  | 1126.1780 | 1150.3979 |                     |
| 1169.1598                                  | 1177.7683 | 1192.9468 |                     |
| 1229.6321                                  | 1245.6990 | 1262.5974 |                     |
| 1289.1790                                  | 1298.5813 | 1312.3803 |                     |
| 1335.5988                                  | 1348.2180 | 1370.8533 |                     |
| 1383.7844                                  | 1396.3973 | 1397.0513 |                     |
| 1411.6710                                  | 1432.2436 | 1432.7258 |                     |
| 1446.8613                                  | 1455.0139 | 1460.6082 |                     |
| 1473.7889                                  | 1480.5686 | 1485.0814 |                     |
| 1604.8745                                  | 1640.1154 | 1860.8458 |                     |
| 2185.3162                                  | 3047.8107 | 3049.7928 |                     |
| 3053.6984                                  | 3064.6981 | 3065.4801 |                     |
| 3077.1572                                  | 3091.9591 | 3116.5227 |                     |
| 3130.2717                                  | 3137.7378 | 3140.1468 |                     |
| 3144.2246                                  | 3146.3067 | 3173.4476 |                     |
| 3191.9307                                  | 3201.2411 | 3847.2037 |                     |
| Zero-point correction (Hartree): 0.271232  |           |           |                     |
| TS.ApineneCI.J.a+H2O.HHP.mpmc              |           |           |                     |
| ~~~~~                                      |           |           |                     |
| E(RM062X/CC-pVDZ) (Hartree): -692.37171629 |           |           |                     |
| Electronic state : 1-A                     |           |           |                     |
| Cartesian coordinates (Angs):              |           |           |                     |
| C                                          | 0.159182  | -0.515821 | -0.595237           |
| H                                          | 0.337543  | -0.766338 | -1.653751           |
| C                                          | 1.405623  | -0.847118 | 0.227751            |
| C                                          | 2.543934  | -0.041748 | -0.279646           |
| H                                          | 1.247052  | -0.607733 | 1.287845            |
| H                                          | 1.669245  | -1.910485 | 0.131629            |
| H                                          | 3.003317  | -0.250233 | -1.250554           |
| C                                          | -1.224930 | -1.104797 | -0.172749           |
| C                                          | -0.430971 | 0.906917  | -0.494077           |
| C                                          | -1.696767 | -2.335037 | -0.928541           |
| C                                          | -1.328831 | -1.325344 | 1.334482            |
| H                                          | -1.039270 | -0.430340 | 1.907425            |
| H                                          | -2.362329 | -1.571424 | 1.608088            |
| H                                          | -0.673591 | -2.154887 | 1.643266            |
| H                                          | -2.754122 | -2.533544 | -0.697843           |
| H                                          | -1.110589 | -3.223037 | -0.642930           |
| H                                          | -1.601371 | -2.195954 | -2.016156           |
| H                                          | -0.125636 | 1.645890  | -1.245090           |
| H                                          | -0.264432 | 1.331756  | 0.507657            |
| C                                          | -1.827264 | 0.256890  | -0.623753           |
| H                                          | -2.104102 | 0.197279  | -1.691498           |
| C                                          | -3.028772 | 0.826220  | 0.097001            |
| C                                          | -3.149161 | 2.331913  | 0.124715            |
| H                                          | -3.009359 | 2.744159  | -0.885999           |
| H                                          | -2.350581 | 2.752867  | 0.754962            |
| H                                          | -4.126478 | 2.620494  | 0.526403            |
| O                                          | -3.856859 | 0.100826  | 0.600925            |
| O                                          | 2.734446  | 1.106166  | 0.217068            |
| O                                          | 4.000585  | 1.587994  | -0.225575           |
| O                                          | 4.353305  | -0.792120 | 0.410859            |
| H                                          | 4.551644  | 0.205534  | 0.171406            |
| H                                          | 4.328980  | -0.789370 | 1.379256            |
| Rotational constants (GHz):                |           |           | 0.3248000 0.2807700 |
| Vibrational harmonic frequencies (cm-1):   |           |           |                     |
| i322.7156                                  | 31.1101   | 36.9181   |                     |
| 46.4890                                    | 72.4323   | 96.1944   |                     |
| 130.9112                                   | 156.4378  | 172.4810  |                     |

|           |           |           |
|-----------|-----------|-----------|
| 218.2324  | 225.6606  | 255.8869  |
| 273.5767  | 296.7359  | 316.9911  |
| 324.6916  | 353.4442  | 397.7389  |
| 403.2221  | 429.5635  | 490.8997  |
| 496.5903  | 517.3852  | 557.1235  |
| 593.9786  | 600.5446  | 614.3262  |
| 650.4451  | 734.5705  | 800.9352  |
| 846.6684  | 898.0829  | 910.1044  |
| 929.6125  | 954.5572  | 966.1476  |
| 974.1751  | 998.8931  | 1014.8129 |
| 1023.4797 | 1037.3585 | 1083.2947 |
| 1105.5503 | 1137.1282 | 1147.9475 |
| 1171.6364 | 1191.8000 | 1212.9084 |
| 1232.2511 | 1240.6573 | 1247.8516 |
| 1275.4538 | 1292.8071 | 1301.7675 |
| 1311.1219 | 1344.4311 | 1359.6359 |
| 1378.8772 | 1382.6485 | 1395.4896 |
| 1405.4676 | 1431.5889 | 1446.0355 |
| 1448.3183 | 1452.7956 | 1463.8883 |
| 1469.9962 | 1476.9844 | 1484.9568 |
| 1619.6011 | 1652.9210 | 1859.3603 |
| 2481.9285 | 3048.2767 | 3051.0630 |
| 3054.6793 | 3064.3955 | 3065.7455 |
| 3082.6530 | 3088.6061 | 3125.3485 |
| 3128.3555 | 3141.0180 | 3141.4684 |
| 3151.2846 | 3153.7810 | 3168.1580 |
| 3192.7337 | 3199.3545 | 3843.0940 |

Zero-point correction (Hartree): 0.271231

TS.ApineneCI.J.a+H2O.HHP.mpmu  
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E(RM062X/CC-pVDZ) (Hartree): -692.37288672

Electronic state : 1-A

Cartesian coordinates (Angs):

C	0.245458	-0.505780	-0.474616
H	0.499133	-0.658803	-1.536364
C	1.406744	-0.975630	0.394019
C	2.716500	-0.456289	-0.075662
H	1.272325	-0.713733	1.452378
H	1.479394	-2.077357	0.328918
H	3.020984	-0.569852	-1.120844
C	-1.174939	-1.095647	-0.209406
C	-0.328032	0.915210	-0.295806
C	-1.609928	-2.248868	-1.097337
C	-1.393891	-1.437915	1.263412
H	-1.127217	-0.601915	1.929212
H	-2.449165	-1.678318	1.442255
H	-0.780996	-2.307158	1.548626
H	-2.683024	-2.447284	-0.956931
H	-1.056763	-3.169157	-0.849413
H	-1.437199	-2.020681	-2.160083
H	0.054758	1.696550	-0.961378
H	-0.240797	1.249092	0.751010
C	-1.721803	0.311026	-0.582898
H	-1.915462	0.350998	-1.669800
C	-2.967147	0.841424	0.090174
C	-3.068848	2.342090	0.237620
H	-2.828535	2.837318	-0.715165
H	-2.328139	2.688568	0.974979
H	-4.075126	2.616516	0.572258
O	-3.842647	0.094599	0.466513
O	3.625482	-0.222355	0.773922
O	4.663925	0.508821	0.122783
O	2.567825	1.527999	-0.641323
H	3.599358	1.368597	-0.430613
H	2.255112	2.026380	0.128790

Rotational constants (GHz): 1.2522700 0.3337600 0.2912600

Vibrational harmonic frequencies (cm-1):

i382.5793	33.3542	44.5682
52.6925	93.9827	105.3752
131.7307	160.8144	165.2345
223.4326	243.2012	264.6453
285.9969	300.6118	317.2742
323.6062	351.3539	388.2868
404.1799	446.3290	483.9695
491.1234	518.1863	569.3027
600.5139	613.0540	621.9637
633.9282	736.3284	808.2132
844.2589	901.3184	920.4066
926.4690	952.9508	960.5107
971.4109	996.9539	1015.3683
1027.7799	1044.0370	1093.7595
1103.6495	1146.7745	1148.4620
1170.4293	1190.3058	1212.0446
1231.1085	1234.0023	1241.6933
1274.2883	1291.5458	1309.4759
1327.6307	1344.1852	1375.5126
1381.4738	1389.2941	1396.5018
1413.1182	1426.9910	1431.8876
1446.6005	1451.4788	1464.1875
1475.0689	1477.8307	1486.6040
1623.9112	1639.5667	1858.8844
2238.3438	3037.8988	3045.9581
3047.0247	3054.1437	3062.6489
3065.6258	3070.6863	3123.9157
3126.1149	3135.3700	3139.2777
3140.5690	3164.9597	3168.7665
3192.4006	3193.3955	3839.1193

Zero-point correction (Hartree): 0.270827

TS.ApineneCI.J.a+H2O.HHP.mppd
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E(RM062X/CC-pVDZ) (Hartree): -692.37257000  
Electronic state : 1-A  
Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.271753  | 0.429465  | 0.333227  |
| H | 0.603637  | 0.489727  | 1.379621  |
| C | 1.401428  | 0.897878  | -0.578561 |
| C | 2.526845  | -0.071744 | -0.574411 |
| H | 1.040494  | 0.939923  | -1.620960 |
| H | 1.776399  | 1.893979  | -0.305365 |
| H | 2.362705  | -1.111741 | -0.873609 |
| C | -1.148670 | 1.065137  | 0.220070  |
| C | -0.345762 | -0.963839 | 0.096591  |
| C | -1.484164 | 2.158822  | 1.220081  |
| C | -1.482360 | 1.514923  | -1.200223 |
| H | -1.291435 | 0.725307  | -1.944581 |
| H | -2.543965 | 1.782219  | -1.271577 |
| H | -0.877524 | 2.394151  | -1.472734 |
| H | -2.562393 | 2.376280  | 1.191747  |
| H | -0.940357 | 3.088079  | 0.986797  |
| H | -1.220628 | 1.855124  | 2.244656  |
| H | 0.077177  | -1.797917 | 0.669096  |
| H | -0.357927 | -1.222891 | -0.974671 |
| C | -1.695306 | -0.355509 | 0.543827  |
| H | -1.796668 | -0.467065 | 1.638099  |
| C | -3.003529 | -0.819691 | -0.054915 |
| C | -3.153401 | -2.306711 | -0.278848 |
| H | -2.857881 | -2.860490 | 0.624966  |
| H | -2.476430 | -2.626628 | -1.086038 |
| H | -4.188011 | -2.539865 | -0.552878 |
| O | -3.887837 | -0.034554 | -0.314768 |
| O | 3.718032  | 0.360447  | -0.601065 |
| O | 4.588312  | -0.735486 | -0.318462 |
| O | 2.746499  | -0.951325 | 1.271597  |
| H | 3.693740  | -1.066112 | 0.782216  |
| H | 2.918016  | -0.257121 | 1.925767  |

Rotational constants (GHz): 1.2750600 0.3250900 0.2937800  
Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i406.8895 | 36.8841   | 43.6954   |
| 47.7212   | 88.4085   | 97.8018   |
| 126.7215  | 154.6624  | 179.9533  |
| 221.5744  | 247.3453  | 262.6041  |
| 285.9385  | 300.8156  | 318.2551  |
| 326.1706  | 349.0105  | 391.6472  |
| 404.3769  | 445.6391  | 489.6025  |
| 504.0524  | 520.1981  | 566.9508  |
| 598.6383  | 607.8194  | 622.7416  |
| 635.9514  | 736.8855  | 795.9235  |
| 861.8017  | 906.4813  | 919.7399  |
| 934.8170  | 951.1502  | 956.1890  |
| 971.4053  | 991.0468  | 1014.8450 |
| 1031.9420 | 1039.7155 | 1096.5318 |
| 1108.7375 | 1147.8030 | 1156.1253 |
| 1172.2944 | 1184.5368 | 1205.1275 |
| 1228.9654 | 1237.3053 | 1252.5519 |
| 1276.3394 | 1295.1096 | 1305.4028 |
| 1324.3525 | 1344.0678 | 1377.6786 |
| 1381.8552 | 1387.9722 | 1395.3472 |
| 1407.4956 | 1432.1432 | 1436.3500 |
| 1446.1244 | 1451.7339 | 1463.8116 |
| 1472.5466 | 1477.2545 | 1485.5929 |
| 1623.0174 | 1640.8596 | 1859.1930 |
| 2165.6878 | 3046.6909 | 3049.1733 |
| 3052.6149 | 3056.7759 | 3065.1672 |
| 3066.7545 | 3097.2277 | 3121.8838 |
| 3127.0235 | 3132.7135 | 3139.1802 |
| 3140.7938 | 3154.3418 | 3167.9952 |
| 3186.7254 | 3192.5348 | 3837.9282 |

Zero-point correction (Hartree): 0.270789

TS.ApineneCI.J.a+H2O.HHP.mppu  
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E(RM062X/CC-pVDZ) (Hartree): -692.37088240
Electronic state : 1-A
Cartesian coordinates (Angs):

C	-0.161178	0.377538	-0.481267
H	-0.411550	0.644046	-1.520214
C	-1.383531	0.611892	0.405970
C	-2.504638	-0.249553	-0.044862
H	-1.162839	0.333862	1.446849
H	-1.701234	1.663817	0.373631
H	-2.421891	-1.340496	-0.013601
C	1.198095	1.048936	-0.106411
C	0.534265	-1.002683	-0.458145
C	1.542101	2.335814	-0.836446
C	1.365543	1.222191	1.401311
H	1.166723	0.290140	1.953792
H	2.393011	1.529009	1.633059
H	0.673486	1.993118	1.774454
H	2.594102	2.600717	-0.652861
H	0.911853	3.168702	-0.486425
H	1.396887	2.228976	-1.922066
H	0.247686	-1.739458	-1.219296
H	0.462566	-1.467571	0.537745
C	1.871118	-0.248368	-0.639100
H	2.079649	-0.134116	-1.717729
C	3.149880	-0.750849	-0.007161
C	3.382026	-2.243539	-0.043189
H	3.210127	-2.632392	-1.058194
H	2.658871	-2.744104	0.619212
H	4.401191	-2.469994	0.288214
O	3.950117	0.016924	0.478125
O	-3.388424	0.243509	-0.804379

O	-4.475111	-0.675498	-0.882574
O	-3.826863	-0.589694	1.505723
H	-4.384857	-0.763911	0.632173
H	-4.153610	0.269463	1.811895
Rotational constants (GHz):	1.2857300	0.2976800	0.2777500
Vibrational harmonic frequencies (cm-1):			
i346.8890	28.4164		36.4380
45.1704	72.0505		93.2054
130.5416	154.9878		185.5744
223.1281	231.2797		258.0566
265.5074	290.8636		316.4970
322.6466	353.5916		396.9190
412.1720	421.6329		493.7945
501.6118	517.8534		566.5202
593.0314	602.2510		617.8254
651.8622	736.6008		798.6454
849.0963	898.9602		912.4955
932.9284	954.9183		963.6913
971.2237	992.6564		1016.1565
1030.1831	1036.7118		1090.1947
1108.7047	1142.7314		1161.2002
1169.8110	1188.0857		1205.7093
1229.8695	1243.3436		1252.7027
1276.0997	1294.6006		1308.9041
1314.7633	1342.1761		1362.3126
1380.5459	1383.4988		1397.0427
1405.1173	1432.0086		1444.9373
1446.8009	1452.8101		1463.9818
1470.2413	1477.5573		1485.2644
1624.4883	1651.5425		1860.1004
2401.4334	3048.9602		3050.1329
3054.1368	3065.9029		3070.4131
3077.1985	3084.5052		3124.5366
3129.7953	3140.8644		3141.0514
3144.3596	3147.1078		3166.9514
3191.2732	3193.3512		3838.1009
Zero-point correction (Hartree):	0.271136		

TS.ApineneCI.J.a+H2O.HHP.mptd

E(RM062X/CC-pVDZ) (Hartree): -692.37351013

Electronic state : 1-A

Cartesian coordinates (Angs):

C	0.326202	-0.688762	-0.307858
H	0.634224	-0.976799	-1.324066
C	1.400765	-1.101458	0.681235
C	2.733001	-0.513764	0.380467
H	1.154111	-0.799284	1.710236
H	1.530454	-2.198782	0.700690
H	3.574156	-0.634357	1.069134
C	-1.151316	-1.134736	-0.082110
C	-0.139925	0.784028	-0.322664
C	-1.623163	-2.346962	-0.866819
C	-1.496492	-1.283182	1.398540
H	-1.204472	-0.398333	1.986335
H	-2.578108	-1.418783	1.522555
H	-0.979972	-2.157974	1.823616
H	-2.716982	-2.439996	-0.792794
H	-1.172812	-3.272082	-0.472903
H	-1.354279	-2.261434	-1.930527
H	0.341475	1.464138	-1.038022
H	-0.103515	1.220170	0.688770
C	-1.554569	0.255233	-0.653089
H	-1.665800	0.180606	-1.749405
C	-2.795442	0.952014	-0.142680
C	-2.781324	2.462991	-0.163677
H	-2.441006	2.828436	-1.144308
H	-2.063404	2.833544	0.584442
H	-3.780832	2.848279	0.065197
O	-3.754530	0.319638	0.239236
O	3.002231	-0.176780	-0.809949
O	4.181344	0.626658	-0.789962
O	2.784761	1.425484	1.082866
H	3.534218	1.383370	0.341186
H	2.075665	1.926863	0.654262
Rotational constants (GHz):	1.1425100	0.3676400	0.3186400
Vibrational harmonic frequencies (cm-1):			
i374.7160	35.3840		47.7889
59.1842	89.8232		105.6999
132.6436	157.6458		164.1440
223.2585	244.1413		266.8595
282.5124	295.6827		315.8041
325.3239	354.5340		390.7644
404.6088	431.0987		474.5965
500.8686	516.0942		564.5304
594.5097	604.2233		618.6775
681.1346	740.3577		809.5082
828.9545	901.1984		923.4481
935.0495	953.6719		959.6698
972.6648	997.3172		998.2155
1021.7328	1037.7419		1055.7261
1099.7244	1128.9577		1156.2551
1170.8294	1187.3128		1203.5767
1230.2178	1240.2787		1255.2417
1290.5131	1303.9261		1313.4132
1332.0596	1344.8452		1361.3285
1381.8293	1392.6751		1397.4873
1411.7187	1431.1428		1432.8873
1446.5680	1452.2993		1464.1331
1477.4488	1480.6606		1486.1392
1614.9547	1648.7176		1859.6543
2352.4383	3047.5120		3050.2523

3052.1027	3054.2717	3063.5982
3065.0445	3092.4908	3120.3672
3123.6744	3127.9480	3137.7440
3139.7398	3140.7068	3167.2593
3192.5264	3193.1138	3849.2745

Zero-point correction (Hartree): 0.271065

TS.ApineneCI.J.a+H2O.HHP.mptu

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E(RM062X/CC-pVDZ) (Hartree): -692.37278609

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.334681 | 0.359582  | -0.155895 |
| H | -0.771198 | 0.508289  | -1.157239 |
| C | -1.377652 | 0.697404  | 0.893952  |
| C | -2.647195 | -0.060003 | 0.741040  |
| H | -1.005045 | 0.496879  | 1.913676  |
| H | -1.652435 | 1.764151  | 0.870275  |
| H | -3.500564 | 0.127723  | 1.398942  |
| C | 1.058342  | 1.061316  | -0.108129 |
| C | 0.372694  | -1.012003 | -0.113096 |
| C | 1.248500  | 2.258404  | -1.024088 |
| C | 1.487938  | 1.402463  | 1.317817  |
| H | 1.406439  | 0.537575  | 1.995293  |
| H | 2.534855  | 1.729940  | 1.328785  |
| H | 0.860164  | 2.212271  | 1.721544  |
| H | 2.311366  | 2.540945  | -1.058176 |
| H | 0.674162  | 3.126941  | -0.663681 |
| H | 0.919267  | 2.031078  | -2.049501 |
| H | -0.047121 | -1.817588 | -0.726082 |
| H | 0.480399  | -1.370393 | 0.922706  |
| C | 1.647968  | -0.289535 | -0.604823 |
| H | 1.664955  | -0.296032 | -1.709477 |
| C | 3.023555  | -0.726583 | -0.155819 |
| C | 3.268494  | -2.216056 | -0.084619 |
| H | 2.935825  | -2.701950 | -1.014241 |
| H | 2.671233  | -2.648067 | 0.733189  |
| H | 4.331685  | -2.411087 | 0.092793  |
| O | 3.884482  | 0.083283  | 0.107453  |
| O | -2.638204 | -1.152034 | 0.099267  |
| O | -3.988897 | -1.523667 | -0.169656 |
| O | -3.848394 | 0.898474  | -0.629851 |
| H | -4.194453 | -0.096879 | -0.620177 |
| H | -3.379194 | 0.967821  | -1.474364 |

Rotational constants (GHz): 1.2408800 0.3424300 0.2977700

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i370.6569 | 34.3442   | 46.8134   |
| 49.4881   | 87.3948   | 92.7924   |
| 132.2861  | 155.3445  | 179.1894  |
| 216.4262  | 240.7089  | 255.5881  |
| 282.4015  | 305.0360  | 318.2268  |
| 324.1312  | 352.0513  | 397.4774  |
| 404.3972  | 426.2302  | 480.1704  |
| 500.9737  | 518.2842  | 557.0186  |
| 593.1539  | 601.1487  | 617.9284  |
| 683.7154  | 737.8637  | 803.4372  |
| 832.0812  | 905.5557  | 919.9155  |
| 931.5550  | 952.9826  | 960.8694  |
| 973.0730  | 997.2730  | 1002.3630 |
| 1020.0258 | 1042.4620 | 1052.6513 |
| 1105.4636 | 1129.4005 | 1153.1977 |
| 1170.7002 | 1190.2244 | 1204.5907 |
| 1229.7143 | 1239.5538 | 1254.2114 |
| 1290.1611 | 1305.1917 | 1312.4224 |
| 1325.7413 | 1346.5277 | 1364.4964 |
| 1381.7954 | 1392.2005 | 1396.6469 |
| 1410.2166 | 1425.5220 | 1432.5277 |
| 1446.4289 | 1451.7920 | 1464.2155 |
| 1471.9294 | 1477.3734 | 1485.3417 |
| 1612.0335 | 1645.5127 | 1858.8203 |
| 2372.3942 | 3046.7598 | 3049.5785 |
| 3052.7851 | 3058.5888 | 3064.7873 |
| 3065.2896 | 3078.6177 | 3108.9967 |
| 3123.3169 | 3126.1619 | 3140.0390 |
| 3140.3081 | 3160.6385 | 3167.1972 |
| 3192.1382 | 3204.1583 | 3842.4526 |

Zero-point correction (Hartree): 0.270995

TS.ApineneCI.J.a+H2O.HHP.mtmd

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E(RM062X/CC-pVDZ) (Hartree): -692.36902029

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-0.001968	0.708558	-1.197412
H	0.255680	1.337853	-2.063613
C	-1.520761	0.786600	-1.030684
C	-2.115368	-0.167276	-0.055995
H	-1.837207	1.804523	-0.758434
H	-1.992363	0.533617	-1.994067
H	-1.803646	-1.214687	-0.016328
C	0.976522	1.082482	-0.041195
C	0.728469	-0.644909	-1.355184
C	1.485550	2.513682	-0.020555
C	0.456008	0.680168	1.337118
H	0.114490	-0.367551	1.373231
H	1.255214	0.785621	2.082059
H	-0.390442	1.317085	1.632885
H	2.319411	2.603497	0.691401
H	0.691192	3.209866	0.292258
H	1.844799	2.824132	-1.013674
H	0.867612	-1.035312	-2.371182
H	0.286275	-1.433502	-0.729082

C	1.933889	0.017046	-0.649141
H	2.581216	0.497637	-1.404138
C	2.851233	-0.769591	0.260784
C	3.152849	-2.195367	-0.138019
H	3.427616	-2.245948	-1.202399
H	2.248784	-2.810688	-0.009433
H	3.958154	-2.594500	0.488113
O	3.331928	-0.258187	1.246908
O	-2.723632	0.294009	0.958297
O	-3.455173	-0.773801	1.553150
O	-3.800351	-0.998886	-0.856254
H	-3.916617	-1.107326	0.199635
H	-4.410888	-0.277753	-1.072334
Rotational constants (GHz): 1.0843300 0.3597000 0.3434300			
Vibrational harmonic frequencies (cm-1):			
i408.2169	35.9646		44.4352
53.3522	72.6726		128.7619
141.5289	154.0971		175.3915
232.3352	242.0828		263.6556
272.1261	287.4162		316.0144
349.1709	360.7126		403.3705
413.8753	438.5870		479.1791
513.3019	542.4612		587.7959
602.4182	605.0810		617.8774
675.9976	721.0842		758.4794
845.6944	899.9070		917.7133
928.6382	950.2946		953.6948
972.1012	987.1749		1010.4310
1026.7232	1036.2538		1098.0117
1126.2958	1141.4002		1153.7211
1170.8566	1185.4008		1206.3624
1234.1111	1237.9679		1257.4401
1295.5515	1299.4328		1311.6196
1321.5051	1343.1103		1370.3583
1381.2052	1395.8279		1396.3207
1410.1636	1429.4346		1431.8305
1446.3987	1452.6986		1464.9403
1472.7514	1476.5128		1490.5645
1614.0925	1646.5993		1860.0021
2220.6393	3047.9172		3050.2690
3055.6994	3065.5578		3066.2057
3076.8560	3088.7125		3127.8444
3128.9551	3131.2446		3140.7367
3140.8767	3149.9324		3166.0277
3193.3790	3200.0157		3834.0999
Zero-point correction (Hartree): 0.271160			
TS.ApineneCI.J.a+H2O.HHP.mtput			
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E(RM062X/CC-pVDZ) (Hartree): -692.36965739			
Electronic state : 1-A			
Cartesian coordinates (Angs):			
C	0.058388	0.945721	1.027306
H	-0.184058	1.658878	1.830884
C	1.572442	1.063108	0.792395
C	2.142479	0.080233	-0.171091
H	1.822403	2.071163	0.432094
H	2.082972	0.909334	1.754753
H	2.252739	0.296301	-1.235577
C	-0.986294	1.153391	-0.111818
C	-0.598083	-0.410291	1.364919
C	-1.565755	2.550632	-0.255413
C	-0.514448	0.628768	-1.466620
H	-0.117814	-0.397972	-1.406210
H	-1.352537	0.614478	-2.175293
H	0.271435	1.283550	-1.875634
H	-2.434007	2.527371	-0.930668
H	-0.822113	3.246542	-0.675898
H	-1.896030	2.947027	0.716784
H	-0.677528	-0.685327	2.424321
H	-0.130169	-1.237778	0.814254
C	-1.862580	0.115510	0.648548
H	-2.507159	0.644543	1.372681
C	-2.769684	-0.806998	-0.135650
C	-2.969309	-2.198969	0.414592
H	-3.194064	-2.157346	1.491001
H	-2.035150	-2.771234	0.303268
H	-3.775075	-2.703097	-0.129836
O	-3.317975	-0.424090	-1.145140
O	2.204669	-1.137254	0.175445
O	3.054000	-1.821237	-0.745263
O	4.194878	0.319002	-0.219954
H	4.030964	-0.661902	-0.552561
H	4.537677	0.197474	0.677938
Rotational constants (GHz): 1.0801400 0.3902200 0.3407300			
Vibrational harmonic frequencies (cm-1):			
i342.4130	35.7095		36.9247
54.3561	79.0714		118.9162
133.9401	154.6305		171.4241
231.3639	231.7625		255.3491
270.9194	295.7234		314.3583
347.3014	376.2673		401.1633
404.3719	440.6907		472.0829
513.8459	529.2743		567.9436
591.5929	599.1643		618.5785
702.8247	726.8748		753.1972
836.2729	899.3937		915.4275
925.7695	954.4175		966.8185
976.5313	990.4520		1008.8630
1026.2699	1051.0964		1071.3788
1102.4054	1132.7713		1159.4971
1170.7553	1188.5672		1216.6507

1232.2021	1237.1492	1257.9200
1297.1704	1297.7811	1307.5512
1322.5461	1340.4927	1353.4374
1381.3250	1386.1870	1394.6691
1406.4412	1431.4658	1445.2597
1449.1274	1454.4172	1464.5675
1476.3900	1481.8352	1490.2765
1610.4636	1649.9999	1858.4119
2433.3943	3046.0261	3048.2460
3051.0277	3065.5784	3068.7873
3082.9418	3096.4178	3121.7295
3126.0439	3137.8579	3140.9794
3141.4900	3157.8183	3162.2739
3193.8217	3218.1894	3842.0836

Zero-point correction (Hartree): 0.271523

TS.ApineneCI.J.a+H2O.HHP.mttd
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 E(RM062X/CC-pVDZ) (Hartree): -692.36855254  
 Electronic state : 1-A  
 Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.098356  | 0.939793  | 1.194205  |
| H | -0.233419 | 1.674843  | 1.944936  |
| C | 1.621373  | 1.063880  | 1.142064  |
| C | 2.477969  | -0.017538 | 0.575127  |
| H | 1.919527  | 1.981889  | 0.607183  |
| H | 2.010413  | 1.199912  | 2.166976  |
| H | 3.559230  | 0.050340  | 0.726735  |
| C | -0.809160 | 1.155170  | -0.056826 |
| C | -0.636655 | -0.391011 | 1.485299  |
| C | -1.346230 | 2.562554  | -0.261731 |
| C | -0.194832 | 0.634784  | -1.353279 |
| H | 0.235289  | -0.372596 | -1.239028 |
| H | -0.958379 | 0.594257  | -2.140781 |
| H | 0.595075  | 1.332471  | -1.676879 |
| H | -2.123291 | 2.556638  | -1.040722 |
| H | -0.545408 | 3.249157  | -0.580864 |
| H | -1.789964 | 2.959341  | 0.663991  |
| H | -0.858963 | -0.622297 | 2.534910  |
| H | -0.136363 | -1.248812 | 1.022682  |
| C | -1.788522 | 0.141713  | 0.604151  |
| H | -2.514367 | 0.693631  | 1.227257  |
| C | -2.602201 | -0.782636 | -0.274279 |
| C | -2.872697 | -2.170165 | 0.256668  |
| H | -3.209965 | -2.122710 | 1.302997  |
| H | -1.937274 | -2.750984 | 0.246234  |
| H | -3.620313 | -2.669244 | -0.369290 |
| O | -3.026489 | -0.404589 | -1.343852 |
| O | 2.012502  | -1.169580 | 0.318371  |
| O | 3.007450  | -1.907232 | -0.391553 |
| O | 3.059577  | 0.352728  | -1.347942 |
| H | 3.215064  | -0.686547 | -1.218630 |
| H | 2.284369  | 0.390828  | -1.926301 |

