

A Structure-Activity Relationship for the rate coefficient of H-migration in substituted alkoxy radicals

– Supporting information –

L. Vereecken,* J. Peeters

Katholieke Universiteit Leuven, Department of chemistry, Celestijnenlaan 200F, B-3001 Leuven, Belgium

Table of contents

- p. 2: Barrier height trends at the B3LYP and CBS-QB3 levels of theory
- p. 5: Approximating $F(\text{SD})$ as $F(\text{rig}) \times F(\text{conf})$
- p. 6: Fall-off corrections
- p. 8: The transition states for H-migration
- p. 19: The impact of heterosubstitution on the H-migration
- p. 29: Testing the framework: predicting relative rate coefficients
- p. 32: Testing the theoretical kinetic values: predicting absolute rate coefficients
- p. 33: Total correction factors at 298K
- p. 34: References
- p. 35 onwards: Raw quantum chemical data

* Email: Luc.Vereecken@chem.kuleuven.be

I. Barrier height trends at the B3LYP and CBS-QB3 levels of theory

For the abstraction of H atoms from hydrocarbons by OH radicals, we have shown earlier that the rate of abstraction is correlated (non-linearly) to the D(C–H) bond strength;^{1,2} it should be stressed that this correlation is non-causal and breaks down for some cases. For H-migration in alkoxy radicals, a similar (non-causal) correlation is expected to exist, and indeed migration of tertiary radicals, with a lower C–H bond strength, is significantly faster than for primary or secondary radicals. The correlation can be described as a Evans-Polanyi type relationship, where within a specific reaction class, larger reaction exothermicity leads to lower reaction barriers. As the newly formed O–H bond is about the same strength in most alkoxy radicals, the bond strength of the breaking C–H bond becomes an interesting metric for the barrier height. The isomerisation reactions of alkoxy radicals are rather exothermic, such that the transition state is reactant-like, and its properties are mostly determined the environment of the migrating H in the reactant, i.e. by the breaking C–H bond.

We have already established earlier that B3LYP/6-31G(d,p) is not an ideal level of theory to calculate D(C–H): while the bond strengths for primary H are fairly close to experimental values, B3LYP tends to underestimate the strength of weaker C–H bonds. This is illustrated in table S1 below.

Table S1: Comparison of B3LYP/6-31G(d,p) D(C–H) bond strengths against experimental values (kJ mol⁻¹) for increasing methyl substitution

| Compound | B3LYP | Experiment ^{3,a} |
|------------------|-------|---------------------------|
| Methane (0° H) | 435.6 | 432.7 ± 0.4 |
| Ethane (1° H) | 415.1 | 416.8 ± 1.6 |
| Propane (2° H) | 398.5 | 402.9 ± 2.0 |
| t-butane (3° H) | 385.3 | 398.1 ± 1.3 |
| ethanol (α-OH H) | 382.9 | 395.2 ± 4 |

^a bond dissociation enthalpies at 298 K rescaled to 0 K

Note, however, that the error is not randomly distributed, but systematic. Because of this, the B3LYP functional is still quite useful for building predictive correlations and SARs where the systematic bias can be incorporated in the model. Also, we have found that B3LYP/6-31G(d,p) is a good method for predicting reactions of alkoxy radicals, both for decomposition¹⁷ and for

isomerisation reactions.⁴ For both reaction types, different levels of quantum chemical theory disagree strongly over the absolute barrier height, and many predictions are irreconcilable with the experimental data. CBS-QB3 does not suffer from a systematic bias in its D(C–H) predictions,⁵ which correlate excellently ($\sigma = 8.4 \text{ kJ mol}^{-1}$) against experimental data.

Due to the (non-causal) correlation between C–H bond strength and barrier height, predictions based on a level of theory that underestimates the bond strength, will lead to lower and earlier transition states. As the B3LYP C–H bond strength for primary H is close to the experimental values, the barrier height for H-migration should be reliable (and indeed⁴ leads to good agreement with experiment), while barrier heights for secondary and even more tertiary H should be underestimated. Much to our surprise, we found that CBS-QB3 calculations predicted an even steeper relative decrease of the barrier height with increasing substitution: -11.5 and $-21.8 \text{ kJ mol}^{-1}$ for 2° and 3° H on average below the barriers for 1° H, versus -10.5 and $-20.4 \text{ kJ mol}^{-1}$ for B3LYP. In hindsight, this is a clear result of the B3LYP geometry optimization used in CBS-QB3, which does suffer from C–H bond strength bias, and hence forces the high-level single point energy calculation to probe the reaction coordinate at a geometry somewhat before the true CBS-QB3 energy maximum on the energy profile. This bias can in principle be circumvented by using IRCMax calculations to construct a CBS-QB3 high-level energy profile and obtain the true energy maximum, but this is computationally very expensive, especially considering the number of isomerisation reactions considered in this work.

As we are developing a SAR relative to experimental data of a comparable degree of substitution, the differences in bond strength against the reference reaction are generally small, and this systematic bias on the barrier heights should have only a minor impact. Furthermore, we found that ring strain is a more dominant factor in driving differences in barrier height. Lastly, as we understand the origin of the bias and know it is systematic rather than random, we can estimate an empirical correction to counteract the effect. For the bond strength bias the bulk of the error can be removed by a simple linear correction; we therefore propose to correct

the isomerisation barrier height increase/decrease caused by the changing C–H bond strengths by a simple linear empirical correction $a + b \times \Delta E_b$ of the predicted difference in barrier height ΔE_b . The parameters in this correction can be derived from the experimentally determined reference rate coefficients. Note that, as the SAR is build on relative rate predictions, the constant factor a cancels out, leaving only a scaling factor for ΔE_b . This scaling factor was determined to be 0.8, as detailed in the error analysis in the main manuscript and elsewhere in the supporting information.

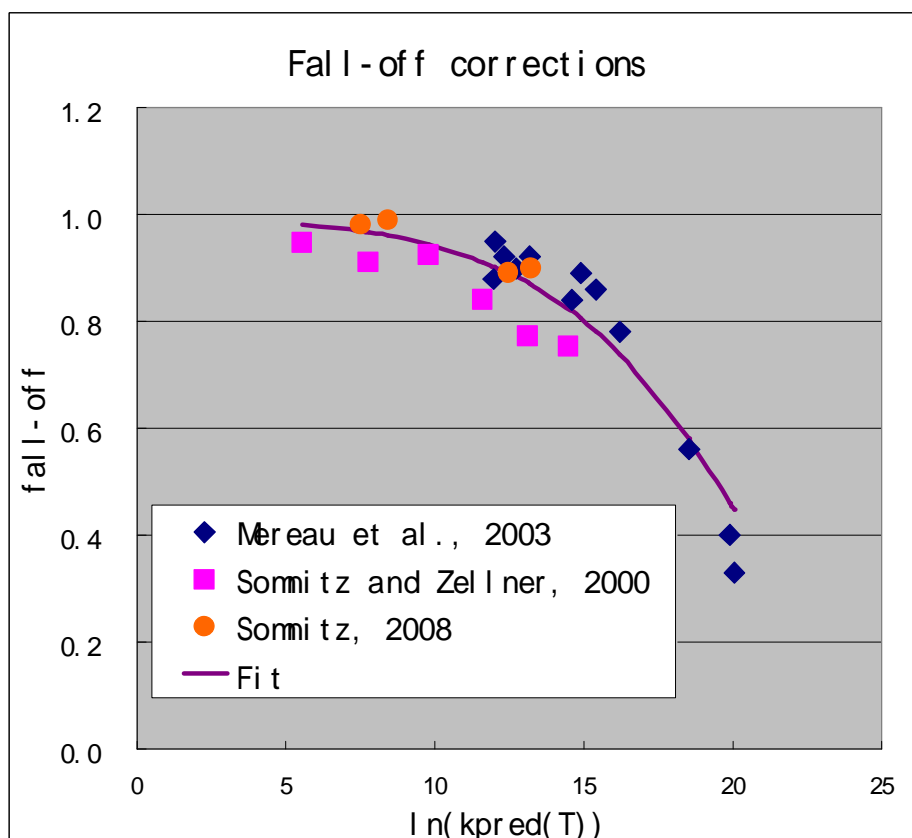
II. Approximating $F(\text{SD})$ as $F(\text{rig}) \times F(\text{conf})$

Table S2: Comparison between $F(\text{SD})$, and its approximation as $F(\text{rig}) \times F(\text{conf})$, based on the multiconformer analysis and lowest-energy-conformer analysis, respectively, of averaged data on 6 primary H-shift, 3 secondary H-shifts, and 2 tertiary H-shifts.

| H-shift | $F(\text{SD})$ | $F(\text{SD})$ | $F(\text{rig}) \times F(\text{conf})$ | $F(\text{rig}) \times F(\text{conf})$ |
|---------|----------------|---|---------------------------------------|---|
| | 298 K | 250K - 350K | 298 K | 250K - 350K |
| 1,4 | 2.21 | $0.359 + 6.19 \times 10^{-3} \text{ T}$ | 2.33 | $0.272 + 6.88 \times 10^{-3} \text{ T}$ |
| 1,5 | 1.00 | 1.00 | 1.00 | 1.00 |
| 1,6 | 0.32 | $0.484 - 5.40 \times 10^{-4} \text{ T}$ | 0.30 | $0.483 - 6.11 \times 10^{-4} \text{ T}$ |
| 1,7 | 0.19 | $0.343 - 5.06 \times 10^{-4} \text{ T}$ | 0.17 | $0.240 - 2.32 \times 10^{-4} \text{ T}$ |
| 1,8 | 0.09 | $0.147 - 1.80 \times 10^{-4} \text{ T}$ | 0.09 | $0.135 - 1.58 \times 10^{-4} \text{ T}$ |

III. Fall-off

Figure S1 Theoretically predicted fall-off correction factors plotted against their predicted rate coefficients. Data by Méreau et al. (2003) is at 298K, data by Somnitz and Zellner (2000), and Somnitz (2008) is at 298K and 220K. Only reactions that have a single, dominant H-migration channel affecting the fall-off are included.



Fall-off is determined by the competition between, on one hand, the chemical reaction(s) that deplete the thermal transition-state population, and on the other hand, collisional energy transfer processes and energy pooling of the reaction coordinate mode with the other (active) vibration modes, which both repopulate the TS. As a consequence, fall-off is more severe as the (H-migration) reaction is faster, as is also borne out by the data shown in Figure S1. Thus, the fall-off factor can be related to the H-migration rate.

However, the impact of fall-off at a given pressure is less severe for larger reactants, with more internal modes contributing to the energy pool. In a Troe fall-off formalism, this translates into

a higher ratio of the low-pressure limit relative to the high-pressure limit, k_0/k_8 , or, alternatively, a fall-off factor closer to 1 at 1 atm for molecules with a higher number of active internal modes. Hence, a correlation between the H-migration rate and the fall-off is valid only in as much as the number of (active) internal modes of all the considered molecules is similar. Unfortunately, the 1 atm fall-off data available (Somnitz 2008; Méreau et al. 2003) for alkoxy-H shifts of different rates pertain all to 1,5-H shifts with varying degrees of substitution, from primary to tertiary migrating H, i.e. for a series of reactants with different number of active internal modes.

In an admittedly first approximation, we still use these available data to estimate the dependence of the fall-off factor on the H-migration rate (see main text). However, one should consider that for larger molecules, the fall-off is then probably overemphasized, as the reference rate coefficients were measured for the smallest possible unsubstituted alkoxy radicals. This overestimation of the fall-off will increase as more internal degrees of freedom are active. At the same time, some forms of substitution, e.g. the presence of double bonds or cycles, can decrease the number of active internal modes, such that fall-off could then become more important compared to the reference reaction. These effects are not accounted for in the proposed fall-off correction factor $F(\text{fall-off})$.

As we currently have insufficient data available to build a predictive correlation including these effects, one would have to resort to Master Equation analyses of the pertaining unimolecular isomerisation mechanism, for each and every reaction examined. This is beyond the scope of the current first-generation SAR. One should consider that for many alkoxy radicals of atmospheric importance, the difference in fall-off relative to the reference reactions is probably not too extreme, except perhaps for the largest of compounds. Also, in many cases the *absolute* rate coefficient is not overly important, e.g. when one channel is clearly dominant.

VI. The transition states for H-migration

a) Ring strain

The ring strain in cycloalkanes has been studied extensively, and depends strongly on the number of atoms in the ring. For cycloalkanes, three-, four-, and five-membered rings are found to have the highest ring strains, while cyclohexane does not have ring strain. For 7-membered and larger rings, ring strain increases again, but to a lesser extent than in the 3- to 5-membered rings, and irregularly decreases again after 9 carbons; there is no easily described trend in the ring strain of these larger rings.

Cyclohexane is strain free because its bond angles are within the fairly narrow range where 6 equally long bonds can make a strain free ring. For the H-migration TS, not all bond lengths are equal, with at least the C–O, C–H, and O–H (partial) bonds being different from the C–C bonds. Likewise, many bond angles differ from those in the proverbial sp^3 -hybridized C tetraeder: C–C–O, C–O–H, O–H–C, and H–C–C. The angles around the C carrying the migrating H is furthermore function of how early/late the TS is, as it changes from sp^3 hybridization to sp^2 . The O–H–C is significantly different from all other angles, with the preferred bond angle for H-migration being close to 180° . As a function of the TS ring size, the O–H–C bond angle is then a nice indicator of how ring strain prevents the active site from attaining the preferred collinear bond:

Table S3: Bond angles around the migrating H.

| H-shift | C–H–O angle |
|---------|-------------|
| 1,4 | 134° |
| 1,5 | 155° |
| 1,6 | 167° |
| 1,7 | 178° |
| 1,8 | 175° |

The above means that one cannot simply transpose the amount of ring strains in cycloalkanes to the cyclic transition states for H-migration. Especially, the O–H–C bond angle clearly

demonstrates that the 6-membered TS rings in 1,5-H-migration is not strain-free, and forces the migration path away from the preferred near-linear reaction path typically found in e.g. H-abstraction by OH from hydrocarbons.

b) Labeling of conformers

The question of how to label the different TS conformers of a given H-migration is rather interesting. We propose here to label the TS rings in accordance to the labeling of the conformers found for the cycloalkanes of the same number of atoms in the ring.^{6,7,8,9,10,11,12} Needless to say, the different angles and bond lengths in the TS compared to a cycloalkane make a one-to-one mapping not always obvious, or even possible. Still, we found that the signs of the dihedral angles through-out the TS ring usually showed the same sequences as in the corresponding alkane. E.g. The signs of the C–C–C–C dihedral angles in sequence through the ring of the chair conformer of cyclohexane are [+ - + - + -], while for the twist-boat conformer one finds [+ + - + + -]. For the 6-membered ring in the 1,5-H-shift in butoxy, on the other hand, we find a sequence of [+ - + - + -], and hence we would label this TS conformer a chair form. One has to trivially account for enantiomers, where all dihedral angles change sign, as well as starting the sequence from a different atom in the ring or rotating through the torsions in the opposite direction. More difficult are dihedral angles close to 0°, where the sign of the dihedral angle can be dependent on the uncertainties in the quantum chemical calculation.

c) 1,4-H-migration TS

Only a single conformer (and its enantiomer) exists for the transition state for 1,4-H-migration, and is best described as a twisted five-membered ring; an example is show below:

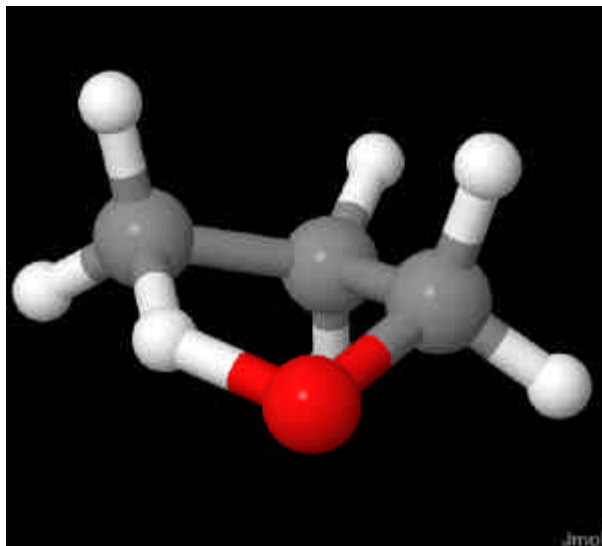


Figure S2: 1,4-H-shift in 1-propoxy

d) 1,5-H-migration TS

We were only able to local a single conformer (and its enantiomer) for the TS for 1,5-H-migration. The $-C-C-H-O-C-$ atoms all lie nearly in a plane, with the remaining carbon pointing upwards (or downwards in the enantiomer). An example is show below:

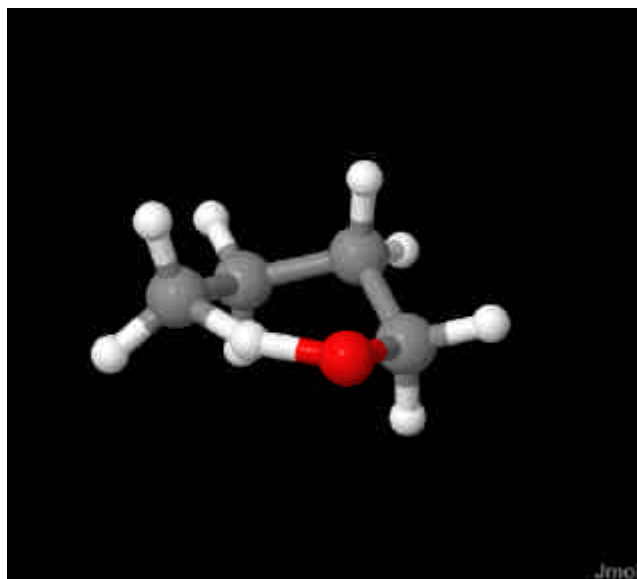


Figure S3: 1,5-H-shift in 1-butoxy

e) 1,6-H-migration TS

Three conformers were found for the 1,6-H-migration: a twist-chair (TC), chair (C), and boat (B) conformer. For B, we find that the signs of the dihedral angles do not correspond to any of the known conformers of cycloheptane, but this might be due to two angles being $\leq 12^\circ$; still, visually, this conformer seems best described as a boat shape. For cycloheptane, only the TC and B conformers are energetic minima, while the chair-form is a transition state; for the H-migration TS, we find three structures with exactly 1 imaginary frequency. The relative energies of the 1,6-H-migration conformers is given below:

Table S4: Relative energies of the TS conformers for 1,6-H-migration

| Conformer | Relative energy (kJ mol^{-1}) | |
|------------------|--|---------|
| | B3LYP/6-31G(d,p) | CBS-QB3 |
| Twist-chair (TC) | 0.0 | 0.0 |
| Chair (C) | 12.5 | 9.9 |
| Boat (B) | 14.1 | |

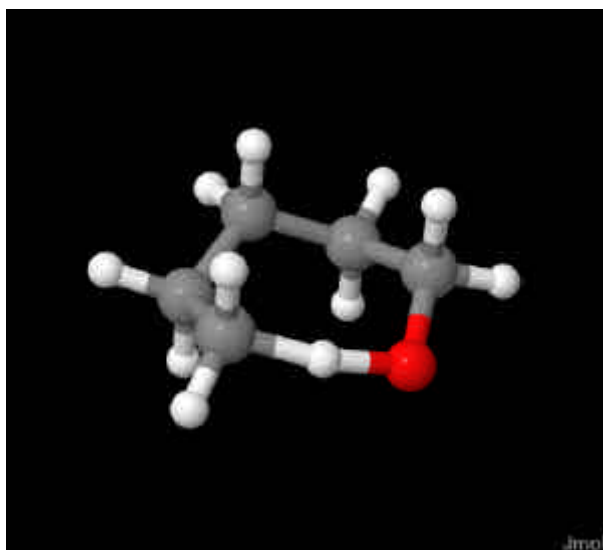


Figure S4: TC conformer of the 1,6-H-shift in 1-pentoxy

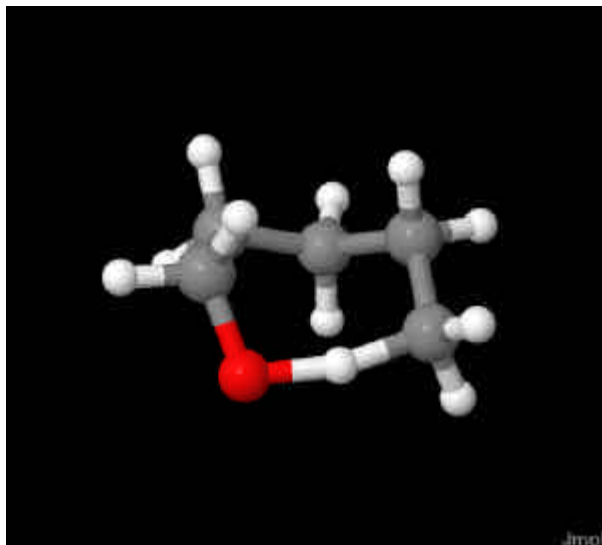


Figure S5: C conformer of the 1,6-H-shift in 1-pentoxy

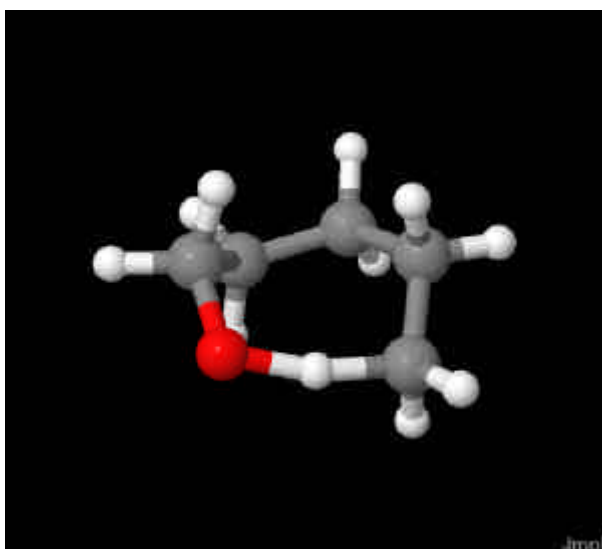


Figure S6: B conformer of the 1,6-H-shift in 1-pentoxy

f) 1,7-H-migration TS

As for the 1,6-H-migration, we found three conformers for the 1,7-H-migration, though for the latter, all three conformers are thermally accessible. The conformers found are labeled crown (CR) (also known as chair-chair), boat-boat (BB), and boat-chair (BC). The relative energies are given below, as are graphical representations of these TS. The B3LYP and CBS-QB3 levels of theory disagree on which conformer is the lowest in energy, by a small margin each way; further IRCMax calculation are needed to settle this matter. As the CR and BB transition state

conformers have also somewhat different rigidities, their different thermal population weights as per the different levels of theory leads to a larger uncertainty on the $F(\text{rig})$, $F(\text{conf})$ and/or $F(\text{SD})$ corrections.

Table S5: Relative energies of the TS conformers for 1,7-H-migration

| Conformer | Relative energy (kJ mol ⁻¹) | |
|-----------------|---|---------|
| | B3LYP/6-31G(d,p) | CBS-QB3 |
| Crown (CR) | 0.0 | 1.0 |
| Boat-boat (BB) | 0.3 | 0.0 |
| Boat-chair (BC) | 4.9 | 3.6 |

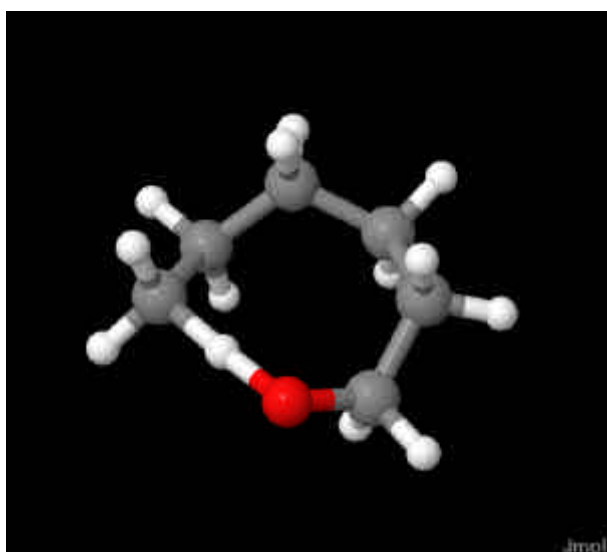


Figure S7: CR conformer of the 1,7-H-shift in 1-hexoxy

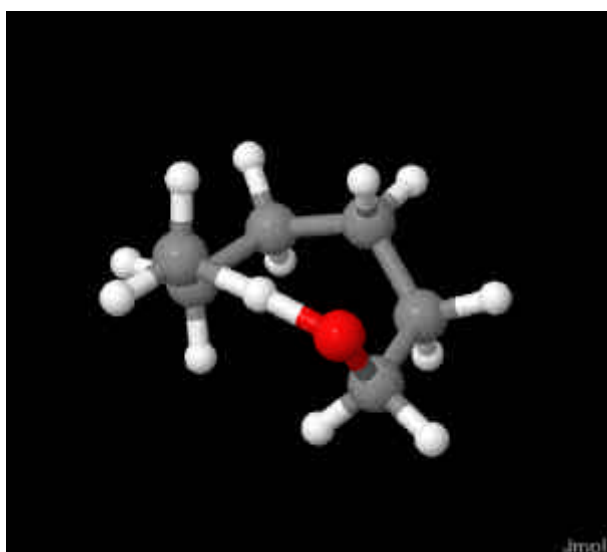


Figure S8: BB conformer of the 1,7-H-shift in 1-hexoxy

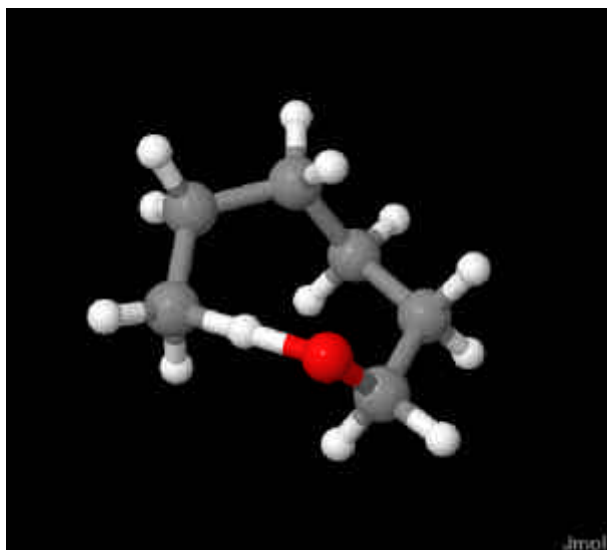


Figure S9: BC conformer of the 1,7-H-shift in 1-hexoxy

g) 1,8-H-migration TS

We characterized 16 conformers for the 1,8-H-migration, all variations of the twist-boat-chair (TBC), twist-chair-boat (TCB), twist-chair-chair (TCC), and skewed-chair-boat (SCB) conformers of cyclononane. The relative energies, and depictions of these structures are given below. The active site can be permuted on multiple (but not all) corners of the 9-membered ring without collapsing the basic geometry of the ring; these variations we label with a lowercase letter. Note that this different positioning also exists for the cycloalkane, but that obviously these are all degenerate given that all carbons are identical.

Table S6: Relative energies of the TS conformers for 1,7-H-migration

| Conformer | Relative energy (kJ mol ⁻¹) | Relative energy (kJ mol ⁻¹) |
|-----------|---|---|
| | B3LYP/6-31G(d,p) | CBS-QB3 |
| TBCa | 0.0 | 0.0 |
| TCBa | 2.0 | 2.3 |
| TBCb | 3.0 | |
| SCBa | 3.6 | |
| TCCa | 3.9 | |
| TBCc | 4.4 | |
| TBCd | 4.4 | |
| TBCe | 5.8 | |
| SCBb | 9.0 | |
| TBCf | 10.2 | |
| TCCb | 11.5 | |
| TBCg | 12.6 | |
| TBCh | 14.7 | |
| TCCc | 20.7 | |
| SCBc | 27.6 | |
| SCBd | 27.7 | |

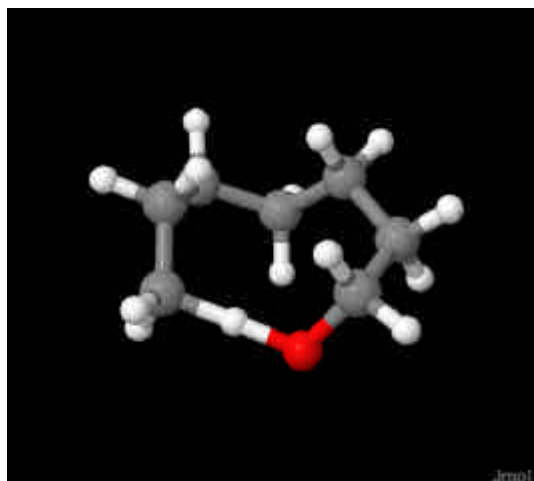


Figure S10: TBCa conformer of the 1,7-H-shift in 1-heptoxy

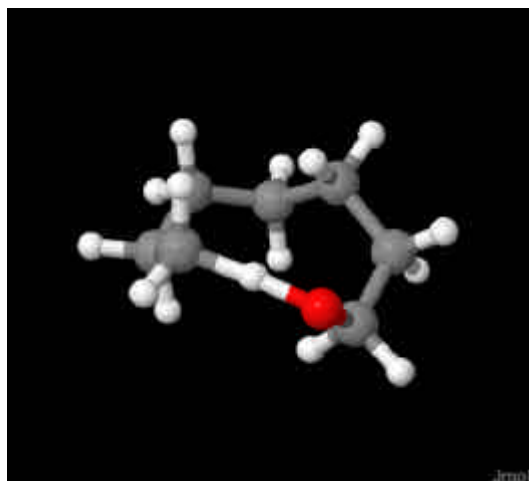


Figure S11: TBCb conformer of the 1,7-H-shift in 1-heptoxy

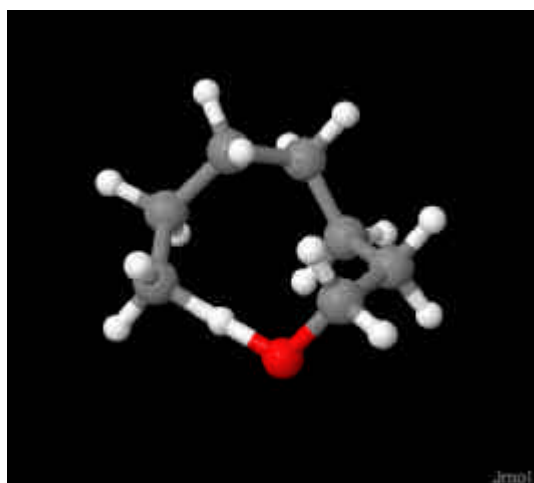


Figure S12: TBCc conformer of the 1,7-H-shift in 1-heptoxy

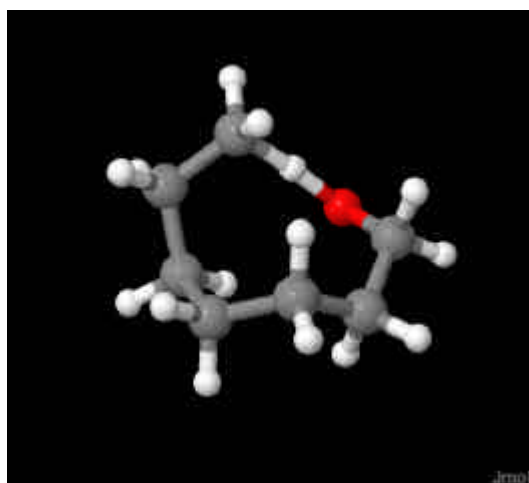


Figure S13: TBCd conformer of the 1,7-H-shift in 1-heptoxy

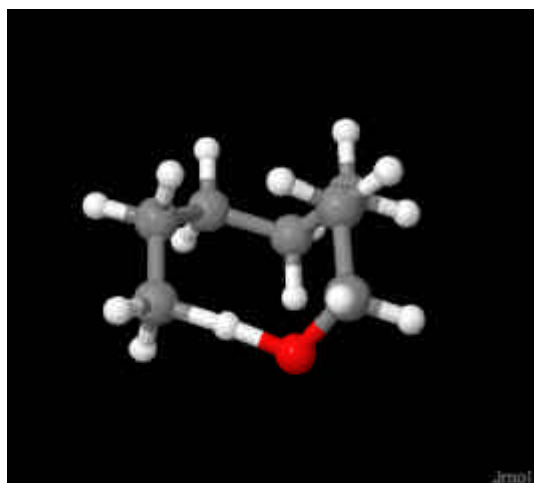


Figure S14: TBCE conformer of the 1,7-H-shift in 1-heptoxy

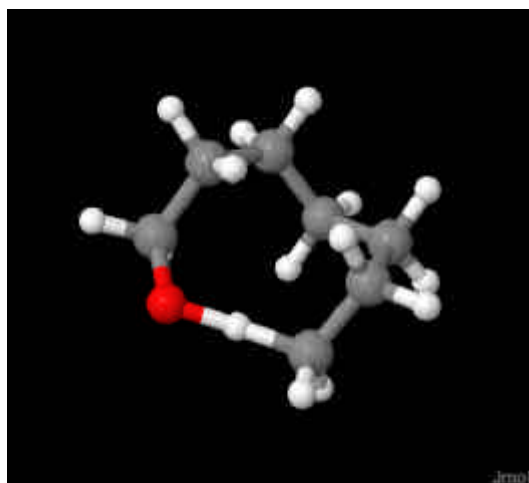


Figure S15: TBCf conformer of the 1,7-H-shift in 1-heptoxy

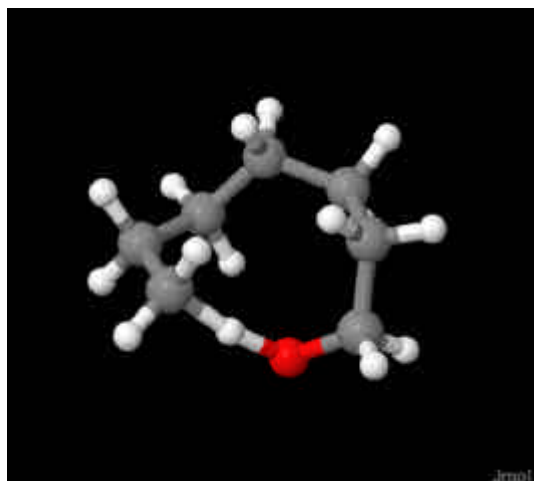


Figure S16: TBCg conformer of the 1,7-H-shift in 1-heptoxy

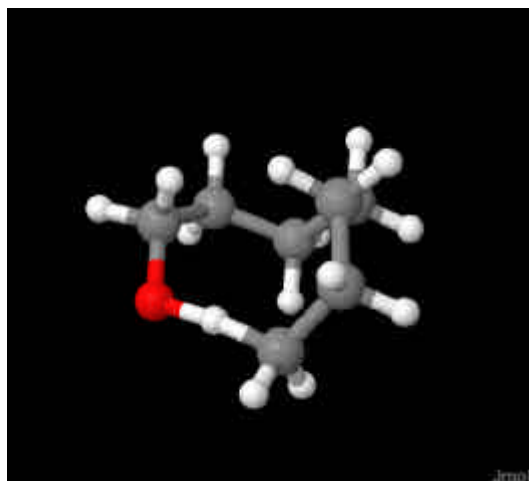


Figure S17: TBCh conformer of the 1,7-H-shift in 1-heptoxy

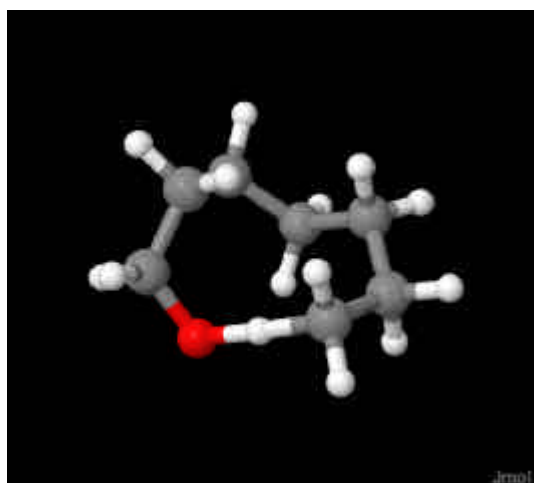


Figure S18: TCBa conformer of the 1,7-H-shift in 1-heptoxy

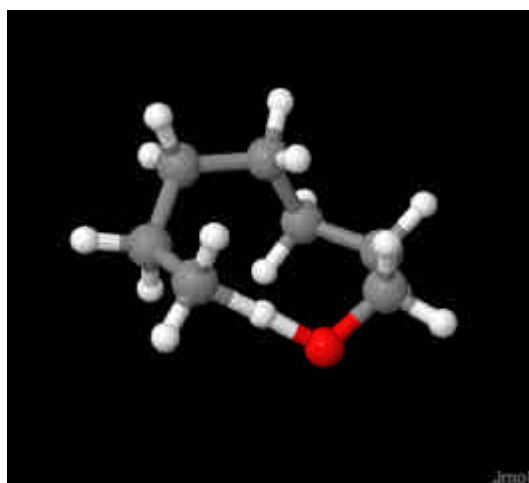


Figure S19: SCBa conformer of the 1,7-H-shift in 1-heptoxy

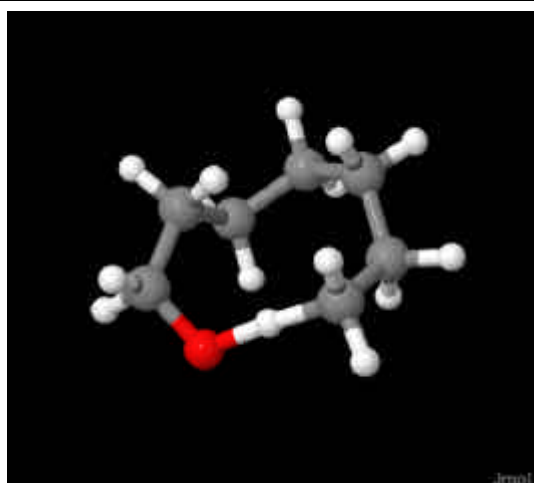


Figure S20: SCBb conformer of the 1,7-H-shift in 1-heptoxy

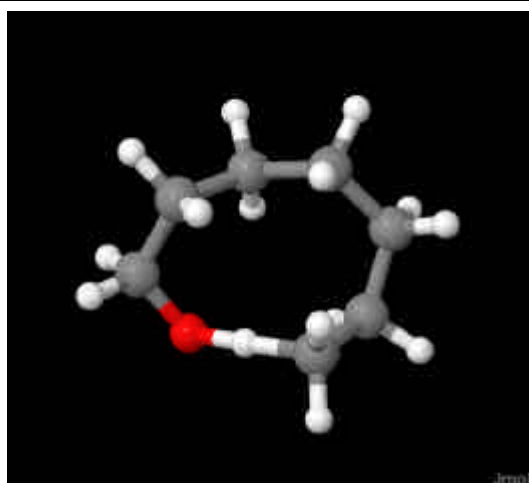


Figure S21: SCBc conformer of the 1,7-H-shift in 1-heptoxy

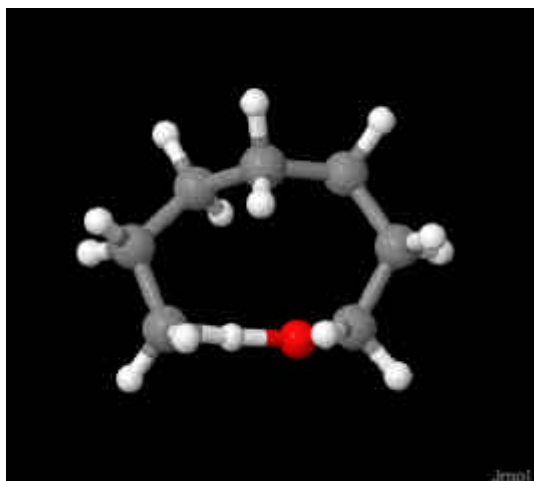


Figure S22: SCBd conformer of the 1,7-H-shift in 1-heptoxy

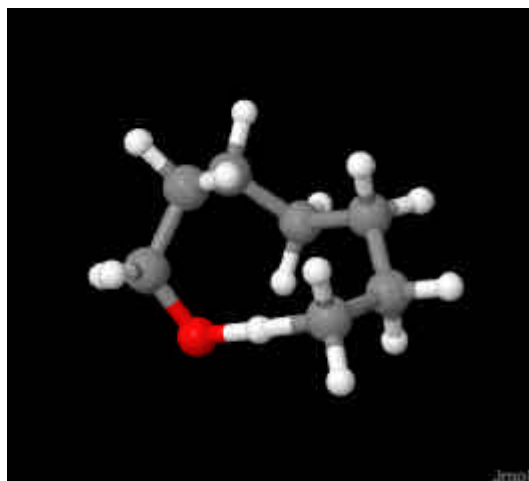


Figure S23: TCCa conformer of the 1,7-H-shift in 1-heptoxy

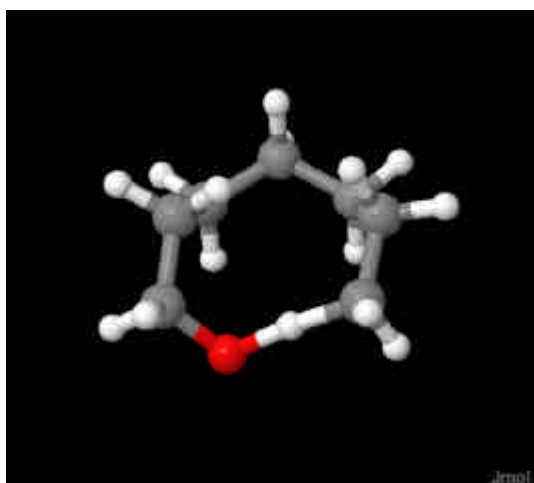


Figure S24: TCCb conformer of the 1,7-H-shift in 1-heptoxy

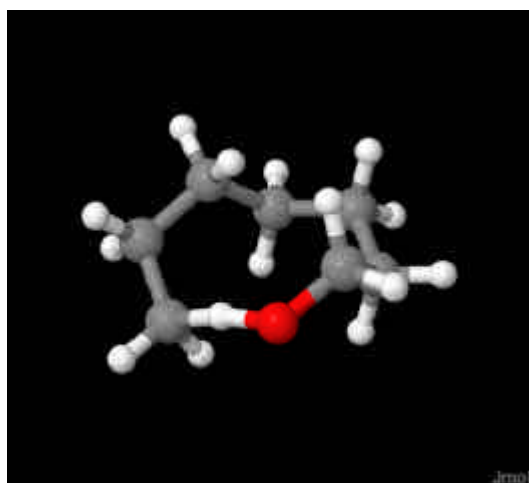


Figure S25: TCCc conformer of the 1,7-H-shift in 1-heptoxy

V. The impact of heterosubstitution on the H-migration.

a) Oxo substitution

a.1) generic exo-oxo alkoxy radicals

These radicals have an oxo substitution outside the TS ring, and not in β -position. As such, these carbonyl groups have little impact on the barrier height, and their contribution to the partition functions should be similar in reactant and TS. Our calculations seem to indicate that there is a slight increase in barrier somewhat, by up to 4 kJ mol^{-1} for oxo-substitution in γ -position relative to the migrating hydrogen, due to the electronegative character of the carbonyl oxygen. However, this effect is small and might be computational noise. At this stage, we propose that exo-(= γ)-oxo substitution does not affect the H-migration appreciably.

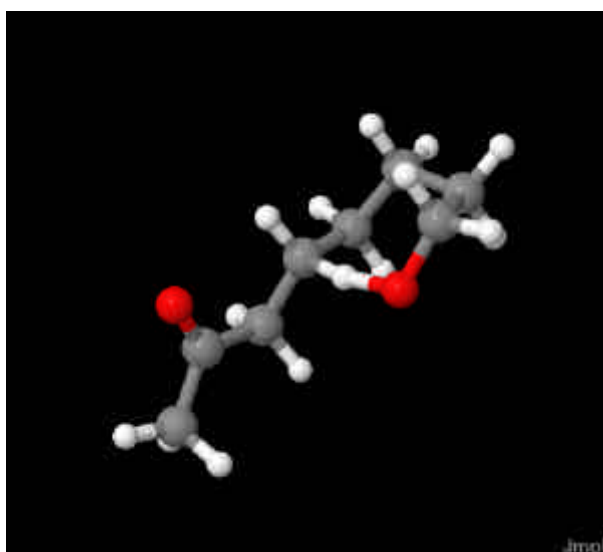


Figure S26: 1,6-H-shift in 7-oxo-1-octoxy

a.2) exo- β -oxo alkoxy radicals

β -Oxo-substitution relative to the migrating hydrogen leads to vinyloxy-resonance stabilized alkyl product radicals, stabilized by $\sim 25 \text{ kJ mol}^{-1}$ compared to their unsubstituted alkyl radical analogues. As the transition state for H-migration is an early transition state, the radical electron is still mostly localized in the TS, such that resonance stabilization is not yet active in the transition state.¹³ This is also borne out e.g. by the near-identical rate coefficient for

H-abstraction by OH for acetone, relative to ethane. Also, the oxo substitution does not alter the TS ring strain significantly, such that this substitution is not expected to alter the rate of H-migration significantly. Our calculations show some small differences relative to the alkyl-substituted analogues, but for the limited set of data available this can not be distinguished from the noise on the calculations.

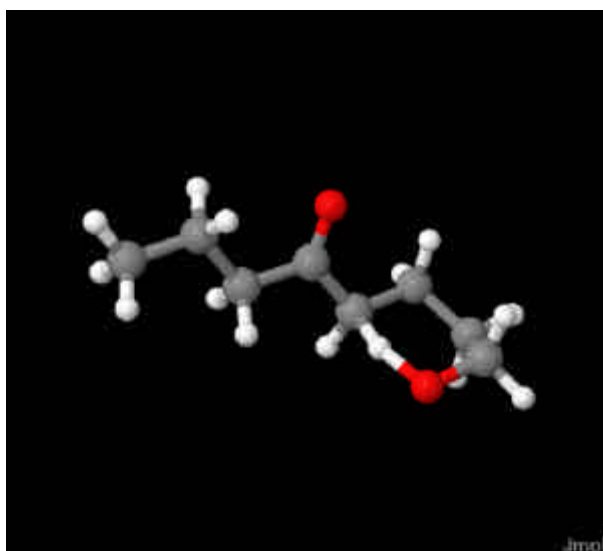


Figure S27: 1,5-H-shift in 5-oxo-1-octoxy

a.3) Aldehydes

Aldehydic hydrogens, with their α -oxo substitution, have a significantly lower $D(\text{C-H})$ bond strength, $\sim 364 \text{ kJ mol}^{-1}$, than the alkyl-substituted tertiary analogues, $\sim 393 \text{ kJ mol}^{-1}$. Abstraction of aldehydic-H leads to the stable acyl radical, $-\dot{\text{C}}=\text{O}$, and given the larger reaction exoergicity one would expect a significantly enhanced H-migration rate. However, for smaller TS rings, ~ 8 -membered or less, the 120° bond angles around the aldehyde carbon increases the TS ring strain significantly, counteracting any lowering of the TS barrier due to larger exoergicity. Furthermore, the fact that during the H-migration the aldehyde carbon does not change its hybridization and hence these angles, forces the migrating hydrogen to remain in a near- 120° angle relative to the substrate C-C bond, whereas in alkylated analogues the substrate carbon changes from sp^3 to sp^2 hybridization, allowing the breaking C-H to point more towards the receiving radical oxygen, further negating any energetic advantage. As a result, we find that aldehydic-H migration has a more curved reaction path, actually increasing

the barrier for migration slightly compared to an alkyl-substituted 3° hydrogen, depending on the span of the migration. This remarkable result is also borne out by the sharper C–H–O angle of 145.3° for 1,5-H-shift in 4-oxo-butoxy, compared to e.g. 153.4° in 1-butoxy and 155.0° in 4-Me-1-pentoxy; strain-free H-migration prefers angles closer to 180°. For larger TS rings, i.e. for 1,8-H-shifts or larger spans where the above geometric constraints are mostly absent due to the flexibility of the longer alkyl backbone, the barrier is expected to decrease again, leading to enhanced aldehydic H-migration. The distinct characteristics of aldehyde-H-migration indicates that one should not expect this reaction to follow a similar Evans-Polanyi relationship as other H-migrations; the usually good correlation between bond strength and H-abstraction rate is non-causal^{14, 15} and the breaks down when the molecular structure is fundamentally different.

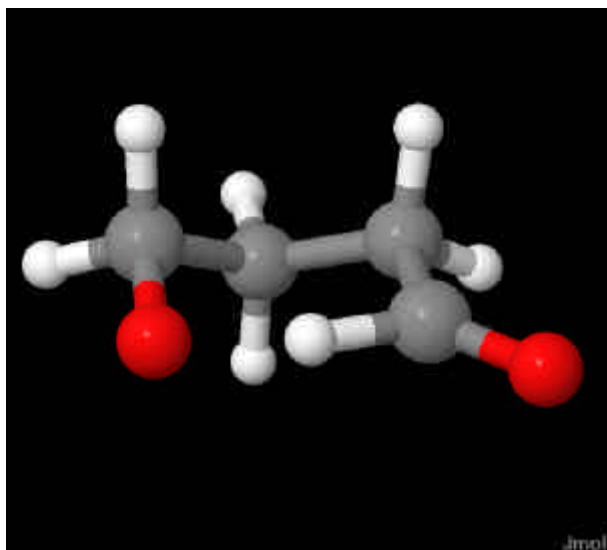


Figure S28: 1,5-H-shift in 4-oxo-1-butoxy

While the two main levels of theory used in this work, B3LYP-DFT and CBS-QB3, tend to agree reasonably well on the barrier height, the migration of aldehydic H is an exception, and more quantum chemical calculations were in order. We find that different levels of theory can strongly disagree on the energy of the barrier for 4-butoxy radicals isomerisation, as shown in table S7 below:

Table S7: barrier heights (kJ mol^{-1}) for 4-oxo-butoxy isomerisation by 1,5-H-shift.

| Geometry | Energy calculations | ZPE calculation | Barrier height |
|-------------------|---------------------|-------------------|-------------------|
| B3LYP/6-31G(d,p) | B3LYP/6-31G(d,p) | B3LYP/6-31G(d,p) | 13.6 |
| B3LYP/CBSB7 | CBS-QB3 | B3LYP/CBSB7 | 25.0 ^a |
| M05-2X/6-31G(d,p) | M05-2X/6-31G(d,p) | M05-2X/6-31G(d,p) | 32.6 |
| | CBS-QB3 | M05-2X/6-31G(d,p) | 21.7 |
| QCISD/6-311G(d,p) | CBS-APNO | HF/6-31G(dp) | 9.8 ^b |
| | | B3LYP/6-31G(d,p) | 16.4 |
| | | M05-2X/6-31G(d,p) | 13.5 |
| | | B3LYP/CBSB7 | 17.1 |
| | CBS-QB3 | B3LYP/CBSB7 | 14.3 |

^a standard CBS-QB3 calculation

^b standard CBS-APNO calculation

From this table, it is clear that the geometry used in single point calculations for this reaction makes a significant difference. E.g. replacing the default B3LYP/CBSB7 geometry in CBS-QB3 energy calculations with more reliable QCISD geometries changes the barrier height by over 10 kJ mol^{-1} . Likewise, the use of HF ZPE corrections is in disagreement with the generally more reliable DFT frequency calculations. Selecting the most reliable level of theory for the migration of aldehydic H from the above table is difficult; as far as CBS-APNO represents the most reliable level of theory in the table, and preferring the more reliable DFT ZPE-corrections over HF, we pragmatically estimate the barrier to be $\sim 16 \text{ kJ mol}^{-1}$, with a sizable uncertainty.

The strongly different barrier heights at the individual levels of theory also influences their barrier width prediction, with B3LYP predicting a low imaginary wavenumber of $\sim i500 \text{ cm}^{-1}$, while the higher M05-2X barrier leads to a $\sim i1100 \text{ cm}^{-1}$ wavenumber. This uncertainty affects the reliability of the tunneling corrections. As imaginary wavenumber, we adopt the average of the B3LYP and M05-2X results at this time.

Costly IRCMax and barrier shape calculations at various high levels of theory are needed to determine the correct barrier height, and even then one might have to conclude that irreconcilable differences remain between different high-level quantum chemical methodologies. Then, direct experimental evidence is required to provide benchmark data.

a.4) endo- β -oxo alkoxy radicals

As for exo- β -oxo alkoxy radicals, vinyloxy resonance in the product radical greatly increases the reaction exoergicity; however, as the transition state is early, this resonance stabilisation is not yet active in the transition state.¹³ The cyclic structure of the transition state forces the carbonyl to point outwards, nearly 180° away from the migrating hydrogen. As such, the carbonyl π -system can not align with the breaking C–H bond at all (this would require a $\sim 90^\circ$ angle), but furthermore also forces unfavourable orientation with respect to the other two substituents on the carbon bearing the migrating H. Combined with the difference in bond lengths and angles imparted by the sp² hybridized carbonyl carbon within the TS ring, we find a significant increase in barrier height for this type of substitution of about 9 kJ mol⁻¹ for 1,6-H-migration, and up to 13 kJ mol⁻¹ for 1,5-H-migration.

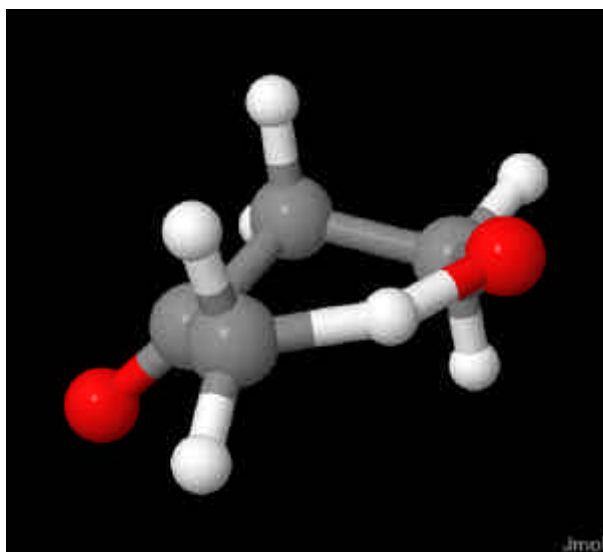


Figure S29: 3-oxo-1-butoxy 1,5-H-migration

The relative rigidity of the H-migration depends on the compound examined, but as we have insufficient data to separate different trends, we use the average as the $F(\text{SD})$ state density correction factor, with an uncertainty of a factor of ~ 2.5 . At this time, we have no data available for tertiary H, we adopt the same correction parameter for 3° H as for 2° H.

a.5) generic endo-oxo alkoxy radicals

For H-migration over a $>C=O$ group, we find an increase of the TS barrier height, 2.1-3.7 kJ mol⁻¹ for a 1,5-H-shift, and 2.8 to 8.8 kJ mol⁻¹ for a 1,6-H-shift. A (slight) increase in barrier is not entirely unexpected considering the $\sim 120^\circ$ bond angle around the sp² hybridized carbon, increasing the TS ring strain. For the 1,5-H-shift, the higher state density correction, $F(SD)$ nearly compensates for the increase in barrier; this is in agreement with the limited experimental data¹⁶ that shows no appreciable difference for isomerisation over a $>C=O$ group.

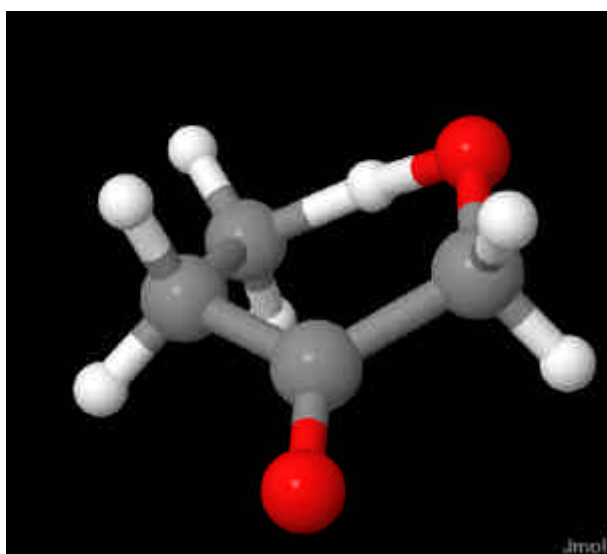


Figure S30: 1,5-H-shift in 2-oxo-1-butoxy

a.6) acyloxy radicals

Acyloxy radicals are characterized by resonance stabilization of the radical electron. Hence, the barrier for H-migration is expected to be higher than for the analogous alkoxy H-migration, but only slightly so, as the TS is early and most of the resonance stabilization is not yet lost. As for all endo-oxo substituted alkoxy radicals, the reaction barrier is also influenced by the sp²-hybridized carbon in the TS ring, but the small barrier difference between 1,5- and 1,6-H-shifts suggests this is a minor effect. B3LYP does not seem to properly account for the acyloxy resonance, and yields inconsistent data. The CBS-QB3 energies are more reliable, but are based on B3LYP geometries, which might affect the accuracy of the barrier height

adversely.