Rotational constants (GHz): 0.9652800 0.4450300 0.3954000  
 Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i390.3781 | 32.5712   | 47.2339   |
| 55.0354   | 117.2432  | 129.4006  |
| 144.7945  | 158.4125  | 174.4141  |
| 223.3235  | 230.9834  | 255.8531  |
| 272.0925  | 284.8895  | 314.0442  |
| 334.2584  | 361.8737  | 390.5265  |
| 405.0559  | 437.8205  | 466.8485  |
| 514.0906  | 525.8968  | 581.0146  |
| 598.7333  | 602.4656  | 618.7154  |
| 717.2184  | 721.1303  | 745.2997  |
| 842.8734  | 900.8514  | 917.8633  |
| 937.7315  | 949.3909  | 963.5172  |
| 972.2448  | 980.9810  | 1004.4933 |
| 1018.7798 | 1039.7356 | 1058.7337 |
| 1136.8229 | 1139.4567 | 1158.6621 |
| 1176.7782 | 1191.0705 | 1217.9514 |
| 1233.3822 | 1244.9406 | 1262.2571 |
| 1302.8829 | 1312.5646 | 1320.1212 |
| 1342.3026 | 1355.3232 | 1374.3463 |
| 1380.9383 | 1390.0957 | 1400.3840 |
| 1405.7706 | 1418.1444 | 1431.9742 |
| 1445.1502 | 1456.7885 | 1462.3599 |
| 1478.0811 | 1483.2982 | 1490.9665 |
| 1611.9459 | 1647.8042 | 1857.0519 |
| 2320.9907 | 3044.4770 | 3047.5506 |
| 3048.0277 | 3050.3949 | 3064.1461 |
| 3068.6581 | 3092.9692 | 3107.8095 |
| 3124.4956 | 3128.8735 | 3138.0296 |
| 3139.4018 | 3161.7141 | 3183.1572 |
| 3191.4037 | 3193.1773 | 3856.3575 |

Zero-point correction (Hartree): 0.271420

TS.ApineneCI.J.a+H2O.HHP.mttu  
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 E(RM062X/CC-pVDZ) (Hartree): -692.36909566
 Electronic state : 1-A
 Cartesian coordinates (Angs):

C	-0.203189	1.095435	-0.853740
H	0.022896	1.698571	-1.746564
C	-1.578360	1.550163	-0.355945
C	-2.461237	0.554156	0.306659
H	-1.469217	2.397154	0.346624
H	-2.182093	1.934605	-1.190859
H	-3.531035	0.757730	0.413740
C	1.067777	1.155495	0.049059
C	0.124788	-0.379317	-1.189910
C	1.899897	2.422859	-0.053584

C	0.802919	0.807360	1.511653
H	0.292042	-0.158022	1.627663
H	1.755230	0.756928	2.056509
H	0.174770	1.578914	1.985571
H	2.873672	2.268278	0.434139
H	1.396458	3.267282	0.444710
H	2.079813	2.700602	-1.103430
H	-0.043363	-0.710022	-2.224523
H	-0.355076	-1.078833	-0.492937
C	1.577895	-0.072129	-0.763581
H	2.162017	0.280108	-1.631112
C	2.436670	-1.092369	-0.047119
C	2.150892	-2.551996	-0.305097
H	2.030942	-2.739394	-1.382712
H	1.198882	-2.822976	0.178370
H	2.956421	-3.167902	0.109229
O	3.317848	-0.725927	0.697858
O	-1.988380	-0.373688	1.024442
O	-3.008166	-1.351838	1.231747
O	-3.147379	-0.732838	-1.169999
H	-3.265481	-1.267638	-0.279243
H	-2.396574	-1.159005	-1.607931
Rotational constants (GHz):			
	0.9751000	0.4575100	0.3904800
Vibrational harmonic frequencies (cm-1):			
i347.0184	20.8860		53.6581
62.6950	73.9934		123.8315
145.2158	160.8185		164.5531
221.9440	228.2145		257.4089
274.1857	303.4093		308.8100
320.9216	356.2494		374.4512
416.4945	427.0871		469.7294
504.7862	531.7517		558.0664
580.4107	597.9088		612.9271
711.9290	724.3772		745.3155
833.5458	896.6227		923.1960
937.6351	949.7226		955.6618
977.8204	982.5501		1003.8571
1017.7688	1033.2858		1049.4147
1096.3466	1137.5502		1161.5662
1172.2118	1189.3042		1212.2544
1231.5822	1242.1692		1258.6659
1298.4139	1300.8900		1316.3183
1339.2009	1343.7606		1372.2536
1379.3762	1393.2503		1399.9755
1404.5275	1415.6878		1432.0388
1444.8211	1450.1841		1463.3949
1476.6257	1481.5044		1487.0013
1619.5655	1639.1071		1858.8017
2478.8462	3045.1642		3045.4405
3058.9744	3060.9195		3063.3107
3073.1246	3084.8405		3119.9555
3123.8363	3138.6840		3140.0111
3142.5785	3156.8868		3169.2192
3192.2504	3192.4999		3852.2005
Zero-point correction (Hartree): 0.271216			
TS.ApineneCI.J.a+H2O.HHP.pmmd			
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E(RM062X/CC-pVDZ) (Hartree): -692.37572649			
Electronic state : 1-A			
Cartesian coordinates (Angs):			
C	-0.103402	-0.809450	-0.699609
H	-0.370894	-0.703361	-1.764321
C	-1.333363	-1.255637	0.075328
C	-2.560375	-0.491103	-0.280999
H	-1.558149	-2.308932	-0.173174
H	-1.184052	-1.224179	1.164608
H	-2.623400	0.066265	-1.222011
C	0.714098	0.451448	-0.276435
C	1.180094	-1.652160	-0.584183
C	0.423852	1.726125	-1.051344
C	0.671666	0.706961	1.226567
H	0.898811	-0.195391	1.812754
H	1.412657	1.471956	1.506376
H	-0.321263	1.083856	1.505854
H	1.156268	2.512365	-0.807048
H	-0.578052	2.099855	-0.789386
H	0.465536	1.548087	-2.136971
H	1.346569	-2.430935	-1.338583
H	1.309391	-2.082043	0.419086
C	2.000579	-0.358639	-0.696125
H	2.264215	-0.110136	-1.735455
C	3.202090	-0.208484	0.208247
C	4.129774	0.944560	-0.093625
H	3.549607	1.873649	-0.206369
H	4.636546	0.764416	-1.054136
H	4.872476	1.050634	0.704572
O	3.379240	-0.948524	1.149904
O	-3.650920	-0.777357	0.293902
O	-4.596145	0.245224	-0.017726
O	-2.530094	1.439158	0.496914
H	-3.560255	1.209507	0.299686
H	-2.482738	1.384663	1.463637
Rotational constants (GHz):			
	1.5545700	0.3263300	0.3036900
Vibrational harmonic frequencies (cm-1):			
i405.6433	27.4290		53.0766
62.3900	88.4266		134.9367
136.8921	160.9426		177.3298
233.8176	257.5161		270.2009
282.5578	297.9599		315.6177
323.8760	366.2739		381.7261
412.7415	425.4179		453.1144

491.1596	565.7778	583.5096
592.6514	606.6898	620.9859
624.7223	717.8529	783.3394
854.4879	905.5012	919.8837
938.9553	955.9054	962.0321
974.4378	988.6825	1007.4654
1032.2356	1076.2703	1082.7628
1116.1335	1121.3140	1158.9535
1169.3169	1187.6947	1189.4331
1206.7059	1249.3781	1257.7615
1266.1870	1287.5226	1320.2921
1326.9766	1351.6624	1377.1996
1385.4286	1391.1398	1399.6675
1412.7436	1419.9017	1432.0473
1446.1630	1450.1032	1468.0672
1472.1028	1478.5385	1486.5433
1624.5582	1647.8952	1861.1164
2140.1885	3044.4628	3051.7672
3056.8477	3062.4047	3063.5756
3086.2027	3091.7858	3122.2039
3123.4166	3135.8047	3138.2233
3142.7501	3155.9940	3165.4130
3183.4239	3193.4335	3834.9887

Zero-point correction (Hartree): 0.270881

TS.ApineneCI.J.a+H2O.HHP.pmmu

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E(RM062X/CC-pVDZ) (Hartree): -692.37589605

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.178769 | -0.497482 | -0.747975 |
| H | -0.578902 | 0.044476  | -1.616025 |
| C | -1.305024 | -1.288160 | -0.088743 |
| C | -2.411781 | -0.425355 | 0.401309  |
| H | -1.717839 | -2.038674 | -0.777530 |
| H | -0.910995 | -1.822441 | 0.793212  |
| H | -2.227505 | 0.368732  | 1.131476  |
| C | 0.687284  | 0.495943  | 0.088371  |
| C | 1.101629  | -1.258336 | -1.138558 |
| C | 0.342553  | 1.969204  | -0.055737 |
| C | 0.807470  | 0.096522  | 1.557156  |
| H | 1.100245  | -0.955975 | 1.681725  |
| H | 1.574982  | 0.707123  | 2.057774  |
| H | -0.141125 | 0.266416  | 2.089484  |
| H | 1.106969  | 2.600110  | 0.425701  |
| H | -0.632386 | 2.193105  | 0.401628  |
| H | 0.272742  | 2.255046  | -1.115759 |
| H | 1.181800  | -1.622106 | -2.170107 |
| H | 1.333872  | -2.077383 | -0.443266 |
| C | 1.918313  | -0.014219 | -0.757113 |
| H | 2.080670  | 0.666126  | -1.606576 |
| C | 3.205395  | -0.226053 | 0.007158  |
| C | 4.119830  | 0.969946  | 0.128553  |
| H | 3.548512  | 1.847519  | 0.469001  |
| H | 4.528913  | 1.218905  | -0.862692 |
| H | 4.937461  | 0.750968  | 0.823885  |
| O | 3.460990  | -1.287783 | 0.529857  |
| O | -3.605878 | -0.833066 | 0.281089  |
| O | -4.475285 | 0.261443  | 0.567456  |
| O | -2.709031 | 1.199550  | -0.831191 |
| H | -3.633706 | 1.061836  | -0.301648 |
| H | -2.911478 | 0.883018  | -1.724501 |

Rotational constants (GHz): 1.5748500 0.3274700 0.3085200

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i413.9513 | 45.7783   | 48.1792   |
| 58.4512   | 67.7020   | 121.8201  |
| 130.7392  | 158.5241  | 206.2197  |
| 215.5148  | 239.7899  | 276.4406  |
| 278.1210  | 307.4557  | 312.1064  |
| 326.8882  | 368.0276  | 380.7231  |
| 411.9306  | 429.7853  | 451.4666  |
| 512.9658  | 558.6182  | 581.8273  |
| 596.3800  | 610.3276  | 618.8297  |
| 629.5076  | 721.9876  | 787.0782  |
| 868.8742  | 905.0438  | 920.9911  |
| 945.7168  | 951.8582  | 962.4372  |
| 975.7428  | 987.0812  | 1002.8812 |
| 1030.3072 | 1073.6172 | 1086.6183 |
| 1112.6264 | 1123.3582 | 1153.2359 |
| 1166.9913 | 1184.0059 | 1200.8332 |
| 1208.9364 | 1247.2220 | 1260.2587 |
| 1262.6756 | 1291.6408 | 1301.5481 |
| 1332.1125 | 1350.3523 | 1378.5387 |
| 1386.9862 | 1390.9701 | 1403.6981 |
| 1407.6629 | 1431.0679 | 1433.6802 |
| 1445.9204 | 1448.6712 | 1456.2270 |
| 1470.4472 | 1473.7201 | 1478.0530 |
| 1621.3757 | 1634.1529 | 1859.8510 |
| 2137.6819 | 3051.3531 | 3054.9409 |
| 3057.8013 | 3062.5845 | 3089.2740 |
| 3093.7096 | 3102.5379 | 3126.2973 |
| 3129.0917 | 3132.3873 | 3137.7278 |
| 3145.2259 | 3146.5568 | 3159.3981 |
| 3189.8992 | 3193.7830 | 3837.4034 |

Zero-point correction (Hartree): 0.270940

TS.ApineneCI.J.a+H2O.HHP.pmpd

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E(RM062X/CC-pVDZ) (Hartree): -692.37713112

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-0.232298	0.949877	0.544461

H	-0.625074	0.792663	1.559956
C	-1.328345	1.599575	-0.296618
C	-2.574490	0.780623	-0.371194
H	-1.578218	2.588205	0.111081
H	-0.975972	1.742329	-1.332152
H	-3.570052	1.199085	-0.199655
C	0.474096	-0.359189	0.075386
C	1.142405	1.634784	0.644851
C	-0.056697	-1.656710	0.666715
C	0.611129	-0.463304	-1.442179
H	1.021946	0.456556	-1.883564
H	1.301662	-1.280548	-1.703663
H	-0.361514	-0.683177	-1.901748
H	0.607797	-2.502789	0.429736
H	-1.051274	-1.894739	0.255547
H	-0.126182	-1.590480	1.765683
H	1.306008	2.322583	1.483174
H	1.445518	2.121083	-0.292664
C	1.779838	0.238840	0.729002
H	1.869452	-0.123450	1.764773
C	3.069218	0.008414	-0.026253
C	3.787545	-1.291167	0.251186
H	3.084583	-2.134698	0.169248
H	4.166043	-1.287285	1.284885
H	4.620218	-1.418107	-0.449175
O	3.475313	0.808352	-0.838627
O	-2.514976	-0.326861	-0.986932
O	-3.669584	-1.099408	-0.668379
O	-2.975982	-0.085345	1.464250
H	-3.456714	-0.705868	0.758559
H	-2.230793	-0.625732	1.765331
Rotational constants (GHz): 1.3977100 0.3774600 0.3586700			
Vibrational harmonic frequencies (cm-1):			
i378.0626	56.2634		63.1041
77.1440	81.8865		129.2759
132.2077	156.4397		222.9608
237.6609	269.4284		281.9763
289.6870	304.5332		314.5786
335.2342	377.2168		380.5552
411.4405	432.8255		455.6669
504.5667	572.4404		576.3875
592.1269	602.1341		622.7933
674.0467	716.1878		782.6768
857.0584	907.7154		927.5259
952.7620	955.2660		963.9697
974.3800	993.6060		1018.7735
1026.6511	1050.2931		1057.5275
1114.3355	1124.3500		1152.5224
1161.8439	1178.9677		1188.0485
1205.0234	1251.6398		1261.1196
1274.7400	1299.2996		1309.2563
1340.4662	1350.2949		1370.5035
1376.4447	1388.7287		1401.7157
1406.7165	1431.6522		1437.3354
1446.5181	1457.1014		1473.5546
1474.5291	1480.9755		1490.9910
1602.8266	1650.0600		1862.6575
2344.4461	3034.6737		3061.2126
3062.7900	3070.0537		3084.3768
3093.3046	3097.5986		3112.7431
3129.2200	3133.4678		3138.2801
3138.7759	3161.8867		3166.8140
3192.2246	3203.4872		3847.3306
Zero-point correction (Hartree): 0.271958			
TS.ApineneCI.J.a+H2O.HHP.pmpu			
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E(RM062X/CC-pVDZ) (Hartree): -692.37591270			
Electronic state : 1-A			
Cartesian coordinates (Angs):			
C	-0.071780	-0.738471	-0.791286
H	-0.317225	-0.566739	-1.852438
C	-1.333229	-1.182784	-0.048191
C	-2.423258	-0.202140	-0.279157
H	-1.675196	-2.151031	-0.442437
H	-1.145553	-1.284089	1.029155
H	-2.863098	-0.076123	-1.273434
C	0.746875	0.482863	-0.271796
C	1.194948	-1.609022	-0.693451
C	0.492198	1.800886	-0.984973
C	0.663976	0.655190	1.243141
H	0.883256	-0.279930	1.778869
H	1.399616	1.401945	1.580758
H	-0.335185	1.009501	1.534968
H	1.215854	2.569414	-0.670186
H	-0.515215	2.178072	-0.746254
H	0.569197	1.684849	-2.076744
H	1.370908	-2.339939	-1.491782
H	1.290538	-2.102560	0.283607
C	2.033420	-0.320983	-0.703421
H	2.332059	-0.015627	-1.717896
C	3.211000	-0.243928	0.241692
C	4.148966	0.924583	0.051172
H	3.575024	1.862341	-0.008692
H	4.682685	0.812889	-0.905166
H	4.868921	0.968110	0.875616
O	3.362437	-1.054293	1.127929
O	-2.589073	0.743022	0.546279
O	-3.819939	1.396983	0.248750
O	-4.277939	-1.048532	0.113776
H	-4.437110	-0.020737	0.189728
H	-4.282055	-1.344942	1.036080

Rotational constants (GHz): 1.5047900 0.3264600 0.3023000
 Vibrational harmonic frequencies (cm-1):
 i322.8441 29.7742 44.9452
 55.8207 66.4873 118.0115
 130.0284 154.1989 190.7075
 228.7697 237.7469 249.2631
 283.0360 309.8362 327.0324
 333.4141 364.7375 378.7611
 409.9219 427.2376 453.3906
 499.9486 549.4871 576.4263
 591.4522 592.6800 622.0407
 643.1001 719.6707 785.3450
 859.8985 905.5789 922.9921
 952.9335 955.0720 963.6157
 973.6673 991.0008 1011.0801
 1029.8719 1055.3985 1071.3322
 1109.6258 1120.2105 1152.7352
 1167.3355 1186.0118 1199.3135
 1208.9756 1242.0996 1256.0185
 1262.8198 1287.5498 1294.9079
 1320.1014 1350.4112 1358.7771
 1382.0371 1388.8134 1403.0878
 1408.2969 1432.2114 1445.9495
 1446.8157 1454.0218 1467.4862
 1471.2533 1478.9576 1488.1209
 1617.6058 1651.8447 1861.9277
 2513.5028 3045.5902 3057.6432
 3059.7092 3062.8947 3087.5071
 3089.7636 3096.7452 3126.4023
 3132.1533 3133.1526 3138.8900
 3152.2182 3156.3722 3162.0982
 3189.9315 3192.9625 3844.9370
 Zero-point correction (Hartree): 0.271611

TS.ApineneCI.J.a+H2O.HHP.pmt

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 E(RM062X/CC-pVDZ) (Hartree): -692.37718149

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.249622 | -0.774374 | -0.453148 |
| H | -0.742579 | -0.637268 | -1.429012 |
| C | -1.270250 | -1.288155 | 0.550032  |
| C | -2.494383 | -0.460901 | 0.689940  |
| H | -1.609561 | -2.298126 | 0.271282  |
| H | -0.828180 | -1.384309 | 1.557502  |
| H | -3.351558 | -0.805832 | 1.275218  |
| C | 0.621495  | 0.488209  | -0.145816 |
| C | 1.038332  | -1.606780 | -0.606130 |
| C | 0.254981  | 1.759696  | -0.894882 |
| C | 0.771323  | 0.753624  | 1.348489  |
| H | 1.105069  | -0.138709 | 1.898185  |
| H | 1.518881  | 1.542377  | 1.526450  |
| H | -0.186317 | 1.100153  | 1.765856  |
| H | 1.047032  | 2.517202  | -0.779859 |
| H | -0.684659 | 2.182834  | -0.513725 |
| H | 0.132630  | 1.560147  | -1.970692 |
| H | 1.083142  | -2.324090 | -1.434666 |
| H | 1.318913  | -2.112233 | 0.329138  |
| C | 1.843838  | -0.308132 | -0.749234 |
| H | 1.995189  | -0.007054 | -1.796641 |
| C | 3.139986  | -0.203905 | 0.021842  |
| C | 4.043175  | 0.952898  | -0.335352 |
| H | 3.466151  | 1.890529  | -0.349535 |
| H | 4.440854  | 0.805533  | -1.351243 |
| H | 4.869052  | 1.021917  | 0.380964  |
| O | 3.412371  | -0.982414 | 0.908425  |
| O | -2.430782 | 0.777144  | 0.432067  |
| O | -3.756827 | 1.294125  | 0.337275  |
| O | -3.773106 | -0.862896 | -0.885333 |
| H | -4.058808 | 0.088425  | -0.550187 |
| H | -3.321753 | -0.682252 | -1.722955 |

Rotational constants (GHz): 1.4773900 0.3513600 0.3269700  
 Vibrational harmonic frequencies (cm-1):  
 i354.3993 37.1179 50.1100  
 60.3499 73.2247 105.7190  
 132.2947 156.0749 212.7015  
 225.6212 237.4738 270.7018  
 287.4353 304.3230 327.7003  
 334.5899 363.6407 374.0136  
 410.2319 428.4255 436.9822  
 493.2147 548.4074 576.4569  
 584.8342 590.2837 620.8028  
 693.4757 714.2769 779.7223  
 852.3545 903.6616 916.8431  
 947.1236 956.1477 963.4631  
 976.5031 990.4246 998.8592  
 1012.6722 1038.7918 1073.3127  
 1109.8245 1121.2801 1158.9745  
 1162.1236 1180.1477 1188.2827  
 1207.2672 1249.4164 1258.2520  
 1275.7090 1301.4506 1305.4232  
 1331.3426 1351.4045 1360.7763  
 1387.6368 1394.7362 1397.4096  
 1408.4338 1419.0920 1431.3014  
 1446.4352 1454.5125 1464.6349  
 1470.2311 1477.9760 1483.2721  
 1612.1599 1647.9960 1859.8795  
 2438.8420 3051.4557 3053.5647  
 3056.5764 3062.2442 3068.6639  
 3087.9501 3090.8813 3109.6485  
 3124.2184 3129.0473 3137.9043  
 3145.5726 3156.8232 3161.5846



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3192.9537          3199.2468          3848.3341
Zero-point correction (Hartree): 0.271314

TS.ApineneCI.J.a+H2O.HHP.pmtu
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E(RM062X/CC-pVDZ) (Hartree): -692.37571322
Electronic state : 1-A
Cartesian coordinates (Angs):
 C -0.131233 -0.703169 -1.040833
 H -0.409284 -0.371305 -2.052621
 C -1.296947 -1.468267 -0.424683
 C -2.567113 -0.699188 -0.295852
 H -1.505266 -2.373571 -1.017089
 H -1.051027 -1.826288 0.588229
 H -3.544297 -1.187754 -0.328737
 C 0.550211 0.489715 -0.293180
 C 1.220981 -1.443059 -1.061170
 C 0.262494 1.883215 -0.830175
 C 0.346486 0.439780 1.216433
 H 0.591165 -0.544255 1.642330
 H 0.984217 1.182572 1.720407
 H -0.700134 0.692078 1.444636
 H 0.974562 2.610590 -0.407531
 H -0.755604 2.203901 -0.569165
 H 0.361354 1.910462 -1.925982
 H 1.503149 -1.959248 -1.986901
 H 1.329695 -2.131607 -0.210804
 C 1.934008 -0.120977 -0.744684
 H 2.289253 0.404707 -1.643349
 C 3.012465 -0.148248 0.314482
 C 3.898997 1.071301 0.404453
 H 3.282294 1.982939 0.437388
 H 4.521422 1.138348 -0.501027
 H 4.538055 1.008635 1.291957
 O 3.123331 -1.081025 1.078852
 O -2.527404 0.545515 -0.554604
 O -3.727003 1.146715 -0.074099
 O -3.099882 -0.464421 1.639724
 H -3.549881 0.373115 1.142021
 H -2.394097 -0.094223 2.188506
Rotational constants (GHz): 1.3254900 0.3717900 0.3586100
Vibrational harmonic frequencies (cm-1):
i450.7298 30.5141 55.2456
 62.8155 84.9354 114.1310
 137.5584 155.8416 216.3752
 226.0562 256.6922 275.8457
 279.4411 294.0114 318.5327
 335.0441 364.1610 376.5654
 425.0745 443.4639 474.1195
 496.1850 569.0117 577.5500
 590.8541 605.7838 621.0419
 678.3427 715.3792 783.0594
 869.4121 903.4167 924.5865
 947.0080 959.3217 965.2857
 977.7873 992.5598 997.2930
 1016.0448 1038.9695 1102.5184
 1112.5554 1119.9219 1155.1555
 1164.2917 1185.2648 1190.1325
 1206.3277 1249.4782 1259.5240
 1275.8759 1296.7879 1313.8117
 1344.1079 1351.0679 1368.0009
 1387.8445 1394.1021 1398.1128
 1413.1987 1421.8946 1431.8127
 1446.7344 1454.1073 1462.8020
 1468.8826 1477.0321 1482.5603
 1584.1986 1607.0341 1859.2885
 2173.5238 3051.1092 3057.1733
 3062.6424 3070.5482 3082.9015
 3087.3498 3090.8756 3110.9935
 3125.6455 3131.8545 3138.4516
 3149.8048 3155.0082 3158.0633
 3192.0060 3200.6416 3854.2339
Zero-point correction (Hartree): 0.271176

TS.ApineneCI.J.a+H2O.HHP.ppmf
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E(RM062X/CC-pVDZ) (Hartree): -692.37343192
Electronic state : 1-A
Cartesian coordinates (Angs):
  C   -0.161104    0.495531   -0.561483
  H   -0.364549    0.899652   -1.566751
  C   -1.375541    0.733888    0.337852
  C   -2.567905    0.100980   -0.278733
  H   -1.214864    0.297285    1.332823
  H   -1.584593    1.809146    0.441146
  H   -3.012858    0.501927   -1.194500
  C    1.238469    1.002629   -0.099067
  C    0.408105   -0.932183   -0.669540
  C    1.710347    2.299504   -0.734982
  C    1.376500    1.054848    1.419279
  H    1.081941    0.108855    1.895103
  H    2.422094    1.250877    1.703640
  H    0.759645    1.867751    1.832590
  H    2.759488    2.511819   -0.474919
  H    1.103305    3.147412   -0.378750
  H    1.629783    2.258609   -1.831457
  H    0.091115   -1.546158   -1.520720
  H    0.272165   -1.504475    0.259099
  C    1.821882   -0.329481   -0.709045
  H    2.175277   -0.137438   -1.733428
  C    2.900945   -1.007631    0.105745
  C    4.323256   -0.586083   -0.179497

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|                                          |           |           |           |
|------------------------------------------|-----------|-----------|-----------|
| H                                        | 4.398413  | 0.512576  | -0.176623 |
| H                                        | 4.609383  | -0.924675 | -1.187138 |
| H                                        | 5.001358  | -1.018473 | 0.564221  |
| O                                        | 2.627985  | -1.809361 | 0.970112  |
| O                                        | -2.840512 | -1.097385 | 0.020786  |
| O                                        | -4.142325 | -1.399098 | -0.475151 |
| O                                        | -4.309883 | 0.852149  | 0.557791  |
| H                                        | -4.581700 | -0.076113 | 0.153784  |
| H                                        | -4.277261 | 0.678961  | 1.510413  |
| Rotational constants (GHz):              | 1.3289100 | 0.3157400 | 0.2842400 |
| Vibrational harmonic frequencies (cm-1): |           |           |           |
| i333.9929                                | 26.5357   |           | 38.5156   |
| 46.2165                                  | 72.4500   |           | 94.2799   |
| 137.9890                                 | 153.1060  |           | 182.1484  |
| 212.2450                                 | 229.3595  |           | 240.0771  |
| 274.8298                                 | 306.7244  |           | 325.6001  |
| 334.8026                                 | 352.1994  |           | 381.0417  |
| 407.4955                                 | 432.5410  |           | 465.6262  |
| 493.6926                                 | 555.6407  |           | 580.0766  |
| 583.8496                                 | 605.0626  |           | 619.9019  |
| 642.4960                                 | 738.9003  |           | 813.8393  |
| 848.8851                                 | 898.6161  |           | 927.7810  |
| 933.1075                                 | 951.7851  |           | 959.4417  |
| 977.1779                                 | 988.6021  |           | 1013.0782 |
| 1019.2318                                | 1040.0945 |           | 1083.6226 |
| 1109.5912                                | 1134.4799 |           | 1154.3194 |
| 1171.1412                                | 1186.6289 |           | 1200.4100 |
| 1222.9106                                | 1239.4243 |           | 1253.3454 |
| 1269.7121                                | 1286.2132 |           | 1306.9231 |
| 1320.6456                                | 1349.5767 |           | 1360.9181 |
| 1382.4441                                | 1387.7240 |           | 1401.2315 |
| 1407.4103                                | 1432.4033 |           | 1445.7612 |
| 1446.9605                                | 1452.9621 |           | 1462.1431 |
| 1469.0270                                | 1477.2931 |           | 1479.4184 |
| 1622.3242                                | 1652.1828 |           | 1862.9358 |
| 2434.1807                                | 3045.8976 |           | 3054.6335 |
| 3061.8955                                | 3064.0338 |           | 3084.4160 |
| 3088.5045                                | 3098.2921 |           | 3122.7735 |
| 3128.1930                                | 3134.0127 |           | 3137.4344 |
| 3149.4932                                | 3152.6518 |           | 3163.7301 |
| 3192.6544                                | 3194.3205 |           | 3842.5418 |
| Zero-point correction (Hartree):         | 0.271300  |           |           |

TS.ApineneCI.J.a+H2O.HHP.ppmu

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E(RM062X/CC-pVDZ) (Hartree): -692.37546339

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-0.250252	0.519111	-0.458207
H	-0.515861	0.841652	-1.478003
C	-1.375790	0.900280	0.498072
C	-2.713318	0.503533	-0.011887
H	-1.231320	0.474498	1.500347
H	-1.407766	2.001123	0.599897
H	-3.042349	0.802475	-1.011957
C	1.192451	1.011372	-0.134354
C	0.269258	-0.930042	-0.492546
C	1.661019	2.233998	-0.905633
C	1.435586	1.182691	1.362748
H	1.139901	0.292149	1.935200
H	2.504186	1.358472	1.562100
H	0.878526	2.050860	1.747166
H	2.730697	2.430647	-0.730505
H	1.104493	3.129911	-0.585613
H	1.507732	2.105509	-1.987499
H	-0.128205	-1.580241	-1.279003
H	0.183853	-1.428658	0.484817
C	1.696123	-0.385423	-0.664087
H	1.992088	-0.292189	-1.719950
C	2.799939	-1.035048	0.139634
C	4.215018	-0.677805	-0.249692
H	4.318995	0.415532	-0.329917
H	4.436206	-1.094725	-1.244253
H	4.921508	-1.076985	0.486142
O	2.554230	-1.766022	1.072770
O	-3.605545	0.152291	0.814175
O	-4.685739	-0.426467	0.083385
O	-2.639072	-1.355157	-0.914265
H	-3.655039	-1.216845	-0.644838
H	-2.308841	-1.986353	-0.256936
Rotational constants (GHz):	1.3328100	0.3284300	0.3000300
Vibrational harmonic frequencies (cm-1):			
i372.8339	39.5734		45.5360
54.0292	94.9842		106.1169
134.5773	157.1874		171.8651
223.3535	232.3130		269.6278
278.0719	314.1801		322.6226
336.9572	350.1470		375.5476
410.3740	448.4409		453.0665
486.1171	561.8871		581.9535
597.4831	613.4858		621.8893
627.0762	741.7665		821.3062
848.7690	908.3059		922.4774
933.7197	949.5937		959.5487
976.8433	988.2729		1014.7319
1020.6050	1047.3965		1094.1910
1106.9228	1143.8159		1153.8986
1172.2389	1187.4915		1200.4929
1221.3217	1236.3494		1248.5508
1271.2231	1283.7631		1317.4178
1326.6089	1350.9592		1370.3828
1387.5714	1389.7137		1400.7887

1412.9861	1429.9361	1431.8144
1446.5963	1452.3817	1461.3945
1474.3450	1477.5970	1479.8104
1623.9938	1637.6657	1861.3869
2291.4537	3039.6168	3044.5405
3055.0742	3061.1434	3067.8706
3086.2205	3091.1082	3120.3751
3127.5805	3133.7022	3135.8624
3136.6190	3149.7910	3173.6541
3191.6934	3192.7428	3838.6700