The reactant has two low-lying conformers, within 1 kJ mol^{-1} , with a strongly differing rigidity, such that we can not use $F(\text{rig}) \times F(\text{conf})$ with the partition function of the lowest energy conformer to approximate the multi-conformer state density correction $F(\text{SD})$.

No data is available for the correction for tertiary H. As a first approximation, we adopt the correction factors for 2° H. CO_2 elimination from acyloxy radicals is predicted to be fast,¹⁷ such that H-migration in acyloxy radicals is probably not competitive.

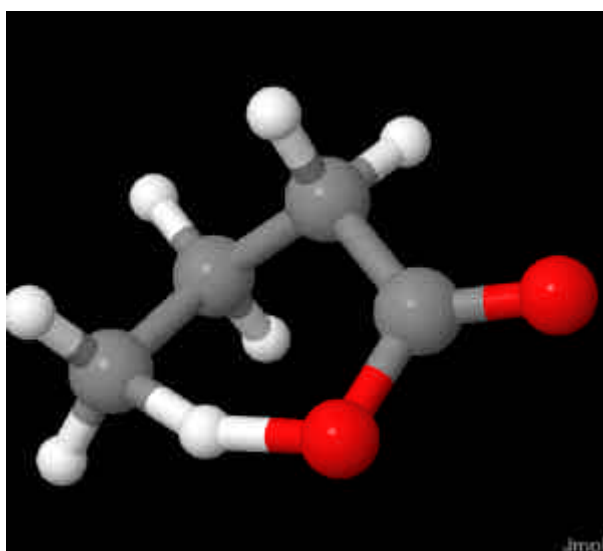


Figure S31: 1,5-H-shift in 1-oxo-1-butoxy

b) Hydroxy substitution

b.1) exo- β -OH alkoxy radicals

For exocyclic β -OH substitution, the positioning of the hydroxy group in the transition state is sufficiently flexible to allow formation of an H-bond between the hydroxy-H and the radical oxygen. The amount of stabilization depends somewhat on the TS geometry, but decreases the barrier by about 2 to 2.5 kJ mol^{-1} . The lowest energy, H-bonded TS conformer is significantly more rigid than for unsubstituted alkoxy radicals, partly negating the energetic advantage of the TS. For those alkoxy radicals where the reactant already has a favorable H-bond between the OH group and the radical oxygen, the H-bond tends to strengthen somewhat due to a more

favorable charge distribution on the oxygen in the newly forming OH group as compared to the oxygen in the alkoxy reactant. For OH-substitutions more than 3 to 4 carbons from the alkoxy radical oxygen, the H-bond in the reactant becomes less favorable due to the energetic and entropic cost of constraining the hydrocarbon chain to accommodate the H-bond.

b.2) α -OH alkoxy radicals

The D(C–H) bond strength is significantly lowered by α -OH substitution. Moreover, there is the possibility of H-bonding between the hydroxyl hydrogen and the radical oxygen even in the TS, where the strength of this H-bond interaction depends on the exact ring structure, and is more pronounced for larger rings. These effects lead to lower barrier heights for H-migration upon substituting a –OH group for an alkyl –R group. The H-bonded transition states are more rigid than for the alkyl-substituted equivalents, but the number of thermally accessible TS conformers also increases due to the H-bond interaction. This leads to strongly enhanced rate of isomerisation, but increasing less with temperature than alkyl-substituted 2°/3° hydrogen migration.

b.3) endo- β -OH alkoxy radicals

The impact of this substitution class depends strongly on the isomerisation examined. For a 1,5-H-shift, the TS geometry does not allow for a strong H-bond between the –OH group and the radical oxygen, leading to a significant increase in the barrier height (7 to 9 kJ mol⁻¹) due to the loss of the H-bond originally present in the reactant; the geometric constraints increase the OH...O distance from 2.0 Å in the reactant to 3.1 Å in the TS. On the other hand, the loss of the H-bond leads to a significantly looser TS, counteracting the effect of the higher barrier to some extent.

For a 1,6-H-shift, we find no net difference in the barrier height as here, the larger flexibility of the TS ring allows the H-bond present in the reactant to remain mostly intact in the transition state. Likewise, for migrations across larger spans (1,7- and 1,8-H-shifts), H-bonding in the TS

remain as strong as in the reactant. However, for these larger spans the H-bond stabilization in the reactant is expected to contribute less to the population due to the entropic penalty for more extensive folding of the hydrocarbon chain. Hence, these H-migrations might enjoy a slight decrease in barrier, but the rate coefficient increase will be moderated by the concomitant increase in TS rigidity.

b.4) generic endo-OH alkoxy radicals

For generic OH-substitution within the TS ring, the impact of the OH substitution is highly dependent on the exact position of the OH relative to the alkoxy radical oxygen, as this determines whether an H-bond can be formed in reactant and/or transition state. In principle, a strong H-bond can be formed between the OH substituent and the alkoxy oxygen in the reactant for spans up to 4 intervening carbons. Beyond that, the additional stabilization by the H-bond in the reactant is mostly lost against the energetically and entropically less favorable constraining of the hydrocarbon chain needed to enable a H-bond to be formed. In the TS, the hydrocarbon chain is necessarily constrained anyway, but the geometric requirements of the active site in the TS might make H-bonding of OH groups near the alkoxy O less or more favorable, while enabling efficient stabilization in the TS for OH groups farther from the alkoxy group.

For a 1,5-H-shift in 2-OH-1-butoxy, we found that the H-bond (across a 5-ring) was retained in the TS, and the TS did not differ appreciably in barrier height compared to 1-butoxy. Preliminary data for H-shifts across other spans and for other natures of H seem to indicate that usually TS geometries exist that retain the H-bond of the reactant. Based on this scarce data, we tentatively propose that the barrier and entropy factor remains largely identical to that of the unsubstituted alkoxy radical.

b.5) $>C(OH)O^\bullet$ -type radicals

For $>\text{C}(\text{OH})\text{O}^\bullet$ -type radicals, a favorable H-bond exists by default in both reactant and transition state. Moreover, the reactant radical oxygen becomes increasingly more charged during the reaction as it transforms into an $-\text{OH}$ substituent, given that the additional H-atom in the $>\text{C}(\text{OH})_2$ moiety provides an additional charge source for the two gemini electronegative oxygen atoms. This charge repositioning increases the H-bond strength significantly in the $>\text{C}(\text{OH})_2$ moiety compared to $>\text{C}(\text{OH})\text{O}^\bullet$, leading to a TS barrier height lowering by 7 kJ mol^{-1} . The stronger H-bonding does lead to an entropic disadvantage for this isomerisation.

b.6) generic exo-OH alkoxy radicals

We have currently no data available for OH-substituents placed outside the TS ring beyond β -position.

VI. Testing the framework: predicting relative rate coefficients for 1,5-H-migration of 1°, 2°, and 3° hydrogens

As we use all of the available experimental data as reference rate coefficients in the SAR, testing the SAR directly is not possible. However, one can use the reference rate coefficients for 1°, 2°, and 3° H-migration to test the SAR framework, i.e. how good does the theoretical kinetic framework and the quantum chemical data perform when we predict the rate of 1,5-H-migration of 2° and 3° H from the experimental rate coefficient for the 1,5-H-shift of a 1° H. This represents a rather stringent test of the SAR model, as the extrapolation required spans two orders of magnitude, much larger than any of the corrections will be within the SAR model (other than the rather unimportant 1,4-H-shifts).

Given the rather large differences between the different levels of quantum chemical theory on the absolute barrier heights, one should at this time accept that any theory used will have some bias. Also, the calculation of relative tunneling, conformer rigidities, conformer energy spacing etc. will undoubtedly have some systematic bias. Hence, pragmatically, we envision that we will have to define some empirical correction on the predictions; in its simplest form this will entail a correction to the temperature dependence of the pre-exponential factor, and a correction to the activation energy. As we work relative to a reference rate coefficient, a significant additional constant correction to the predicted rates appears unlikely.

To derive the rate coefficients for 1,5-H-migration of 2° and 3° H from that for a 1° H, we first need to derive $C(\text{subst})$, $F_{\text{subst}}(\text{tunnel})$, $F_{\text{subst}}(\text{rig})$ and $F_{\text{subst}}(\text{conf})$ for methyl substitution around the migrating H (α -Me H substitution) from the available data. We will derive the rate coefficient per migrating H. The correction factors are shown in the table below.

Table S8: Correction factors for α -Me substitution substitution around the migrating H, without empirical correction.

| Nature of H | Correction | |
|-------------|-----------------------------------|--|
| 1° → 2° | $C(\text{subst})$ | -1193 |
| | $F_{\text{subst}}(\text{rig})$ | $0.79 + 1.22 \times 10^{-4} T$ |
| | $F_{\text{subst}}(\text{conf})$ | $0.98 - 1.36 \times 10^{-4} T$ |
| | $F_{\text{subst}}(\text{tunnel})$ | $1.42 \times \exp(-163 \text{ K} / T)$ |
| 1° → 3° | $C(\text{subst})$ | -2365 |
| | $F_{\text{subst}}(\text{rig})$ | $0.62 + 9.02 \times 10^{-4} T$ |
| | $F_{\text{subst}}(\text{conf})$ | $0.46 + 9.84 \times 10^{-5} T$ |
| | $F_{\text{subst}}(\text{tunnel})$ | $2.05 \times \exp(-346 \text{ K} / T)$ |

Applying these SAR parameters leads to a k_{sec} per H that is a factor 1.9 too high, and a k_{tert} per H that is a factor 4.5 too high, but with a fairly good temperature dependence. As already discussed earlier in the analysis of the quantum chemical data, one contributing factor to this is that the CBS-QB3 barrier heights underestimate the barrier heights with increasing substitution owing to the B3LYP geometries used in this method. A correction to this specific problem was possible by scaling the barrier energy difference, i.e. $C(\text{subst})$, by a constant factor, the same for all substitutions. Based on the rate coefficient ratios, we derive a scaling correction for $C(\text{subst})$ of 0.8; this scaling factor does not apply to all $C(\text{subst})$ in the SAR, only to those where $C(\text{subst})$ is driven by differences in the C–H bonding. Applying this correction, we find that the predicted rate coefficients are within 30% of the experimental rate coefficient (after fall-off correction which is based on the total rate coefficient, not the per-H rate coefficient). This is shown in the graph below. The temperature dependence is remarkably good, and further empirical correction is not warranted within the intrinsic uncertainty of the SAR. As such, it seems that the SAR framework performs remarkably good, and that the quantum chemical data used is sufficient to get reliable relative rate coefficients, at least after the D(C–H) bond strength bias is corrected for. This latter empirical correction should be straightforward to eliminate or at least reduce by using a better geometry optimization method for the CBS-Q energy calculations.

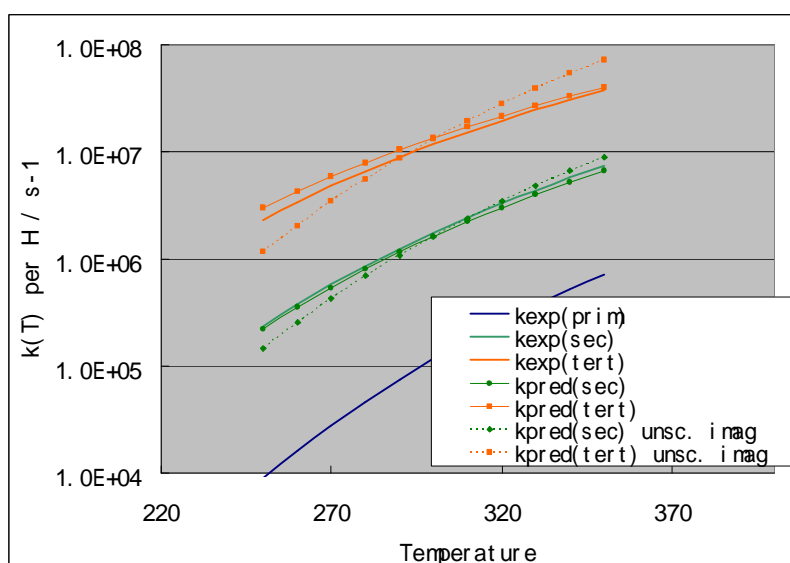
Some authors (Méreau et al, 2003; Somnitz, 2007) spent a significant effort in determining the tunneling factors, and found that the imaginary wavenumber of the TS should not be used as-is

as it underestimates the barrier width. While the current SAR uses a relative tunneling correction, and is as such not overly affected by bias in the predicted tunneling corrections, an incorrect tunneling correction does lead to an erroneous temperature dependence. To show the effect of the scaling of the imaginary wavenumber on the temperature dependence, we also show the predicted rate coefficients when using unscaled B3LYP imaginary wavenumber to estimate the Eckart tunneling correction. Clearly, the scaling factor of 0.6 as proposed by Méreau does a remarkably good job in improving the temperature dependence.

Table S9: Correction factors for α -Me substitution around the migrating H, with empirical correction.

| Nature of H | Correction | |
|-------------------------------|-----------------------------------|--|
| $1^\circ \rightarrow 2^\circ$ | $C(\text{subst})$ | -956 |
| | $F_{\text{subst}}(\text{rig})$ | $0.79 + 1.22 \times 10^{-4} T$ |
| | $F_{\text{subst}}(\text{conf})$ | $0.98 - 1.36 \times 10^{-4} T$ |
| | $F_{\text{subst}}(\text{tunnel})$ | $1.42 \times \exp(-163 \text{ K} / T)$ |
| $1^\circ \rightarrow 3^\circ$ | $C(\text{subst})$ | -1892 |
| | $F_{\text{subst}}(\text{rig})$ | $0.62 + 9.02 \times 10^{-4} T$ |
| | $F_{\text{subst}}(\text{conf})$ | $0.46 + 9.84 \times 10^{-5} T$ |
| | $F_{\text{subst}}(\text{tunnel})$ | $2.05 \times \exp(-346 \text{ K} / T)$ |

Figure S32: Comparison between the k_{exp} reference rate coefficients (thick solid lines), and the rate coefficients k_{pred} for 2° and 3° H-migration predicted from the 1° reference reaction (thin solid line) after empirical correction. Also shown (dashed line) are the predicted where Eckart tunneling correction uses an unscaled imaginary wavenumber..



VII. Testing the theoretical kinetic values: predicting absolute rate coefficients for 1,5-H-migration of 1°, 2°, and 3° hydrogens

A fundamental advantage of the current SAR framework is that it predicts rate coefficients relative to an experimentally measured reaction, chosen to be similar to the reaction studied. This leads to significant cancellation of error, thereby improving the reliability of the predictions. It is, however, useful to assess the reliability of the underlying quantum chemical data by also predicting absolute rate coefficients. To this end, we applied MC-TST based on the B3LYP rovibrational data, and the CBS-QB3 barrier heights to predict the absolute rate coefficients for 1,5-H-shift in 1-butoxy, 1-pentoxy, and 4-Me-1-pentoxy. Tunneling corrections (ZCT) are done using asymmetric Eckart corrections, using B3LYP imaginary wavenumbers scaled by 0.6 (see Méreau et al., 2003). Fall-off corrections are done using the crude fall-off correction developed in the main paper. The CBS-QB3 absolute barrier heights for 1-pentoxy and 4-Me-1-pentoxy were corrected upwards by 1.97 and 3.93 kJ mol⁻¹, respectively, i.e. applying the 0.8 empirical scaling factor for the barrier height relative to the 1-butoxy TS as discussed and derived elsewhere in this work.

At 298K, the predicted absolute rate coefficients are a factor 2.58, 3.41, and 7.23 times higher than the reference rate coefficients, while the temperature dependence is quite good. These results suggest firstly that the CBS-QB3 barrier heights are systematically low. Méreau et al. (2003) have likewise significantly overpredicted the rate coefficient for tertiary H-migration by a factor of 40 relative to the experimental data; theoretical kinetic work by other authors has only examined 1° and 2° H-migration. The B3LYP barriers are typically about 4 kJ mol⁻¹ higher than the CBS-QB3 results; this would lead to a systematic underestimation of the rate coefficients though with a smaller absolute error. Considering the difficulty many (affordable) quantum chemical methodologies have in predicting the barrier height for H-migration in alkoxy radicals, with tens of kJ mol⁻¹ spread on the available values, and in view of the crude fall-off model used, we consider these absolute predictions sufficiently good. At any rate, it shows that the quantum chemical data should be sufficiently reliable for relative predictions.

VIII. Total correction factors at 298 K

Table S10 Total correction factors (without fall-off correction) at 298K relative to the reference 1,5-H-migration rate coefficient of identical nature of migrating H. These correction factors are estimated directly from the quantum chemical data rather than the (averaged) fits listed in Table 5, and include both the corrections for the migration span as for the substitution.

| Substitution | Span | 1° | 2° | 3° |
|--------------------|------|------------------------------------|----------------------|----------------------|
| alkyl only | 1,4 | 5.8×10^{-8} | 5.6×10^{-8} | 5.5×10^{-8} |
| | 1,5 | 1.0 | 1.0 | 1.0 |
| | 1,6 | 0.18 | 0.16 | 0.16 |
| | 1,7 | 1.9×10^{-3} | 1.7×10^{-3} | 1.7×10^{-3} |
| | 1,8 | 5.9×10^{-5} | 5.7×10^{-5} | 5.8×10^{-5} |
| acyloxy | 1,5 | 2.7×10^{-2} | 8.0×10^{-3} | 8.0×10^{-3} |
| | 1,6 | 2.3×10^{-2} | 1.3×10^{-3} | 1.3×10^{-3} |
| aldehyde H | 1,5 | – | – | 1.16 |
| | 1,6 | – | – | 4.5×10^{-2} |
| | 1,7 | – | – | 2.1×10^{-3} |
| endo- β -oxo | 1,5 | 5.6×10^{-4} | 3.8×10^{-3} | 3.8×10^{-3} |
| | 1,6 | 4.4×10^{-3} | 7.9×10^{-3} | 7.9×10^{-3} |
| generic endo-oxo | 1,5 | 0.74 | 0.74 | 0.74 |
| | 1,6 | 0.13 | 0.13 | 0.13 |
| exo- β -oxo | all | same as alkyl-only alkoxy radicals | | |
| generic exo-oxo | all | same as alkyl-only alkoxy radicals | | |
| $>C(OH)O^\bullet$ | 1,5 | 3.0 | 3.0 | 3.0 |
| α -OH | 1,5 | – | 8.4 | 8.4 |
| | 1,6 | – | 6.4 | 6.4 |
| endo- β -OH | 1,5 | 0.22 | 0.22 | 0.22 |
| | 1,6 | 0.21 | 0.19 | 0.19 |
| exo- β -OH | 1,5 | – | 1.6 | 1.6 |
| | 1,6 | – | 0.38 | 0.38 |
| generic endo-OH | 1,5 | same as alkyl-only alkoxy radicals | | |

References

- ¹ L. Vereecken, and J. Peeters, *Chem. Phys. Lett.*, **333**, 162-168 (2001).
- ² L. Vereecken, and J. Peeters, *Phys. Chem. Chem. Phys.*, **4**, 467-472 (2002).
- ³ D.R. Lide, (Ed.), CRC Handbook of Chemistry and Physics, 82th Edition (2001), CRC Press, Boca Raton.
- ⁴ L. Vereecken, and J. Peeters, *J. Chem. Phys.*, **119**, 5159-5170 (2003).
- ⁵ X.-J. Qi, Y. Feng, L. Liu, Q.-X. Guo, *Chin. J. Chem.*, **23**, 194-199 (2005).
- ⁶ K. B. Wiberg, *J. Org. Chem.*, **68**, 9322-9329 (2003).
- ⁷ I. Yavari, A. Jabbari, and S. Moradi, *J. Molec. Struct. (Theochem)*, **631**, 225-229 (2003).
- ⁸ C. P. A. Anconi, C. S. Nascimento Jr, H. F. Dos Santos, and W.B. De Almeida, *Chem. Phys. Lett.*, **418**, 456-466 (2006).
- ⁹ R. K. Bharadwaj, *Molec. Physics*, **98**, 211-218 (2000).
- ¹⁰ H. F. Dos Santos, W. R. Rocha, and W. B. De Almeida, *Chem. Phys. Lett.*, **280**, 31 (2002).
- ¹¹ F. D. Suvire, L. N. Santagata, J. A. Bombasaro, and R. D. Enriz, *J. Comput. Chem.*, **27**, 188-202 (2006).
- ¹² M. L. Franco, D. E. C. Ferreira, H. F. Dos Santos, and W. B. De Almeida, *Int. J. Quantum Chem.*, **107**, 545-555 (2007).
- ¹³ L. Vereecken, and J. Peeters, *Phys. Chem. Chem. Phys.*, **4**, 467-472 (2002).
- ¹⁴ N. M. Donahue, *J. Phys. Chem. A*, 2001, **105**, 1489.
- ¹⁵ H. A. Rypkema, N. M. Donahue, J. G. Anderson, *J. Phys. Chem. A*, 2001, **105**, 1498.
- ¹⁶ R. Atkinson. and S.M. Aschmann, *Int. J. Chem. Kinet.*, **27**, 261-275 (1995).
- ¹⁷ L. Vereecken, and J. Peeters, *Phys. Chem. Chem. Phys.*, **11**, 9062-9074 (2009).

Raw quantum chemical data

Below, the DFT quantum chemical data is listed. Contrary to chemical convention, positions of substitutions are marked with the radical oxygen numbered as atom 1, such that e.g. a 1,5-H-shift in a 5-Me-substituted alkoxy radical abstract a hydrogen on the carbon bearing the methyl substituent.

The compounds are listed in the same order as given in Table 1, and Table 2.

C3H7O.p

```
-----  
E(UB+HF-LYP/6-31G(d,p)) (Hartree): -193.69110288  
Electronic state : 2-A  
Cartesian coordinates (Angs):  
  O      1.468654      -0.691118      -0.191145  
  C      0.856114      0.448090      0.257415  
  C     -0.574337      0.669461     -0.251685  
  C     -1.512140     -0.485599      0.106162  
  H      0.854378      0.346140      1.366268  
  H      1.503610      1.328387      0.075827  
  H     -0.947407      1.616198      0.160426  
  H     -0.533738      0.796713     -1.340616  
  H     -1.635622     -0.574523      1.191896  
  H     -1.103973     -1.430808     -0.263149  
  H     -2.504302     -0.344875     -0.332844  
Rotational constants (GHz):  15.1846700      5.2305300      4.4046000  
Vibrational harmonic frequencies (cm-1):  
  140.9177      220.9098      302.2827  
  489.7225      558.2123      793.8727  
  868.1653      983.5863      995.8827  
 1095.8776      1103.1990     1216.2184  
 1292.2221      1341.9913     1367.5187  
 1386.3877      1428.4374     1496.6179  
 1510.7593      1522.6559     2877.0517  
 2936.7775      3039.1962     3045.3088  
 3077.1552      3114.7580     3132.8767  
Zero-point correction (Hartree): 0.094176
```

C3H7O.t

```
-----  
E(UB+HF-LYP/6-31G(d,p)) (Hartree): -193.69059801  
Electronic state : 2-A  
Cartesian coordinates (Angs):  
  O      1.949504      0.144794      0.007236  
  C      0.706209     -0.426505     -0.013672  
  C     -0.475349      0.549299     -0.008750  
  C     -1.828754     -0.166880      0.007940  
  H      0.640196     -1.144815     -0.856911  
  H      0.668933     -1.086163      0.881982  
  H     -0.376710      1.207202      0.862585  
  H     -0.396766      1.190365     -0.895107  
  H     -1.941228     -0.789751      0.903106  
  H     -1.947166     -0.819574     -0.864843  
  H     -2.655928      0.548898     -0.001804  
Rotational constants (GHz):  27.8688800      3.9002100      3.6519100  
Vibrational harmonic frequencies (cm-1):  
  123.1946      232.2213      269.7336  
  365.1619      478.1039      770.5089  
  888.0619      963.3229     1036.4483  
 1083.0162      1124.2283     1234.0799  
 1297.5540      1324.0646     1369.2975  
 1406.2066      1428.8014     1502.1722  
 1514.6000      1519.7158     2882.5589  
 2917.9395      3039.8634     3050.1755  
 3084.8011      3108.8568     3121.6907  
Zero-point correction (Hartree): 0.093716
```

C3H7O-1-4-Hshift

```
-----  
E(UB+HF-LYP/6-31G(d,p)) (Hartree): -193.65385325
```

Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 1.069597 | -0.826456 | -0.164411 |
| H | -0.127897 | -1.177200 | -0.092454 |
| C | -1.245028 | -0.537726 | 0.116964 |
| C | -0.596509 | 0.817184 | -0.180618 |
| C | 0.867894 | 0.536309 | 0.193211 |
| H | -2.010206 | -0.907671 | -0.565294 |
| H | -1.479043 | -0.734742 | 1.165145 |
| H | -0.673624 | 1.033784 | -1.250764 |
| H | -1.046598 | 1.653669 | 0.366363 |
| H | 1.591125 | 1.152142 | -0.356575 |
| H | 1.031332 | 0.697072 | 1.271526 |

 Rotational constants (GHz): 12.4810600 7.3775300 5.2742900
 Vibrational harmonic frequencies (cm-1):

| | | |
|------------|-----------|-----------|
| i1866.5568 | 213.8598 | 424.4380 |
| 586.1923 | 618.3793 | 850.3965 |
| 896.8026 | 916.2221 | 984.7712 |
| 1040.1448 | 1087.8406 | 1162.8128 |
| 1179.7986 | 1224.4976 | 1245.3904 |
| 1331.1471 | 1375.6929 | 1470.5145 |
| 1501.8457 | 1532.9603 | 1747.4192 |
| 2983.5416 | 3054.6285 | 3061.6769 |
| 3101.4486 | 3108.5818 | 3190.3728 |

 Zero-point correction (Hartree): 0.090879

C4H9O.mm

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -233.00587531
 Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| C | 1.893592 | -0.587074 | 0.307311 |
| C | 1.030138 | 0.283897 | -0.613258 |
| C | -0.136468 | 0.985758 | 0.096781 |
| C | -1.260439 | 0.032286 | 0.531198 |
| O | -1.818022 | -0.706625 | -0.477632 |
| H | 1.319152 | -1.403612 | 0.758881 |
| H | 2.326411 | 0.004268 | 1.122776 |
| H | 2.720204 | -1.043977 | -0.246112 |
| H | 1.664101 | 1.043502 | -1.086276 |
| H | 0.619045 | -0.327059 | -1.425491 |
| H | 0.221979 | 1.528155 | 0.982675 |
| H | -0.576027 | 1.736210 | -0.571797 |
| H | -0.868407 | -0.729622 | 1.240871 |
| H | -2.043222 | 0.555931 | 1.113339 |

 Rotational constants (GHz): 8.8556222 2.9250279 2.7152182
 Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 69.3202 | 160.5017 | 240.1176 |
| 271.6353 | 387.7346 | 508.8217 |
| 646.5783 | 769.2552 | 842.8621 |
| 877.9827 | 951.2510 | 1038.4948 |
| 1045.7267 | 1099.3378 | 1118.5098 |
| 1179.0072 | 1259.0512 | 1306.6187 |
| 1336.0849 | 1371.4788 | 1379.9768 |
| 1405.3553 | 1429.8651 | 1494.3179 |
| 1503.6669 | 1516.3137 | 1519.8618 |
| 2889.0709 | 2942.1265 | 3031.5905 |
| 3040.0437 | 3046.6525 | 3076.4172 |
| 3082.8757 | 3108.9557 | 3113.9743 |

 Zero-point correction (Hartree): 0.123161

C4H9O.mp

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -233.00589171
 Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| C | -1.585458 | -0.852456 | -0.054042 |
| C | -1.191698 | 0.599310 | 0.234547 |
| C | 0.163420 | 1.015550 | -0.359538 |
| C | 1.351698 | 0.256217 | 0.254646 |
| O | 1.447896 | -1.062522 | -0.100213 |
| H | -0.844785 | -1.557788 | 0.338910 |
| H | -1.663882 | -1.033762 | -1.131450 |
| H | -2.552223 | -1.093764 | 0.400443 |
| H | -1.964650 | 1.271674 | -0.159258 |
| H | -1.170623 | 0.767090 | 1.320548 |
| H | 0.170943 | 0.848156 | -1.443597 |
| H | 0.321464 | 2.089252 | -0.194004 |
| H | 2.294733 | 0.699566 | -0.135803 |
| H | 1.398084 | 0.398026 | 1.352231 |

 Rotational constants (GHz): 7.5387426 3.7036824 2.7702648
 Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 102.1040 | 140.0611 | 226.7865 |
| 324.7265 | 353.4424 | 467.8185 |
| 767.6812 | 785.8787 | 854.4958 |
| 903.4339 | 925.8398 | 1047.1854 |
| 1057.4912 | 1081.2772 | 1102.9331 |

| | | |
|-----------|-----------|-----------|
| 1158.3926 | 1237.8458 | 1301.3731 |
| 1330.4437 | 1371.5884 | 1382.6230 |
| 1408.9598 | 1434.2596 | 1483.7290 |
| 1496.0101 | 1511.5866 | 1514.5803 |
| 2880.8453 | 2939.4597 | 3024.7167 |
| 3034.9670 | 3040.7885 | 3061.1564 |
| 3085.9241 | 3109.3832 | 3114.3624 |

Zero-point correction (Hartree): 0.123167

C4H9O.mt

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -233.00514356
 Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| C | -2.006428 | -0.683991 | -0.164045 |
| C | -1.283895 | 0.599341 | 0.264056 |
| C | 0.149587 | 0.728357 | -0.273201 |
| C | 1.122374 | -0.308806 | 0.308316 |
| O | 2.404070 | -0.225017 | -0.162949 |
| H | -1.512562 | -1.583828 | 0.219590 |
| H | -2.045740 | -0.769121 | -1.256037 |
| H | -3.035999 | -0.698100 | 0.207616 |
| H | -1.862214 | 1.466303 | -0.077442 |
| H | -1.268584 | 0.663302 | 1.361069 |
| H | 0.159267 | 0.639523 | -1.366543 |
| H | 0.543016 | 1.723928 | -0.035299 |
| H | 1.098148 | -0.315911 | 1.416507 |
| H | 0.802282 | -1.335372 | 0.023374 |

Rotational constants (GHz): 12.3814136 2.4127878 2.2152235
 Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 100.5243 | 118.6543 | 210.8997 |
| 286.8978 | 349.2839 | 480.5311 |
| 679.5842 | 766.1400 | 871.0001 |
| 892.7703 | 958.6864 | 1040.2842 |
| 1076.0058 | 1085.7868 | 1112.0110 |
| 1191.9458 | 1256.6931 | 1302.4061 |
| 1340.9245 | 1367.4117 | 1384.5253 |
| 1389.9575 | 1430.4178 | 1498.9555 |
| 1502.1174 | 1517.0354 | 1519.9827 |
| 2885.5809 | 2930.3640 | 3028.5022 |
| 3040.8167 | 3044.5790 | 3068.6313 |
| 3090.0734 | 3108.1395 | 3115.0606 |

Zero-point correction (Hartree): 0.123119

C4H9O.tm

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -233.00690307
 Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| C | 2.355101 | -0.120736 | -0.135067 |
| C | 0.914557 | -0.348547 | 0.330798 |
| C | -0.063470 | 0.712173 | -0.186049 |
| C | -1.518672 | 0.419676 | 0.198211 |
| O | -2.017823 | -0.773256 | -0.254594 |
| H | 2.736015 | 0.849714 | 0.203810 |
| H | 2.424680 | -0.138264 | -1.228679 |
| H | 3.026051 | -0.894236 | 0.252384 |
| H | 0.562780 | -1.332045 | -0.002098 |
| H | 0.881092 | -0.365711 | 1.429383 |
| H | 0.208990 | 1.705389 | 0.197173 |
| H | -0.001310 | 0.772711 | -1.280651 |
| H | -1.621410 | 0.367395 | 1.305406 |
| H | -2.199405 | 1.245690 | -0.087342 |

Rotational constants (GHz): 13.1455519 2.3954176 2.2125704
 Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 99.8711 | 139.8021 | 243.0933 |
| 251.0681 | 343.1993 | 514.9544 |
| 606.9308 | 758.3746 | 855.2640 |
| 882.3787 | 959.0166 | 1033.8680 |
| 1051.2572 | 1095.4209 | 1127.8606 |
| 1207.1767 | 1266.4083 | 1321.0320 |
| 1332.7833 | 1363.8306 | 1373.8618 |
| 1415.0197 | 1430.2585 | 1494.2030 |
| 1508.9612 | 1514.2096 | 1524.1629 |
| 2881.3085 | 2935.7101 | 3024.2657 |
| 3030.1379 | 3039.7796 | 3064.7534 |
| 3082.0562 | 3108.5278 | 3113.9084 |

Zero-point correction (Hartree): 0.123009

C4H9O.tt

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -233.00513911
 Point group : CS
 Electronic state : 2-A'
 Cartesian coordinates (Angs):

| | | | |
|---|----------|-----------|----------|
| C | 2.413874 | -0.424263 | 0.000000 |
| C | 0.937327 | -0.833367 | 0.000000 |

| | | | |
|--|-----------------|-----------------|-----------|
| C | 0.000000 | 0.381809 | 0.000000 |
| C | -1.501599 | -0.052599 | 0.000000 |
| O | -2.242864 | 1.095093 | 0.000000 |
| H | 2.660480 | 0.173620 | 0.884369 |
| H | 2.660480 | 0.173620 | -0.884369 |
| H | 3.066385 | -1.303345 | 0.000000 |
| H | 0.726480 | -1.455846 | -0.878798 |
| H | 0.726480 | -1.455846 | 0.878798 |
| H | 0.176803 | 1.005415 | 0.882617 |
| H | 0.176803 | 1.005415 | -0.882617 |
| H | -1.674305 | -0.666633 | -0.901788 |
| H | -1.674305 | -0.666633 | 0.901788 |
| Rotational constants (GHz): | 18.7531523 | 2.0719850 | 1.9575088 |
| Vibrational harmonic frequencies (cm-1): | | | |
| 103.1257 (A") | 117.6323 (A") | 192.3474 (A') | |
| 238.8098 (A") | 382.4811 (A') | 412.3140 (A') | |
| 617.7789 (A") | 759.1551 (A") | 880.8563 (A') | |
| 884.3755 (A") | 932.9132 (A') | 1039.5327 (A') | |
| 1066.8829 (A") | 1079.6901 (A') | 1146.5359 (A') | |
| 1236.5829 (A") | 1280.7275 (A') | 1284.7557 (A") | |
| 1315.1741 (A') | 1326.5124 (A") | 1385.0260 (A') | |
| 1426.7627 (A') | 1503.4869 (A') | 1509.9677 (A") | |
| 1509.9799 (A') | 1522.3132 (A') | 1555.1528 (A') | |
| 2942.3046 (A') | 2984.4201 (A") | 3036.6518 (A') | |
| 3042.1557 (A') | 3064.0083 (A') | 3069.0814 (A") | |
| 3108.7300 (A") | 3116.0328 (A') | 3119.7621 (A") | |
| Zero-point correction (Hartree): | 0.123463 | | |

C4H9O.1-4Hshift.d

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -232.97430468
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | |
|--|-----------|-----------|-----------|
| O | 1.256044 | -1.034264 | -0.259875 |
| H | 0.060147 | -0.867717 | -0.686198 |
| C | -0.800502 | 0.081882 | -0.603646 |
| C | 0.267434 | 1.088506 | -0.137506 |
| C | 1.321251 | 0.164640 | 0.498032 |
| H | -1.182765 | 0.238947 | -1.615593 |
| C | -1.867336 | -0.314618 | 0.391007 |
| H | 0.692456 | 1.601153 | -1.006045 |
| H | -0.123186 | 1.852104 | 0.546436 |
| H | 2.342074 | 0.565181 | 0.436352 |
| H | 1.094997 | -0.016437 | 1.561797 |
| H | -2.558199 | 0.524302 | 0.560086 |
| H | -1.437489 | -0.584457 | 1.361099 |
| H | -2.461470 | -1.161419 | 0.033743 |
| Rotational constants (GHz): | 8.2123400 | 3.6160300 | 3.1220200 |
| Vibrational harmonic frequencies (cm-1): | | | |
| i1747.5347 | 147.4165 | 195.9146 | |
| 211.8048 | 354.3480 | 595.9572 | |
| 621.1732 | 791.6247 | 834.2034 | |
| 904.1379 | 949.7643 | 994.5452 | |
| 1010.0260 | 1080.7768 | 1126.2329 | |
| 1149.2646 | 1190.9610 | 1209.8608 | |
| 1254.3022 | 1324.6748 | 1360.3227 | |
| 1381.4222 | 1419.5634 | 1491.9894 | |
| 1502.1826 | 1503.3497 | 1534.2178 | |
| 1746.9164 | 2979.8177 | 3018.1122 | |
| 3045.1263 | 3053.3728 | 3089.7201 | |
| 3100.7471 | 3110.9667 | 3127.9542 | |
| Zero-point correction (Hartree): | 0.119405 | | |

C4H9O.1-5Hshift

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -232.98794288
 Cartesian coordinates (Angs):

| | | | |
|--|-----------|-----------|-----------|
| C | 1.332927 | -0.875706 | -0.067310 |
| C | 1.175624 | 0.602008 | 0.231825 |
| C | -0.163342 | 1.121311 | -0.324006 |
| C | -1.302089 | 0.247036 | 0.231491 |
| O | -1.116744 | -1.105561 | -0.090688 |
| H | 1.606453 | -1.116375 | -1.096871 |
| H | 1.892674 | -1.466099 | 0.659864 |
| H | 2.006737 | 1.176459 | -0.202811 |
| H | 1.206593 | 0.771098 | 1.315119 |
| H | -0.164496 | 1.053692 | -1.418776 |
| H | -0.323778 | 2.171496 | -0.053919 |
| H | -2.256587 | 0.556882 | -0.221757 |
| H | -1.386627 | 0.404394 | 1.322033 |
| H | 0.094268 | -1.274961 | -0.009381 |
| Rotational constants (GHz): | 7.0366311 | 4.6870173 | 3.1659676 |
| Vibrational harmonic frequencies (cm-1): | | | |
| i1589.6047 | 163.7621 | 308.5696 | |
| 416.6012 | 458.1826 | 493.7680 | |

| | | |
|-----------|-----------|-----------|
| 623.4732 | 824.1825 | 846.4153 |
| 889.9720 | 939.0235 | 968.3479 |
| 1037.8063 | 1076.3274 | 1106.6449 |
| 1166.4646 | 1188.3235 | 1202.0431 |
| 1252.6247 | 1263.7479 | 1349.5533 |
| 1370.0791 | 1385.9130 | 1467.3684 |
| 1487.4904 | 1497.6308 | 1510.3606 |
| 1553.6282 | 2953.7254 | 3014.1619 |
| 3016.4069 | 3049.4213 | 3069.4387 |
| 3095.3991 | 3098.7133 | 3177.0717 |

Zero-point correction (Hartree): 0.119200

C5H11O.pmm

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -272.32100436

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -1.345482 | -1.363145 | -0.185724 |
| C | -1.776227 | -0.068483 | -0.062196 |
| C | -0.778516 | 0.894058 | 0.600499 |
| C | 0.440636 | 1.205365 | -0.284478 |
| C | 1.310572 | -0.003271 | -0.668009 |
| C | 1.969634 | -0.714166 | 0.518622 |
| H | -2.155751 | 0.333353 | -1.022064 |
| H | -2.675402 | -0.154519 | 0.587795 |
| H | -1.304486 | 1.830082 | 0.829720 |
| H | -0.465882 | 0.462116 | 1.557778 |
| H | 0.089570 | 1.696467 | -1.202896 |
| H | 1.064092 | 1.945842 | 0.235094 |
| H | 0.704355 | -0.729385 | -1.226911 |
| H | 2.086133 | 0.342884 | -1.363684 |
| H | 1.221994 | -1.188835 | 1.160406 |
| H | 2.552215 | -0.014608 | 1.130208 |
| H | 2.650421 | -1.499262 | 0.173721 |

Rotational constants (GHz): 4.8653700 2.4611800 1.9736100

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 68.2720 | 120.2910 | 145.5302 |
| 240.1342 | 263.0878 | 354.4040 |
| 415.2694 | 487.5247 | 748.1656 |
| 761.4589 | 830.2153 | 855.4979 |
| 904.9407 | 960.0571 | 982.2360 |
| 1071.0018 | 1072.5764 | 1101.3137 |
| 1111.4190 | 1164.8349 | 1201.2228 |
| 1270.8896 | 1319.6062 | 1338.0763 |
| 1363.2069 | 1387.8295 | 1398.6322 |
| 1405.4330 | 1426.5446 | 1485.2982 |
| 1497.8410 | 1500.6766 | 1514.1999 |
| 1524.9777 | 2881.0814 | 2940.2103 |
| 3018.3672 | 3022.2028 | 3040.4253 |
| 3042.5665 | 3054.3048 | 3064.2684 |
| 3093.5318 | 3107.4599 | 3126.4703 |

Zero-point correction (Hartree): 0.151916

C5H11O.pmp

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -272.31778877

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 1.323104 | -1.287381 | -0.348333 |
| C | 1.619783 | -0.071249 | 0.319204 |
| C | 0.829607 | 1.140591 | -0.191266 |
| C | -0.650770 | 1.238043 | 0.221744 |
| C | -1.604689 | 0.171886 | -0.360887 |
| C | -1.560638 | -1.163695 | 0.305037 |
| H | 1.487750 | -0.166829 | 1.411169 |
| H | 2.687188 | 0.104293 | 0.144818 |
| H | 1.336558 | 2.044011 | 0.175047 |
| H | 0.910447 | 1.160949 | -1.286154 |
| H | -0.726136 | 1.221973 | 1.318741 |
| H | -1.018891 | 2.223317 | -0.089184 |
| H | -2.636406 | 0.561965 | -0.277135 |
| H | -1.428285 | 0.061122 | -1.439001 |
| H | -1.470760 | -1.226023 | 1.387355 |
| H | 0.409749 | -1.533615 | -0.114834 |
| H | -1.935801 | -2.045577 | -0.207154 |

Rotational constants (GHz): 4.4388400 2.8303900 1.9477400

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 90.3209 | 128.4284 | 188.6472 |
| 278.3834 | 295.2508 | 319.0407 |
| 415.8619 | 473.1137 | 508.1138 |
| 618.1969 | 765.3245 | 812.6101 |
| 860.3385 | 889.1925 | 957.5988 |
| 996.1985 | 1031.3144 | 1100.5602 |
| 1111.4136 | 1143.4694 | 1201.1630 |

| | | |
|-----------|-----------|-----------|
| 1219.5720 | 1281.9471 | 1294.5207 |
| 1375.6375 | 1393.6165 | 1399.1407 |
| 1408.6230 | 1437.7223 | 1467.0640 |
| 1477.6436 | 1487.1664 | 1502.0205 |
| 1516.5895 | 2939.1011 | 2968.0960 |
| 3020.2261 | 3025.7583 | 3051.3483 |
| 3066.3092 | 3073.8647 | 3079.0280 |
| 3139.8187 | 3241.3614 | 3601.0546 |

Zero-point correction (Hartree): 0.151844

C5H11O.pmt

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -272.32182779
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 1.687107 | -1.324609 | -0.117088 |
| C | 1.895999 | -0.051305 | 0.340873 |
| C | 1.007560 | 1.029606 | -0.297192 |
| C | -0.461310 | 0.946274 | 0.145705 |
| C | -1.193904 | -0.323433 | -0.305994 |
| C | -2.650463 | -0.370406 | 0.167207 |
| H | 1.868747 | 0.003644 | 1.446845 |
| H | 2.955075 | 0.152597 | 0.066928 |
| H | 1.416121 | 2.011517 | -0.025098 |
| H | 1.082360 | 0.937196 | -1.387658 |
| H | -0.510254 | 1.024970 | 1.241984 |
| H | -0.994256 | 1.825175 | -0.241970 |
| H | -1.157662 | -0.389612 | -1.401352 |
| H | -0.658652 | -1.209513 | 0.060904 |
| H | -3.220681 | 0.484119 | -0.215747 |
| H | -2.714270 | -0.344859 | 1.261234 |
| H | -3.150667 | -1.282779 | -0.172960 |

Rotational constants (GHz): 6.2481900 1.9078000 1.5874400
 Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 87.4484 | 101.4117 | 124.2835 |
| 246.6965 | 256.8233 | 313.6911 |
| 389.9796 | 483.2040 | 742.3896 |
| 785.3365 | 828.3781 | 862.7443 |
| 917.2204 | 949.8767 | 1002.6981 |
| 1059.7778 | 1074.5319 | 1091.8837 |
| 1111.1655 | 1162.8773 | 1224.6047 |
| 1276.3570 | 1321.7928 | 1335.5991 |
| 1347.9875 | 1374.5046 | 1405.6512 |
| 1413.2214 | 1426.0830 | 1484.9989 |
| 1491.1772 | 1504.6969 | 1513.7477 |
| 1520.8479 | 2881.3390 | 2939.4649 |
| 3012.3711 | 3026.1940 | 3035.6341 |
| 3037.7864 | 3046.9743 | 3067.0116 |
| 3085.8219 | 3104.6377 | 3114.2462 |

Zero-point correction (Hartree): 0.151692

C5H11O.ppm

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -272.31832924
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 2.165171 | -0.529445 | -0.744738 |
| C | 1.538407 | -0.406367 | 0.464963 |
| C | 0.656735 | 0.845507 | 0.619306 |
| C | -0.436401 | 0.991842 | -0.456782 |
| C | -1.805008 | 0.377346 | -0.114584 |
| C | -1.822117 | -1.141579 | 0.095512 |
| H | 0.924503 | -1.329321 | 0.542963 |
| H | 2.265439 | -0.498283 | 1.295381 |
| H | 0.218056 | 0.845076 | 1.626758 |
| H | 1.327440 | 1.712203 | 0.579055 |
| H | -0.591327 | 2.058764 | -0.656777 |
| H | -0.052846 | 0.564853 | -1.392716 |
| H | -2.202289 | 0.868544 | 0.784616 |
| H | -2.501671 | 0.627145 | -0.925118 |
| H | -1.251890 | -1.439944 | 0.982451 |
| H | -1.401152 | -1.669333 | -0.768045 |
| H | -2.845328 | -1.504635 | 0.238844 |

Rotational constants (GHz): 5.4992100 2.0232400 1.7827200
 Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 58.3156 | 115.0023 | 159.2589 |
| 258.6235 | 275.0527 | 303.0738 |
| 434.2745 | 494.0240 | 662.3546 |
| 772.6566 | 795.6285 | 852.1173 |
| 903.6133 | 934.0340 | 1002.0590 |
| 1060.5363 | 1075.8287 | 1110.9461 |
| 1123.3714 | 1166.5342 | 1231.4977 |
| 1292.0407 | 1313.0886 | 1331.3644 |
| 1367.8116 | 1380.4838 | 1390.5529 |
| 1406.8280 | 1427.9809 | 1492.6231 |

| | | |
|-----------|-----------|-----------|
| 1502.3200 | 1505.6243 | 1517.2801 |
| 1523.0159 | 2901.5884 | 2939.4177 |
| 3024.1732 | 3032.0179 | 3036.5612 |
| 3038.7669 | 3060.2694 | 3075.7143 |
| 3079.3971 | 3106.0587 | 3109.8008 |

Zero-point correction (Hartree): 0.151825

C5H11O.ppp

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -272.32034256
Electronic state : 2-A
Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -2.399054 | -0.575024 | -0.380211 |
| C | -1.608559 | 0.542478 | -0.409842 |
| C | -0.581836 | 0.646361 | 0.728900 |
| C | 0.369670 | -0.557205 | 0.813937 |
| C | 1.397895 | -0.675311 | -0.325034 |
| C | 2.436047 | 0.452808 | -0.364002 |
| H | -1.090634 | 0.481229 | -1.392690 |
| H | -2.225025 | 1.458383 | -0.493192 |
| H | -0.027431 | 1.586304 | 0.612208 |
| H | -1.137691 | 0.733551 | 1.670537 |
| H | 0.906731 | -0.516812 | 1.770573 |
| H | -0.244085 | -1.465191 | 0.840237 |
| H | 1.919491 | -1.634372 | -0.216096 |
| H | 0.882138 | -0.732202 | -1.293303 |
| H | 2.983902 | 0.516257 | 0.583452 |
| H | 1.976627 | 1.430900 | -0.543426 |
| H | 3.169112 | 0.287358 | -1.160365 |

Rotational constants (GHz): 6.8844800 1.7235600 1.6961600
Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 39.3439 | 99.1035 | 184.3612 |
| 222.2077 | 266.2821 | 346.5288 |
| 428.1725 | 520.4424 | 632.3260 |
| 740.8010 | 806.6955 | 841.8377 |
| 914.3506 | 939.8745 | 1005.0018 |
| 1060.9724 | 1064.9485 | 1095.4327 |
| 1124.8707 | 1174.1341 | 1224.5691 |
| 1279.2955 | 1321.4659 | 1334.4903 |
| 1371.4327 | 1374.7584 | 1397.3224 |
| 1410.7503 | 1429.4940 | 1492.7500 |
| 1500.2463 | 1504.9347 | 1517.6101 |
| 1522.9114 | 2886.0064 | 2942.2933 |
| 3030.2871 | 3035.5066 | 3039.5341 |
| 3045.5274 | 3065.2548 | 3078.1049 |
| 3087.6439 | 3108.6173 | 3112.5300 |

Zero-point correction (Hartree): 0.151774

C5H11O.ppt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -272.32164847
Electronic state : 2-A
Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 2.150571 | -1.064146 | -0.393846 |
| C | 1.845883 | -0.063259 | 0.489022 |
| C | 0.918223 | 1.032513 | -0.059792 |
| C | -0.424628 | 0.504329 | -0.583767 |
| C | -1.390875 | 0.022036 | 0.507466 |
| C | -2.728657 | -0.467653 | -0.056621 |
| H | 1.359839 | -0.590719 | 1.339491 |
| H | 2.766509 | 0.361478 | 0.933958 |
| H | 0.758028 | 1.779837 | 0.729719 |
| H | 1.452288 | 1.545272 | -0.869192 |
| H | -0.915072 | 1.295658 | -1.165399 |
| H | -0.221815 | -0.314933 | -1.285068 |
| H | -0.929483 | -0.789381 | 1.086062 |
| H | -1.570657 | 0.839577 | 1.219571 |
| H | -2.583920 | -1.309591 | -0.742837 |
| H | -3.237422 | 0.327610 | -0.613377 |
| H | -3.402551 | -0.799433 | 0.739989 |

Rotational constants (GHz): 7.0380800 1.6373700 1.5172900
Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 61.4485 | 79.1985 | 171.9914 |
| 235.0198 | 251.5238 | 290.6503 |
| 420.6845 | 516.5237 | 628.4794 |
| 743.8324 | 826.2448 | 839.8731 |
| 906.6870 | 951.5365 | 1022.5887 |
| 1055.5872 | 1069.7313 | 1101.4876 |
| 1118.8765 | 1176.4979 | 1244.7093 |
| 1289.9785 | 1318.6605 | 1343.1730 |
| 1347.1578 | 1373.2850 | 1398.1126 |
| 1414.4368 | 1428.0118 | 1492.3939 |
| 1499.3694 | 1507.2465 | 1513.5357 |
| 1522.6168 | 2888.1722 | 2941.8532 |
| 3021.1918 | 3031.4895 | 3036.3821 |

3041.1187 3051.3681 3075.5626
3082.7249 3109.1964 3113.8473
Zero-point correction (Hartree): 0.151621

C5H11O.ptm

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -272.32156493
Electronic state : 2-A
Cartesian coordinates (Angs):
O 2.656848 -0.583483 -0.128317
C 1.965445 0.563935 0.157907
C 0.498664 0.579486 -0.291148
C -0.321247 -0.554295 0.336373
C -1.749038 -0.691520 -0.214242
C -2.661460 0.505266 0.080994
H 2.028980 0.662797 1.264877
H 2.524242 1.444645 -0.215060
H 0.072738 1.560197 -0.043936
H 0.473490 0.493569 -1.385833
H 0.223118 -1.491706 0.172209
H -0.365104 -0.409205 1.426134
H -1.701683 -0.856529 -1.299340
H -2.200735 -1.597356 0.209567
H -2.297688 1.423862 -0.391593
H -2.729742 0.692517 1.159223
H -3.676586 0.327838 -0.289016
Rotational constants (GHz): 9.7461400 1.4760100 1.3692000
Vibrational harmonic frequencies (cm-1):
58.0964 110.2490 156.1264
210.8463 263.5921 295.1254
429.8280 511.6452 557.7771
749.6587 797.8297 869.9887
910.1495 938.3977 1000.7632
1052.6044 1079.1040 1095.8230
1122.4476 1203.0453 1230.1629
1289.4656 1328.4786 1336.6367
1363.7726 1370.5284 1388.3205
1416.1164 1429.5338 1493.1305
1502.6108 1509.7774 1517.2828
1522.4434 2880.6897 2936.6605
3014.1649 3028.4775 3035.4660
3040.4860 3063.9114 3068.7912
3086.9992 3107.6825 3114.7537
Zero-point correction (Hartree): 0.151474

C5H11O.ptp

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -272.32129205
Electronic state : 2-A
Cartesian coordinates (Angs):
O 2.387846 0.771664 -0.552912
C 2.032029 -0.208364 0.335995
C 0.540879 -0.269410 0.688157
C -0.344373 -0.519024 -0.538730
C -1.853689 -0.547740 -0.248803
C -2.439356 0.793716 0.208830
H 2.356277 -1.159879 -0.141948
H 2.670251 -0.141737 1.239312
H 0.389422 -1.060670 1.435866
H 0.268960 0.675774 1.172987
H -0.124882 0.253594 -1.286489
H -0.052762 -1.476605 -0.993123
H -2.375452 -0.869777 -1.158914
H -2.064156 -1.316647 0.507627
H -2.248024 1.579512 -0.530985
H -2.011922 1.125458 1.160738
H -3.523425 0.722587 0.345540
Rotational constants (GHz): 7.7940700 1.5305000 1.4861300
Vibrational harmonic frequencies (cm-1):
56.0983 108.4034 145.5875
206.3955 264.2329 303.8672
402.9330 429.0665 537.6318
752.4214 789.7673 866.4883
895.2571 946.4768 989.4047
1054.7513 1077.1276 1098.9418
1133.4204 1181.6656 1240.4913
1299.4017 1318.2735 1338.1225
1362.5742 1373.4819 1386.6257
1413.7953 1427.5022 1492.9349
1501.9432 1507.8694 1516.9638
1521.8791 2881.7712 2933.1472
3018.3451 3026.9053 3030.4704
3042.4176 3059.4311 3068.2253
3086.7393 3110.7599 3115.0117
Zero-point correction (Hartree): 0.151077

C5H11O.ptt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -272.32272531
Electronic state : 2-A
Cartesian coordinates (Angs):
O 2.460978 -0.965456 -0.314921
C 2.151206 0.230587 0.277176
C 0.793588 0.826920 -0.113376
C -0.382190 -0.095891 0.223777
C -1.738001 0.437368 -0.254330
C -2.905794 -0.492334 0.091102
H 2.180855 0.022754 1.370274
H 2.980429 0.949680 0.126779
H 0.678811 1.796723 0.390371
H 0.806482 1.035044 -1.191336
H -0.190465 -1.078869 -0.224498
H -0.417812 -0.256346 1.311627
H -1.915815 1.428170 0.186149
H -1.701679 0.591506 -1.341331
H -2.989471 -0.638127 1.174178
H -2.773191 -1.479925 -0.364893
H -3.858823 -0.086862 -0.264050
Rotational constants (GHz): 9.5061800 1.3840400 1.2867800
Vibrational harmonic frequencies (cm-1):
84.6276 94.1872 146.3148
185.4233 244.8360 313.4792
395.0498 473.1371 524.2294
743.6897 799.5354 894.3621
902.8200 945.5774 1006.4760
1053.5028 1079.9857 1094.7966
1130.8940 1200.4128 1245.7016
1293.8687 1320.5650 1338.3948
1359.0307 1364.7479 1389.2840
1420.5236 1427.3944 1494.2410
1502.5441 1512.6249 1513.7579
1525.9089 2881.6491 2935.3893
3014.4935 3023.5316 3030.6972
3039.8723 3051.4834 3063.8622
3082.9859 3108.2997 3113.2170
Zero-point correction (Hartree): 0.151196