Zero-point correction (Hartree): 0.271177

TS.ApineneCI.J.a+H2O.HHP.pppd

E(RM062X/CC-pVDZ) (Hartree): -692.37493418

Electronic state : 1-A

Cartesian coordinates (Angs):

C	0.277004	0.423689	0.289712
H	0.626213	0.733845	1.284624
C	1.372699	0.704838	-0.733975
C	2.537647	-0.191987	-0.521064
H	0.996153	0.476095	-1.746204
H	1.710735	1.750531	-0.720235
H	2.409333	-1.278858	-0.535118
C	-1.159954	0.979897	0.062996
C	-0.301351	-1.000296	0.378388
C	-1.511054	2.232040	0.849755
C	-1.514834	1.144202	-1.411341
H	-1.311613	0.233042	-1.992238
H	-2.586488	1.369393	-1.527304
H	-0.948846	1.980006	-1.851292
H	-2.583635	2.468670	0.765556
H	-0.949737	3.099352	0.466533
H	-1.268665	2.112538	1.916228
H	0.132551	-1.662752	1.136194
H	-0.321623	-1.511328	-0.596080
C	-1.682566	-0.385540	0.657505
H	-1.885205	-0.263398	1.732094
C	-2.877423	-0.991682	-0.043315
C	-4.237681	-0.572515	0.462330
H	-4.286525	0.524248	0.547772
H	-4.392392	-0.980173	1.473180
H	-5.020340	-0.940130	-0.210144
O	-2.743510	-1.735877	-0.988640
O	3.707745	0.261287	-0.699181
O	4.632279	-0.691049	-0.173172
O	2.839491	-0.548203	1.483244
H	3.776680	-0.755966	1.008401
H	3.000447	0.299753	1.924069

Rotational constants (GHz): 1.3663600 0.3165300 0.3009900

Vibrational harmonic frequencies (cm-1):

1402.8171	35.9294	43.2479
51.0143	86.8700	97.6185
135.3513	152.8346	189.5016
217.6677	236.6854	266.9523
278.1403	308.2802	327.4455
340.4885	350.3471	379.8282
408.5582	445.7940	454.5179
507.6994	559.5502	581.9074
593.6531	612.4033	623.9203
627.6541	741.7337	806.0047
867.8416	903.8406	928.5052
939.2270	948.5475	957.4548
976.1517	987.2670	1008.8794
1015.4333	1046.8371	1099.1620
1113.6244	1147.1363	1160.3413
1167.4059	1183.4083	1200.7325
1211.1952	1243.1425	1253.7686
1267.2865	1291.8595	1314.4986
1322.4397	1350.2426	1380.2239
1387.3707	1387.7145	1400.0485
1408.5095	1431.6455	1435.3235
1446.4585	1452.6701	1461.5467
1470.5384	1477.0981	1478.3931
1623.4971	1640.9413	1861.5344
2177.7894	3046.0616	3052.5750
3056.7597	3061.4277	3085.6874
3089.8665	3101.8115	3122.3098
3126.9731	3131.2074	3134.9531
3136.8908	3144.8815	3164.4541
3192.8493	3195.7864	3837.2788

Zero-point correction (Hartree): 0.271036

TS.ApineneCI.J.a+H2O.HHP.pppu

E(RM062X/CC-pVDZ) (Hartree): -692.37333214

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-0.166149	0.487451	-0.373567
H	-0.433540	1.143924	-1.216381
C	-1.358794	0.388658	0.578629
C	-2.521765	-0.191183	-0.138377
H	-1.126805	-0.285622	1.415712
H	-1.637284	1.376183	0.973824
H	-2.491844	-1.215133	-0.523548
C	1.216703	0.934446	0.189666
C	0.486207	-0.808401	-0.897656
C	1.585450	2.388387	-0.053306
C	1.408918	0.556674	1.654999
H	1.187870	-0.503596	1.843264
H	2.451368	0.731388	1.963670
H	0.762248	1.173317	2.298016

H	2.630100	2.587525	0.233949
H	0.944363	3.054601	0.545953
H	1.462361	2.658990	-1.112453
H	0.179839	-1.173361	-1.885539
H	0.428980	-1.630652	-0.169460
C	1.857269	-0.122827	-0.789586
H	2.157550	0.378049	-1.722249
C	3.005156	-0.931065	-0.226844
C	4.385651	-0.339727	-0.387515
H	4.386199	0.711529	-0.059777
H	4.662340	-0.343653	-1.453029
H	5.114527	-0.920975	0.187619
O	2.814122	-1.972352	0.359710
O	-3.383738	0.592281	-0.632570
O	-4.516106	-0.177020	-1.029115
O	-3.853258	-1.034703	1.200197
H	-4.422980	-0.840776	0.340241
H	-4.135335	-0.341855	1.815758
Rotational constants (GHz):			
Vibrational harmonic frequencies (cm-1):			
i342.1498	29.8033		38.4555
51.8218	76.5154		83.8020
126.8937	151.8364		191.3886
216.7331	233.3925		242.3794
270.1154	294.8503		325.6195
339.9679	352.4803		383.6538
408.3353	432.7779		460.3934
504.4843	557.3450		578.1008
585.7805	607.5593		620.8850
644.8912	741.7564		809.3898
852.4812	900.7253		927.4051
934.8764	951.1870		958.2923
979.4539	988.4839		1008.7971
1016.3018	1042.6144		1091.9491
1111.8003	1142.1566		1163.3913
1166.7523	1184.3422		1201.2345
1212.6378	1247.7694		1255.4791
1266.4566	1288.8452		1308.4294
1323.2888	1348.4795		1359.8959
1380.9697	1388.9373		1402.1218
1405.9245	1430.8641		1445.6141
1446.8324	1453.3309		1462.1692
1469.7044	1478.1232		1479.6412
1623.5606	1651.1026		1862.5917
2421.0131	3046.4713		3055.0929
3062.2660	3073.1975		3082.8510
3090.1002	3091.6350		3123.2373
3128.8376	3135.7585		3137.4791
3146.4226	3150.0718		3157.6688
3193.4854	3197.4350		3843.0168
Zero-point correction (Hartree): 0.271358			
TS.ApineneCI.J.a+H2O.HHP.pptd			
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E(RM062X/CC-pVDZ) (Hartree): -692.37620752			
Electronic state : 1-A			
Cartesian coordinates (Angs):			
C	-0.333464	0.711823	-0.227741
H	-0.640261	1.221458	-1.153163
C	-1.382890	0.945335	0.844373
C	-2.732393	0.461767	0.447272
H	-1.134723	0.426796	1.782957
H	-1.483349	2.017241	1.093389
H	-3.571400	0.478547	1.148660
C	1.158085	1.050067	0.064420
C	0.078046	-0.738328	-0.550315
C	1.660051	2.365389	-0.507630
C	1.517192	0.922351	1.542141
H	1.198992	-0.041167	1.965426
H	2.606910	0.995545	1.682774
H	1.050897	1.733985	2.121728
H	2.751800	2.459385	-0.394541
H	1.198902	3.216542	0.018826
H	1.415583	2.453299	-1.576574
H	-0.417798	-1.227484	-1.398316
H	0.042921	-1.389064	0.336658
C	1.521131	-0.250062	-0.752377
H	1.736137	0.022014	-1.796645
C	2.635518	-1.098018	-0.182402
C	4.037969	-0.747846	-0.620042
H	4.208652	0.334171	-0.507725
H	4.155301	-0.981723	-1.689347
H	4.769307	-1.314338	-0.033415
O	2.410962	-1.979110	0.616813
O	-3.006381	0.356060	-0.783940
O	-4.207525	-0.402084	-0.913946
O	-2.839250	-1.567878	0.791858
H	-3.574488	-1.385305	0.065979
H	-2.131295	-2.010680	0.300866
Rotational constants (GHz):			
Vibrational harmonic frequencies (cm-1):			
i364.1212	38.7636		50.9374
59.1178	92.4491		100.7337
133.1371	151.9983		174.9044
222.5819	232.4032		264.3772
285.4843	299.0098		320.7560
339.0558	353.5890		380.3222
398.5854	437.1624		460.8355
485.3454	557.9446		581.6540
586.7115	597.6562		625.3163
673.7373	749.5494		817.5486
833.8785	908.7495		927.4357

938.4470	950.1471	959.1670
976.0688	986.8357	998.8112
1023.2401	1025.5620	1058.7900
1103.0253	1138.3180	1152.0826
1166.5584	1184.2908	1202.6244
1212.5611	1244.1582	1254.2499
1277.0436	1301.2170	1321.2365
1327.2785	1347.9871	1357.3941
1388.4274	1397.5964	1401.8926
1411.2692	1429.3057	1431.4896
1446.9458	1453.3825	1462.2984
1475.7965	1478.6457	1481.3668
1614.0471	1640.7576	1861.2353
2424.1803	3045.9241	3050.6440
3053.9222	3062.1610	3081.0791
3089.8030	3093.0513	3119.7044
3121.6677	3127.8003	3136.2538
3137.7219	3145.1641	3153.0245
3193.2303	3203.5420	3847.0363

Zero-point correction (Hartree): 0.271351

TS.ApineneCI.J.a+H2O.HHP.pptu

E(RM062X/CC-pVDZ) (Hartree): -692.37476333

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-0.341179	0.310773	-0.143846
H	-0.793937	0.658790	-1.086598
C	-1.350158	0.477566	0.978502
C	-2.656065	-0.177433	0.705674
H	-0.970752	0.057123	1.926055
H	-1.578962	1.537102	1.177205
H	-3.484920	-0.102345	1.415336
C	1.069479	0.954774	0.002670
C	0.326156	-1.060961	-0.362153
C	1.274022	2.267910	-0.734595
C	1.519615	1.068980	1.456476
H	1.422036	0.116241	1.996170
H	2.578922	1.364939	1.510149
H	0.931706	1.837306	1.981954
H	2.329591	2.581754	-0.705769
H	0.677888	3.069558	-0.269153
H	0.969559	2.184029	-1.788583
H	-0.110906	-1.716590	-1.123156
H	0.444359	-1.620816	0.576865
C	1.639160	-0.336799	-0.701127
H	1.754615	-0.145170	-1.778688
C	2.921685	-0.889177	-0.121189
C	4.208919	-0.356559	-0.705723
H	4.182560	0.744039	-0.733421
H	4.307748	-0.701283	-1.746527
H	5.063918	-0.704531	-0.115921
O	2.910668	-1.680452	0.794872
O	-2.712270	-1.102987	-0.157468
O	-4.085187	-1.345009	-0.460216
O	-3.836337	1.104902	-0.388482
H	-4.228840	0.142317	-0.581768
H	-3.379378	1.331453	-1.211925

Rotational constants (GHz): 1.3322000 0.3341400 0.3030700

Vibrational harmonic frequencies (cm-1):

1377.9188	38.1370	42.4218
50.4862	80.2157	95.3827
135.0774	152.0184	187.7028
210.7051	239.8734	248.3786
279.9924	311.9224	326.8887
336.8201	352.4328	379.8764
413.0536	432.3739	461.4927
489.1263	555.4631	578.4473
585.2219	603.9053	620.3893
676.8807	745.2268	807.2768
841.2335	903.6540	933.2820
936.7675	949.0291	957.6665
976.0950	986.7575	999.6867
1021.8130	1031.6847	1054.5305
1107.7413	1135.5519	1147.2066
1166.8583	1186.4699	1199.8527
1211.2099	1241.6744	1254.5386
1275.2297	1311.4873	1319.0478
1328.5116	1351.5061	1367.0070
1386.8621	1396.8298	1400.4468
1409.8344	1423.3760	1431.7014
1446.5777	1453.5764	1461.1025
1469.5727	1478.0424	1479.4154
1613.4709	1646.3231	1860.6549
2338.3763	3043.0384	3053.8133
3057.9622	3061.6034	3065.1840
3086.7437	3098.5364	3108.4519
3119.6719	3127.5421	3132.3039
3137.0190	3149.1272	3171.4521
3192.2247	3195.6812	3841.8213

Zero-point correction (Hartree): 0.271037

TS.ApineneCI.J.a+H2O.HHP.ptmd

E(RM062X/CC-pVDZ) (Hartree): -692.37182685

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-0.007791	1.140522	0.875640
H	-0.262171	2.074787	1.400106
C	1.499801	1.178558	0.619001
C	2.096099	-0.073170	0.078612
H	1.772372	2.008904	-0.049541

H	2.010243	1.341110	1.582260
H	1.823216	-1.056312	0.472388
C	-1.035038	0.961601	-0.282361
C	-0.669119	-0.036655	1.621390
C	-1.622770	2.247376	-0.840465
C	-0.535529	0.059993	-1.407639
H	-0.143550	-0.899431	-1.038531
H	-1.359493	-0.177263	-2.098939
H	0.255988	0.558334	-1.985981
H	-2.446967	2.038353	-1.540659
H	-0.855830	2.811940	-1.394718
H	-2.009550	2.892073	-0.036980
H	-0.777167	0.048345	2.709446
H	-0.230695	-1.013770	1.376764
C	-1.922956	0.177492	0.757952
H	-2.644181	0.869769	1.218584
C	-2.628848	-1.053310	0.234488
C	-3.980731	-0.833491	-0.402407
H	-3.921412	-0.019270	-1.141300
H	-4.700671	-0.516955	0.367911
H	-4.327423	-1.757272	-0.878125
O	-2.112173	-2.146239	0.288626
O	2.649709	-0.034673	-1.063399
O	3.405437	-1.230338	-1.228383
O	3.844547	-0.477365	1.058581
H	3.927301	-0.992817	0.129360
H	4.431127	0.284913	0.939290
Rotational constants (GHz): 1.1267700 0.3713700 0.3495800			
Vibrational harmonic frequencies (cm-1):			
i404.3167	41.7486	46.8084	
49.4537	76.8398	128.8546	
131.3794	150.1911	184.6611	
228.1576	234.4864	246.0581	
281.4900	284.4298	342.8297	
346.7116	362.7631	383.4914	
409.4877	432.0653	460.3989	
537.5976	572.1239	581.5215	
592.8421	600.7187	622.7773	
675.4959	718.2021	772.4947	
847.5035	903.2845	931.4531	
942.1737	948.6734	953.8530	
972.6343	987.2219	992.6875	
1010.7633	1044.3595	1097.1590	
1134.5716	1138.6467	1156.4134	
1164.5487	1182.9219	1199.5571	
1214.9200	1245.3230	1254.8693	
1290.5800	1295.5414	1311.6334	
1325.0702	1351.2197	1368.4684	
1388.2359	1395.7901	1402.7447	
1410.6504	1428.9149	1432.0204	
1446.7327	1453.8124	1460.4653	
1471.8900	1474.9435	1484.2690	
1612.2501	1645.0096	1862.6410	
2241.8242	3047.3978	3056.9036	
3062.7908	3064.6382	3076.8770	
3088.2488	3100.8973	3124.8389	
3125.5050	3130.8947	3134.6169	
3138.8305	3149.9307	3162.9020	
3191.9177	3198.2332	3835.1650	
Zero-point correction (Hartree): 0.271250			
TS.ApineneCI.J.a+H2O.HHP.ptpd			
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E(RM062X/CC-pVDZ) (Hartree): -692.37624306			
Electronic state : 1-A			
Cartesian coordinates (Angs):			
C	-0.142620	1.404038	-0.591866
H	-0.007787	2.266869	-1.258307
C	-1.398698	1.650297	0.265206
C	-2.405567	0.553522	0.351798
H	-1.129174	1.931897	1.291800
H	-1.972457	2.500946	-0.141586
H	-3.063335	0.466689	1.221035
C	1.218758	1.124801	0.134221
C	0.020203	0.090440	-1.392857
C	2.235950	2.248617	-0.004565
C	1.092937	0.703028	1.594359
H	0.287541	-0.024400	1.757078
H	2.036261	0.259442	1.950145
H	0.892242	1.583538	2.224364
H	3.220695	1.937586	0.379875
H	1.914683	3.132472	0.569307
H	2.358222	2.549847	-1.055858
H	-0.098762	0.178111	-2.478866
H	-0.614127	-0.726240	-1.040376
C	1.461796	-0.064821	-0.877985
H	2.236414	0.201890	-1.610439
C	1.797960	-1.383656	-0.224981
C	3.255770	-1.757629	-0.150554
H	3.835285	-0.913500	0.254570
H	3.633606	-1.946577	-1.167159
H	3.388359	-2.649983	0.470322
O	0.938982	-2.093178	0.261709
O	-2.798982	0.010478	-0.723104
O	-3.557562	-1.151720	-0.391792
O	-1.637774	-1.153357	1.179957
H	-2.449255	-1.492079	0.616656
H	-0.844670	-1.566113	0.786627
Rotational constants (GHz): 1.0001800 0.5115900 0.4136100			
Vibrational harmonic frequencies (cm-1):			
i359.9607	62.6648	75.2347	
102.5004	135.1837	143.8716	

153.2738	174.1449	196.1052
207.2685	260.5506	281.9367
291.0190	308.8735	336.4427
346.4806	359.5056	385.5729
403.7733	433.4996	490.9718
529.0186	585.9852	592.6885
623.9782	691.3212	725.4677
741.4252	762.5625	783.2784
837.7294	883.6789	928.6235
951.3236	959.8021	965.5710
980.7047	993.7358	1000.0588
1022.8455	1036.6496	1071.2214
1097.2913	1145.8148	1163.3247
1169.1681	1194.2033	1199.7030
1214.9203	1250.2672	1269.2733
1271.3354	1281.4427	1314.1659
1328.8235	1352.2084	1366.4355
1384.9720	1386.6957	1403.0613
1406.8657	1425.9433	1432.2750
1445.6329	1456.6060	1460.7439
1466.5389	1477.6736	1487.2763
1597.3418	1637.5715	1838.0685
2489.7074	3043.1208	3057.6618
3061.2927	3063.5151	3092.0551
3100.3668	3120.8275	3125.3583
3128.6024	3131.6179	3136.4998
3139.1617	3176.5435	3190.3457
3196.4751	3215.1343	3685.0047