C5H11O.tpm

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -272.31750786
Electronic state : 2-A
Cartesian coordinates (Angs):
O 2.700926 0.515484 -0.215579
C 1.480135 0.276056 0.352310
C 0.641487 -0.814232 -0.332874
C -0.722958 -1.088003 0.332901
C -1.912393 -0.270657 -0.202555
C -1.824931 1.246857 -0.002048
H 1.594731 0.073950 1.437162
H 0.961744 1.258187 0.329895
H 0.511381 -0.547453 -1.389130
H 1.245557 -1.729163 -0.321387
H -0.966136 -2.149290 0.204161
H -0.636735 -0.936676 1.419415
H -2.035468 -0.485954 -1.272606
H -2.824343 -0.638398 0.285059
H -1.009835 1.691469 -0.583026
H -1.666310 1.502711 1.052291
H -2.750036 1.736622 -0.323606
Rotational constants (GHz): 6.2381400 1.7871300 1.5135500
Vibrational harmonic frequencies (cm-1):
56.0890 94.9569 114.0072
251.0429 267.1972 307.5427
389.0286 477.9877 534.1650
765.2390 793.0453 844.7232
887.6658 971.1735 1008.8198
1052.6226 1082.6109 1102.5067
1120.7189 1189.3464 1246.1812
1291.2973 1313.5066 1336.0317
1372.1298 1387.8225 1390.7083
1392.4623 1427.1320 1496.9705
1500.8017 1505.4253 1515.3837
1523.1770 2904.3120 2921.9591
3014.3076 3028.2933 3038.6480
3042.6158 3062.9801 3070.5536
3086.6282 3107.3729 3111.6501
Zero-point correction (Hartree): 0.151268

C5H11O.tpp

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -272.31971714
Electronic state : 2-A
Cartesian coordinates (Angs):
O -2.715924 -0.638886 -0.049142
C -1.567120 -0.070108 0.428226
C -0.621691 0.480595 -0.650468
C 0.662471 1.106255 -0.082155
C 1.626547 0.132874 0.620500
C 2.213189 -0.947739 -0.295169
H -1.782117 0.686909 1.208839
H -1.073328 -0.898718 0.982918
H -0.392408 -0.325234 -1.356542
H -1.171866 1.240518 -1.218294
H 1.198988 1.603308 -0.900961
H 0.386750 1.903094 0.622504
H 2.447193 0.718107 1.053994
H 1.124636 -0.344081 1.473468
H 2.734947 -0.499948 -1.148909
H 1.440477 -1.613240 -0.693854
H 2.933744 -1.570885 0.244374
Rotational constants (GHz): 6.7099300 1.6532100 1.5290100
Vibrational harmonic frequencies (cm-1):
60.0622 94.5084 156.7538
237.7943 267.5449 320.7446
407.3600 497.4353 669.3603
747.0326 816.3753 851.2774
922.2210 966.5033 996.8368
1055.1367 1081.7899 1096.9828
1122.8018 1176.4027 1230.7949
1276.6652 1325.9749 1332.0090
1360.4515 1384.3885 1395.0005
1397.6507 1432.7916 1494.2228
1504.9976 1506.8523 1518.7112
1526.0882 2885.4433 2930.8409
3022.8127 3029.3578 3043.8553
3051.8815 3059.9048 3068.9667
3098.4088 3111.5407 3117.8955
Zero-point correction (Hartree): 0.151845

C5H11O.tpt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -272.32097201
Electronic state : 2-A
Cartesian coordinates (Angs):
O -2.988563 -0.393757 -0.109299
C -1.681517 -0.389653 0.293906
C -0.843661 0.783789 -0.236441
C 0.618995 0.764172 0.232608
C 1.461791 -0.386192 -0.337213
C 2.928301 -0.324417 0.102542
H -1.599231 -0.485956 1.395313
H -1.281793 -1.353535 -0.091606
H -0.896451 0.781804 -1.332119
H -1.323621 1.711255 0.098174
H 1.088331 1.716435 -0.046620
H 0.650564 0.727224 1.331501
H 1.037644 -1.352038 -0.031798
H 1.405732 -0.363336 -1.434109
H 3.017597 -0.377230 1.193623
H 3.398183 0.611100 -0.221516
H 3.508087 -1.151860 -0.318861
Rotational constants (GHz): 10.5412300 1.3456600 1.2730000
Vibrational harmonic frequencies (cm-1):
80.8737 94.1740 118.1202
241.6682 256.1787 287.2970
344.9640 524.9450 657.6774
741.5477 825.2453 846.7114
923.3537 966.7208 1026.2602
1054.9068 1073.4253 1087.2165
1123.0490 1188.2844 1247.7264
1282.5740 1318.9925 1339.2278
1344.8824 1368.0010 1389.5357
1409.9113 1427.8743 1496.7852
1502.4268 1507.9181 1513.4178
1523.1664 2888.9458 2927.7455
3016.5840 3027.6853 3040.4216
3042.3648 3050.6960 3070.5344
3089.8544 3108.6223 3115.3034
Zero-point correction (Hartree): 0.151530

C5H11O.ttp

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -272.32087084
Electronic state : 2-A
Cartesian coordinates (Angs):

| | | | |
|--|-----------|-----------|-----------|
| O | 2.963386 | -0.577447 | -0.117793 |
| C | 1.942459 | 0.273770 | 0.207733 |
| C | 0.545649 | -0.157465 | -0.254854 |
| C | -0.549502 | 0.815907 | 0.200071 |
| C | -1.957165 | 0.482119 | -0.320982 |
| C | -2.531009 | -0.837735 | 0.206668 |
| H | 1.973930 | 0.344738 | 1.318331 |
| H | 2.184216 | 1.305040 | -0.120866 |
| H | 0.550588 | -0.227932 | -1.350570 |
| H | 0.358867 | -1.168429 | 0.124010 |
| H | -0.571566 | 0.852047 | 1.299407 |
| H | -0.283739 | 1.830143 | -0.129734 |
| H | -2.633744 | 1.301190 | -0.046084 |
| H | -1.937563 | 0.460508 | -1.419071 |
| H | -2.563600 | -0.843575 | 1.302530 |
| H | -1.934984 | -1.699006 | -0.111504 |
| H | -3.552082 | -0.994719 | -0.155914 |
| Rotational constants (GHz): | 9.6529700 | 1.3606100 | 1.2695400 |
| Vibrational harmonic frequencies (cm-1): | | | |
| 80.6598 | 89.2797 | | 140.0436 |
| 168.2458 | 261.9692 | | 307.2489 |
| 425.3227 | 459.8988 | | 518.0891 |
| 747.7997 | 788.6429 | | 875.2162 |
| 911.8056 | 984.0135 | | 1013.4378 |
| 1031.4239 | 1083.9064 | | 1088.7894 |
| 1132.5792 | 1203.3856 | | 1255.7744 |
| 1277.1941 | 1320.8895 | | 1328.4957 |
| 1367.4132 | 1380.2803 | | 1387.0042 |
| 1408.3162 | 1430.6166 | | 1495.6135 |
| 1502.2347 | 1511.7857 | | 1516.2775 |
| 1521.4521 | 2878.3339 | | 2923.0687 |
| 3010.1059 | 3027.1305 | | 3041.1851 |
| 3042.9961 | 3048.9500 | | 3065.1901 |
| 3096.8289 | 3110.0197 | | 3119.1013 |
| Zero-point correction (Hartree): | 0.151220 | | |

C5H11O.ttt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -272.32214276

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|--|------------|-----------|-----------|
| O | 3.205868 | 0.194257 | 0.013885 |
| C | 2.000772 | -0.453838 | -0.018171 |
| C | 0.760715 | 0.446563 | -0.007712 |
| C | -0.550741 | -0.347137 | 0.003809 |
| C | -1.802134 | 0.540191 | -0.005791 |
| C | -3.108507 | -0.259736 | 0.007202 |
| H | 1.981170 | -1.169299 | -0.865624 |
| H | 2.004064 | -1.118422 | 0.874586 |
| H | 0.817151 | 1.104812 | 0.868109 |
| H | 0.797930 | 1.097393 | -0.890743 |
| H | -0.580025 | -1.020253 | -0.865561 |
| H | -0.577214 | -0.998440 | 0.889909 |
| H | -1.773960 | 1.212308 | 0.862301 |
| H | -1.776902 | 1.188566 | -0.891908 |
| H | -3.177698 | -0.891797 | 0.899943 |
| H | -3.180493 | -0.915905 | -0.867745 |
| H | -3.981597 | 0.400725 | -0.000371 |
| Rotational constants (GHz): | 16.3930200 | 1.1554000 | 1.1164000 |
| Vibrational harmonic frequencies (cm-1): | | | |
| 79.6511 | 108.4106 | | 133.9379 |
| 150.9395 | 244.9430 | | 316.5513 |
| 354.4458 | 411.6192 | | 512.3309 |
| 738.7307 | 784.2668 | | 899.6367 |
| 902.1462 | 1011.1707 | | 1023.3504 |
| 1031.0979 | 1067.3989 | | 1089.2999 |
| 1135.4345 | 1220.5227 | | 1257.5912 |
| 1278.3165 | 1320.4834 | | 1340.5104 |
| 1346.8061 | 1372.5833 | | 1399.3630 |
| 1415.2552 | 1427.5135 | | 1499.3727 |
| 1502.4487 | 1512.7697 | | 1513.8045 |
| 1525.8121 | 2882.4467 | | 2921.3953 |
| 3009.1918 | 3028.6825 | | 3037.0615 |
| 3039.6186 | 3042.1144 | | 3064.3004 |
| 3087.7851 | 3107.5976 | | 3114.1027 |
| Zero-point correction (Hartree): | 0.150958 | | |

C5H11O-1-5Hshift.m

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -272.30713560

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| C | 1.091606 | -0.073308 | 0.597448 |
| C | 0.265387 | 1.194235 | 0.403039 |
| C | -0.929196 | 0.939004 | -0.536130 |

| | | | |
|---|-----------|-----------|-----------|
| C | -1.732838 | -0.262070 | -0.007411 |
| O | -0.931322 | -1.406071 | 0.105920 |
| C | 2.102143 | -0.413997 | -0.480254 |
| H | 1.491376 | -0.188681 | 1.609719 |
| H | 0.892998 | 2.001919 | -0.001701 |
| H | -0.112910 | 1.541480 | 1.372071 |
| | | | |
| H | -0.573842 | 0.712216 | -1.548189 |
| H | -1.571270 | 1.825025 | -0.603542 |
| H | -2.539676 | -0.503847 | -0.717595 |
| H | -2.209309 | 0.007714 | 0.952910 |
| H | 0.177388 | -0.955297 | 0.509521 |
| H | 2.925477 | 0.314410 | -0.484068 |
| H | 1.648015 | -0.405335 | -1.475988 |
| H | 2.539717 | -1.404222 | -0.320649 |
| Rotational constants (GHz): | 5.0594600 | 2.6898800 | 2.1102300 |
| Vibrational harmonic frequencies (cm ⁻¹): | | | |
| i1448.9990 | 123.4208 | | 153.0741 |
| 193.1764 | 286.2410 | | 371.4786 |
| 481.1305 | 489.6958 | | 625.2061 |
| 799.1905 | 827.8091 | | 856.3193 |
| 903.2987 | 919.8335 | | 999.2918 |
| 1008.0505 | 1065.7100 | | 1085.1202 |
| 1138.0439 | 1160.6540 | | 1178.1196 |
| 1215.9870 | 1232.5540 | | 1271.8986 |
| 1347.8888 | 1358.3521 | | 1376.4700 |
| 1386.3502 | 1420.0730 | | 1483.8338 |
| 1493.6488 | 1499.2960 | | 1505.5531 |
| 1509.5569 | 1560.0466 | | 2949.4178 |
| 3007.1427 | 3014.1540 | | 3022.8817 |
| 3051.3114 | 3068.5355 | | 3091.2725 |
| 3095.3465 | 3099.4718 | | 3127.5538 |
| Zero-point correction (Hartree): | 0.147747 | | |

C5H11O-1-5Hshift.p

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -272.30791328
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| C | 1.065976 | 0.005988 | -0.444112 |
| C | 0.259964 | 1.166117 | 0.121651 |
| C | -1.237975 | 0.983369 | -0.174353 |
| C | -1.688334 | -0.389330 | 0.359385 |
| O | -0.934678 | -1.430187 | -0.199306 |
| H | 1.156777 | 0.049704 | -1.535118 |
| C | 2.362860 | -0.355314 | 0.248503 |
| H | 0.614501 | 2.120185 | -0.295715 |
| H | 0.410141 | 1.223015 | 1.208295 |
| H | -1.411846 | 1.018379 | -1.256783 |
| H | -1.832890 | 1.781647 | 0.284417 |
| H | -2.739358 | -0.563266 | 0.078838 |
| H | -1.637898 | -0.386377 | 1.463733 |
| H | 0.223301 | -0.942772 | -0.309462 |
| H | 2.206366 | -0.546476 | 1.315655 |
| H | 3.089500 | 0.466433 | 0.167296 |
| H | 2.823882 | -1.243955 | -0.193150 |
| Rotational constants (GHz): | 5.4362900 | 2.4805500 | 1.9020400 |
| Vibrational harmonic frequencies (cm ⁻¹): | | | |
| i1457.7076 | 115.5798 | | 175.5158 |
| 211.3206 | 304.5566 | | 355.1072 |
| 437.8605 | 482.0788 | | 574.8974 |
| 783.8837 | 831.3756 | | 872.8566 |
| 902.0359 | 921.9634 | | 996.5256 |
| 1016.3463 | 1073.6481 | | 1092.2653 |
| 1130.8211 | 1171.7708 | | 1191.8139 |
| 1237.9417 | 1249.4459 | | 1274.5486 |
| 1327.1756 | 1363.1226 | | 1385.6926 |
| 1391.8206 | 1421.4922 | | 1484.8038 |
| 1493.0258 | 1498.0612 | | 1503.2108 |
| 1511.7761 | 1563.9069 | | 2948.7557 |
| 3007.5493 | 3011.1023 | | 3017.3592 |
| 3045.9494 | 3056.8825 | | 3080.6267 |
| 3089.1439 | 3096.6742 | | 3123.6723 |
| Zero-point correction (Hartree): | 0.147684 | | |

C5H11O-1-6Hshift.a

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -272.30441346
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 1.147240 | -1.297468 | -0.306485 |
| H | -0.040227 | -1.419666 | -0.038666 |
| C | -1.277734 | -1.201761 | 0.235885 |
| C | 1.574324 | -0.089418 | 0.274790 |
| C | -1.584731 | 0.182068 | -0.293231 |

| | | | |
|--|-----------|-----------|-----------|
| C | 0.825799 | 1.154989 | -0.224457 |
| C | -0.636098 | 1.273220 | 0.240842 |
| H | -1.322006 | -1.298983 | 1.324331 |
| H | -1.789705 | -2.024359 | -0.268475 |
| H | 1.540031 | -0.130435 | 1.378398 |
| H | 2.636446 | -0.008457 | -0.002283 |
| H | -1.547208 | 0.171655 | -1.390112 |
| H | -2.619370 | 0.447021 | -0.026201 |
| H | 1.373956 | 2.040213 | 0.124364 |
| H | 0.869192 | 1.166182 | -1.321433 |
| H | -1.021543 | 2.251464 | -0.071319 |
| H | -0.666846 | 1.270507 | 1.340309 |
| Rotational constants (GHz): | 4.4028000 | 3.2295300 | 2.0888000 |
| Vibrational harmonic frequencies (cm-1): | | | |
| i1538.4981 | 132.9520 | | 189.6435 |
| | | | |
| 313.5285 | 337.8795 | | 401.6662 |
| 468.8153 | 558.1475 | | 591.4324 |
| 780.2944 | 796.6193 | | 863.4988 |
| 884.9886 | 935.0388 | | 1000.3268 |
| 1010.9301 | 1045.6565 | | 1093.3979 |
| 1110.9268 | 1158.1055 | | 1199.9163 |
| 1239.2289 | 1257.3513 | | 1287.1132 |
| 1301.2119 | 1376.7539 | | 1387.2455 |
| 1396.7069 | 1409.0229 | | 1452.5870 |
| 1466.0365 | 1482.2314 | | 1484.1583 |
| 1491.4031 | 1504.4531 | | 2958.1820 |
| 3004.5769 | 3018.8824 | | 3020.3110 |
| 3034.7879 | 3059.7867 | | 3070.0263 |
| 3077.4632 | 3081.5910 | | 3161.2039 |
| Zero-point correction (Hartree): | 0.147844 | | |

C5H11O-1-6Hshift.b

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -272.29987605
Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|--|-----------|-----------|-----------|
| O | -0.996306 | -1.327663 | -0.432166 |
| H | 0.216931 | -1.382778 | -0.262736 |
| C | 1.447864 | -1.066692 | -0.027545 |
| C | -1.428127 | -0.308890 | 0.436028 |
| C | 1.453387 | 0.390993 | 0.395996 |
| C | -1.013853 | 1.107822 | -0.004021 |
| C | 0.464815 | 1.240875 | -0.431883 |
| H | 1.900187 | -1.249520 | -1.005970 |
| H | 1.784213 | -1.789136 | 0.719401 |
| H | -2.525477 | -0.382105 | 0.459586 |
| H | -1.089227 | -0.500353 | 1.468002 |
| H | 1.225561 | 0.481649 | 1.465455 |
| H | 2.469557 | 0.792324 | 0.269285 |
| H | -1.649476 | 1.430920 | -0.836541 |
| H | -1.221201 | 1.788762 | 0.832711 |
| H | 0.750953 | 2.297352 | -0.378824 |
| H | 0.563905 | 0.949543 | -1.484489 |
| Rotational constants (GHz): | 4.3422900 | 3.3068200 | 2.1919800 |
| Vibrational harmonic frequencies (cm-1): | | | |
| i1568.7492 | 113.5971 | | 239.4037 |
| 254.1062 | 338.5221 | | 399.8314 |
| 459.6999 | 559.2925 | | 600.0393 |
| 766.7001 | 794.3400 | | 857.6228 |
| 889.8290 | 955.0359 | | 1000.6548 |
| 1024.7493 | 1054.6985 | | 1091.9357 |
| 1118.7240 | 1149.2938 | | 1191.2588 |
| 1248.9514 | 1255.6433 | | 1266.2745 |
| 1303.6977 | 1356.8802 | | 1383.6098 |
| 1388.1635 | 1415.4552 | | 1462.1889 |
| 1480.0519 | 1482.3899 | | 1494.0412 |
| 1505.0179 | 1511.7208 | | 2975.4234 |
| 3014.1425 | 3026.9812 | | 3035.0101 |
| 3045.6119 | 3065.7496 | | 3077.3840 |
| 3083.2242 | 3092.0382 | | 3163.8075 |
| Zero-point correction (Hartree): | 0.148064 | | |

C5H11O-1-6Hshift.c

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -272.29896178
Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| C | 1.476480 | 0.011748 | 0.474027 |
| C | 0.771368 | 1.285269 | -0.043708 |
| C | -0.716704 | 1.113829 | -0.434923 |
| C | -1.495800 | 0.074806 | 0.390738 |
| O | -1.283091 | -1.249205 | -0.039314 |
| H | -0.088071 | -1.385631 | -0.255533 |

| | | | | |
|--|-----------|-----------|-----------|--|
| C | 1.191539 | -1.222561 | -0.350335 | |
| H | 1.173716 | -0.183813 | 1.510571 | |
| H | 2.560022 | 0.198556 | 0.514183 | |
| H | 0.858793 | 2.055655 | 0.732006 | |
| H | 1.316098 | 1.670511 | -0.914687 | |
| H | -1.214161 | 2.087621 | -0.353010 | |
| H | -0.805586 | 0.806862 | -1.483501 | |
| H | -1.286946 | 0.200242 | 1.467985 | |
| H | -2.574703 | 0.245716 | 0.255787 | |
| H | 1.593739 | -2.155592 | 0.050357 | |
| H | 1.370531 | -1.125034 | -1.424440 | |
| Rotational constants (GHz): | 4.3487700 | 3.2703900 | 2.1706900 | |
| Vibrational harmonic frequencies (cm-1): | | | | |
| i1579.8053 | 96.4874 | | 215.3359 | |
| 264.2258 | 331.4598 | | 407.9223 | |
| 449.0566 | 547.8796 | | 588.6216 | |
| 760.0368 | 789.6922 | | 877.4929 | |
| 880.7932 | 949.1472 | | 1002.8164 | |
| 1011.2729 | 1052.7241 | | 1109.2189 | |
| 1120.2952 | 1153.6146 | | 1174.0838 | |
| 1237.9837 | 1243.0376 | | 1269.5326 | |
| 1303.8734 | 1360.9313 | | 1386.9599 | |
| 1395.3677 | 1399.1537 | | 1462.4553 | |
| 1478.9438 | 1489.6512 | | 1493.2162 | |
| 1505.4297 | 1512.2744 | | 2961.1410 | |
| 3012.3781 | 3017.1795 | | 3036.8720 | |
| 3050.7665 | 3053.5610 | | 3073.4631 | |
| 3083.8896 | 3094.2126 | | 3164.0530 | |
| Zero-point correction (Hartree): | 0.147781 | | | |

C6H13O.pmmm

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -311.63551279

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | | |
|--|-----------|-----------|-----------|--|
| O | 1.866266 | -1.329266 | -0.054563 | |
| C | 2.216239 | -0.012649 | -0.196644 | |
| C | 1.069726 | 0.933214 | -0.588466 | |
| C | 0.053721 | 1.152746 | 0.545181 | |
| C | -0.687372 | -0.107917 | 1.024207 | |
| C | -1.556296 | -0.818406 | -0.027106 | |
| C | -2.683984 | 0.042092 | -0.608965 | |
| H | 2.771700 | 0.364693 | 0.684192 | |
| H | 2.962698 | -0.029341 | -1.021781 | |
| H | 1.505329 | 1.899826 | -0.873499 | |
| H | 0.578578 | 0.528736 | -1.480702 | |
| H | 0.578107 | 1.595837 | 1.403331 | |
| H | -0.671977 | 1.908272 | 0.218917 | |
| H | 0.044795 | -0.829971 | 1.411116 | |
| H | -1.317880 | 0.172444 | 1.879675 | |
| H | -0.916947 | -1.194576 | -0.834269 | |
| H | -1.993832 | -1.708982 | 0.441763 | |
| H | -2.299030 | 0.901541 | -1.168622 | |
| H | -3.335783 | 0.430622 | 0.182715 | |
| H | -3.308091 | -0.539464 | -1.295576 | |
| Rotational constants (GHz): | 4.1887300 | 1.4647400 | 1.3197400 | |
| Vibrational harmonic frequencies (cm-1): | | | | |
| 48.1521 | 82.1203 | | 123.9079 | |
| 166.8050 | 221.0800 | | 261.6841 | |
| 329.3353 | 373.3592 | | 444.0831 | |
| 502.7110 | 729.6546 | | 753.2458 | |
| 804.0180 | 843.7721 | | 858.4957 | |
| 913.2526 | 957.0431 | | 984.4343 | |
| 1020.6305 | 1076.5135 | | 1082.0175 | |
| 1106.5305 | 1118.2044 | | 1161.3764 | |
| 1186.9595 | 1240.9180 | | 1287.8412 | |
| 1330.1292 | 1336.2551 | | 1366.0141 | |
| 1373.7964 | 1399.4276 | | 1402.4733 | |
| 1409.7262 | 1429.9725 | | 1482.5577 | |
| 1490.2757 | 1500.6632 | | 1510.0784 | |
| 1516.6514 | 1524.5081 | | 2880.7756 | |
| 2939.7160 | 3013.2836 | | 3025.1588 | |
| 3038.5127 | 3039.1682 | | 3042.8593 | |
| 3050.1826 | 3068.0172 | | 3078.0155 | |
| 3092.0270 | 3107.0599 | | 3110.9444 | |
| Zero-point correction (Hartree): | 0.180514 | | | |

Rotational constants (GHz): 4.1887300 1.4647400 1.3197400

Vibrational harmonic frequencies (cm-1):

| | | | | |
|-----------|-----------|--|-----------|--|
| 48.1521 | 82.1203 | | 123.9079 | |
| 166.8050 | 221.0800 | | 261.6841 | |
| 329.3353 | 373.3592 | | 444.0831 | |
| 502.7110 | 729.6546 | | 753.2458 | |
| 804.0180 | 843.7721 | | 858.4957 | |
| 913.2526 | 957.0431 | | 984.4343 | |
| 1020.6305 | 1076.5135 | | 1082.0175 | |
| 1106.5305 | 1118.2044 | | 1161.3764 | |
| 1186.9595 | 1240.9180 | | 1287.8412 | |
| 1330.1292 | 1336.2551 | | 1366.0141 | |
| 1373.7964 | 1399.4276 | | 1402.4733 | |
| 1409.7262 | 1429.9725 | | 1482.5577 | |
| 1490.2757 | 1500.6632 | | 1510.0784 | |
| 1516.6514 | 1524.5081 | | 2880.7756 | |
| 2939.7160 | 3013.2836 | | 3025.1588 | |
| 3038.5127 | 3039.1682 | | 3042.8593 | |
| 3050.1826 | 3068.0172 | | 3078.0155 | |
| 3092.0270 | 3107.0599 | | 3110.9444 | |

Zero-point correction (Hartree): 0.180514

C6H13O.pmp

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -311.63309294

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | | |
|---|-----------|-----------|-----------|--|
| O | -1.482169 | -1.297619 | -0.722230 | |
| C | -2.082215 | -0.279874 | -0.027325 | |
| C | -1.146484 | 0.502711 | 0.910936 | |

| | | | |
|---|-----------|-----------|-----------|
| C | -0.160786 | 1.412295 | 0.153869 |
| C | 0.793376 | 0.730364 | -0.846251 |
| C | 2.066734 | 0.084794 | -0.269854 |
| C | 1.857092 | -1.124064 | 0.652070 |
| H | -2.655789 | 0.399011 | -0.687275 |
| H | -2.841378 | -0.801734 | 0.596113 |
| H | -1.767752 | 1.124353 | 1.569155 |
| H | -0.623142 | -0.216055 | 1.547232 |
| H | -0.754978 | 2.158651 | -0.391424 |
| H | 0.427393 | 1.980230 | 0.887993 |
| H | 0.240375 | -0.023905 | -1.425466 |
| H | 1.109879 | 1.489224 | -1.573747 |
| H | 2.688731 | -0.227839 | -1.118674 |
| H | 2.648604 | 0.852570 | 0.259631 |
| H | 1.164492 | -1.844757 | 0.205407 |
| H | 1.447545 | -0.831648 | 1.624230 |
| H | 2.807067 | -1.634500 | 0.843999 |

Rotational constants (GHz): 3.4645000 1.6901400 1.4555600
 Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 53.5405 | 94.5622 | 122.0532 |
| 160.4162 | 266.0750 | 277.6060 |
| 309.3851 | 356.6286 | 429.9697 |
| 489.1998 | 745.1802 | 776.6564 |
| 808.6181 | 834.3985 | 865.6782 |
| 913.4612 | 955.1937 | 990.1915 |
| 1023.2433 | 1080.3867 | 1083.3595 |
| 1108.7213 | 1130.7744 | 1148.7929 |
| 1196.0136 | 1246.0137 | 1309.2530 |
| 1317.3086 | 1335.5910 | 1363.9598 |
| 1388.0899 | 1395.9982 | 1404.1035 |
| 1417.3201 | 1432.9527 | 1485.1694 |
| 1494.5341 | 1495.4869 | 1504.8461 |
| 1515.9608 | 1528.7440 | 2883.9580 |
| 2946.8921 | 3005.2324 | 3016.6486 |
| 3020.1886 | 3042.6403 | 3045.6644 |
| 3053.5036 | 3055.6738 | 3059.4806 |
| 3108.3988 | 3120.6511 | 3124.1025 |

Zero-point correction (Hartree): 0.180746

C6H13O.pmmt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -311.63680785

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -1.310317 | -1.623939 | -0.188363 |
| C | -2.150660 | -0.549829 | -0.057911 |
| C | -1.532629 | 0.689138 | 0.608316 |
| C | -0.492850 | 1.395951 | -0.278811 |
| C | 0.732675 | 0.553380 | -0.667737 |
| C | 1.616134 | 0.115856 | 0.507904 |
| C | 2.885876 | -0.611765 | 0.054007 |
| H | -2.645569 | -0.294057 | -1.015194 |
| H | -2.966644 | -0.935530 | 0.593065 |
| H | -2.341897 | 1.392595 | 0.843884 |
| H | -1.087983 | 0.383121 | 1.561776 |
| H | -0.992642 | 1.739769 | -1.195199 |
| H | -0.155933 | 2.303903 | 0.239687 |
| H | 0.406901 | -0.341602 | -1.217445 |
| H | 1.339647 | 1.136521 | -1.374415 |
| H | 1.891238 | 0.997325 | 1.104499 |
| H | 1.042006 | -0.543578 | 1.168796 |
| H | 3.501880 | 0.026863 | -0.589964 |
| H | 2.639382 | -1.515290 | -0.514955 |
| H | 3.500877 | -0.914921 | 0.907763 |

Rotational constants (GHz): 3.9409600 1.4783200 1.2202500

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 62.8368 | 76.5077 | 114.8021 |
| 167.0137 | 232.2380 | 255.4527 |
| 300.6086 | 347.9484 | 442.3113 |
| 501.2055 | 734.1241 | 764.3318 |
| 806.2439 | 848.6700 | 862.0395 |
| 924.9904 | 957.5135 | 988.4091 |
| 1037.2604 | 1071.8747 | 1091.4788 |
| 1107.1648 | 1114.6079 | 1166.8264 |
| 1194.1178 | 1255.2736 | 1305.1627 |
| 1329.6683 | 1336.8725 | 1345.7891 |
| 1374.3286 | 1389.9568 | 1405.7215 |
| 1416.7112 | 1426.5380 | 1488.4887 |
| 1494.3891 | 1500.8755 | 1506.1938 |
| 1514.0965 | 1521.6920 | 2881.3877 |
| 2940.2573 | 3009.1711 | 3019.3830 |
| 3025.1435 | 3038.1128 | 3041.5941 |
| 3045.8671 | 3060.0254 | 3079.3739 |

3095.5588 3108.6315 3112.1036
Zero-point correction (Hartree): 0.180520

C6H13O.pmpm

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -311.62700010

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 1.204681 | -1.668066 | -0.409472 |
| C | 1.856685 | -0.688706 | 0.392450 |
| C | 1.742359 | 0.745730 | -0.140362 |
| C | 0.424332 | 1.498017 | 0.124785 |
| C | -0.859775 | 0.871598 | -0.464508 |
| C | -1.642232 | -0.021240 | 0.520841 |
| C | -2.837497 | -0.677050 | -0.082619 |
| H | 1.513531 | -0.732620 | 1.439862 |
| H | 2.911017 | -0.984746 | 0.393135 |
| H | 2.557343 | 1.332365 | 0.305527 |
| H | 1.939589 | 0.712000 | -1.219742 |
| H | 0.294336 | 1.630585 | 1.208513 |
| H | 0.542750 | 2.509386 | -0.282315 |
| H | -1.539385 | 1.668807 | -0.790397 |
| H | -0.615784 | 0.302080 | -1.370300 |
| H | -0.989416 | -0.783934 | 0.973722 |
| H | -1.942662 | 0.607633 | 1.380150 |
| H | 0.251830 | -1.537986 | -0.342207 |
| H | -3.360112 | -0.214249 | -0.914209 |
| H | -3.303720 | -1.534890 | 0.390507 |

Rotational constants (GHz): 3.5466800 1.6020000 1.2250300

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 59.4893 | 77.8477 | 107.3303 |
| 131.9439 | 180.1058 | 250.9815 |
| 269.9878 | 294.8545 | 345.0141 |
| 438.4042 | 471.7530 | 491.1347 |
| 738.9161 | 773.2717 | 827.6784 |
| 883.3850 | 901.6299 | 969.2716 |
| 983.5196 | 1056.2511 | 1091.0090 |
| 1094.1016 | 1101.0435 | 1123.6198 |
| 1164.2831 | 1209.0213 | 1262.7523 |
| 1286.3535 | 1319.7403 | 1334.4587 |
| 1387.5656 | 1390.9552 | 1400.5961 |
| 1402.3194 | 1431.4183 | 1478.1320 |
| 1484.4156 | 1492.6721 | 1502.6418 |
| 1514.6405 | 1518.1485 | 2937.7752 |
| 2980.1664 | 3004.9725 | 3020.5845 |
| 3027.5855 | 3036.1995 | 3063.9657 |
| 3075.5309 | 3076.4938 | 3085.8272 |
| 3158.4868 | 3261.7587 | 3848.4150 |

Zero-point correction (Hartree): 0.179566

C6H13O.pmpm

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -311.63868588

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 1.187666 | -1.525276 | -0.567997 |
| C | 1.739123 | -0.676518 | 0.424811 |
| C | 1.591092 | 0.822368 | 0.134024 |
| C | 0.194166 | 1.440079 | 0.332930 |
| C | -0.896769 | 1.039953 | -0.691660 |
| C | -1.523161 | -0.316127 | -0.532016 |
| C | -2.248970 | -0.707332 | 0.716519 |
| H | 1.324369 | -0.899948 | 1.423755 |
| H | 2.805434 | -0.925986 | 0.463534 |
| H | 2.286078 | 1.355364 | 0.797633 |
| H | 1.936789 | 1.007645 | -0.891689 |
| H | -0.156678 | 1.226144 | 1.351615 |
| H | 0.301743 | 2.530469 | 0.281644 |
| H | -1.700775 | 1.796070 | -0.622346 |
| H | -0.485857 | 1.136123 | -1.703677 |
| H | -1.795580 | -0.846159 | -1.444265 |
| H | 0.224883 | -1.373858 | -0.577481 |
| H | -3.226702 | -0.198193 | 0.784184 |
| H | -1.698181 | -0.437212 | 1.624384 |
| H | -2.449732 | -1.782788 | 0.749030 |

Rotational constants (GHz): 3.1971400 1.8575200 1.4373900

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 47.4816 | 68.2661 | 106.4300 |
| 161.2691 | 199.6487 | 253.7155 |
| 319.1008 | 349.7101 | 448.2930 |
| 469.4372 | 521.4277 | 581.7088 |
| 754.6696 | 816.6475 | 848.7590 |
| 901.2277 | 935.1866 | 956.9060 |
| 1008.8794 | 1040.1761 | 1060.9427 |
| 1107.6900 | 1142.3170 | 1154.2638 |

| | | |
|-----------|-----------|-----------|
| 1200.8135 | 1225.6823 | 1279.6481 |
| 1293.6458 | 1370.5887 | 1378.5701 |
| 1396.2451 | 1400.7839 | 1408.8932 |
| 1422.3589 | 1440.7118 | 1475.4778 |
| 1485.3060 | 1490.1239 | 1494.7100 |
| 1501.7473 | 1519.6586 | 2942.0436 |
| 2963.0922 | 2966.9189 | 3022.7933 |
| 3032.0491 | 3063.0791 | 3067.2721 |
| 3069.4208 | 3076.2312 | 3079.1131 |
| 3115.1147 | 3154.4582 | 3596.2030 |

Zero-point correction (Hartree): 0.180401

C6H130.pmpm

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -311.63408912

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 1.110235 | -1.689719 | -0.305450 |
| C | 1.918844 | -0.753344 | 0.285865 |
| C | 1.788494 | 0.680637 | -0.248545 |
| C | 0.547939 | 1.466526 | 0.215373 |
| C | -0.820893 | 0.994152 | -0.315163 |
| C | -1.454389 | -0.190010 | 0.429663 |
| C | -2.845262 | -0.546437 | -0.104333 |
| H | 1.848846 | -0.788433 | 1.390159 |
| H | 2.941923 | -1.126608 | 0.057172 |
| H | 2.682753 | 1.233237 | 0.069548 |
| H | 1.815599 | 0.636144 | -1.344550 |
| H | 0.524167 | 1.490925 | 1.314778 |
| H | 0.696686 | 2.507092 | -0.099427 |
| H | -1.518745 | 1.840867 | -0.257957 |
| H | -0.732968 | 0.749216 | -1.382653 |
| H | -0.809558 | -1.075023 | 0.355162 |
| H | -1.522325 | 0.054459 | 1.499169 |
| H | -2.800386 | -0.832608 | -1.161223 |
| H | -3.532992 | 0.303778 | -0.021314 |
| H | -3.283283 | -1.384437 | 0.447576 |

Rotational constants (GHz): 3.6489700 1.5993000 1.2119000

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 48.9808 | 84.6731 | 113.8136 |
| 154.1965 | 242.0058 | 245.9607 |
| 311.6158 | 328.0313 | 440.4379 |
| 474.8566 | 727.9684 | 763.6868 |
| 776.8707 | 851.8218 | 881.5901 |
| 922.6955 | 965.7486 | 978.1254 |
| 1043.5945 | 1075.0199 | 1090.2500 |
| 1108.2220 | 1125.2742 | 1178.0761 |
| 1220.4888 | 1277.6499 | 1287.7497 |
| 1340.8696 | 1344.1006 | 1348.5677 |
| 1381.3195 | 1393.3812 | 1404.5365 |
| 1412.5329 | 1425.1116 | 1480.7190 |
| 1494.5281 | 1498.9315 | 1504.9348 |
| 1512.3218 | 1519.5445 | 2882.5905 |
| 2946.1056 | 3012.3555 | 3018.6525 |
| 3021.8063 | 3030.6413 | 3036.4354 |
| 3043.3102 | 3062.3843 | 3065.9186 |
| 3080.7801 | 3103.7863 | 3112.8799 |

Zero-point correction (Hartree): 0.180427

C6H130.pmtm

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -311.63622277

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 2.034068 | -1.362813 | -0.301965 |
| C | 2.248197 | -0.260851 | 0.481965 |
| C | 1.572515 | 1.032059 | -0.004944 |
| C | 0.044519 | 1.017705 | 0.160232 |
| C | -0.674745 | -0.014595 | -0.718763 |
| C | -2.206671 | -0.006330 | -0.580381 |
| C | -2.724526 | -0.463873 | 0.788821 |
| H | 2.023656 | -0.457412 | 1.548735 |
| H | 3.351409 | -0.121925 | 0.438689 |
| H | 1.993655 | 1.871374 | 0.563750 |
| H | 1.840715 | 1.185195 | -1.057549 |
| H | -0.193781 | 0.844848 | 1.218600 |
| H | -0.341272 | 2.019014 | -0.076228 |
| H | -0.408578 | 0.172368 | -1.767427 |
| H | -0.296258 | -1.021838 | -0.493263 |
| H | -2.584181 | 1.002945 | -0.796450 |
| H | -2.629042 | -0.659068 | -1.354670 |
| H | -2.397642 | 0.201006 | 1.595135 |
| H | -2.367790 | -1.472789 | 1.026422 |
| H | -3.819170 | -0.485909 | 0.808397 |

Rotational constants (GHz): 4.5534300 1.2314100 1.1342400

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 41.8106 | 91.1102 | 121.1475 |
| 135.0605 | 206.8131 | 278.5306 |
| 305.2669 | 332.2352 | 424.9557 |
| 498.0414 | 740.1648 | 777.7948 |
| 802.8856 | 842.3250 | 869.9873 |
| 918.0084 | 956.3639 | 987.8422 |
| 1025.7333 | 1073.9403 | 1090.8732 |
| 1097.7834 | 1115.1867 | 1161.6183 |
| 1195.2702 | 1255.6011 | 1305.2909 |
| 1321.7144 | 1334.1324 | 1352.8387 |
| 1373.7062 | 1383.9502 | 1405.9778 |
| 1413.6637 | 1427.6705 | 1485.4249 |
| 1489.5333 | 1501.5616 | 1507.2258 |
| 1513.8350 | 1521.5956 | 2881.2705 |
| 2939.6743 | 3014.1612 | 3022.2707 |
| 3026.3140 | 3036.0622 | 3041.5873 |
| 3048.7210 | 3062.6629 | 3070.5595 |
| 3086.3258 | 3109.4457 | 3114.3692 |

Zero-point correction (Hartree): 0.180289

C6H13O.pmtp

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -311.63624678
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 2.309599 | -1.215270 | -0.217547 |
| C | 2.432064 | 0.048731 | 0.294450 |
| C | 1.429390 | 1.077080 | -0.258205 |
| C | -0.007457 | 0.849616 | 0.237770 |
| C | -0.642262 | -0.460444 | -0.248003 |
| C | -2.048728 | -0.729893 | 0.312566 |
| C | -3.120591 | 0.264488 | -0.151170 |
| H | 2.445021 | 0.054298 | 1.401865 |
| H | 3.455904 | 0.356718 | -0.013209 |
| H | 1.766598 | 2.077278 | 0.043339 |
| H | 1.465241 | 1.038090 | -1.353772 |
| H | -0.014036 | 0.870732 | 1.337940 |
| H | -0.619614 | 1.701371 | -0.083756 |
| | | | |
| H | -0.680723 | -0.457047 | -1.346481 |
| H | 0.013534 | -1.299562 | 0.021453 |
| H | -2.352563 | -1.742204 | 0.017822 |
| H | -2.005379 | -0.735428 | 1.410568 |
| H | -3.185215 | 0.291627 | -1.245288 |
| H | -2.912322 | 1.282822 | 0.193132 |
| H | -4.107735 | -0.014001 | 0.232315 |

Rotational constants (GHz): 5.6871700 1.1515100 1.0217700

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 48.2574 | 95.1410 | 120.9395 |
| 132.3144 | 213.8437 | 285.9035 |
| 289.8468 | 344.9496 | 432.4873 |
| 490.1630 | 743.2245 | 767.0804 |
| 813.6638 | 837.1382 | 888.5043 |
| 905.8123 | 966.3415 | 979.1764 |
| 1025.7658 | 1077.3396 | 1083.7042 |
| 1094.2968 | 1112.0615 | 1153.8348 |
| 1212.7320 | 1250.5536 | 1294.0822 |
| 1327.3804 | 1332.4837 | 1352.1922 |
| 1373.9403 | 1386.3933 | 1408.9828 |
| 1414.1981 | 1429.2742 | 1485.0372 |
| 1488.2170 | 1502.2448 | 1507.0378 |
| 1514.9775 | 1522.0660 | 2882.9060 |
| 2942.1265 | 3011.8589 | 3018.5164 |
| 3025.6417 | 3036.4244 | 3041.2838 |
| 3049.3725 | 3063.4846 | 3074.3875 |
| 3086.8251 | 3108.5304 | 3116.0257 |

Zero-point correction (Hartree): 0.180342

C6H13O.pmtt

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -311.63760269
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -1.854215 | 1.551891 | -0.061994 |
| C | -2.376612 | 0.344127 | 0.316684 |
| C | -1.744723 | -0.884000 | -0.359816 |
| C | -0.314261 | -1.171185 | 0.123211 |
| C | 0.710449 | -0.089439 | -0.239293 |
| C | 2.120714 | -0.393629 | 0.282862 |
| C | 3.145844 | 0.683062 | -0.086682 |
| H | -2.405504 | 0.228247 | 1.417860 |
| H | -3.442138 | 0.412190 | 0.003391 |
| H | -2.382112 | -1.753416 | -0.152494 |
| H | -1.755632 | -0.724029 | -1.444891 |

| | | | | |
|--|-----------|-----------|-----------|--|
| H | -0.326693 | -1.311686 | 1.214244 | |
| H | 0.010871 | -2.131717 | -0.299090 | |
| H | 0.740995 | 0.029667 | -1.331314 | |
| H | 0.378669 | 0.882303 | 0.153531 | |
| H | 2.085453 | -0.506315 | 1.375175 | |
| H | 2.451463 | -1.365012 | -0.110525 | |
| H | 2.859791 | 1.658740 | 0.322116 | |
| H | 3.229390 | 0.793792 | -1.173837 | |
| H | 4.140702 | 0.438499 | 0.299990 | |
| Rotational constants (GHz): | 4.7922800 | 1.1784400 | 1.0052200 | |
| Vibrational harmonic frequencies (cm-1): | | | | |
| 65.6832 | 79.9893 | | 111.6323 | |
| 135.9817 | 186.1244 | | 251.0175 | |
| 309.7666 | 370.2420 | | 395.7760 | |
| 475.3248 | 734.7896 | | 778.1345 | |
| 803.9876 | 845.3084 | | 884.5335 | |
| 927.4231 | 963.6170 | | 985.3541 | |
| 1041.2584 | 1068.5465 | | 1081.7615 | |
| 1098.9017 | 1115.6000 | | 1160.5502 | |
| 1218.4047 | 1255.8063 | | 1297.6940 | |
| 1320.8789 | 1335.4269 | | 1336.7007 | |
| 1373.1734 | 1382.3630 | | 1408.0316 | |
| 1415.4087 | 1427.8346 | | 1483.8825 | |
| 1490.1277 | 1499.3591 | | 1510.8056 | |
| 1513.5440 | 1523.8364 | | 2881.8544 | |
| 2940.3552 | 3010.3844 | | 3014.0455 | |
| 3024.1267 | 3034.2860 | | 3039.3233 | |
| 3039.9183 | 3051.7339 | | 3069.6931 | |
| 3086.3637 | 3108.2642 | | 3112.4088 | |
| Zero-point correction (Hartree): | 0.180151 | | | |

C6H13O.ppm

```

-----
E(UB+HF-LYP/6-31G(d,p)) (Hartree): -311.63334345
Electronic state : 2-A
Cartesian coordinates (Angs):
O      1.796190    -1.331911    -0.483650
C      1.725882    -0.456185     0.564293
C      1.368820     0.995469     0.196288
C      0.131386     1.163463    -0.703374
C     -1.240516     1.169460    -0.001898
C     -1.714755    -0.140283     0.653667
C     -1.820200    -1.331718    -0.305030
H      0.945891    -0.895607     1.223003
H      2.646162    -0.501450     1.178711
H      1.257410     1.572069     1.125101
H      2.240343     1.416193    -0.320764
H      0.228428     2.120503    -1.230365
H      0.164160     0.390827    -1.479724
H     -1.243222     1.963694     0.757829
H     -1.992810     1.465383    -0.746246
H     -1.061659    -0.400857     1.497906
H     -2.699329     0.045721     1.102490
H     -0.845774    -1.616589    -0.714487
H     -2.477520    -1.097139    -1.150651
H     -2.235292    -2.208695     0.202727
Rotational constants (GHz):      3.2322700      1.8107200      1.3801500
Vibrational harmonic frequencies (cm-1):
50.1279      83.7383      149.6756
203.4508     236.4279     263.9678
294.1709     387.4823     457.0028
518.6859     653.8820     747.8320
775.6564     834.7525     875.6290
888.7808     943.5741     997.9941
1021.3093    1081.9923    1087.5711
1114.3448    1123.5806    1173.2981
1203.0513    1273.1615    1299.2274
1306.7456    1337.4377    1366.3541
1374.7482    1393.5392    1400.6061
1411.2852    1434.0583    1491.6014
1498.3540    1506.8368    1508.9941
1518.1408    1530.2358    2897.3117
2939.4248    3015.7629    3023.3555
3029.2386    3040.5793    3045.6222
3050.5515    3060.3536    3072.4962
3091.6933    3107.4565    3118.9432
Zero-point correction (Hartree): 0.180686

```

C6H13O.pmp

```

-----
E(UB+HF-LYP/6-31G(d,p)) (Hartree): -311.62971361
Electronic state : 2-A
Cartesian coordinates (Angs):
O      2.407757    -0.556217    -0.865567
C      1.631192    -0.783364     0.237949

```

| | | | |
|---|-----------|-----------|-----------|
| C | 1.065685 | 0.482511 | 0.906411 |
| C | 0.247538 | 1.388019 | -0.034519 |
| C | -1.273085 | 1.151978 | -0.118054 |
| C | -1.759441 | -0.207656 | -0.668621 |
| C | -1.979910 | -1.295903 | 0.391532 |
| H | -1.069177 | -1.533888 | 0.950622 |
| H | 2.159294 | -1.429127 | 0.966180 |
| H | 0.479102 | 0.189813 | 1.787186 |
| H | 1.926385 | 1.045029 | 1.288226 |
| H | 0.393714 | 2.429013 | 0.278387 |
| H | 0.689841 | 1.316270 | -1.036667 |
| H | -1.720887 | 1.316259 | 0.872758 |
| H | -1.677176 | 1.946276 | -0.758265 |
| H | -2.713506 | -0.052436 | -1.187495 |
| H | -1.062813 | -0.563846 | -1.439501 |
| H | -2.730350 | -0.975472 | 1.123054 |
| H | 0.809508 | -1.426118 | -0.144295 |
| H | -2.337873 | -2.225547 | -0.063845 |
| Rotational constants (GHz): | 3.4699400 | 1.5566200 | 1.3200100 |
| Vibrational harmonic frequencies (cm ⁻¹): | | | |
| 52.5972 | 101.8283 | 132.8740 | |
| 145.6050 | 209.2627 | 262.9131 | |
| 289.3368 | 357.5806 | 443.1119 | |
| 489.3059 | 676.5751 | 745.8632 | |
| 789.4569 | 839.8200 | 870.2085 | |
| 887.1227 | 951.9977 | 996.6568 | |
| 1035.3118 | 1080.2702 | 1092.6612 | |
| 1111.0856 | 1131.6188 | 1155.1817 | |
| 1213.5857 | 1287.5537 | 1287.9309 | |
| 1319.5259 | 1330.1414 | 1369.2348 | |
| 1379.1104 | 1387.0062 | 1398.2026 | |
| 1412.6344 | 1429.7139 | 1492.2122 | |
| 1500.0877 | 1506.2014 | 1509.3548 | |
| 1513.1895 | 1520.6069 | 2905.1314 | |
| 2941.3890 | 3018.1675 | 3030.2339 | |
| 3034.7576 | 3038.3553 | 3043.6793 | |
| 3059.5949 | 3066.0195 | 3076.7793 | |
| 3078.0391 | 3109.3174 | 3115.0793 | |
| Zero-point correction (Hartree): | 0.180479 | | |

C6H13O.ppmf

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -311.63418517
Electronic state : 2-A
Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 2.514836 | -0.916471 | -0.738200 |
| C | 1.896141 | -0.698191 | 0.462073 |
| C | 1.360241 | 0.729156 | 0.670700 |
| C | 0.382885 | 1.208811 | -0.419977 |
| C | -1.109711 | 0.951693 | -0.148743 |
| C | -1.537476 | -0.519545 | -0.049211 |
| C | -3.054600 | -0.687574 | 0.089208 |
| H | 1.062548 | -1.433192 | 0.470691 |
| H | 2.543145 | -1.018173 | 1.302068 |
| H | 0.897882 | 0.789378 | 1.665704 |
| H | 2.231869 | 1.394087 | 0.698609 |
| H | 0.514375 | 2.288553 | -0.557802 |
| H | 0.679987 | 0.747838 | -1.370969 |
| H | -1.401555 | 1.470364 | 0.776185 |
| H | -1.689273 | 1.426099 | -0.952730 |
| H | -1.187694 | -1.061773 | -0.938306 |
| H | -1.050142 | -0.993764 | 0.813432 |
| H | -3.578528 | -0.267281 | -0.776733 |
| H | -3.429504 | -0.174000 | 0.981983 |
| H | -3.336676 | -1.742471 | 0.169171 |
| Rotational constants (GHz): | 4.3923900 | 1.2276000 | 1.0878400 |
| Vibrational harmonic frequencies (cm ⁻¹): | | | |
| 48.8133 | 99.0734 | 122.1229 | |
| 150.4463 | 230.9344 | 250.8362 | |
| 281.0986 | 335.0077 | 456.6773 | |
| 500.3131 | 675.8657 | 753.0864 | |
| 787.2659 | 842.1383 | 882.9970 | |
| 898.7512 | 948.8828 | 1004.2285 | |
| 1031.3228 | 1071.8904 | 1088.8810 | |
| 1108.9167 | 1126.2721 | 1166.2571 | |
| 1225.0801 | 1286.2399 | 1291.3081 | |
| 1321.0496 | 1337.7802 | 1346.1863 | |
| 1368.2986 | 1382.4879 | 1403.5976 | |
| 1413.5828 | 1427.9493 | 1491.1456 | |
| 1500.7611 | 1507.0368 | 1510.0129 | |
| 1514.0546 | 1524.0011 | 2901.7374 | |
| 2939.8910 | 3012.4347 | 3024.2329 | |
| 3031.9581 | 3036.1730 | 3039.6861 | |
| 3045.9477 | 3064.8106 | 3076.6912 | |

3079.7580 3108.1637 3113.5511
 Zero-point correction (Hartree): 0.180403

C6H13O.pppm

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -311.63200558

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -2.652607 | 0.188240 | -0.744553 |
| C | -1.725088 | 0.829039 | 0.032275 |
| C | -0.954396 | -0.074286 | 1.007299 |
| C | -0.242610 | -1.256153 | 0.331704 |
| C | 0.908672 | -0.929548 | -0.639616 |
| C | 2.155772 | -0.256259 | -0.024582 |
| C | 2.138924 | 1.278594 | -0.019797 |
| H | -1.027162 | 1.286622 | -0.703405 |
| H | -2.175356 | 1.700272 | 0.546324 |
| H | -0.251320 | 0.544556 | 1.578208 |
| H | -1.674717 | -0.466221 | 1.736567 |
| H | 0.143488 | -1.921592 | 1.115006 |
| H | -1.001869 | -1.829268 | -0.213341 |
| H | 1.214858 | -1.880426 | -1.092945 |
| H | 0.540045 | -0.318314 | -1.475117 |
| H | 2.303372 | -0.628675 | 0.998480 |
| H | 3.040402 | -0.579460 | -0.587322 |
| H | 1.317661 | 1.686948 | 0.577247 |
| H | 2.032941 | 1.670021 | -1.038372 |
| H | 3.070862 | 1.681296 | 0.391395 |

Rotational constants (GHz): 4.0484700 1.3930100 1.2468200

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 47.2585 | 57.3267 | 112.8813 |
| 193.5210 | 220.8866 | 230.4761 |
| 336.5479 | 355.8904 | 447.9517 |
| 526.2306 | 632.8710 | 739.7018 |
| 772.7789 | 811.1272 | 876.1518 |
| 900.1699 | 955.7322 | 998.3256 |
| 1040.0131 | 1068.6428 | 1087.2348 |
| 1102.1114 | 1135.4687 | 1158.1488 |
| 1217.6513 | 1253.7333 | 1303.5100 |
| 1322.2120 | 1336.6031 | 1371.1497 |
| 1375.4267 | 1387.3278 | 1400.7172 |
| 1414.7069 | 1426.7487 | 1492.3138 |
| 1496.1174 | 1504.9873 | 1506.7457 |
| 1517.2359 | 1521.8604 | 2890.9911 |
| 2941.0601 | 3026.2440 | 3027.4443 |
| 3032.5557 | 3042.0589 | 3045.4931 |
| 3061.7745 | 3067.8714 | 3075.6814 |
| 3087.3069 | 3106.7461 | 3121.6693 |

Zero-point correction (Hartree): 0.180393

C6H13O.pppp

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -311.63477051

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -2.859069 | -0.528921 | 0.049133 |
| C | -1.994718 | 0.237146 | -0.686155 |
| C | -0.936109 | 0.995675 | 0.128656 |
| C | -0.085252 | 0.097740 | 1.041050 |
| C | 0.765818 | -0.967823 | 0.325258 |
| C | 1.799652 | -0.437900 | -0.684167 |
| C | 2.862737 | 0.484769 | -0.077167 |
| H | -1.505913 | -0.489072 | -1.372583 |
| H | -2.548442 | 0.911665 | -1.367803 |
| H | -0.306355 | 1.564525 | -0.567646 |
| H | -1.458004 | 1.737186 | 0.746178 |
| H | 0.566044 | 0.737183 | 1.648898 |
| H | -0.758758 | -0.408007 | 1.742056 |
| H | 1.291567 | -1.553802 | 1.091188 |
| H | 0.105779 | -1.681183 | -0.185184 |
| H | 2.297969 | -1.298348 | -1.148757 |
| H | 1.290182 | 0.085676 | -1.504406 |
| H | 3.412637 | -0.022077 | 0.724433 |
| H | 2.422353 | 1.392399 | 0.348540 |
| H | 3.590723 | 0.797592 | -0.832830 |

Rotational constants (GHz): 5.4422200 1.1849600 1.1635300

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 36.5743 | 60.0496 | 118.6673 |
| 186.5574 | 222.2435 | 284.9586 |
| 316.8123 | 392.2796 | 460.0177 |
| 546.0268 | 613.9743 | 727.8047 |
| 772.4089 | 822.2752 | 879.6294 |
| 893.7503 | 960.6121 | 991.2718 |
| 1028.3179 | 1071.0174 | 1080.8800 |
| 1097.0671 | 1130.4014 | 1176.6795 |

| | | |
|-----------|-----------|-----------|
| 1203.9678 | 1260.0304 | 1301.0668 |
| 1310.5180 | 1340.6736 | 1370.1673 |
| 1376.9975 | 1388.1351 | 1403.6810 |
| 1413.8206 | 1432.7116 | 1488.5216 |
| 1498.8431 | 1507.5246 | 1511.0434 |
| 1519.8371 | 1524.9725 | 2890.4171 |
| 2940.1146 | 3027.6245 | 3029.7161 |
| 3038.6994 | 3042.4958 | 3051.0720 |
| 3060.4336 | 3068.0351 | 3078.6363 |
| 3092.8951 | 3109.8134 | 3116.3850 |

Zero-point correction (Hartree): 0.180588

C6H130.pppt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -311.63611600

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 2.837556 | -0.597175 | -0.655109 |
| C | 2.029890 | -0.679758 | 0.447352 |
| C | 1.240583 | 0.597062 | 0.775719 |
| C | 0.351084 | 1.087306 | -0.377912 |
| C | -0.870644 | 0.208825 | -0.700109 |
| C | -1.938597 | 0.156509 | 0.402002 |
| C | -3.168237 | -0.666842 | 0.004128 |
| H | 1.333543 | -1.514640 | 0.210716 |
| H | 2.597142 | -1.049914 | 1.323230 |
| H | 0.652828 | 0.418323 | 1.685122 |
| H | 1.965821 | 1.380272 | 1.028399 |
| H | 0.005137 | 2.103914 | -0.149978 |
| H | 0.980771 | 1.167595 | -1.271632 |
| H | -1.334465 | 0.590402 | -1.619551 |
| H | -0.548104 | -0.814455 | -0.940390 |
| H | -1.510209 | -0.260475 | 1.322781 |
| H | -2.248254 | 1.181143 | 0.650103 |
| H | -2.895419 | -1.704497 | -0.220367 |
| H | -3.649099 | -0.253172 | -0.889616 |
| H | -3.914618 | -0.685706 | 0.804982 |

Rotational constants (GHz): 5.3974400 1.0675700 1.0395900

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 28.6672 | 78.0256 | 102.7500 |
| 187.5220 | 225.1406 | 253.4346 |
| 284.1272 | 355.9525 | 456.4316 |
| 528.5627 | 624.5912 | 730.6827 |
| 786.3913 | 824.0719 | 887.3881 |
| 898.3579 | 949.9435 | 1007.2844 |
| 1041.1479 | 1068.5878 | 1075.0714 |
| 1104.4062 | 1122.7119 | 1177.0548 |
| 1217.5144 | 1264.4121 | 1310.4931 |
| 1315.6499 | 1337.9080 | 1348.3710 |
| 1372.7683 | 1387.6792 | 1407.0738 |
| 1416.4988 | 1429.3068 | 1496.9878 |
| 1498.1426 | 1502.8778 | 1509.6290 |
| 1514.1291 | 1524.2388 | 2886.0933 |
| 2941.5822 | 3018.6417 | 3027.2714 |
| 3034.6580 | 3039.4015 | 3041.8882 |
| 3050.4869 | 3067.9433 | 3079.2929 |
| 3087.8899 | 3107.1198 | 3113.0558 |

Zero-point correction (Hartree): 0.180311

C6H130.pptm

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -311.63600888

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 2.703726 | -0.873925 | -0.679106 |
| C | 2.413874 | -0.068449 | 0.389126 |
| C | 1.380324 | 1.034906 | 0.112538 |
| C | 0.030020 | 0.507825 | -0.395628 |
| C | -0.820447 | -0.184661 | 0.680069 |
| C | -2.142012 | -0.776346 | 0.160886 |
| C | -3.146826 | 0.262306 | -0.352359 |
| H | 2.032739 | -0.771265 | 1.162868 |
| H | 3.340921 | 0.338814 | 0.837072 |
| H | 1.245144 | 1.624130 | 1.030121 |
| H | 1.813642 | 1.714478 | -0.631539 |
| H | -0.532863 | 1.345340 | -0.823548 |
| H | 0.222962 | -0.190628 | -1.220063 |
| H | -0.240720 | -0.995503 | 1.141628 |
| H | -1.036259 | 0.531026 | 1.486889 |
| H | -1.922280 | -1.498072 | -0.637539 |
| H | -2.609003 | -1.352542 | 0.969832 |
| H | -2.765455 | 0.806078 | -1.222545 |
| H | -3.382241 | 1.000709 | 0.423301 |
| H | -4.085993 | -0.214646 | -0.651419 |

Rotational constants (GHz): 6.0861200 1.0299900 0.9876500

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 43.8475 | 66.0785 | 113.1344 |
| 169.2646 | 222.6973 | 235.4806 |
| 291.3710 | 356.3496 | 458.9622 |
| 512.2684 | 632.6819 | 736.6404 |
| 775.9650 | 856.4078 | 862.4944 |
| 898.1759 | 956.7087 | 993.3118 |
| 1037.2698 | 1075.5146 | 1085.9750 |
| 1101.8452 | 1121.4959 | 1167.4926 |
| 1219.9264 | 1275.0603 | 1295.5636 |
| 1324.0778 | 1340.4924 | 1351.9109 |
| 1372.5413 | 1387.3783 | 1399.1050 |
| 1412.0688 | 1430.0312 | 1492.8160 |
| 1495.3788 | 1502.6992 | 1508.5717 |
| 1517.3901 | 1522.3087 | 2886.5865 |
| 2941.9114 | 3013.2161 | 3027.1326 |
| 3032.0999 | 3041.0847 | 3043.6624 |
| 3050.3625 | 3063.7940 | 3076.8153 |
| 3088.1683 | 3108.5022 | 3118.1433 |

Zero-point correction (Hartree): 0.180226

C6H130.pptp

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -311.63617269

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 2.301124 | 1.378446 | 0.062547 |
| C | 2.279392 | 0.113447 | -0.460316 |
| C | 1.529385 | -0.929347 | 0.383754 |
| C | 0.066491 | -0.559928 | 0.669733 |
| C | -0.858664 | -0.661228 | -0.552584 |
| C | -2.341188 | -0.388465 | -0.247056 |
| C | -2.643482 | 1.047976 | 0.196051 |
| H | 1.785319 | 0.237081 | -1.449417 |
| H | 3.302601 | -0.222982 | -0.716844 |
| H | 1.589833 | -1.899680 | -0.128543 |
| H | 2.071763 | -1.042692 | 1.330452 |
| H | -0.317940 | -1.219762 | 1.458657 |
| H | 0.048601 | 0.456936 | 1.077936 |
| H | -0.527316 | 0.037022 | -1.334390 |
| H | -0.765939 | -1.667832 | -0.983850 |
| H | -2.931279 | -0.616749 | -1.143882 |
| H | -2.683007 | -1.089747 | 0.526771 |
| H | -2.314811 | 1.771269 | -0.559363 |
| H | -2.140659 | 1.300911 | 1.134846 |
| H | -3.717764 | 1.193927 | 0.349767 |

Rotational constants (GHz): 4.5858400 1.1921200 1.0590100

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 42.8414 | 63.4974 | 126.3400 |
| 167.8645 | 223.7733 | 243.5944 |
| 295.2964 | 350.3655 | 456.1641 |
| 520.9230 | 629.1252 | 747.4124 |
| 784.9416 | 835.5746 | 866.6470 |
| 905.9760 | 951.4880 | 1002.4549 |
| 1035.1112 | 1080.0188 | 1085.6104 |
| 1103.8336 | 1118.6665 | 1169.7444 |
| 1218.7293 | 1273.4110 | 1306.9669 |
| 1315.6517 | 1342.2409 | 1354.2488 |
| 1372.7381 | 1387.7695 | 1398.0470 |
| 1414.0959 | 1433.2744 | 1493.5008 |
| 1497.5438 | 1502.2276 | 1509.5053 |
| 1517.1234 | 1522.5689 | 2888.4287 |
| 2941.7679 | 3013.7894 | 3024.3299 |
| 3030.6514 | 3037.6805 | 3043.3711 |
| 3050.7737 | 3062.3742 | 3075.5808 |
| 3091.9497 | 3109.5302 | 3119.8169 |

Zero-point correction (Hartree): 0.180333

C6H130.pptt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -311.63746364

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 2.612572 | -1.087826 | -0.612083 |
| C | 2.317953 | -0.383436 | 0.524058 |
| C | 1.596628 | 0.954438 | 0.295421 |
| C | 0.279388 | 0.824029 | -0.482660 |
| C | -0.865417 | 0.172240 | 0.305355 |
| C | -2.175595 | 0.091388 | -0.489088 |
| C | -3.319617 | -0.560311 | 0.293884 |
| H | 1.673672 | -1.074132 | 1.112090 |
| H | 3.219282 | -0.262286 | 1.155598 |
| H | 1.423503 | 1.427535 | 1.271896 |
| H | 2.282615 | 1.612349 | -0.252096 |
| H | -0.038984 | 1.822243 | -0.809776 |

| | | | |
|--|-----------|-----------|-----------|
| H | 0.475913 | 0.246986 | -1.394916 |
| H | -0.579968 | -0.842299 | 0.617722 |
| H | -1.038736 | 0.738035 | 1.232544 |
| H | -2.471953 | 1.103157 | -0.797925 |
| H | -1.999463 | -0.469121 | -1.416989 |
| H | -3.538503 | -0.004657 | 1.213094 |
| H | -3.068216 | -1.587565 | 0.581906 |
| H | -4.239783 | -0.597723 | -0.298300 |
| Rotational constants (GHz): | 5.6037700 | 0.9973900 | 0.9458000 |
| Vibrational harmonic frequencies (cm-1): | | | |
| 48.6237 | 70.6149 | | 115.0886 |
| 148.2356 | 209.2564 | | 246.2375 |
| 263.8534 | 394.7193 | | 404.6419 |
| 514.2544 | 632.7756 | | 735.9580 |
| 782.3655 | 853.9578 | | 869.5263 |
| 915.7593 | 946.2824 | | 1018.8640 |
| 1040.1536 | 1062.8269 | | 1089.6276 |
| 1100.7315 | 1121.7087 | | 1171.3728 |
| 1234.0460 | 1272.7540 | | 1295.9491 |
| 1321.5277 | 1337.5931 | | 1338.7015 |
| 1373.0912 | 1382.0081 | | 1401.1619 |
| 1414.8744 | 1427.6945 | | 1493.6329 |
| 1498.3466 | 1500.7606 | | 1512.1818 |
| 1513.4671 | 1524.4388 | | 2887.9627 |
| 2941.7226 | 3010.2012 | | 3025.8228 |
| 3031.7437 | 3036.4190 | | 3038.4076 |
| 3040.7112 | 3062.2406 | | 3076.2791 |
| 3084.2412 | 3106.0552 | | 3112.4853 |
| Zero-point correction (Hartree): | 0.180098 | | |

C6H13O.ptmm

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -311.63606502
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | |
|--|-----------|-----------|-----------|
| O | 3.147093 | 0.323055 | -0.314421 |
| C | 2.331166 | -0.690944 | 0.112901 |
| C | 0.943051 | -0.257770 | 0.601994 |
| C | 0.140941 | 0.474144 | -0.480966 |
| C | -1.168659 | 1.109545 | 0.014114 |
| C | -2.224521 | 0.132953 | 0.562048 |
| C | -2.750645 | -0.873089 | -0.468694 |
| H | 2.234606 | -1.365398 | -0.767372 |
| H | 2.861317 | -1.312616 | 0.860903 |
| H | 0.409510 | -1.148641 | 0.957758 |
| H | 1.075060 | 0.396818 | 1.473948 |
| H | 0.781485 | 1.260537 | -0.897227 |
| H | -0.066037 | -0.218586 | -1.308483 |
| H | -0.928581 | 1.843539 | 0.795413 |
| H | -1.613961 | 1.680778 | -0.811829 |
| H | -1.818626 | -0.407962 | 1.426866 |
| H | -3.067363 | 0.720151 | 0.948328 |
| H | -1.963180 | -1.546353 | -0.823820 |
| H | -3.164584 | -0.360125 | -1.344714 |
| H | -3.544379 | -1.495609 | -0.042784 |
| Rotational constants (GHz): | 6.1249200 | 1.0365000 | 0.9869300 |
| Vibrational harmonic frequencies (cm-1): | | | |
| 53.6258 | 60.8268 | | 123.1298 |
| 165.0976 | 231.2751 | | 245.1726 |
| 270.3375 | 369.4862 | | 465.4727 |
| 509.2666 | 545.2253 | | 732.1056 |
| 783.7988 | 835.8451 | | 851.5450 |
| 915.6314 | 958.8822 | | 987.3917 |
| 1028.1275 | 1059.1827 | | 1090.9903 |
| 1104.1549 | 1128.6194 | | 1181.3381 |
| 1220.5475 | 1266.3734 | | 1303.3621 |
| 1326.5646 | 1339.2764 | | 1363.0540 |
| 1366.7779 | 1387.1661 | | 1397.1031 |
| 1417.7558 | 1427.9826 | | 1491.2551 |
| 1499.9969 | 1504.9303 | | 1510.1889 |
| 1517.1254 | 1524.4446 | | 2880.7387 |
| 2936.4348 | 3021.3518 | | 3024.7249 |
| 3032.6021 | 3036.0451 | | 3041.1125 |
| 3058.3369 | 3066.5278 | | 3069.5403 |
| 3086.8047 | 3108.6451 | | 3113.2442 |
| Zero-point correction (Hartree): | 0.180058 | | |

C6H13O.ptmp

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -311.63345248
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -3.117797 | 0.246009 | -0.393002 |
| C | -2.322018 | -0.625437 | 0.302078 |

| | | | |
|--|-----------|-----------|-----------|
| C | -0.824031 | -0.556456 | -0.028095 |
| C | -0.234938 | 0.834366 | 0.239353 |
| C | 1.182256 | 1.098522 | -0.297707 |
| C | 2.332011 | 0.301033 | 0.353499 |
| C | 2.589812 | -1.092221 | -0.236121 |
| H | -2.487919 | -0.361967 | 1.370964 |
| H | -2.719691 | -1.655703 | 0.219696 |
| H | -0.311132 | -1.328110 | 0.558639 |
| H | -0.692744 | -0.823950 | -1.084729 |
| H | -0.917443 | 1.566967 | -0.208707 |
| H | -0.248197 | 1.027080 | 1.322479 |
| H | 1.197122 | 0.935037 | -1.384836 |
| H | 1.384331 | 2.167794 | -0.155844 |
| H | 3.255722 | 0.884832 | 0.252491 |
| H | 2.150042 | 0.219619 | 1.434264 |
| H | 2.800311 | -1.027616 | -1.309943 |
| H | 1.738100 | -1.766459 | -0.109771 |
| H | 3.455325 | -1.564440 | 0.241272 |
| Rotational constants (GHz): | 5.7304800 | 1.0838100 | 0.9768900 |
| Vibrational harmonic frequencies (cm-1): | | | |
| 38.7569 | 59.0793 | | 117.8177 |
| 154.2392 | 216.7295 | | 230.5116 |
| 280.2630 | 356.2655 | | 449.0307 |
| 518.1569 | 583.1311 | | 755.1678 |
| 777.2607 | 803.1925 | | 878.6216 |
| 923.8131 | 955.3304 | | 995.6490 |
| 1031.7292 | 1067.5569 | | 1088.5909 |
| 1100.8108 | 1127.4407 | | 1188.4039 |
| 1227.4679 | 1260.2760 | | 1307.7351 |
| 1328.5798 | 1336.6000 | | 1365.9606 |
| 1369.5670 | 1383.8501 | | 1394.4904 |
| 1419.9026 | 1429.8372 | | 1490.3251 |
| 1499.1716 | 1503.4956 | | 1509.8581 |
| 1515.0437 | 1522.3483 | | 2879.1813 |
| 2939.7790 | 3013.2281 | | 3020.2436 |
| 3024.1856 | 3039.2536 | | 3044.7529 |
| 3059.8204 | 3063.5289 | | 3067.0416 |
| 3088.1029 | 3106.8036 | | 3127.9088 |
| Zero-point correction (Hartree): | 0.180057 | | |

C6H13O.ptmt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -311.63732950
Electronic state : 2-A
Cartesian coordinates (Angs):

| | | | |
|--|-----------|-----------|-----------|
| O | -3.267193 | 0.527434 | -0.230903 |
| C | -2.563312 | -0.591465 | 0.128517 |
| C | -1.077300 | -0.585945 | -0.252575 |
| C | -0.314960 | 0.589951 | 0.370810 |
| C | 1.131351 | 0.750857 | -0.120886 |
| C | 2.074866 | -0.397988 | 0.262960 |
| C | 3.519540 | -0.160152 | -0.188700 |
| H | -2.675260 | -0.652083 | 1.234347 |
| H | -3.083366 | -1.498760 | -0.236649 |
| H | -0.640846 | -1.546695 | 0.048655 |
| H | -1.003289 | -0.537361 | -1.347295 |
| H | -0.876473 | 1.505598 | 0.151025 |
| H | -0.316988 | 0.482882 | 1.465771 |
| H | 1.131331 | 0.869418 | -1.214077 |
| H | 1.537054 | 1.688301 | 0.283291 |
| H | 2.049451 | -0.534687 | 1.353206 |
| H | 1.712944 | -1.339591 | -0.169717 |
| H | 3.929011 | 0.753461 | 0.257473 |
| H | 3.580830 | -0.050042 | -1.277509 |
| H | 4.172027 | -0.991454 | 0.097947 |
| Rotational constants (GHz): | 8.9141600 | 0.8847800 | 0.8471100 |
| Vibrational harmonic frequencies (cm-1): | | | |
| 50.9541 | 80.9747 | | 97.9696 |
| 153.5425 | 239.2887 | | 244.7046 |
| 262.8867 | 300.8387 | | 455.1538 |
| 525.1654 | 573.3636 | | 737.2909 |
| 775.0535 | 838.6481 | | 868.3775 |
| 918.8443 | 956.1689 | | 1003.9880 |
| 1039.7593 | 1062.8741 | | 1084.4807 |
| 1099.2263 | 1127.4072 | | 1202.6114 |
| 1223.5700 | 1271.3104 | | 1315.5147 |
| 1321.1098 | 1342.2415 | | 1347.4169 |
| 1366.1198 | 1371.4673 | | 1409.7489 |
| 1417.6969 | 1427.6366 | | 1493.6390 |
| 1498.6248 | 1508.0415 | | 1512.0572 |
| 1513.5937 | 1523.6705 | | 2881.0952 |
| 2936.8596 | 3013.8746 | | 3015.6393 |
| 3026.3664 | 3034.7628 | | 3038.8151 |
| 3045.9502 | 3066.8578 | | 3070.1784 |
| 3086.3478 | 3106.9090 | | 3111.9534 |

Zero-point correction (Hartree): 0.179972

C6H13O.ptpm

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -311.63338358

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 2.472677 | 0.932788 | -0.723365 |
| C | 2.400086 | -0.002036 | 0.276304 |
| C | 0.982066 | -0.342996 | 0.749755 |
| C | 0.108791 | -0.921773 | -0.372259 |
| C | -1.377059 | -1.127031 | -0.002694 |
| C | -2.317345 | 0.034528 | -0.371639 |
| C | -2.022428 | 1.373383 | 0.314405 |
| H | 2.892377 | -0.905964 | -0.147961 |
| H | 3.062680 | 0.287552 | 1.115300 |
| H | 1.051858 | -1.057946 | 1.581160 |
| H | 0.532730 | 0.567341 | 1.161758 |
| H | 0.188394 | -0.266475 | -1.248951 |
| H | 0.542788 | -1.884224 | -0.676144 |
| H | -1.746966 | -2.024985 | -0.512864 |
| H | -1.462362 | -1.340134 | 1.072554 |
| H | -2.288602 | 0.176395 | -1.460671 |
| H | -3.345796 | -0.267825 | -0.134349 |
| H | -1.049650 | 1.777351 | 0.016620 |
| H | -2.024750 | 1.271706 | 1.406169 |
| H | -2.778778 | 2.120459 | 0.051066 |

Rotational constants (GHz): 4.2906900 1.2561100 1.1134100

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 36.1995 | 86.8160 | 126.6587 |
| 160.0255 | 233.7673 | 267.1698 |
| 305.4172 | 332.2779 | 434.7550 |
| 512.1776 | 558.9038 | 746.6430 |
| 788.8692 | 818.5919 | 864.3014 |
| 923.2326 | 947.2527 | 1004.5442 |
| 1030.4610 | 1073.3826 | 1089.4272 |
| 1110.0651 | 1135.5884 | 1169.1581 |
| 1226.3795 | 1273.4929 | 1307.5567 |
| 1327.3935 | 1332.3364 | 1364.9011 |
| 1366.5859 | 1389.5327 | 1392.9832 |
| 1413.1190 | 1432.8048 | 1496.0439 |
| 1499.6099 | 1504.1881 | 1516.1516 |
| 1519.4293 | 1527.3023 | 2878.9664 |
| 2937.7009 | 3018.5105 | 3024.3397 |
| 3025.3725 | 3036.0636 | 3040.0163 |
| 3059.0639 | 3066.2337 | 3070.7392 |
| 3096.9580 | 3106.0295 | 3118.4363 |

Zero-point correction (Hartree): 0.180258

C6H13O.ptpp

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -311.63594329

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 2.522871 | 1.169578 | -0.281952 |
| C | 2.443422 | -0.092266 | 0.246325 |
| C | 1.027042 | -0.579970 | 0.573121 |
| C | 0.120339 | -0.620793 | -0.662716 |
| C | -1.327703 | -1.057706 | -0.383080 |
| C | -2.150165 | -0.121505 | 0.520539 |
| C | -2.349591 | 1.288750 | -0.047019 |
| H | 2.915277 | -0.752833 | -0.515091 |
| H | 3.123764 | -0.174233 | 1.117073 |
| H | 1.094366 | -1.576403 | 1.031919 |
| H | 0.608390 | 0.087429 | 1.336027 |
| H | 0.137241 | 0.367554 | -1.136220 |
| H | 0.556637 | -1.313399 | -1.396348 |
| H | -1.849870 | -1.162162 | -1.343993 |
| H | -1.316201 | -2.061192 | 0.064880 |
| H | -3.132145 | -0.582978 | 0.685906 |
| H | -1.684612 | -0.053552 | 1.512309 |
| H | -2.814457 | 1.252481 | -1.039351 |
| H | -1.402076 | 1.828166 | -0.146196 |
| H | -2.999350 | 1.885436 | 0.601688 |

Rotational constants (GHz): 4.4608100 1.2139800 1.0760700

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 45.7235 | 54.5000 | 136.5972 |
| 162.2102 | 232.0197 | 261.2820 |
| 273.9264 | 366.3532 | 449.6555 |
| 456.8036 | 549.0942 | 732.7578 |
| 786.6012 | 836.0838 | 842.0616 |
| 924.3198 | 941.1106 | 1002.4013 |
| 1016.9045 | 1074.5294 | 1088.2775 |
| 1105.2025 | 1133.1567 | 1175.4196 |
| 1217.1394 | 1278.7540 | 1310.5093 |

| | | |
|-----------|-----------|-----------|
| 1319.3764 | 1342.0713 | 1361.5858 |
| 1372.2285 | 1388.5945 | 1397.2554 |
| 1418.3844 | 1430.3786 | 1493.2573 |
| 1499.3231 | 1505.8593 | 1511.1479 |
| 1518.8890 | 1527.1146 | 2882.4810 |
| 2932.8456 | 3016.0074 | 3025.8606 |
| 3031.1472 | 3035.6791 | 3041.6442 |
| 3053.5436 | 3065.7093 | 3076.6221 |
| 3090.4872 | 3108.6107 | 3117.4952 |

Zero-point correction (Hartree): 0.180014

C6H130.ptpt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -311.63707948

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -2.930391 | -0.827961 | -0.607573 |
| C | -2.620847 | 0.046197 | 0.401092 |
| C | -1.126722 | 0.187013 | 0.715527 |
| C | -0.314851 | 0.677088 | -0.489767 |
| C | 1.198292 | 0.790906 | -0.245224 |
| C | 1.919225 | -0.547594 | -0.028443 |
| C | 3.433725 | -0.387258 | 0.139942 |
| H | -3.041167 | 1.022933 | 0.072141 |
| H | -3.214402 | -0.200209 | 1.303681 |
| H | -1.009783 | 0.879036 | 1.561340 |
| H | -0.759435 | -0.788309 | 1.056398 |
| H | -0.504794 | 0.000906 | -1.332859 |
| H | -0.699364 | 1.660791 | -0.794560 |
| H | 1.654162 | 1.296866 | -1.107126 |
| H | 1.381541 | 1.445875 | 0.619202 |
| H | 1.510958 | -1.055187 | 0.854516 |
| H | 1.712144 | -1.208284 | -0.881336 |
| H | 3.671781 | 0.243826 | 1.004003 |
| H | 3.883206 | 0.081446 | -0.743082 |
| H | 3.925352 | -1.354110 | 0.289507 |

Rotational constants (GHz): 6.8739900 0.9272500 0.9051700

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 47.3746 | 69.8074 | 117.8184 |
| 141.1888 | 229.8875 | 244.4025 |
| 274.1969 | 294.9758 | 436.4755 |
| 466.8303 | 567.5925 | 739.0363 |
| 774.8886 | 835.9695 | 859.5038 |
| 917.4111 | 951.0069 | 1009.2013 |
| 1029.5753 | 1066.7573 | 1089.2974 |
| 1097.7557 | 1140.5649 | 1177.4127 |
| 1232.8933 | 1288.2755 | 1308.9931 |
| 1322.3669 | 1340.6641 | 1353.1105 |
| 1362.4553 | 1375.1905 | 1410.3278 |
| 1419.3650 | 1426.0566 | 1494.1319 |
| 1497.6637 | 1507.8732 | 1511.7418 |
| 1512.9684 | 1523.2753 | 2881.2789 |
| 2933.6200 | 3012.2090 | 3022.2195 |
| 3030.4686 | 3032.3081 | 3038.0942 |
| 3047.0378 | 3063.6281 | 3074.6855 |
| 3087.9796 | 3106.4159 | 3112.0342 |

Zero-point correction (Hartree): 0.179766

C6H130.pttm

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -311.63725655

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -2.698055 | 1.241585 | -0.151848 |
| C | -2.636216 | -0.077527 | 0.213006 |
| C | -1.384914 | -0.831574 | -0.252971 |
| C | -0.085532 | -0.212661 | 0.273575 |
| C | 1.175589 | -0.895824 | -0.271959 |
| C | 2.495914 | -0.334572 | 0.281697 |
| C | 2.790103 | 1.113295 | -0.129459 |
| H | -2.687073 | -0.066540 | 1.324944 |
| H | -3.569282 | -0.595016 | -0.085059 |
| H | -1.469031 | -1.880299 | 0.064062 |
| H | -1.376022 | -0.837807 | -1.350865 |
| H | -0.087730 | 0.852285 | 0.015343 |
| H | -0.078722 | -0.264280 | 1.372729 |
| H | 1.124454 | -1.969621 | -0.044504 |
| H | 1.182458 | -0.818489 | -1.368811 |
| H | 2.488245 | -0.409652 | 1.377905 |
| H | 3.318911 | -0.975674 | -0.059131 |
| H | 2.034198 | 1.807810 | 0.250556 |
| H | 2.813343 | 1.215196 | -1.220805 |
| H | 3.761027 | 1.442592 | 0.255080 |

Rotational constants (GHz): 5.4547500 1.0237400 0.9102800

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 55.8147 | 72.2230 | 126.7708 |
| 148.2198 | 173.2651 | 249.2744 |
| 304.8952 | 324.8252 | 453.5730 |
| 488.4018 | 528.1618 | 744.3243 |
| 778.0820 | 831.3783 | 887.2613 |
| 914.5538 | 952.5552 | 1000.1140 |
| 1021.0088 | 1080.1150 | 1088.9504 |
| 1095.5920 | 1130.1859 | 1198.9712 |
| 1216.4724 | 1275.5235 | 1311.8719 |
| 1320.9603 | 1337.4994 | 1359.2114 |
| 1365.3896 | 1387.2001 | 1392.4558 |
| 1418.8586 | 1429.1662 | 1494.6810 |
| 1497.9467 | 1502.7232 | 1515.6288 |
| 1519.6496 | 1522.3824 | 2881.0183 |
| 2935.5037 | 3011.4469 | 3017.6590 |
| 3025.1930 | 3030.0271 | 3042.0102 |
| 3051.5972 | 3062.6923 | 3066.9418 |
| 3091.3994 | 3108.9083 | 3118.0003 |

Zero-point correction (Hartree): 0.179881

C6H13O.pttp

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -311.63719559

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 2.904895 | -0.812161 | -0.702024 |
| C | 2.600148 | -0.111585 | 0.435362 |
| C | 1.354063 | 0.777468 | 0.347087 |
| C | 0.082303 | -0.009691 | 0.012210 |
| C | -1.149757 | 0.884394 | -0.180028 |
| C | -2.429247 | 0.133341 | -0.584726 |
| C | -2.969521 | -0.824341 | 0.484251 |
| H | 2.463517 | -0.889796 | 1.219435 |
| H | 3.489836 | 0.451238 | 0.780310 |
| H | 1.236232 | 1.311428 | 1.300193 |
| H | 1.530749 | 1.543603 | -0.419353 |
| H | 0.265287 | -0.589788 | -0.901285 |
| H | -0.104107 | -0.741466 | 0.810100 |
| H | -1.339474 | 1.448638 | 0.744886 |
| H | -0.922673 | 1.634119 | -0.950173 |
| H | -3.205416 | 0.870663 | -0.826326 |
| H | -2.240889 | -0.423504 | -1.512785 |
| H | -3.169442 | -0.294974 | 1.423453 |
| H | -2.263966 | -1.632260 | 0.703239 |
| H | -3.906750 | -1.288133 | 0.159556 |

Rotational constants (GHz): 6.0820200 0.9491500 0.9133400

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 50.3462 | 85.9592 | 119.0007 |
| 142.0751 | 178.2935 | 261.6228 |
| 310.8089 | 316.9347 | 454.3763 |
| 483.9594 | 528.8368 | 743.5291 |
| 776.3738 | 843.1582 | 874.1187 |
| 914.3742 | 961.8375 | 987.9584 |
| 1027.9682 | 1076.3698 | 1093.4323 |
| 1095.5163 | 1137.0201 | 1184.0251 |
| 1228.2193 | 1280.8125 | 1299.9494 |
| 1328.7977 | 1336.6076 | 1360.7348 |
| 1364.9491 | 1388.1645 | 1393.2026 |
| 1418.8072 | 1428.5464 | 1494.9848 |
| 1496.8090 | 1503.1961 | 1515.9627 |
| 1519.6532 | 1523.0407 | 2881.6728 |
| 2935.4148 | 3013.4027 | 3025.2002 |
| 3028.0853 | 3033.2712 | 3041.3027 |
| 3050.5381 | 3061.7525 | 3065.6344 |
| 3085.6607 | 3108.2143 | 3117.0826 |

Zero-point correction (Hartree): 0.179924

C6H13O.pttt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -311.63852343

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 3.080036 | -0.949569 | -0.384001 |
| C | 2.784387 | 0.241403 | 0.225213 |
| C | 1.405181 | 0.825372 | -0.103791 |
| C | 0.254234 | -0.111106 | 0.279091 |
| C | -1.125534 | 0.409623 | -0.139973 |
| C | -2.275711 | -0.529382 | 0.245851 |
| C | -3.651626 | -0.006581 | -0.179447 |
| H | 2.863646 | 0.030477 | 1.315267 |
| H | 3.598932 | 0.969513 | 0.041542 |
| H | 1.302337 | 1.791809 | 0.408820 |
| H | 1.369588 | 1.038107 | -1.180327 |
| H | 0.438092 | -1.090094 | -0.180863 |
| H | 0.266858 | -0.275516 | 1.366715 |

| | | | | |
|--|-----------|-----------|-----------|-----------|
| H | -1.297729 | 1.397445 | 0.311706 | |
| H | -1.137646 | 0.568819 | -1.227752 | |
| H | -2.102270 | -1.515670 | -0.205286 | |
| H | -2.264065 | -0.687527 | 1.332935 | |
| H | -3.705823 | 0.128365 | -1.265798 | |
| H | -3.867950 | 0.962960 | 0.283894 | |
| H | -4.449837 | -0.698113 | 0.109493 | |
| Rotational constants (GHz): | 8.7979300 | | 0.8308100 | 0.7965900 |
| Vibrational harmonic frequencies (cm-1): | | | | |
| 62.3274 | 79.7145 | | | 119.3926 |
| 143.4397 | 161.3491 | | | 246.2495 |
| 257.6238 | 356.7204 | | | 407.5949 |
| 469.1992 | 539.4219 | | | 738.6120 |
| 766.5946 | 846.0041 | | | 892.2991 |
| 921.7245 | 956.5111 | | | 1005.8808 |
| 1037.9693 | 1069.8700 | | | 1086.8161 |
| 1094.7561 | 1134.0905 | | | 1197.0368 |
| 1235.1481 | 1274.8811 | | | 1300.5123 |
| 1334.1860 | 1336.1429 | | | 1341.3080 |
| 1363.8929 | 1372.5946 | | | 1404.5670 |
| 1419.7811 | 1428.8686 | | | 1493.8634 |
| 1500.8375 | 1505.4818 | | | 1512.9132 |
| 1517.8216 | 1526.9816 | | | 2881.1208 |
| 2935.2145 | 3011.2074 | | | 3015.6931 |
| 3026.8203 | 3030.1911 | | | 3038.7619 |
| 3040.1656 | 3059.0291 | | | 3066.2277 |
| 3084.0833 | 3106.4839 | | | 3112.5109 |
| Zero-point correction (Hartree): | 0.179676 | | | |

C6H13O.tpmmm

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -311.63189751
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | | |
|--|-----------|-----------|-----------|-----------|
| O | -2.894334 | -0.849966 | -0.291938 | |
| C | -1.655889 | -0.537970 | 0.197873 | |
| C | -1.211581 | 0.914726 | -0.031529 | |
| C | 0.162005 | 1.280072 | 0.567228 | |
| C | 1.385621 | 1.040216 | -0.338835 | |
| C | 1.725186 | -0.415270 | -0.704775 | |
| C | 2.086241 | -1.303798 | 0.491696 | |
| H | -1.585429 | -0.818876 | 1.268910 | |
| H | -0.969978 | -1.254959 | -0.301318 | |
| H | -1.231050 | 1.123002 | -1.108556 | |
| H | -1.983315 | 1.551671 | 0.417023 | |
| H | 0.151558 | 2.347763 | 0.816513 | |
| H | 0.294065 | 0.762162 | 1.527603 | |
| H | 1.242153 | 1.610197 | -1.266787 | |
| H | 2.262989 | 1.482515 | 0.153113 | |
| H | 0.897427 | -0.866729 | -1.267604 | |
| H | 2.573193 | -0.399763 | -1.401322 | |
| H | 1.249165 | -1.418340 | 1.188397 | |
| H | 2.925488 | -0.879980 | 1.055175 | |
| H | 2.378904 | -2.306782 | 0.164399 | |
| Rotational constants (GHz): | 3.7205600 | | 1.3866400 | 1.1471200 |
| Vibrational harmonic frequencies (cm-1): | | | | |
| 54.0594 | 70.9497 | | | 99.0046 |
| 167.0211 | 210.8707 | | | 257.9712 |
| 291.9566 | 368.4821 | | | 424.8868 |
| 493.3725 | 543.8546 | | | 748.3334 |
| 761.4926 | 839.6408 | | | 867.0798 |
| 885.4647 | 961.6564 | | | 1007.6919 |
| 1034.7444 | 1068.6006 | | | 1083.5425 |
| 1104.3708 | 1126.0691 | | | 1183.9851 |
| 1222.1888 | 1274.9992 | | | 1295.9937 |
| 1319.6167 | 1342.0275 | | | 1370.2056 |
| 1372.4809 | 1391.7073 | | | 1398.2708 |
| 1402.4728 | 1427.4436 | | | 1492.8777 |
| 1500.1191 | 1505.1855 | | | 1507.2990 |
| 1516.6198 | 1522.5280 | | | 2903.6405 |
| 2921.5340 | 3020.3167 | | | 3027.3282 |
| 3033.8273 | 3042.1080 | | | 3042.9386 |
| 3057.2065 | 3066.1892 | | | 3072.0743 |
| 3086.5186 | 3110.3760 | | | 3115.0256 |
| Zero-point correction (Hartree): | 0.180012 | | | |

C6H13O.tpmmp

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -311.62894474
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | | |
|---|-----------|-----------|-----------|--|
| O | -2.734619 | -0.916750 | -0.060093 | |
| C | -1.694219 | -0.194100 | 0.454817 | |
| C | -1.031826 | 0.790375 | -0.521228 | |
| C | 0.167204 | 1.558191 | 0.074318 | |

| | | | |
|--|-----------|-----------|-----------|
| C | 1.570161 | 0.949141 | -0.121226 |
| C | 1.849020 | -0.427170 | 0.523869 |
| C | 1.552322 | -1.637707 | -0.372577 |
| H | -1.995836 | 0.312606 | 1.393977 |
| H | 0.504056 | -1.691186 | -0.681850 |
| H | -0.740743 | 0.250348 | -1.429508 |
| H | -1.807658 | 1.503330 | -0.824712 |
| H | 0.188079 | 2.561798 | -0.366909 |
| H | -0.005363 | 1.718029 | 1.149345 |
| H | 1.787932 | 0.889605 | -1.196852 |
| H | 2.286854 | 1.673646 | 0.285645 |
| H | 2.908760 | -0.471495 | 0.804027 |
| H | 1.295216 | -0.510407 | 1.469414 |
| H | 2.155656 | -1.596532 | -1.286508 |
| H | -0.968508 | -0.962337 | 0.797666 |
| H | 1.792544 | -2.575787 | 0.139172 |
| Rotational constants (GHz): | 3.3939200 | 1.5477100 | 1.1840900 |
| Vibrational harmonic frequencies (cm-1): | | | |
| 52.7789 | 78.5641 | | 101.5373 |
| 155.6124 | 216.3541 | | 265.6189 |
| 281.9084 | 349.0511 | | 411.8689 |
| 471.7329 | 557.7977 | | 745.0440 |
| 780.9406 | 821.4476 | | 865.8253 |
| 901.5820 | 956.6502 | | 1007.7464 |
| 1046.1660 | 1061.9805 | | 1082.5871 |
| 1120.5118 | 1128.8116 | | 1169.8572 |
| 1225.3935 | 1281.8338 | | 1290.5892 |
| 1316.2966 | 1338.3225 | | 1367.8694 |
| 1378.4148 | 1382.5350 | | 1394.6115 |
| 1400.9587 | 1432.0882 | | 1495.0203 |
| 1499.1633 | 1504.7229 | | 1507.2962 |
| 1515.1178 | 1522.3673 | | 2903.3704 |
| 2925.3944 | 3013.0794 | | 3022.5193 |
| 3025.0545 | 3045.3610 | | 3046.7919 |
| 3059.2496 | 3066.4902 | | 3069.9086 |
| 3092.5169 | 3109.6912 | | 3122.7947 |
| Zero-point correction (Hartree): | 0.179945 | | |

C6H13O.tpm

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -311.63336993

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|--|-----------|-----------|-----------|
| O | -2.973278 | -1.096177 | -0.224888 |
| C | -1.891882 | -0.492006 | 0.354435 |
| C | -1.349917 | 0.736174 | -0.392874 |
| C | -0.144773 | 1.420841 | 0.284687 |
| C | 1.247646 | 0.922544 | -0.141836 |
| C | 1.581431 | -0.536599 | 0.200098 |
| C | 3.031489 | -0.905333 | -0.132112 |
| H | -2.107963 | -0.254779 | 1.416441 |
| H | -1.125228 | -1.292949 | 0.423453 |
| H | -1.102058 | 0.443063 | -1.420605 |
| H | -2.179826 | 1.448537 | -0.469956 |
| H | -0.190881 | 2.494902 | 0.069710 |
| H | -0.242879 | 1.336763 | 1.377453 |
| H | 1.361967 | 1.069966 | -1.225258 |
| H | 2.000255 | 1.569612 | 0.329547 |
| H | 1.395424 | -0.713193 | 1.268777 |
| H | 0.910913 | -1.211911 | -0.347065 |
| H | 3.735966 | -0.280641 | 0.428704 |
| H | 3.241053 | -0.762784 | -1.198353 |
| H | 3.245520 | -1.950893 | 0.111865 |
| Rotational constants (GHz): | 4.3663300 | 1.1532400 | 0.9735400 |
| Vibrational harmonic frequencies (cm-1): | | | |
| 51.5764 | 86.5325 | | 92.4107 |
| 130.1461 | 220.4902 | | 249.0138 |
| 289.6430 | 305.3958 | | 437.4017 |
| 490.3509 | 542.6953 | | 748.9650 |
| 780.6813 | 840.7859 | | 872.2008 |
| 906.0418 | 968.2228 | | 1008.8627 |
| 1044.3300 | 1067.7762 | | 1085.3539 |
| 1100.5551 | 1131.6974 | | 1190.3914 |
| 1236.7729 | 1287.0155 | | 1288.0628 |
| 1333.7048 | 1335.5123 | | 1345.0556 |
| 1372.7819 | 1388.9441 | | 1393.2849 |
| 1413.0843 | 1426.2450 | | 1494.2523 |
| 1502.5152 | 1504.4108 | | 1508.7299 |
| 1513.6731 | 1523.2505 | | 2902.7684 |
| 2921.9876 | 3014.1728 | | 3015.7861 |
| 3025.1178 | 3040.3054 | | 3043.2223 |
| 3045.9308 | 3067.0645 | | 3071.6161 |
| 3087.6027 | 3108.9889 | | 3114.6245 |
| Zero-point correction (Hartree): | 0.179902 | | |

C6H13O.tppm

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -311.63149428

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 2.788493 | 0.948288 | 0.018082 |
| C | 1.792440 | 0.111440 | 0.440892 |
| C | 0.997611 | -0.566201 | -0.685626 |
| C | -0.116680 | -1.497712 | -0.182776 |
| C | -1.272054 | -0.858335 | 0.613356 |
| C | -2.158196 | 0.146215 | -0.155599 |
| C | -1.697829 | 1.609416 | -0.099341 |
| H | 2.165209 | -0.626392 | 1.179021 |
| H | 1.123306 | 0.774945 | 1.032215 |
| H | 0.601314 | 0.208171 | -1.350771 |
| H | 1.705747 | -1.151655 | -1.284846 |
| H | -0.542988 | -2.021376 | -1.048400 |
| H | 0.338076 | -2.279710 | 0.441773 |
| H | -1.905103 | -1.682599 | 0.964892 |
| H | -0.888814 | -0.380009 | 1.525870 |
| H | -2.245841 | -0.175159 | -1.202476 |
| H | -3.174297 | 0.097479 | 0.255197 |
| H | -0.712206 | 1.758488 | -0.550103 |
| H | -1.644241 | 1.961320 | 0.937645 |
| H | -2.399864 | 2.261257 | -0.630121 |

Rotational constants (GHz): 3.6343700 1.4434900 1.1612500

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 49.9534 | 67.5818 | 117.7454 |
| 186.4651 | 211.3986 | 242.1497 |
| 312.4126 | 356.3849 | 426.3383 |
| 497.7225 | 682.9687 | 747.2312 |
| 778.9334 | 822.0937 | 885.2400 |
| 919.4214 | 967.3551 | 1001.4197 |
| 1047.0295 | 1071.4977 | 1084.4083 |
| 1117.8569 | 1119.3254 | 1167.9934 |
| 1219.5840 | 1252.1675 | 1309.0818 |
| 1319.6505 | 1335.0249 | 1360.3012 |
| 1378.4985 | 1392.4535 | 1399.0123 |
| 1402.6552 | 1429.0756 | 1496.9498 |
| 1499.1997 | 1506.0206 | 1510.8804 |
| 1520.3953 | 1522.1048 | 2890.3058 |
| 2932.0468 | 3019.2182 | 3025.9651 |
| 3028.2215 | 3042.8537 | 3049.6000 |
| 3057.2460 | 3065.8577 | 3068.9193 |
| 3099.9924 | 3107.1903 | 3124.0293 |

Zero-point correction (Hartree): 0.180534

C6H13O.tppp

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -311.63423516

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -3.084395 | -0.840240 | -0.006811 |
| C | -2.063170 | 0.006951 | 0.326244 |
| C | -1.002097 | 0.200107 | -0.767782 |
| C | 0.131589 | 1.158369 | -0.366574 |
| C | 1.016179 | 0.693412 | 0.806041 |
| C | 1.772344 | -0.629572 | 0.591204 |
| C | 2.772534 | -0.603892 | -0.570346 |
| H | -2.445795 | 0.977158 | 0.701434 |
| H | -1.606443 | -0.469856 | 1.221777 |
| H | -0.609991 | -0.784127 | -1.047895 |
| H | -1.508675 | 0.594554 | -1.656778 |
| H | 0.759244 | 1.341267 | -1.246821 |
| H | -0.302569 | 2.134018 | -0.107705 |
| H | 1.746673 | 1.485921 | 1.018041 |
| H | 0.405989 | 0.607134 | 1.715439 |
| H | 2.307343 | -0.872116 | 1.518126 |
| H | 1.057873 | -1.449058 | 0.438475 |
| H | 3.503171 | 0.203931 | -0.444969 |
| H | 2.276843 | -0.453392 | -1.535022 |
| H | 3.327228 | -1.545760 | -0.632339 |

Rotational constants (GHz): 4.9506900 1.1218300 1.0822200

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 41.8236 | 85.7774 | 98.4725 |
| 179.0333 | 209.0414 | 276.0322 |
| 301.5780 | 370.6167 | 440.2969 |
| 517.1253 | 674.2445 | 730.8696 |
| 776.1232 | 845.2628 | 888.1671 |
| 905.7641 | 962.9529 | 1004.0626 |
| 1031.4581 | 1072.8462 | 1082.2092 |
| 1103.8015 | 1125.7260 | 1176.8504 |
| 1207.3266 | 1256.2243 | 1295.9636 |
| 1325.2345 | 1339.7614 | 1361.6452 |

| | | |
|-----------|-----------|-----------|
| 1375.6440 | 1389.2116 | 1402.2061 |
| 1404.6917 | 1429.9244 | 1493.8709 |
| 1500.7154 | 1508.9064 | 1511.9911 |
| 1517.3421 | 1525.4996 | 2885.3955 |
| 2931.4038 | 3021.6127 | 3029.4807 |
| 3035.6525 | 3041.8258 | 3050.3403 |
| 3055.5825 | 3066.8548 | 3076.8013 |
| 3095.7126 | 3109.3144 | 3116.1224 |

Zero-point correction (Hartree): 0.180573

C6H13O.tppt

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -311.63542351
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 3.024737 | -1.096471 | 0.098947 |
| C | 2.016916 | -0.337023 | -0.429055 |
| C | 1.283405 | 0.556727 | 0.582449 |
| C | 0.148604 | 1.388195 | -0.038627 |
| C | -1.054806 | 0.589194 | -0.570894 |
| C | -1.849547 | -0.168117 | 0.502322 |
| C | -3.072729 | -0.895671 | -0.065538 |
| H | 2.362372 | 0.240275 | -1.310005 |
| H | 1.315893 | -1.088394 | -0.855837 |
| H | 0.914499 | -0.073450 | 1.399235 |
| H | 2.023998 | 1.233319 | 1.025682 |
| H | -0.208555 | 2.105384 | 0.711916 |
| H | 0.561509 | 1.993857 | -0.857247 |
| H | -1.731779 | 1.286125 | -1.083008 |
| H | -0.726822 | -0.119668 | -1.344851 |
| H | -1.200800 | -0.894692 | 1.007581 |
| H | -2.171002 | 0.541150 | 1.277375 |
| H | -2.778881 | -1.635820 | -0.818785 |
| H | -3.763664 | -0.193732 | -0.546410 |
| H | -3.625723 | -1.422416 | 0.718835 |

Rotational constants (GHz): 4.7044000 1.0810100 0.9714700
 Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 48.0121 | 79.9735 | 95.1201 |
| 174.7855 | 214.0131 | 251.5179 |
| 289.6763 | 319.1016 | 441.7473 |
| 504.2237 | 672.4973 | 733.9577 |
| 787.1010 | 847.0073 | 891.7121 |
| 902.5311 | 971.7064 | 1001.6396 |
| 1040.0583 | 1076.8906 | 1085.0533 |
| 1092.9069 | 1125.9848 | 1172.4407 |
| 1221.5542 | 1259.8304 | 1305.2226 |
| 1319.2236 | 1336.3124 | 1344.9039 |
| 1367.2193 | 1392.3565 | 1394.4360 |
| 1409.8768 | 1428.9551 | 1497.4076 |
| 1501.9124 | 1505.9870 | 1509.2817 |
| 1514.5324 | 1524.4894 | 2885.6620 |
| 2930.6102 | 3014.5367 | 3024.0704 |
| 3030.2266 | 3039.2322 | 3047.0771 |
| 3049.6187 | 3064.4214 | 3072.1935 |
| 3096.8722 | 3107.3552 | 3114.1015 |

Zero-point correction (Hartree): 0.180269

C6H13O.tptm

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -311.63534196
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -3.554534 | -0.202638 | -0.210210 |
| C | -2.269003 | -0.352127 | 0.232082 |
| C | -1.318338 | 0.795869 | -0.140841 |
| C | 0.119431 | 0.601965 | 0.365909 |
| C | 0.882652 | -0.545817 | -0.313559 |
| C | 2.324606 | -0.735311 | 0.188080 |
| C | 3.271635 | 0.424040 | -0.144621 |
| H | -2.238258 | -0.570943 | 1.318510 |
| H | -1.932823 | -1.299696 | -0.244052 |
| H | -1.329199 | 0.917099 | -1.230991 |
| H | -1.734040 | 1.719200 | 0.280255 |
| H | 0.664247 | 1.541366 | 0.217320 |
| H | 0.104016 | 0.432570 | 1.452800 |
| H | 0.339876 | -1.488553 | -0.162436 |
| H | 0.896483 | -0.375131 | -1.399753 |
| H | 2.309908 | -0.896457 | 1.274830 |
| H | 2.727155 | -1.658314 | -0.248098 |
| H | 2.961639 | 1.358544 | 0.334112 |
| H | 3.310882 | 0.602604 | -1.225601 |
| H | 4.290490 | 0.207100 | 0.192489 |

Rotational constants (GHz): 8.5690400 0.8884700 0.8482300
 Vibrational harmonic frequencies (cm-1):

| | | |
|---------|---------|---------|
| 38.9358 | 92.7074 | 99.5633 |
|---------|---------|---------|

| | | |
|-----------|-----------|-----------|
| 131.7483 | 215.4035 | 247.7180 |
| 286.4276 | 318.0896 | 413.5244 |
| 528.9460 | 659.0680 | 737.2468 |
| 775.4625 | 847.0431 | 882.8061 |
| 911.0021 | 962.9168 | 1003.8369 |
| 1050.5565 | 1071.3081 | 1081.7476 |
| 1092.4141 | 1120.8023 | 1188.0960 |
| 1221.5699 | 1269.8135 | 1294.4035 |
| 1326.7670 | 1343.1147 | 1350.9266 |

| | | |
|-----------|-----------|-----------|
| 1367.5261 | 1387.4784 | 1391.0016 |
| 1411.5251 | 1429.5686 | 1494.0803 |
| 1501.3034 | 1503.2828 | 1509.9710 |
| 1515.9038 | 1522.4417 | 2887.3334 |
| 2928.7966 | 3013.6752 | 3020.9064 |
| 3026.3778 | 3042.0265 | 3044.2316 |
| 3052.3389 | 3063.5447 | 3079.9495 |
| 3089.5749 | 3109.6356 | 3117.4910 |

Zero-point correction (Hartree): 0.180144

C6H130.tptp

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -311.63546096

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 3.443181 | -0.466144 | 0.230237 |
| C | 2.094061 | -0.561107 | 0.025864 |
| C | 1.402742 | 0.755919 | -0.358535 |
| C | -0.110363 | 0.617924 | -0.586480 |
| C | -0.915186 | 0.300293 | 0.683800 |
| C | -2.440066 | 0.297200 | 0.483134 |
| C | -2.960109 | -0.824879 | -0.423380 |
| H | 1.850729 | -1.373885 | -0.687833 |
| H | 1.703319 | -0.931806 | 0.999331 |
| H | 1.608304 | 1.498019 | 0.422682 |
| H | 1.879696 | 1.125043 | -1.274468 |
| H | -0.485909 | 1.556651 | -1.014633 |
| H | -0.290137 | -0.152499 | -1.348468 |
| H | -0.610887 | -0.675059 | 1.089611 |
| H | -0.660471 | 1.042023 | 1.453211 |
| H | -2.922165 | 0.213139 | 1.465304 |
| H | -2.749609 | 1.269622 | 0.075970 |
| H | -2.671539 | -1.809646 | -0.037239 |
| H | -2.570440 | -0.741978 | -1.443107 |
| H | -4.052813 | -0.802571 | -0.488678 |

Rotational constants (GHz): 6.6030200 0.9305000 0.9064600

Vibrational harmonic frequencies (cm⁻¹):

| | | |
|-----------|-----------|-----------|
| 44.9101 | 90.5721 | 107.0265 |
| 133.9394 | 206.0360 | 256.9220 |
| 293.2315 | 313.6162 | 406.0703 |
| 536.9055 | 656.2657 | 747.5870 |
| 780.3277 | 831.0814 | 893.4212 |
| 902.4677 | 974.2912 | 995.6261 |
| 1052.1286 | 1071.0364 | 1085.3976 |
| 1094.0707 | 1131.7185 | 1173.6774 |
| 1228.0127 | 1268.9655 | 1310.6057 |
| 1313.7076 | 1344.9387 | 1350.0084 |
| 1368.3205 | 1384.5814 | 1392.2963 |
| 1411.4446 | 1429.7413 | 1494.9619 |
| 1502.5244 | 1502.9720 | 1511.1488 |
| 1516.1432 | 1521.6186 | 2886.9325 |
| 2927.8895 | 3015.8597 | 3025.5359 |
| 3029.8155 | 3041.0442 | 3043.1763 |
| 3049.7855 | 3063.0783 | 3073.6379 |
| 3090.0858 | 3108.5413 | 3116.0067 |

Zero-point correction (Hartree): 0.180207

C6H130.tptt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -311.63676907

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -3.455901 | -0.739801 | -0.094916 |
| C | -2.185694 | -0.465146 | 0.331812 |
| C | -1.520809 | 0.741592 | -0.347858 |
| C | -0.097880 | 1.029862 | 0.154582 |
| C | 0.940115 | -0.041566 | -0.208998 |
| C | 2.361593 | 0.312608 | 0.247679 |
| C | 3.397148 | -0.756986 | -0.113284 |
| H | -2.139121 | -0.388667 | 1.436850 |
| H | -1.621294 | -1.395833 | 0.101812 |
| H | -1.519342 | 0.573894 | -1.431829 |
| H | -2.157631 | 1.615891 | -0.167223 |
| H | 0.228971 | 1.993283 | -0.257618 |

| | | | | |
|--|-----------|-----------|-----------|-----------|
| H | -0.115861 | 1.163292 | 1.246172 | |
| H | 0.658611 | -1.007598 | 0.233429 | |
| H | 0.935872 | -0.194781 | -1.297807 | |
| H | 2.654102 | 1.272565 | -0.198992 | |
| H | 2.362176 | 0.471968 | 1.334573 | |
| H | 3.445003 | -0.912861 | -1.197079 | |
| H | 3.149858 | -1.720338 | 0.347415 | |
| H | 4.399027 | -0.474583 | 0.226023 | |
| Rotational constants (GHz): | | | | 7.0515900 |
| Vibrational harmonic frequencies (cm-1): | | | | 0.8761300 |
| | | | | 0.8187900 |
| 62.4218 | | 82.2489 | | 86.2754 |
| 130.7089 | | 196.1348 | | 244.2779 |
| 269.0717 | | 327.5913 | | 399.9723 |
| 515.2970 | | 659.7379 | | 734.5402 |
| 778.9416 | | 849.1048 | | 894.1545 |
| 918.1071 | | 971.6645 | | 1006.4821 |
| 1056.3060 | | 1069.5032 | | 1082.1965 |
| 1087.1059 | | 1127.7612 | | 1184.5628 |
| 1237.3399 | | 1266.4160 | | 1298.0902 |
| 1317.9929 | | 1334.2919 | | 1343.8955 |
| 1367.3897 | | 1381.8689 | | 1389.2875 |
| 1412.6871 | | 1427.9822 | | 1495.5212 |
| 1499.9392 | | 1502.4593 | | 1512.5006 |
| 1513.5917 | | 1524.3089 | | 2888.0014 |
| 2928.3879 | | 3011.9610 | | 3017.8300 |
| 3027.7015 | | 3038.1573 | | 3039.5109 |
| 3044.1510 | | 3057.8586 | | 3072.9195 |
| 3090.1456 | | 3107.1203 | | 3113.6315 |
| Zero-point correction (Hartree): | | | | 0.179969 |