Zero-point correction (Hartree): 0.273142

TS.ApineneCI.J.a+H2O.HHP.ptpu

~~~~~  
E(RM062X/CC-pVDZ) (Hartree): -692.37075390

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.012989 | 0.887203  | 1.124062  |
| H | -0.296379 | 1.683406  | 1.830053  |
| C | 1.496848  | 0.989039  | 0.929498  |
| C | 2.153946  | -0.173409 | 0.265463  |
| H | 1.728200  | 1.874689  | 0.313833  |
| H | 2.012204  | 1.134387  | 1.891061  |
| H | 1.611903  | -0.900702 | -0.342731 |
| C | -1.001102 | 0.977554  | -0.077271 |
| C | -0.698684 | -0.421121 | 1.565403  |
| C | -1.545039 | 2.367582  | -0.364366 |
| C | -0.485459 | 0.323341  | -1.358508 |
| H | -0.277285 | -0.747392 | -1.222873 |
| H | -1.246345 | 0.398149  | -2.151330 |
| H | 0.433360  | 0.809612  | -1.720419 |
| H | -2.359133 | 2.332687  | -1.105324 |
| H | -0.752368 | 3.011137  | -0.779437 |
| H | -1.930497 | 2.844325  | 0.549385  |
| H | -0.830044 | -0.594418 | 2.640358  |
| H | -0.256392 | -1.316950 | 1.105868  |
| C | -1.930852 | 0.008955  | 0.751006  |
| H | -2.638784 | 0.607219  | 1.345059  |
| C | -2.665637 | -1.052952 | -0.034623 |
| C | -4.000566 | -0.654739 | -0.618725 |
| H | -3.901047 | 0.292799  | -1.170826 |
| H | -4.720039 | -0.478788 | 0.195589  |
| H | -4.372579 | -1.444743 | -1.280010 |
| O | -2.183312 | -2.147849 | -0.218229 |
| O | 3.287986  | -0.530701 | 0.712275  |
| O | 3.874854  | -1.409673 | -0.241390 |
| O | 2.890027  | 0.380096  | -1.564383 |
| H | 3.477052  | -0.471788 | -1.263367 |
| H | 3.498937  | 1.122668  | -1.432703 |

Rotational constants (GHz): 1.1273900 0.3709300 0.3460700

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i442.3456 | 43.1112   | 47.2197   |
| 60.5933   | 76.7924   | 129.3232  |
| 134.2857  | 154.1487  | 185.3020  |
| 231.3633  | 234.1602  | 257.0020  |
| 280.8487  | 285.5985  | 336.5309  |
| 350.2111  | 364.5832  | 381.6755  |
| 406.0575  | 440.5014  | 464.0043  |
| 532.9862  | 577.2375  | 582.6114  |
| 591.6134  | 605.2237  | 623.3806  |
| 673.4412  | 719.1350  | 777.1334  |
| 828.2286  | 908.9644  | 928.0229  |
| 944.8080  | 951.8885  | 961.5269  |
| 971.9604  | 991.1153  | 995.8015  |
| 1023.0973 | 1047.1033 | 1069.9607 |
| 1121.7797 | 1138.7680 | 1158.4270 |
| 1164.9415 | 1185.3988 | 1201.0091 |
| 1217.3691 | 1235.7474 | 1253.4877 |
| 1291.2719 | 1305.4514 | 1320.7053 |
| 1325.1289 | 1350.4479 | 1373.4729 |
| 1387.9436 | 1399.9980 | 1404.1467 |
| 1411.7878 | 1422.8561 | 1431.5312 |
| 1446.8131 | 1458.0573 | 1462.4858 |
| 1474.2945 | 1481.4737 | 1494.3606 |
| 1612.7611 | 1636.6702 | 1861.3767 |
| 2123.7334 | 3044.9812 | 3056.8481 |
| 3062.8625 | 3063.1164 | 3075.0799 |
| 3083.7573 | 3093.6228 | 3117.1457 |
| 3121.9855 | 3131.1263 | 3132.8300 |
| 3138.8620 | 3151.5603 | 3157.5938 |
| 3193.8803 | 3222.2659 | 3833.0605 |

Zero-point correction (Hartree): 0.271108

TS.ApineneCI.J.a+H2O.HHP.pttd

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E(RM062X/CC-pVDZ) (Hartree): -692.36895732
Electronic state : 1-A
Cartesian coordinates (Angs):
C -0.082669 1.155199 -1.015634
H 0.264146 2.023657 -1.598577
C -1.588232 1.355869 -0.844658
C -2.495016 0.229922 -0.479050
H -1.797725 2.148861 -0.106261
H -2.010331 1.738450 -1.791127
H -3.573525 0.400554 -0.546353
C 0.890431 1.032133 0.193593
C 0.549663 -0.112588 -1.632152
C 1.519445 2.335111 0.661779
C 0.306598 0.265043 1.375527
H -0.181648 -0.670419 1.065494
H 1.097555 0.007192 2.097295
H -0.416024 0.910840 1.900330
H 2.294880 2.153423 1.422897
H 0.758450 2.989481 1.117524
H 1.980833 2.879754 -0.175413
H 0.709441 -0.116586 -2.717360
H 0.048107 -1.037335 -1.327068
C 1.777921 0.122892 -0.737418
H 2.548385 0.743095 -1.220722
C 2.407848 -1.080384 -0.072336
C 3.758276 -0.860409 0.569932
H 3.728732 0.031946 1.214640
H 4.508127 -0.666402 -0.212404
H 4.047440 -1.743081 1.150716
O 1.836766 -2.145166 -0.020563
O -2.108611 -0.977566 -0.512332
O -3.130798 -1.781196 0.077610
O -2.960199 0.191599 1.508651
H -3.205490 -0.782481 1.146794
H -2.164208 0.030952 2.035177
Rotational constants (GHz): 1.0217100 0.4499100 0.3972700
Vibrational harmonic frequencies (cm-1):
i410.2407 39.0484 50.1134
55.4901 117.4787 137.6939
140.2599 156.6545 185.1718
205.3333 230.4739 261.6180
274.0938 282.6454 341.5059
344.2641 363.1508 380.3797
420.1477 426.0405 452.8937
525.2099 565.8363 583.7913
601.6821 608.7171 623.2357
712.6274 721.8557 765.3354
843.2605 907.3226 930.6643
942.2012 950.2051 962.9829
975.5295 981.6881 993.8748
1019.2678 1028.6271 1058.5124
1139.8591 1143.0287 1161.2337
1169.4860 1189.2072 1201.2408
1223.7505 1245.6376 1259.7885
1298.5274 1319.2261 1322.9918
1351.4939 1365.5478 1376.8691
1388.4851 1396.8540 1402.7167
1408.4897 1420.7970 1432.3450
1447.6674 1455.6976 1461.6655
1476.3656 1480.9033 1490.2855
1617.5078 1651.9159 1866.7904
2223.1089 3042.7963 3045.7578
3047.1719 3061.2119 3064.7051
3081.8066 3087.4441 3110.7256
3117.3495 3121.0876 3132.8565
3136.3310 3152.8132 3189.3483
3191.4427 3192.6664 3859.7891
Zero-point correction (Hartree): 0.271539

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TS.ApineneCI.J.a+H2O.HHP.pttu

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E(RM062X/CC-pVDZ) (Hartree): -692.37040995
Electronic state : 1-A
Cartesian coordinates (Angs):
C      -0.197473      1.179658      -0.742715
H       0.057433      1.911735      -1.524993
C      -1.572881      1.585638      -0.209021
C      -2.473957      0.533800      0.333054
H      -1.468710      2.352991      0.580767
H      -2.161712      2.062107      -1.006502
H      -3.542286      0.742171      0.445475
C       1.059617      1.072403      0.171982
C       0.108999      -0.228352      -1.295292
C       1.899493      2.336783      0.261016
C       0.775159      0.510281      1.561732
H       0.260759      -0.457365      1.524991
H       1.718951      0.374488      2.113477
H       0.152965      1.209682      2.142947
H       2.849215      2.149647      0.786434
H       1.361966      3.116563      0.825156
H       2.131457      2.736418      -0.737692
H      -0.058366      -0.400759      -2.367037
H      -0.350846      -1.031451      -0.704139
C       1.561042      -0.038715      -0.826633
H       2.198210      0.425158      -1.595647
C       2.262273      -1.230042      -0.213953
C       3.735929      -1.062638      0.076644
H       3.909111      -0.125907      0.628628
H       4.289105      -0.984657      -0.872000
H       4.104816      -1.918853      0.651766
O       1.663126      -2.244837      0.057318

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|                                          |           |           |                               |
|------------------------------------------|-----------|-----------|-------------------------------|
| O                                        | -2.025884 | -0.465925 | 0.962531                      |
| O                                        | -3.071570 | -1.432278 | 1.070431                      |
| O                                        | -3.153529 | -0.595754 | -1.270062                     |
| H                                        | -3.301971 | -1.205636 | -0.434483                     |
| H                                        | -2.396449 | -0.998891 | -1.719781                     |
| Rotational constants (GHz):              |           |           | 1.0289900 0.4542100 0.3920400 |
| Vibrational harmonic frequencies (cm-1): |           |           |                               |
| i347.8510                                | 42.1808   |           | 52.8641                       |
| 61.1943                                  | 80.1075   |           | 118.2985                      |
| 124.0579                                 | 145.9617  |           | 176.1048                      |
| 207.8652                                 | 230.5319  |           | 253.4243                      |
| 282.6101                                 | 292.6701  |           | 311.0712                      |
| 340.0710                                 | 354.0053  |           | 379.0835                      |
| 392.3983                                 | 434.6076  |           | 438.0270                      |
| 527.7576                                 | 559.7565  |           | 568.0815                      |
| 579.6974                                 | 590.4474  |           | 625.4009                      |
| 706.2640                                 | 724.9101  |           | 762.4198                      |
| 835.4059                                 | 912.1454  |           | 923.2693                      |
| 947.2616                                 | 948.4274  |           | 956.8540                      |
| 971.3029                                 | 984.5223  |           | 1000.7602                     |
| 1016.7478                                | 1018.8217 |           | 1051.5480                     |
| 1097.6493                                | 1142.4996 |           | 1164.3338                     |
| 1167.0311                                | 1185.2494 |           | 1201.2371                     |
| 1217.6278                                | 1241.7834 |           | 1254.6536                     |
| 1294.8497                                | 1299.2493 |           | 1321.3940                     |
| 1343.2835                                | 1350.2846 |           | 1373.9234                     |
| 1388.3354                                | 1398.5132 |           | 1404.3481                     |
| 1409.2635                                | 1418.0603 |           | 1431.2636                     |
| 1445.7633                                | 1454.6506 |           | 1461.3208                     |
| 1477.1579                                | 1479.6202 |           | 1486.4058                     |
| 1625.3860                                | 1644.2112 |           | 1866.4764                     |
| 2481.8486                                | 3043.6131 |           | 3047.3829                     |
| 3054.5047                                | 3062.3875 |           | 3068.2544                     |
| 3080.4058                                | 3088.2993 |           | 3115.1267                     |
| 3118.2313                                | 3121.8477 |           | 3131.5794                     |
| 3138.0906                                | 3160.7312 |           | 3181.5194                     |
| 3190.6154                                | 3193.2950 |           | 3846.9443                     |

Zero-point correction (Hartree): 0.271328

TS.ApineneCI.J.a+H2O.HHP.tmpd

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E(RM062X/CC-pVDZ) (Hartree): -692.37396849

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-0.183096	1.014173	0.266234
H	-0.529016	1.144952	1.302351
C	-1.276151	1.514556	-0.674911
C	-2.572388	0.791972	-0.502987
H	-1.446256	2.588171	-0.518011
H	-0.967599	1.369317	-1.723630
H	-3.524460	1.311235	-0.363913
C	0.422485	-0.418621	0.116428
C	1.236035	1.606487	0.147489
C	-0.159329	-1.513608	0.996974
C	0.500631	-0.882860	-1.337872
H	0.950595	-0.119491	-1.993316
H	1.126429	-1.781934	-1.405153
H	-0.502921	-1.118762	-1.716648
H	0.491974	-2.399894	0.968808
H	-1.162112	-1.812592	0.651110
H	-0.220747	-1.184474	2.048910
H	1.478148	2.479250	0.766850
H	1.496301	1.822887	-0.899496
C	1.760045	0.221521	0.591050
H	1.808857	0.190154	1.694333
C	3.078082	-0.326147	0.090859
C	4.209404	0.663548	-0.066562
H	4.304445	1.282192	0.838594
H	3.985821	1.346637	-0.900663
H	5.144851	0.130760	-0.268918
O	3.214261	-1.505621	-0.143942
O	-2.627373	-0.417306	-0.880193
O	-3.805991	-1.014870	-0.347454
O	-2.893464	0.346498	1.491416
H	-3.465695	-0.360674	0.957640
H	-2.162395	-0.183467	1.842322

Rotational constants (GHz): 1.4468600 0.3712900 0.3472100

Vibrational harmonic frequencies (cm-1):

i376.9891	36.3944		67.7527
72.4320	89.8362		127.2767
142.2683	156.9102		219.5407
241.2633	259.7448		283.9233
290.5749	307.6793		327.1181
330.3716	380.3742		398.1794
407.0850	411.9629		479.5831
510.5131	527.5023		582.7889
595.0556	605.1433		616.5975
675.6120	719.7912		769.0635
853.6426	899.1352		919.2319
947.9400	955.7330		964.2354
983.2181	1008.1570		1018.7612
1032.3875	1049.4504		1055.8858
1110.1306	1125.0174		1151.0487
1168.0150	1177.5182		1192.9675
1231.4027	1245.0301		1263.9503
1286.9554	1300.1397		1306.7977
1334.0916	1346.1351		1368.5016
1378.1274	1381.6072		1395.6948
1404.7837	1432.2437		1438.7110
1446.7332	1460.7677		1471.8527
1474.0671	1486.4598		1491.0705
1605.2944	1650.8129		1860.5596

2355.2559	3031.7531	3047.1522
3059.9908	3065.5926	3069.6083
3081.2719	3094.9107	3112.9566
3136.2405	3138.5535	3140.5032
3142.4898	3147.8034	3174.1859
3192.0997	3199.7887	3839.6186

Zero-point correction (Hartree): 0.271868

TS.ApineneCI.J.a+H2O.HHP.tmtu

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E(RM062X/CC-pVDZ) (Hartree): -692.37227300

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.097533  | 0.950434  | -0.625717 |
| H | 0.346835  | 0.991202  | -1.697105 |
| C | 1.245059  | 1.542810  | 0.182361  |
| C | 2.566685  | 0.887262  | -0.031208 |
| H | 1.360264  | 2.613406  | -0.052961 |
| H | 1.049219  | 1.492988  | 1.265781  |
| H | 3.504664  | 1.429685  | 0.112979  |
| C | -0.493223 | -0.465120 | -0.308816 |
| C | -1.298600 | 1.566115  | -0.390747 |
| C | -0.086868 | -1.618972 | -1.211718 |
| C | -0.317780 | -0.846830 | 1.157466  |
| H | -0.661042 | -0.057696 | 1.845517  |
| H | -0.884098 | -1.757585 | 1.387170  |
| H | 0.749214  | -1.035402 | 1.351016  |
| H | -0.788895 | -2.454456 | -1.067004 |
| H | 0.931950  | -1.965755 | -0.989990 |
| H | -0.119940 | -1.320972 | -2.271003 |
| H | -1.622775 | 2.375232  | -1.057627 |
| H | -1.414629 | 1.894896  | 0.653969  |
| C | -1.886906 | 0.155566  | -0.611324 |
| H | -2.117244 | 0.021004  | -1.683249 |
| C | -3.110013 | -0.302856 | 0.149360  |
| C | -4.232634 | 0.701042  | 0.285848  |
| H | -4.468245 | 1.144431  | -0.693386 |
| H | -3.912998 | 1.524516  | 0.943012  |
| H | -5.117563 | 0.214364  | 0.710057  |
| O | -3.189496 | -1.422925 | 0.601548  |
| O | 2.596438  | -0.147352 | -0.769418 |
| O | 3.861333  | -0.781989 | -0.603682 |
| O | 3.226985  | -0.055405 | 1.628525  |
| H | 3.708161  | -0.575042 | 0.817976  |
| H | 2.595530  | -0.690152 | 1.996024  |

Rotational constants (GHz): 1.4294400 0.3551300 0.3381200

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i457.2429 | 19.3522   | 44.7205   |
| 64.8876   | 86.0614   | 118.9769  |
| 130.6415  | 152.6359  | 212.3525  |
| 230.9247  | 256.2279  | 265.0049  |
| 278.9540  | 307.5731  | 316.9501  |
| 318.9034  | 362.6987  | 392.5975  |
| 407.0076  | 460.5329  | 474.0728  |
| 506.0960  | 525.7906  | 562.6491  |
| 596.0290  | 598.6261  | 617.6663  |
| 678.9312  | 719.9716  | 768.0586  |
| 862.0004  | 907.7880  | 923.6623  |
| 925.7114  | 955.9751  | 962.2890  |
| 979.9174  | 993.1027  | 1009.1199 |
| 1021.8778 | 1031.1931 | 1104.7095 |
| 1114.9547 | 1118.4728 | 1149.5432 |
| 1169.3861 | 1181.5976 | 1193.6084 |
| 1229.8771 | 1241.7745 | 1260.8486 |
| 1290.0617 | 1294.0385 | 1310.0135 |
| 1339.5948 | 1347.2792 | 1368.8218 |
| 1380.5564 | 1395.0689 | 1395.2869 |
| 1413.8091 | 1421.5710 | 1432.5600 |
| 1446.6857 | 1451.5634 | 1462.4389 |
| 1469.3789 | 1477.0206 | 1481.6355 |
| 1589.5171 | 1614.5195 | 1860.1855 |
| 2146.6371 | 3048.6881 | 3053.9809 |
| 3058.5258 | 3064.7936 | 3068.0021 |
| 3070.5325 | 3084.1838 | 3110.0469 |
| 3132.6334 | 3132.9067 | 3139.0880 |
| 3141.4675 | 3155.1421 | 3172.6653 |
| 3191.8974 | 3199.0214 | 3854.8169 |

Zero-point correction (Hartree): 0.270826

TS.ApineneCI.J.a+H2O.HHP.ttpd

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E(RM062X/CC-pVDZ) (Hartree): -692.36927511

Electronic state : 1-A

Cartesian coordinates (Angs):

C	0.027712	1.198124	0.923555
H	-0.255139	2.045376	1.567827
C	1.530083	1.366844	0.674480
C	2.259415	0.400859	-0.197558
H	1.689028	2.342324	0.176050
H	2.065163	1.411151	1.634497
H	1.965828	0.219149	-1.232041
C	-1.039551	1.121522	-0.213713
C	-0.546965	-0.092493	1.542067
C	-1.756594	2.418074	-0.551915
C	-0.572711	0.427401	-1.491143
H	-0.060080	-0.524181	-1.283755
H	-1.441232	0.217441	-2.132182
H	0.107275	1.080926	-2.060904
H	-2.644007	2.200511	-1.165218
H	-1.101975	3.098140	-1.120679
H	-2.089997	2.939012	0.358191
H	-0.637795	-0.126514	2.635451

H	-0.013238	-0.976895	1.182517
C	-1.831187	0.144994	0.724135
H	-2.584433	0.715022	1.288495
C	-2.549645	-0.990521	0.021314
C	-2.041888	-2.397374	0.225400
H	-2.012799	-2.637736	1.299536
H	-1.007626	-2.480082	-0.147561
H	-2.690411	-3.101658	-0.306557
O	-3.480668	-0.738869	-0.711650
O	3.471751	0.161847	0.103241
O	3.927604	-0.898660	-0.732897
O	1.731697	-1.594602	-0.040999
H	2.761806	-1.565786	-0.450008
H	1.874558	-1.878517	0.875052
Rotational constants (GHz):			
	1.0705600	0.4264400	0.3628300
Vibrational harmonic frequencies (cm-1):			
i531.7553	22.0422		44.9456
78.3755	88.6115		143.2693
169.7836	181.9682		220.5126
230.0683	253.3130		256.2664
288.8980	305.2234		323.3755
353.0703	386.4626		404.2973
434.8303	469.9993		481.6388
493.2425	537.8690		586.9994
609.0601	624.3596		643.5632
658.4350	717.4190		763.7630
831.9146	890.7561		923.8532
939.1413	957.0142		967.6845
985.5370	993.0979		1007.0600
1029.1999	1053.5247		1072.4188
1099.7770	1144.3660		1172.7361
1177.3638	1192.7902		1216.6719
1234.6096	1243.7211		1252.5183
1268.9927	1298.0038		1317.7332
1327.4429	1344.4436		1365.4097
1378.6200	1390.0685		1397.3797
1410.4706	1426.5979		1436.8223
1445.6612	1457.5237		1465.0400
1471.5089	1487.9930		1497.1804
1609.8214	1623.0640		1854.9398
1883.4750	3031.4271		3045.3065
3050.1434	3055.0328		3069.4048
3093.9714	3107.7322		3117.5912
3125.8138	3129.1640		3130.4808
3140.4981	3148.9478		3191.1865
3203.2580	3235.4664		3829.0566
Zero-point correction (Hartree): 0.271148			

Z-pinonaldehyde-A-oxide
#####

Population analysis as 298K (%)
Total partition function, Relative energy (kcal/mol), Boltzmann-weighted Q(T)

Compound	Qtot	Erel	Erel2	n*Q*MB	%
TS.ApineneCI.J.b+H2O.HHP.pmpd	9.975e+44	0.00	0.00	9.975e+44	66.6
TS.ApineneCI.J.b+H2O.HHP.pppu	2.210e+45	1.98	1.98	7.836e+43	5.23
TS.ApineneCI.J.b+H2O.HHP.pmpu	9.238e+44	1.53	1.53	7.011e+43	4.68
TS.ApineneCI.J.b+H2O.HHP.pppd	3.090e+45	2.40	2.40	5.382e+43	3.59
TS.ApineneCI.J.b+H2O.HHP.ppmu	2.449e+45	2.29	2.29	5.162e+43	3.44
TS.ApineneCI.J.b+H2O.HHP.mmpd	1.423e+45	2.02	2.02	4.657e+43	3.11
TS.ApineneCI.J.b+H2O.HHP.mpmu	1.943e+45	2.30	2.30	4.013e+43	2.68
TS.ApineneCI.J.b+H2O.HHP.pmmu	1.468e+45	2.17	2.17	3.736e+43	2.49
TS.ApineneCI.J.b+H2O.HHP.pppd	2.495e+45	2.71	2.71	2.579e+43	1.72
TS.ApineneCI.J.b+H2O.HHP.pmmu	2.274e+45	2.67	2.67	2.496e+43	1.67
TS.ApineneCI.J.b+H2O.HHP.pmtu	1.033e+45	2.38	2.38	1.857e+43	1.24
TS.ApineneCI.J.b+H2O.HHP.pmtu	5.323e+44	2.28	2.28	1.137e+43	0.758
TS.ApineneCI.J.b+H2O.HHP.mppd	2.169e+45	3.41	3.41	6.879e+42	0.459
TS.ApineneCI.J.b+H2O.HHP.mmmu	2.257e+45	3.52	3.52	5.961e+42	0.398
TS.ApineneCI.J.b+H2O.HHP.mmmu	2.690e+45	3.77	3.77	4.621e+42	0.308
TS.ApineneCI.J.b+H2O.HHP.mmpu	1.420e+45	3.46	3.46	4.145e+42	0.277
TS.ApineneCI.J.b+H2O.HHP.mppu	2.761e+45	3.86	3.86	4.101e+42	0.274
TS.ApineneCI.J.b+H2O.HHP.ptmu	8.037e+44	3.13	3.13	4.081e+42	0.272
TS.ApineneCI.J.b+H2O.HHP.pptu	9.321e+44	3.28	3.28	3.656e+42	0.244
TS.ApineneCI.J.b+H2O.HHP.pptd	1.736e+45	3.73	3.73	3.208e+42	0.214
TS.ApineneCI.J.b+H2O.HHP.mppd	3.036e+45	4.30	4.30	2.140e+42	0.143
TS.ApineneCI.J.b+H2O.HHP.mptu	1.047e+45	4.02	4.02	1.189e+42	0.0794
TS.ApineneCI.J.b+H2O.HHP.mmtu	7.479e+44	4.26	4.26	5.620e+41	0.0375
TS.ApineneCI.J.b+H2O.HHP.mptd	1.928e+45	4.87	4.87	5.133e+41	0.0342
TS.ApineneCI.J.b+H2O.HHP.mtpd	8.463e+44	4.46	4.46	4.555e+41	0.0304
TS.ApineneCI.J.b+H2O.HHP.ptmd	1.050e+45	4.60	4.60	4.431e+41	0.0296
TS.ApineneCI.J.b+H2O.HHP.ptpd	7.822e+44	4.46	4.46	4.196e+41	0.028
TS.ApineneCI.J.b+H2O.HHP.mtmu	1.652e+45	5.34	5.34	1.989e+41	0.0133
TS.ApineneCI.J.b+H2O.HHP.mtpu	1.174e+45	6.08	6.08	4.066e+40	0.00271
TS.ApineneCI.J.b+H2O.HHP.mtmd	1.407e+45	6.77	6.77	1.534e+40	0.00102
TS.ApineneCI.J.b+H2O.HHP.pttd	1.102e+45	9.79	9.79	7.285e+37	4.86e-06
TS.ApineneCI.J.b+H2O.HHP.tttu	3.892e+44	9.19	9.19	7.096e+37	4.73e-06
TS.ApineneCI.J.b+H2O.HHP.tttu	1.229e+45	10.65	10.65	1.904e+37	1.27e-06
TS.ApineneCI.J.b+H2O.HHP.pttu	1.140e+45	11.45	11.45	4.598e+36	3.07e-07
Total				1.499e+45	100

TS.ApineneCI.J.b+H2O.HHP.mmmu
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E(RM062X/CC-pVDZ) (Hartree): -692.36924228  
Electronic state : 1-A  
Cartesian coordinates (Angs):

|   |          |           |           |
|---|----------|-----------|-----------|
| C | 0.245379 | -0.462879 | 0.394027  |
| H | 0.593466 | -0.397969 | 1.434204  |
| C | 1.448363 | -0.709848 | -0.497595 |
| C | 2.448953 | 0.396030  | -0.459256 |

|                                                           |           |           |           |
|-----------------------------------------------------------|-----------|-----------|-----------|
| H                                                         | 1.950347  | -1.655926 | -0.270732 |
| H                                                         | 1.140589  | -0.748938 | -1.560367 |
| H                                                         | 2.078945  | 1.431240  | -0.477452 |
| C                                                         | -0.742469 | 0.719719  | 0.117033  |
| C                                                         | -0.941032 | -1.445260 | 0.303242  |
| C                                                         | -0.567491 | 1.984314  | 0.943653  |
| C                                                         | -0.861648 | 1.056632  | -1.368522 |
| H                                                         | -1.049812 | 0.163225  | -1.984610 |
| H                                                         | -1.694424 | 1.752134  | -1.532571 |
| H                                                         | 0.062607  | 1.529516  | -1.738190 |
| H                                                         | -1.470374 | 2.608332  | 0.861904  |
| H                                                         | 0.288330  | 2.585070  | 0.594590  |
| H                                                         | -0.404899 | 1.745222  | 2.005399  |
| H                                                         | -0.956251 | -2.293962 | 0.998270  |
| H                                                         | -1.073708 | -1.819329 | -0.723716 |
| C                                                         | -1.866148 | -0.243058 | 0.594868  |
| H                                                         | -1.989471 | -0.139356 | 1.687738  |
| C                                                         | -3.251635 | -0.147091 | -0.001484 |
| C                                                         | -4.055388 | -1.425882 | -0.054047 |
| H                                                         | -4.031930 | -1.931221 | 0.923239  |
| H                                                         | -3.600788 | -2.115364 | -0.782163 |
| H                                                         | -5.087078 | -1.206088 | -0.349365 |
| O                                                         | -3.694614 | 0.910197  | -0.392143 |
| O                                                         | 3.653624  | 0.304624  | -0.856959 |
| O                                                         | 4.197807  | -0.947376 | -0.437416 |
| O                                                         | 2.962914  | -0.013043 | 1.483712  |
| H                                                         | 3.634121  | -0.597947 | 0.905349  |
| H                                                         | 3.511170  | 0.720094  | 1.799401  |
| Rotational constants (GHz): 1.5242500 0.3199500 0.3053100 |           |           |           |
| Vibrational harmonic frequencies (cm-1):                  |           |           |           |
| i443.8849                                                 | 26.9280   | 43.4356   |           |
| 62.0142                                                   | 64.4959   | 125.4784  |           |
| 137.0250                                                  | 168.0032  | 209.1424  |           |
| 215.4837                                                  | 220.2403  | 268.5105  |           |
| 293.4301                                                  | 303.5104  | 316.7625  |           |
| 332.9295                                                  | 363.4904  | 396.9249  |           |
| 408.3890                                                  | 434.3918  | 475.0669  |           |
| 514.2094                                                  | 533.6003  | 589.2444  |           |
| 601.3956                                                  | 615.4121  | 638.5725  |           |
| 659.3353                                                  | 725.2194  | 784.6533  |           |
| 825.3531                                                  | 872.1254  | 902.1079  |           |
| 923.2398                                                  | 950.7407  | 961.4757  |           |
| 970.7234                                                  | 984.5735  | 1013.5126 |           |
| 1024.7657                                                 | 1028.2664 | 1080.9173 |           |
| 1113.0415                                                 | 1119.7916 | 1154.1273 |           |
| 1171.4386                                                 | 1189.5112 | 1202.4646 |           |
| 1231.7135                                                 | 1241.4826 | 1264.4618 |           |
| 1267.2111                                                 | 1295.6114 | 1321.9532 |           |
| 1336.5950                                                 | 1346.4698 | 1366.1529 |           |
| 1381.0451                                                 | 1384.3974 | 1396.9970 |           |
| 1409.2802                                                 | 1431.5178 | 1432.1063 |           |
| 1445.9516                                                 | 1449.6901 | 1465.0189 |           |
| 1472.7256                                                 | 1474.8655 | 1485.4338 |           |
| 1613.5265                                                 | 1644.3613 | 1857.7225 |           |
| 2268.8497                                                 | 3037.3839 | 3045.1940 |           |
| 3049.5952                                                 | 3053.3637 | 3065.8751 |           |
| 3076.0303                                                 | 3113.9293 | 3121.3412 |           |
| 3123.1473                                                 | 3138.9347 | 3141.1081 |           |
| 3148.1570                                                 | 3156.1024 | 3165.8668 |           |
| 3175.3785                                                 | 3192.1226 | 3843.1483 |           |
| Zero-point correction (Hartree): 0.270982                 |           |           |           |
| TS.ApineneCI.J.b+H2O.HHP.mmmu                             |           |           |           |
| ~~~~~                                                     |           |           |           |
| E(RM062X/CC-pVDZ) (Hartree): -692.37011206                |           |           |           |
| Electronic state : 1-A                                    |           |           |           |
| Cartesian coordinates (Angs):                             |           |           |           |
| C                                                         | -0.287527 | -0.479835 | -0.300233 |
| H                                                         | -0.695549 | -0.416654 | -1.320451 |
| C                                                         | -1.460390 | -0.750305 | 0.642815  |
| C                                                         | -2.428207 | 0.382577  | 0.503671  |
| H                                                         | -1.935563 | -1.692188 | 0.353315  |
| H                                                         | -1.141647 | -0.814165 | 1.691906  |
| H                                                         | -2.417948 | 1.196505  | 1.241177  |
| C                                                         | 0.690230  | 0.711901  | -0.054649 |
| C                                                         | 0.911450  | -1.449358 | -0.272498 |
| C                                                         | 0.438611  | 1.979240  | -0.854825 |
| C                                                         | 0.860654  | 1.033219  | 1.428890  |
| H                                                         | 1.086979  | 0.137090  | 2.027877  |
| H                                                         | 1.684130  | 1.743928  | 1.572441  |
| H                                                         | -0.061375 | 1.483778  | 1.831878  |
| H                                                         | 1.306656  | 2.651506  | -0.778578 |
| H                                                         | -0.447385 | 2.517293  | -0.480974 |
| H                                                         | 0.265394  | 1.749010  | -1.916583 |
| H                                                         | 0.903703  | -2.288011 | -0.979699 |
| H                                                         | 1.095601  | -1.833813 | 0.742632  |
| C                                                         | 1.806434  | -0.229128 | -0.590271 |
| H                                                         | 1.881550  | -0.113782 | -1.686141 |
| C                                                         | 3.214123  | -0.128912 | -0.050188 |
| C                                                         | 4.042501  | -1.392972 | -0.092980 |
| H                                                         | 3.989641  | -1.849141 | -1.093027 |
| H                                                         | 3.629675  | -2.126850 | 0.616340  |
| H                                                         | 5.081067  | -1.167404 | 0.172481  |
| O                                                         | 3.655889  | 0.916962  | 0.370963  |
| O                                                         | -2.916071 | 0.747677  | -0.614946 |
| O                                                         | -3.229707 | -0.424566 | -1.369741 |
| O                                                         | -4.036005 | -0.761617 | 0.970128  |
| H                                                         | -3.939879 | -0.883602 | -0.065328 |
| H                                                         | -4.805164 | -0.179716 | 1.061094  |
| Rotational constants (GHz): 1.5059500 0.3353800 0.3188700 |           |           |           |
| Vibrational harmonic frequencies (cm-1):                  |           |           |           |
| i415.1280                                                 | 40.3573   | 46.2382   |           |

|                                                           |           |           |           |
|-----------------------------------------------------------|-----------|-----------|-----------|
| 55.8813                                                   | 63.9828   | 119.7290  |           |
| 128.4552                                                  | 156.8884  | 200.1019  |           |
| 210.4781                                                  | 215.0565  | 268.2747  |           |
| 285.9728                                                  | 305.2908  | 310.0628  |           |
| 322.5016                                                  | 375.6171  | 392.0833  |           |
| 395.8588                                                  | 430.3937  | 494.5363  |           |
| 514.6404                                                  | 537.2792  | 590.6302  |           |
| 605.8135                                                  | 617.0232  | 642.2615  |           |
| 679.1651                                                  | 730.5556  | 770.2209  |           |
| 865.7705                                                  | 884.9503  | 909.9847  |           |
| 933.6664                                                  | 949.8031  | 957.3317  |           |
| 971.2983                                                  | 987.9646  | 999.6203  |           |
| 1017.5828                                                 | 1027.3861 | 1058.4279 |           |
| 1102.8835                                                 | 1115.2986 | 1148.6962 |           |
| 1170.3328                                                 | 1188.4773 | 1202.1387 |           |
| 1230.6303                                                 | 1242.1166 | 1265.8683 |           |
| 1277.9258                                                 | 1297.1632 | 1315.0539 |           |
| 1325.1141                                                 | 1341.2193 | 1358.8052 |           |
| 1380.0597                                                 | 1383.0687 | 1394.5694 |           |
| 1403.0676                                                 | 1432.2056 | 1440.5003 |           |
| 1446.4808                                                 | 1450.9769 | 1460.5151 |           |
| 1470.7680                                                 | 1473.1358 | 1483.1559 |           |
| 1598.1982                                                 | 1653.4110 | 1858.1971 |           |
| 2454.7002                                                 | 3046.6310 | 3049.1528 |           |
| 3052.3783                                                 | 3064.6186 | 3075.1451 |           |
| 3093.8746                                                 | 3112.4291 | 3118.8944 |           |
| 3126.5240                                                 | 3139.5878 | 3139.9534 |           |
| 3148.8048                                                 | 3162.3597 | 3165.6860 |           |
| 3185.4741                                                 | 3191.5186 | 3843.9744 |           |
| Zero-point correction (Hartree): 0.271446                 |           |           |           |
| TS.ApineneCI.J.b+H2O.HHP.mmpd                             |           |           |           |
| ~~~~~                                                     |           |           |           |
| E(RM062X/CC-pVDZ) (Hartree): -692.37270986                |           |           |           |
| Electronic state : 1-A                                    |           |           |           |
| Cartesian coordinates (Angs):                             |           |           |           |
| C                                                         | -0.147559 | 0.743837  | 0.782104  |
| H                                                         | -0.276425 | 0.763656  | 1.878475  |
| C                                                         | -1.470904 | 1.091583  | 0.096901  |
| C                                                         | -2.520263 | 0.181323  | 0.636420  |
| H                                                         | -1.758743 | 2.123185  | 0.340355  |
| H                                                         | -1.410511 | 0.975177  | -0.989926 |
| H                                                         | -2.765376 | 0.258472  | 1.705456  |
| C                                                         | 0.631302  | -0.555908 | 0.404282  |
| C                                                         | 1.103179  | 1.574963  | 0.421883  |
| C                                                         | 0.443850  | -1.757308 | 1.315303  |
| C                                                         | 0.438033  | -0.949820 | -1.059401 |
| H                                                         | 0.650890  | -0.108736 | -1.740233 |
| H                                                         | 1.130762  | -1.762052 | -1.316756 |
| H                                                         | -0.597563 | -1.273255 | -1.245950 |
| H                                                         | 1.208890  | -2.515389 | 1.090841  |
| H                                                         | -0.547725 | -2.211140 | 1.162610  |
| H                                                         | 0.541636  | -1.474096 | 2.375432  |
| H                                                         | 1.335761  | 2.444804  | 1.049310  |
| H                                                         | 1.077956  | 1.886337  | -0.632689 |
| C                                                         | 1.925796  | 0.282560  | 0.620106  |
| H                                                         | 2.241055  | 0.205023  | 1.675902  |
| C                                                         | 3.148120  | -0.026144 | -0.215790 |
| C                                                         | 3.982853  | 1.146070  | -0.677524 |
| H                                                         | 4.175325  | 1.834781  | 0.158934  |
| H                                                         | 3.424390  | 1.712741  | -1.438890 |
| H                                                         | 4.924081  | 0.786646  | -1.107579 |
| O                                                         | 3.441119  | -1.170370 | -0.479957 |
| O                                                         | -2.819240 | -0.962200 | 0.159434  |
| O                                                         | -2.860357 | -0.894598 | -1.264903 |
| O                                                         | -4.011317 | 1.126292  | -0.389752 |
| H                                                         | -3.702666 | 0.376364  | -1.051318 |
| H                                                         | -4.859822 | 0.797553  | -0.058256 |
| Rotational constants (GHz): 1.4224100 0.3544700 0.3297400 |           |           |           |
| Vibrational harmonic frequencies (cm-1):                  |           |           |           |
| i407.5676                                                 | 26.3302   | 48.7247   |           |
| 65.8645                                                   | 92.9756   | 135.8475  |           |
| 151.6543                                                  | 162.7711  | 195.9822  |           |
| 223.2860                                                  | 239.0052  | 259.8410  |           |
| 279.8295                                                  | 314.7310  | 324.3982  |           |
| 341.1827                                                  | 378.4098  | 392.9379  |           |
| 409.3502                                                  | 427.7259  | 497.6698  |           |
| 510.5124                                                  | 532.5195  | 575.6952  |           |
| 603.6127                                                  | 619.0215  | 629.9083  |           |
| 648.5256                                                  | 723.4661  | 771.5023  |           |
| 868.8288                                                  | 888.9600  | 910.4699  |           |
| 923.9089                                                  | 956.6256  | 962.8041  |           |
| 975.7921                                                  | 994.8581  | 1017.0159 |           |
| 1021.8907                                                 | 1037.6313 | 1051.1069 |           |
| 1101.9303                                                 | 1116.4005 | 1149.7221 |           |
| 1168.6027                                                 | 1190.8135 | 1205.1363 |           |
| 1232.6710                                                 | 1237.2853 | 1258.5680 |           |
| 1266.2063                                                 | 1294.2681 | 1306.4630 |           |
| 1319.6605                                                 | 1340.7485 | 1363.6892 |           |
| 1377.5406                                                 | 1384.1535 | 1401.6055 |           |
| 1411.0538                                                 | 1431.7357 | 1440.8659 |           |
| 1445.6363                                                 | 1457.5681 | 1468.1553 |           |
| 1470.6113                                                 | 1486.2267 | 1490.1464 |           |
| 1599.4908                                                 | 1652.8989 | 1860.2526 |           |
| 2456.1276                                                 | 3043.0625 | 3045.9601 |           |
| 3048.6192                                                 | 3051.3028 | 3065.1782 |           |
| 3082.9799                                                 | 3109.5036 | 3125.4721 |           |
| 3127.0734                                                 | 3140.0395 | 3140.6593 |           |
| 3146.5471                                                 | 3155.7047 | 3162.3530 |           |
| 3191.4064                                                 | 3192.0436 | 3841.0262 |           |
| Zero-point correction (Hartree): 0.271668                 |           |           |           |

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TS.ApineneCI.J.b+H2O.HHP.mmpu
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E(RM062X/CC-pVDZ) (Hartree): -692.36965652
Electronic state : 1-A
Cartesian coordinates (Angs):
C -0.171638 0.643967 0.712820
H -0.339418 0.596200 1.803228
C -1.458965 1.041717 0.008714
C -2.698305 0.518789 0.652022
H -1.589346 2.139283 0.098744
H -1.463360 0.817113 -1.062478
H -2.699567 0.391491 1.744551
C 0.657582 -0.617610 0.295994
C 1.076337 1.515197 0.452826
C 0.478291 -1.872720 1.132270
C 0.536286 -0.936808 -1.192198
H 0.692611 -0.046113 -1.822579
H 1.295055 -1.678271 -1.474678
H -0.462004 -1.343039 -1.402397
H 1.275700 -2.592705 0.894203
H -0.495148 -2.335979 0.918777
H 0.535185 -1.643826 2.208458
H 1.264818 2.356612 1.132605
H 1.086871 1.883004 -0.584491
C 1.921851 0.234774 0.611234
H 2.192760 0.104131 1.674413
C 3.191830 0.016678 -0.179701
C 4.043220 1.234989 -0.455624
H 4.186869 1.818867 0.466069
H 3.523714 1.889354 -1.172777
H 5.008524 0.928048 -0.872739
O 3.512883 -1.090435 -0.549611
O -3.870219 0.640057 0.175682
O -3.827544 0.405674 -1.232344
O -2.477134 -1.354822 -0.163565
H -3.056767 -0.816585 -0.878272
H -3.119314 -1.945222 0.257917
Rotational constants (GHz): 1.4743400 0.3406300 0.3160600
Vibrational harmonic frequencies (cm-1):
i453.0725 31.4278 40.1643
70.1194 93.1295 135.9609
152.7352 164.6797 187.6880
225.5621 252.8093 256.1675
278.8842 312.0353 323.3619
329.2393 362.2686 395.6941
416.9008 429.9921 479.6885
512.5209 520.5106 591.6175
605.2530 616.3392 634.2332
673.0746 718.0871 771.1286
830.0609 874.4355 899.6403
917.2701 955.6612 959.9582
969.8899 988.6536 1017.7000
1024.1135 1042.8610 1069.7165
1111.0359 1116.0670 1157.0786
1168.7492 1189.3902 1199.2171
1231.6188 1242.5840 1255.2848
1269.5705 1293.7691 1316.6568
1341.9666 1343.4085 1367.5904
1377.6755 1382.9094 1390.7348
1412.8655 1418.0896 1431.5129
1445.7190 1453.5064 1467.1676
1473.4889 1481.3973 1490.5487
1618.0451 1639.3450 1859.1462
2219.0674 3018.6802 3038.9151
3045.3363 3052.2950 3059.8433
3064.1941 3077.4459 3129.3199
3138.2668 3140.9205 3144.7750
3154.1324 3161.3956 3176.8999
3180.4437 3191.1687 3839.2690
Zero-point correction (Hartree): 0.270896

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TS.ApineneCI.J.b+H2O.HHP.mmtD
~~~~~
E(RM062X/CC-pVDZ) (Hartree): -692.36868404
Electronic state : 1-A
Cartesian coordinates (Angs):
C      0.343769      0.809808     -0.251498
H      0.731490      0.871545     -1.274121
C      1.425402      1.230807      0.731132
C      2.861740      0.881651      0.514802
H      1.468979      2.339753      0.743013
H      1.180574      0.939127      1.764147
H      3.559424      1.280725      1.265160
C      -0.441726     -0.536521     -0.096472
C      -0.996738      1.571229     -0.154918
C      -0.024214     -1.710499     -0.966927
C      -0.592738     -0.973541      1.360135
H      -0.971312     -0.161801      2.003612
H      -1.309321     -1.802719      1.425677
H      0.380528     -1.304451      1.748629
H      -0.863394     -2.419993     -1.034538
H      0.836293     -2.241282     -0.534238
H      0.249126     -1.379414     -1.979641
H      -1.122765      2.463493     -0.782590
H      -1.244616      1.826001      0.887541
C      -1.682054      0.260016     -0.593897
H      -1.715366      0.222009     -1.697559
C      -3.064975     -0.107751     -0.109363
C      -4.064263      1.021757      0.008796
H      -4.066870      1.626284     -0.910804
H      -3.766631      1.690308      0.831402
H      -5.062812      0.616807      0.206540