C6H130.ttpm

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -311.63272345
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | | |
|--|-----------|-----------|-----------|-----------|
| O | -3.200373 | 0.891339 | -0.003796 | |
| C | -2.369951 | -0.190145 | 0.109635 | |
| C | -0.884389 | 0.084219 | -0.156933 | |
| C | -0.015403 | -1.159807 | 0.067676 | |
| C | 1.462755 | -1.041517 | -0.344995 | |
| C | 2.313825 | -0.021077 | 0.442116 | |
| C | 2.321465 | 1.404675 | -0.125999 | |
| H | -2.510866 | -0.544807 | 1.155664 | |
| H | -2.748202 | -1.034605 | -0.501566 | |
| H | -0.778275 | 0.437516 | -1.190802 | |
| H | -0.571404 | 0.908314 | 0.492681 | |
| H | -0.064899 | -1.446041 | 1.128671 | |
| H | -0.455909 | -1.999957 | -0.488492 | |
| H | 1.911212 | -2.035660 | -0.224265 | |
| H | 1.524702 | -0.815213 | -1.418909 | |
| H | 1.982103 | -0.002544 | 1.489563 | |
| H | 3.350273 | -0.380234 | 0.467005 | |
| H | 1.326052 | 1.857293 | -0.135277 | |
| H | 2.694072 | 1.410118 | -1.156793 | |
| H | 2.974313 | 2.057020 | 0.463886 | |
| Rotational constants (GHz): | | | | 4.8401600 |
| Vibrational harmonic frequencies (cm-1): | | | | 1.0878700 |
| | | | | 0.9389700 |
| 46.3749 | | 86.2353 | | 105.9995 |
| 117.8822 | | 196.7500 | | 218.5268 |
| 295.3446 | | 362.0101 | | 422.3109 |
| 470.4704 | | 530.9920 | | 751.3267 |
| 767.6151 | | 822.5693 | | 862.7247 |
| 947.1083 | | 964.4194 | | 1019.5765 |
| 1040.7615 | | 1053.0375 | | 1087.2958 |
| 1098.4949 | | 1130.8499 | | 1195.4423 |
| 1247.5832 | | 1255.9289 | | 1302.7758 |
| 1320.6785 | | 1333.6817 | | 1370.8870 |
| 1375.0004 | | 1382.4192 | | 1394.8080 |
| 1412.9709 | | 1430.4784 | | 1492.5744 |
| 1501.3483 | | 1504.0615 | | 1510.2820 |
| 1516.2316 | | 1522.2570 | | 2876.8166 |
| 2924.2811 | | 3007.9767 | | 3021.1381 |
| 3025.5243 | | 3041.3078 | | 3044.4484 |
| 3046.9305 | | 3062.3089 | | 3066.1925 |
| 3101.1376 | | 3108.1252 | | 3128.9629 |
| Zero-point correction (Hartree): | | | | 0.179800 |

C6H130.ttpm

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -311.63542098
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | |
|---|----------|-----------|-----------|
| O | 3.320729 | -0.663672 | -0.361497 |
| C | 2.344437 | -0.042820 | 0.369320 |
| C | 0.998744 | 0.142115 | -0.341777 |

| | | | |
|--|-----------|-----------|-----------|
| C | -0.059521 | 0.786594 | 0.562821 |
| C | -1.395669 | 1.091388 | -0.136718 |
| C | -2.169956 | -0.129350 | -0.664481 |
| C | -2.613991 | -1.114567 | 0.423130 |
| H | 2.216155 | -0.679633 | 1.273432 |
| H | 2.726208 | 0.912853 | 0.782734 |
| H | 1.159448 | 0.764794 | -1.231582 |
| H | 0.667380 | -0.838431 | -0.701745 |
| H | -0.234186 | 0.142672 | 1.435681 |
| H | 0.340785 | 1.727900 | 0.964645 |
| H | -2.039164 | 1.639554 | 0.564961 |
| H | -1.204951 | 1.777706 | -0.972972 |
| H | -3.056239 | 0.234131 | -1.199835 |
| H | -1.566849 | -0.658314 | -1.413361 |
| H | -3.228552 | -0.615668 | 1.181710 |
| H | -1.760850 | -1.569636 | 0.937507 |
| H | -3.209286 | -1.928709 | -0.002964 |
| Rotational constants (GHz): | 5.4051800 | 1.0059600 | 0.9460800 |
| Vibrational harmonic frequencies (cm-1): | | | |
| 50.3888 | 77.1330 | | 110.1274 |
| 138.4771 | 205.4054 | | 262.9630 |
| 283.3426 | 385.2163 | | 433.0794 |
| 491.4928 | 517.9111 | | 729.8989 |
| 777.9915 | 828.2889 | | 864.5483 |
| 940.3185 | 971.0334 | | 1008.6215 |
| 1028.5572 | 1050.4795 | | 1086.6061 |
| 1103.3866 | 1142.1537 | | 1176.4522 |
| 1253.5107 | 1259.2750 | | 1297.9761 |
| 1312.9352 | 1338.7181 | | 1365.1900 |
| 1377.1949 | 1389.6583 | | 1397.9470 |
| 1411.7073 | 1430.3908 | | 1493.6725 |
| 1503.4484 | 1505.3878 | | 1511.2903 |
| 1518.6754 | 1526.2997 | | 2878.0435 |
| 2923.1417 | 3017.8959 | | 3024.2256 |
| 3036.7401 | 3042.0301 | | 3042.3159 |
| 3051.1201 | 3061.4222 | | 3071.9389 |
| 3094.4538 | 3109.8067 | | 3115.2777 |
| Zero-point correction (Hartree): | 0.180033 | | |

C6H130.ttpt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -311.63663285

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|--|-----------|-----------|-----------|
| O | 3.477966 | -0.819273 | -0.116347 |
| C | 2.566870 | 0.162417 | 0.164614 |
| C | 1.117833 | -0.143695 | -0.231627 |
| C | 0.149701 | 0.976369 | 0.170830 |
| C | -1.301059 | 0.764530 | -0.291323 |
| C | -2.015559 | -0.430546 | 0.355500 |
| C | -3.476867 | -0.560131 | -0.086575 |
| H | 2.640297 | 0.314136 | 1.265055 |
| H | 2.910900 | 1.132029 | -0.249757 |
| H | 1.080859 | -0.296070 | -1.318335 |
| H | 0.833006 | -1.096179 | 0.228730 |
| H | 0.166749 | 1.098149 | 1.264017 |
| H | 0.514535 | 1.926812 | -0.243244 |
| H | -1.874603 | 1.675993 | -0.074706 |
| H | -1.319038 | 0.649193 | -1.384551 |
| H | -1.483523 | -1.359692 | 0.115763 |
| H | -1.970741 | -0.327293 | 1.448677 |
| H | -3.551542 | -0.697591 | -1.171421 |
| H | -4.050892 | 0.337187 | 0.171672 |
| H | -3.965252 | -1.416147 | 0.390360 |
| Rotational constants (GHz): | 7.6597600 | 0.8561200 | 0.8067600 |
| Vibrational harmonic frequencies (cm-1): | | | |
| 71.8236 | 74.9561 | | 83.7404 |
| 130.1629 | 206.9998 | | 245.2016 |
| 266.1280 | 301.6548 | | 434.0725 |
| 500.9379 | 514.1205 | | 737.4200 |
| 762.2045 | 850.5908 | | 857.6688 |
| 942.7105 | 981.1538 | | 1012.6040 |
| 1036.6009 | 1055.2867 | | 1084.0362 |
| 1091.6506 | 1138.3640 | | 1198.5585 |
| 1254.0664 | 1262.4072 | | 1305.7968 |
| 1313.7899 | 1337.9412 | | 1349.1837 |
| 1368.1417 | 1382.3549 | | 1406.7933 |
| 1412.3649 | 1428.6920 | | 1495.7011 |
| 1498.8723 | 1508.1533 | | 1512.4563 |
| 1513.4836 | 1523.7493 | | 2878.7272 |
| 2921.8477 | 3010.3314 | | 3016.5154 |
| 3027.6842 | 3039.0405 | | 3041.7320 |
| 3046.7659 | 3049.3375 | | 3072.1077 |
| 3095.3705 | 3107.6013 | | 3113.2014 |
| Zero-point correction (Hartree): | 0.179686 | | |

C6H13O.tttt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -311.63659905

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 3.711010 | 0.094107 | -0.182595 |
| C | 2.462563 | 0.468317 | 0.235487 |
| C | 1.311976 | -0.440180 | -0.211216 |
| C | -0.059485 | 0.064756 | 0.252724 |
| C | -1.214513 | -0.854058 | -0.169629 |
| C | -2.600343 | -0.411566 | 0.328476 |
| C | -3.097033 | 0.911828 | -0.265997 |
| H | 2.463398 | 0.619062 | 1.334450 |
| H | 2.319496 | 1.497906 | -0.162289 |
| H | 1.339575 | -0.522062 | -1.304854 |
| H | 1.494094 | -1.448443 | 0.182474 |
| H | -0.061707 | 0.163407 | 1.348420 |
| H | -0.223240 | 1.076336 | -0.142935 |
| H | -1.231714 | -0.931606 | -1.266144 |
| H | -1.010940 | -1.867096 | 0.202512 |
| H | -3.324353 | -1.201340 | 0.091224 |
| H | -2.582753 | -0.336896 | 1.424571 |
| H | -3.127106 | 0.865186 | -1.360939 |
| H | -2.453721 | 1.753236 | 0.011576 |
| H | -4.108090 | 1.144878 | 0.083620 |

Rotational constants (GHz): 8.5304700 0.8263000 0.7910200

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 57.2001 | 75.3320 | 118.5054 |
| 134.7635 | 148.4679 | 235.2749 |
| 288.2264 | 340.4886 | 351.6183 |
| 415.6611 | 522.5163 | 739.0828 |
| 771.9179 | 817.3401 | 878.2900 |
| 942.1140 | 974.4365 | 1026.8202 |
| 1037.1622 | 1047.4848 | 1083.8568 |
| 1093.8960 | 1136.0192 | 1200.1409 |
| 1247.9803 | 1267.5862 | 1298.4778 |
| 1321.8728 | 1339.9552 | 1352.1716 |
| 1373.1888 | 1386.9176 | 1398.3362 |
| 1415.5079 | 1429.5845 | 1496.8295 |
| 1500.5498 | 1502.8335 | 1515.4951 |
| 1519.2560 | 1522.2715 | 2881.2766 |
| 2920.5078 | 3010.9884 | 3020.4905 |
| 3026.1409 | 3040.0589 | 3041.3672 |
| 3045.0126 | 3061.2410 | 3067.3748 |
| 3088.9332 | 3109.2808 | 3115.5863 |

Zero-point correction (Hartree): 0.179414

C6H13O.tttt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -311.63793173

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 3.827200 | -0.330728 | -0.013538 |
| C | 2.665610 | 0.392389 | 0.019178 |
| C | 1.370965 | -0.427711 | 0.006880 |
| C | 0.112571 | 0.447998 | -0.003922 |
| C | -1.192279 | -0.358247 | 0.004797 |
| C | -2.452510 | 0.516264 | -0.008680 |
| C | -3.751039 | -0.296673 | 0.001071 |
| H | 2.690674 | 1.106939 | 0.867259 |
| H | 2.711463 | 1.056159 | -0.873054 |
| H | 1.385923 | -1.086898 | -0.869869 |
| H | 1.366406 | -1.080941 | 0.888873 |
| H | 0.126912 | 1.120767 | 0.865975 |
| H | 0.128513 | 1.100325 | -0.889403 |
| H | -1.208289 | -1.031636 | -0.863879 |
| H | -1.210772 | -1.008173 | 0.891170 |
| H | -2.434876 | 1.189280 | 0.859434 |
| H | -2.432938 | 1.165030 | -0.895043 |
| H | -3.816131 | -0.928737 | 0.894093 |
| H | -3.813098 | -0.954694 | -0.873216 |
| H | -4.631304 | 0.354291 | -0.009985 |

Rotational constants (GHz): 13.5535900 0.7293700 0.7102700

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 65.0232 | 87.0330 | 100.5470 |
| 141.4152 | 152.1772 | 245.6221 |
| 250.8086 | 304.7248 | 411.7973 |
| 433.3873 | 517.2018 | 737.1650 |
| 757.3901 | 831.8146 | 900.1620 |
| 939.0907 | 998.7633 | 1032.0423 |
| 1037.3426 | 1053.8241 | 1071.3650 |
| 1088.2976 | 1138.9416 | 1217.6043 |
| 1247.8134 | 1265.4897 | 1303.0976 |
| 1322.5444 | 1339.1238 | 1341.1964 |

| | | |
|-----------|-----------|-----------|
| 1365.7400 | 1385.4528 | 1404.8326 |
| 1417.5643 | 1427.7276 | 1499.2457 |
| 1500.4536 | 1507.0888 | 1512.7497 |
| 1517.9871 | 1527.3188 | 2881.7677 |
| 2921.1375 | 3009.2540 | 3016.8072 |
| 3027.4453 | 3035.1730 | 3039.5381 |
| 3042.4881 | 3047.8453 | 3069.0076 |
| 3088.7439 | 3107.4986 | 3113.0870 |

Zero-point correction (Hartree): 0.179517

C6H13O-1-6Hshift.a.a

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -311.62284963
Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 0.781082 | -1.547180 | -0.595380 |
| H | -0.364012 | -1.009724 | -0.606708 |
| C | -1.354807 | -0.239115 | -0.532533 |
| C | 1.542129 | -0.861969 | 0.364982 |
| C | -0.770874 | 1.164668 | -0.624227 |
| C | 1.668198 | 0.648846 | 0.119003 |
| C | 0.382506 | 1.460414 | 0.356642 |
| C | -2.114236 | -0.599695 | 0.730510 |
| H | -1.903674 | -0.518231 | -1.438745 |
| H | 1.175048 | -1.045202 | 1.391654 |
| H | 2.541784 | -1.321329 | 0.307159 |
| H | -0.415016 | 1.335584 | -1.647937 |
| H | -1.577365 | 1.894883 | -0.453966 |
| H | 2.450576 | 1.034817 | 0.785866 |
| H | 2.021402 | 0.802276 | -0.909136 |
| H | 0.626832 | 2.526985 | 0.280385 |
| H | 0.043733 | 1.305148 | 1.390156 |
| H | -3.008771 | 0.031372 | 0.833497 |
| H | -1.511493 | -0.455773 | 1.632915 |
| H | -2.445196 | -1.642267 | 0.711636 |

Rotational constants (GHz): 3.1686700 2.1335100 1.5788200

Vibrational harmonic frequencies (cm-1):

| | | |
|------------|-----------|-----------|
| i1352.9602 | 95.1521 | 125.2958 |
| 193.9564 | 233.2572 | 306.7826 |
| 340.2409 | 372.7452 | 451.8005 |
| 515.3989 | 601.9856 | 771.6233 |
| 805.3169 | 830.6097 | 874.0745 |
| 907.0478 | 945.0210 | 964.8288 |
| 1030.0139 | 1044.5734 | 1065.2475 |
| 1109.5377 | 1136.2457 | 1156.8905 |
| 1178.5068 | 1213.5320 | 1250.2410 |
| 1282.4372 | 1298.3667 | 1362.7083 |
| 1378.4506 | 1385.5640 | 1399.0189 |
| 1407.2248 | 1422.7528 | 1453.9126 |
| 1480.8010 | 1483.3667 | 1489.0742 |
| 1500.2197 | 1503.3430 | 1513.3661 |
| 2950.2475 | 3002.7762 | 3008.9634 |
| 3021.2881 | 3029.8681 | 3033.6431 |
| 3060.3510 | 3069.8273 | 3078.4231 |
| 3080.9940 | 3094.5078 | 3126.2969 |

Zero-point correction (Hartree): 0.176416

C6H13O-1-6Hshift.a.e

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -311.62442124

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 0.493542 | -1.661929 | -0.222002 |
| H | -0.495064 | -0.948784 | 0.120669 |
| C | -1.284018 | -0.016108 | 0.407569 |
| C | 1.638663 | -0.993830 | 0.241616 |
| C | -0.659874 | 1.224762 | -0.206624 |
| C | 1.813758 | 0.426438 | -0.314808 |
| C | 0.804425 | 1.463897 | 0.209009 |
| H | -1.244828 | -0.001827 | 1.503931 |
| C | -2.640076 | -0.428536 | -0.129484 |
| H | 1.684799 | -0.972282 | 1.345819 |
| H | 2.481557 | -1.619576 | -0.092234 |
| H | -0.721441 | 1.155905 | -1.301432 |
| H | -1.262251 | 2.101862 | 0.077138 |
| H | 2.826241 | 0.766680 | -0.059815 |
| H | 1.761035 | 0.376635 | -1.410261 |
| H | 1.109542 | 2.454925 | -0.148501 |
| H | 0.866399 | 1.505254 | 1.306403 |
| H | -2.609436 | -0.572454 | -1.214787 |
| H | -3.390951 | 0.347778 | 0.077747 |
| H | -2.991207 | -1.358421 | 0.327669 |

Rotational constants (GHz): 3.5394800 1.9233800 1.3608100

Vibrational harmonic frequencies (cm-1):

| | | |
|------------|---------|----------|
| i1333.8945 | 96.8710 | 153.7091 |
|------------|---------|----------|

| | | |
|-----------|-----------|-----------|
| 205.2348 | 213.0884 | 267.9379 |
| 332.8820 | 339.6531 | 437.9693 |
| 497.7494 | 593.8913 | 778.0398 |
| 785.9383 | 836.8813 | 861.7355 |
| 913.3950 | 954.1957 | 969.4564 |
| 1026.6068 | 1060.1280 | 1077.2046 |
| 1105.5347 | 1121.7362 | 1163.7447 |
| 1220.9837 | 1230.1629 | 1274.0945 |
| 1279.4382 | 1294.9397 | 1335.5607 |
| 1382.2487 | 1395.7022 | 1398.0085 |
| 1405.8346 | 1415.8425 | 1454.2159 |
| 1480.6898 | 1482.6108 | 1490.7155 |
| 1498.5207 | 1501.9589 | 1505.2882 |
| 2952.2097 | 3000.5696 | 3010.4782 |
| 3018.3382 | 3019.4042 | 3033.0711 |
| 3047.5252 | 3065.3190 | 3069.0011 |
| 3077.8230 | 3090.1639 | 3124.6368 |

Zero-point correction (Hartree): 0.176214

C6H13O-1-6Hshift.b.a

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -311.61888901

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -0.656341 | -1.586719 | -0.282366 |
| H | 0.420844 | -1.065413 | 0.134682 |
| C | 1.306808 | -0.265711 | 0.543533 |
| C | -1.657603 | -0.808013 | 0.320933 |
| C | 0.612870 | 1.093111 | 0.642052 |
| C | -1.778050 | 0.613500 | -0.260665 |
| C | -0.424585 | 1.323697 | -0.478904 |
| C | 2.435049 | -0.372653 | -0.465498 |
| H | 1.576888 | -0.686432 | 1.518266 |
| H | -2.599767 | -1.355123 | 0.164522 |
| H | -1.514341 | -0.760209 | 1.413988 |
| H | 0.129675 | 1.201289 | 1.620854 |
| H | 1.378419 | 1.881409 | 0.592954 |
| H | -2.308502 | 0.573256 | -1.219250 |
| H | -2.404420 | 1.204501 | 0.421581 |
| H | -0.607662 | 2.397858 | -0.595778 |
| H | 0.006589 | 0.983371 | -1.427203 |
| H | 3.283908 | 0.255328 | -0.158984 |
| H | 2.123327 | -0.038983 | -1.460608 |
| H | 2.798833 | -1.400689 | -0.554808 |

Rotational constants (GHz): 3.5812800 1.9753000 1.5094100

Vibrational harmonic frequencies (cm-1):

| | | |
|------------|-----------|-----------|
| i1386.0777 | 95.2321 | 150.0011 |
| 202.4005 | 215.3993 | 258.2316 |
| 308.1629 | 378.6831 | 430.1421 |
| 561.8145 | 609.9713 | 766.4035 |
| 781.9336 | 822.3648 | 850.7543 |
| 899.6832 | 954.5557 | 981.6434 |
| 1029.7506 | 1053.4626 | 1067.7981 |
| 1116.2638 | 1123.9392 | 1153.0815 |
| 1204.0712 | 1223.7663 | 1266.3755 |
| 1284.6890 | 1300.3562 | 1350.4272 |
| 1358.9388 | 1382.6830 | 1388.5939 |
| 1414.4154 | 1419.9021 | 1468.4586 |
| 1478.2221 | 1493.1264 | 1494.7013 |
| 1504.0086 | 1506.8338 | 1511.3938 |
| 2968.8928 | 3013.6015 | 3021.1398 |
| 3021.6884 | 3031.9283 | 3050.4060 |
| 3064.9147 | 3076.2191 | 3081.6383 |
| 3092.3970 | 3096.1158 | 3125.5577 |

Zero-point correction (Hartree): 0.176574

C6H13O-1-6Hshift.b.e

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -311.62003123

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -0.508790 | -1.548487 | -0.617625 |
| H | 0.521227 | -0.811015 | -0.597009 |
| C | 1.333773 | 0.142143 | -0.433146 |
| C | -1.283318 | -1.082246 | 0.456524 |
| C | 0.529439 | 1.251957 | 0.233368 |
| C | -1.892969 | 0.314044 | 0.230899 |
| C | -0.902562 | 1.358654 | -0.330517 |
| H | 1.559757 | 0.380236 | -1.479608 |
| C | 2.529565 | -0.397998 | 0.322750 |
| H | -2.088710 | -1.820893 | 0.589324 |
| H | -0.706059 | -1.097090 | 1.397231 |
| H | 0.498446 | 1.094822 | 1.320133 |
| H | 1.056110 | 2.206109 | 0.083512 |
| H | -2.744092 | 0.233799 | -0.455197 |

| | | | | |
|--|-----------|-----------|-----------|--|
| H | -2.295216 | 0.661989 | 1.192230 | |
| H | -1.304223 | 2.360160 | -0.139673 | |
| H | -0.848815 | 1.253492 | -1.420786 | |
| H | 2.241599 | -0.771492 | 1.311779 | |
| H | 3.279011 | 0.391523 | 0.479610 | |
| H | 3.017713 | -1.213070 | -0.219809 | |
| Rotational constants (GHz): | 3.4858700 | 1.9854700 | 1.4620600 | |
| Vibrational harmonic frequencies (cm-1): | | | | |
| i1386.5580 | 82.8442 | | 137.6770 | |
| 193.9680 | 234.8289 | | 259.1737 | |
| 336.0360 | 354.5241 | | 422.9987 | |
| 564.6091 | 568.2897 | | 758.9119 | |
| 792.1230 | 831.9220 | | 863.8329 | |
| 895.4185 | 965.9117 | | 984.2561 | |
| 1026.2054 | 1057.6075 | | 1076.7001 | |
| 1108.5502 | 1125.6816 | | 1155.2361 | |
| 1215.8409 | 1235.2998 | | 1253.6759 | |
| 1268.8311 | 1296.8023 | | 1329.4940 | |
| 1373.7390 | 1384.9689 | | 1394.1219 | |
| 1412.1975 | 1419.8454 | | 1466.3588 | |
| 1478.8685 | 1492.3565 | | 1495.9862 | |
| 1502.3424 | 1505.6436 | | 1509.1084 | |
| 2964.9479 | 3010.1929 | | 3017.6941 | |
| 3018.9541 | 3032.1324 | | 3042.4958 | |
| 3052.6925 | 3070.7767 | | 3077.0718 | |
| 3086.2448 | 3091.1436 | | 3122.5293 | |
| Zero-point correction (Hartree): | 0.176375 | | | |

C6H13O-1-6Hshift.c.a

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -311.61788996
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | | |
|--|-----------|-----------|-----------|--|
| C | -0.716627 | 0.895036 | -0.910580 | |
| C | 0.228191 | 1.553536 | 0.121765 | |
| C | 1.306892 | 0.630930 | 0.742164 | |
| C | 1.789110 | -0.519250 | -0.158483 | |
| O | 0.911648 | -1.617106 | -0.174444 | |
| H | -0.258984 | -1.166553 | -0.324106 | |
| C | -1.287064 | -0.452021 | -0.498540 | |
| H | -0.180239 | 0.761476 | -1.857939 | |
| H | -1.537341 | 1.595073 | -1.129779 | |
| H | 0.717095 | 2.398638 | -0.377884 | |
| H | -0.363412 | 1.992267 | 0.933969 | |
| H | 2.166876 | 1.246379 | 1.032769 | |
| H | 0.933656 | 0.166335 | 1.662199 | |
| H | 2.014910 | -0.149392 | -1.174698 | |
| H | 2.732507 | -0.917526 | 0.247092 | |
| H | -1.769639 | -0.968051 | -1.335915 | |
| C | -2.110959 | -0.514801 | 0.772694 | |
| H | -3.033025 | 0.074569 | 0.663085 | |
| H | -1.569186 | -0.114381 | 1.635176 | |
| H | -2.403667 | -1.542569 | 1.007465 | |
| Rotational constants (GHz): | 3.1844700 | 2.1199600 | 1.6437000 | |
| Vibrational harmonic frequencies (cm-1): | | | | |
| i1406.8567 | 97.2148 | | 143.0492 | |
| 175.8633 | 211.0842 | | 271.3142 | |
| 309.2804 | 379.7338 | | 435.9071 | |
| 576.8198 | 590.3455 | | 744.9192 | |
| 770.4036 | 824.9411 | | 859.7950 | |
| 924.8681 | 950.5003 | | 957.4859 | |
| 1036.9016 | 1046.7366 | | 1065.5582 | |
| 1111.2713 | 1142.1936 | | 1156.5721 | |
| 1187.8422 | 1225.1571 | | 1257.0531 | |
| 1262.6119 | 1303.3407 | | 1353.6018 | |
| 1365.5560 | 1393.3206 | | 1393.7492 | |
| 1402.4183 | 1419.9679 | | 1465.1173 | |
| 1486.8713 | 1489.9967 | | 1499.0106 | |
| 1504.9440 | 1506.1564 | | 1516.7902 | |
| 2957.6372 | 3008.0508 | | 3009.5210 | |
| 3019.1426 | 3039.6943 | | 3050.4077 | |
| 3057.3886 | 3075.0357 | | 3080.2289 | |
| 3092.2755 | 3095.0166 | | 3127.0953 | |
| Zero-point correction (Hartree): | 0.176393 | | | |

C6H13O-1-6Hshift.c.e

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -311.61908353
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | | |
|---|-----------|-----------|-----------|--|
| C | 0.568492 | 1.136529 | 0.437178 | |
| C | -0.855167 | 1.511379 | -0.027144 | |
| C | -1.777273 | 0.323613 | -0.397606 | |
| C | -1.533465 | -0.967683 | 0.403515 | |
| O | -0.444362 | -1.717346 | -0.075212 | |

| | | | | |
|--|-----------|-----------|-----------|--|
| H | 0.487661 | -0.905733 | -0.337686 | |
| C | 1.252481 | 0.095255 | -0.428026 | |
| H | 0.535123 | 0.758593 | 1.468024 | |
| H | 1.180968 | 2.050154 | 0.478361 | |
| H | -1.323250 | 2.099949 | 0.771210 | |
| H | -0.788387 | 2.180310 | -0.894301 | |
| H | -2.820237 | 0.637565 | -0.270173 | |
| H | -1.659059 | 0.059819 | -1.454925 | |
| H | -1.444601 | -0.743492 | 1.481715 | |
| H | -2.407159 | -1.628696 | 0.289912 | |
| C | 2.618730 | -0.372700 | 0.030608 | |
| H | 1.216566 | 0.334352 | -1.497767 | |
| H | 2.588273 | -0.727743 | 1.066263 | |
| H | 3.346730 | 0.450209 | -0.014242 | |
| H | 2.999478 | -1.184871 | -0.595852 | |
| Rotational constants (GHz): | 3.4705600 | 1.9790000 | 1.4049800 | |
| Vibrational harmonic frequencies (cm-1): | | | | |
| i1404.1398 | 80.1020 | | 151.3131 | |
| 176.2402 | 218.6601 | | 257.9802 | |
| 287.0176 | 344.8911 | | 428.1143 | |
| 542.7504 | 592.8195 | | 749.9221 | |
| 793.2117 | 810.6250 | | 868.4600 | |
| 921.8911 | 962.9810 | | 966.7290 | |
| 1028.3360 | 1061.5504 | | 1075.9924 | |
| 1110.2845 | 1133.6114 | | 1159.5303 | |
| 1209.1728 | 1229.5838 | | 1260.5756 | |
| 1269.6323 | 1297.0176 | | 1330.8744 | |
| 1368.9839 | 1387.6845 | | 1395.9368 | |
| 1407.2044 | 1418.6408 | | 1466.1234 | |
| 1488.0270 | 1492.3705 | | 1499.3457 | |
| 1503.3292 | 1506.5382 | | 1511.0030 | |
| 2955.2639 | 3006.6592 | | 3007.7098 | |
| 3019.8499 | 3035.1418 | | 3043.7514 | |
| 3050.3825 | 3068.1289 | | 3072.6803 | |
| 3090.5948 | 3094.2051 | | 3124.5752 | |
| Zero-point correction (Hartree): | 0.176180 | | | |

C6H13O-1-7Hshift.BB

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -311.61539959
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | | |
|--|-----------|-----------|-----------|--|
| O | -1.193660 | -1.396578 | -0.441468 | |
| H | 0.025369 | -1.440181 | -0.480451 | |
| C | 1.318647 | -1.352863 | -0.347519 | |
| C | -1.547691 | -0.475033 | 0.557144 | |
| C | 1.607468 | -0.217523 | 0.608683 | |
| C | -1.385956 | 1.002534 | 0.145641 | |
| C | 1.244138 | 1.185622 | 0.078678 | |
| C | -0.107554 | 1.322960 | -0.647046 | |
| H | 1.655286 | -1.195001 | -1.375892 | |
| H | 1.592675 | -2.343913 | 0.021117 | |
| H | -2.606879 | -0.678489 | 0.780789 | |
| H | -1.009408 | -0.681864 | 1.496058 | |
| H | 1.099726 | -0.410556 | 1.562200 | |
| H | 2.681042 | -0.228626 | 0.857192 | |
| H | -2.238747 | 1.281381 | -0.485752 | |
| H | -1.448780 | 1.628001 | 1.047125 | |
| H | 1.288594 | 1.896470 | 0.914386 | |
| H | 2.025266 | 1.501072 | -0.625979 | |
| H | -0.184405 | 2.356185 | -1.007871 | |
| H | -0.104774 | 0.693966 | -1.544662 | |
| Rotational constants (GHz): | 3.0688900 | 2.3785100 | 1.6163900 | |
| Vibrational harmonic frequencies (cm-1): | | | | |
| i1597.6849 | 92.7374 | | 232.3139 | |
| 257.3145 | 267.8991 | | 286.5569 | |
| 361.8300 | 456.2221 | | 506.2817 | |
| 555.8910 | 561.7129 | | 737.1147 | |
| 777.9918 | 817.5559 | | 851.2996 | |
| 900.2202 | 943.5004 | | 972.5709 | |
| 1021.1316 | 1035.1175 | | 1086.7244 | |
| 1116.9089 | 1130.7769 | | 1152.7002 | |
| 1183.5393 | 1205.8867 | | 1234.0362 | |
| 1269.0981 | 1306.2995 | | 1310.2874 | |
| 1366.7214 | 1389.7584 | | 1397.2463 | |
| 1398.8727 | 1417.9472 | | 1447.1874 | |
| 1468.9028 | 1473.5659 | | 1492.9612 | |
| 1495.0135 | 1505.7028 | | 1512.9240 | |
| 2983.0131 | 2994.2664 | | 3012.2593 | |
| 3026.5246 | 3028.3619 | | 3044.6705 | |
| 3049.6472 | 3067.2796 | | 3071.3581 | |
| 3082.3543 | 3089.9361 | | 3161.3309 | |
| Zero-point correction (Hartree): | 0.176807 | | | |

C6H13O-1-7Hshift.BC

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -311.61351601

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -0.927032 | -1.419751 | -0.645458 |
| H | 0.210724 | -1.456616 | -0.184818 |
| C | 1.299192 | -1.289313 | 0.476063 |
| C | -1.706015 | -0.618492 | 0.209018 |
| C | 1.971595 | -0.025087 | -0.029029 |
| C | -1.525906 | 0.893762 | 0.033702 |
| C | 1.012307 | 1.062873 | -0.556463 |
| C | -0.142008 | 1.469314 | 0.395635 |
| H | 1.850604 | -2.217256 | 0.310309 |
| H | 0.921143 | -1.235827 | 1.500124 |
| H | -2.749074 | -0.883051 | -0.028067 |
| H | -1.557714 | -0.899728 | 1.266089 |
| H | 2.574873 | 0.398198 | 0.789241 |
| H | 2.676502 | -0.276825 | -0.829583 |
| H | -1.756818 | 1.149828 | -1.008545 |
| H | -2.287160 | 1.389572 | 0.652533 |
| H | 1.616702 | 1.946388 | -0.793887 |
| H | 0.587053 | 0.717239 | -1.505075 |
| H | -0.233853 | 2.561788 | 0.388554 |
| H | 0.108288 | 1.205950 | 1.433237 |

Rotational constants (GHz): 3.1754400 2.2633200 1.5416900

Vibrational harmonic frequencies (cm-1):

| | | |
|------------|-----------|-----------|
| i1535.6870 | 122.1403 | 146.8611 |
| 176.2178 | 255.1433 | 319.8221 |
| 338.7461 | 452.8124 | 486.5396 |
| 557.6422 | 600.0625 | 748.3075 |
| 782.0487 | 844.1394 | 867.2494 |
| 895.4731 | 946.3127 | 958.1300 |
| 1041.1924 | 1045.8226 | 1077.6851 |
| 1098.5045 | 1114.5600 | 1151.2002 |
| 1206.4469 | 1225.2269 | 1253.9289 |
| 1284.2505 | 1293.6363 | 1313.8859 |
| 1360.1261 | 1372.8082 | 1390.0298 |
| 1401.7534 | 1413.1829 | 1450.5199 |
| 1466.2989 | 1473.5054 | 1487.4278 |
| 1497.3537 | 1506.9613 | 1509.4555 |
| 2967.6525 | 3000.6330 | 3008.3863 |
| 3022.1761 | 3027.1807 | 3043.1548 |
| 3065.2406 | 3072.0864 | 3075.6047 |
| 3085.6338 | 3093.3316 | 3161.4737 |

Zero-point correction (Hartree): 0.176685

C6H13O-1-7Hshift.CR

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -311.61465160

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -1.168349 | -1.565082 | -0.260791 |
| H | 0.046702 | -1.547136 | -0.195336 |
| C | 1.332064 | -1.473001 | -0.154016 |
| C | -1.686051 | -0.444809 | 0.405316 |
| C | 1.769845 | -0.141299 | 0.412245 |
| C | -1.411524 | 0.912488 | -0.264312 |
| C | 1.238156 | 1.104579 | -0.325926 |
| C | -0.124018 | 1.654820 | 0.141995 |
| H | 1.583960 | -1.617327 | -1.208583 |
| H | 1.610364 | -2.342705 | 0.446229 |
| H | -2.773661 | -0.623350 | 0.404915 |
| H | -1.386967 | -0.416050 | 1.468535 |
| H | 1.512652 | -0.077925 | 1.478012 |
| H | 2.871596 | -0.122052 | 0.378829 |
| H | -1.442146 | 0.760408 | -1.350833 |
| H | -2.251474 | 1.577858 | -0.022014 |
| H | 1.969248 | 1.911214 | -0.190391 |
| H | 1.208560 | 0.905955 | -1.406220 |
| H | -0.208733 | 2.678334 | -0.245738 |
| H | -0.104131 | 1.756759 | 1.237109 |

Rotational constants (GHz): 2.9154000 2.3447600 1.4451400

Vibrational harmonic frequencies (cm-1):

| | | |
|------------|-----------|-----------|
| i1521.6519 | 67.2376 | 117.9654 |
| 238.6784 | 292.1792 | 302.9979 |
| 376.0523 | 406.1550 | 459.9603 |
| 470.3709 | 554.5236 | 728.8286 |
| 801.1106 | 816.8336 | 866.1938 |
| 911.5676 | 948.5184 | 974.3382 |
| 1019.5069 | 1050.3354 | 1095.7456 |
| 1115.7280 | 1119.7225 | 1148.8289 |
| 1170.3427 | 1222.8639 | 1254.4036 |
| 1278.5965 | 1304.3682 | 1306.7555 |
| 1372.2056 | 1387.3488 | 1396.6410 |

| | | |
|-----------|-----------|-----------|
| 1402.2372 | 1408.5149 | 1425.0569 |
| 1470.2555 | 1474.1698 | 1483.5179 |
| 1486.6278 | 1499.5038 | 1503.6003 |
| 2958.0246 | 2985.7936 | 3001.7836 |
| 3014.2227 | 3026.9586 | 3029.4559 |
| 3049.0004 | 3059.3658 | 3068.0422 |
| 3076.4905 | 3079.0266 | 3156.6960 |

Zero-point correction (Hartree): 0.175955

C7H15O.pmmmm

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.95007977

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 2.427329 | -1.237916 | 0.066909 |
| C | 2.696776 | 0.089160 | -0.140145 |
| C | 1.506232 | 0.934253 | -0.620247 |
| C | 0.433037 | 1.137824 | 0.462488 |
| C | -0.242246 | -0.145332 | 0.977671 |
| C | -1.017662 | -0.964866 | -0.069807 |
| C | -2.157819 | -0.227072 | -0.792591 |
| C | -3.285785 | 0.251046 | 0.129453 |
| H | 3.197649 | 0.550560 | 0.733422 |
| H | 3.469813 | 0.075266 | -0.940533 |
| H | 1.887815 | 1.913722 | -0.937160 |
| H | 1.078561 | 0.455822 | -1.508513 |
| H | 0.891083 | 1.657131 | 1.315924 |
| H | -0.326400 | 1.826324 | 0.070457 |
| H | 0.521510 | -0.800298 | 1.418795 |
| H | -0.910990 | 0.129442 | 1.803621 |
| H | -0.309786 | -1.353888 | -0.810948 |
| H | -1.434844 | -1.848380 | 0.432705 |
| H | -1.756168 | 0.629351 | -1.350385 |
| H | -2.577765 | -0.901871 | -1.549579 |
| H | -2.933396 | 0.988907 | 0.858183 |
| H | -3.716565 | -0.586054 | 0.691246 |
| H | -4.094351 | 0.717205 | -0.443440 |

Rotational constants (GHz): 3.9631900 0.9448300 0.8827600

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 47.1515 | 63.1195 | 104.4051 |
| 121.6649 | 193.8168 | 208.0898 |
| 264.6733 | 325.0315 | 355.4225 |
| 406.6811 | 460.7391 | 519.7847 |
| 719.9744 | 745.7694 | 783.9982 |
| 828.1122 | 855.7938 | 867.8874 |
| 916.4002 | 955.2232 | 994.2136 |
| 1006.3975 | 1044.1953 | 1083.9180 |
| 1093.9642 | 1107.3235 | 1122.5432 |
| 1158.9906 | 1190.6498 | 1216.7478 |
| 1267.8643 | 1304.5012 | 1334.6580 |
| 1342.4906 | 1362.2938 | 1376.7700 |
| 1384.4943 | 1401.2257 | 1410.1151 |
| 1411.7901 | 1429.1746 | 1481.6020 |
| 1492.9999 | 1499.3154 | 1509.0947 |
| 1512.1068 | 1518.4062 | 1525.3126 |
| 2880.4859 | 2940.8580 | 3018.9322 |
| 3024.3749 | 3030.6988 | 3032.8256 |
| 3040.0546 | 3041.3123 | 3055.7062 |
| 3061.7396 | 3069.9978 | 3080.1807 |
| 3092.0743 | 3107.9441 | 3112.1761 |

Zero-point correction (Hartree): 0.209401

C7H15O.pmmmp

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.94715948

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 2.286964 | -0.867920 | -0.922178 |
| C | 2.512083 | 0.328118 | -0.293242 |
| C | 1.249885 | 1.129417 | 0.062784 |
| C | 0.433916 | 0.493101 | 1.200681 |
| C | -0.109455 | -0.918514 | 0.919674 |
| C | -1.099229 | -1.086738 | -0.248408 |
| C | -2.467143 | -0.386324 | -0.099680 |
| C | -2.530146 | 1.063071 | -0.601378 |
| H | 3.183414 | 0.216218 | 0.580555 |
| H | 3.103176 | 0.906234 | -1.038058 |
| H | 1.558470 | 2.139681 | 0.362180 |
| H | 0.642258 | 1.235966 | -0.842535 |
| H | 1.068944 | 0.443670 | 2.096745 |
| H | -0.390554 | 1.167192 | 1.462107 |
| H | 0.740628 | -1.590460 | 0.735432 |
| H | -0.587411 | -1.286721 | 1.838370 |
| H | -0.621880 | -0.779602 | -1.187156 |
| H | -1.276241 | -2.164637 | -0.352670 |

| | | | | |
|--|-----------|-----------|-----------|--|
| H | -3.214030 | -0.965589 | -0.657308 | |
| H | -2.785843 | -0.428010 | 0.951383 | |
| H | -2.244249 | 1.122079 | -1.658041 | |
| H | -1.866230 | 1.730061 | -0.043586 | |
| H | -3.545635 | 1.464493 | -0.512573 | |
| Rotational constants (GHz): | 3.1052300 | 1.0596300 | 0.9943700 | |
| Vibrational harmonic frequencies (cm-1): | | | | |
| 47.3024 | 56.1427 | | 88.7797 | |
| 126.5673 | 177.2785 | | 218.7783 | |
| 237.5419 | 329.2309 | | 354.2030 | |
| 382.1482 | 454.5804 | | 501.0258 | |
| 731.0092 | 748.6987 | | 778.9219 | |
| 810.0837 | 861.9359 | | 873.7855 | |
| 907.3907 | 962.4892 | | 989.4719 | |
| 1010.4962 | 1055.9141 | | 1084.9911 | |
| 1094.8522 | 1110.2421 | | 1128.1796 | |
| 1163.7160 | 1174.3943 | | 1227.8464 | |
| 1264.7633 | 1313.8834 | | 1329.1913 | |
| 1340.8713 | 1367.2691 | | 1374.2115 | |
| 1385.2950 | 1398.8871 | | 1407.1903 | |
| 1411.2322 | 1426.3232 | | 1485.1751 | |
| 1492.3843 | 1495.9507 | | 1504.5402 | |
| 1509.7366 | 1518.5815 | | 1521.4247 | |
| 2881.2068 | 2940.6045 | | 3010.3479 | |
| 3022.6656 | 3023.2458 | | 3036.0771 | |
| 3041.3214 | 3042.6520 | | 3046.5378 | |
| 3060.9321 | 3071.2911 | | 3077.3227 | |
| 3096.9154 | 3105.5087 | | 3123.2786 | |
| Zero-point correction (Hartree): | 0.209170 | | | |

C7H15O.pmmmt

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.95127487

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | | |
|--|-----------|-----------|-----------|--|
| O | 2.157106 | -1.439470 | 0.348573 | |
| C | 2.616147 | -0.367051 | -0.369013 | |
| C | 1.525897 | 0.536194 | -0.968086 | |
| C | 0.768891 | 1.355089 | 0.090974 | |
| C | 0.004221 | 0.532930 | 1.143125 | |
| C | -1.109150 | -0.382187 | 0.607169 | |
| C | -2.242338 | 0.340993 | -0.133927 | |
| C | -3.367467 | -0.604056 | -0.568724 | |
| H | 3.364939 | 0.219455 | 0.198078 | |
| H | 3.186137 | -0.836333 | -1.201662 | |
| H | 2.004166 | 1.222550 | -1.679059 | |
| H | 0.835527 | -0.090799 | -1.543775 | |
| H | 1.487884 | 2.003036 | 0.611590 | |
| H | 0.077415 | 2.033205 | -0.424700 | |
| H | 0.718561 | -0.086949 | 1.702194 | |
| H | -0.426146 | 1.231624 | 1.874176 | |
| H | -0.670686 | -1.149050 | -0.043415 | |
| H | -1.538666 | -0.928962 | 1.457757 | |
| H | -2.654181 | 1.128567 | 0.512740 | |
| H | -1.845229 | 0.854427 | -1.019286 | |
| H | -3.820953 | -1.104410 | 0.294533 | |
| H | -2.990606 | -1.384834 | -1.239431 | |
| H | -4.162224 | -0.067238 | -1.097434 | |
| Rotational constants (GHz): | 3.3814000 | 0.9262600 | 0.8760600 | |
| Vibrational harmonic frequencies (cm-1): | | | | |
| 42.7003 | 77.8995 | | 90.7314 | |
| 126.8272 | 177.4925 | | 219.0418 | |
| 255.0378 | 275.7210 | | 345.3057 | |
| 383.5020 | 459.0785 | | 520.4076 | |
| 726.5613 | 760.1436 | | 773.3470 | |
| 827.6409 | 867.3165 | | 875.6283 | |
| 910.5886 | 964.5904 | | 995.8844 | |
| 1013.2606 | 1047.5694 | | 1084.4713 | |
| 1099.4397 | 1112.5401 | | 1116.6427 | |
| 1160.4764 | 1189.6289 | | 1233.0713 | |
| 1271.6460 | 1320.3684 | | 1327.8645 | |
| 1336.5045 | 1347.1440 | | 1367.5111 | |
| 1391.0350 | 1401.0875 | | 1409.0383 | |
| 1415.8848 | 1426.7092 | | 1483.0698 | |
| 1491.7718 | 1503.0123 | | 1506.6511 | |
| 1511.9065 | 1514.0223 | | 1526.2463 | |
| 2880.9541 | 2942.1834 | | 3012.5654 | |
| 3021.8436 | 3026.7637 | | 3032.0561 | |
| 3038.1846 | 3040.3276 | | 3047.8767 | |
| 3053.3001 | 3071.9811 | | 3077.7468 | |
| 3091.3127 | 3106.6086 | | 3110.2078 | |
| Zero-point correction (Hartree): | 0.209222 | | | |

C7H15O.pmmpm

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.94474197

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -1.796192 | -0.734973 | -1.317470 |
| C | -2.311255 | -0.562058 | -0.059027 |
| C | -1.260393 | -0.329118 | 1.040679 |
| C | -0.621447 | 1.070563 | 0.972294 |
| C | 0.102253 | 1.446119 | -0.336747 |
| C | 1.561197 | 0.983161 | -0.517005 |
| C | 1.813617 | -0.538787 | -0.642740 |
| C | 2.291153 | -1.209184 | 0.652384 |
| H | -3.106789 | 0.206939 | -0.031435 |
| H | -2.821872 | -1.528234 | 0.148891 |
| H | -1.753983 | -0.445802 | 2.014509 |
| H | 1.584296 | -1.071466 | 1.477438 |
| H | -1.422865 | 1.803052 | 1.141559 |
| H | 0.068645 | 1.186394 | 1.819177 |
| H | -0.490459 | 1.093409 | -1.193937 |
| H | 0.100752 | 2.541669 | -0.409987 |
| H | 1.933408 | 1.475923 | -1.423809 |
| H | 2.168511 | 1.386842 | 0.306170 |
| H | 0.906430 | -1.029019 | -1.015140 |
| H | 2.579626 | -0.708510 | -1.409536 |
| H | -0.510076 | -1.120661 | 0.964795 |
| H | 3.249880 | -0.788139 | 0.976839 |
| H | 2.433282 | -2.286788 | 0.515200 |

Rotational constants (GHz): 2.5192500 1.2151900 1.1372900

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 49.9704 | 85.9889 | 114.6799 |
| 130.2408 | 149.4155 | 223.7828 |
| 259.5684 | 304.9539 | 345.7713 |
| 377.0456 | 431.7187 | 484.5380 |
| 723.5991 | 775.9144 | 806.8439 |
| 824.7267 | 834.3145 | 895.0380 |
| 902.7182 | 961.9928 | 992.9300 |
| 1018.6461 | 1050.5888 | 1088.5945 |
| 1095.4095 | 1117.1958 | 1135.7184 |
| 1148.9373 | 1184.2189 | 1224.0163 |
| 1295.2237 | 1300.6540 | 1323.8195 |
| 1337.5641 | 1364.6333 | 1376.0297 |
| 1392.4862 | 1397.7515 | 1408.6121 |

| | | |
|-----------|-----------|-----------|
| 1417.4150 | 1427.3889 | 1487.3606 |
| 1491.8015 | 1495.0596 | 1503.6965 |
| 1512.3237 | 1515.4897 | 1525.6661 |
| 2884.0895 | 2949.3657 | 3002.1227 |
| 3015.7773 | 3018.0663 | 3037.6569 |
| 3039.6338 | 3044.1255 | 3053.1735 |
| 3056.4950 | 3064.1553 | 3078.2260 |
| 3106.0384 | 3112.7210 | 3123.7300 |

Zero-point correction (Hartree): 0.209358

C7H15O.pmmpp

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.94507299

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 1.555754 | 1.281872 | -0.807706 |
| C | 2.246798 | 0.450081 | 0.116423 |
| C | 1.355201 | -0.496654 | 0.927734 |
| C | 0.602669 | -1.576527 | 0.124638 |
| C | -0.488172 | -1.116156 | -0.866930 |
| C | -1.873487 | -0.791015 | -0.276484 |
| C | -1.982042 | 0.428082 | 0.661127 |
| C | -1.544064 | 1.725395 | 0.067425 |
| H | 2.959166 | -0.130447 | -0.482878 |
| H | 2.841427 | 1.060351 | 0.817239 |
| H | 2.005963 | -1.002358 | 1.654794 |
| H | 0.660071 | 0.103848 | 1.527864 |
| H | 1.354374 | -2.145701 | -0.439335 |
| H | 0.160890 | -2.292279 | 0.832768 |
| H | -0.111912 | -0.267237 | -1.444328 |
| H | -0.641067 | -1.930821 | -1.586890 |
| H | -2.566017 | -0.632874 | -1.114635 |
| H | -2.250227 | -1.671224 | 0.262123 |
| H | -3.041134 | 0.518245 | 0.968714 |
| H | -1.445104 | 0.243761 | 1.600985 |
| H | -1.643648 | 1.902178 | -1.000413 |
| H | 0.778621 | 1.651616 | -0.358197 |
| H | -1.408857 | 2.598734 | 0.700239 |

Rotational constants (GHz): 2.4207600 1.4316500 1.1149800

Vibrational harmonic frequencies (cm-1):

| | | |
|----------|----------|----------|
| 66.7443 | 96.0554 | 117.9620 |
| 157.9603 | 215.8422 | 235.1891 |
| 254.8477 | 290.9616 | 332.0253 |

| | | |
|-----------|-----------|-----------|
| 391.8580 | 424.4757 | 474.6076 |
| 509.3474 | 574.1428 | 748.7459 |
| 769.5412 | 809.7246 | 844.4450 |
| 877.7883 | 905.4563 | 934.3530 |
| 992.9048 | 1022.3573 | 1053.1289 |
| 1070.3333 | 1111.8536 | 1121.6953 |
| 1148.7575 | 1168.7358 | 1203.2405 |
| 1224.7911 | 1292.7711 | 1317.6354 |
| 1322.4058 | 1367.5004 | 1383.7886 |
| 1389.0039 | 1401.9781 | 1405.1011 |
| 1412.0966 | 1437.2883 | 1472.2611 |
| 1477.0903 | 1495.3144 | 1499.3768 |
| 1503.3646 | 1510.5234 | 1527.8088 |
| 2936.5519 | 2973.5964 | 3012.4633 |
| 3020.3747 | 3030.0458 | 3038.6222 |
| 3040.8063 | 3050.6896 | 3057.9522 |
| 3062.3260 | 3080.9677 | 3114.9892 |
| 3142.6815 | 3243.0387 | 3707.8808 |

Zero-point correction (Hartree): 0.209314

C7H15O.pmmpt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.94895900

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -1.610302 | -1.433810 | -0.890330 |
| C | -2.382715 | -0.769790 | 0.026716 |
| C | -1.599927 | 0.099188 | 1.026645 |
| C | -1.019607 | 1.374098 | 0.386149 |
| C | -0.035376 | 1.181309 | -0.784253 |
| C | 1.430182 | 0.873526 | -0.427639 |
| C | 1.708649 | -0.481915 | 0.240551 |
| C | 3.204085 | -0.812981 | 0.293863 |
| H | -3.203733 | -0.200123 | -0.449714 |
| H | -2.878647 | -1.589723 | 0.591817 |
| H | -2.285019 | 0.388759 | 1.834374 |
| H | -0.816318 | -0.517879 | 1.474927 |

| | | | |
|---|-----------|-----------|-----------|
| H | -1.865892 | 1.977004 | 0.028712 |
| H | -0.538549 | 1.973963 | 1.171160 |
| H | -0.412901 | 0.396157 | -1.455933 |
| H | -0.041320 | 2.105400 | -1.376955 |
| H | 2.011851 | 0.920750 | -1.358868 |
| H | 1.823759 | 1.679672 | 0.209126 |
| H | 1.309747 | -0.483995 | 1.262452 |
| H | 1.167717 | -1.269253 | -0.298737 |
| H | 3.762190 | -0.047060 | 0.845348 |
| H | 3.632494 | -0.869641 | -0.713561 |
| H | 3.385287 | -1.774152 | 0.786290 |

Rotational constants (GHz): 2.8147900 1.0776500 0.9390500

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 45.8249 | 81.2364 | 107.9000 |
| 124.3290 | 146.7324 | 238.2150 |
| 262.6172 | 279.3589 | 340.6855 |
| 366.2879 | 445.3780 | 498.4536 |
| 750.4474 | 754.8897 | 804.7003 |
| 827.6550 | 842.0004 | 885.2640 |
| 916.5097 | 967.8327 | 982.6223 |
| 1017.3859 | 1044.1688 | 1081.6459 |
| 1098.4109 | 1110.1258 | 1128.9426 |
| 1151.1659 | 1193.6659 | 1233.9581 |
| 1290.1666 | 1303.5977 | 1333.5533 |
| 1337.6170 | 1349.5578 | 1365.7966 |
| 1391.9778 | 1403.2490 | 1415.2228 |
| 1416.4119 | 1426.5700 | 1486.2295 |
| 1494.3996 | 1496.9340 | 1503.7632 |
| 1509.5086 | 1513.9872 | 1524.7021 |
| 2883.5443 | 2946.6161 | 3006.0070 |
| 3010.1023 | 3017.2685 | 3036.2246 |
| 3037.9250 | 3043.9568 | 3046.5439 |
| 3054.9697 | 3056.9069 | 3078.3317 |
| 3106.1950 | 3110.5984 | 3119.6152 |

Zero-point correction (Hartree): 0.209242

C7H15O.pmmtm

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.95117657

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -1.290148 | 1.735168 | -0.026053 |
| C | -2.356717 | 0.877014 | 0.024367 |
| C | -2.080689 | -0.543751 | -0.492243 |
| C | -1.172612 | -1.361830 | 0.442217 |
| C | 0.234954 | -0.787185 | 0.673116 |
| C | 1.107207 | -0.711352 | -0.588000 |

| | | | |
|--|-----------|-----------|-----------|
| C | 2.573292 | -0.331984 | -0.318773 |
| C | 2.768382 | 1.075700 | 0.257829 |
| H | -2.828243 | 0.862498 | 1.026487 |
| H | -3.108873 | 1.358154 | -0.639849 |
| H | -3.042320 | -1.061903 | -0.602261 |
| H | -1.642618 | -0.467777 | -1.493636 |
| H | -1.676533 | -1.468457 | 1.413034 |
| H | -1.084142 | -2.378175 | 0.034620 |
| H | 0.150051 | 0.212330 | 1.120150 |
| H | 0.740816 | -1.412721 | 1.422327 |
| H | 1.082557 | -1.685621 | -1.096695 |
| H | 0.675040 | 0.016930 | -1.285458 |
| H | 3.019450 | -1.071030 | 0.361560 |
| H | 3.132450 | -0.411820 | -1.259965 |
| H | 2.313434 | 1.178448 | 1.248235 |
| H | 2.314819 | 1.833592 | -0.390811 |
| H | 3.832391 | 1.314527 | 0.359609 |
| Rotational constants (GHz): | 2.9900700 | 1.0937600 | 0.8935300 |
| Vibrational harmonic frequencies (cm-1): | | | |
| 39.6265 | 47.7086 | | 110.5735 |
| 121.6971 | 163.3632 | | 212.3068 |
| 241.4896 | 297.6289 | | 342.8977 |
| 372.8053 | 462.1314 | | 507.5857 |
| 733.2324 | 765.5746 | | 781.7228 |
| 821.4808 | 858.4489 | | 884.0312 |
| 902.0950 | 963.0715 | | 984.9064 |
| 1014.2111 | 1056.1984 | | 1084.3987 |
| 1099.1245 | 1109.7218 | | 1117.3805 |
| 1164.9547 | 1182.9190 | | 1230.0053 |
| 1283.6800 | 1313.0741 | | 1324.0276 |
| 1338.4885 | 1346.7393 | | 1375.3054 |
| 1385.1865 | 1391.3795 | | 1405.4755 |
| 1415.0388 | 1428.0232 | | 1486.6477 |
| 1493.0212 | 1501.1073 | | 1502.3316 |
| 1507.9156 | 1515.3068 | | 1521.8464 |
| 2880.7390 | 2940.2023 | | 3011.9779 |
| 3018.1431 | 3021.9531 | | 3025.5232 |
| 3041.0653 | 3043.1173 | | 3047.2667 |
| 3056.2654 | 3061.1924 | | 3078.6584 |
| 3095.0612 | 3111.1171 | | 3115.9000 |
| Zero-point correction (Hartree): | 0.209036 | | |