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|                                                           |           |           |           |
|-----------------------------------------------------------|-----------|-----------|-----------|
| O                                                         | -3.359395 | -1.253984 | 0.146977  |
| O                                                         | 3.456820  | 0.609982  | -0.574199 |
| O                                                         | 2.684855  | -0.306627 | -1.348300 |
| O                                                         | 2.607130  | -1.127969 | 0.977801  |
| H                                                         | 2.541973  | -1.092457 | -0.073288 |
| H                                                         | 3.474201  | -1.526895 | 1.142093  |
| Rotational constants (GHz): 1.4284900 0.3849500 0.3577400 |           |           |           |
| Vibrational harmonic frequencies (cm-1):                  |           |           |           |
| i415.1299                                                 | 35.3706   |           | 54.7782   |
| 74.1356                                                   | 100.6354  |           | 134.7728  |
| 149.2531                                                  | 161.2290  |           | 210.9747  |
| 219.7154                                                  | 261.8240  |           | 272.8536  |
| 285.9125                                                  | 307.2812  |           | 317.0413  |
| 336.0333                                                  | 378.9810  |           | 387.3991  |
| 401.0506                                                  | 418.7465  |           | 463.4616  |
| 498.2523                                                  | 526.4665  |           | 573.1547  |
| 591.1233                                                  | 599.3745  |           | 617.2585  |
| 710.5343                                                  | 746.7542  |           | 776.9403  |
| 841.6466                                                  | 869.0157  |           | 903.8308  |
| 921.8296                                                  | 934.7845  |           | 958.3429  |
| 965.2794                                                  | 975.3415  |           | 997.4623  |
| 1025.3581                                                 | 1027.8232 |           | 1044.2011 |
| 1108.7132                                                 | 1121.6572 |           | 1158.6279 |
| 1169.2370                                                 | 1182.9181 |           | 1195.7453 |
| 1232.5424                                                 | 1240.2996 |           | 1268.8538 |
| 1295.2648                                                 | 1296.4947 |           | 1331.3843 |
| 1337.7924                                                 | 1350.9467 |           | 1370.0496 |
| 1378.4825                                                 | 1391.4381 |           | 1394.6853 |
| 1405.4643                                                 | 1431.6933 |           | 1432.9372 |
| 1443.7151                                                 | 1445.9624 |           | 1470.5744 |
| 1472.7977                                                 | 1478.9068 |           | 1489.7737 |
| 1613.7946                                                 | 1638.2157 |           | 1858.4523 |
| 2361.1847                                                 | 3005.8971 |           | 3046.8990 |
| 3052.9454                                                 | 3055.9878 |           | 3063.7467 |
| 3068.3674                                                 | 3107.7800 |           | 3130.1791 |
| 3137.7070                                                 | 3138.1077 |           | 3139.3809 |
| 3147.4845                                                 | 3148.2756 |           | 3152.4596 |
| 3171.3425                                                 | 3190.1567 |           | 3843.0476 |
| Zero-point correction (Hartree): 0.271204                 |           |           |           |
| TS.ApineneCI.J.b+H2O.HHP.mpm                              |           |           |           |
| ~~~~~                                                     |           |           |           |
| E(RM062X/CC-pVDZ) (Hartree): -692.36962186                |           |           |           |
| Electronic state : 1-A                                    |           |           |           |
| Cartesian coordinates (Angs):                             |           |           |           |
| C                                                         | -0.268441 | 0.500259  | -0.659689 |
| H                                                         | -0.385621 | 0.831657  | -1.706679 |
| C                                                         | -1.558540 | 0.742577  | 0.103166  |
| C                                                         | -2.772890 | 0.270895  | -0.620912 |
| H                                                         | -1.551060 | 0.331140  | 1.117018  |
| H                                                         | -1.729825 | 1.834081  | 0.199355  |
| H                                                         | -2.795821 | 0.377388  | -1.715467 |
| C                                                         | 1.055311  | 1.118200  | -0.108267 |
| C                                                         | 0.399681  | -0.891599 | -0.638770 |
| C                                                         | 1.499293  | 2.437019  | -0.717750 |
| C                                                         | 1.060862  | 1.201804  | 1.417314  |
| H                                                         | 0.774501  | 0.247330  | 1.885628  |
| H                                                         | 2.064260  | 1.462120  | 1.777082  |
| H                                                         | 0.351826  | 1.971161  | 1.760135  |
| H                                                         | 2.526238  | 2.670808  | -0.399263 |
| H                                                         | 0.844298  | 3.262286  | -0.394705 |
| H                                                         | 1.481054  | 2.394295  | -1.817650 |
| H                                                         | 0.171980  | -1.581916 | -1.459711 |
| H                                                         | 0.197923  | -1.406458 | 0.310659  |
| C                                                         | 1.761417  | -0.162059 | -0.637324 |
| H                                                         | 2.091151  | 0.007381  | -1.678328 |
| C                                                         | 2.956033  | -0.720649 | 0.100998  |
| C                                                         | 3.147762  | -2.218593 | 0.043222  |
| H                                                         | 3.070277  | -2.573003 | -0.995783 |
| H                                                         | 2.343107  | -2.711680 | 0.610202  |
| H                                                         | 4.119632  | -2.487702 | 0.471011  |
| O                                                         | 3.726248  | 0.006385  | 0.688314  |
| O                                                         | -3.937891 | 0.188968  | -0.117923 |
| O                                                         | -3.841424 | -0.334074 | 1.207548  |
| O                                                         | -2.362620 | -1.695997 | -0.215973 |
| H                                                         | -2.970503 | -1.378179 | 0.597744  |
| H                                                         | -2.960848 | -2.240097 | -0.748902 |
| Rotational constants (GHz): 1.2204600 0.3541800 0.3119700 |           |           |           |
| Vibrational harmonic frequencies (cm-1):                  |           |           |           |
| i453.2886                                                 | 28.4528   |           | 44.8392   |
| 58.2961                                                   | 96.8305   |           | 122.3352  |
| 138.6256                                                  | 161.0895  |           | 179.2548  |
| 224.2838                                                  | 243.0526  |           | 256.9065  |
| 275.8360                                                  | 310.6859  |           | 316.6881  |
| 339.0624                                                  | 350.4607  |           | 382.9556  |
| 414.1862                                                  | 447.1211  |           | 484.4329  |
| 513.4934                                                  | 520.1236  |           | 588.3396  |
| 597.7431                                                  | 625.4415  |           | 643.0853  |
| 674.4493                                                  | 730.6464  |           | 801.9164  |
| 824.4822                                                  | 872.1962  |           | 901.9177  |
| 913.7435                                                  | 947.0891  |           | 954.9484  |
| 969.9173                                                  | 985.6573  |           | 1003.4549 |
| 1020.0198                                                 | 1038.8024 |           | 1064.9582 |
| 1103.2008                                                 | 1141.8330 |           | 1151.9192 |
| 1167.9586                                                 | 1191.9733 |           | 1213.5672 |
| 1226.7807                                                 | 1236.2794 |           | 1246.2773 |
| 1278.2553                                                 | 1294.4547 |           | 1311.8150 |
| 1342.3405                                                 | 1345.2135 |           | 1368.6259 |
| 1380.3374                                                 | 1386.1920 |           | 1396.3381 |
| 1412.6060                                                 | 1422.8618 |           | 1432.2792 |
| 1445.2612                                                 | 1451.8389 |           | 1463.9211 |
| 1465.2196                                                 | 1477.4279 |           | 1485.1576 |

|           |           |           |
|-----------|-----------|-----------|
| 1615.7952 | 1641.7312 | 1858.1720 |
| 2238.7173 | 3019.1323 | 3039.2104 |
| 3043.0188 | 3044.9255 | 3058.7330 |
| 3065.0782 | 3099.4303 | 3122.7046 |
| 3130.2981 | 3137.6900 | 3140.2886 |
| 3150.7874 | 3159.1049 | 3166.8452 |
| 3184.7158 | 3192.0871 | 3843.6893 |

Zero-point correction (Hartree): 0.270783

TS.ApineneCI.J.b+H2O.HHP.mpmu

~~~~~  
E(RM062X/CC-pVDZ) (Hartree): -692.37223806

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-0.279603	0.717630	-0.745990
H	-0.335121	1.164642	-1.752776
C	-1.596935	0.928289	0.006550
C	-2.632546	0.116632	-0.692881
H	-1.505293	0.577822	1.037191
H	-1.904476	1.982408	-0.002744
H	-3.093517	0.514955	-1.607469
C	1.054688	1.178510	-0.069609
C	0.284404	-0.719208	-0.838531
C	1.633044	2.501655	-0.540937
C	0.985313	1.130241	1.454320
H	0.605167	0.162963	1.819319
H	1.986664	1.277936	1.878454
H	0.320381	1.921998	1.832830
H	2.660632	2.614522	-0.163915
H	1.034795	3.349300	-0.170109
H	1.661965	2.555387	-1.640042
H	0.076056	-1.285428	-1.755160
H	-0.041533	-1.317704	0.024983
C	1.691524	-0.106594	-0.672998
H	2.115048	0.127868	-1.666006
C	2.781050	-0.823219	0.093167
C	2.809259	-2.329351	-0.013450
H	2.730834	-2.639295	-1.066506
H	1.933243	-2.746058	0.507198
H	3.728398	-2.718908	0.437482
O	3.595577	-0.204292	0.741821
O	-2.690667	-1.155694	-0.639392
O	-2.425509	-1.583876	0.699795
O	-3.985546	0.364140	0.800549
H	-3.466498	-0.494557	1.092242
H	-4.838765	0.022414	0.494991

Rotational constants (GHz): 1.1310500 0.3949700 0.3388900

Vibrational harmonic frequencies (cm-1):

i402.0570	36.0676	40.4426
53.8372	95.2760	115.0016
143.5454	160.1289	181.3253
229.1102	237.0678	260.8597
278.4893	302.0991	324.2788
336.6246	352.2527	402.7798
411.3414	438.1326	503.1546
509.4950	527.6537	585.2211
597.1753	628.4913	633.9877
660.2622	733.3221	794.2785
869.7205	878.6723	902.3892
918.9982	953.9228	962.9446
973.2808	996.0100	997.9223
1012.1985	1034.2560	1043.4693
1098.4785	1132.6964	1146.0578
1167.8501	1190.9894	1215.7351
1235.4180	1242.9010	1259.0179
1281.3325	1290.7472	1309.2388
1313.6208	1341.8226	1362.0254
1376.0167	1381.3560	1394.8303
1402.3248	1432.2328	1436.5632
1444.9317	1452.5289	1463.7519
1473.3118	1477.5776	1485.9421
1596.7214	1654.0060	1856.6947
2484.4947	3045.9044	3047.3275
3052.3289	3055.8295	3064.3161
3089.4699	3113.7112	3125.4176
3128.5700	3138.7679	3139.2208
3151.0350	3157.3645	3164.5780
3192.7230	3207.6801	3841.1717

Zero-point correction (Hartree): 0.271631

TS.ApineneCI.J.b+H2O.HHP.mppd

~~~~~  
E(RM062X/CC-pVDZ) (Hartree): -692.36901687

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.335232 | 0.039345  | -0.264205 |
| H | -0.733677 | 0.110657  | -1.287944 |
| C | -1.510678 | 0.217510  | 0.696513  |
| C | -2.480228 | -0.885089 | 0.414794  |
| H | -1.199427 | 0.146268  | 1.747252  |
| H | -1.979156 | 1.190561  | 0.520442  |
| H | -2.437031 | -1.803616 | 1.015595  |
| C | 0.907521  | 0.972044  | -0.130819 |
| C | 0.593358  | -1.189461 | -0.140035 |
| C | 0.945710  | 2.178560  | -1.052686 |
| C | 1.175633  | 1.387665  | 1.314005  |
| H | 1.199735  | 0.524842  | 1.998702  |
| H | 2.145958  | 1.894339  | 1.388559  |
| H | 0.388754  | 2.074921  | 1.661662  |
| H | 1.942481  | 2.644078  | -1.022936 |
| H | 0.203776  | 2.931728  | -0.743911 |
| H | 0.725624  | 1.891252  | -2.091617 |



|                                                           |           |           |           |
|-----------------------------------------------------------|-----------|-----------|-----------|
| H                                                         | 0.375421  | -2.065765 | -0.764393 |
| H                                                         | 0.700960  | -1.509168 | 0.909032  |
| C                                                         | 1.752035  | -0.259443 | -0.567647 |
| H                                                         | 1.834759  | -0.270613 | -1.669009 |
| C                                                         | 3.150897  | -0.453572 | -0.029856 |
| C                                                         | 3.643005  | -1.879927 | 0.070483  |
| H                                                         | 3.459844  | -2.413311 | -0.874505 |
| H                                                         | 3.078231  | -2.409927 | 0.852981  |
| H                                                         | 4.710378  | -1.889197 | 0.316712  |
| O                                                         | 3.843732  | 0.489897  | 0.279298  |
| O                                                         | -3.006789 | -1.079434 | -0.728048 |
| O                                                         | -3.347786 | 0.191291  | -1.285878 |
| O                                                         | -4.067547 | 0.168675  | 1.103836  |
| H                                                         | -4.007115 | 0.446074  | 0.094555  |
| H                                                         | -4.834534 | -0.422352 | 1.131874  |
| Rotational constants (GHz): 1.3559400 0.3314100 0.3088100 |           |           |           |
| Vibrational harmonic frequencies (cm-1):                  |           |           |           |
| i419.1583                                                 | 32.9920   |           | 43.9102   |
| 47.1062                                                   | 91.2811   |           | 95.9269   |
| 131.4720                                                  | 154.4882  |           | 199.3727  |
| 213.9101                                                  | 225.7534  |           | 260.4881  |
| 276.5382                                                  | 309.1585  |           | 316.9923  |
| 327.3452                                                  | 354.7167  |           | 389.1062  |
| 410.3218                                                  | 440.7248  |           | 507.9443  |
| 516.9696                                                  | 522.2865  |           | 596.3136  |
| 602.5914                                                  | 627.1489  |           | 644.9201  |
| 675.5739                                                  | 737.2812  |           | 790.3311  |
| 869.1342                                                  | 882.8146  |           | 907.5101  |
| 932.2795                                                  | 950.4835  |           | 955.7549  |
| 970.0424                                                  | 989.7579  |           | 1003.6646 |
| 1022.9536                                                 | 1023.4954 |           | 1045.1150 |
| 1100.2064                                                 | 1139.7644 |           | 1146.3124 |
| 1171.4704                                                 | 1189.9177 |           | 1214.0504 |
| 1231.2362                                                 | 1243.3351 |           | 1256.3241 |
| 1283.4625                                                 | 1297.6764 |           | 1316.2529 |
| 1325.7859                                                 | 1342.3132 |           | 1359.5811 |
| 1379.1027                                                 | 1382.9692 |           | 1395.8673 |
| 1404.4569                                                 | 1432.4696 |           | 1443.6655 |
| 1447.0403                                                 | 1453.1550 |           | 1462.7301 |
| 1471.2317                                                 | 1477.7037 |           | 1485.2858 |
| 1603.5651                                                 | 1655.2417 |           | 1860.0362 |
| 2438.8170                                                 | 3050.0221 |           | 3050.9139 |
| 3055.0666                                                 | 3064.4611 |           | 3065.5676 |
| 3091.4143                                                 | 3111.5803 |           | 3125.0069 |
| 3132.4599                                                 | 3137.3925 |           | 3139.8717 |
| 3140.8796                                                 | 3161.2305 |           | 3167.5621 |
| 3186.7679                                                 | 3191.7256 |           | 3838.4225 |
| Zero-point correction (Hartree): 0.271597                 |           |           |           |
| TS.ApineneCI.J.b+H2O.HHP.mppu                             |           |           |           |
| ~~~~~                                                     |           |           |           |
| E(RM062X/CC-pVDZ) (Hartree): -692.36902098                |           |           |           |
| Electronic state : 1-A                                    |           |           |           |
| Cartesian coordinates (Angs):                             |           |           |           |
| C                                                         | -0.292278 | 0.085607  | -0.360963 |
| H                                                         | -0.637691 | 0.254214  | -1.390658 |
| C                                                         | -1.491286 | 0.171279  | 0.565329  |
| C                                                         | -2.493193 | -0.899814 | 0.301800  |
| H                                                         | -1.182743 | -0.016829 | 1.612088  |
| H                                                         | -1.986332 | 1.147721  | 0.540928  |
| H                                                         | -2.119769 | -1.912127 | 0.087612  |
| C                                                         | 0.954486  | 0.982233  | -0.086414 |
| C                                                         | 0.621141  | -1.162845 | -0.316587 |
| C                                                         | 1.049265  | 2.270524  | -0.885929 |
| C                                                         | 1.164800  | 1.256087  | 1.401423  |
| H                                                         | 1.151432  | 0.332490  | 2.002280  |
| H                                                         | 2.136663  | 1.738947  | 1.563582  |
| H                                                         | 0.372117  | 1.919291  | 1.780897  |
| H                                                         | 2.049315  | 2.714359  | -0.768724 |
| H                                                         | 0.303619  | 3.003143  | -0.538971 |
| H                                                         | 0.873684  | 2.086617  | -1.956591 |
| H                                                         | 0.430555  | -1.974133 | -1.031809 |
| H                                                         | 0.676453  | -1.584669 | 0.700130  |
| C                                                         | 1.806995  | -0.212609 | -0.600160 |
| H                                                         | 1.941679  | -0.119576 | -1.692517 |
| C                                                         | 3.178679  | -0.471998 | -0.020605 |
| C                                                         | 3.645696  | -1.909914 | -0.001001 |
| H                                                         | 3.486947  | -2.376515 | -0.984943 |
| H                                                         | 3.047393  | -2.480729 | 0.725945  |
| H                                                         | 4.703688  | -1.953915 | 0.279497  |
| O                                                         | 3.870595  | 0.435691  | 0.382871  |
| O                                                         | -3.690953 | -0.905439 | 0.729959  |
| O                                                         | -4.241601 | 0.406814  | 0.607062  |
| O                                                         | -3.039880 | -0.072537 | -1.491284 |
| H                                                         | -3.700192 | 0.368700  | -0.784904 |
| H                                                         | -3.597937 | -0.714517 | -1.954071 |
| Rotational constants (GHz): 1.3753800 0.3190300 0.2977800 |           |           |           |
| Vibrational harmonic frequencies (cm-1):                  |           |           |           |
| i449.6342                                                 | 32.6466   |           | 42.8349   |
| 48.6824                                                   | 90.6327   |           | 110.1762  |
| 133.0476                                                  | 158.9993  |           | 199.2336  |
| 215.5796                                                  | 228.4364  |           | 251.2103  |
| 277.7433                                                  | 317.8025  |           | 320.6335  |
| 339.8333                                                  | 351.4029  |           | 381.9187  |
| 411.8654                                                  | 443.6665  |           | 491.8629  |
| 511.4403                                                  | 521.4784  |           | 586.7669  |
| 598.3079                                                  | 626.0748  |           | 643.2532  |
| 661.5546                                                  | 735.9511  |           | 813.3296  |
| 825.3803                                                  | 867.0568  |           | 902.8570  |
| 920.1818                                                  | 942.2516  |           | 954.9598  |
| 969.9576                                                  | 987.9809  |           | 1000.8801 |
| 1023.0777                                                 | 1033.7056 |           | 1064.5754 |

|           |           |           |
|-----------|-----------|-----------|
| 1108.3672 | 1150.7777 | 1155.0353 |
| 1169.7560 | 1187.5248 | 1201.8176 |
| 1230.0725 | 1244.0649 | 1253.1593 |
| 1278.6804 | 1295.9939 | 1319.9920 |
| 1336.2013 | 1344.8243 | 1366.6242 |
| 1380.1891 | 1384.7387 | 1396.7608 |
| 1408.8480 | 1428.2196 | 1432.0697 |
| 1446.8958 | 1452.5157 | 1462.8962 |
| 1470.1894 | 1478.0325 | 1485.2560 |
| 1614.9516 | 1644.8828 | 1860.0181 |
| 2259.0130 | 3033.3935 | 3047.7955 |
| 3050.2931 | 3054.4572 | 3062.9017 |
| 3065.3275 | 3110.0635 | 3124.9425 |
| 3129.7271 | 3133.7179 | 3138.4009 |
| 3140.5194 | 3149.8957 | 3166.2733 |
| 3175.3020 | 3192.5586 | 3847.2498 |

Zero-point correction (Hartree): 0.270898

TS.ApineneCI.J.b+H2O.HHP.mptd

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E(RM062X/CC-pVDZ) (Hartree): -692.36752513

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-0.469583	0.288762	-0.160261
H	-0.902981	0.385505	-1.163975
C	-1.516244	0.638185	0.880707
C	-2.822890	-0.086036	0.931759
H	-1.108812	0.475563	1.898206
H	-1.773889	1.707804	0.830196
H	-3.509048	0.250686	1.722506
C	0.886318	1.067826	-0.119368
C	0.308176	-1.036358	-0.062438
C	1.015699	2.246022	-1.070103
C	1.299242	1.474426	1.294509
H	1.260265	0.628598	1.999529
H	2.329577	1.851418	1.293116
H	0.635164	2.266709	1.674915
H	2.060677	2.589365	-1.108579
H	0.388839	3.090158	-0.739830
H	0.703807	1.969289	-2.088476
H	-0.084727	-1.875644	-0.644059
H	0.434338	-1.348278	0.987350
C	1.547091	-0.264131	-0.573512
H	1.565557	-0.304149	-1.677576
C	2.939939	-0.621332	-0.112367
C	3.256768	-2.096831	-0.018223
H	2.948482	-2.612142	-0.940304
H	2.677794	-2.543589	0.804746
H	4.327751	-2.238066	0.163929
O	3.762107	0.230572	0.145028
O	-3.105314	-1.265675	0.550586
O	-2.548775	-1.524807	-0.734630
O	-3.489852	0.756952	-0.829796
H	-3.114819	-0.179004	-1.127664
H	-4.450409	0.646237	-0.877756

Rotational constants (GHz): 1.1999900 0.3828700 0.3341300

Vibrational harmonic frequencies (cm-1):

i421.2245	32.2992	43.7612
68.9414	88.9134	107.2898
134.1472	166.5012	187.7010
216.2602	242.3615	251.8666
279.6784	314.5980	322.4507
332.6783	354.0910	382.3874
403.0389	446.2173	462.5702
505.9657	520.8244	572.5156
596.0326	603.9835	625.9630
722.3710	740.8557	807.2810
850.3936	871.1122	903.3776
921.7709	949.4916	954.1960
963.5025	973.2217	997.1781
1010.4851	1027.1993	1041.2971
1096.3173	1122.0226	1154.2577
1169.4616	1188.3317	1206.5299
1227.5357	1230.5133	1263.8169
1289.6857	1303.7206	1319.9982
1343.6385	1353.8572	1373.2753
1380.9438	1392.1586	1395.9007
1406.8646	1430.0555	1432.6322
1445.8080	1451.2192	1463.2683
1474.3544	1477.2467	1485.4400
1610.5944	1641.1793	1856.3016
2391.2048	3027.4490	3045.1002
3045.8993	3052.5452	3064.8955
3066.2526	3104.7841	3120.8370
3123.1676	3124.9757	3137.7314
3140.7259	3147.9713	3167.0209
3182.5798	3190.6995	3848.0986

Zero-point correction (Hartree): 0.271024

TS.ApineneCI.J.b+H2O.HHP.mptu

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E(RM062X/CC-pVDZ) (Hartree): -692.36891834

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |          |           |
|---|-----------|----------|-----------|
| C | 0.477674  | 0.522899 | 0.304878  |
| H | 0.825355  | 0.721065 | 1.326494  |
| C | 1.555069  | 0.924409 | -0.685690 |
| C | 2.961698  | 0.447328 | -0.520514 |
| H | 1.271431  | 0.673270 | -1.718704 |
| H | 1.673262  | 2.027426 | -0.667324 |
| H | 3.670751  | 0.808176 | -1.279639 |
| C | -0.948282 | 1.135137 | 0.109536  |

|                                                           |           |           |           |
|-----------------------------------------------------------|-----------|-----------|-----------|
| C                                                         | -0.142103 | -0.887152 | 0.253852  |
| C                                                         | -1.283284 | 2.352019  | 0.955570  |
| C                                                         | -1.289982 | 1.390095  | -1.357648 |
| H                                                         | -1.090508 | 0.509448  | -1.988785 |
| H                                                         | -2.354502 | 1.635151  | -1.460614 |
| H                                                         | -0.696278 | 2.230928  | -1.750027 |
| H                                                         | -2.360708 | 2.568886  | 0.897082  |
| H                                                         | -0.736083 | 3.241710  | 0.603336  |
| H                                                         | -1.019918 | 2.185259  | 2.010891  |
| H                                                         | 0.276344  | -1.631053 | 0.942146  |
| H                                                         | -0.136545 | -1.294556 | -0.768029 |
| C                                                         | -1.493256 | -0.229462 | 0.616163  |
| H                                                         | -1.596798 | -0.195400 | 1.715534  |
| C                                                         | -2.798017 | -0.772092 | 0.083322  |
| C                                                         | -2.935612 | -2.277342 | 0.050513  |
| H                                                         | -2.641955 | -2.707420 | 1.019935  |
| H                                                         | -2.247686 | -2.690576 | -0.703128 |
| H                                                         | -3.966319 | -2.553130 | -0.197881 |
| O                                                         | -3.691284 | -0.036331 | -0.275274 |
| O                                                         | 3.563065  | 0.089728  | 0.540860  |
| O                                                         | 2.732121  | -0.772804 | 1.314846  |
| O                                                         | 2.487505  | -1.494139 | -1.032295 |
| H                                                         | 2.467504  | -1.495694 | 0.022722  |
| H                                                         | 3.307981  | -1.960160 | -1.248990 |
| Rotational constants (GHz): 1.1448900 0.4010000 0.3495800 |           |           |           |
| Vibrational harmonic frequencies (cm-1):                  |           |           |           |
| i426.0437                                                 | 40.4861   |           | 55.7982   |
| 68.5580                                                   | 108.7585  |           | 111.2818  |
| 132.7962                                                  | 165.1212  |           | 179.7591  |
| 222.0721                                                  | 248.4960  |           | 262.9458  |
| 271.0940                                                  | 304.1467  |           | 315.5934  |
| 339.0274                                                  | 349.1905  |           | 388.3661  |
| 405.0972                                                  | 441.4715  |           | 466.1884  |
| 504.1489                                                  | 520.0874  |           | 584.1522  |
| 598.5548                                                  | 605.3269  |           | 625.9323  |
| 724.3488                                                  | 750.4700  |           | 793.1798  |
| 847.1730                                                  | 872.1968  |           | 905.0100  |
| 921.0204                                                  | 946.7333  |           | 953.5475  |
| 964.8709                                                  | 972.1271  |           | 994.7313  |
| 1018.4713                                                 | 1022.4861 |           | 1046.4436 |
| 1087.8908                                                 | 1122.9145 |           | 1156.8007 |
| 1170.3240                                                 | 1187.4751 |           | 1208.2476 |
| 1230.5629                                                 | 1233.5687 |           | 1263.5934 |
| 1288.7605                                                 | 1302.2186 |           | 1332.6942 |
| 1342.7884                                                 | 1351.6946 |           | 1370.7360 |
| 1380.3787                                                 | 1391.8195 |           | 1395.6051 |
| 1409.0025                                                 | 1431.8718 |           | 1434.6399 |
| 1445.4630                                                 | 1451.7658 |           | 1463.5675 |
| 1471.1132                                                 | 1476.4569 |           | 1484.3257 |
| 1612.1186                                                 | 1642.8591 |           | 1856.5192 |
| 2344.6451                                                 | 3013.2152 |           | 3044.7911 |
| 3048.0506                                                 | 3053.7151 |           | 3064.5171 |
| 3087.8806                                                 | 3110.7813 |           | 3122.5584 |
| 3124.7030                                                 | 3129.6523 |           | 3138.4831 |
| 3140.0399                                                 | 3148.3804 |           | 3159.4372 |
| 3164.8241                                                 | 3190.0981 |           | 3845.6151 |
| Zero-point correction (Hartree): 0.271048                 |           |           |           |
| TS.ApineneCI.J.b+H2O.HHP.mtmd                             |           |           |           |
| ~~~~~                                                     |           |           |           |
| E(RM062X/CC-pVDZ) (Hartree): -692.36460334                |           |           |           |
| Electronic state : 1-A                                    |           |           |           |
| Cartesian coordinates (Angs):                             |           |           |           |
| C                                                         | 0.131503  | 0.047559  | 1.191653  |
| H                                                         | -0.001636 | 0.336581  | 2.246380  |
| C                                                         | 1.635744  | 0.012641  | 0.945025  |
| C                                                         | 2.066411  | -0.665527 | -0.322073 |
| H                                                         | 2.041875  | 1.031672  | 0.986272  |
| H                                                         | 2.159950  | -0.542895 | 1.739338  |
| H                                                         | 1.319513  | -1.005171 | -1.049183 |
| C                                                         | -0.835880 | 0.945567  | 0.359534  |
| C                                                         | -0.794977 | -1.162322 | 0.927190  |
| C                                                         | -1.094486 | 2.338333  | 0.908937  |
| C                                                         | -0.469306 | 1.023011  | -1.123323 |
| H                                                         | -0.460131 | 0.030644  | -1.603201 |
| H                                                         | -1.217562 | 1.618769  | -1.661619 |
| H                                                         | 0.523770  | 1.480082  | -1.249337 |
| H                                                         | -1.943688 | 2.799577  | 0.382884  |
| H                                                         | -0.212792 | 2.983582  | 0.768082  |
| H                                                         | -1.329055 | 2.306124  | 1.983947  |
| H                                                         | -0.938741 | -1.886834 | 1.738901  |
| H                                                         | -0.523743 | -1.708979 | 0.010457  |
| C                                                         | -1.917397 | -0.132716 | 0.651146  |
| H                                                         | -2.427508 | 0.106744  | 1.601382  |
| C                                                         | -3.003187 | -0.409287 | -0.363337 |
| C                                                         | -3.585004 | -1.804746 | -0.368563 |
| H                                                         | -3.863844 | -2.104662 | 0.652913  |
| H                                                         | -2.824135 | -2.520664 | -0.716176 |
| H                                                         | -4.456382 | -1.842877 | -1.031297 |
| O                                                         | -3.395803 | 0.456086  | -1.113261 |
| O                                                         | 3.155109  | -1.326687 | -0.403728 |
| O                                                         | 4.160749  | -0.571254 | 0.269001  |
| O                                                         | 2.894498  | 0.992580  | -1.134347 |
| H                                                         | 3.673609  | 0.567174  | -0.535068 |
| H                                                         | 3.163542  | 0.790269  | -2.043135 |
| Rotational constants (GHz): 1.2400600 0.3553200 0.3313400 |           |           |           |
| Vibrational harmonic frequencies (cm-1):                  |           |           |           |
| i487.0174                                                 | 39.2352   |           | 47.1507   |
| 64.9724                                                   | 78.6444   |           | 121.7455  |
| 143.1600                                                  | 167.5868  |           | 196.4978  |
| 221.9246                                                  | 238.6915  |           | 250.4526  |
| 275.7173                                                  | 308.1999  |           | 316.4286  |

|           |           |           |
|-----------|-----------|-----------|
| 335.0419  | 355.7770  | 394.9055  |
| 411.2621  | 456.0110  | 498.3821  |
| 519.9043  | 586.3314  | 586.5388  |
| 613.1313  | 619.8053  | 668.7432  |
| 675.0380  | 727.0950  | 781.8122  |
| 817.2782  | 884.4494  | 900.9250  |
| 920.0990  | 952.6405  | 956.8958  |
| 970.7344  | 990.7550  | 1000.9832 |
| 1026.9473 | 1034.6965 | 1046.0556 |
| 1101.6208 | 1127.4683 | 1150.3597 |
| 1173.6839 | 1186.6134 | 1211.5989 |
| 1229.7650 | 1235.0784 | 1253.1098 |
| 1299.9867 | 1310.0771 | 1316.1100 |
| 1333.0018 | 1345.1867 | 1370.2335 |
| 1381.9961 | 1390.1363 | 1397.1643 |
| 1410.2166 | 1414.7352 | 1431.8069 |
| 1446.4269 | 1457.0738 | 1463.3226 |
| 1472.7539 | 1481.3881 | 1489.1687 |
| 1601.6921 | 1635.6492 | 1860.3572 |
| 2176.5791 | 3047.0883 | 3048.9009 |
| 3054.0553 | 3064.5557 | 3065.5645 |
| 3075.2569 | 3088.5108 | 3127.6962 |
| 3130.4446 | 3138.8747 | 3139.1707 |
| 3140.5326 | 3142.2468 | 3164.5526 |
| 3191.7789 | 3193.9800 | 3836.6955 |

Zero-point correction (Hartree): 0.271118

TS.ApineneCI.J.b+H2O.HHP.mtmu

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E(RM062X/CC-pVDZ) (Hartree): -692.36735917

Electronic state : 1-A

Cartesian coordinates (Angs):

C	0.166657	0.242729	1.259320
H	0.003323	0.696876	2.249315
C	1.687769	0.188672	1.052251
C	2.115661	-0.870449	0.089769
H	2.060312	1.158668	0.703313
H	2.180610	-0.052019	2.003114
H	1.926257	-1.917851	0.363291
C	-0.771225	0.989221	0.263149
C	-0.754317	-0.997849	1.160100
C	-1.036318	2.454044	0.563859
C	-0.372021	0.805239	-1.199969
H	-0.311390	-0.257242	-1.484252
H	-1.125898	1.271825	-1.848086
H	0.614009	1.252082	-1.401257
H	-1.874117	2.815102	-0.050837
H	-0.150698	3.066113	0.330535
H	-1.293353	2.606085	1.623701
H	-0.918734	-1.595302	2.066398
H	-0.462325	-1.667305	0.336720
C	-1.866300	-0.025485	0.703796
H	-2.397595	0.366268	1.589379
C	-2.928872	-0.435137	-0.291424
C	-3.393658	-1.872968	-0.253344
H	-3.608187	-2.180679	0.781193
H	-2.588097	-2.526099	-0.623819
H	-4.280384	-1.994417	-0.885007
O	-3.389997	0.371476	-1.066780
O	2.265289	-0.726763	-1.169034
O	2.890260	0.528929	-1.428452
O	4.071578	-0.522231	0.469368
H	3.864734	0.118647	-0.344042
H	4.580228	-1.240142	0.064477

Rotational constants (GHz): 1.2132000 0.3746600 0.3613000

Vibrational harmonic frequencies (cm-1):

1437.2282	23.9024	49.4968
66.1765	95.9349	128.8897
144.0625	152.0125	198.6032
228.1544	234.7053	255.6278
275.0393	313.2317	319.5545
349.8436	366.8248	396.9179
413.1977	444.6660	498.1729
512.0563	577.3256	582.5494
608.0130	620.1995	644.2332
655.3892	726.3942	755.7402
871.2124	879.1174	905.3973
919.8399	932.3166	957.9893
971.6838	988.5357	1012.1607
1026.3378	1031.3001	1039.2151
1122.7420	1134.7971	1152.7194
1169.2632	1186.4723	1211.1944
1233.4071	1237.4291	1259.0496
1299.8301	1302.3061	1315.6903
1328.3911	1341.9391	1363.2452
1378.5658	1385.8788	1398.4585
1411.2693	1430.5732	1437.2062
1445.4550	1453.5609	1465.1559
1470.0003	1482.0134	1489.0298
1602.7489	1649.5811	1861.0920
2347.1140	3046.5681	3048.5133
3057.7031	3063.3204	3068.1968
3075.7405	3112.9637	3126.3099
3132.5802	3137.3692	3140.4440
3141.8037	3156.6724	3161.0031
3178.8864	3191.5143	3843.8187

Zero-point correction (Hartree): 0.271607

TS.ApineneCI.J.b+H2O.HHP.mtpd

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E(RM062X/CC-pVDZ) (Hartree): -692.36913123

Electronic state : 1-A

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Cartesian coordinates (Angs):
C      -0.282988      0.693027      -0.981803
H      -0.168354      1.168898      -1.969197
C      -1.758465      0.894616      -0.602105
C      -2.154723      0.206040      0.667461
H      -1.978108      1.965502      -0.483615
H      -2.369780      0.503542      -1.420542
H      -2.150359      0.764693      1.610764
C      0.911121      1.177962      -0.103028
C      0.352950      -0.711089      -1.052274
C      1.465002      2.558976      -0.412862
C      0.660271      1.031092      1.396450
H      0.294707      0.026135      1.659785
H      1.591090      1.198488      1.953156
H      -0.080518      1.776228      1.730485
H      2.422180      2.706717      0.109506
H      0.769230      3.347804      -0.083702
H      1.638561      2.685003      -1.492354
H      0.276019      -1.249713      -2.004430
H      -0.009933      -1.370360      -0.253492
C      1.694476      -0.030570      -0.693461
H      2.208793      0.287000      -1.618334
C      2.730804      -0.740762      0.146492
C      2.934589      -2.210520      -0.137728
H      3.058533      -2.375312      -1.218720
H      2.036715      -2.769047      0.168657
H      3.807292      -2.580150      0.411537
O      3.374020      -0.149773      0.986213
O      -2.078555      -1.053492      0.851495
O      -2.484712      -1.712995      -0.352369
O      -4.104152      0.121900      0.128481
H      -3.706567      -0.762464      -0.269829
H      -4.610525      -0.180739      0.896926
Rotational constants (GHz):      1.1308400      0.4199800      0.3612900
Vibrational harmonic frequencies (cm-1):
i411.3903      42.6618      57.4065
61.4473      103.2884      130.1066
142.9700      159.2009      180.8716
230.9705      238.9957      258.5046
269.8941      306.0007      327.7031
345.3268      368.8254      395.6059
404.5968      440.5998      490.4737
518.7063      580.4921      592.1885
612.1828      622.1956      651.4901
678.3605      730.2133      757.9513
858.9021      876.9361      901.3364
918.6699      953.7673      962.6709
969.4727      982.6390      1002.1729
1013.5728      1036.1080      1060.1305
1076.1168      1132.1819      1158.8079
1170.0601      1188.8738      1219.3527
1236.3484      1239.0499      1267.2512
1300.2852      1302.0272      1319.2175
1323.2594      1344.6118      1358.0942
1380.8410      1383.5591      1393.1917
1405.9684      1432.1896      1437.2579
1444.8854      1454.3356      1463.4827
1466.8998      1479.9747      1486.9948
1597.7966      1653.0045      1855.5428
2435.0806      3044.1177      3046.2527
3049.1218      3062.6027      3066.3152
3101.3034      3113.0435      3122.2749
3124.6957      3137.6919      3141.6364
3159.4229      3172.3298      3175.4910
3186.5667      3193.3363      3840.9346
Zero-point correction (Hartree): 0.271966