C7H15O.pmmtp

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.95114222

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|--|-----------|-----------|-----------|
| O | -1.836149 | -1.598229 | -0.276137 |
| C | -2.656865 | -0.505361 | -0.180671 |
| C | -2.059601 | 0.698591 | 0.564106 |
| C | -0.938558 | 1.399172 | -0.223303 |
| C | 0.292226 | 0.535370 | -0.546653 |
| C | 1.077897 | 0.055707 | 0.681945 |
| C | 2.344502 | -0.750625 | 0.347547 |
| C | 3.453075 | 0.053030 | -0.343026 |
| H | -3.070619 | -0.211748 | -1.165229 |
| H | -3.529415 | -0.884900 | 0.396285 |
| H | -2.865952 | 1.418178 | 0.757228 |
| H | -1.696806 | 0.356133 | 1.539483 |
| H | -1.360287 | 1.780466 | -1.163806 |
| H | -0.618555 | 2.283818 | 0.343900 |
| H | -0.017310 | -0.342873 | -1.132051 |
| H | 0.948971 | 1.120502 | -1.202781 |
| H | 1.353894 | 0.923066 | 1.300474 |
| H | 0.424323 | -0.572348 | 1.297813 |
| H | 2.743096 | -1.174837 | 1.278045 |
| H | 2.067071 | -1.608504 | -0.279858 |
| H | 3.755154 | 0.913141 | 0.266493 |
| H | 3.137136 | 0.434940 | -1.319243 |
| H | 4.342441 | -0.564494 | -0.507329 |
| Rotational constants (GHz): | 3.6982300 | 0.9165800 | 0.8149800 |
| Vibrational harmonic frequencies (cm-1): | | | |
| 42.8836 | 62.2658 | | 111.4901 |
| 125.6583 | 163.2286 | | 216.1618 |
| 238.2090 | 292.7947 | | 340.6475 |
| 386.4908 | 460.4621 | | 503.6814 |
| 730.6237 | 753.3064 | | 782.5292 |
| 836.1268 | 858.2983 | | 874.6158 |
| 912.7509 | 959.4000 | | 988.7413 |
| 1012.4235 | 1060.7347 | | 1082.8930 |
| 1100.5118 | 1107.7151 | | 1115.3676 |
| 1162.0972 | 1189.9670 | | 1228.0572 |
| 1292.7358 | 1299.6722 | | 1333.5603 |
| 1343.6977 | 1348.9121 | | 1377.3194 |
| 1387.5568 | 1392.7948 | | 1406.5532 |

| | | |
|-----------|-----------|-----------|
| 1418.2999 | 1430.3955 | 1487.7186 |
| 1493.5527 | 1498.6212 | 1502.6293 |
| 1506.7771 | 1516.3342 | 1522.0256 |
| 2881.3986 | 2940.6226 | 3007.4974 |
| 3016.9885 | 3019.5898 | 3029.8132 |
| 3039.7517 | 3041.6638 | 3055.9810 |
| 3060.9164 | 3064.5179 | 3084.0785 |
| 3096.4378 | 3106.5748 | 3115.0186 |

Zero-point correction (Hartree): 0.209182

C7H15O.pmmtt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.95257450

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 1.610173 | 1.674708 | -0.389935 |
| C | 2.557231 | 0.771659 | 0.015370 |
| C | 2.020165 | -0.433216 | 0.803409 |
| C | 1.218978 | -1.416990 | -0.066424 |
| C | -0.041112 | -0.842924 | -0.734428 |
| C | -1.129626 | -0.370255 | 0.237798 |
| C | -2.414388 | 0.078190 | -0.471133 |
| C | -3.502631 | 0.555815 | 0.495555 |
| H | 3.210090 | 0.454689 | -0.821345 |
| H | 3.217267 | 1.369477 | 0.682819 |
| H | 2.873996 | -0.960762 | 1.248405 |
| H | 1.409324 | -0.058631 | 1.632266 |
| H | 1.883705 | -1.814771 | -0.846001 |
| H | 0.935860 | -2.276754 | 0.555930 |
| H | 0.236752 | -0.005097 | -1.390018 |
| H | -0.459726 | -1.615388 | -1.394577 |
| H | -1.368492 | -1.180087 | 0.943216 |
| H | -0.746600 | 0.464520 | 0.837601 |
| H | -2.171706 | 0.884157 | -1.176503 |
| H | -2.802424 | -0.751186 | -1.078669 |
| H | -3.157206 | 1.409648 | 1.089583 |
| H | -3.787915 | -0.238435 | 1.195212 |
| H | -4.406004 | 0.867284 | -0.039320 |

Rotational constants (GHz): 3.3205800 0.9117400 0.8068700

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 43.0879 | 56.3925 | 97.8830 |
| 116.3676 | 150.5696 | 189.2726 |
| 247.0458 | 265.7419 | 342.7561 |
| 395.2204 | 429.6372 | 492.2950 |
| 729.6350 | 763.2851 | 769.1903 |
| 834.4994 | 858.8876 | 897.4126 |
| 909.4351 | 968.1914 | 980.7305 |
| 1026.2418 | 1058.7559 | 1076.9484 |
| 1100.1079 | 1109.7005 | 1115.1964 |
| 1166.2543 | 1187.7148 | 1241.5938 |
| 1285.8995 | 1303.9104 | 1326.9528 |
| 1337.8629 | 1340.9773 | 1366.8256 |
| 1388.6456 | 1393.8229 | 1406.2317 |
| 1416.3655 | 1426.9286 | 1486.6436 |
| 1492.4952 | 1499.0405 | 1500.0938 |
| 1509.7317 | 1513.8246 | 1523.3590 |
| 2880.4789 | 2940.3987 | 3007.9854 |
| 3014.2414 | 3019.2706 | 3024.9211 |
| 3037.7735 | 3040.7663 | 3044.4329 |
| 3052.8912 | 3059.2096 | 3078.2104 |
| 3094.7440 | 3106.1488 | 3110.7121 |

Zero-point correction (Hartree): 0.208798

C7H15O.pmpmm

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.94944811

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -0.917255 | -1.361296 | -0.439386 |
| C | 2.031335 | -1.322941 | 0.462353 |
| C | 2.187595 | -0.235339 | -0.548838 |
| C | 1.703289 | 1.166947 | -0.124546 |
| C | 0.180959 | 1.402841 | -0.173729 |
| C | -0.652193 | 0.676572 | 0.912003 |
| C | -1.599951 | -0.419747 | 0.386127 |
| C | -2.761524 | 0.122772 | -0.442098 |
| H | 2.160434 | -1.109932 | 1.520530 |
| H | 2.129216 | -2.362737 | 0.159372 |
| H | 3.262534 | -0.156592 | -0.800428 |
| H | 1.695503 | -0.527023 | -1.485961 |
| H | 2.080394 | 1.390175 | 0.883668 |
| H | 2.177557 | 1.897860 | -0.791355 |
| H | 0.013169 | 2.483025 | -0.092248 |
| H | -0.178585 | 1.114867 | -1.168407 |
| H | 0.019403 | 0.220327 | 1.650827 |

| | | | |
|--|-----------|-----------|-----------|
| H | -1.256101 | 1.399495 | 1.474863 |
| H | -0.109377 | -1.631786 | 0.028416 |
| H | -2.025239 | -0.934520 | 1.265717 |
| H | -2.400703 | 0.677458 | -1.313597 |
| H | -3.389031 | 0.788077 | 0.159677 |
| H | -3.378202 | -0.704958 | -0.803613 |
| Rotational constants (GHz): | 3.0215100 | 1.2939600 | 1.0615800 |
| Vibrational harmonic frequencies (cm-1): | | | |
| 68.4351 | 94.1679 | | 111.0641 |
| 163.1621 | 218.3749 | | 248.4973 |
| 267.0881 | 286.6160 | | 335.8250 |
| 357.8512 | 422.2842 | | 457.1765 |
| 495.6537 | 602.1607 | | 611.1065 |
| 737.5749 | 811.3338 | | 820.8747 |
| 856.5548 | 896.9352 | | 955.5937 |
| 968.3476 | 974.3560 | | 1042.0975 |
| 1075.3620 | 1078.2517 | | 1117.4239 |
| 1144.3449 | 1152.1464 | | 1199.5546 |
| 1243.9111 | 1264.3847 | | 1306.4026 |
| 1311.1237 | 1350.0451 | | 1375.2763 |
| 1379.3888 | 1397.3287 | | 1409.9007 |
| 1414.2190 | 1459.6425 | | 1466.4749 |
| 1477.2030 | 1496.2375 | | 1499.2172 |
| 1503.7053 | 1504.9404 | | 1517.9673 |
| 2930.9559 | 2956.2353 | | 3022.3414 |
| 3033.8331 | 3044.2202 | | 3052.2665 |
| 3053.5888 | 3064.1996 | | 3072.6103 |
| 3088.8934 | 3127.2825 | | 3132.0509 |
| 3138.7365 | 3237.5896 | | 3679.2024 |
| Zero-point correction (Hartree): | 0.208638 | | |

C7H15O.pmpmt

```

-----
E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.94868065
Electronic state : 2-A
Cartesian coordinates (Angs):
O      -1.221643    -1.831460    -0.200857
C      -2.252284    -0.863316    -0.058108
C      -1.755116     0.461868     0.524333
C      -0.918889     1.309688    -0.472666
C       0.395418     1.895516     0.089762
C       1.636284     1.014323    -0.157818
C       1.582754    -0.367693     0.413950
C       2.520284    -1.434257    -0.052557
H      -2.753817    -0.675502    -1.023709
H      -2.998999    -1.310641     0.608285
H      -2.618363     1.046500     0.865687
H      -1.170814     0.231279     1.422712
H      -0.677709     0.708611    -1.361030
H      -1.546895     2.127075    -0.844321
H       0.587425     2.873207    -0.367971
H       0.284675     2.084293     1.165884
H       1.818104     0.949244    -1.241420
H       2.520867     1.545086     0.244562
H       1.132435    -0.494135     1.397201
H      -0.407199    -1.371074    -0.455546
H       3.525084    -1.318812     0.391714
H       2.659239    -1.406396    -1.140309
H       2.168407    -2.433828     0.223735
Rotational constants (GHz): 2.2345400 1.4074800 0.9363900
Vibrational harmonic frequencies (cm-1):
33.8015 48.1982 68.3138
106.5753 151.7563 163.4866
230.6224 264.4053 300.5043
324.1940 367.5610 453.3965
505.0943 541.9756 730.8558
806.2806 836.8692 859.5354
917.4760 957.1141 982.9837
1014.4057 1047.9141 1070.2761
1090.1298 1104.7068 1133.1335
1152.1306 1186.1046 1226.0284
1246.3477 1264.2282 1299.1052
1338.8567 1349.3990 1375.9875
1383.2979 1395.0331 1415.3110
1425.0373 1443.0196 1476.7959
1490.9163 1496.5109 1498.8419
1506.0468 1510.8121 1533.7656
2927.6016 2962.0660 2967.2727
3014.9074 3020.3750 3035.6220
3041.0656 3057.0463 3066.8438
3072.5974 3074.5537 3089.5745
3107.8127 3163.8657 3731.6648
Zero-point correction (Hartree): 0.208357
    
```

C7H15O.pmppm

```

-----
E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.95475743
Electronic state : 2-A
Cartesian coordinates (Angs):
O      -0.657114      -1.709020      0.747628
C      -1.489660      -1.348476      -0.343059
C      -2.150445      0.031299      -0.218617
C      -1.267578      1.259035      -0.516303
C      -0.205971      1.637383      0.546173
C      0.989490      0.737834      0.674253
C      1.920779      0.456458      -0.466329
C      2.725029      -0.841015      -0.288935
H      -0.945534      -1.406601      -1.302597
H      -2.270954      -2.115867      -0.377757
H      -2.991735      0.053982      -0.924799
H      -2.586957      0.115597      0.785665
H      -0.784243      1.126216      -1.493680
H      -1.927741      2.127700      -0.630187
H      0.148876      2.655261      0.298981
H      -0.699139      1.727331      1.521821
H      1.395899      0.589153      1.675833
H      0.010388      -1.004699      0.851437
H      1.366111      0.421579      -1.412440
H      2.624153      1.303046      -0.575701
H      2.055698      -1.704268      -0.218358
H      3.325283      -0.808598      0.627164
H      3.406940      -1.002778      -1.129507
Rotational constants (GHz):      2.4045600      1.3983600      1.0395200
Vibrational harmonic frequencies (cm-1):
      56.7651      66.6765      67.5265
      163.8532      188.3865      217.5554
      259.8779      312.6029      327.6791
      379.2692      461.8569      484.4108
      541.6017      583.7225      754.8798
      778.5860      813.0064      866.4799
      889.9105      936.2799      960.7288
      1016.4992      1053.8069      1061.7077
      1072.1498      1106.4704      1130.1768
      1163.5169      1207.8036      1221.3979
      1272.2653      1280.2318      1289.7046
      1322.0321      1378.0187      1385.6989
      1395.8666      1399.7246      1423.4412
      1428.5261      1444.4051      1476.6566
      1482.3142      1486.7355      1501.1734
      1513.6661      1522.5620      1524.3325
      2940.5855      2945.2656      2961.2611
      3023.4040      3032.0362      3045.3777
      3056.4945      3059.8750      3066.5765
      3075.6519      3078.4730      3115.2587
      3125.2764      3138.1083      3563.3725
Zero-point correction (Hartree): 0.209363
    
```

C7H15O.pmppp

```

-----
E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.94697330
Electronic state : 2-A
Cartesian coordinates (Angs):
O      -1.969539      -1.456575      0.409388
C      -2.220750      -0.550469      -0.588508
C      -1.987070      0.925694      -0.232379
C      -0.520304      1.394589      -0.209408
C      0.372153      0.844778      0.923538
C      0.943179      -0.574517      0.739076
C      1.882456      -0.772010      -0.463742
C      3.156996      0.080115      -0.422372
H      -1.717348      -0.829242      -1.534478
H      -3.304452      -0.699740      -0.792570
H      -2.527680      1.531416      -0.972048
H      -2.458049      1.116361      0.740269
H      -0.061183      1.190115      -1.186270
H      -0.539377      2.488199      -0.120831
H      1.207690      1.541886      1.064100
H      -0.196190      0.871929      1.862386
H      1.490263      -0.838352      1.654990
H      0.121745      -1.299706      0.671749
H      2.164033      -1.831879      -0.504933
H      1.343871      -0.574176      -1.400050
H      3.719441      -0.096588      0.502018
H      2.936376      1.151421      -0.473674
H      3.817215      -0.158120      -1.262989
Rotational constants (GHz):      3.1302700      1.0795900      0.9456000
Vibrational harmonic frequencies (cm-1):
      37.6564      56.3350      91.1431
      137.3767      179.2102      226.1933
      267.3121      318.4323      348.4588
    
```

| | | |
|-----------|-----------|-----------|
| 404.3672 | 463.1532 | 478.6412 |
| 712.6101 | 759.2259 | 766.5908 |
| 817.9418 | 853.8936 | 881.7570 |
| 922.8246 | 943.4043 | 1001.4094 |
| 1006.4682 | 1050.3885 | 1082.2911 |
| 1101.5498 | 1119.1002 | 1123.9176 |
| 1171.2106 | 1195.6791 | 1240.2692 |
| 1279.3448 | 1295.6624 | 1335.6373 |
| 1348.3889 | 1371.8210 | 1381.3318 |
| 1386.1934 | 1400.5848 | 1405.3303 |
| 1407.9010 | 1429.9628 | 1480.3517 |
| 1492.6160 | 1497.0865 | 1506.7215 |
| 1509.8813 | 1519.8518 | 1525.0284 |
| 2882.3563 | 2944.4419 | 3013.0008 |
| 3024.7024 | 3027.8366 | 3032.1018 |
| 3037.3431 | 3041.7351 | 3050.4421 |
| 3061.9546 | 3066.8075 | 3072.2475 |
| 3080.8077 | 3108.1497 | 3114.3773 |

Zero-point correction (Hartree): 0.209343

C7H15O.pmppt

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.95475747
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -0.658105 | -1.708852 | 0.747595 |
| C | -1.490494 | -1.348126 | -0.343135 |
| C | -2.150686 | 0.031946 | -0.218867 |
| C | -1.267179 | 1.259271 | -0.516281 |
| C | -0.205582 | 1.636970 | 0.546437 |
| C | 0.989671 | 0.737116 | 0.674348 |
| C | 1.921193 | 0.456239 | -0.466162 |
| C | 2.725650 | -0.841126 | -0.289052 |
| H | -0.946427 | -1.406630 | -1.302684 |
| H | -2.272136 | -2.115171 | -0.377711 |
| H | -2.991782 | 0.055011 | -0.925268 |
| H | -2.587408 | 0.116432 | 0.785306 |
| H | -0.783743 | 1.126344 | -1.493596 |
| H | -1.926906 | 2.128267 | -0.630171 |
| H | 0.149556 | 2.654846 | 0.299646 |
| H | -0.698835 | 1.726704 | 1.522060 |
| H | 1.395825 | 0.587870 | 1.675949 |
| H | 0.010206 | -1.005198 | 0.850803 |
| H | 1.366673 | 0.421557 | -1.412372 |
| H | 2.624420 | 1.303001 | -0.575180 |
| H | 2.056480 | -1.704535 | -0.218827 |
| H | 3.325776 | -0.808893 | 0.627135 |
| H | 3.407698 | -1.002533 | -1.129582 |

Rotational constants (GHz): 2.4050300 1.3978300 1.0393300
 Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 56.5827 | 66.5073 | 67.4345 |
| 163.9127 | 188.3844 | 217.5908 |
| 259.8324 | 312.5358 | 327.6840 |
| 379.2682 | 461.8888 | 484.3978 |
| 541.4724 | 583.7552 | 754.9118 |
| 778.5904 | 813.0144 | 866.4983 |
| 889.9151 | 936.2826 | 960.7391 |
| 1016.5349 | 1053.8201 | 1061.7091 |
| 1072.1467 | 1106.4889 | 1130.1843 |
| 1163.5004 | 1207.7846 | 1221.4291 |
| 1272.2813 | 1280.2467 | 1289.7140 |
| 1322.0410 | 1378.0174 | 1385.7080 |
| 1395.8852 | 1399.7649 | 1423.4520 |
| 1428.5218 | 1444.3835 | 1476.6603 |
| 1482.3090 | 1486.7332 | 1501.1803 |
| 1513.6588 | 1522.5542 | 1524.3038 |
| 2940.5580 | 2945.2278 | 2961.2668 |
| 3023.4028 | 3032.0269 | 3045.3760 |
| 3056.4642 | 3059.8747 | 3066.5800 |
| 3075.6461 | 3078.4642 | 3115.2590 |
| 3125.2377 | 3138.1058 | 3563.2101 |

Zero-point correction (Hartree): 0.209361

C7H15O.pmpptm

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.95512868
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 1.394774 | -1.693769 | -0.261533 |
| C | 2.336117 | -0.802321 | 0.313536 |
| C | 2.279246 | 0.624439 | -0.246615 |
| C | 1.095127 | 1.504096 | 0.197208 |
| C | -0.303523 | 1.103252 | -0.320537 |
| C | -0.964873 | -0.035560 | 0.394890 |

| | | | | |
|---|-----------|-----------|-----------|-------------------------------|
| C | -2.168263 | -0.726064 | -0.174501 | |
| C | -3.488629 | 0.041082 | 0.078796 | |
| H | 2.243501 | -0.770766 | 1.413585 | |
| H | 3.319838 | -1.231344 | 0.092233 | |
| H | 3.204276 | 1.134961 | 0.055315 | |
| H | 2.302425 | 0.561023 | -1.342633 | |
| H | 1.068728 | 1.553843 | 1.295499 | |
| H | 1.296935 | 2.527247 | -0.142497 | |
| H | -0.957346 | 1.992037 | -0.238178 | |
| H | -0.254400 | 0.886436 | -1.397500 | |
| H | 0.507677 | -1.378424 | -0.008046 | |
| H | -0.826048 | -0.088309 | 1.476745 | |
| H | -2.040319 | -0.861640 | -1.256449 | |
| H | -2.263033 | -1.729856 | 0.259774 | |
| H | -3.463437 | 1.034726 | -0.379802 | |
| H | -3.668645 | 0.170450 | 1.151072 | |
| H | -4.339560 | -0.503780 | -0.343519 | |
| Rotational constants (GHz): | | | | 3.3525800 1.0134200 0.8293300 |
| Vibrational harmonic frequencies (cm-1): | | | | |
| 38.4757 | | 64.4838 | 78.2190 | |
| 126.1635 | | 176.1053 | 209.2251 | |
| 262.2174 | | 311.7096 | 327.6241 | |
| 368.3827 | | 460.3261 | 481.4462 | |
| 517.8204 | | 612.5283 | 754.4005 | |
| 790.8225 | | 834.4033 | 849.2575 | |
| 908.8829 | | 942.3318 | 962.2362 | |
| 990.6038 | | 1035.2196 | 1057.7181 | |
| 1083.4675 | | 1109.5227 | 1147.4573 | |
| 1151.5882 | | 1197.3229 | 1221.7604 | |
| 1270.6049 | | 1283.7235 | 1302.8651 | |
| 1331.5914 | | 1356.1893 | 1391.0965 | |
| 1396.7675 | | 1406.8790 | 1412.0401 | |
| 1429.7316 | | 1439.7710 | 1472.5520 | |
| 1486.1512 | | 1495.6373 | 1500.5193 | |
| 1510.7443 | | 1518.4221 | 1519.1123 | |
| 2933.4744 | | 2964.5496 | 3018.7946 | |
| 3024.3454 | | 3027.1431 | 3034.8307 | |
| 3044.4393 | | 3064.8204 | 3066.0799 | |
| 3071.9603 | | 3077.6667 | 3117.0583 | |
| 3121.6301 | | 3130.6796 | 3588.0913 | |
| Zero-point correction (Hartree): 0.209322 | | | | |

C7H15O.pmpm

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.92737068
Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 2.020616 | -1.611466 | -0.675464 |
| C | 2.381008 | -0.668476 | 0.422236 |
| C | 2.289153 | 0.803671 | 0.011903 |
| C | 0.899772 | 1.501398 | -0.027617 |
| C | -0.369238 | 0.694667 | -0.402635 |
| C | -1.081526 | -0.089668 | 0.716088 |
| C | -2.343595 | -0.827753 | 0.245488 |
| C | -3.428973 | 0.089378 | -0.341359 |
| H | 1.715104 | -0.867738 | 1.255162 |
| H | 3.414042 | -0.897299 | 0.694474 |
| H | 2.917054 | 1.338492 | 0.727560 |
| H | 2.702670 | 0.862409 | -0.997092 |
| H | 0.732550 | 1.943414 | 0.957448 |
| H | 1.007850 | 2.273343 | -0.791760 |
| H | -1.089000 | 1.428597 | -0.770015 |
| H | -0.078833 | -0.001908 | -1.194181 |
| H | -0.396422 | -0.830582 | 1.110142 |
| H | -1.365507 | 0.631839 | 1.487185 |
| H | -2.034757 | -1.541067 | -0.522288 |
| H | -2.757786 | -1.343092 | 1.114959 |
| H | -3.011739 | 0.607622 | -1.205431 |
| H | -3.725649 | 0.802059 | 0.430509 |
| H | -4.274112 | -0.533666 | -0.637587 |
| Rotational constants (GHz): 3.3400432 0.9171589 0.7960337 | | | |

C7H15O.pmpmp

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.94851096
Electronic state : 2-A
Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -1.170644 | 1.775876 | -0.019358 |
| C | -2.200352 | 0.925409 | 0.293289 |
| C | -2.225793 | -0.407155 | -0.469318 |
| C | -1.204207 | -1.465796 | -0.013940 |
| C | 0.283902 | -1.159819 | -0.283550 |
| C | 0.973337 | -0.269565 | 0.762277 |
| C | 2.482645 | -0.084493 | 0.533778 |
| C | 2.839503 | 0.688904 | -0.741673 |
| H | -2.291807 | 0.775517 | 1.386260 |

| | | | |
|--|-----------|-----------|-----------|
| H | -3.103024 | 1.513093 | 0.013633 |
| H | -3.232864 | -0.831436 | -0.359149 |
| H | -2.087824 | -0.188675 | -1.535742 |
| H | -1.347657 | -1.671291 | 1.057025 |
| H | -1.462848 | -2.398310 | -0.531150 |
| H | 0.826983 | -2.114272 | -0.323965 |
| H | 0.380365 | -0.714094 | -1.281327 |
| H | 0.500975 | 0.722011 | 0.788864 |
| H | 0.816396 | -0.712861 | 1.755854 |
| H | 2.903759 | 0.443514 | 1.398896 |
| H | 2.969325 | -1.070150 | 0.513898 |
| H | 2.351465 | 1.669911 | -0.754262 |
| H | 2.527519 | 0.154227 | -1.644686 |
| H | 3.920175 | 0.850902 | -0.814472 |
| Rotational constants (GHz): | 2.9131700 | 1.0994400 | 0.9109600 |
| Vibrational harmonic frequencies (cm-1): | | | |
| 32.6534 | 61.9100 | | 101.1358 |
| 126.4193 | 149.1248 | | 205.0573 |
| 270.7589 | 300.3885 | | 314.0084 |
| 370.6765 | 453.1108 | | 492.9125 |
| 735.9688 | 750.9937 | | 777.5523 |
| 802.2959 | 869.7369 | | 889.4450 |
| 931.5078 | 943.6064 | | 991.0995 |
| 1015.0252 | 1061.6289 | | 1087.1813 |
| 1101.0014 | 1107.7826 | | 1132.2387 |
| 1171.7182 | 1203.2705 | | 1260.9489 |
| 1274.1863 | 1309.1717 | | 1334.3589 |
| 1345.2657 | 1355.5861 | | 1380.9604 |
| 1385.3709 | 1393.8804 | | 1404.4226 |
| 1413.7303 | 1429.4976 | | 1480.9766 |
| 1491.1989 | 1499.6154 | | 1501.2073 |
| 1508.1973 | 1515.2443 | | 1522.0914 |
| 2882.9519 | 2947.1211 | | 3005.6795 |
| 3017.4104 | 3018.6975 | | 3023.6004 |
| 3030.4770 | 3043.2201 | | 3045.8326 |
| 3059.3266 | 3062.5201 | | 3074.4703 |
| 3081.1124 | 3111.7168 | | 3115.7913 |
| Zero-point correction (Hartree): | 0.209081 | | |

C7H15O.pmpptt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.94987210

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|--|-----------|-----------|-----------|
| O | -1.178606 | 1.764455 | -0.434200 |
| C | -2.142744 | 1.104298 | 0.283573 |
| C | -2.406766 | -0.351736 | -0.127121 |
| C | -1.357072 | -1.383622 | 0.325770 |
| C | 0.037054 | -1.297020 | -0.329061 |
| C | 0.999772 | -0.269368 | 0.282648 |
| C | 2.391641 | -0.296880 | -0.361782 |
| C | 3.365000 | 0.711553 | 0.256358 |
| H | -1.980874 | 1.200865 | 1.374459 |
| H | -3.058703 | 1.703023 | 0.081275 |
| H | -3.378207 | -0.642053 | 0.295117 |
| H | -2.513112 | -0.380832 | -1.218854 |
| H | -1.250487 | -1.336938 | 1.419505 |
| H | -1.775675 | -2.375098 | 0.112052 |
| H | 0.508274 | -2.286810 | -0.256951 |
| H | -0.078500 | -1.096186 | -1.402888 |
| H | 0.588646 | 0.744639 | 0.185646 |
| H | 1.095405 | -0.462242 | 1.361546 |
| H | 2.809284 | -1.310134 | -0.276691 |
| H | 2.293646 | -0.098778 | -1.437673 |
| H | 3.508423 | 0.519758 | 1.326105 |
| H | 2.991209 | 1.736349 | 0.152304 |
| H | 4.348210 | 0.665452 | -0.223658 |
| Rotational constants (GHz): | 3.0520500 | 1.0098200 | 0.8163200 |
| Vibrational harmonic frequencies (cm-1): | | | |
| 47.3368 | 71.1592 | | 79.5560 |
| 131.4394 | 154.8668 | | 178.7489 |
| 247.6620 | 302.8146 | | 309.3286 |
| 395.7433 | 429.2494 | | 470.0448 |
| 727.9903 | 755.8461 | | 789.2067 |
| 790.7431 | 880.2461 | | 899.1233 |
| 934.8045 | 947.1626 | | 990.7300 |
| 1029.4627 | 1064.3519 | | 1073.1775 |
| 1104.5043 | 1106.2421 | | 1130.5158 |
| 1175.7631 | 1216.9219 | | 1263.2968 |
| 1271.3584 | 1314.3189 | | 1324.9781 |
| 1341.8747 | 1347.1027 | | 1381.1435 |
| 1383.7099 | 1393.3584 | | 1405.0153 |
| 1415.9397 | 1427.4378 | | 1480.2760 |
| 1493.7124 | 1498.0549 | | 1500.2216 |
| 1511.1908 | 1513.2182 | | 1523.6340 |

| | | |
|-----------|-----------|-----------|
| 2882.4363 | 2946.6073 | 3004.3063 |
| 3016.6323 | 3018.9333 | 3024.1334 |
| 3030.2456 | 3035.2827 | 3038.7326 |
| 3054.4157 | 3062.1249 | 3070.2200 |
| 3080.1205 | 3106.8022 | 3111.5204 |

Zero-point correction (Hartree): 0.208924

C7H15O.pmtmm

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.95077645

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 2.115447 | 1.345939 | 0.742987 |
| C | 2.453619 | 0.647477 | -0.385133 |
| C | 2.078540 | -0.844213 | -0.368771 |
| C | 0.564143 | -1.085800 | -0.472498 |
| C | -0.233718 | -0.597775 | 0.744425 |
| C | -1.747335 | -0.864330 | 0.658784 |
| C | -2.502157 | -0.113571 | -0.452933 |
| C | -2.473671 | 1.413330 | -0.314470 |
| H | 2.093518 | 1.142842 | -1.308093 |
| H | 3.562419 | 0.732854 | -0.421622 |
| H | 2.586137 | -1.331601 | -1.211370 |
| H | 2.473918 | -1.290183 | 0.552097 |
| H | 0.194285 | -0.603168 | -1.387684 |
| H | 0.388891 | -2.161967 | -0.607893 |
| H | 0.159116 | -1.093834 | 1.641726 |
| H | -0.049171 | 0.473036 | 0.903367 |
| H | -1.908980 | -1.943661 | 0.529372 |
| H | -2.200772 | -0.603875 | 1.624795 |
| H | -2.103771 | -0.399306 | -1.434976 |
| H | -3.546054 | -0.452589 | -0.447310 |
| H | -1.457659 | 1.813659 | -0.392624 |
| H | -2.876873 | 1.728655 | 0.654993 |
| H | -3.075105 | 1.890914 | -1.095102 |

Rotational constants (GHz): 3.0256800 0.9945900 0.8689600

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 28.5536 | 43.1863 | 99.7999 |
| 118.2282 | 158.0594 | 232.9699 |
| 260.8629 | 290.6637 | 321.6807 |
| 383.2723 | 446.6779 | 509.2406 |
| 723.7187 | 772.3491 | 792.3290 |
| 825.2016 | 846.0474 | 879.3759 |
| 906.3372 | 976.9253 | 981.3303 |
| 1015.5388 | 1034.2160 | 1083.8639 |
| 1093.5820 | 1104.8693 | 1118.8198 |
| 1159.6483 | 1179.7495 | 1234.7908 |
| 1281.5474 | 1311.2462 | 1319.4187 |
| 1339.5593 | 1347.9362 | 1373.4118 |
| 1385.0062 | 1394.8080 | 1408.4929 |
| 1414.5927 | 1427.7722 | 1485.0233 |
| 1488.8504 | 1498.9528 | 1504.6809 |
| 1507.0850 | 1516.2380 | 1523.5520 |
| 2881.9388 | 2939.8002 | 3016.2525 |
| 3019.2005 | 3028.2487 | 3033.0122 |
| 3037.4065 | 3042.3434 | 3048.6147 |
| 3054.8030 | 3068.6460 | 3071.6823 |
| 3086.6920 | 3108.9097 | 3116.9469 |

Zero-point correction (Hartree): 0.208918

C7H15O.pmtmp

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.94816388

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -2.186306 | 0.993853 | -1.131680 |
| C | -2.451181 | 0.708436 | 0.180826 |
| C | -2.025608 | -0.693536 | 0.647971 |
| C | -0.501813 | -0.860281 | 0.756562 |
| C | 0.234939 | -0.811065 | -0.591044 |
| C | 1.769054 | -0.975737 | -0.496966 |
| C | 2.581650 | 0.329445 | -0.418730 |
| C | 2.333814 | 1.195286 | 0.821568 |
| H | -2.071443 | 1.493984 | 0.863409 |
| H | -3.559829 | 0.781985 | 0.243772 |
| H | -2.484290 | -0.879008 | 1.628018 |
| H | -2.441236 | -1.430771 | -0.050109 |
| H | -0.107370 | -0.094906 | 1.437378 |
| H | -0.290878 | -1.825162 | 1.237523 |
| H | -0.176124 | -1.606854 | -1.225465 |
| H | -0.002549 | 0.125690 | -1.115221 |
| H | 2.016610 | -1.611969 | 0.365097 |
| H | 2.116206 | -1.525061 | -1.380851 |
| H | 3.648048 | 0.071869 | -0.462590 |
| H | 2.378403 | 0.925074 | -1.319105 |

| | | | | |
|---|-----------|-----------|-----------|-----------|
| H | 2.504076 | 0.628546 | 1.744573 | |
| H | 1.309639 | 1.580538 | 0.850441 | |
| H | 3.006054 | 2.059932 | 0.835451 | |
| Rotational constants (GHz): | 3.0230000 | | 0.9599100 | 0.9058600 |
| Vibrational harmonic frequencies (cm ⁻¹): | | | | |
| | 29.3567 | 70.6008 | | 101.2134 |
| | 117.1841 | 127.6336 | | 243.5616 |
| | 256.9702 | 306.3252 | | 314.9173 |
| | 360.2226 | 440.2594 | | 498.6964 |
| | 737.1368 | 772.0769 | | 779.4415 |
| | 823.8393 | 848.9020 | | 881.2478 |
| | 907.5588 | 981.4095 | | 983.9347 |
| | 1019.1252 | 1043.5013 | | 1081.4709 |
| | 1096.8580 | 1109.1866 | | 1119.9369 |
| | 1160.6706 | 1183.0036 | | 1238.7484 |
| | 1280.6338 | 1311.2840 | | 1326.2524 |
| | 1332.0115 | 1349.4686 | | 1373.6929 |
| | 1386.6410 | 1392.1117 | | 1403.9310 |
| | 1410.4406 | 1427.7110 | | 1484.8835 |
| | 1490.9226 | 1498.6917 | | 1502.2598 |
| | 1509.6204 | 1516.5063 | | 1522.9059 |
| | 2880.2893 | 2937.7518 | | 3015.1699 |
| | 3017.7749 | 3025.5435 | | 3029.1757 |
| | 3037.5570 | 3040.1102 | | 3048.9429 |
| | 3060.4239 | 3066.2442 | | 3073.1239 |
| | 3086.9450 | 3105.9006 | | 3116.5547 |
| Zero-point correction (Hartree): | 0.208900 | | | |

C7H15O.pmtmt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.95199506
Electronic state : 2-A
Cartesian coordinates (Angs):

| | | | | |
|---|-----------|-----------|-----------|-----------|
| O | -2.540765 | -1.404513 | 0.336621 | |
| C | -2.750934 | -0.394727 | -0.563962 | |
| C | -2.179644 | 0.974813 | -0.159234 | |
| C | -0.644777 | 1.030747 | -0.211693 | |
| C | 0.053464 | 0.125552 | 0.812871 | |
| C | 1.588784 | 0.216007 | 0.797940 | |
| C | 2.258396 | -0.336343 | -0.468631 | |
| C | 3.788492 | -0.283258 | -0.404431 | |
| H | -2.436987 | -0.676736 | -1.588102 | |
| H | -3.859819 | -0.315775 | -0.611739 | |
| H | -2.596542 | 1.731229 | -0.836929 | |
| H | -2.535186 | 1.211600 | 0.851105 | |
| H | -0.317645 | 0.774470 | -1.228514 | |
| H | -0.327268 | 2.069412 | -0.045309 | |
| H | -0.309914 | 0.387778 | 1.815152 | |
| H | -0.251897 | -0.918461 | 0.653850 | |
| H | 1.892500 | 1.263637 | 0.940390 | |
| H | 1.979563 | -0.331440 | 1.666272 | |
| H | 1.933561 | -1.374622 | -0.622207 | |
| H | 1.916182 | 0.222817 | -1.348693 | |
| H | 4.169691 | -0.867027 | 0.441319 | |
| H | 4.144127 | 0.746150 | -0.280137 | |
| H | 4.243064 | -0.683684 | -1.316600 | |
| Rotational constants (GHz): | 4.1757900 | | 0.7585300 | 0.7229600 |
| Vibrational harmonic frequencies (cm ⁻¹): | | | | |
| | 39.8397 | 74.2020 | | 96.5490 |
| | 114.3533 | 135.9477 | | 246.9901 |
| | 258.2508 | 284.4782 | | 294.5140 |
| | 337.9642 | 444.2573 | | 531.3071 |
| | 734.7833 | 761.3037 | | 790.9096 |
| | 836.7119 | 849.3909 | | 874.6533 |
| | 915.3920 | 975.1887 | | 997.6148 |
| | 1020.9786 | 1041.6661 | | 1083.3197 |
| | 1091.5663 | 1101.1440 | | 1120.5091 |
| | 1163.2567 | 1190.6389 | | 1245.8537 |
| | 1293.1584 | 1312.8146 | | 1320.3208 |
| | 1337.8380 | 1346.1312 | | 1357.3813 |
| | 1374.8598 | 1404.8847 | | 1411.0858 |
| | 1415.2646 | 1427.8180 | | 1484.4437 |
| | 1491.0414 | 1498.7259 | | 1508.3231 |
| | 1509.7562 | 1514.3841 | | 1524.6125 |
| | 2881.7679 | 2939.7912 | | 3012.8659 |
| | 3015.8572 | 3025.6809 | | 3030.0210 |
| | 3036.2529 | 3038.5043 | | 3046.4965 |
| | 3050.2777 | 3070.9720 | | 3071.3762 |
| | 3086.5694 | 3107.0207 | | 3111.6512 |
| Zero-point correction (Hartree): | 0.208934 | | | |

C7H15O.pmtpm

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.94811124


```

Electronic state : 2-A
Cartesian coordinates (Angs):
O      -2.900200   -1.040634   -0.086876
C      -2.820536    0.297035   -0.367210
C      -1.762719    1.069824    0.440750
C      -0.319872    0.748270    0.016553
C       0.104740   -0.699360    0.295485
C       1.484136   -1.117454   -0.246395
C       2.708701   -0.397921    0.361433
C       3.127885    0.897752   -0.346663
H      -2.722427    0.495830   -1.452220
H      -3.825001    0.683491   -0.085333
H      -1.950902    2.143281    0.309581
H      -1.907612    0.841582    1.503727
H      -0.204705    0.966965   -1.055298
H       0.349369    1.440281    0.541591
H       0.076038   -0.875693    1.380005
H      -0.648291   -1.378314   -0.129227
H       1.587836   -2.194105   -0.062966
H       1.500207   -0.999434   -1.339423
H       2.520234   -0.196194    1.425049
H       3.563235   -1.085923    0.338105
H       2.343507    1.659570   -0.322484
H       3.365570    0.705928   -1.399422
H       4.020537    1.328931    0.119605
Rotational constants (GHz):   4.2905100   0.8279600   0.7403500
Vibrational harmonic frequencies (cm-1):
  40.1410           65.2140           99.7438
 113.5615          129.1246          221.6889
 244.7562          286.6029          337.0527
 367.0833          445.4643          490.7920
 749.9371          754.7490          786.4122
 826.5922          860.1615          870.3399
 918.9340          979.3881          994.7409
1011.1905          1045.6285         1082.4978
1094.1485          1096.5251         1123.8968
1151.2003          1199.2608         1247.8826
1267.6172          1308.6567         1327.7737
1336.2405          1355.3788         1372.5191
1382.0480          1392.2995         1412.2003
1418.6172          1429.3665         1483.6421
1486.0640          1500.4560         1504.5293
1506.3907          1516.9736         1522.8673
2882.2137          2942.0843         3008.3483
3018.7917          3020.8343         3026.1895
3036.7492          3043.4361         3044.5886
3061.5283          3066.8010         3076.7695
3087.6845          3106.3220         3126.5256
Zero-point correction (Hartree): 0.208924

```

C7H15O.pmtpp

```

-----
E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.95079936
Electronic state : 2-A
Cartesian coordinates (Angs):
O      -2.749439   -1.091070    0.568884
C      -2.899932    0.073954   -0.134791
C      -1.805606    1.128472    0.107375
C      -0.449477    0.746229   -0.507513
C       0.198666   -0.494835    0.119414
C       1.499707   -0.944704   -0.569115
C       2.670230    0.054102   -0.518107
C       3.176318    0.362277    0.895872
H      -3.054089   -0.105046   -1.216776
H      -3.866609    0.480189    0.237094
H      -2.147831    2.078899   -0.322307
H      -1.705056    1.278291    1.189345
H      -0.579056    0.583508   -1.587974
H       0.224311    1.607050   -0.412135
H       0.378338   -0.309002    1.186312
H      -0.515805   -1.328736    0.087800

H       1.825981   -1.889736   -0.114214
H       1.279755   -1.175680   -1.620660
H       3.497466   -0.357416   -1.110571
H       2.385681    0.989754   -1.016672
H       3.476399   -0.555033    1.415898
H       2.410788    0.851171    1.507546
H       4.045806    1.027378    0.867431
Rotational constants (GHz):   4.2784900   0.8019600   0.7621300
Vibrational harmonic frequencies (cm-1):
  38.4854           60.0020           93.1883
 118.1133          158.9048          235.0225
 248.2191          285.9373          330.1341
 385.7232          456.1588          503.9146

```

| | | |
|-----------|-----------|-----------|
| 726.1285 | 765.0740 | 797.3550 |
| 821.9280 | 857.5596 | 876.1778 |
| 913.6736 | 975.9512 | 984.9313 |
| 1007.5456 | 1038.6033 | 1078.6818 |
| 1094.3575 | 1105.7356 | 1120.8148 |
| 1156.0067 | 1183.4924 | 1246.9103 |
| 1270.7988 | 1307.6139 | 1323.4929 |
| 1339.3059 | 1349.2582 | 1373.2228 |
| 1386.2559 | 1395.2203 | 1410.8143 |
| 1416.4625 | 1429.4649 | 1484.2934 |
| 1487.4860 | 1500.3058 | 1504.9989 |
| 1506.1035 | 1516.0803 | 1523.1530 |
| 2882.9591 | 2942.4794 | 3012.9639 |
| 3018.4405 | 3024.1811 | 3035.2322 |
| 3035.9641 | 3040.6158 | 3050.8855 |
| 3057.0403 | 3070.1256 | 3074.3032 |
| 3086.2717 | 3108.4213 | 3112.8078 |

Zero-point correction (Hartree): 0.209003

C7H15O.pmtpt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.95201978

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 2.878848 | -1.235886 | -0.177477 |
| C | 3.002903 | 0.022371 | 0.348032 |
| C | 2.036474 | 1.069869 | -0.231808 |
| C | 0.579400 | 0.863205 | 0.211654 |
| C | -0.057838 | -0.435397 | -0.301705 |
| C | -1.486686 | -0.687720 | 0.207359 |
| C | -2.539226 | 0.309164 | -0.299208 |
| C | -3.957495 | -0.032124 | 0.169777 |
| H | 2.977575 | 0.019968 | 1.455240 |
| H | 4.041558 | 0.316374 | 0.078505 |
| H | 2.378539 | 2.062767 | 0.088022 |
| H | 2.109871 | 1.037501 | -1.325725 |
| H | 0.533087 | 0.880780 | 1.310895 |
| H | -0.006733 | 1.725993 | -0.128429 |
| H | -0.056000 | -0.428574 | -1.400734 |
| H | 0.575866 | -1.284864 | -0.012443 |
| H | -1.791143 | -1.699710 | -0.092186 |
| H | -1.487060 | -0.686985 | 1.307200 |
| H | -2.285319 | 1.323739 | 0.032866 |
| H | -2.511834 | 0.332682 | -1.397513 |
| H | -4.023376 | -0.033008 | 1.263946 |
| H | -4.261368 | -1.026040 | -0.178385 |
| H | -4.689637 | 0.690256 | -0.206056 |

Rotational constants (GHz): 5.4282700 0.7066000 0.6563700

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 41.9852 | 72.1668 | 85.0498 |
| 119.9947 | 127.5870 | 238.8427 |
| 259.5129 | 272.8420 | 296.4951 |
| 342.4899 | 450.9784 | 524.3948 |
| 734.3074 | 755.6499 | 793.5537 |
| 834.5960 | 856.6766 | 880.8662 |
| 914.0355 | 979.5771 | 1004.4085 |
| 1009.2886 | 1042.2064 | 1080.9266 |
| 1087.1449 | 1100.0036 | 1119.1827 |
| 1154.5920 | 1209.1171 | 1247.8185 |
| 1274.8631 | 1314.8607 | 1321.7134 |
| 1337.0249 | 1345.4784 | 1357.0324 |
| 1375.6852 | 1406.3267 | 1411.2066 |
| 1416.8752 | 1425.2673 | 1485.1984 |
| 1488.7608 | 1498.0495 | 1507.1766 |
| 1507.9374 | 1512.6786 | 1523.4862 |
| 2882.4819 | 2942.0171 | 3010.8432 |
| 3015.5547 | 3019.1347 | 3028.0347 |
| 3036.0893 | 3037.8228 | 3046.7043 |
| 3048.6615 | 3071.1057 | 3074.5971 |
| 3086.7204 | 3106.5392 | 3111.0819 |

Zero-point correction (Hartree): 0.208824

C7H15O.pmttm

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.95210583

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 2.166494 | 1.624460 | -0.207130 |
| C | 2.830024 | 0.427286 | -0.242901 |
| C | 2.215816 | -0.690006 | 0.617097 |
| C | 0.890305 | -1.227559 | 0.055658 |
| C | -0.261352 | -0.214447 | 0.056979 |
| C | -1.561697 | -0.791334 | -0.521255 |
| C | -2.726428 | 0.208928 | -0.603311 |
| C | -3.239535 | 0.701752 | 0.755154 |

| | | | | |
|--|-----------|-----------|-----------|--|
| H | 3.014585 | 0.083752 | -1.279689 | |
| H | 3.835835 | 0.675534 | 0.163272 | |
| H | 2.943918 | -1.509039 | 0.682414 | |
| H | 2.070162 | -0.302855 | 1.633022 | |
| H | 1.056766 | -1.591128 | -0.969146 | |
| H | 0.595045 | -2.108484 | 0.641747 | |
| H | -0.425563 | 0.135621 | 1.083928 | |
| H | 0.027739 | 0.677048 | -0.517856 | |
| H | -1.358156 | -1.178808 | -1.529109 | |
| H | -1.871622 | -1.659319 | 0.079369 | |
| H | -2.418071 | 1.070539 | -1.211071 | |
| H | -3.555188 | -0.263495 | -1.146258 | |
| H | -2.473853 | 1.259983 | 1.303145 | |
| H | -3.554193 | -0.137731 | 1.386529 | |
| H | -4.102153 | 1.364977 | 0.632222 | |
| Rotational constants (GHz): | 3.6354400 | 0.8142800 | 0.7378000 | |
| Vibrational harmonic frequencies (cm-1): | | | | |
| 36.4984 | 75.1013 | | 94.7114 | |
| 120.5432 | 139.1210 | | 168.4634 | |
| 256.4124 | 304.5716 | | 315.0792 | |
| 370.8393 | 455.3535 | | 475.2762 | |
| 736.2911 | 763.0580 | | 795.4391 | |
| 823.0682 | 860.4589 | | 877.6524 | |
| 922.1958 | 982.2484 | | 987.3688 | |
| 1005.2079 | 1055.2772 | | 1082.3582 | |
| 1091.3050 | 1099.7653 | | 1120.8723 | |
| 1160.7604 | 1196.8121 | | 1242.5361 | |
| 1289.6785 | 1301.4597 | | 1326.5536 | |
| 1336.4122 | 1341.1297 | | 1373.4228 | |
| 1385.7710 | 1387.8894 | | 1407.2150 | |
| 1416.3835 | 1429.5263 | | 1484.0647 | |
| 1490.8462 | 1496.9929 | | 1501.1121 | |
| 1513.6814 | 1517.2647 | | 1521.7964 | |
| 2880.8910 | 2939.2945 | | 3009.6609 | |
| 3012.2669 | 3021.4324 | | 3025.2999 | |
| 3035.3646 | 3040.8282 | | 3046.0833 | |
| 3051.2971 | 3061.6706 | | 3076.5210 | |
| 3086.2320 | 3107.5068 | | 3118.0327 | |
| Zero-point correction (Hartree): | 0.208790 | | | |

C7H15O.pmttp

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.95217857

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | | |
|--|-----------|-----------|-----------|--|
| O | -1.948061 | 1.678074 | -0.201253 | |
| C | -2.678489 | 0.632532 | 0.297268 | |
| C | -2.309662 | -0.750475 | -0.266004 | |
| C | -0.942323 | -1.256676 | 0.219008 | |
| C | 0.253332 | -0.428964 | -0.268862 | |
| C | 1.597838 | -0.961380 | 0.246994 | |
| C | 2.829850 | -0.207667 | -0.280514 | |
| C | 2.928489 | 1.251154 | 0.181404 | |
| H | -2.696653 | 0.625852 | 1.404732 | |
| H | -3.720609 | 0.873262 | -0.009500 | |
| H | -3.090722 | -1.460534 | 0.035541 | |
| H | -2.327651 | -0.692770 | -1.361220 | |
| H | -0.941549 | -1.287216 | 1.318623 | |
| H | -0.818747 | -2.297414 | -0.109976 | |
| H | 0.261395 | -0.418730 | -1.367953 | |
| H | 0.120123 | 0.617297 | 0.035996 | |
| H | 1.601294 | -0.934409 | 1.346469 | |
| H | 1.687492 | -2.021287 | -0.029384 | |
| H | 3.731773 | -0.744916 | 0.040037 | |
| H | 2.830598 | -0.244054 | -1.378687 | |
| H | 2.930169 | 1.318754 | 1.275784 | |
| H | 2.091979 | 1.854058 | -0.185698 | |
| H | 3.851400 | 1.716367 | -0.180502 | |
| Rotational constants (GHz): | 3.3247600 | 0.8953000 | 0.7449000 | |
| Vibrational harmonic frequencies (cm-1): | | | | |
| 44.1778 | 63.1557 | | 109.8149 | |
| 126.2727 | 137.1754 | | 172.4824 | |
| 259.9596 | 296.9698 | | 325.2893 | |
| 369.2916 | 456.9417 | | 475.2351 | |
| 736.0545 | 770.9863 | | 797.5409 | |
| 819.8422 | 854.4532 | | 889.8784 | |
| 915.6352 | 979.9205 | | 991.8790 | |
| 1004.3413 | 1050.6897 | | 1083.6963 | |
| 1089.6984 | 1099.2260 | | 1119.3487 | |
| 1156.0253 | 1208.2104 | | 1237.3999 | |
| 1280.5271 | 1313.1234 | | 1321.6082 | |
| 1338.4639 | 1341.3321 | | 1372.8823 | |
| 1385.8066 | 1389.2291 | | 1408.9768 | |
| 1416.6574 | 1430.3689 | | 1484.8683 | |
| 1489.6084 | 1497.2052 | | 1502.3323 | |

| | | |
|-----------|-----------|-----------|
| 1513.5609 | 1517.7716 | 1522.2726 |
| 2881.7535 | 2940.2463 | 3010.8010 |
| 3013.2758 | 3023.7605 | 3026.1249 |
| 3034.3305 | 3041.2130 | 3042.8230 |
| 3050.8875 | 3060.9714 | 3074.1681 |
| 3086.4815 | 3107.6518 | 3119.8408 |

Zero-point correction (Hartree): 0.208868

C7H15O.pmttt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.95337853

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -2.390620 | 1.589318 | -0.051061 |
| C | -2.936447 | 0.406776 | 0.371502 |
| C | -2.372741 | -0.854087 | -0.305148 |
| C | -0.933414 | -1.179413 | 0.124421 |
| C | 0.109559 | -0.140183 | -0.304772 |
| C | 1.530188 | -0.480759 | 0.163516 |
| C | 2.580513 | 0.549520 | -0.270402 |
| C | 3.996177 | 0.206705 | 0.204294 |
| H | -2.925200 | 0.312180 | 1.475030 |
| H | -4.010850 | 0.504412 | 0.098961 |
| H | -3.028764 | -1.697872 | -0.054544 |
| H | -2.423377 | -0.714344 | -1.391913 |
| H | -0.904195 | -1.296701 | 1.217832 |
| H | -0.658286 | -2.158872 | -0.289778 |
| H | 0.095853 | -0.045047 | -1.399441 |
| H | -0.173838 | 0.849536 | 0.080453 |
| H | 1.540973 | -0.568774 | 1.259643 |
| H | 1.813559 | -1.471442 | -0.221302 |
| H | 2.571479 | 0.635016 | -1.365547 |
| H | 2.294933 | 1.538756 | 0.112039 |
| H | 4.323393 | -0.762395 | -0.189907 |
| H | 4.044671 | 0.150155 | 1.297906 |
| H | 4.721592 | 0.959495 | -0.121410 |

Rotational constants (GHz): 4.5423600 0.7138400 0.6466000

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 43.7175 | 61.2975 | 94.4472 |
| 125.6161 | 134.3252 | 148.9887 |
| 245.1639 | 275.8834 | 322.0522 |
| 363.6170 | 427.7127 | 491.8572 |
| 733.1842 | 753.6278 | 796.1946 |
| 826.6963 | 860.6490 | 901.2730 |
| 914.7736 | 981.1303 | 998.4838 |
| 1020.8709 | 1057.0564 | 1069.0971 |
| 1086.4638 | 1101.3784 | 1121.0624 |
| 1159.2158 | 1214.6492 | 1242.9737 |
| 1278.4588 | 1302.2090 | 1329.6505 |
| 1332.9094 | 1336.1308 | 1354.8262 |
| 1373.5330 | 1400.8044 | 1409.1887 |
| 1414.9490 | 1425.7208 | 1484.2185 |
| 1489.5368 | 1497.1129 | 1503.7629 |
| 1512.4630 | 1513.8800 | 1524.6401 |
| 2881.5955 | 2940.2920 | 3007.7203 |
| 3010.6437 | 3018.4429 | 3027.5723 |
| 3032.9835 | 3035.3575 | 3037.7296 |
| 3045.5847 | 3059.9493 | 3072.0728 |
| 3086.1116 | 3105.2652 | 3111.3767 |

Zero-point correction (Hartree): 0.208521

C7H15O.pppmm

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.94781154

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 1.758462 | -1.677824 | -0.413176 |
| C | 2.085822 | -0.672789 | 0.454575 |
| C | 1.966039 | 0.756142 | -0.105090 |
| C | 0.633840 | 1.088329 | -0.800764 |
| C | -0.540719 | 1.501291 | 0.106884 |
| C | -1.137330 | 0.426451 | 1.036089 |
| C | -1.652886 | -0.848881 | 0.346386 |
| C | -2.792952 | -0.607977 | -0.650455 |
| H | 1.388873 | -0.820511 | 1.307677 |
| H | 3.085042 | -0.848059 | 0.899028 |
| H | 2.167137 | 1.466139 | 0.709059 |
| H | 2.781022 | 0.883578 | -0.828686 |
| H | 0.817877 | 1.921999 | -1.489548 |
| H | 0.354405 | 0.236887 | -1.431995 |
| H | -0.224689 | 2.353655 | 0.724555 |
| H | -1.340570 | 1.887802 | -0.537543 |
| H | -0.400251 | 0.146371 | 1.800825 |
| H | -1.966696 | 0.885304 | 1.592457 |
| H | -0.826222 | -1.359762 | -0.163216 |

| | | | | |
|--|-----------|-----------|-----------|--|
| H | -2.000727 | -1.541518 | 1.123742 | |
| H | -2.472296 | 0.007683 | -1.497280 | |
| H | -3.637661 | -0.098109 | -0.171918 | |
| H | -3.163822 | -1.554266 | -1.057508 | |
| Rotational constants (GHz): | 2.6572500 | 1.2168200 | 1.0071200 | |
| Vibrational harmonic frequencies (cm-1): | | | | |
| 48.0861 | 60.4351 | | 80.0668 | |
| 155.5475 | 195.2366 | | 218.0005 | |
| 247.6199 | 292.6189 | | 350.6443 | |
| 417.7971 | 482.8910 | | 520.7454 | |
| 639.4140 | 726.8250 | | 766.3171 | |
| 805.1776 | 841.2190 | | 880.5069 | |
| 907.9827 | 939.6474 | | 981.8862 | |
| 1029.6248 | 1038.6935 | | 1089.6898 | |
| 1099.5538 | 1118.2704 | | 1123.8887 | |
| 1167.8827 | 1198.4143 | | 1246.2160 | |
| 1289.0247 | 1298.8592 | | 1323.1872 | |
| 1342.7254 | 1367.2010 | | 1376.2657 | |
| 1387.0693 | 1396.5494 | | 1411.2594 | |
| 1414.6133 | 1426.5920 | | 1490.2260 | |
| 1494.7156 | 1500.1466 | | 1509.2109 | |
| 1511.3198 | 1517.5270 | | 1524.0557 | |
| 2897.0689 | 2938.0317 | | 3016.6377 | |
| 3024.6953 | 3029.2239 | | 3035.0498 | |
| 3039.6478 | 3043.5715 | | 3048.5201 | |
| 3064.5329 | 3070.9367 | | 3073.0110 | |
| 3089.1440 | 3107.3373 | | 3114.5974 | |
| Zero-point correction (Hartree): | 0.209235 | | | |

C7H15O.ppmmp

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.94499653

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | | |
|--|-----------|-----------|-----------|--|
| O | 1.833191 | 1.653714 | 0.227537 | |
| C | 2.344784 | 0.519872 | -0.344348 | |
| C | 2.028838 | -0.791722 | 0.394101 | |
| C | 0.539668 | -1.040939 | 0.681957 | |
| C | -0.352723 | -1.173046 | -0.575674 | |
| C | -1.071162 | 0.119989 | -1.033838 | |
| C | -2.486718 | 0.309669 | -0.458910 | |
| C | -2.563330 | 0.466765 | 1.064016 | |
| H | 1.878053 | 0.501264 | -1.354109 | |
| H | 3.428183 | 0.621262 | -0.545032 | |
| H | 2.441772 | -1.617624 | -0.201761 | |
| H | 2.584067 | -0.786450 | 1.340696 | |
| H | 0.472031 | -1.960435 | 1.276012 | |
| H | 0.169399 | -0.234711 | 1.322557 | |
| H | 0.261415 | -1.561445 | -1.399977 | |
| H | -1.113007 | -1.945416 | -0.400544 | |
| H | -0.462469 | 0.995699 | -0.776787 | |
| H | -1.156261 | 0.112915 | -2.128183 | |
| H | -2.934095 | 1.195169 | -0.929076 | |
| H | -3.109664 | -0.542191 | -0.766112 | |
| H | -1.956455 | 1.312299 | 1.407329 | |
| H | -2.209749 | -0.429068 | 1.584872 | |
| H | -3.594887 | 0.645487 | 1.385996 | |
| Rotational constants (GHz): | 2.9378800 | 1.0581000 | 0.9732000 | |
| Vibrational harmonic frequencies (cm-1): | | | | |
| 47.0058 | 70.2331 | | 77.4893 | |
| 126.5856 | 179.0714 | | 209.1644 | |
| 258.5567 | 305.0256 | | 331.3916 | |
| 396.9014 | 449.5331 | | 511.2120 | |
| 671.6554 | 758.9951 | | 784.0692 | |
| 795.3776 | 855.6545 | | 899.0871 | |
| 911.7852 | 934.8354 | | 989.9527 | |
| 1033.0642 | 1049.0464 | | 1085.4208 | |
| 1105.7352 | 1107.5071 | | 1123.6644 | |
| 1162.2887 | 1195.1687 | | 1244.2047 | |
| 1271.3528 | 1297.5538 | | 1317.2561 | |
| 1322.6819 | 1363.4611 | | 1385.0427 | |
| 1392.7470 | 1394.6093 | | 1398.3832 | |
| 1405.9612 | 1431.1231 | | 1494.0587 | |
| 1497.0480 | 1502.2976 | | 1506.4337 | |
| 1510.5276 | 1519.1349 | | 1523.4523 | |
| 2886.0797 | 2949.7668 | | 3017.6672 | |
| 3021.3384 | 3027.9055 | | 3032.5321 | |
| 3042.2589 | 3045.5984 | | 3056.8869 | |
| 3060.6806 | 3071.9003 | | 3079.4912 | |
| 3104.4364 | 3109.6528 | | 3116.8620 | |
| Zero-point correction (Hartree): | 0.209195 | | | |

C7H15O.ppmmt

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.94912467

Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 1.368387 | -1.866169 | -0.551785 |
| C | 1.678828 | -1.122461 | 0.552945 |
| C | 2.101063 | 0.332496 | 0.279950 |
| C | 1.160667 | 1.133162 | -0.638308 |
| C | -0.075796 | 1.774327 | 0.021295 |
| C | -1.165248 | 0.834466 | 0.568667 |
| C | -1.786893 | -0.109853 | -0.469162 |
| C | -2.938500 | -0.946125 | 0.099036 |
| H | 0.750089 | -1.153297 | 1.162816 |
| H | 2.423901 | -1.646491 | 1.182953 |
| H | 2.232660 | 0.843101 | 1.244039 |
| H | 3.095341 | 0.294033 | -0.182550 |
| H | 1.744632 | 1.946602 | -1.086047 |
| H | 0.861499 | 0.487510 | -1.471575 |
| H | 0.261110 | 2.431871 | 0.834828 |
| H | -0.542674 | 2.435192 | -0.722012 |
| H | -0.775442 | 0.246690 | 1.412207 |
| H | -1.961965 | 1.456125 | 1.000686 |
| H | -2.150407 | 0.484324 | -1.319179 |
| H | -1.019327 | -0.780473 | -0.874645 |
| H | -3.746039 | -0.308709 | 0.477580 |
| H | -2.599971 | -1.575576 | 0.930491 |
| H | -3.365225 | -1.607634 | -0.661843 |

Rotational constants (GHz): 2.4036700 1.2754500 0.9488600
 Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 48.0645 | 58.3585 | 110.1726 |
| 141.6812 | 211.9522 | 218.5090 |
| 261.4814 | 269.2341 | 303.9028 |
| 399.8253 | 479.6859 | 523.3998 |
| 654.4971 | 740.3531 | 785.1853 |
| 796.8305 | 841.2928 | 890.1858 |
| 920.4598 | 930.8680 | 992.5356 |
| 1040.3628 | 1044.3192 | 1087.4259 |
| 1094.1162 | 1120.4351 | 1127.8154 |
| 1176.0267 | 1201.1282 | 1256.9411 |
| 1296.4773 | 1300.9500 | 1333.3199 |
| 1335.5811 | 1350.6616 | 1370.1055 |
| 1385.7243 | 1401.5247 | 1411.7514 |
| 1417.3209 | 1426.7745 | 1490.2132 |
| 1497.9025 | 1505.0284 | 1507.8082 |
| 1512.3735 | 1513.5531 | 1525.2995 |
| 2898.3821 | 2938.1739 | 3012.4052 |
| 3017.6028 | 3028.3824 | 3029.4300 |
| 3037.0893 | 3042.0562 | 3046.0328 |
| 3057.0484 | 3071.8670 | 3073.3317 |
| 3095.7322 | 3104.3009 | 3112.8508 |

Zero-point correction (Hartree): 0.209305

C7H15O.ppmppm

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.94786890
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 2.058642 | -1.396057 | -0.870395 |
| C | 2.004691 | -0.981013 | 0.432847 |
| C | 2.109939 | 0.537492 | 0.646823 |
| C | 1.115755 | 1.383966 | -0.163567 |
| C | -0.378014 | 1.150596 | 0.165609 |
| C | -1.102154 | 0.195817 | -0.799410 |
| C | -2.588199 | -0.029196 | -0.475464 |
| C | -2.846578 | -0.801862 | 0.824134 |
| H | -2.475304 | -0.264102 | 1.702852 |
| H | 2.731427 | -1.531344 | 1.060577 |
| H | 1.986413 | 0.734805 | 1.720750 |
| H | 3.133101 | 0.842774 | 0.393091 |
| H | 1.365560 | 2.436806 | 0.013235 |
| H | 1.289763 | 1.204265 | -1.230868 |
| H | -0.470601 | 0.790557 | 1.199560 |
| H | -0.906623 | 2.112716 | 0.143576 |
| H | -1.019345 | 0.609702 | -1.813107 |
| H | -0.587608 | -0.772866 | -0.837290 |
| H | -3.099952 | 0.942345 | -0.430912 |
| H | -3.048929 | -0.574981 | -1.308627 |
| H | 1.013516 | -1.342022 | 0.785887 |
| H | -2.355692 | -1.782231 | 0.802916 |
| H | -3.917512 | -0.972762 | 0.975676 |

Rotational constants (GHz): 2.9004700 0.9920400 0.8857000
 Vibrational harmonic frequencies (cm-1):

| | | |
|----------|----------|----------|
| 34.0785 | 70.1337 | 77.9453 |
| 130.9400 | 171.7990 | 205.1234 |
| 234.3673 | 286.8309 | 325.0101 |
| 372.7468 | 464.0706 | 526.9173 |
| 649.9697 | 735.2651 | 757.1407 |

| | | |
|-----------|-----------|-----------|
| 819.0072 | 863.3258 | 881.3213 |
| 912.1486 | 949.1814 | 989.4466 |
| 1032.5454 | 1054.8339 | 1083.3101 |
| 1093.3631 | 1114.3919 | 1119.8834 |
| 1174.3541 | 1199.0451 | 1236.5734 |
| 1282.8543 | 1296.1748 | 1318.6761 |
| 1337.3708 | 1347.5644 | 1378.3204 |
| 1386.5523 | 1389.8821 | 1405.8759 |
| 1408.7811 | 1429.5035 | 1493.5228 |
| 1498.3663 | 1501.8169 | 1503.7845 |
| 1514.8504 | 1517.8621 | 1523.1407 |
| 2888.6198 | 2945.8196 | 3020.1823 |
| 3025.6870 | 3028.1802 | 3033.8529 |
| 3039.9676 | 3042.8408 | 3053.6308 |
| 3061.6770 | 3071.0650 | 3079.4735 |
| 3088.3406 | 3106.6000 | 3115.3072 |

Zero-point correction (Hartree): 0.208911

C7H15O.ppmpp

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.94419297

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 2.778752 | -0.828511 | -0.741676 |
| C | 1.879935 | -0.999856 | 0.275258 |
| C | 1.474796 | 0.288939 | 1.012804 |
| C | 0.931829 | 1.408339 | 0.103838 |
| C | -0.583802 | 1.433043 | -0.176080 |
| C | -1.169430 | 0.257205 | -0.993093 |
| C | -1.753810 | -0.907530 | -0.169649 |
| C | -3.074447 | -0.566329 | 0.531735 |
| H | -1.028544 | -1.246859 | 0.581379 |
| H | 2.226687 | -1.780396 | 0.980280 |
| H | 0.754713 | 0.035643 | 1.802417 |
| H | 2.373596 | 0.651064 | 1.526946 |
| H | 1.191049 | 2.371574 | 0.560035 |
| H | 1.484095 | 1.369923 | -0.844003 |
| H | -1.122765 | 1.526037 | 0.776627 |
| H | -0.788132 | 2.365332 | -0.716885 |
| H | -1.971949 | 0.637106 | -1.639243 |
| H | -0.400505 | -0.122033 | -1.679020 |
| H | -1.920429 | -1.763169 | -0.836809 |
| H | 1.000171 | -1.461822 | -0.221319 |
| H | -3.841054 | -0.279983 | -0.197405 |
| H | -2.961705 | 0.266027 | 1.234662 |
| H | -3.455675 | -1.423220 | 1.096870 |

Rotational constants (GHz): 2.9443000 1.0285500 0.9176200

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 37.8753 | 72.0317 | 97.5261 |
| 112.6664 | 161.1812 | 228.3046 |
| 258.1714 | 272.4744 | 323.8310 |
| 411.4830 | 439.1087 | 494.4627 |
| 665.3160 | 735.7352 | 785.5527 |
| 831.7014 | 843.8465 | 862.7240 |
| 907.7800 | 934.4473 | 992.9973 |
| 1023.1933 | 1051.2663 | 1093.7157 |
| 1097.1092 | 1111.6411 | 1134.8933 |
| 1158.7125 | 1189.4466 | 1268.0375 |
| 1278.0228 | 1302.8373 | 1326.3461 |
| 1329.8363 | 1366.7284 | 1369.8273 |
| 1385.3271 | 1389.8229 | 1399.6082 |
| 1411.8501 | 1428.1778 | 1492.4941 |
| 1496.1476 | 1500.8362 | 1507.2625 |
| 1509.8553 | 1517.3230 | 1520.8912 |
| 2907.3524 | 2939.8375 | 3023.7135 |
| 3026.3511 | 3032.5909 | 3033.8592 |
| 3038.4259 | 3042.1661 | 3060.3347 |
| 3063.8700 | 3068.2366 | 3076.6510 |
| 3078.7338 | 3111.1118 | 3113.9165 |

Zero-point correction (Hartree): 0.209016

C7H15O.ppmpt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.94565426

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 2.331028 | -1.372859 | -0.858379 |
| C | 1.591649 | -1.194958 | 0.279045 |
| C | 1.641806 | 0.224218 | 0.872641 |
| C | 1.232106 | 1.341120 | -0.106557 |
| C | -0.252380 | 1.754168 | -0.142998 |
| C | -1.276530 | 0.698476 | -0.617152 |
| C | -1.909914 | -0.147228 | 0.499209 |
| C | -2.908694 | -1.182859 | -0.027211 |
| H | -1.134158 | -0.655880 | 1.085789 |

| | | | |
|--|-----------|-----------|-----------|
| H | 1.841353 | -1.963386 | 1.036299 |
| H | 1.029662 | 0.250584 | 1.783936 |
| H | 2.676372 | 0.391271 | 1.196419 |
| H | 1.810246 | 2.240426 | 0.138246 |
| H | 1.558938 | 1.043690 | -1.111429 |
| H | -0.550551 | 2.122348 | 0.849245 |
| H | -0.318884 | 2.622801 | -0.809945 |
| H | -2.092926 | 1.210024 | -1.144116 |
| H | -0.812469 | 0.043147 | -1.367952 |
| H | 0.557273 | -1.453755 | -0.033714 |
| H | -2.416699 | 0.525601 | 1.204063 |
| H | -2.422329 | -1.900055 | -0.698629 |
| H | -3.714966 | -0.701208 | -0.592182 |
| H | -3.367345 | -1.750361 | 0.789139 |
| Rotational constants (GHz): | 2.4360700 | 1.1470900 | 0.9066200 |
| Vibrational harmonic frequencies (cm-1): | | | |
| 49.2454 | 87.6377 | 97.7314 | |
| 135.5066 | 168.2736 | 236.0932 | |
| 254.4373 | 276.2180 | 291.0277 | |
| 382.8590 | 467.5089 | 493.4796 | |
| 674.7341 | 738.6522 | 771.8898 | |
| 835.8064 | 848.3069 | 873.8149 | |
| 906.6333 | 941.6068 | 1000.1765 | |
| 1032.4657 | 1055.0471 | 1083.2232 | |
| 1097.7197 | 1119.2064 | 1131.4678 | |
| 1159.4406 | 1209.3760 | 1271.2787 | |
| 1279.4780 | 1303.2833 | 1327.7149 | |
| 1336.4670 | 1343.0705 | 1371.6583 | |
| 1385.6588 | 1394.8724 | 1405.9746 | |
| 1413.7801 | 1426.3899 | 1495.2095 | |
| 1500.5844 | 1506.4024 | 1507.1320 | |
| 1512.0034 | 1512.4820 | 1526.8679 | |
| 2902.8246 | 2940.8348 | 3017.9709 | |
| 3019.9816 | 3033.1770 | 3034.5890 | |
| 3038.5281 | 3039.5236 | 3047.7960 | |
| 3062.8811 | 3070.5865 | 3077.1666 | |
| 3078.2885 | 3106.4987 | 3113.1391 | |
| Zero-point correction (Hartree): | 0.209190 | | |

C7H15O.ppmtn

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.94865562
Electronic state : 2-A
Cartesian coordinates (Angs):

| | | | |
|--|-----------|-----------|-----------|
| O | 3.024129 | -0.967819 | -0.542143 |
| C | 2.286963 | -0.721900 | 0.583518 |
| C | 1.776679 | 0.722665 | 0.728037 |
| C | 0.939724 | 1.227525 | -0.463070 |
| C | -0.578910 | 0.993361 | -0.371188 |
| C | -1.032882 | -0.474496 | -0.357773 |
| C | -2.554926 | -0.663175 | -0.480491 |
| C | -3.359780 | -0.115561 | 0.704419 |
| H | 1.434943 | -1.431063 | 0.506125 |
| H | 2.830065 | -1.055237 | 1.489410 |
| H | 1.210792 | 0.803809 | 1.666427 |
| H | 2.660577 | 1.360624 | 0.848086 |
| H | 1.103013 | 2.306469 | -0.570562 |
| H | 1.339376 | 0.771349 | -1.378159 |
| H | -0.961087 | 1.505760 | 0.521850 |
| H | -1.051754 | 1.491620 | -1.229243 |
| H | -0.543132 | -1.006072 | -1.185109 |
| H | -0.695758 | -0.963824 | 0.567467 |
| H | -2.900333 | -0.187108 | -1.408514 |
| H | -2.768416 | -1.733913 | -0.591706 |
| H | -3.248568 | 0.968525 | 0.809114 |
| H | -3.036078 | -0.574088 | 1.646464 |
| H | -4.427871 | -0.324817 | 0.584780 |
| Rotational constants (GHz): | 3.7297100 | 0.8211600 | 0.7702200 |
| Vibrational harmonic frequencies (cm-1): | | | |
| 44.7066 | 50.6323 | 102.2774 | |
| 128.9215 | 151.7945 | 209.8909 | |
| 263.5966 | 275.3686 | 310.3127 | |
| 390.0704 | 473.4187 | 510.3566 | |
| 665.5204 | 747.8560 | 778.1062 | |
| 808.6710 | 856.9240 | 875.7879 | |
| 920.2824 | 935.5431 | 994.1602 | |
| 1022.2963 | 1054.7389 | 1085.9795 | |
| 1095.9359 | 1111.8467 | 1127.6653 | |
| 1167.3538 | 1202.2501 | 1265.9192 | |
| 1283.3390 | 1308.3478 | 1327.9281 | |
| 1333.1582 | 1358.6020 | 1367.2230 | |
| 1381.9773 | 1385.6157 | 1405.9274 | |
| 1414.8281 | 1430.0094 | 1490.0186 | |
| 1498.2383 | 1502.4306 | 1505.2084 | |
| 1510.9322 | 1517.1827 | 1522.5768 | |

| | | |
|-----------|-----------|-----------|
| 2903.0624 | 2939.2304 | 3010.4845 |
| 3021.2086 | 3026.1368 | 3032.1010 |
| 3037.5301 | 3041.6688 | 3046.5248 |
| 3061.0731 | 3067.8027 | 3077.7129 |
| 3080.1652 | 3107.8077 | 3118.6655 |

Zero-point correction (Hartree): 0.209006

C7H15O.ppmtp

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.94848492

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 2.917060 | -1.000199 | -0.866694 |
| C | 2.418233 | -0.724848 | 0.376828 |
| C | 1.945342 | 0.724851 | 0.583829 |
| C | 0.881561 | 1.198271 | -0.426286 |
| C | -0.585675 | 1.020498 | 0.003639 |
| C | -1.046280 | -0.426277 | 0.235294 |
| C | -2.538421 | -0.567395 | 0.586075 |
| C | -3.498404 | -0.213914 | -0.556332 |
| H | 1.566916 | -1.431066 | 0.484797 |
| H | 3.129340 | -1.039428 | 1.165446 |
| H | 1.583066 | 0.833107 | 1.615519 |
| H | 2.834180 | 1.362156 | 0.504321 |
| H | 1.040764 | 2.263959 | -0.628946 |
| H | 1.063314 | 0.683982 | -1.378986 |
| H | -0.762204 | 1.598326 | 0.922912 |
| H | -1.217572 | 1.480392 | -0.766332 |
| H | -0.827606 | -1.028584 | -0.658620 |
| H | -0.462249 | -0.866370 | 1.054746 |
| H | -2.727631 | -1.602209 | 0.898746 |
| H | -2.763175 | 0.058403 | 1.460818 |
| H | -3.300654 | -0.829717 | -1.441499 |
| H | -3.412173 | 0.835037 | -0.857211 |
| H | -4.538930 | -0.383513 | -0.260445 |

Rotational constants (GHz): 3.8605400 0.7987700 0.7476400

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 38.4796 | 55.8539 | 102.8025 |
| 129.2301 | 146.3787 | 202.4993 |
| 253.7232 | 279.4563 | 302.6246 |
| 406.3587 | 466.5457 | 501.4784 |
| 682.5692 | 745.1345 | 767.2373 |
| 809.3974 | 871.2034 | 878.4138 |
| 913.0709 | 947.1061 | 984.9240 |
| 1030.2755 | 1053.2968 | 1087.3374 |
| 1097.6962 | 1113.6773 | 1127.1994 |
| 1157.9156 | 1213.4231 | 1262.8023 |
| 1278.5769 | 1306.9032 | 1323.5999 |
| 1340.5174 | 1357.3489 | 1368.6319 |
| 1382.9902 | 1387.7327 | 1403.9654 |
| 1416.8798 | 1429.9122 | 1489.9343 |
| 1498.1786 | 1500.9978 | 1506.9104 |
| 1511.5575 | 1516.8395 | 1522.0129 |
| 2900.9652 | 2940.0264 | 3010.8702 |
| 3018.5038 | 3025.1252 | 3031.9677 |
| 3037.9992 | 3042.0638 | 3049.7827 |
| 3061.8697 | 3070.6922 | 3078.1283 |
| 3079.8319 | 3109.4599 | 3116.8174 |

Zero-point correction (Hartree): 0.209012

C7H15O.ppmtt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.95002858

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 2.705529 | -1.314651 | -0.758750 |
| C | 2.155160 | -0.979306 | 0.447799 |
| C | 1.990354 | 0.530558 | 0.693592 |
| C | 1.169410 | 1.267738 | -0.381905 |
| C | -0.344130 | 1.372029 | -0.125338 |
| C | -1.122657 | 0.049030 | -0.094832 |
| C | -2.640122 | 0.246676 | 0.022635 |
| C | -3.421982 | -1.070030 | 0.065339 |
| H | 1.165360 | -1.484455 | 0.440327 |
| H | 2.699118 | -1.470799 | 1.278016 |
| H | 1.553455 | 0.679877 | 1.690700 |
| H | 3.000067 | 0.956506 | 0.736179 |
| H | 1.559639 | 2.287763 | -0.479571 |
| H | 1.358136 | 0.782100 | -1.348094 |
| H | -0.511164 | 1.906471 | 0.821223 |
| H | -0.777844 | 2.009237 | -0.908359 |
| H | -0.902283 | -0.527561 | -1.004784 |
| H | -0.786429 | -0.568507 | 0.750322 |
| H | -2.859024 | 0.833026 | 0.925481 |
| H | -2.989356 | 0.853219 | -0.823957 |

| | | | | |
|---|-----------|-----------|-----------|-----------|
| H | -3.122734 | -1.682410 | 0.923916 | |
| H | -3.247678 | -1.663831 | -0.839227 | |
| H | -4.499696 | -0.893595 | 0.144092 | |
| Rotational constants (GHz): | 3.1694100 | | 0.8493600 | 0.7337600 |
| Vibrational harmonic frequencies (cm ⁻¹): | | | | |
| | 45.5707 | 70.2487 | | 98.8144 |
| | 128.5882 | 148.3447 | | 192.1239 |
| | 249.7691 | 278.9409 | | 307.5907 |
| | 393.9019 | 449.8818 | | 498.6384 |
| | 662.8907 | 743.8599 | | 787.0266 |
| | 802.2242 | 872.7780 | | 877.5184 |
| | 927.0743 | 941.0559 | | 1000.8089 |
| | 1029.1686 | 1056.1136 | | 1072.3659 |
| | 1100.3034 | 1115.9249 | | 1129.2653 |
| | 1165.1391 | 1220.2393 | | 1264.6528 |
| | 1280.5475 | 1309.1998 | | 1326.0653 |
| | 1335.9943 | 1338.6348 | | 1367.9638 |
| | 1381.3359 | 1389.0344 | | 1407.0248 |
| | 1415.9703 | 1430.1426 | | 1492.1967 |
| | 1500.7992 | 1501.0533 | | 1507.9167 |
| | 1513.5713 | 1514.4412 | | 1525.2249 |
| | 2899.9080 | 2939.2326 | | 3009.9061 |
| | 3015.3099 | 3027.3089 | | 3031.9174 |
| | 3034.5566 | 3039.0814 | | 3040.6202 |
| | 3053.1233 | 3069.2633 | | 3077.0220 |
| | 3079.7805 | 3106.5031 | | 3112.7979 |
| Zero-point correction (Hartree): | 0.208918 | | | |

C7H15O.pppmm

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.94676823
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | | |
|---|-----------|-----------|-----------|-----------|
| O | -3.297077 | 0.087654 | -0.406573 | |
| C | -2.197085 | 0.866872 | -0.167580 | |
| C | -1.204806 | 0.294569 | 0.858145 | |
| C | -0.655868 | -1.086129 | 0.460784 | |
| C | 0.402859 | -1.094156 | -0.665546 | |
| C | 1.870297 | -1.045524 | -0.196499 | |
| C | 2.338328 | 0.233038 | 0.519911 | |
| C | 2.332685 | 1.489594 | -0.358608 | |
| H | -1.709047 | 0.955643 | -1.164002 | |
| H | -2.493721 | 1.904678 | 0.077854 | |
| H | -0.399369 | 1.024144 | 1.002673 | |
| H | -1.731127 | 0.217662 | 1.817605 | |
| H | -0.238778 | -1.580152 | 1.347632 | |
| H | -1.517799 | -1.691061 | 0.156305 | |
| H | 0.281721 | -2.014127 | -1.250213 | |
| H | 0.209727 | -0.277175 | -1.374464 | |
| H | 2.043419 | -1.902237 | 0.469145 | |
| H | 2.517456 | -1.208052 | -1.069782 | |
| H | 1.730648 | 0.404088 | 1.417524 | |
| H | 3.359868 | 0.064238 | 0.884407 | |
| H | 1.325664 | 1.747025 | -0.704011 | |
| H | 2.957175 | 1.348989 | -1.248524 | |
| H | 2.722313 | 2.355522 | 0.186788 | |
| Rotational constants (GHz): | 3.3171100 | | 0.9558200 | 0.8470900 |
| Vibrational harmonic frequencies (cm ⁻¹): | | | | |
| | 36.3184 | 77.9811 | | 81.8440 |
| | 159.0967 | 162.6115 | | 214.4940 |
| | 239.1457 | 274.9913 | | 369.9759 |
| | 392.6663 | 467.3700 | | 498.3858 |
| | 646.0603 | 744.7845 | | 768.2500 |
| | 811.2720 | 830.3019 | | 883.9023 |
| | 926.6566 | 939.1512 | | 983.5638 |
| | 1023.9427 | 1047.7207 | | 1080.4739 |
| | 1092.2028 | 1109.7631 | | 1133.5597 |
| | 1159.2209 | 1204.7429 | | 1230.0307 |
| | 1278.3344 | 1306.6205 | | 1325.9882 |
| | 1334.1228 | 1362.1180 | | 1373.8865 |
| | 1383.7639 | 1397.8022 | | 1402.7914 |
| | 1406.0392 | 1429.1685 | | 1490.9967 |
| | 1494.7397 | 1502.6867 | | 1505.3332 |
| | 1509.9765 | 1517.2410 | | 1520.7174 |
| | 2880.7790 | 2945.3559 | | 3017.3359 |
| | 3024.2978 | 3034.5001 | | 3037.4311 |
| | 3040.9426 | 3049.5294 | | 3054.9956 |
| | 3065.8452 | 3069.4658 | | 3080.6176 |
| | 3093.8361 | 3108.0887 | | 3112.0031 |
| Zero-point correction (Hartree): | 0.209017 | | | |

C7H15O.pppmp

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.94391401

Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 3.386678 | 0.083996 | 0.033492 |
| C | 2.344435 | -0.500894 | -0.633782 |
| C | 1.110003 | -0.811138 | 0.229656 |
| C | 0.515639 | 0.439245 | 0.899980 |
| C | -0.298523 | 1.366520 | -0.030431 |
| C | -1.822628 | 1.143396 | -0.099222 |
| C | -2.331427 | -0.193328 | -0.681659 |
| C | -2.483511 | -1.335531 | 0.332155 |
| H | 2.081777 | 0.238626 | -1.423130 |
| H | 2.685526 | -1.387977 | -1.201159 |
| H | -1.534915 | -1.611464 | 0.800841 |
| H | 1.417992 | -1.532397 | 0.996755 |
| H | -0.106159 | 0.141816 | 1.752828 |
| H | 1.358529 | 0.997987 | 1.323155 |
| H | -0.143706 | 2.403158 | 0.293587 |
| H | 0.109783 | 1.320262 | -1.050847 |
| H | -2.249650 | 1.280434 | 0.904700 |
| H | -2.233298 | 1.959572 | -0.707505 |
| H | -3.314473 | -0.017953 | -1.136789 |
| H | -1.678526 | -0.507572 | -1.507716 |
| H | -3.174208 | -1.050444 | 1.133956 |
| H | 0.371440 | -1.321372 | -0.400204 |
| H | -2.887465 | -2.234266 | -0.146584 |

Rotational constants (GHz): 3.5502900 0.9233600 0.8284200
 Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 44.7823 | 74.1276 | 97.3047 |
| 127.1688 | 162.2253 | 217.2479 |
| 236.5782 | 297.9334 | 335.8282 |
| 391.8705 | 449.4299 | 497.4358 |
| 663.6741 | 739.7892 | 782.4155 |
| 817.4987 | 836.8150 | 867.1087 |
| 930.8722 | 944.8381 | 983.0738 |
| 1033.0119 | 1055.7834 | 1084.0972 |
| 1098.7031 | 1103.5102 | 1135.4572 |
| 1169.7179 | 1197.3321 | 1239.1338 |
| 1291.8538 | 1304.7090 | 1322.4629 |
| 1330.7300 | 1368.1869 | 1376.1159 |
| 1383.6784 | 1396.2271 | 1405.5369 |
| 1406.7143 | 1429.2824 | 1492.9362 |
| 1495.6691 | 1499.3249 | 1504.9016 |
| 1509.9096 | 1516.6855 | 1523.0868 |
| 2883.1462 | 2945.9872 | 3014.9424 |
| 3017.7279 | 3023.9529 | 3042.3711 |
| 3044.4655 | 3047.8576 | 3056.6656 |
| 3062.1514 | 3065.0436 | 3083.3770 |
| 3090.9185 | 3106.7666 | 3129.4775 |

Zero-point correction (Hartree): 0.209108

C7H15O.pppmt

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.94795492
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 3.057051 | -0.634233 | -0.688452 |
| C | 1.950582 | -1.091944 | -0.024824 |
| C | 1.366349 | -0.123324 | 1.015064 |
| C | 1.011396 | 1.259441 | 0.448448 |
| C | -0.127110 | 1.326070 | -0.588556 |
| C | -1.529112 | 0.905598 | -0.094204 |
| C | -1.888520 | -0.573926 | -0.303196 |
| C | -3.306692 | -0.915771 | 0.165797 |
| H | 1.209706 | -1.279557 | -0.833240 |
| H | 2.134247 | -2.095803 | 0.404635 |
| H | 0.496073 | -0.597364 | 1.485606 |
| H | 2.112252 | 0.000724 | 1.810285 |
| H | 0.757330 | 1.922143 | 1.286101 |
| H | 1.918848 | 1.672533 | -0.007486 |
| H | -0.175488 | 2.365500 | -0.935434 |
| H | 0.136411 | 0.739076 | -1.479565 |
| H | -1.635608 | 1.161751 | 0.969947 |
| H | -2.284068 | 1.506482 | -0.618589 |
| H | -1.789448 | -0.814925 | -1.370718 |
| H | -1.172211 | -1.219004 | 0.220540 |
| H | -4.053384 | -0.312223 | -0.362909 |
| H | -3.427084 | -0.722607 | 1.237924 |
| H | -3.545341 | -1.969729 | -0.010651 |

Rotational constants (GHz): 3.1899800 0.9284400 0.8222700
 Vibrational harmonic frequencies (cm-1):

| | | |
|----------|----------|----------|
| 47.7622 | 57.2483 | 98.5585 |
| 104.0699 | 198.6869 | 205.3044 |
| 249.0487 | 277.4191 | 329.8199 |
| 382.0077 | 466.2933 | 530.6344 |

| | | |
|-----------|-----------|-----------|
| 626.3288 | 729.5641 | 764.9795 |
| 797.7521 | 855.9387 | 872.5079 |
| 918.7791 | 958.1846 | 987.8838 |
| 1037.2542 | 1052.1880 | 1078.3116 |
| 1092.3798 | 1102.1759 | 1137.1188 |
| 1162.4834 | 1212.5898 | 1249.4834 |
| 1278.3089 | 1311.7378 | 1327.8592 |
| 1337.7781 | 1343.4827 | 1374.6585 |
| 1380.0426 | 1400.4941 | 1405.7779 |
| 1415.4502 | 1426.5785 | 1492.8086 |
| 1493.9312 | 1505.1962 | 1507.1174 |
| 1509.0986 | 1513.0070 | 1524.6327 |
| 2888.8430 | 2941.9284 | 3016.1690 |
| 3026.0915 | 3029.8651 | 3032.2394 |
| 3039.1995 | 3044.8810 | 3049.4810 |
| 3067.3580 | 3071.5533 | 3077.0237 |
| 3088.6095 | 3108.2219 | 3112.5928 |

Zero-point correction (Hartree): 0.208964

C7H15O.ppppm

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.94648069

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -3.327403 | -0.204990 | 0.087681 |
| C | -2.354760 | 0.371261 | -0.684528 |
| C | -1.157027 | 0.945368 | 0.088527 |
| C | -0.467270 | -0.068345 | 1.013896 |
| C | 0.229406 | -1.250148 | 0.314775 |
| C | 1.372240 | -0.930631 | -0.669363 |
| C | 2.638151 | -0.289078 | -0.060080 |
| C | 2.636293 | 1.244153 | 0.005575 |
| H | -2.023098 | -0.450387 | -1.357614 |
| H | -2.791656 | 1.117267 | -1.376375 |
| H | -0.450852 | 1.369853 | -0.636105 |
| H | -1.521440 | 1.787903 | 0.689529 |
| H | 0.252155 | 0.462493 | 1.648080 |
| H | -1.229107 | -0.471349 | 1.691519 |
| H | 0.624888 | -1.916769 | 1.093068 |
| H | -0.525260 | -1.844860 | -0.217503 |
| H | 1.659219 | -1.880119 | -1.138859 |
| H | 1.005338 | -0.299166 | -1.490820 |
| H | 2.804735 | -0.702396 | 0.944243 |
| H | 3.506075 | -0.599520 | -0.655431 |
| H | 1.832571 | 1.634518 | 0.636235 |
| H | 2.510937 | 1.676961 | -0.993922 |
| H | 3.582513 | 1.620009 | 0.409702 |

Rotational constants (GHz): 3.8463100 0.9056200 0.8368000

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 28.2913 | 64.6561 | 77.0180 |
| 125.9527 | 181.4859 | 223.0566 |
| 239.1415 | 309.2102 | 351.5939 |
| 396.5332 | 468.0557 | 535.3761 |
| 616.3766 | 736.8957 | 740.0667 |
| 800.8636 | 848.2221 | 858.3687 |
| 937.3460 | 939.5878 | 985.5551 |
| 1030.0089 | 1052.0662 | 1083.1779 |
| 1095.5721 | 1096.5912 | 1134.7967 |
| 1169.8315 | 1196.2467 | 1238.3049 |
| 1282.8666 | 1306.0795 | 1322.1606 |
| 1340.9876 | 1370.6737 | 1376.2600 |
| 1384.8376 | 1392.9244 | 1409.3128 |
| 1415.6487 | 1427.3650 | 1491.6832 |
| 1497.9092 | 1498.3510 | 1507.0442 |
| 1511.2567 | 1516.4619 | 1522.2687 |
| 2885.0353 | 2941.0008 | 3019.7786 |
| 3023.9883 | 3026.1787 | 3041.7150 |
| 3042.8731 | 3047.6870 | 3056.6975 |
| 3063.6489 | 3064.4129 | 3080.8722 |
| 3089.6891 | 3105.1308 | 3129.6002 |

Zero-point correction (Hartree): 0.209028

C7H15O.ppppp

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.94934741

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 3.354923 | -0.545232 | 0.253848 |
| C | 2.578034 | 0.576829 | 0.145479 |
| C | 1.417533 | 0.476284 | -0.856766 |
| C | 0.476214 | -0.711098 | -0.600825 |
| C | -0.334208 | -0.652545 | 0.707565 |
| C | -1.276845 | 0.555884 | 0.863372 |
| C | -2.362217 | 0.701536 | -0.217652 |
| C | -3.356374 | -0.464454 | -0.275313 |

| | | | | |
|---|-----------|-----------|-----------|--|
| H | 2.186180 | 0.734300 | 1.174840 | |
| H | 3.202933 | 1.472168 | -0.038490 | |
| H | 0.870528 | 1.427835 | -0.848734 | |
| H | 1.850197 | 0.380365 | -1.860336 | |
| H | -0.208323 | -0.805063 | -1.452502 | |
| H | 1.082920 | -1.623871 | -0.594303 | |
| H | -0.915730 | -1.579129 | 0.789310 | |
| H | 0.352051 | -0.669363 | 1.564483 | |
| H | -1.766000 | 0.485538 | 1.844624 | |
| H | -0.685911 | 1.481108 | 0.893797 | |
| H | -2.913703 | 1.631236 | -0.027615 | |
| H | -1.893983 | 0.830028 | -1.202143 | |
| H | -3.846727 | -0.613175 | 0.693974 | |
| H | -2.867293 | -1.406320 | -0.545029 | |
| H | -4.139354 | -0.278416 | -1.017824 | |
| Rotational constants (GHz): | 4.8700600 | 0.7942700 | 0.7883600 | |
| Vibrational harmonic frequencies (cm ⁻¹): | | | | |
| 31.8628 | 46.6635 | | 74.2714 | |
| 144.5643 | 174.7217 | | 224.6932 | |
| 284.8206 | 299.0170 | | 362.6056 | |
| 411.8302 | 481.0032 | | 544.5079 | |
| 617.9947 | 713.1387 | | 751.8069 | |
| 812.3090 | 832.2060 | | 876.5760 | |
| 927.2134 | 946.9028 | | 983.7291 | |
| 1026.0183 | 1041.5839 | | 1075.8694 | |
| 1090.2650 | 1106.5927 | | 1132.1727 | |
| 1166.3584 | 1198.7083 | | 1235.2225 | |
| 1279.2710 | 1305.3538 | | 1320.5825 | |
| 1344.7665 | 1368.7299 | | 1374.2746 | |
| 1386.2224 | 1394.2676 | | 1409.4484 | |
| 1416.0221 | 1429.7319 | | 1487.4666 | |
| 1495.3129 | 1503.4433 | | 1510.9677 | |
| 1512.3696 | 1518.4734 | | 1525.8990 | |
| 2886.6723 | 2941.3591 | | 3021.8464 | |
| 3031.2937 | 3037.4649 | | 3040.1466 | |
| 3042.2851 | 3047.8291 | | 3055.8654 | |
| 3066.7623 | 3072.6583 | | 3079.6457 | |
| 3090.5666 | 3108.5252 | | 3115.1252 | |
| Zero-point correction (Hartree): | 0.209218 | | | |

C7H15O.ppppt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.95058621
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | | |
|---|-----------|-----------|-----------|--|
| O | 3.463591 | 0.164021 | -0.272966 | |
| C | 2.454941 | -0.746145 | -0.443242 | |
| C | 1.379555 | -0.744040 | 0.653898 | |
| C | 0.720512 | 0.626346 | 0.874585 | |
| C | -0.127540 | 1.157155 | -0.297240 | |
| C | -1.326803 | 0.288109 | -0.714434 | |
| C | -2.397743 | 0.109382 | 0.370408 | |
| C | -3.613981 | -0.685418 | -0.116007 | |
| H | 2.007555 | -0.476114 | -1.425397 | |
| H | 2.867189 | -1.759794 | -0.613306 | |
| H | 0.633797 | -1.511617 | 0.409966 | |
| H | 1.856184 | -1.066506 | 1.587861 | |
| H | 0.104115 | 0.577900 | 1.780106 | |
| H | 1.516347 | 1.349977 | 1.085271 | |
| H | -0.496413 | 2.155025 | -0.024131 | |
| H | 0.516690 | 1.314701 | -1.172390 | |
| H | -1.793683 | 0.746139 | -1.597175 | |
| H | -0.981544 | -0.701599 | -1.045218 | |
| H | -1.964106 | -0.394107 | 1.243782 | |
| H | -2.722358 | 1.098807 | 0.721162 | |
| H | -3.324917 | -1.690406 | -0.444883 | |
| H | -4.098542 | -0.188940 | -0.964685 | |
| H | -4.362691 | -0.797977 | 0.674946 | |
| Rotational constants (GHz): | 4.6891500 | 0.7583700 | 0.7388500 | |
| Vibrational harmonic frequencies (cm ⁻¹): | | | | |
| 26.1299 | 54.4036 | | 81.3511 | |
| 120.0256 | 188.8309 | | 233.4831 | |
| 255.9696 | 287.1746 | | 326.4090 | |
| 400.9243 | 478.6179 | | 543.0538 | |
| 621.5283 | 720.1748 | | 760.6353 | |
| 803.8447 | 846.8125 | | 877.5277 | |
| 926.4295 | 954.7067 | | 986.4673 | |
| 1035.9994 | 1044.7757 | | 1078.2091 | |
| 1084.1362 | 1106.4382 | | 1131.7591 | |
| 1175.8810 | 1198.8379 | | 1247.9901 | |
| 1283.1050 | 1312.1547 | | 1328.5663 | |
| 1335.2749 | 1348.1166 | | 1373.4396 | |
| 1380.4698 | 1399.8530 | | 1410.2984 | |
| 1417.1802 | 1428.3239 | | 1489.6810 | |
| 1499.9242 | 1503.1467 | | 1506.9590 | |

| | | |
|-----------|-----------|-----------|
| 1513.1328 | 1515.0144 | 1524.0030 |
| 2888.6193 | 2939.6431 | 3017.6166 |
| 3026.2182 | 3028.8724 | 3038.1362 |
| 3040.0701 | 3046.7933 | 3048.1986 |
| 3062.7995 | 3070.5216 | 3079.3029 |
| 3091.0413 | 3106.1207 | 3112.0370 |

Zero-point correction (Hartree): 0.209052

C7H15O.ppptm

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.95049299

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 3.291878 | -0.967702 | -0.374622 |
| C | 2.589198 | -0.400204 | 0.654740 |
| C | 1.839374 | 0.893592 | 0.297533 |
| C | 0.842974 | 0.727194 | -0.861759 |
| C | -0.416982 | -0.100419 | -0.548641 |
| C | -1.379690 | 0.555453 | 0.453577 |
| C | -2.643366 | -0.268540 | 0.755066 |
| C | -3.597736 | -0.430397 | -0.435011 |
| H | 1.868469 | -1.191621 | 0.957777 |
| H | 3.232276 | -0.271041 | 1.546424 |
| H | 1.344043 | 1.269937 | 1.201735 |
| H | 2.589097 | 1.645781 | 0.023729 |
| H | 0.534810 | 1.721134 | -1.210924 |
| H | 1.381333 | 0.260153 | -1.694658 |
| H | -0.944689 | -0.280402 | -1.492780 |
| H | -0.132505 | -1.095766 | -0.177616 |
| H | -0.854551 | 0.740654 | 1.399510 |
| H | -1.675763 | 1.544247 | 0.073818 |
| H | -2.347694 | -1.260578 | 1.123663 |
| H | -3.184871 | 0.210947 | 1.580447 |
| H | -3.134332 | -0.978800 | -1.261454 |
| H | -3.913563 | 0.545769 | -0.821583 |
| H | -4.499722 | -0.978876 | -0.144145 |

Rotational constants (GHz): 4.6523500 0.7127200 0.7078400

Vibrational harmonic frequencies (cm⁻¹):

| | | |
|-----------|-----------|-----------|
| 31.8774 | 43.3226 | 92.1928 |
| 128.6909 | 183.4871 | 220.6891 |
| 241.3745 | 290.6965 | 321.4242 |
| 407.7781 | 470.2234 | 526.1403 |
| 619.3821 | 730.7040 | 758.1589 |
| 822.7187 | 841.1939 | 876.8659 |
| 921.2676 | 948.1839 | 977.7725 |
| 1036.6852 | 1053.4972 | 1077.7129 |
| 1087.4592 | 1105.6005 | 1122.5664 |
| 1168.7350 | 1211.0060 | 1239.0220 |
| 1295.2422 | 1302.5592 | 1320.8958 |
| 1344.4801 | 1353.9269 | 1373.0189 |
| 1386.9875 | 1388.8619 | 1405.7329 |
| 1418.0077 | 1429.3139 | 1495.9834 |
| 1497.8172 | 1501.6552 | 1503.0601 |
| 1514.0669 | 1516.9687 | 1522.7373 |
| 2890.3678 | 2944.3001 | 3015.2429 |
| 3023.2158 | 3025.9711 | 3037.7364 |
| 3042.3131 | 3045.2821 | 3056.5085 |
| 3062.2263 | 3076.7518 | 3081.4421 |
| 3088.8271 | 3108.5615 | 3118.8919 |

Zero-point correction (Hartree): 0.209011

C7H15O.ppptp

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.95054248

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -3.045089 | 1.002980 | -0.598727 |
| C | -2.282074 | 0.795918 | 0.519087 |
| C | -1.771995 | -0.641686 | 0.705319 |
| C | -0.961209 | -1.171158 | -0.488542 |
| C | 0.407187 | -0.505047 | -0.717503 |
| C | 1.427742 | -0.737770 | 0.406859 |
| C | 2.839510 | -0.209109 | 0.101448 |
| C | 2.931734 | 1.315475 | -0.036086 |
| H | -1.426226 | 1.496067 | 0.395471 |
| H | -2.799474 | 1.169362 | 1.423929 |
| H | -1.189389 | -0.685301 | 1.634330 |
| H | -2.645119 | -1.287380 | 0.860467 |
| H | -0.812414 | -2.251355 | -0.360537 |
| H | -1.574512 | -1.046483 | -1.388399 |
| H | 0.824336 | -0.896764 | -1.655285 |
| H | 0.272369 | 0.571403 | -0.884965 |
| H | 1.073201 | -0.277929 | 1.339973 |
| H | 1.489981 | -1.816555 | 0.606436 |
| H | 3.516518 | -0.535336 | 0.901313 |

| | | | | |
|---|-----------|-----------|-----------|---------------------|
| H | 3.209209 | -0.681171 | -0.819316 | |
| H | 2.565273 | 1.816205 | 0.868136 | |
| H | 2.344247 | 1.687223 | -0.881848 | |
| H | 3.967337 | 1.634443 | -0.193378 | |
| Rotational constants (GHz): | | | 3.4979400 | 0.8358400 0.7609800 |
| Vibrational harmonic frequencies (cm ⁻¹): | | | | |
| | 31.7277 | 43.7945 | | 94.3761 |
| | 127.3282 | 179.5250 | | 224.6256 |
| | 238.5657 | 294.7379 | | 320.4862 |
| | 393.1946 | 474.9664 | | 535.3700 |
| | 630.6699 | 730.1298 | | 773.7805 |
| | 809.1620 | 842.7932 | | 873.9651 |
| | 924.2616 | 941.8286 | | 987.0561 |
| | 1031.7587 | 1058.9840 | | 1076.2780 |
| | 1086.8115 | 1106.8469 | | 1124.7296 |
| | 1176.3325 | 1197.1895 | | 1243.9089 |
| | 1292.1251 | 1304.0985 | | 1329.8568 |
| | 1335.0427 | 1351.8069 | | 1373.2785 |
| | 1384.8140 | 1388.0055 | | 1406.5362 |
| | 1415.7719 | 1431.0573 | | 1493.9453 |
| | 1496.8058 | 1501.7376 | | 1503.3480 |
| | 1513.8244 | 1517.3566 | | 1522.4443 |
| | 2887.8279 | 2941.7574 | | 3013.9834 |
| | 3024.7831 | 3028.8303 | | 3033.6820 |
| | 3040.4876 | 3043.2392 | | 3048.9281 |
| | 3061.0527 | 3070.6758 | | 3079.8001 |
| | 3088.3980 | 3107.1257 | | 3116.9247 |
| Zero-point correction (Hartree): 0.208964 | | | | |

C7H15O.ppptt

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.95189267

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | | |
|---|-----------|-----------|-----------|---------------------|
| O | 3.376607 | -0.411620 | -0.773035 | |
| C | 2.462142 | -0.946601 | 0.094378 | |
| C | 1.744922 | 0.069123 | 0.996796 | |
| C | 1.021920 | 1.182192 | 0.221594 | |
| C | -0.210910 | 0.741247 | -0.587256 | |
| C | -1.388654 | 0.232839 | 0.256023 | |
| C | -2.628784 | -0.111983 | -0.579310 | |
| C | -3.804988 | -0.616289 | 0.262749 | |
| H | 1.730521 | -1.462195 | -0.566425 | |
| H | 2.913288 | -1.771177 | 0.679782 | |
| H | 1.052365 | -0.475182 | 1.651322 | |
| H | 2.498240 | 0.520123 | 1.654378 | |
| H | 0.718959 | 1.965228 | 0.928864 | |
| H | 1.750234 | 1.641770 | -0.456603 | |
| H | -0.550977 | 1.597075 | -1.185591 | |
| H | 0.072932 | -0.029829 | -1.317344 | |
| H | -1.089538 | -0.655792 | 0.828884 | |
| H | -1.654976 | 0.996244 | 1.001440 | |
| H | -2.938609 | 0.775487 | -1.147733 | |
| H | -2.361462 | -0.871123 | -1.327214 | |
| H | -4.117617 | 0.135411 | 0.996558 | |
| H | -3.537011 | -1.524121 | 0.815610 | |
| H | -4.673093 | -0.852123 | -0.361483 | |
| Rotational constants (GHz): | | | 4.5073400 | 0.6965700 0.6831400 |
| Vibrational harmonic frequencies (cm ⁻¹): | | | | |
| | 18.7777 | 56.3752 | | 82.5879 |
| | 123.6980 | 147.1935 | | 232.8809 |
| | 237.9606 | 253.5372 | | 347.3553 |
| | 396.5114 | 447.6619 | | 529.9219 |
| | 626.9402 | 730.6908 | | 760.3165 |
| | 824.3963 | 841.5144 | | 892.2303 |
| | 924.4291 | 954.9842 | | 982.5213 |
| | 1047.1630 | 1061.3539 | | 1070.0448 |
| | 1080.6909 | 1105.0330 | | 1128.8304 |
| | 1177.3834 | 1213.5417 | | 1249.9306 |
| | 1293.5682 | 1301.9702 | | 1328.2672 |
| | 1337.1416 | 1341.8180 | | 1372.4748 |
| | 1377.8077 | 1394.0690 | | 1409.8518 |
| | 1417.8417 | 1426.0091 | | 1497.1774 |
| | 1498.1282 | 1500.7965 | | 1505.0596 |
| | 1511.9767 | 1515.0297 | | 1525.0436 |
| | 2890.7994 | 2940.5902 | | 3013.6511 |
| | 3021.3341 | 3029.0688 | | 3034.9356 |
| | 3038.0087 | 3038.2861 | | 3046.7061 |
| | 3055.7837 | 3071.7177 | | 3079.7470 |
| | 3088.5102 | 3105.9659 | | 3112.0636 |
| Zero-point correction (Hartree): 0.208834 | | | | |

C7H15O.pptmm

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.95058317

```

Electronic state : 2-A
Cartesian coordinates (Angs):
O      3.281917   -0.812392   -0.426487
C      2.861518    0.178092    0.419752
C      1.734477    1.068458   -0.127776
C      0.469110    0.292865   -0.524145
C     -0.352579   -0.218603    0.668578
C     -1.562217   -1.088045    0.280879
C     -2.650651   -0.393316   -0.557113
C     -3.326122    0.792247    0.141829
H      2.517528   -0.368030    1.326006
H      3.719861    0.776258    0.782090
H      1.499364    1.834696    0.623805
H      2.129215    1.601124   -1.001592
H     -0.156487    0.940535   -1.149485
H      0.769593   -0.552178   -1.157022
H      0.290423   -0.816504    1.328504
H     -0.684093    0.636772    1.272979
H     -1.200362   -1.966410   -0.270328
H     -2.022716   -1.475101    1.200331
H     -2.229585   -0.062059   -1.514847
H     -3.414078   -1.139744   -0.810962
H     -2.621671    1.607495    0.337847
H     -3.757538    0.490723    1.103660
H     -4.136014    1.201368   -0.471108
Rotational constants (GHz):   4.8076700   0.7429600   0.7058500
Vibrational harmonic frequencies (cm-1):
   31.5107           52.4596           69.6408
  146.7152          188.9075          226.0053
  239.0108          268.4659          333.9006
  398.3950          487.6711          517.5589
  638.3505          726.0199          767.4616
  831.1427          835.7475          873.3759
  902.3029          969.6678          995.5761
 1016.6203         1046.9555         1093.6418
 1097.8871         1103.3405         1124.1549
 1170.8416         1190.9689         1265.7278
 1280.1188         1303.4553         1331.0414
 1342.9785         1351.7329         1373.4286
 1387.6163         1394.8636         1401.9252
 1417.1530         1430.2624         1491.8470
 1492.1577         1502.9637         1508.0625
 1509.3811         1518.4538         1526.0359
 2886.3108         2942.3600         3018.1242
 3024.7692         3032.4374         3037.2515
 3041.0181         3043.2460         3050.7634
 3061.1682         3071.9993         3077.7327
 3087.8709         3108.4969         3114.1807
Zero-point correction (Hartree): 0.209070
  
```

C7H15O.pptmp

```

-----
E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.94790255
Electronic state : 2-A
Cartesian coordinates (Angs):
O      3.267954   -0.533238   -0.765146
C      2.856654    0.003809    0.424889
C      1.699552    1.010387    0.321699
C      0.439520    0.445748   -0.350835
C     -0.322615   -0.585352    0.498259
C     -1.606176   -1.142411   -0.158961
C     -2.913818   -0.408789    0.189855
C     -3.004319    1.053163   -0.262719
H      2.549132   -0.878731    1.028459
H      3.715459    0.420257    0.986129
H      1.467724    1.378333    1.330873
H      2.062500    1.874654   -0.248040
H     -0.223949    1.277740   -0.609138
H      0.736572   -0.017197   -1.300234
H      0.348828   -1.426302    0.714393
H     -0.572861   -0.146071    1.475204
H     -1.476213   -1.159469   -1.250239
H     -1.729737   -2.190385    0.141247
H     -3.746820   -0.967637   -0.256407
H     -3.067488   -0.459150    1.276810
H     -2.827938    1.148333   -1.340430
H     -2.274598    1.687060    0.251207
H     -3.997032    1.465143   -0.051799
Rotational constants (GHz):   4.5706300   0.7586100   0.7099500
Vibrational harmonic frequencies (cm-1):
   25.9254           63.0709           85.9113
  103.9563          176.9599          208.1513
  272.7334          285.8240          311.2825
  384.0659          469.0200          515.3697
  
```


| | | |
|-----------|-----------|-----------|
| 635.9723 | 733.1958 | 775.6112 |
| 805.5271 | 852.4892 | 869.3602 |
| 905.1333 | 975.4378 | 992.8749 |
| 1027.2628 | 1050.9303 | 1085.2563 |
| 1099.1742 | 1110.1812 | 1124.3741 |
| 1163.0060 | 1207.8670 | 1260.2466 |
| 1282.7130 | 1310.6515 | 1321.4271 |
| 1343.7170 | 1352.2020 | 1373.4406 |
| 1390.1538 | 1392.8524 | 1398.4736 |
| 1410.9472 | 1430.1945 | 1493.1399 |
| 1496.6421 | 1499.2795 | 1503.6338 |
| 1511.6410 | 1516.6818 | 1524.3821 |
| 2889.5113 | 2941.5063 | 3014.4543 |
| 3022.2506 | 3023.6351 | 3031.5311 |
| 3041.0918 | 3048.5204 | 3052.2365 |
| 3060.3409 | 3067.6130 | 3077.2269 |
| 3098.8061 | 3107.4690 | 3117.1021 |