TS.ApineneCI.J.b+H2O.HHP.mtpu
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E(RM062X/CC-pVDZ) (Hartree): -692.36565700
Electronic state : 1-A
Cartesian coordinates (Angs):
C -0.240542 0.513585 -0.938948
H -0.157763 0.832518 -1.989445
C -1.676162 0.789150 -0.504126
C -2.163940 0.020782 0.679067
H -1.772990 1.848612 -0.194169
H -2.391436 0.647541 -1.318733
H -1.466671 -0.215376 1.492833
C 0.987764 1.129122 -0.195149
C 0.416769 -0.878730 -0.821161
C 1.489697 2.464526 -0.718731
C 0.812750 1.190470 1.322457
H 0.607100 0.201671 1.762027
H 1.734448 1.555328 1.792875
H -0.010401 1.872539 1.591063
H 2.469070 2.701038 -0.276438
H 0.792196 3.277163 -0.458538
H 1.599571 2.446567 -1.813612
H 0.289620 -1.577533 -1.656109
H 0.122077 -1.390419 0.106588
C 1.764054 -0.137292 -0.652887
H 2.205126 0.045286 -1.649284
C 2.864914 -0.708232 0.209787
C 3.144053 -2.185563 0.050717
H 3.262345 -2.437481 -1.013945
H 2.284193 -2.764140 0.422226
H 4.044124 -2.458344 0.612337
O 3.498143 -0.010726 0.970796
O -3.376209 0.002478 1.069174
O -4.237167 -0.085956 -0.066380
O -2.396591 -1.678039 -0.431528

```

|                                          |           |           |           |  |
|------------------------------------------|-----------|-----------|-----------|--|
| H                                        | -3.338429 | -1.181490 | -0.506971 |  |
| H                                        | -2.573727 | -2.412445 | 0.174642  |  |
| Rotational constants (GHz):              | 1.1890100 | 0.3731500 | 0.3303900 |  |
| Vibrational harmonic frequencies (cm-1): |           |           |           |  |
| i465.4499                                | 40.7458   |           | 56.5311   |  |
| 67.6143                                  | 75.6984   |           | 126.1309  |  |
| 148.4755                                 | 165.5244  |           | 174.8100  |  |
| 227.7723                                 | 234.3894  |           | 258.5263  |  |
| 280.6542                                 | 302.9725  |           | 330.8709  |  |
| 334.3809                                 | 354.4276  |           | 385.7687  |  |
| 409.3825                                 | 463.9779  |           | 473.5080  |  |
| 524.5444                                 | 576.9053  |           | 591.7065  |  |
| 609.0111                                 | 619.2553  |           | 643.1244  |  |
| 679.7469                                 | 726.2862  |           | 780.2486  |  |
| 805.9590                                 | 878.8183  |           | 901.0875  |  |
| 918.0270                                 | 945.6404  |           | 953.1777  |  |
| 966.8261                                 | 981.8285  |           | 996.3586  |  |
| 1022.4771                                | 1032.6618 |           | 1064.2419 |  |
| 1080.9893                                | 1127.5912 |           | 1163.9853 |  |
| 1173.3924                                | 1185.4589 |           | 1217.9881 |  |
| 1222.1688                                | 1236.3362 |           | 1254.7316 |  |
| 1299.3009                                | 1309.8961 |           | 1317.1637 |  |
| 1343.3996                                | 1346.3442 |           | 1371.3877 |  |
| 1382.0274                                | 1387.2085 |           | 1393.9360 |  |
| 1411.8167                                | 1426.3191 |           | 1432.0979 |  |
| 1446.6225                                | 1453.2968 |           | 1463.3638 |  |
| 1471.1847                                | 1475.4329 |           | 1487.9685 |  |
| 1609.8899                                | 1644.0010 |           | 1858.9037 |  |
| 2202.5696                                | 3032.0474 |           | 3046.3532 |  |
| 3048.8683                                | 3051.5301 |           | 3066.2111 |  |
| 3073.6721                                | 3093.0636 |           | 3122.1119 |  |
| 3126.0095                                | 3139.9121 |           | 3141.4441 |  |
| 3158.3991                                | 3163.1584 |           | 3178.9656 |  |
| 3188.0994                                | 3192.9603 |           | 3841.1234 |  |
| Zero-point correction (Hartree):         | 0.271081  |           |           |  |

TS.ApineneCI.J.b+H2O.HHP.pmm

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E(RM062X/CC-pVDZ) (Hartree): -692.37117669

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.268778 | -0.230455 | -0.635254 |
| H | -0.641720 | 0.362388  | -1.481237 |
| C | -1.461241 | -0.846371 | 0.074802  |
| C | -2.406777 | 0.150139  | 0.655859  |
| H | -2.019482 | -1.530147 | -0.573165 |
| H | -1.123601 | -1.430082 | 0.953171  |
| H | -1.989603 | 1.000082  | 1.214908  |
| C | 0.786430  | 0.616641  | 0.145386  |
| C | 0.861599  | -1.168807 | -1.097552 |
| C | 0.660605  | 2.127070  | 0.019225  |
| C | 0.940980  | 0.195195  | 1.604404  |
| H | 1.086096  | -0.889381 | 1.709262  |
| H | 1.817963  | 0.684921  | 2.056329  |
| H | 0.061028  | 0.490069  | 2.197881  |
| H | 1.551617  | 2.635370  | 0.421632  |
| H | -0.210177 | 2.502150  | 0.581669  |
| H | 0.536685  | 2.427372  | -1.031647 |
| H | 0.824091  | -1.537497 | -2.129537 |
| H | 1.013849  | -2.014752 | -0.412367 |
| C | 1.873718  | -0.058433 | -0.776180 |
| H | 2.073140  | 0.595655  | -1.638491 |
| C | 3.166403  | -0.452468 | -0.098600 |
| C | 4.257810  | 0.592004  | -0.068566 |
| H | 3.853489  | 1.549106  | 0.296275  |
| H | 4.623670  | 0.767985  | -1.091812 |
| H | 5.083208  | 0.257157  | 0.569103  |
| O | 3.298043  | -1.533792 | 0.429673  |
| O | -3.614526 | -0.089512 | 0.975584  |
| O | -4.222579 | -0.896265 | -0.033793 |
| O | -2.947935 | 0.871385  | -1.189495 |
| H | -3.642808 | 0.091587  | -0.995705 |
| H | -3.465969 | 1.676394  | -1.043164 |

|                             |           |           |           |
|-----------------------------|-----------|-----------|-----------|
| Rotational constants (GHz): | 1.5454100 | 0.3240200 | 0.3120400 |
|-----------------------------|-----------|-----------|-----------|

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i445.5454 | 22.5486   | 52.5183   |
| 57.6626   | 75.4783   | 138.9317  |
| 141.5268  | 160.2123  | 208.0094  |
| 218.5374  | 224.6248  | 270.7887  |
| 276.7247  | 309.3575  | 316.0005  |
| 338.7283  | 365.9788  | 387.3913  |
| 400.4753  | 448.3628  | 459.8025  |
| 507.5110  | 573.6606  | 586.0141  |
| 601.8204  | 621.2805  | 634.5387  |
| 651.9503  | 725.9861  | 796.6018  |
| 826.3974  | 873.6144  | 906.6040  |
| 938.8541  | 949.3347  | 961.3159  |
| 971.6439  | 986.8113  | 991.0384  |
| 1025.3101 | 1029.4850 | 1081.3781 |
| 1117.4942 | 1119.1969 | 1156.8667 |
| 1168.0143 | 1184.4842 | 1202.8419 |
| 1209.9178 | 1249.7577 | 1260.8554 |
| 1266.9426 | 1288.3324 | 1329.4308 |
| 1341.9723 | 1350.7284 | 1370.4125 |
| 1383.4649 | 1389.7007 | 1403.4307 |
| 1410.6247 | 1429.6373 | 1432.0369 |
| 1446.5803 | 1451.6912 | 1460.7675 |
| 1471.4793 | 1474.8654 | 1478.5362 |
| 1613.1776 | 1645.7776 | 1861.1497 |
| 2257.8742 | 3034.0050 | 3043.1884 |
| 3052.6966 | 3062.5626 | 3089.6040 |
| 3094.0653 | 3115.0000 | 3121.0627 |

|           |           |           |
|-----------|-----------|-----------|
| 3122.4407 | 3135.5699 | 3138.6643 |
| 3147.8943 | 3155.1931 | 3161.1781 |
| 3174.8983 | 3191.0939 | 3846.0820 |

Zero-point correction (Hartree): 0.271166

TS.ApineneCI.J.b+H2O.HHP.pmmu

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E(RM062X/CC-pVDZ) (Hartree): -692.37255444

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.314037 | -0.293936 | -0.569103 |
| H | -0.751112 | 0.278188  | -1.401038 |
| C | -1.471559 | -0.946669 | 0.188851  |
| C | -2.378611 | 0.134127  | 0.687117  |
| H | -2.008720 | -1.605403 | -0.500331 |
| H | -1.121260 | -1.536788 | 1.046441  |
| H | -2.317593 | 0.451413  | 1.737050  |
| C | 0.736403  | 0.586118  | 0.172712  |
| C | 0.824197  | -1.201331 | -1.070409 |
| C | 0.548545  | 2.089445  | 0.048306  |
| C | 0.938418  | 0.174283  | 1.627969  |
| H | 1.116312  | -0.905251 | 1.734191  |
| H | 1.807725  | 0.692926  | 2.062062  |
| H | 0.058965  | 0.448261  | 2.233162  |
| H | 1.417089  | 2.635898  | 0.449963  |
| H | -0.341757 | 2.418662  | 0.607861  |
| H | 0.407057  | 2.384057  | -1.001793 |
| H | 0.760090  | -1.566665 | -2.102268 |
| H | 1.022747  | -2.044302 | -0.393437 |
| C | 1.814293  | -0.062542 | -0.779039 |
| H | 1.971892  | 0.594847  | -1.647139 |
| C | 3.133710  | -0.418123 | -0.134118 |
| C | 4.189842  | 0.662500  | -0.124763 |
| H | 3.759787  | 1.605833  | 0.246344  |
| H | 4.530346  | 0.849223  | -1.154835 |
| H | 5.037882  | 0.356382  | 0.497483  |
| O | 3.313145  | -1.495896 | 0.387809  |
| O | -2.860908 | 1.042346  | -0.065210 |
| O | -3.250021 | 0.439260  | -1.301049 |
| O | -4.043395 | -1.019007 | 0.567836  |
| H | -3.968412 | -0.598543 | -0.386707 |
| H | -4.778821 | -0.535590 | 0.972759  |

Rotational constants (GHz): 1.5261400 0.3413000 0.3250300

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| 1412.4195 | 44.2197   | 50.0061   |
| 54.4566   | 73.8524   | 123.7583  |
| 138.9917  | 157.2308  | 208.0480  |
| 213.4671  | 228.6968  | 263.2430  |
| 278.8505  | 309.2668  | 317.4071  |
| 333.1694  | 368.9480  | 386.2967  |
| 393.6615  | 433.1534  | 478.3059  |
| 518.8980  | 577.1792  | 588.1734  |
| 599.9730  | 620.2010  | 640.9378  |
| 682.9501  | 726.6817  | 785.2038  |
| 865.8811  | 892.9469  | 906.3870  |
| 945.0277  | 949.0018  | 958.7486  |
| 976.4833  | 987.7987  | 995.7806  |
| 1000.8180 | 1028.3805 | 1063.3996 |
| 1104.9019 | 1115.0617 | 1152.8479 |
| 1164.7751 | 1184.7621 | 1200.2743 |
| 1209.3370 | 1249.1744 | 1261.2634 |
| 1275.9571 | 1289.5387 | 1311.7596 |
| 1331.1042 | 1348.7278 | 1359.1456 |
| 1379.1612 | 1389.3821 | 1401.0318 |
| 1405.2251 | 1431.8166 | 1440.6634 |
| 1446.3672 | 1453.1141 | 1460.3043 |
| 1469.3702 | 1474.7206 | 1477.8622 |
| 1596.6052 | 1653.3036 | 1860.0303 |
| 2466.7909 | 3045.3608 | 3049.0281 |
| 3061.8806 | 3090.3830 | 3094.4903 |
| 3098.7814 | 3113.6360 | 3116.9524 |
| 3121.9148 | 3137.3723 | 3138.4848 |
| 3146.9392 | 3161.5984 | 3162.2427 |
| 3182.3975 | 3190.5552 | 3842.1071 |

Zero-point correction (Hartree): 0.271750

TS.ApineneCI.J.b+H2O.HHP.pmpd

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E(RM062X/CC-pVDZ) (Hartree): -692.37605071

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.178416 | -0.683062 | -0.894816 |
| H | -0.333242 | -0.542617 | -1.979003 |
| C | -1.507764 | -1.039927 | -0.223754 |
| C | -2.527338 | -0.047270 | -0.663612 |
| H | -1.836075 | -2.033162 | -0.558678 |
| H | -1.426176 | -1.032236 | 0.867675  |
| H | -2.812192 | -0.043722 | -1.725564 |
| C | 0.682271  | 0.505321  | -0.365436 |
| C | 1.022983  | -1.624597 | -0.679940 |
| C | 0.562678  | 1.806662  | -1.141845 |
| C | 0.510109  | 0.741023  | 1.132788  |
| H | 0.665021  | -0.182815 | 1.710113  |
| H | 1.253301  | 1.473072  | 1.487232  |
| H | -0.498512 | 1.122493  | 1.355485  |
| H | 1.320828  | 2.535768  | -0.814448 |
| H | -0.426241 | 2.260701  | -0.972378 |
| H | 0.691822  | 1.641596  | -2.222888 |
| H | 1.201263  | -2.399453 | -1.435468 |
| H | 1.022200  | -2.080119 | 0.319700  |
| C | 1.939343  | -0.391867 | -0.684973 |
| H | 2.318118  | -0.148338 | -1.689964 |

|                                            |           |           |           |
|--------------------------------------------|-----------|-----------|-----------|
| C                                          | 3.062502  | -0.348168 | 0.325007  |
| C                                          | 4.045963  | 0.790524  | 0.183721  |
| H                                          | 3.504936  | 1.746298  | 0.106123  |
| H                                          | 4.619160  | 0.667547  | -0.748023 |
| H                                          | 4.727908  | 0.806745  | 1.040918  |
| O                                          | 3.141903  | -1.159450 | 1.219503  |
| O                                          | -2.752689 | 1.076936  | -0.106480 |
| O                                          | -2.748605 | 0.923301  | 1.312000  |
| O                                          | -4.031313 | -0.984423 | 0.351800  |
| H                                          | -3.667369 | -0.299175 | 1.049049  |
| H                                          | -4.873110 | -0.595328 | 0.072697  |
| Rotational constants (GHz):                |           |           |           |
| 1.4012900      0.3590300      0.3413500    |           |           |           |
| Vibrational harmonic frequencies (cm-1):   |           |           |           |
| i398.4049                                  | 44.4173   |           | 52.5123   |
| 59.0989                                    | 94.3678   |           | 120.0142  |
| 144.7147                                   | 163.6520  |           | 193.6743  |
| 223.6998                                   | 243.9471  |           | 249.4443  |
| 283.8259                                   | 319.3320  |           | 328.0000  |
| 338.7315                                   | 377.0554  |           | 385.5927  |
| 392.4929                                   | 437.2864  |           | 485.6605  |
| 510.0160                                   | 565.2375  |           | 580.6744  |
| 600.7142                                   | 621.6326  |           | 627.3568  |
| 647.7143                                   | 721.3250  |           | 786.4172  |
| 869.4770                                   | 904.9318  |           | 908.8848  |
| 939.2326                                   | 954.5974  |           | 961.2499  |
| 969.1944                                   | 994.1631  |           | 997.9661  |
| 1017.4599                                  | 1041.9204 |           | 1050.7020 |
| 1104.9915                                  | 1115.4373 |           | 1150.4830 |
| 1164.4797                                  | 1186.3361 |           | 1198.5565 |
| 1207.9930                                  | 1240.2389 |           | 1255.7240 |
| 1263.5346                                  | 1285.6163 |           | 1299.6269 |
| 1321.3456                                  | 1348.8081 |           | 1362.3978 |
| 1380.8885                                  | 1389.2418 |           | 1407.6330 |
| 1413.6078                                  | 1431.8208 |           | 1438.7270 |
| 1445.0444                                  | 1456.7922 |           | 1467.6718 |
| 1472.1788                                  | 1481.6664 |           | 1491.4309 |
| 1598.0077                                  | 1653.1471 |           | 1862.7195 |
| 2503.1371                                  | 3039.7245 |           | 3044.3374 |
| 3047.0958                                  | 3063.2282 |           | 3078.3474 |
| 3096.1251                                  | 3112.0380 |           | 3124.0890 |
| 3126.6072                                  | 3132.2802 |           | 3139.5868 |
| 3143.3676                                  | 3151.5867 |           | 3160.5382 |
| 3192.0730                                  | 3193.4257 |           | 3846.4852 |
| Zero-point correction (Hartree): 0.271782  |           |           |           |
| TS.ApineneCI.J.b+H2O.HHP.pmpu              |           |           |           |
| ~~~~~                                      |           |           |           |
| E(RM062X/CC-pVDZ) (Hartree): -692.37280738 |           |           |           |
| Electronic state : 1-A                     |           |           |           |
| Cartesian coordinates (Angs):              |           |           |           |
| C                                          | -0.203332 | 0.533040  | 0.879821  |
| H                                          | -0.408570 | 0.251066  | 1.927250  |
| C                                          | -1.486957 | 0.999775  | 0.209489  |
| C                                          | -2.727640 | 0.341488  | 0.705067  |
| H                                          | -1.657735 | 2.060258  | 0.486399  |
| H                                          | -1.451789 | 0.967777  | -0.883907 |
| H                                          | -2.783316 | 0.083963  | 1.773039  |
| C                                          | 0.706342  | -0.571539 | 0.247281  |
| C                                          | 0.995129  | 1.501379  | 0.843289  |
| C                                          | 0.604246  | -1.958060 | 0.860444  |
| C                                          | 0.601386  | -0.633993 | -1.273082 |
| H                                          | 0.701021  | 0.358819  | -1.735971 |
| H                                          | 1.405766  | -1.265170 | -1.683310 |
| H                                          | -0.362536 | -1.074718 | -1.560531 |
| H                                          | 1.401230  | -2.616765 | 0.479346  |
| H                                          | -0.364672 | -2.406576 | 0.600839  |
| H                                          | 0.694950  | -1.915260 | 1.957087  |
| H                                          | 1.132767  | 2.173625  | 1.699690  |
| H                                          | 1.024793  | 2.086030  | -0.087125 |
| C                                          | 1.936181  | 0.296607  | 0.719204  |
| H                                          | 2.291236  | -0.071631 | 1.694153  |
| C                                          | 3.086904  | 0.403784  | -0.254318 |
| C                                          | 4.120950  | -0.696654 | -0.195964 |
| H                                          | 3.625760  | -1.679817 | -0.217517 |
| H                                          | 4.669413  | -0.633563 | 0.756490  |
| H                                          | 4.819669  | -0.601604 | -1.034333 |
| O                                          | 3.149993  | 1.301926  | -1.063387 |
| O                                          | -3.877149 | 0.455763  | 0.174071  |
| O                                          | -3.745789 | 0.385589  | -1.246195 |
| O                                          | -2.354541 | -1.409254 | -0.316606 |
| H                                          | -2.929581 | -0.809285 | -0.994414 |
| H                                          | -2.987767 | -2.074307 | -0.007632 |
| Rotational constants (GHz):                |           |           |           |
| 1.4475600      0.3473500      0.3294300    |           |           |           |
| Vibrational harmonic frequencies (cm-1):   |           |           |           |
| i462.6613                                  | 34.6106   |           | 58.2533   |
| 65.4974                                    | 96.2711   |           | 131.3078  |
| 148.9388                                   | 165.5673  |           | 190.1882  |
| 233.1349                                   | 243.2124  |           | 263.2881  |
| 279.7166                                   | 321.2367  |           | 322.1654  |
| 340.0704                                   | 368.8834  |           | 386.3796  |
| 418.9804                                   | 435.5405  |           | 464.7078  |
| 501.5221                                   | 576.2713  |           | 589.5389  |
| 602.0785                                   | 619.9718  |           | 633.5742  |
| 669.5286                                   | 719.9897  |           | 779.5584  |
| 840.7091                                   | 876.2606  |           | 905.9117  |
| 929.3495                                   | 954.5388  |           | 958.5744  |
| 973.2015                                   | 990.0101  |           | 991.1896  |
| 1024.8555                                  | 1045.4941 |           | 1071.4275 |
| 1113.5679                                  | 1117.0995 |           | 1155.5422 |
| 1168.1127                                  | 1185.5165 |           | 1196.8058 |
| 1209.1657                                  | 1246.3716 |           | 1251.6687 |
| 1267.1590                                  | 1287.3900 |           | 1317.8883 |



|           |           |           |
|-----------|-----------|-----------|
| 1346.7277 | 1350.9915 | 1367.9327 |
| 1382.0265 | 1387.8589 | 1398.0156 |
| 1413.3508 | 1419.2864 | 1431.9437 |
| 1445.8857 | 1450.4705 | 1468.4678 |
| 1471.4943 | 1476.5496 | 1491.0082 |
| 1618.5754 | 1637.4173 | 1861.5701 |
| 2151.1937 | 3014.4995 | 3040.5064 |
| 3050.0871 | 3058.2178 | 3062.4414 |
| 3082.8579 | 3088.5731 | 3121.5123 |
| 3130.9263 | 3138.5137 | 3151.9721 |
| 3152.2399 | 3162.3389 | 3165.7740 |
| 3184.1919 | 3191.0794 | 3838.7110 |

Zero-point correction (Hartree): 0.270972

TS.ApineneCI.J.b+H2O.HHP.pmtd

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E(RM062X/CC-pVDZ) (Hartree): -692.37204656

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.385390 | -0.724893 | -0.531390 |
| H | -0.808031 | -0.450332 | -1.503630 |
| C | -1.468935 | -1.348879 | 0.334041  |
| C | -2.882198 | -0.868411 | 0.297545  |
| H | -1.589995 | -2.406279 | 0.018917  |
| H | -1.175453 | -1.398142 | 1.393952  |
| H | -3.585826 | -1.433710 | 0.925665  |
| C | 0.496357  | 0.459604  | -0.017348 |
| C | 0.895867  | -1.559997 | -0.722775 |
| C | 0.146502  | 1.850990  | -0.519610 |
| C | 0.688285  | 0.457797  | 1.497254  |
| H | 1.018794  | -0.521952 | 1.873566  |
| H | 1.461726  | 1.189084  | 1.782299  |
| H | -0.252070 | 0.740187  | 1.990513  |
| H | 1.003593  | 2.531840  | -0.387944 |
| H | -0.696970 | 2.271691  | 0.046797  |
| H | -0.130018 | 1.833693  | -1.583709 |
| H | 0.947967  | -2.211725 | -1.604337 |
| H | 1.170025  | -2.134924 | 0.173430  |
| C | 1.696820  | -0.251508 | -0.753583 |
| H | 1.791225  | 0.162350  | -1.769261 |
| C | 3.028181  | -0.223687 | -0.041417 |
| C | 3.894615  | 0.991481  | -0.279334 |
| H | 3.313252  | 1.906886  | -0.088149 |
| H | 4.204746  | 1.023236  | -1.334898 |
| H | 4.776679  | 0.957925  | 0.369539  |
| O | 3.361636  | -1.109616 | 0.714186  |
| O | -3.487300 | -0.250471 | -0.634395 |
| O | -2.678628 | 0.816108  | -1.129519 |
| O | -2.486558 | 0.895380  | 1.321750  |
| H | -2.460601 | 1.168752  | 0.300026  |
| H | -3.322860 | 1.265215  | 1.640741  |

Rotational constants (GHz): 1.4164500 0.3886100 0.3678700

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i424.6983 | 49.7802   | 58.3774   |
| 65.6825   | 101.9237  | 125.7456  |
| 154.4070  | 166.5623  | 199.0873  |
| 233.2081  | 267.5669  | 279.8214  |
| 291.5407  | 306.6933  | 323.8101  |
| 335.3277  | 375.8870  | 382.7961  |
| 413.8017  | 427.3627  | 469.6749  |
| 471.1425  | 570.4857  | 576.1279  |
| 591.1560  | 596.4356  | 624.8305  |
| 704.6016  | 759.2769  | 778.8339  |
| 846.8693  | 871.7670  | 906.9493  |
| 925.0190  | 946.2476  | 957.2160  |
| 968.8212  | 974.2787  | 992.8893  |
| 1004.7406 | 1030.3355 | 1050.5156 |
| 1112.6156 | 1125.0067 | 1157.7965 |
| 1165.1674 | 1181.8484 | 1190.0907 |
| 1207.2662 | 1248.9303 | 1265.1984 |
| 1281.3632 | 1301.4970 | 1344.8152 |
| 1348.0814 | 1352.3413 | 1369.1558 |
| 1388.4237 | 1394.4794 | 1400.8116 |
| 1406.8138 | 1430.8184 | 1433.0015 |
| 1445.0612 | 1447.6437 | 1469.0249 |
| 1473.3232 | 1477.9496 | 1490.7925 |
| 1611.9905 | 1629.2359 | 1858.7127 |
| 2302.3124 | 3007.2084 | 3049.7201 |
| 3056.1208 | 3062.1448 | 3083.2129 |
| 3087.1905 | 3109.7436 | 3126.5088 |
| 3127.9383 | 3138.2530 | 3142.5579 |
| 3147.9811 | 3151.3001 | 3156.0579 |
| 3164.2566 | 3190.5761 | 3844.4169 |

Zero-point correction (Hartree): 0.271408

TS.ApineneCI.J.b+H2O.HHP.pmtu

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E(RM062X/CC-pVDZ) (Hartree): -692.37223649

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.401042 | -0.584432 | -0.631891 |
| H | -0.945163 | -0.314236 | -1.545545 |
| C | -1.353711 | -1.271919 | 0.339565  |
| C | -2.654223 | -0.698440 | 0.799609  |
| H | -1.609920 | -2.259008 | -0.076528 |
| H | -0.832292 | -1.487349 | 1.293308  |
| H | -3.314650 | -1.403282 | 1.325168  |
| C | 0.539603  | 0.583948  | -0.183381 |
| C | 0.839425  | -1.456572 | -0.933830 |
| C | 0.327872  | 1.925558  | -0.870903 |
| C | 0.608857  | 0.756172  | 1.328506  |
| H | 0.874795  | -0.178386 | 1.844722  |

|                                            |           |           |           |
|--------------------------------------------|-----------|-----------|-----------|
| H                                          | 1.369021  | 1.505829  | 1.600598  |
| H                                          | -0.367654 | 1.115334  | 1.687317  |
| H                                          | 1.226612  | 2.553153  | -0.747923 |
| H                                          | -0.534503 | 2.450351  | -0.441809 |
| H                                          | 0.160816  | 1.789259  | -1.951089 |
| H                                          | 0.855324  | -1.984427 | -1.895513 |
| H                                          | 1.057871  | -2.168090 | -0.123882 |
| C                                          | 1.748242  | -0.228701 | -0.801141 |
| H                                          | 2.038162  | 0.213799  | -1.765348 |
| C                                          | 2.957985  | -0.363053 | 0.092806  |
| C                                          | 3.986031  | 0.740752  | -0.002331 |
| H                                          | 3.491283  | 1.722169  | 0.061540  |
| H                                          | 4.480714  | 0.693774  | -0.984742 |
| H                                          | 4.730278  | 0.633099  | 0.794393  |
| O                                          | 3.075625  | -1.279718 | 0.876563  |
| O                                          | -2.931222 | 0.505462  | 1.100398  |
| O                                          | -2.361909 | 1.374698  | 0.125733  |
| O                                          | -3.398361 | -0.518883 | -1.098319 |
| H                                          | -2.993960 | 0.426530  | -0.906115 |
| H                                          | -4.354036 | -0.380867 | -1.025604 |
| Rotational constants (GHz):                |           |           |           |
|                                            | 1.3706200 | 0.3966000 | 0.3727200 |
| Vibrational harmonic frequencies (cm-1):   |           |           |           |
| i408.4260                                  | 26.1648   |           | 59.0922   |
| 60.6222                                    | 91.8092   |           | 131.6466  |
| 147.0792                                   | 177.6452  |           | 206.1408  |
| 227.1400                                   | 264.4809  |           | 280.1979  |
| 286.9466                                   | 313.5746  |           | 330.4405  |
| 348.8285                                   | 362.5535  |           | 373.5801  |
| 415.8030                                   | 430.8598  |           | 470.0081  |
| 480.1937                                   | 571.5546  |           | 578.7479  |
| 598.3882                                   | 617.7869  |           | 621.0028  |
| 700.6844                                   | 747.6754  |           | 797.2094  |
| 861.6998                                   | 884.8237  |           | 897.3638  |
| 929.9722                                   | 947.3976  |           | 958.9801  |
| 970.2140                                   | 982.9597  |           | 993.3833  |
| 1011.7849                                  | 1032.4620 |           | 1044.0876 |
| 1097.4740                                  | 1126.9626 |           | 1161.4597 |
| 1171.3137                                  | 1185.9378 |           | 1189.9584 |
| 1207.9176                                  | 1251.9622 |           | 1265.1597 |
| 1279.9735                                  | 1300.3340 |           | 1308.9018 |
| 1349.5604                                  | 1354.6847 |           | 1373.2901 |
| 1379.7532                                  | 1390.7542 |           | 1393.7531 |
| 1406.2517                                  | 1417.3455 |           | 1431.4865 |
| 1446.0083                                  | 1450.8499 |           | 1462.4202 |
| 1469.6863                                  | 1478.8166 |           | 1489.5043 |
| 1612.9537                                  | 1646.4493 |           | 1855.2218 |
| 2474.6520                                  | 3027.2697 |           | 3043.0698 |
| 3050.6930                                  | 3063.0247 |           | 3082.2643 |
| 3090.5737                                  | 3099.6006 |           | 3112.1472 |
| 3125.7736                                  | 3127.2258 |           | 3138.9152 |
| 3146.4849                                  | 3150.7927 |           | 3152.0992 |
| 3177.4942                                  | 3191.7671 |           | 3845.9509 |
| Zero-point correction (Hartree): 0.271760  |           |           |           |
| TS.ApineneCI.J.b+H2O.HHP.ppm               |           |           |           |
| ~~~~~                                      |           |           |           |
| E(RM062X/CC-pVDZ) (Hartree): -692.37098396 |           |           |           |
| Electronic state : 1-A                     |           |           |           |
| Cartesian coordinates (Angs):              |           |           |           |
| C                                          | -0.264279 | 0.566143  | -0.609495 |
| H                                          | -0.384556 | 1.102727  | -1.567339 |
| C                                          | -1.529922 | 0.710318  | 0.217206  |
| C                                          | -2.774096 | 0.445611  | -0.560582 |
| H                                          | -1.526814 | 0.102299  | 1.126984  |
| H                                          | -1.650245 | 1.766361  | 0.534053  |
| H                                          | -2.799086 | 0.751989  | -1.616676 |
| C                                          | 1.087986  | 1.016224  | 0.020708  |
| C                                          | 0.347988  | -0.824929 | -0.866887 |
| C                                          | 1.572785  | 2.402354  | -0.370746 |
| C                                          | 1.116773  | 0.834539  | 1.536064  |
| H                                          | 0.801099  | -0.174198 | 1.836750  |
| H                                          | 2.136100  | 0.989103  | 1.923294  |
| H                                          | 0.458657  | 1.568968  | 2.024974  |
| H                                          | 2.591724  | 2.590387  | 0.003521  |
| H                                          | 0.916556  | 3.176646  | 0.059085  |
| H                                          | 1.579785  | 2.528742  | -1.463887 |
| H                                          | 0.095285  | -1.327402 | -1.807644 |
| H                                          | 0.159144  | -1.516862 | -0.036528 |
| C                                          | 1.745625  | -0.199687 | -0.735363 |
| H                                          | 2.151878  | 0.149062  | -1.697587 |
| C                                          | 2.797950  | -0.964508 | 0.034159  |
| C                                          | 4.216304  | -0.453851 | -0.078560 |
| H                                          | 4.242086  | 0.630586  | 0.111350  |
| H                                          | 4.580844  | -0.608571 | -1.105726 |
| H                                          | 4.864578  | -0.981669 | 0.629434  |
| O                                          | 2.509372  | -1.906071 | 0.737545  |
| O                                          | -3.936883 | 0.334260  | -0.060231 |
| O                                          | -3.858894 | -0.420419 | 1.149576  |
| O                                          | -2.462383 | -1.577198 | -0.534510 |
| H                                          | -3.039220 | -1.394861 | 0.332531  |
| H                                          | -3.090198 | -1.991166 | -1.144653 |
| Rotational constants (GHz):                |           |           |           |
|                                            | 1.3012500 | 0.3503800 | 0.3169400 |
| Vibrational harmonic frequencies (cm-1):   |           |           |           |
| i439.8510                                  | 24.6004   |           | 47.1615   |
| 56.2126                                    | 105.7297  |           | 116.2899  |
| 126.5322                                   | 157.5343  |           | 182.7918  |
| 223.1930                                   | 233.0236  |           | 248.9566  |
| 290.2718                                   | 313.3541  |           | 320.7421  |
| 341.2130                                   | 354.5190  |           | 377.0214  |
| 391.4959                                   | 455.3000  |           | 468.4215  |
| 499.7400                                   | 576.9457  |           | 590.0292  |
| 596.4346                                   | 623.4163  |           | 637.0069  |

|           |           |           |
|-----------|-----------|-----------|
| 673.7182  | 736.4973  | 802.0870  |
| 837.1014  | 870.6265  | 906.0929  |
| 931.6858  | 947.5795  | 956.3902  |
| 966.6005  | 986.6085  | 987.6663  |
| 1015.2684 | 1039.3789 | 1065.2482 |
| 1107.1667 | 1144.7351 | 1151.5869 |
| 1169.8274 | 1188.0763 | 1199.0118 |
| 1218.6819 | 1236.1366 | 1251.6136 |
| 1269.7537 | 1290.9363 | 1320.5521 |
| 1333.2822 | 1350.2070 | 1363.0263 |
| 1387.4734 | 1389.4780 | 1401.9383 |
| 1414.1121 | 1423.1624 | 1430.8078 |
| 1446.2601 | 1451.8875 | 1462.1318 |
| 1467.4046 | 1476.9981 | 1479.8433 |
| 1615.0322 | 1643.6307 | 1863.3546 |
| 2316.2207 | 3018.3923 | 3039.4429 |
| 3044.2850 | 3056.2100 | 3060.9984 |
| 3079.8516 | 3114.0117 | 3119.9115 |
| 3128.5329 | 3132.6802 | 3136.7492 |
| 3146.7931 | 3152.9795 | 3176.2469 |
| 3184.4538 | 3190.9679 | 3841.2003 |

Zero-point correction (Hartree): 0.271030

TS.ApineneCI.J.b+H2O.HHP.ppmu

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E(RM062X/CC-pVDZ) (Hartree): -692.37214026

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.273090 | 0.744637  | -0.649229 |
| H | -0.342951 | 1.339849  | -1.575696 |
| C | -1.560232 | 0.883834  | 0.167308  |
| C | -2.658367 | 0.308748  | -0.659854 |
| H | -1.481369 | 0.321531  | 1.100996  |
| H | -1.793572 | 1.935806  | 0.380986  |
| H | -3.082773 | 0.915613  | -1.471943 |
| C | 1.088156  | 1.068749  | 0.042128  |
| C | 0.246924  | -0.673822 | -0.964004 |
| C | 1.681535  | 2.430346  | -0.278924 |
| C | 1.060654  | 0.821752  | 1.547066  |
| H | 0.670526  | -0.175950 | 1.793281  |
| H | 2.077812  | 0.889264  | 1.964107  |
| H | 0.440460  | 1.578962  | 2.050860  |
| H | 2.703917  | 2.523736  | 0.120715  |
| H | 1.075567  | 3.232053  | 0.173310  |
| H | 1.720895  | 2.602281  | -1.365093 |
| H | 0.004963  | -1.094020 | -1.947648 |
| H | -0.042687 | -1.394556 | -0.186730 |
| C | 1.679035  | -0.159331 | -0.748868 |
| H | 2.145694  | 0.200162  | -1.679207 |
| C | 2.645421  | -1.033701 | 0.017835  |
| C | 4.100340  | -0.624107 | -0.027966 |
| H | 4.198550  | 0.446386  | 0.211086  |
| H | 4.487807  | -0.762225 | -1.049090 |
| H | 4.683822  | -1.228017 | 0.675577  |
| O | 2.265947  | -1.981087 | 0.666945  |
| O | -2.824677 | -0.938780 | -0.852440 |
| O | -2.600222 | -1.638048 | 0.373896  |
| O | -3.982924 | 0.367756  | 0.887465  |
| H | -3.531255 | -0.574497 | 0.986028  |
| H | -4.862658 | 0.162267  | 0.538583  |

Rotational constants (GHz): 1.2187900 0.3823800 0.3380500

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i410.9976 | 33.9151   | 46.4860   |
| 47.6338   | 94.0582   | 102.6958  |
| 126.6656  | 155.1942  | 185.8137  |
| 222.9583  | 232.0014  | 248.8775  |
| 282.0276  | 312.8640  | 329.7407  |
| 339.8397  | 351.3398  | 384.2478  |
| 414.0380  | 444.0568  | 479.6162  |
| 517.6436  | 579.1272  | 586.7151  |
| 599.9122  | 619.9434  | 629.6515  |
| 659.4240  | 736.1075  | 805.9610  |
| 869.9815  | 882.4708  | 912.8013  |
| 930.4111  | 950.2081  | 956.6797  |
| 973.8602  | 987.4516  | 996.4252  |
| 1006.3381 | 1036.7333 | 1037.7418 |
| 1099.3123 | 1131.0475 | 1147.6787 |
| 1168.9747 | 1185.1778 | 1197.4675 |
| 1220.6690 | 1248.3896 | 1254.8808 |
| 1270.3103 | 1289.5848 | 1317.7722 |
| 1321.6644 | 1349.4201 | 1364.7274 |
| 1378.4083 | 1386.9803 | 1400.9741 |
| 1406.2268 | 1431.4906 | 1439.6402 |
| 1446.0673 | 1453.5326 | 1461.5106 |
| 1472.4254 | 1477.7089 | 1479.2518 |
| 1603.9370 | 1653.4662 | 1865.5163 |
| 2416.5152 | 3043.2578 | 3048.4019 |
| 3052.4035 | 3061.7803 | 3077.1078 |
| 3103.2707 | 3111.5716 | 3119.6936 |
| 3125.8929 | 3131.2037 | 3137.4043 |
| 3148.4442 | 3159.9004 | 3167.1424 |
| 3191.3328 | 3207.0654 | 3844.4113 |

Zero-point correction (Hartree): 0.271514

TS.ApineneCI.J.b+H2O.HHP.pppd

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E(RM062X/CC-pVDZ) (Hartree): -692.37211045

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.339482 | 0.110732  | -0.303193 |
| H | -0.754215 | 0.616703  | -1.188425 |
| C | -1.484248 | -0.069473 | 0.694413  |

|                                                           |           |           |           |
|-----------------------------------------------------------|-----------|-----------|-----------|
| C                                                         | -2.517318 | -0.913402 | 0.020057  |
| H                                                         | -1.155866 | -0.586021 | 1.606094  |
| H                                                         | -1.903710 | 0.906786  | 0.955465  |
| H                                                         | -2.502208 | -2.001118 | 0.171524  |
| C                                                         | 0.949303  | 0.853147  | 0.156254  |
| C                                                         | 0.523350  | -1.098875 | -0.717001 |
| C                                                         | 1.040370  | 2.314408  | -0.249683 |
| C                                                         | 1.239750  | 0.677036  | 1.643578  |
| H                                                         | 1.221018  | -0.379385 | 1.947558  |
| H                                                         | 2.237895  | 1.070827  | 1.892013  |
| H                                                         | 0.502192  | 1.230510  | 2.244707  |
| H                                                         | 2.034544  | 2.731613  | -0.022198 |
| H                                                         | 0.294725  | 2.911757  | 0.298656  |
| H                                                         | 0.848830  | 2.440086  | -1.325344 |
| H                                                         | 0.266233  | -1.613417 | -1.651378 |
| H                                                         | 0.635194  | -1.837090 | 0.090972  |
| C                                                         | 1.750019  | -0.173820 | -0.734677 |
| H                                                         | 1.933663  | 0.269891  | -1.724771 |
| C                                                         | 3.037264  | -0.697128 | -0.140865 |
| C                                                         | 4.276680  | 0.129412  | -0.392931 |
| H                                                         | 4.078890  | 1.186531  | -0.156760 |
| H                                                         | 4.535299  | 0.082573  | -1.461968 |
| H                                                         | 5.111036  | -0.248382 | 0.208100  |
| O                                                         | 3.060248  | -1.699628 | 0.537800  |
| O                                                         | -3.086571 | -0.583865 | -1.070362 |
| O                                                         | -3.377674 | 0.814477  | -1.019850 |
| O                                                         | -4.025588 | -0.197488 | 1.166580  |
| H                                                         | -3.982152 | 0.479296  | 0.366338  |
| H                                                         | -4.818806 | -0.721361 | 0.980358  |
| Rotational constants (GHz): 1.4215500 0.3290100 0.3154200 |           |           |           |
| Vibrational harmonic frequencies (cm-1):                  |           |           |           |
| i421.3068                                                 | 32.2570   | 42.3999   |           |
| 53.8658                                                   | 78.5989   | 99.9300   |           |
| 132.1341                                                  | 150.5935  | 201.1702  |           |
| 205.3351                                                  | 230.0203  | 247.7328  |           |
| 277.5420                                                  | 312.4861  | 321.9944  |           |
| 338.8663                                                  | 351.5819  | 385.6631  |           |
| 400.3010                                                  | 443.2805  | 482.5492  |           |
| 516.1050                                                  | 582.1540  | 590.6971  |           |
| 602.2286                                                  | 621.5683  | 647.1474  |           |
| 674.8804                                                  | 740.5065  | 801.2364  |           |
| 873.3276                                                  | 886.2792  | 910.2335  |           |
| 937.2530                                                  | 949.8621  | 957.5757  |           |
| 976.7340                                                  | 987.7784  | 996.7632  |           |
| 1006.8193                                                 | 1024.8455 | 1051.2704 |           |
| 1102.8583                                                 | 1139.9063 | 1149.9305 |           |
| 1164.1849                                                 | 1184.7053 | 1203.4877 |           |
| 1220.2033                                                 | 1249.5894 | 1253.8227 |           |
| 1271.7857                                                 | 1294.3412 | 1320.8256 |           |
| 1331.2055                                                 | 1348.9070 | 1358.9886 |           |
| 1381.0117                                                 | 1389.1373 | 1400.3094 |           |
| 1405.3333                                                 | 1432.0854 | 1442.8756 |           |
| 1446.4973                                                 | 1452.5032 | 1460.7822 |           |
| 1468.3982                                                 | 1476.9033 | 1478.6479 |           |
| 1603.3437                                                 | 1653.3189 | 1860.1600 |           |
| 2425.7378                                                 | 3046.0697 | 3052.8964 |           |
| 3063.3247                                                 | 3084.6282 | 3089.4880 |           |
| 3091.0995                                                 | 3111.9448 | 3122.0960 |           |
| 3126.7812                                                 | 3138.2413 | 3139.3402 |           |
| 3146.0765                                                 | 3152.0278 | 3166.1677 |           |
| 3187.0808                                                 | 3191.6396 | 3842.5261 |           |
| Zero-point correction (Hartree): 0.271664                 |           |           |           |
| TS.ApineneCI.J.b+H2O.HHP.pppu                             |           |           |           |
| ~~~~~                                                     |           |           |           |
| E(RM062X/CC-pVDZ) (Hartree): -692.37217240                |           |           |           |
| Electronic state : 1-A                                    |           |           |           |
| Cartesian coordinates (Angs):                             |           |           |           |
| C                                                         | -0.299160 | 0.196384  | -0.369752 |
| H                                                         | -0.660754 | 0.763833  | -1.238353 |
| C                                                         | -1.469130 | -0.027017 | 0.571799  |
| C                                                         | -2.524047 | -0.889878 | -0.030274 |
| H                                                         | -1.140931 | -0.607102 | 1.456151  |
| H                                                         | -1.922568 | 0.901559  | 0.934299  |
| H                                                         | -2.201242 | -1.768265 | -0.608118 |
| C                                                         | 0.996408  | 0.865792  | 0.176479  |
| C                                                         | 0.543916  | -1.011547 | -0.833639 |
| C                                                         | 1.148216  | 2.346010  | -0.132140 |
| C                                                         | 1.232997  | 0.589535  | 1.658466  |
| H                                                         | 1.174107  | -0.482442 | 1.896372  |
| H                                                         | 2.234028  | 0.935052  | 1.961076  |
| H                                                         | 0.493796  | 1.127933  | 2.271096  |
| H                                                         | 2.147604  | 2.713777  | 0.150494  |
| H                                                         | 0.405800  | 2.933210  | 0.431421  |
| H                                                         | 0.996212  | 2.545593  | -1.203171 |
| H                                                         | 0.310584  | -1.458659 | -1.808482 |
| H                                                         | 0.605622  | -1.804180 | -0.072748 |
| C                                                         | 1.797594  | -0.126912 | -0.750428 |
| H                                                         | 2.030213  | 0.371624  | -1.703509 |
| C                                                         | 3.046297  | -0.730120 | -0.149783 |
| C                                                         | 4.317982  | 0.071477  | -0.301042 |
| H                                                         | 4.144109  | 1.114910  | 0.004700  |
| H                                                         | 4.612461  | 0.092733  | -1.361560 |
| H                                                         | 5.118921  | -0.374994 | 0.298248  |
| O                                                         | 3.014166  | -1.776617 | 0.458163  |
| O                                                         | -3.713724 | -1.005223 | 0.406088  |
| O                                                         | -4.204920 | 0.282244  | 0.782992  |
| O                                                         | -3.063758 | 0.552668  | -1.382080 |
| H                                                         | -3.691696 | 0.729208  | -0.540965 |
| H                                                         | -3.656806 | 0.139296  | -2.026380 |
| Rotational constants (GHz): 1.4365200 0.3201000 0.3038600 |           |           |           |
| Vibrational harmonic frequencies (cm-1):                  |           |           |           |

|           |           |           |
|-----------|-----------|-----------|
| i453.1312 | 32.8499   | 43.6333   |
| 57.4412   | 89.5096   | 113.7398  |
| 134.4111  | 153.5854  | 201.9745  |
| 210.1825  | 232.2948  | 243.1226  |
| 282.8505  | 321.3311  | 333.0349  |
| 344.4647  | 352.1943  | 381.8070  |
| 395.8145  | 450.4251  | 471.1798  |
| 503.7399  | 577.4749  | 593.3374  |
| 603.6398  | 622.1172  | 642.2670  |
| 657.6764  | 742.3510  | 824.5038  |
| 826.8580  | 869.5942  | 905.7905  |
| 933.9743  | 946.6086  | 955.3357  |
| 968.3760  | 988.1556  | 989.6683  |
| 1011.7404 | 1032.9140 | 1066.4836 |
| 1114.4403 | 1150.0500 | 1157.9862 |
| 1164.2457 | 1184.9256 | 1199.5411 |
| 1208.7507 | 1248.0203 | 1254.4700 |
| 1270.1353 | 1290.5913 | 1328.0228 |
| 1336.8023 | 1351.0344 | 1368.2675 |
| 1383.6672 | 1388.2355 | 1400.1820 |
| 1408.4539 | 1427.8357 | 1431.7103 |
| 1446.9958 | 1453.3869 | 1460.9915 |
| 1470.3570 | 1478.1935 | 1478.7401 |
| 1614.4448 | 1644.3223 | 1861.3419 |
| 2237.7611 | 3033.9681 | 3045.9780 |
| 3054.1819 | 3062.0811 | 3081.6130 |
| 3088.3868 | 3114.4041 | 3122.8411 |
| 3128.2071 | 3135.4201 | 3137.8335 |
| 3145.3287 | 3148.0404 | 3151.1327 |
| 3172.5668 | 3191.3055 | 3843.6980 |

Zero-point correction (Hartree): 0.271055

TS.ApineneCI.J.b+H2O.HHP.pptd  
 ~~~~~  
 E(RM062X/CC-pVDZ) (Hartree): -692.36942236  
 Electronic state : 1-A  
 Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.473563 | 0.270015  | -0.151828 |
| H | -0.920756 | 0.599198  | -1.098044 |
| C | -1.481291 | 0.434543  | 0.970578  |
| C | -2.810767 | -0.245556 | 0.900206  |
| H | -1.056945 | 0.041991  | 1.915521  |
| H | -1.702084 | 1.497268  | 1.157032  |
| H | -3.452810 | -0.103591 | 1.781632  |
| C | 0.917083  | 0.959325  | 0.018316  |
| C | 0.238077  | -1.078802 | -0.344538 |
| C | 1.088972  | 2.274644  | -0.723639 |
| C | 1.355873  | 1.096198  | 1.473810  |
| H | 1.285329  | 0.144479  | 2.019746  |
| H | 2.405783  | 1.424219  | 1.531045  |
| H | 0.744150  | 1.850923  | 1.992236  |
| H | 2.133616  | 2.623510  | -0.685558 |
| H | 0.460604  | 3.058451  | -0.270114 |
| H | 0.796095  | 2.175104  | -1.779269 |
| H | -0.187997 | -1.745038 | -1.100315 |
| H | 0.365361  | -1.624061 | 0.602749  |
| C | 1.533078  | -0.317517 | -0.673578 |
| H | 1.650976  | -0.125930 | -1.750920 |
| C | 2.828346  | -0.821611 | -0.082356 |
| C | 4.101276  | -0.260356 | -0.673812 |
| H | 4.042307  | 0.838531  | -0.716659 |
| H | 4.210884  | -0.615917 | -1.709862 |
| H | 4.965612  | -0.574942 | -0.078691 |
| O | 2.843312  | -1.596982 | 0.847991  |
| O | -3.149944 | -1.282217 | 0.246217  |
| O | -2.658815 | -1.214150 | -1.089120 |
| O | -3.516565 | 1.033377  | -0.555954 |
| H | -3.185110 | 0.191050  | -1.097560 |
| H | -4.481423 | 0.959232  | -0.584990 |

Rotational constants (GHz): 1.2768000 0.3731600 0.3417600  
 Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i429.7402 | 31.8811   | 50.4068   |
| 64.5794   | 76.4815   | 122.6063  |
| 135.7089  | 162.0166  | 191.6247  |
| 216.0065  | 239.4350  | 250.2756  |
| 284.4717  | 325.1613  | 330.3943  |
| 341.2768  | 352.9107  | 380.2583  |
| 399.4598  | 449.1103  | 462.0219  |
| 479.1480  | 571.1223  | 579.4390  |
| 592.9532  | 607.0185  | 621.3935  |
| 717.2714  | 751.4940  | 814.9490  |
| 851.0493  | 873.2634  | 905.2957  |
| 934.2681  | 946.8426  | 952.3784  |
| 966.4484  | 974.3614  | 986.7339  |
| 1006.9164 | 1021.3703 | 1038.7026 |
| 1096.8381 | 1133.2483 | 1147.1871 |
| 1168.5303 | 1183.9100 | 1197.7211 |
| 1213.4977 | 1232.6225 | 1262.5523 |
| 1273.7828 | 1314.9168 | 1327.3772 |
| 1346.7108 | 1354.0314 | 1372.4954 |
| 1385.7752 | 1396.3246 | 1399.0479 |
| 1406.8501 | 1428.0738 | 1431.4109 |
| 1446.2692 | 1453.1335 | 1461.2186 |
| 1472.3380 | 1477.7005 | 1479.4334 |
| 1609.8980 | 1642.3637 | 1857.9975 |
| 2346.3528 | 3026.3343 | 3042.0720 |
| 3051.0978 | 3060.2405 | 3085.0794 |
| 3093.0840 | 3104.0670 | 3116.5591 |
| 3122.5068 | 3126.6479 | 3134.3668 |
| 3136.0804 | 3145.7160 | 3148.9703 |
| 3187.6446 | 3190.2021 | 3847.3916 |

Zero-point correction (Hartree): 0.271093

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TS.ApineneCI.J.b+H2O.HHP.pptu
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E(RM062X/CC-pVDZ) (Hartree): -692.37046737
Electronic state : 1-A
Cartesian coordinates (Angs):
  C   -0.480802   0.528728   -0.230372
  H   -0.836094   0.966841   -1.171078
  C   -1.523563   0.743060   0.852451
  C   -2.955056   0.384998   0.612472
  H   -1.240383   0.242294   1.790521
  H   -1.586851   1.824263   1.093793
  H   -3.636169   0.588807   1.451282
  C    0.968883   1.028138   0.062848
  C    0.081130   -0.878061   -0.499586
  C    1.335463   2.370796   -0.547946
  C    1.337700   0.982556   1.543216
  H    1.113657   0.005568   1.994769
  H    2.415780   1.163363   1.678260
  H    0.798289   1.763828   2.101187
  H    2.410582   2.584213   -0.434009
  H    0.783311   3.185558   -0.051232
  H    1.089258   2.398532   -1.619653
  H   -0.362129   -1.425834   -1.339194
  H    0.082809   -1.513020   0.396715
  C    1.468532   -0.251053   -0.710923
  H    1.660073   0.012950   -1.762078
  C    2.667367   -0.951247   -0.115916
  C    4.023501   -0.480617   -0.590520
  H    4.084075   0.617055   -0.525436
  H    4.152233   -0.746217   -1.651057
  H    4.815275   -0.944289   0.008093
  O    2.548311   -1.809488   0.729942
  O   -3.583847   0.315247   -0.489047
  O   -2.804307   -0.370665   -1.466243
  O   -2.574350   -1.643270   0.649510
  H   -2.556827   -1.407680   -0.371555
  H   -3.412289   -2.114615   0.763024
Rotational constants (GHz): 1.2201000 0.3911000 0.3560600
Vibrational harmonic frequencies (cm-1):
  i409.7235 49.2427 51.5089
    62.4739 103.4679 123.2974
   134.5401 164.7845 180.1876
   224.9931 236.9366 261.6822
   283.7763 300.8437 328.0003
   343.4629 358.4178 376.6578
   393.9968 444.6157 463.7492
   476.5048 575.6594 580.2262
   592.7682 600.5054 622.7771
   719.9566 764.5794 793.9775
   855.6608 870.1685 904.8752
   932.9444 946.5454 952.9810
   970.0857 977.6479 989.0971
  1009.1158 1022.5237 1044.1478
  1089.3967 1134.2650 1152.4827
  1169.9270 1186.3781 1200.7340
  1219.2154 1244.0777 1262.4399
  1274.6595 1312.1173 1317.9552
  1343.5332 1352.8391 1371.5685
  1385.8819 1397.4648 1399.5255
  1408.1021 1431.4513 1434.4265
  1446.5502 1452.9161 1461.4128
  1470.2263 1476.9572 1479.6050
  1613.0654 1643.9085 1860.2917
  2441.1467 3009.3858 3042.0324
  3051.7292 3059.9016 3085.9764
  3104.6700 3112.6307 3114.9836
  3122.6805 3131.7500 3135.2011
  3136.3964 3147.1034 3156.1478
  3172.8668 3189.3542 3846.5346
Zero-point correction (Hartree): 0.271428

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TS.ApineneCI.J.b+H2O.HHP.ptmd
~~~~~
E(RM062X/CC-pVDZ) (Hartree): -692.36827721
Electronic state : 1-A
Cartesian coordinates (Angs):
 C 0.136436 0.431892 1.177581
 H 0.009368 1.066038 2.069216
 C 1.633006 0.398093 0.886809
 C 2.079191 -0.672144 -0.065679
 H 1.975339 1.382356 0.542108
 H 2.209916 0.195307 1.804000
 H 1.340733 -1.319774 -0.553481
 C -0.902267 0.927556 0.127469
 C -0.706867 -0.844897 1.381249
 C -1.266959 2.400183 0.218429
 C -0.553477 0.548663 -1.310156
 H -0.443297 -0.538274 -1.437106
 H -1.359695 0.863594 -1.991778
 H 0.380025 1.038518 -1.623283
 H -2.117055 2.643412 -0.438689
 H -0.416053 3.024227 -0.098699
 H -1.534668 2.682900 1.247611
 H -0.802186 -1.235225 2.401918
 H -0.434835 -1.668884 0.706248
 C -1.909670 -0.091149 0.788934
 H -2.501448 0.430020 1.556760
 C -2.814183 -0.841622 -0.160099
 C -4.124401 -0.176081 -0.508955
 H -3.944610 0.865404 -0.818093
 H -4.766516 -0.139636 0.384394

```

|                                                           |           |           |           |
|-----------------------------------------------------------|-----------|-----------|-----------|
| H                                                         | -4.628588 | -0.730839 | -1.307658 |
| O                                                         | -2.479428 | -1.897818 | -0.649672 |
| O                                                         | 3.224335  | -1.228522 | 0.025641  |
| O                                                         | 4.174603  | -0.199404 | 0.295368  |
| O                                                         | 2.716181  | 0.619018  | -1.490820 |
| H                                                         | 3.555367  | 0.505498  | -0.827344 |
| H                                                         | 2.967826  | 0.106199  | -2.273747 |
| Rotational constants (GHz): 1.2770700 0.3619200 0.3437200 |           |           |           |
| Vibrational harmonic frequencies (cm-1):                  |           |           |           |
| i497.3608                                                 | 44.3865   | 48.7328   |           |
| 61.0643                                                   | 82.0918   | 130.9468  |           |
| 147.1936                                                  | 176.7631  | 190.6468  |           |
| 220.2691                                                  | 237.0076  | 240.3009  |           |
| 283.6052                                                  | 313.7766  | 337.7616  |           |
| 349.7615                                                  | 362.5674  | 380.4821  |           |
| 409.5702                                                  | 433.7724  | 501.3155  |           |
| 566.3657                                                  | 578.5563  | 591.5391  |           |
| 617.1231                                                  | 625.4648  | 667.7749  |           |
| 672.8072                                                  | 730.5592  | 791.6483  |           |
| 817.8136                                                  | 884.8698  | 907.1297  |           |
| 939.1976                                                  | 952.9423  | 960.1461  |           |
| 970.7384                                                  | 991.9470  | 994.7810  |           |
| 1004.2509                                                 | 1037.6972 | 1051.4398 |           |
| 1104.7074                                                 | 1140.8673 | 1148.7647 |           |
| 1164.9800                                                 | 1185.0041 | 1200.5997 |           |
| 1216.3656                                                 | 1238.1470 | 1254.5584 |           |
| 1290.2221                                                 | 1308.9136 | 1324.2263 |           |
| 1335.5072                                                 | 1350.8202 | 1371.2508 |           |
| 1386.7130                                                 | 1389.8617 | 1403.5772 |           |
| 1410.0066                                                 | 1415.8723 | 1431.7517 |           |
| 1446.4650                                                 | 1457.7202 | 1462.3276 |           |
| 1473.3970                                                 | 1482.0223 | 1490.6784 |           |
| 1602.5529                                                 | 1637.0273 | 1857.7600 |           |
| 2132.4200                                                 | 3044.0219 | 3055.3227 |           |
| 3061.9755                                                 | 3065.6388 | 3082.5361 |           |
| 3087.2364                                                 | 3094.5386 | 3121.7252 |           |
| 3128.7829                                                 | 3132.0968 | 3137.7532 |           |
| 3140.7556                                                 | 3156.2623 | 3156.6965 |           |
| 3189.1114                                                 | 3192.6037 | 3836.3535 |           |
| Zero-point correction (Hartree): 0.271342                 |           |           |           |

TS.ApineneCI.J.b+H2O.HHP.ptmu

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E(RM062X/CC-pVDZ) (Hartree): -692.37128312

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.167763  | 0.709268  | 1.117404  |
| H | 0.015209  | 1.532122  | 1.833516  |
| C | 1.682929  | 0.620951  | 0.887903  |
| C | 2.129626  | -0.703729 | 0.358226  |
| H | 2.016668  | 1.407933  | 0.201897  |
| H | 2.202465  | 0.752671  | 1.846153  |
| H | 1.976223  | -1.588663 | 0.990922  |
| C | -0.828068 | 0.946829  | -0.056055 |
| C | -0.691287 | -0.488402 | 1.578236  |
| C | -1.170716 | 2.402922  | -0.324217 |
| C | -0.441679 | 0.233251  | -1.348572 |
| H | -0.320666 | -0.849415 | -1.204059 |
| H | -1.228998 | 0.375141  | -2.106168 |
| H | 0.505353  | 0.625749  | -1.751122 |
| H | -1.994775 | 2.492350  | -1.049645 |
| H | -0.299696 | 2.925281  | -0.751256 |
| H | -1.466287 | 2.923496  | 0.599468  |
| H | -0.818713 | -0.645564 | 2.656665  |
| H | -0.411063 | -1.439371 | 1.103301  |
| C | -1.866312 | 0.119528  | 0.795975  |
| H | -2.471010 | 0.808049  | 1.406565  |
| C | -2.760256 | -0.827392 | 0.029720  |
| C | -4.000476 | -0.225596 | -0.588757 |
| H | -3.734529 | 0.673879  | -1.165174 |
| H | -4.689508 | 0.093961  | 0.208079  |
| H | -4.493418 | -0.960726 | -1.234177 |
| O | -2.473194 | -1.995016 | -0.110447 |
| O | 2.253929  | -1.014375 | -0.873656 |
| O | 2.828018  | 0.084945  | -1.579033 |
| O | 4.073381  | -0.195685 | 0.534058  |
| H | 3.832727  | 0.109495  | -0.449137 |
| H | 4.593789  | -1.001120 | 0.397593  |

Rotational constants (GHz): 1.2407000 0.3829300 0.3695400

Vibrational harmonic frequencies (cm-1):

|           |           |           |  |
|-----------|-----------|-----------|--|
| i442.3699 | 50.0596   | 52.1290   |  |
| 59.7026   | 99.4352   | 121.1111  |  |
| 143.0296  | 154.8783  | 204.4491  |  |
| 229.1767  | 230.1362  | 246.4330  |  |
| 282.9268  | 316.4343  | 343.3718  |  |
| 347.3374  | 382.7851  | 391.1153  |  |
| 399.9616  | 440.7757  | 489.6660  |  |
| 564.5525  | 580.2851  | 591.5749  |  |
| 607.0902  | 625.3459  | 649.5888  |  |
| 660.5050  | 722.9335  | 769.6112  |  |
| 873.6436  | 888.5238  | 906.1882  |  |
| 933.6074  | 945.4946  | 958.9495  |  |
| 970.8911  | 987.5258  | 994.0040  |  |
| 1012.6921 | 1034.7493 | 1047.5364 |  |
| 1126.9311 | 1141.2358 | 1153.1850 |  |
| 1164.9986 | 1183.2055 | 1200.5920 |  |
| 1219.0058 | 1244.8713 | 1256.6493 |  |
| 1293.6456 | 1300.9128 | 1318.1342 |  |
| 1330.5743 | 1350.3977 | 1362.3534 |  |
| 1384.4571 | 1389.8470 | 1405.6142 |  |
| 1413.2568 | 1431.5366 | 1436.4377 |  |
| 1445.5543 | 1455.8091 | 1464.3651 |  |

|           |           |           |
|-----------|-----------|-----------|
| 1473.3295 | 1485.1665 | 1487.9127 |
| 1600.1637 | 1650.4908 | 1861.2211 |
| 2329.1361 | 3044.6866 | 3053.0838 |
| 3063.6725 | 3065.9620 | 3081.4963 |
| 3092.3166 | 3111.8077 | 3123.3181 |
| 3130.3711 | 3131.0800 | 3139.8358 |
| 3152.0875 | 3155.2192 | 3163.6737 |
| 3179.5596 | 3192.5682 | 3842.2404 |

Zero-point correction (Hartree): 0.272000

TS.ApineneCI.J.b+H2O.HHP.ptpd

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E(RM062X/CC-pVDZ) (Hartree): -692.36923702

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.270361 | 0.828614  | -0.870481 |
| H | -0.158540 | 1.477943  | -1.753742 |
| C | -1.714080 | 1.041229  | -0.389048 |
| C | -2.126842 | 0.099358  | 0.700080  |
| H | -1.847288 | 2.067272  | -0.015948 |
| H | -2.376330 | 0.896031  | -1.246944 |
| H | -2.038384 | 0.408505  | 1.748411  |
| C | 0.971341  | 1.077622  | 0.033847  |
| C | 0.283189  | -0.566603 | -1.218902 |
| C | 1.592609  | 2.461882  | -0.060503 |
| C | 0.752435  | 0.680498  | 1.490827  |
| H | 0.343789  | -0.336256 | 1.583611  |
| H | 1.704369  | 0.696745  | 2.044682  |
| H | 0.075123  | 1.397311  | 1.983230  |
| H | 2.546817  | 2.510825  | 0.488009  |
| H | 0.920975  | 3.218249  | 0.377568  |
| H | 1.783161  | 2.741815  | -1.107240 |
| H | 0.156141  | -0.913519 | -2.250569 |
| H | -0.063578 | -1.351492 | -0.536489 |
| C | 1.675078  | -0.068324 | -0.790449 |
| H | 2.240769  | 0.382388  | -1.620247 |
| C | 2.556078  | -1.004189 | 0.004738  |
| C | 4.019143  | -0.635229 | 0.097650  |
| H | 4.121908  | 0.417036  | 0.406302  |
| H | 4.483375  | -0.724210 | -0.896538 |
| H | 4.530486  | -1.294315 | 0.807767  |
| O | 2.101598  | -1.969399 | 0.576436  |
| O | -2.157046 | -1.168114 | 0.570435  |
| O | -2.664801 | -1.473584 | -0.731507 |
| O | -4.090048 | 0.304110  | 0.259960  |
| H | -3.777953 | -0.489362 | -0.360152 |
| H | -4.593993 | -0.138213 | 0.959147  |

Rotational constants (GHz): 1.2215300 0.4151000 0.3632100

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i427.6069 | 47.5622   | 52.5910   |
| 57.8789   | 101.2440  | 136.5220  |
| 145.1857  | 163.3018  | 182.1282  |
| 224.8619  | 233.7222  | 241.0685  |
| 281.8367  | 318.7110  | 348.2715  |
| 351.5042  | 381.1241  | 382.7281  |
| 403.4322  | 435.4628  | 478.4572  |
| 567.1970  | 584.6854  | 593.6300  |
| 617.5377  | 624.0818  | 655.3060  |
| 680.3166  | 726.0538  | 772.0230  |
| 862.0572  | 877.5208  | 906.4963  |
| 938.2226  | 950.3473  | 961.3843  |
| 974.8131  | 980.1098  | 987.4043  |
| 1016.5792 | 1033.0213 | 1063.8359 |
| 1073.6052 | 1138.9866 | 1155.5123 |
| 1165.9132 | 1185.5680 | 1199.3067 |
| 1229.8153 | 1241.3236 | 1260.3874 |
| 1299.0360 | 1303.3889 | 1326.0474 |
| 1328.3601 | 1349.5879 | 1359.2375 |
| 1385.6446 | 1387.5219 | 1398.4975 |
| 1407.5886 | 1432.4905 | 1436.6377 |
| 1446.7162 | 1455.8418 | 1460.9816 |
| 1466.7645 | 1478.1984 | 1485.4041 |
| 1601.4452 | 1655.3670 | 1862.2528 |
| 2359.9161 | 3042.5039 | 3045.6277 |
| 3059.7461 | 3060.4695 | 3081.8659 |
| 3100.7598 | 3114.8642 | 3119.3836 |
| 3123.1535 | 3133.5809 | 3135.1607 |
| 3145.0602 | 3178.6805 | 3187.8136 |
| 3189.8685 | 3190.7294 | 3840.2933 |

Zero-point correction (Hartree): 0.272075

TS.ApineneCI.J.b+H2O.HHP.pttd

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E(RM062X/CC-pVDZ) (Hartree): -692.35990622

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.373252 | 0.966945  | -0.855589 |
| H | -0.203025 | 1.714044  | -1.649393 |
| C | -1.791159 | 1.281392  | -0.375312 |
| C | -2.721682 | 0.446117  | 0.453754  |
| H | -1.735672 | 2.216500  | 0.220483  |
| H | -2.415516 | 1.545215  | -1.242409 |
| H | -3.669168 | 0.965150  | 0.663490  |
| C | 0.855941  | 1.083251  | 0.092876  |
| C | 0.164020  | -0.377657 | -1.383979 |
| C | 1.497539  | 2.461839  | 0.145877  |
| C | 0.602402  | 0.547163  | 1.497825  |
| H | 0.159024  | -0.457268 | 1.479677  |
| H | 1.541655  | 0.519035  | 2.073567  |
| H | -0.086898 | 1.218953  | 2.037497  |
| H | 2.442990  | 2.440485  | 0.711179  |
| H | 0.831699  | 3.179173  | 0.654060  |



|                                                           |           |           |           |
|-----------------------------------------------------------|-----------|-----------|-----------|
| H                                                         | 1.709627  | 2.847768  | -0.862985 |
| H                                                         | 0.067011  | -0.561944 | -2.460780 |
| H                                                         | -0.198646 | -1.235101 | -0.811444 |
| C                                                         | 1.548875  | 0.030889  | -0.852111 |
| H                                                         | 2.159657  | 0.563140  | -1.599106 |
| C                                                         | 2.383749  | -1.031731 | -0.175153 |
| C                                                         | 3.777234  | -0.615554 | 0.244241  |
| H                                                         | 3.739661  | 0.332545  | 0.802372  |
| H                                                         | 4.390900  | -0.438559 | -0.652587 |
| H                                                         | 4.234343  | -1.401140 | 0.856042  |
| O                                                         | 1.955325  | -2.141139 | 0.041491  |
| O                                                         | -2.533674 | -0.485061 | 1.298382  |
| O                                                         | -1.617309 | -1.450248 | 0.800878  |
| O                                                         | -3.092742 | -0.860693 | -1.085861 |
| H                                                         | -2.398003 | -1.379039 | -0.494895 |
| H                                                         | -3.924441 | -1.327757 | -0.918463 |
| Rotational constants (GHz): 1.0777600 0.4736800 0.4145600 |           |           |           |
| Vibrational harmonic frequencies (cm-1):                  |           |           |           |
| i429.8426                                                 | 45.6580   | 47.8202   |           |
| 60.5737                                                   | 97.9603   | 117.4406  |           |
| 149.3927                                                  | 169.7003  | 179.7916  |           |
| 192.5440                                                  | 229.1813  | 259.5198  |           |
| 289.9833                                                  | 301.8306  | 307.9013  |           |
| 340.0130                                                  | 359.2180  | 386.6978  |           |
| 390.9046                                                  | 429.6041  | 456.3263  |           |
| 545.5181                                                  | 558.4831  | 572.9514  |           |
| 584.8433                                                  | 597.6541  | 622.4188  |           |
| 702.0351                                                  | 737.8671  | 772.8470  |           |
| 841.0382                                                  | 878.5553  | 912.6512  |           |
| 916.6180                                                  | 943.7480  | 954.9328  |           |
| 967.8931                                                  | 981.9837  | 991.3419  |           |
| 1015.3038                                                 | 1022.1459 | 1051.4861 |           |
| 1071.5659                                                 | 1146.9268 | 1166.5606 |           |
| 1177.2864                                                 | 1192.1392 | 1201.7145 |           |
| 1227.1336                                                 | 1251.8207 | 1262.8063 |           |
| 1301.2571                                                 | 1307.6955 | 1332.1825 |           |
| 1348.2543                                                 | 1372.0768 | 1384.4731 |           |
| 1386.8488                                                 | 1397.4084 | 1404.8576 |           |
| 1417.8327                                                 | 1421.5162 | 1431.9863 |           |
| 1445.9052                                                 | 1455.1606 | 1460.6142 |           |
| 1472.5591                                                 | 1478.0082 | 1488.7640 |           |
| 1612.5496                                                 | 1644.7053 | 1868.7995 |           |
| 2425.0933                                                 | 3005.3655 | 3037.2678 |           |
| 3039.4785                                                 | 3044.2074 | 3061.7864 |           |
| 3070.4370                                                 | 3104.3017 | 3105.8999 |           |
| 3113.7917                                                 | 3116.4438 | 3126.9648 |           |
| 3138.2796                                                 | 3138.5631 | 3163.9878 |           |
| 3188.9424                                                 | 3216.2914 | 3847.2359 |           |
| Zero-point correction (Hartree): 0.271239                 |           |           |           |

TS.ApineneCI.J.b+H2O.HHP.pttu

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E(RM062X/CC-pVDZ) (Hartree): -692.35749996

Electronic state : 1-A

Cartesian coordinates (Angs):

|                                                           |           |           |           |
|-----------------------------------------------------------|-----------|-----------|-----------|
| C                                                         | 0.345380  | 0.820928  | 1.043400  |
| H                                                         | 0.088997  | 1.605770  | 1.776253  |
| C                                                         | 1.861476  | 0.998149  | 0.886249  |
| C                                                         | 2.868472  | -0.056400 | 0.530343  |
| H                                                         | 2.077266  | 1.855524  | 0.228180  |
| H                                                         | 2.246771  | 1.310664  | 1.875646  |
| H                                                         | 3.898477  | 0.199487  | 0.816740  |
| C                                                         | -0.713411 | 1.019408  | -0.085048 |
| C                                                         | -0.389771 | -0.453782 | 1.501011  |
| C                                                         | -1.163515 | 2.461221  | -0.274097 |
| C                                                         | -0.397275 | 0.385101  | -1.435665 |
| H                                                         | -0.220866 | -0.693384 | -1.352236 |
| H                                                         | -1.244518 | 0.545462  | -2.122595 |
| H                                                         | 0.491454  | 0.853833  | -1.884984 |
| H                                                         | -2.038067 | 2.522950  | -0.941098 |
| H                                                         | -0.358663 | 3.056010  | -0.736857 |
| H                                                         | -1.429645 | 2.930819  | 0.685232  |
| H                                                         | -0.457759 | -0.635887 | 2.581436  |
| H                                                         | -0.034134 | -1.346027 | 0.974248  |
| C                                                         | -1.642656 | 0.103085  | 0.800749  |
| H                                                         | -2.249736 | 0.742313  | 1.462454  |
| C                                                         | -2.539571 | -0.862210 | 0.062210  |
| C                                                         | -3.826154 | -0.285453 | -0.488500 |
| H                                                         | -3.614517 | 0.627949  | -1.065624 |
| H                                                         | -4.485210 | 0.004235  | 0.344407  |
| H                                                         | -4.329241 | -1.026736 | -1.119141 |
| O                                                         | -2.234814 | -2.020175 | -0.105584 |
| O                                                         | 2.729753  | -1.309437 | 0.379565  |
| O                                                         | 1.605649  | -1.565081 | -0.453074 |
| O                                                         | 2.830886  | 0.303486  | -1.505368 |
| H                                                         | 2.176534  | -0.507474 | -1.376882 |
| H                                                         | 3.613218  | -0.096117 | -1.913402 |
| Rotational constants (GHz): 1.1010300 0.4599900 0.4140000 |           |           |           |
| Vibrational harmonic frequencies (cm-1):                  |           |           |           |
| i421.9827                                                 | 46.3090   | 50.1691   |           |
| 59.2053                                                   | 80.7646   | 118.7931  |           |
| 145.3544                                                  | 174.2915  | 184.6540  |           |
| 214.6361                                                  | 227.6359  | 240.7726  |           |
| 288.5098                                                  | 303.1758  | 331.2010  |           |
| 346.4877                                                  | 357.6078  | 379.0210  |           |
| 393.4613                                                  | 437.7498  | 455.1793  |           |
| 549.3571                                                  | 562.3785  | 576.0512  |           |
| 588.8853                                                  | 609.0239  | 623.0762  |           |
| 684.2662                                                  | 746.6647  | 802.5380  |           |
| 814.6969                                                  | 879.9899  | 916.4220  |           |
| 920.9495                                                  | 941.7055  | 954.4465  |           |
| 963.2361                                                  | 974.3484  | 991.9139  |           |

|           |           |           |
|-----------|-----------|-----------|
| 1012.1281 | 1023.1141 | 1045.5760 |
| 1090.9643 | 1141.8797 | 1168.3433 |
| 1174.8743 | 1196.2704 | 1203.0582 |
| 1233.5953 | 1250.2455 | 1260.2294 |
| 1302.7903 | 1320.4287 | 1329.9070 |
| 1350.1946 | 1375.0176 | 1384.8284 |
| 1387.3626 | 1400.2971 | 1401.1614 |
| 1410.1998 | 1428.1912 | 1432.0663 |
| 1446.0098 | 1455.5071 | 1462.2458 |
| 1474.5210 | 1485.2853 | 1490.7141 |
| 1616.8491 | 1646.6570 | 1867.3302 |
| 2412.5109 | 3019.5610 | 3038.4559 |
| 3041.0565 | 3054.2808 | 3061.0028 |
| 3069.5799 | 3098.7277 | 3101.0835 |
| 3115.4938 | 3127.3088 | 3128.6670 |
| 3136.9618 | 3155.6921 | 3183.0169 |
| 3188.6815 | 3189.5386 | 3837.8901 |

Zero-point correction (Hartree): 0.271472

TS.ApineneCI.J.b+H2O.HHP.tttdd

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E(RM062X/CC-pVDZ) (Hartree): -692.36185157

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.318135  | 1.137763  | 0.843343  |
| H | 0.199230  | 1.966800  | 1.559618  |
| C | 1.722986  | 1.352945  | 0.278704  |
| C | 2.549204  | 0.429428  | -0.571183 |
| H | 1.679948  | 2.259981  | -0.358821 |
| H | 2.413548  | 1.621566  | 1.092826  |
| H | 3.472667  | 0.909492  | -0.928067 |
| C | -0.933696 | 1.169265  | -0.086959 |
| C | -0.194669 | -0.152253 | 1.520548  |
| C | -1.679933 | 2.494978  | -0.116431 |
| C | -0.691682 | 0.675507  | -1.509256 |
| H | -0.205265 | -0.308476 | -1.523085 |
| H | -1.650140 | 0.602975  | -2.043927 |
| H | -0.054982 | 1.389933  | -2.058099 |
| H | -2.660221 | 2.358597  | -0.597869 |
| H | -1.118807 | 3.252896  | -0.688130 |
| H | -1.848949 | 2.883753  | 0.899544  |
| H | -0.173890 | -0.154817 | 2.617629  |
| H | 0.293828  | -1.047796 | 1.134719  |
| C | -1.569593 | 0.090041  | 0.858834  |
| H | -2.288070 | 0.573377  | 1.537329  |
| C | -2.318513 | -1.016117 | 0.139219  |
| C | -1.717790 | -2.398583 | 0.110329  |
| H | -1.518575 | -2.749605 | 1.134664  |
| H | -0.746886 | -2.361944 | -0.411996 |
| H | -2.402316 | -3.083004 | -0.402569 |
| O | -3.355383 | -0.749206 | -0.429582 |
| O | 2.258843  | -0.565336 | -1.313026 |
| O | 1.400199  | -1.472854 | -0.631878 |
| O | 3.121553  | -0.747438 | 0.991194  |
| H | 2.367117  | -1.315590 | 0.550572  |
| H | 3.933367  | -1.217310 | 0.749124  |

Rotational constants (GHz): 1.0037000 0.5182100 0.4366000

Vibrational harmonic frequencies (cm-1):

|           |           |           |
|-----------|-----------|-----------|
| i420.0332 | 38.6630   | 55.5998   |
| 84.7479   | 103.8036  | 153.5366  |
| 164.9846  | 179.1558  | 202.4968  |
| 249.2008  | 254.9689  | 270.5879  |
| 299.3767  | 311.2064  | 342.6865  |
| 348.5593  | 354.8374  | 378.9252  |
| 424.8955  | 459.0722  | 468.9566  |
| 488.4041  | 549.5260  | 569.3029  |
| 594.5453  | 604.4962  | 621.7984  |
| 702.1418  | 736.3773  | 774.5915  |
| 833.3794  | 881.0995  | 895.0381  |
| 907.7584  | 929.1688  | 955.5516  |
| 980.9632  | 993.4759  | 1006.5278 |
| 1016.5767 | 1032.6164 | 1059.0326 |
| 1075.5955 | 1149.6045 | 1166.2229 |
| 1174.2592 | 1199.2499 | 1225.1068 |
| 1246.8346 | 1255.4303 | 1263.7518 |
| 1286.1480 | 1302.4045 | 1329.7959 |
| 1336.9826 | 1367.5916 | 1378.1973 |
| 1382.7591 | 1389.0449 | 1398.4149 |
| 1409.3985 | 1417.9494 | 1439.4202 |
| 1445.2194 | 1456.1222 | 1463.8446 |
| 1465.4888 | 1479.7403 | 1500.8578 |
| 1598.1299 | 1642.5062 | 1850.8096 |
| 2517.0736 | 3011.8029 | 3040.8811 |
| 3046.7928 | 3052.0786 | 3057.7653 |
| 3093.0220 | 3105.8668 | 3113.2312 |
| 3120.5430 | 3126.0475 | 3129.8258 |
| 3136.0127 | 3141.7011 | 3171.9932 |
| 3188.0284 | 3227.1773 | 3838.6122 |

Zero-point correction (Hartree): 0.272227

TS.ApineneCI.J.b+H2O.HHP.ttttu

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E(RM062X/CC-pVDZ) (Hartree): -692.35934825

Electronic state : 1-A

Cartesian coordinates (Angs):

|   |          |           |           |
|---|----------|-----------|-----------|
| C | 0.318368 | 1.064496  | 1.014390  |
| H | 0.162474 | 1.932447  | 1.674625  |
| C | 1.829828 | 1.086270  | 0.751080  |
| C | 2.685763 | -0.127541 | 0.509913  |
| H | 2.073531 | 1.805938  | -0.046394 |
| H | 2.312614 | 1.502678  | 1.654061  |
| H | 3.737422 | -0.002764 | 0.803361  |

|                                           |           |           |           |
|-------------------------------------------|-----------|-----------|-----------|
| C                                         | -0.772538 | 1.198311  | -0.099711 |
| C                                         | -0.426162 | -0.139061 | 1.635170  |
| C                                         | -1.356801 | 2.601746  | -0.208642 |
| C                                         | -0.429320 | 0.697440  | -1.499438 |
| H                                         | -0.201018 | -0.373465 | -1.516109 |
| H                                         | -1.287595 | 0.868807  | -2.164560 |
| H                                         | 0.439542  | 1.240766  | -1.904057 |
| H                                         | -2.279677 | 2.575415  | -0.807456 |
| H                                         | -0.645542 | 3.285185  | -0.701701 |
| H                                         | -1.602348 | 3.014638  | 0.782025  |
| H                                         | -0.587337 | -0.091770 | 2.720277  |
| H                                         | 0.022271  | -1.096723 | 1.359534  |
| C                                         | -1.644559 | 0.207201  | 0.749408  |
| H                                         | -2.419129 | 0.766291  | 1.296487  |
| C                                         | -2.365719 | -0.861665 | -0.051493 |
| C                                         | -1.988644 | -2.303847 | 0.170902  |
| H                                         | -2.070902 | -2.556851 | 1.239550  |
| H                                         | -0.931205 | -2.448415 | -0.107664 |
| H                                         | -2.640325 | -2.949964 | -0.427408 |
| O                                         | -3.199588 | -0.525989 | -0.864772 |
| O                                         | 2.370749  | -1.360694 | 0.464678  |
| O                                         | 1.234165  | -1.534188 | -0.375203 |
| O                                         | 2.761899  | 0.057795  | -1.527413 |
| H                                         | 1.990740  | -0.621705 | -1.392916 |
| H                                         | 3.487389  | -0.485990 | -1.869454 |
| Rotational constants (GHz):               |           |           |           |
|                                           | 0.9711900 | 0.5273100 | 0.4524800 |
| Vibrational harmonic frequencies (cm-1):  |           |           |           |
| i404.6737                                 | 25.3057   |           | 34.7709   |
| 74.3555                                   | 86.7720   |           | 147.7376  |
| 168.0969                                  | 190.6008  |           | 214.4768  |
| 222.1577                                  | 244.2372  |           | 269.3498  |
| 293.6178                                  | 307.2068  |           | 320.3523  |
| 345.9204                                  | 355.6396  |           | 362.2866  |
| 432.7209                                  | 449.2829  |           | 475.0422  |
| 486.1116                                  | 545.9594  |           | 565.1769  |
| 592.2241                                  | 603.2837  |           | 623.8402  |
| 689.5743                                  | 740.5408  |           | 793.8993  |
| 822.0634                                  | 883.3944  |           | 897.1878  |
| 914.4509                                  | 928.4108  |           | 950.2347  |
| 967.4370                                  | 993.7450  |           | 999.0140  |
| 1011.1806                                 | 1031.5872 |           | 1051.4504 |
| 1096.6832                                 | 1149.8022 |           | 1164.2693 |
| 1174.4963                                 | 1203.4794 |           | 1232.3072 |
| 1241.5134                                 | 1244.3243 |           | 1254.4274 |
| 1263.6593                                 | 1309.5793 |           | 1321.4412 |
| 1341.8193                                 | 1371.4315 |           | 1379.2153 |
| 1380.7228                                 | 1388.8434 |           | 1395.3725 |
| 1409.6161                                 | 1416.0856 |           | 1437.1596 |
| 1445.9374                                 | 1454.2458 |           | 1459.5517 |
| 1464.9446                                 | 1473.6894 |           | 1489.8940 |
| 1598.0022                                 | 1646.0556 |           | 1851.5147 |
| 2607.1313                                 | 3034.8015 |           | 3040.2832 |
| 3051.2261                                 | 3060.2947 |           | 3064.5434 |
| 3085.1839                                 | 3100.5424 |           | 3104.0135 |
| 3119.7989                                 | 3127.6270 |           | 3134.4819 |
| 3140.3955                                 | 3156.3605 |           | 3188.5772 |
| 3189.1944                                 | 3206.5673 |           | 3834.1820 |
| Zero-point correction (Hartree): 0.272050 |           |           |           |