Zero-point correction (Hartree): 0.208957

C7H15O.pptmt

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.95179121
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 3.207664 | -1.045166 | -0.639010 |
| C | 3.014677 | -0.074828 | 0.307089 |
| C | 2.003678 | 1.017709 | -0.075988 |
| C | 0.607445 | 0.478637 | -0.421304 |
| C | -0.196492 | -0.012241 | 0.792481 |
| C | -1.573384 | -0.604073 | 0.446551 |
| C | -2.589495 | 0.404090 | -0.108996 |
| C | -3.963842 | -0.220316 | -0.372511 |
| H | 2.660889 | -0.634214 | 1.201415 |
| H | 3.982100 | 0.355071 | 0.631526 |
| H | 1.945642 | 1.743291 | 0.747163 |
| H | 2.412488 | 1.558287 | -0.938406 |
| H | 0.047486 | 1.266724 | -0.937788 |
| H | 0.725638 | -0.341481 | -1.141034 |
| H | 0.380174 | -0.778586 | 1.327729 |
| H | -0.326619 | 0.818348 | 1.501634 |
| H | -1.443179 | -1.423057 | -0.275347 |
| H | -1.996408 | -1.063343 | 1.350465 |
| H | -2.695341 | 1.236041 | 0.601295 |
| H | -2.210695 | 0.844831 | -1.039497 |
| H | -4.391142 | -0.640077 | 0.545517 |
| H | -3.895658 | -1.032847 | -1.104919 |
| H | -4.672211 | 0.518468 | -0.761604 |

Rotational constants (GHz): 5.4782400 0.6564400 0.6401600
 Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 36.7012 | 63.2793 | 83.5384 |
| 105.5665 | 179.8334 | 223.3668 |
| 241.6272 | 259.4813 | 292.8139 |
| 355.2772 | 488.8892 | 532.0734 |
| 631.9763 | 732.7032 | 757.4115 |
| 824.5656 | 850.2370 | 882.2133 |
| 896.2312 | 981.2858 | 997.8389 |
| 1028.8597 | 1044.6035 | 1078.9858 |
| 1098.9596 | 1103.1907 | 1121.0529 |
| 1167.3987 | 1212.1291 | 1269.8994 |
| 1278.1357 | 1309.3710 | 1331.6409 |
| 1334.5555 | 1346.5687 | 1358.3041 |
| 1373.7313 | 1397.6527 | 1409.1795 |
| 1415.4273 | 1427.0112 | 1492.7272 |
| 1496.1676 | 1500.5300 | 1509.6829 |
| 1510.0468 | 1512.6328 | 1525.0017 |
| 2885.4645 | 2941.6148 | 3012.4103 |
| 3017.1859 | 3028.0916 | 3031.8113 |
| 3038.6884 | 3043.0200 | 3048.4448 |
| 3050.3651 | 3072.4322 | 3077.4345 |
| 3088.5516 | 3107.4466 | 3111.8958 |

Zero-point correction (Hartree): 0.208738

C7H15O.pptpm

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.94803210
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 2.527257 | 1.414258 | -0.555168 |
| C | 2.708800 | 0.069889 | -0.371067 |
| C | 1.941208 | -0.536516 | 0.814546 |
| C | 0.424137 | -0.303273 | 0.756957 |
| C | -0.290179 | -1.108217 | -0.339868 |
| C | -1.829617 | -1.061637 | -0.321055 |
| C | -2.482840 | 0.303302 | -0.627870 |
| C | -2.678964 | 1.228255 | 0.580930 |

| | | | |
|---|-----------|-----------|-----------|
| H | 2.364611 | -0.383476 | -1.326953 |
| H | 3.786921 | -0.179438 | -0.334178 |
| H | 2.166223 | -1.611146 | 0.861228 |
| H | 2.345361 | -0.093734 | 1.733254 |
| H | -0.010578 | -0.561868 | 1.731127 |
| H | 0.256987 | 0.769503 | 0.613487 |
| H | 0.052711 | -0.773682 | -1.329105 |
| H | 0.017602 | -2.160386 | -0.254371 |
| H | -2.182627 | -1.787445 | -1.064747 |
| H | -2.193743 | -1.428952 | 0.649343 |
| H | -1.895827 | 0.820688 | -1.399216 |
| H | -3.467464 | 0.121164 | -1.076960 |
| H | -1.731654 | 1.509494 | 1.048445 |
| H | -3.293537 | 0.742044 | 1.347588 |
| H | -3.188318 | 2.152352 | 0.286964 |

Rotational constants (GHz): 3.2061300 0.8864800 0.8084000

Vibrational harmonic frequencies (cm⁻¹):

| | | |
|-----------|-----------|-----------|
| 33.8627 | 47.7870 | 71.0439 |
| 121.2832 | 169.9030 | 220.8869 |
| 236.0992 | 263.2193 | 334.5678 |
| 378.3894 | 462.4067 | 524.3533 |
| 643.0804 | 748.2783 | 774.6186 |
| 801.3350 | 831.4203 | 884.8843 |
| 901.6655 | 976.3037 | 985.2114 |
| 1037.6885 | 1049.9353 | 1082.8907 |
| 1096.0166 | 1115.0304 | 1121.9567 |
| 1160.0454 | 1211.4645 | 1252.7992 |
| 1294.4482 | 1306.3035 | 1321.9965 |
| 1343.1105 | 1356.3847 | 1373.2850 |
| 1382.2617 | 1395.6187 | 1398.5952 |
| 1415.2844 | 1429.9713 | 1490.8897 |
| 1495.1803 | 1500.9557 | 1504.5169 |
| 1508.0632 | 1515.7077 | 1522.7248 |
| 2886.7677 | 2942.1870 | 3009.8215 |
| 3018.6712 | 3025.6284 | 3030.0573 |
| 3039.7863 | 3044.0101 | 3047.3214 |
| 3062.0433 | 3063.2810 | 3075.0133 |
| 3098.2368 | 3106.2389 | 3133.6738 |

Zero-point correction (Hartree): 0.208854

C7H15O.pptpp

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.95080821

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -2.221819 | 1.572392 | -0.254173 |
| C | -2.514077 | 0.420719 | 0.425252 |
| C | -2.040158 | -0.877802 | -0.248611 |
| C | -0.544762 | -0.886371 | -0.595787 |
| C | 0.385873 | -0.939666 | 0.624862 |
| C | 1.881566 | -1.028641 | 0.273774 |
| C | 2.453908 | 0.158087 | -0.522460 |
| C | 2.330823 | 1.513292 | 0.184002 |
| H | -2.003190 | 0.552874 | 1.405011 |
| H | -3.588005 | 0.377693 | 0.690521 |
| H | -2.290891 | -1.720226 | 0.410831 |
| H | -2.629165 | -1.013535 | -1.164130 |
| H | -0.335124 | -1.749773 | -1.240802 |
| H | -0.332685 | 0.007093 | -1.193323 |
| H | 0.216673 | -0.062632 | 1.262742 |
| H | 0.120372 | -1.812395 | 1.237757 |
| H | 2.452819 | -1.134588 | 1.206271 |
| H | 2.056444 | -1.951931 | -0.295764 |
| H | 3.513043 | -0.046501 | -0.725065 |
| H | 1.969091 | 0.215873 | -1.505107 |
| H | 2.792052 | 1.485507 | 1.178520 |
| H | 1.285500 | 1.813998 | 0.309757 |
| H | 2.828589 | 2.301698 | -0.390017 |

Rotational constants (GHz): 2.9460600 1.0158500 0.8396800

Vibrational harmonic frequencies (cm⁻¹):

| | | |
|-----------|-----------|-----------|
| 25.9226 | 37.2936 | 79.7284 |
| 158.9873 | 182.0747 | 237.5145 |
| 243.5175 | 266.6414 | 326.0621 |
| 395.8950 | 483.2925 | 534.2958 |
| 649.2147 | 727.3797 | 786.8811 |
| 813.1504 | 833.8266 | 878.0505 |
| 899.1522 | 975.3534 | 986.3005 |
| 1025.8303 | 1045.0108 | 1086.1771 |
| 1098.7113 | 1107.7754 | 1119.7052 |
| 1170.8404 | 1193.3105 | 1256.4151 |
| 1289.7409 | 1292.8441 | 1327.1416 |
| 1341.2668 | 1350.3195 | 1375.4236 |
| 1386.2486 | 1394.9082 | 1400.7695 |
| 1417.9022 | 1430.2511 | 1491.4102 |
| 1495.5049 | 1502.3924 | 1506.4464 |

| | | |
|-----------|-----------|-----------|
| 1509.2054 | 1517.5331 | 1526.6928 |
| 2883.8457 | 2943.7859 | 3016.0389 |
| 3024.1255 | 3030.4956 | 3036.7401 |
| 3039.3448 | 3040.2904 | 3051.0908 |
| 3062.2759 | 3072.5981 | 3074.4931 |
| 3095.1861 | 3107.9366 | 3115.7885 |

Zero-point correction (Hartree): 0.209077

C7H15O.pptpt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.95192310

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 2.652035 | 1.584088 | 0.022987 |
| C | 2.813402 | 0.301036 | -0.426403 |
| C | 2.179221 | -0.784376 | 0.457804 |
| C | 0.671401 | -0.598332 | 0.680919 |
| C | -0.192246 | -0.906423 | -0.552183 |
| C | -1.706977 | -0.809042 | -0.304163 |
| C | -2.221960 | 0.605936 | -0.004238 |
| C | -3.743067 | 0.660662 | 0.172170 |
| H | 2.339978 | 0.304425 | -1.433084 |
| H | 3.879716 | 0.090072 | -0.636950 |
| H | 2.386432 | -1.765307 | 0.008001 |
| H | 2.697851 | -0.769394 | 1.424262 |
| H | 0.351559 | -1.248828 | 1.505551 |
| H | 0.505277 | 0.431998 | 1.015182 |
| H | 0.073768 | -0.230883 | -1.377720 |
| H | 0.043574 | -1.920946 | -0.902514 |
| H | -2.234394 | -1.193906 | -1.187736 |
| H | -1.980900 | -1.477555 | 0.525040 |
| H | -1.739482 | 0.996181 | 0.900267 |
| H | -1.923432 | 1.277562 | -0.821080 |
| H | -4.068921 | 0.025338 | 1.003878 |
| H | -4.259770 | 0.312150 | -0.729626 |
| H | -4.086172 | 1.679622 | 0.379198 |

Rotational constants (GHz): 3.9073900 0.7600100 0.6898600

Vibrational harmonic frequencies (cm⁻¹):

| | | |
|-----------|-----------|-----------|
| 36.2202 | 56.9124 | 78.8885 |
| 119.5153 | 169.3754 | 228.9971 |
| 245.8332 | 266.9471 | 293.6173 |
| 351.7702 | 483.4700 | 539.2011 |
| 628.5407 | 737.9024 | 764.5413 |
| 822.9646 | 832.9206 | 888.2996 |
| 896.2889 | 979.9366 | 993.5158 |
| 1038.5453 | 1050.7181 | 1080.6879 |
| 1092.8950 | 1102.5823 | 1123.0837 |
| 1170.9187 | 1209.9774 | 1260.5346 |
| 1298.9082 | 1301.9141 | 1328.4806 |
| 1333.5976 | 1348.7046 | 1358.8719 |
| 1372.9622 | 1397.3910 | 1409.9658 |
| 1413.7592 | 1427.4861 | 1493.7366 |
| 1497.4502 | 1499.2176 | 1508.7566 |
| 1511.3754 | 1513.9013 | 1524.0528 |
| 2886.9155 | 2942.2549 | 3011.8994 |
| 3015.6834 | 3029.3579 | 3030.7388 |
| 3037.8113 | 3038.3334 | 3046.4596 |
| 3050.5990 | 3072.7893 | 3075.9988 |
| 3091.8533 | 3106.4792 | 3112.3674 |

Zero-point correction (Hartree): 0.208761

C7H15O.ppttm

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.95190775

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 2.883688 | 1.160498 | 0.806966 |
| C | 2.639434 | 0.670448 | -0.447726 |
| C | 2.150253 | -0.785721 | -0.496407 |
| C | 0.871246 | -1.038566 | 0.314398 |
| C | -0.403355 | -0.443532 | -0.301324 |
| C | -1.660330 | -0.744205 | 0.527599 |
| C | -2.974506 | -0.232473 | -0.084911 |
| C | -3.087842 | 1.294736 | -0.165244 |
| H | 1.863386 | 1.353127 | -0.859439 |
| H | 3.511849 | 0.833969 | -1.109624 |
| H | 2.003902 | -1.068805 | -1.548008 |
| H | 2.958997 | -1.420129 | -0.113357 |
| H | 0.735192 | -2.121225 | 0.433518 |
| H | 1.018790 | -0.632718 | 1.323119 |
| H | -0.290295 | 0.642702 | -0.412391 |
| H | -0.536877 | -0.842509 | -1.317845 |
| H | -1.735752 | -1.831288 | 0.667577 |
| H | -1.539449 | -0.317337 | 1.533572 |
| H | -3.095679 | -0.661463 | -1.089353 |

| | | | |
|---|-----------|-----------|-----------|
| H | -3.811174 | -0.619177 | 0.510893 |
| H | -2.324791 | 1.728738 | -0.819612 |
| H | -2.972636 | 1.751166 | 0.824846 |
| H | -4.064365 | 1.596838 | -0.557938 |
| Rotational constants (GHz): | 3.6744000 | 0.7613700 | 0.6925200 |
| Vibrational harmonic frequencies (cm ⁻¹): | | | |
| 33.7841 | 59.0999 | 99.8335 | |
| 118.6989 | 150.2042 | 202.5925 | |
| 243.3494 | 274.8918 | 315.8657 | |
| 404.3983 | 457.1183 | 512.7040 | |
| 628.9960 | 736.1478 | 775.2793 | |
| 808.9110 | 869.0431 | 881.6594 | |
| 890.8083 | 979.5730 | 988.6464 | |
| 1033.8719 | 1045.0838 | 1083.9117 | |
| 1099.5803 | 1101.7706 | 1125.6220 | |
| 1166.4844 | 1212.0136 | 1263.4782 | |
| 1280.8487 | 1311.6400 | 1326.0473 | |
| 1340.1164 | 1342.0221 | 1373.3286 | |
| 1386.3115 | 1386.6097 | 1403.6720 | |
| 1416.4651 | 1428.5062 | 1493.6243 | |
| 1496.6636 | 1500.1038 | 1503.3419 | |
| 1514.6794 | 1519.1832 | 1522.8372 | |
| 2888.8940 | 2941.4644 | 3012.5409 | |
| 3019.6353 | 3024.4626 | 3031.1867 | |
| 3036.9397 | 3041.2667 | 3047.0901 | |
| 3059.9063 | 3065.8708 | 3076.3739 | |
| 3085.2187 | 3108.5754 | 3115.6637 | |
| Zero-point correction (Hartree): | 0.208827 | | |

C7H15O.ppttp

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.95194754

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -3.147914 | -1.167065 | -0.036093 |
| C | -2.735640 | -0.083946 | -0.764719 |
| C | -2.046491 | 1.025576 | 0.045133 |
| C | -0.830360 | 0.544982 | 0.849733 |
| C | 0.388550 | 0.160503 | -0.001667 |
| C | 1.593224 | -0.270726 | 0.847346 |
| C | 2.818977 | -0.728812 | 0.039986 |
| C | 3.478226 | 0.373883 | -0.797201 |
| H | -2.030426 | -0.511777 | -1.511256 |
| H | -3.564718 | 0.312357 | -1.382428 |
| H | -1.759195 | 1.831736 | -0.644121 |
| H | -2.792186 | 1.451434 | 0.727812 |
| H | -0.536410 | 1.336414 | 1.551270 |
| H | -1.138372 | -0.312288 | 1.461024 |
| H | 0.128328 | -0.661647 | -0.683283 |
| H | 0.663489 | 1.011614 | -0.639117 |
| H | 1.884530 | 0.558255 | 1.508577 |
| H | 1.279581 | -1.089476 | 1.508871 |
| H | 3.562389 | -1.138943 | 0.735448 |
| H | 2.527840 | -1.561211 | -0.615674 |
| H | 3.783169 | 1.218057 | -0.167472 |
| H | 2.803370 | 0.762941 | -1.566623 |
| H | 4.373009 | 0.000293 | -1.305953 |
| Rotational constants (GHz): | 4.3552000 | 0.6947300 | 0.6840400 |
| Vibrational harmonic frequencies (cm ⁻¹): | | | |
| 37.7002 | 63.4812 | 97.2540 | |
| 120.3408 | 141.8935 | 202.9230 | |
| 253.5071 | 268.8375 | 315.1725 | |
| 404.3617 | 457.5808 | 517.7452 | |
| 636.8650 | 739.6953 | 766.2346 | |
| 823.7409 | 860.2087 | 885.1127 | |
| 894.3235 | 977.5778 | 988.6303 | |
| 1031.2215 | 1049.4980 | 1087.7022 | |
| 1101.1604 | 1103.2848 | 1123.9976 | |
| 1168.0522 | 1211.2881 | 1264.8616 | |
| 1288.5980 | 1304.4278 | 1335.2657 | |
| 1336.1233 | 1342.7066 | 1373.4471 | |
| 1387.1381 | 1389.5903 | 1404.3258 | |
| 1417.4513 | 1430.1618 | 1495.1614 | |
| 1497.3776 | 1500.2631 | 1502.9827 | |
| 1514.8891 | 1519.6791 | 1522.6410 | |
| 2888.2486 | 2941.2932 | 3015.0754 | |
| 3021.3253 | 3025.6707 | 3031.8196 | |
| 3038.9261 | 3041.1833 | 3047.0068 | |
| 3060.2196 | 3066.4021 | 3075.2659 | |
| 3087.2021 | 3107.9017 | 3115.9140 | |
| Zero-point correction (Hartree): | 0.208953 | | |

C7H15O.ppttt

```

-----
E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.95326545
Electronic state : 2-A
Cartesian coordinates (Angs):
O      3.123209      -1.249697      -0.549620
C      2.914608      -0.406905      0.508913
C      2.254626      0.935128      0.154455
C      0.896727      0.792587      -0.547865
C      -0.243860     0.314370      0.361739
C      -1.591442     0.209388     -0.363968
C      -2.739713     -0.263452     0.536613
C      -4.081584     -0.361695     -0.196164
H      2.261292     -0.990033      1.195129
H      3.847380     -0.266761      1.088718
H      2.153838      1.527563      1.074394
H      2.947912      1.484236     -0.494461
H      0.619612      1.760918     -0.984065
H      1.016646      0.097349     -1.388117
H      0.002464     -0.666610      0.792101
H      -0.342870      1.003255      1.213238
H      -1.848210      1.188127     -0.794344
H      -1.491533     -0.478279     -1.215636
H      -2.483950     -1.242524      0.964449
H      -2.837413      0.423068      1.388780
H      -4.025492     -1.067613     -1.032636
H      -4.381927      0.609889     -0.605090
H      -4.879594     -0.701535      0.472167
Rotational constants (GHz):  5.0991900      0.6330500      0.6099200
Vibrational harmonic frequencies (cm-1):
  46.3482          52.3390          102.6844
 120.7836         132.6888         195.2976
 236.7703         247.4616         328.6339
 366.6567         453.8306         521.9137
 639.5513         735.2796         757.2029
 823.9108         869.5241         883.1935
 909.0232         975.5697        1014.2986
1036.0954        1051.0313        1069.9065
1100.4479        1102.4548        1125.6439
1167.7675        1228.0024        1261.2675
1282.7086        1307.4203        1326.5833
1338.5183        1345.1411        1357.4286
1374.0133        1394.2714        1409.6645
1416.4255        1427.1343        1494.7602
1498.8817        1499.4043        1506.1186
1512.9922        1516.5114        1525.9385
2887.4050        2941.9778        3010.4568
3014.6940        3025.7752        3031.1879
3035.0557        3038.5209        3039.7555
3047.5917        3067.3098        3075.9304
3085.3868        3106.9927        3111.9573
Zero-point correction (Hartree): 0.208702
    
```

C7H15O.ptmmm

```

-----
E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.95062590
Electronic state : 2-A
Cartesian coordinates (Angs):
O      3.540469      -0.245542      -0.608922
C      2.760850      -0.554794      0.474180
C      1.471104      0.263947      0.613452
C      0.548224      0.118057     -0.602633
C      -0.665345      1.062056     -0.601238
C      -1.655555      0.879024      0.564257
C      -2.327791     -0.501996      0.661313
C      -3.198044     -0.868813     -0.546593

H      2.518080     -1.633813      0.348062
H      3.371394     -0.531065      1.398165
H      0.963850     -0.046491      1.536071
H      1.746038      1.318768      0.747583
H      1.145953      0.308801     -1.501646
H      0.212470     -0.925813     -0.677922
H      -0.303239      2.099022     -0.586623
H      -1.198104      0.947540     -1.553462
H      -1.144013      1.089459      1.512504
H      -2.438574      1.644263      0.472991
H      -1.566267     -1.278881      0.810512
H      -2.948876     -0.518633      1.566114
H      -2.608952     -0.954426     -1.465613
H      -3.971287     -0.111174     -0.720135
H      -3.702882     -1.828105     -0.391658
Rotational constants (GHz):  4.3893800      0.7431200      0.7341700
Vibrational harmonic frequencies (cm-1):
  46.7546          48.9660          86.9496
 140.3860         177.1616         217.7410
    
```

| | | |
|-----------|-----------|-----------|
| 245.2181 | 287.9288 | 333.8977 |
| 411.5023 | 484.0100 | 516.8672 |
| 552.1031 | 720.7766 | 757.0873 |
| 814.0339 | 841.6992 | 884.8874 |
| 916.6285 | 949.5318 | 988.0750 |
| 1029.0255 | 1046.5872 | 1067.9368 |
| 1094.1151 | 1113.7862 | 1133.4121 |
| 1171.2130 | 1218.0884 | 1240.5758 |
| 1283.5954 | 1315.4772 | 1326.6826 |
| 1344.3334 | 1362.9769 | 1368.1291 |
| 1378.8386 | 1396.3736 | 1406.8777 |
| 1420.3780 | 1431.5236 | 1490.0449 |
| 1498.0015 | 1502.2781 | 1506.2700 |
| 1516.0106 | 1519.4825 | 1526.1825 |
| 2880.6040 | 2936.4422 | 3021.2757 |
| 3025.9236 | 3028.6541 | 3035.1745 |
| 3036.5805 | 3042.0667 | 3056.6759 |
| 3064.9329 | 3067.6354 | 3074.8291 |
| 3087.0127 | 3108.5235 | 3115.4063 |

Zero-point correction (Hartree): 0.208936

C7H15O.ptmmp

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.94775541

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -3.471412 | -0.026709 | -0.372245 |
| C | -2.533087 | 0.763579 | 0.237415 |
| C | -1.235071 | 0.053657 | 0.643282 |
| C | -0.516655 | -0.587895 | -0.549616 |
| C | 0.672427 | -1.487296 | -0.173233 |
| C | 1.857548 | -0.838413 | 0.569119 |
| C | 2.683936 | 0.196605 | -0.224382 |
| C | 2.171345 | 1.642142 | -0.166279 |
| H | -2.316922 | 1.566346 | -0.502844 |
| H | -2.991741 | 1.308693 | 1.085697 |
| H | -0.588962 | 0.780462 | 1.151439 |
| H | -1.482683 | -0.717445 | 1.385172 |
| H | -1.251835 | -1.192121 | -1.094649 |
| H | -0.195095 | 0.195976 | -1.248128 |
| H | 0.293103 | -2.310605 | 0.447908 |
| H | 1.055674 | -1.956815 | -1.089515 |
| H | 1.513462 | -0.386366 | 1.509579 |
| H | 2.527898 | -1.654938 | 0.866272 |
| H | 3.710416 | 0.189458 | 0.163599 |
| H | 2.760702 | -0.126959 | -1.271644 |
| H | 2.114582 | 1.994321 | 0.870413 |
| H | 1.176230 | 1.751689 | -0.607108 |
| H | 2.843809 | 2.317706 | -0.706065 |

Rotational constants (GHz): 3.5500600 0.8766900 0.7714800

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 43.8741 | 59.4379 | 67.5111 |
| 131.8661 | 182.8853 | 220.5430 |
| 242.5089 | 249.1762 | 350.9446 |
| 382.0013 | 473.6224 | 509.7272 |
| 546.4756 | 744.4363 | 748.2449 |
| 818.0856 | 828.1198 | 875.5224 |
| 924.6432 | 947.5603 | 984.7715 |
| 1033.4369 | 1057.7320 | 1077.1319 |
| 1094.1235 | 1112.2631 | 1129.5364 |
| 1181.1214 | 1213.0581 | 1245.1943 |
| 1294.4993 | 1313.2019 | 1332.4186 |
| 1340.9389 | 1364.2512 | 1367.0069 |
| 1382.3590 | 1395.7375 | 1405.4122 |
| 1420.0599 | 1426.5145 | 1491.2461 |
| 1498.9317 | 1500.9450 | 1504.5148 |
| 1511.7908 | 1520.4279 | 1521.9870 |
| 2880.1845 | 2936.1943 | 3018.0021 |
| 3024.3858 | 3025.8548 | 3032.2802 |
| 3038.8049 | 3042.1012 | 3055.0513 |
| 3062.5227 | 3066.2250 | 3070.0816 |
| 3088.4124 | 3105.3626 | 3122.1647 |

Zero-point correction (Hartree): 0.208761

C7H15O.ptmmt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.95184203

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 3.689659 | -0.037213 | -0.297119 |
| C | 2.713682 | -0.916619 | 0.091188 |
| C | 1.412106 | -0.277630 | 0.592127 |
| C | 0.751571 | 0.616386 | -0.463957 |
| C | -0.448648 | 1.430194 | 0.048434 |
| C | -1.654818 | 0.613181 | 0.544634 |

| | | | |
|--|-----------|-----------|-----------|
| C | -2.342910 | -0.236597 | -0.532526 |
| C | -3.580800 | -0.974031 | -0.010946 |
| H | 2.514559 | -1.534974 | -0.812785 |
| H | 3.127835 | -1.643052 | 0.817724 |
| H | 0.735722 | -1.080673 | 0.912606 |
| H | 1.641942 | 0.313496 | 1.488731 |
| H | 1.514229 | 1.307731 | -0.841325 |
| H | 0.449902 | 0.000830 | -1.322673 |
| H | -0.106386 | 2.082254 | 0.863515 |
| H | -0.783728 | 2.101398 | -0.754003 |
| H | -1.350845 | -0.035538 | 1.377783 |
| H | -2.393010 | 1.308633 | 0.966991 |
| H | -2.628623 | 0.410548 | -1.373362 |
| H | -1.634597 | -0.968302 | -0.942006 |
| H | -4.330781 | -0.270456 | 0.368386 |
| H | -3.321068 | -1.651561 | 0.810747 |
| H | -4.053521 | -1.571934 | -0.797107 |
| Rotational constants (GHz): | 4.4985300 | 0.7138600 | 0.6657400 |
| Vibrational harmonic frequencies (cm-1): | | | |
| 48.5751 | 50.7411 | | 70.9050 |
| 131.5517 | 193.7232 | | 217.0045 |
| 243.4773 | 263.0952 | | 297.1868 |
| 391.0006 | 485.6244 | | 511.9978 |
| 544.6497 | 726.1587 | | 764.3635 |
| 823.1072 | 843.4301 | | 879.0355 |
| 929.1834 | 949.3976 | | 986.3244 |
| 1037.3730 | 1047.9857 | | 1076.1764 |
| 1090.2839 | 1104.1235 | | 1136.3648 |
| 1177.6090 | 1220.4361 | | 1252.3301 |
| 1289.3112 | 1319.4459 | | 1326.3275 |
| 1335.5307 | 1350.0526 | | 1365.1591 |
| 1371.9111 | 1398.8290 | | 1411.4480 |
| 1419.7451 | 1427.9421 | | 1493.6792 |
| 1499.3285 | 1504.0256 | | 1509.4026 |
| 1514.0785 | 1517.1837 | | 1524.1837 |
| 2880.9134 | 2936.8308 | | 3018.6574 |
| 3023.7806 | 3028.8429 | | 3030.3315 |
| 3035.9534 | 3038.4543 | | 3047.8622 |
| 3061.7091 | 3067.1004 | | 3071.8204 |
| 3087.3493 | 3106.0784 | | 3111.5723 |
| Zero-point correction (Hartree): | 0.208721 | | |

C7H15O.ptmpm

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.94475167
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | |
|--|-----------|-----------|-----------|
| O | -3.460726 | -0.088955 | -0.192898 |
| C | -2.460484 | 0.809987 | 0.069341 |
| C | -1.144491 | 0.204193 | 0.574506 |
| C | -0.545431 | -0.807668 | -0.411636 |
| C | 0.701756 | -1.563513 | 0.093980 |
| C | 2.083140 | -0.931955 | -0.172090 |
| C | 2.384718 | 0.436136 | 0.481647 |
| C | 2.077063 | 1.651961 | -0.402917 |
| H | -2.295192 | 1.337179 | -0.897093 |
| H | -2.835922 | 1.607731 | 0.739990 |
| H | 1.025546 | 1.694466 | -0.703070 |
| H | -1.342685 | -0.295030 | 1.532101 |
| H | -1.336223 | -1.532527 | -0.636700 |
| H | -0.316148 | -0.309085 | -1.364479 |
| H | 0.594414 | -1.748347 | 1.172447 |
| H | 0.712523 | -2.556101 | -0.373854 |
| H | 2.831364 | -1.655697 | 0.175359 |
| H | 2.236016 | -0.849750 | -1.257700 |
| H | 1.845565 | 0.516915 | 1.434701 |
| H | 3.449650 | 0.473765 | 0.742992 |
| H | -0.447328 | 1.022164 | 0.789120 |
| H | 2.674560 | 1.622115 | -1.321279 |
| H | 2.312033 | 2.589000 | 0.113661 |
| Rotational constants (GHz): | 3.3341900 | 0.9226900 | 0.7820200 |
| Vibrational harmonic frequencies (cm-1): | | | |
| 35.0074 | 74.4452 | | 97.8169 |
| 121.2694 | 147.7464 | | 216.5937 |
| 233.8875 | 279.5054 | | 317.2148 |
| 372.7722 | 449.8079 | | 502.2124 |
| 539.2431 | 737.6101 | | 767.4625 |
| 788.7651 | 845.9436 | | 883.8885 |
| 931.4660 | 939.1624 | | 981.7120 |
| 1036.1773 | 1054.2598 | | 1079.7758 |
| 1093.4722 | 1108.6082 | | 1131.9176 |
| 1182.0479 | 1217.6555 | | 1245.2217 |
| 1296.1114 | 1306.5265 | | 1328.4742 |
| 1335.3939 | 1363.3303 | | 1368.8394 |
| 1378.3335 | 1394.7521 | | 1402.0393 |

| | | |
|-----------|-----------|-----------|
| 1413.7003 | 1427.7314 | 1492.3976 |
| 1496.7123 | 1502.7149 | 1504.2073 |
| 1509.8765 | 1514.5864 | 1524.1100 |
| 2880.1734 | 2936.4283 | 3018.1780 |
| 3019.3347 | 3021.7060 | 3030.5818 |
| 3042.9766 | 3043.5984 | 3056.5014 |
| 3065.1465 | 3065.7363 | 3073.7495 |
| 3093.8960 | 3107.2446 | 3120.3254 |

Zero-point correction (Hartree): 0.208562

C7H15O.ptmpp

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.94786618

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -3.522511 | 0.011671 | -0.313485 |
| C | -2.596282 | -0.725992 | 0.375410 |
| C | -1.138469 | -0.528691 | -0.062039 |
| C | -0.681977 | 0.930866 | 0.074488 |
| C | 0.693474 | 1.274674 | -0.531495 |
| C | 1.927142 | 1.008458 | 0.353881 |
| C | 2.288961 | -0.455649 | 0.661250 |
| C | 2.615701 | -1.300429 | -0.575633 |
| H | -2.722587 | -0.415121 | 1.436915 |
| H | -2.888773 | -1.794319 | 0.379228 |
| H | -0.509740 | -1.208479 | 0.524514 |
| H | -1.051165 | -0.846174 | -1.109427 |
| H | -1.446511 | 1.545290 | -0.415577 |
| H | -0.695462 | 1.220951 | 1.135743 |
| H | 0.803064 | 0.766115 | -1.498658 |
| H | 0.697289 | 2.346900 | -0.764866 |
| H | 2.795371 | 1.477039 | -0.130524 |
| H | 1.790926 | 1.543042 | 1.304244 |
| H | 3.160286 | -0.454219 | 1.329217 |
| H | 1.483057 | -0.933446 | 1.231784 |
| H | 3.428317 | -0.848728 | -1.156572 |
| H | 1.752585 | -1.401962 | -1.241286 |
| H | 2.932135 | -2.309689 | -0.292024 |

Rotational constants (GHz): 3.6749700 0.8470900 0.7576400

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 29.7552 | 59.3502 | 89.4758 |
| 138.3611 | 168.9277 | 209.7245 |
| 249.5702 | 281.4148 | 322.4503 |
| 399.9356 | 473.6743 | 514.1819 |
| 548.6172 | 747.9226 | 755.0511 |
| 783.6717 | 858.5983 | 873.5946 |
| 929.1139 | 944.5251 | 980.7373 |
| 1030.1281 | 1042.9238 | 1076.3298 |
| 1091.5835 | 1111.0108 | 1132.5123 |
| 1176.8215 | 1220.8125 | 1242.4481 |
| 1282.8907 | 1316.9355 | 1332.7548 |
| 1339.3610 | 1364.2648 | 1370.1599 |
| 1376.1922 | 1399.5777 | 1403.6733 |
| 1415.1177 | 1430.7087 | 1491.8695 |
| 1494.1306 | 1502.2977 | 1506.9563 |
| 1513.2032 | 1518.4716 | 1524.5622 |
| 2879.6885 | 2937.6825 | 3014.5146 |
| 3015.6129 | 3030.2267 | 3036.4481 |
| 3041.8441 | 3043.4686 | 3051.5285 |
| 3068.7606 | 3069.5784 | 3072.3167 |
| 3094.2501 | 3109.4476 | 3117.8096 |

Zero-point correction (Hartree): 0.208793

C7H15O.ptmpt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.94931723

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -3.652667 | -0.126656 | -0.313545 |
| C | -2.684715 | -0.897194 | 0.274060 |
| C | -1.239105 | -0.532324 | -0.092063 |
| C | -0.891439 | 0.913203 | 0.283922 |
| C | 0.445310 | 1.456772 | -0.249288 |
| C | 1.726768 | 0.803533 | 0.311712 |
| C | 2.234727 | -0.431358 | -0.449472 |
| C | 3.532921 | -0.996931 | 0.135742 |
| H | -2.846324 | -0.763835 | 1.367437 |
| H | -2.898350 | -1.970874 | 0.106153 |
| H | -0.571222 | -1.246051 | 0.405829 |
| H | -1.110809 | -0.680683 | -1.172314 |
| H | -1.701819 | 1.551157 | -0.089407 |
| H | -0.904965 | 1.011678 | 1.379646 |
| H | 0.453848 | 1.392399 | -1.346688 |
| H | 0.472719 | 2.528340 | -0.015352 |
| H | 2.531894 | 1.550700 | 0.306570 |

| | | | | |
|--|-----------|-----------|-----------|--|
| H | 1.571512 | 0.545004 | 1.369573 | |
| H | 1.469959 | -1.216528 | -0.458969 | |
| H | 2.397345 | -0.156820 | -1.500737 | |
| H | 3.394209 | -1.314898 | 1.175576 | |
| H | 4.331658 | -0.246279 | 0.125841 | |
| H | 3.884869 | -1.864264 | -0.432477 | |
| Rotational constants (GHz): | 4.2132900 | 0.7419100 | 0.6663200 | |
| Vibrational harmonic frequencies (cm-1): | | | | |
| 30.6642 | 52.9657 | | 90.9427 | |
| 113.9124 | 154.4857 | | 218.3396 | |
| 245.2693 | 249.2527 | | 292.5393 | |
| 382.0929 | 471.7451 | | 518.0586 | |
| 586.8876 | 733.9023 | | 769.2487 | |
| 792.3669 | 864.6647 | | 888.6245 | |
| 927.5769 | 952.1430 | | 984.5750 | |
| 1037.8544 | 1048.5253 | | 1081.6660 | |
| 1092.3374 | 1101.3464 | | 1133.1490 | |
| 1186.5456 | 1223.5937 | | 1252.5503 | |
| 1281.2692 | 1324.1838 | | 1329.5021 | |
| 1339.5156 | 1343.0190 | | 1366.8222 | |
| 1371.0687 | 1392.7123 | | 1406.1751 | |
| 1420.3202 | 1426.7454 | | 1491.0810 | |
| 1499.5536 | 1501.9370 | | 1506.7347 | |
| 1511.9650 | 1513.1630 | | 1523.9636 | |
| 2880.0002 | 2938.7873 | | 3012.4087 | |
| 3014.1079 | 3021.9127 | | 3032.0062 | |
| 3037.3435 | 3038.3571 | | 3049.7530 | |
| 3064.9114 | 3067.0759 | | 3079.2347 | |
| 3087.9234 | 3107.7397 | | 3112.1744 | |
| Zero-point correction (Hartree): | 0.208615 | | | |

C7H15O.ptmtm

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.95177352
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | | |
|--|-----------|-----------|-----------|--|
| O | 3.724406 | 0.172006 | -0.658240 | |
| C | 3.052310 | 0.290762 | 0.529392 | |
| C | 1.533081 | 0.466957 | 0.414083 | |
| C | 0.858741 | -0.700799 | -0.317090 | |
| C | -0.633431 | -0.491291 | -0.618029 | |
| C | -1.527012 | -0.413905 | 0.629517 | |
| C | -3.034249 | -0.352362 | 0.330198 | |
| C | -3.485470 | 0.920265 | -0.397051 | |
| H | 3.289017 | -0.646245 | 1.082107 | |
| H | 3.517201 | 1.082117 | 1.149855 | |
| H | 1.123106 | 0.591817 | 1.424373 | |
| H | 1.335481 | 1.404195 | -0.123160 | |
| H | 1.399981 | -0.863657 | -1.256448 | |
| H | 0.984719 | -1.619252 | 0.275427 | |
| H | -0.749852 | 0.419681 | -1.219810 | |
| H | -0.982943 | -1.319579 | -1.249708 | |
| H | -1.326999 | -1.293219 | 1.257693 | |
| H | -1.250353 | 0.460912 | 1.234128 | |
| H | -3.320278 | -1.232391 | -0.262279 | |
| H | -3.582921 | -0.433618 | 1.277217 | |
| H | -3.032953 | 1.005620 | -1.390233 | |
| H | -3.210063 | 1.816827 | 0.170878 | |
| H | -4.572212 | 0.932988 | -0.530235 | |
| Rotational constants (GHz): | 5.8042000 | 0.6313900 | 0.6295700 | |
| Vibrational harmonic frequencies (cm-1): | | | | |
| 44.1474 | 46.7577 | | 94.7737 | |
| 126.4152 | 153.2474 | | 218.8794 | |
| 239.8062 | 265.2113 | | 297.8842 | |
| 378.0663 | 471.2076 | | 528.1618 | |
| 576.0429 | 739.9486 | | 774.2562 | |
| 786.5058 | 866.3637 | | 873.4473 | |
| 926.1493 | 946.6106 | | 981.9088 | |
| 1037.2416 | 1055.4833 | | 1078.8446 | |
| 1088.1277 | 1101.3190 | | 1132.2135 | |
| 1186.7442 | 1218.4351 | | 1249.6128 | |
| 1295.5686 | 1314.4536 | | 1328.6403 | |
| 1340.1766 | 1352.1701 | | 1366.5224 | |
| 1371.4976 | 1385.4754 | | 1411.4535 | |
| 1417.8523 | 1428.6874 | | 1492.7826 | |
| 1495.4586 | 1501.4102 | | 1511.3410 | |
| 1513.1527 | 1516.6407 | | 1522.6544 | |
| 2879.2341 | 2935.1630 | | 3013.5521 | |
| 3017.0797 | 3025.3424 | | 3025.8462 | |
| 3035.4912 | 3041.1260 | | 3048.1139 | |
| 3060.8739 | 3068.0981 | | 3074.6801 | |
| 3087.2162 | 3108.3257 | | 3117.1841 | |
| Zero-point correction (Hartree): | 0.208651 | | | |

C7H15O.ptmtp

```

-----
E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.95164981
Electronic state : 2-A
Cartesian coordinates (Angs):
O      3.777053      -0.656259      -0.243307
C      3.141337      0.456515      0.240637
C      1.674625      0.614716      -0.179842
C      0.805463      -0.570566      0.259063
C     -0.632784     -0.551701     -0.283386
C     -1.497048      0.604382      0.241616
C     -2.939398      0.616896     -0.293925
C     -3.803293     -0.562464      0.169588
H      3.215506      0.365298      1.347618
H      3.738894      1.361192      0.013413
H      1.299099      1.558975      0.234478
H      1.639316      0.715953     -1.272862
H      1.304468     -1.489334     -0.070652
H      0.778862     -0.612553      1.358164
H     -0.603627     -0.510603     -1.382019
H     -1.107950     -1.506815     -0.028759
H     -1.520852      0.566478      1.340867
H     -1.023574      1.559506     -0.018775
H     -3.420394      1.552327      0.019425
H     -2.915386      0.643014     -1.392151
H     -3.848381     -0.611742      1.263968
H     -3.416181     -1.521638     -0.188795
H     -4.829632     -0.466660     -0.199972
Rotational constants (GHz):   7.0776800   0.6151600   0.5905900
Vibrational harmonic frequencies (cm-1):
    40.5707          49.8714          84.3265
   131.0432         151.3919         214.2783
   243.8908         253.4451         287.3869
   390.3140         468.3366         509.0414
   562.4801         735.2298         757.0788
   801.3585         859.3368         890.8954
   916.2465         949.4071         981.3982
  1035.4675        1059.9189        1069.3650
  1090.9343        1099.9641        1126.8115
  1196.6650        1221.2432        1241.9417
  1293.8252        1310.8093        1328.7131
  1343.5504        1352.1951        1367.0813
  1371.8584        1385.6228        1410.3267
  1419.1885        1430.0595        1493.3045
  1495.2417        1501.5902        1510.9776
  1511.8647        1516.6955        1522.0313
  2880.9119        2936.3209        3012.8221
  3014.0238        3023.3160        3026.4127
  3036.7765        3042.1722        3056.0251
  3061.5214        3069.5379        3079.4924
  3087.5193        3108.3747        3118.1942
Zero-point correction (Hartree): 0.208539
    
```

C7H15O.ptmtt

```

-----
E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.95312116
Electronic state : 2-A
Cartesian coordinates (Angs):
O     -3.890200      0.295062      -0.178386
C     -3.060946     -0.756801      0.108920
C     -1.591350     -0.565203     -0.287556
C     -0.952458      0.650127      0.395527
C      0.459493      0.997427     -0.100840
C      1.527473     -0.063882      0.198783
C      2.936551      0.350956     -0.244918
C      4.001551     -0.709065      0.053756
H     -3.146242     -0.890093      1.210811
H     -3.484241     -1.694839     -0.300838
H     -1.046986     -1.487412     -0.047552
H     -1.542200     -0.446825     -1.378338
H     -1.614223      1.509319      0.234928
H     -0.924874      0.481508      1.482345
H      0.425738      1.182301     -1.184114
H      0.767535      1.946983      0.357319
H      1.535679     -0.274686      1.278387
H      1.265216     -1.010525     -0.292890
H      2.926746      0.567061     -1.322012
H      3.208025      1.293379      0.249888
H      3.774646     -1.653314     -0.454656
H      4.060807     -0.919810      1.127767
H      4.994085     -0.384903     -0.275991
Rotational constants (GHz):   6.7677700   0.5965000   0.5695300
Vibrational harmonic frequencies (cm-1):
    45.6366          68.3241          79.7156
   127.6019         142.1103         204.3263
   236.5937         249.1410         279.7284
    
```

| | | |
|-----------|-----------|-----------|
| 396.2217 | 445.8827 | 524.3860 |
| 573.8819 | 734.9726 | 761.9028 |
| 799.5833 | 872.6677 | 893.3090 |
| 926.8539 | 959.1329 | 976.6410 |
| 1048.6326 | 1062.2607 | 1072.0294 |
| 1084.6532 | 1098.1682 | 1131.7175 |
| 1202.7020 | 1219.3335 | 1253.8583 |
| 1293.9433 | 1309.0175 | 1332.4247 |
| 1335.7949 | 1343.6664 | 1365.1148 |
| 1371.2310 | 1385.3520 | 1413.4065 |
| 1418.4949 | 1427.2816 | 1492.8332 |
| 1497.8454 | 1501.6995 | 1512.1242 |
| 1513.2188 | 1513.7540 | 1525.4110 |
| 2880.6384 | 2937.2276 | 3011.7421 |
| 3014.7900 | 3018.9546 | 3027.9273 |
| 3035.2442 | 3038.2458 | 3042.0147 |
| 3054.7058 | 3068.0549 | 3074.2920 |
| 3086.7868 | 3106.0123 | 3111.7704 |

Zero-point correction (Hartree): 0.208527

C7H15O.ptpmm

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.94771837

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 2.855102 | -0.632262 | 1.012309 |
| C | 2.663976 | -0.430268 | -0.329558 |
| C | 1.217302 | -0.143264 | -0.749905 |
| C | 0.652520 | 1.120936 | -0.087718 |
| C | -0.831730 | 1.421954 | -0.392039 |
| C | -1.852020 | 0.846710 | 0.609726 |
| C | -1.957177 | -0.684648 | 0.712004 |
| C | -2.438298 | -1.375415 | -0.569363 |
| H | 3.315726 | 0.437239 | -0.578965 |
| H | 3.108342 | -1.265519 | -0.905594 |
| H | 1.184407 | -0.043742 | -1.843771 |
| H | 0.610255 | -1.020129 | -0.499789 |
| H | 0.803852 | 1.044465 | 0.996362 |
| H | 1.263668 | 1.972773 | -0.417110 |
| H | -0.969457 | 2.510316 | -0.397826 |
| H | -1.073357 | 1.092616 | -1.411490 |
| H | -1.614953 | 1.246405 | 1.605136 |
| H | -2.844175 | 1.244810 | 0.353949 |
| H | -0.993021 | -1.105484 | 1.023489 |
| H | -2.656694 | -0.922347 | 1.523909 |
| H | -1.741773 | -1.231322 | -1.402000 |
| H | -3.412306 | -0.983599 | -0.885400 |
| H | -2.548766 | -2.454420 | -0.418249 |

Rotational constants (GHz): 2.9364600 0.9537400 0.8616800

Vibrational harmonic frequencies (cm⁻¹):

| | | |
|-----------|-----------|-----------|
| 31.8462 | 72.3845 | 79.6962 |
| 148.1079 | 165.5829 | 206.2140 |
| 256.3196 | 259.6859 | 331.5213 |
| 387.5862 | 459.7323 | 511.4961 |
| 555.9035 | 741.3335 | 752.0133 |
| 797.0504 | 859.9085 | 873.7142 |
| 909.8001 | 964.1030 | 979.8812 |
| 1021.1006 | 1049.4285 | 1086.8933 |
| 1094.1334 | 1114.3679 | 1131.1323 |
| 1172.9312 | 1202.3484 | 1263.6324 |
| 1278.4345 | 1313.5736 | 1329.1512 |
| 1338.1036 | 1364.5764 | 1366.9543 |
| 1376.0614 | 1398.7975 | 1404.0002 |
| 1412.8927 | 1427.4154 | 1491.9459 |
| 1494.2924 | 1504.4413 | 1508.2689 |
| 1515.1585 | 1517.2838 | 1524.1428 |
| 2878.9797 | 2937.0084 | 3016.4486 |
| 3020.0918 | 3029.5552 | 3034.5220 |
| 3036.8377 | 3040.9813 | 3054.2023 |
| 3066.3130 | 3068.9990 | 3073.3350 |
| 3096.6013 | 3107.3664 | 3113.6596 |

Zero-point correction (Hartree): 0.208726

C7H15O.ptpmp

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.94579114

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 2.438261 | 1.117340 | -0.587450 |
| C | 2.558209 | 0.049955 | 0.265513 |
| C | 1.235985 | -0.573433 | 0.720709 |
| C | 0.434297 | -1.165864 | -0.447562 |
| C | -1.004032 | -1.599415 | -0.091482 |
| C | -2.125731 | -0.566343 | -0.318266 |
| C | -2.087334 | 0.735370 | 0.512835 |

| | | | |
|---|-----------|-----------|-----------|
| C | -1.299425 | 1.893840 | -0.116420 |
| H | 3.181808 | -0.696048 | -0.275059 |
| H | 3.198615 | 0.345516 | 1.120505 |
| H | 1.446371 | -1.354609 | 1.464092 |
| H | -0.241361 | 1.664007 | -0.270536 |
| H | 0.412399 | -0.440786 | -1.270309 |
| H | 0.988649 | -2.034657 | -0.828571 |
| H | -1.258986 | -2.482125 | -0.691492 |
| H | -1.032350 | -1.937814 | 0.954321 |
| H | -2.159809 | -0.305756 | -1.385726 |
| H | -3.073109 | -1.080261 | -0.109719 |
| H | -3.119524 | 1.076854 | 0.662831 |
| H | -1.703409 | 0.518018 | 1.519075 |
| H | -1.720602 | 2.156392 | -1.093893 |
| H | 0.657191 | 0.199171 | 1.238488 |
| H | -1.353778 | 2.788721 | 0.513632 |
| Rotational constants (GHz): | 2.6115600 | 1.1851300 | 0.9175600 |
| Vibrational harmonic frequencies (cm ⁻¹): | | | |
| 62.1187 | 75.8448 | 105.4695 | |
| 140.6848 | 168.6957 | 224.9994 | |
| 249.4806 | 283.9206 | 321.6464 | |
| 371.3459 | 398.2957 | 440.0939 | |
| 542.1864 | 738.3346 | 765.7520 | |
| 795.9963 | 854.8399 | 879.8789 | |
| 905.2315 | 960.9841 | 980.7258 | |
| 1033.2005 | 1053.9922 | 1086.7308 | |
| 1091.7518 | 1128.7647 | 1137.8441 | |
| 1159.8359 | 1210.8522 | 1263.5343 | |
| 1293.4805 | 1311.9944 | 1330.2319 | |
| 1334.9106 | 1355.7848 | 1379.2505 | |
| 1385.1023 | 1395.9180 | 1402.1752 | |
| 1410.2224 | 1436.7420 | 1492.8983 | |
| 1498.4641 | 1502.5800 | 1506.7517 | |
| 1513.4829 | 1520.7161 | 1530.6162 | |
| 2887.3738 | 2930.3155 | 3015.9539 | |
| 3018.8321 | 3023.9765 | 3025.1746 | |
| 3036.7701 | 3042.4446 | 3055.6937 | |
| 3061.1598 | 3063.1494 | 3072.6550 | |
| 3096.2279 | 3103.3908 | 3131.5493 | |
| Zero-point correction (Hartree): | 0.208678 | | |

C7H15O.ptpmt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.94919840

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -2.608200 | -1.375870 | -0.721757 |
| C | -2.783013 | -0.457472 | 0.280377 |
| C | -1.505817 | 0.251162 | 0.747414 |
| C | -0.825836 | 1.042866 | -0.377754 |
| C | 0.543526 | 1.655715 | -0.008386 |
| C | 1.771842 | 0.798180 | -0.361850 |
| C | 1.873520 | -0.562365 | 0.342201 |
| C | 3.173383 | -1.302953 | 0.009480 |
| H | -3.501017 | 0.282435 | -0.139934 |
| H | -3.339671 | -0.914235 | 1.121925 |
| H | -1.760564 | 0.921362 | 1.579948 |
| H | -0.825553 | -0.504628 | 1.155398 |
| H | -0.717835 | 0.386668 | -1.250682 |
| H | -1.509536 | 1.845215 | -0.687525 |
| H | 0.651923 | 2.615283 | -0.528802 |
| H | 0.560822 | 1.897222 | 1.064051 |
| H | 1.787770 | 0.635862 | -1.449265 |
| H | 2.676054 | 1.379241 | -0.132103 |
| H | 1.803773 | -0.417143 | 1.429400 |
| H | 1.020582 | -1.191483 | 0.059353 |
| H | 4.050505 | -0.720849 | 0.315047 |
| H | 3.258931 | -1.486441 | -1.067691 |
| H | 3.223788 | -2.272349 | 0.516045 |
| Rotational constants (GHz): | 2.9069100 | 0.9031800 | 0.7614300 |
| Vibrational harmonic frequencies (cm ⁻¹): | | | |
| 27.2501 | 79.9522 | 95.0305 | |
| 127.1210 | 160.0561 | 212.0240 | |
| 243.5845 | 254.5991 | 307.6348 | |
| 356.8714 | 465.1179 | 519.6404 | |
| 570.3297 | 743.3300 | 764.6799 | |
| 804.4540 | 864.5263 | 884.0073 | |
| 918.1198 | 963.4142 | 994.1325 | |
| 1024.1730 | 1048.8037 | 1087.3795 | |
| 1095.6472 | 1105.1774 | 1139.2238 | |
| 1169.2004 | 1222.2877 | 1261.8505 | |
| 1285.8062 | 1320.0474 | 1327.0142 | |
| 1340.9648 | 1347.1490 | 1364.8028 | |
| 1367.2856 | 1390.6550 | 1411.4538 | |
| 1416.3683 | 1426.0637 | 1496.0082 | |

| | | |
|-----------|-----------|-----------|
| 1498.3946 | 1504.7013 | 1509.1063 |
| 1513.3590 | 1517.4072 | 1523.5870 |
| 2878.4490 | 2938.1901 | 3013.2841 |
| 3018.6363 | 3024.1106 | 3025.9965 |
| 3036.2375 | 3038.3356 | 3047.1354 |
| 3064.6942 | 3069.5622 | 3073.9100 |
| 3097.9718 | 3107.4571 | 3112.3917 |

Zero-point correction (Hartree): 0.208717

C7H15O.ptppm

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.94843630

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 2.387505 | 1.299051 | -0.354505 |
| C | 2.597339 | 0.067046 | 0.210066 |
| C | 1.328052 | -0.698634 | 0.596788 |
| C | 0.441474 | -1.007705 | -0.616171 |
| C | -0.939980 | -1.588129 | -0.273944 |
| C | -1.913741 | -0.669137 | 0.489998 |
| C | -2.305843 | 0.641765 | -0.229423 |
| C | -1.440581 | 1.862825 | 0.115234 |
| H | 3.188302 | -0.503314 | -0.540511 |
| H | 3.298679 | 0.173225 | 1.061419 |
| H | 1.612808 | -1.628231 | 1.108610 |
| H | 0.781735 | -0.093228 | 1.329303 |
| H | 0.328133 | -0.093638 | -1.210298 |
| H | 0.969792 | -1.722054 | -1.263390 |
| H | -1.424434 | -1.893170 | -1.211440 |
| H | -0.803610 | -2.511171 | 0.307090 |
| H | -2.822199 | -1.255753 | 0.676068 |
| H | -1.512837 | -0.431055 | 1.484562 |
| H | -2.297580 | 0.475786 | -1.315619 |
| H | -3.345939 | 0.882448 | 0.023995 |
| H | -0.387782 | 1.728839 | -0.149599 |

| | | | |
|---|-----------|----------|-----------|
| H | -1.485447 | 2.075817 | 1.190033 |
| H | -1.799968 | 2.754904 | -0.409465 |

Rotational constants (GHz): 2.6359400 1.1730800 0.9017900

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 57.6377 | 73.0635 | 96.4254 |
| 143.3499 | 191.6624 | 216.2926 |
| 254.1446 | 267.7338 | 356.2313 |
| 367.6843 | 445.4385 | 465.0608 |
| 549.9202 | 747.1255 | 749.5213 |
| 815.9542 | 826.5989 | 888.4027 |
| 903.7442 | 959.7251 | 983.6178 |
| 1040.6031 | 1050.6943 | 1081.8882 |
| 1089.2072 | 1115.0444 | 1137.5867 |
| 1162.8039 | 1212.3496 | 1247.6726 |
| 1301.9107 | 1309.0404 | 1325.2663 |
| 1343.4844 | 1357.3657 | 1372.9673 |
| 1384.6609 | 1393.8694 | 1402.7758 |
| 1417.1132 | 1433.7363 | 1494.7721 |
| 1497.9365 | 1502.0192 | 1508.5872 |
| 1513.0136 | 1522.7486 | 1529.9622 |
| 2885.7928 | 2932.4496 | 3014.7325 |
| 3023.8693 | 3025.1729 | 3030.5003 |
| 3035.9640 | 3040.4357 | 3050.5369 |
| 3062.2209 | 3066.9347 | 3078.5892 |
| 3091.6536 | 3102.7802 | 3128.8538 |

Zero-point correction (Hartree): 0.208860

C7H15O.ptppp

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.95046754

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 2.695775 | 1.467524 | -0.038008 |
| C | 2.863410 | 0.114984 | 0.104108 |
| C | 1.581755 | -0.680681 | 0.378647 |
| C | 0.549143 | -0.533755 | -0.745397 |
| C | -0.775882 | -1.276872 | -0.504825 |
| C | -1.603324 | -0.798300 | 0.703246 |
| C | -2.037601 | 0.677740 | 0.673054 |
| C | -2.939106 | 1.047546 | -0.510710 |
| H | 3.328435 | -0.218086 | -0.850629 |
| H | 3.649115 | -0.085791 | 0.859100 |
| H | 1.846647 | -1.737977 | 0.519560 |
| H | 1.165898 | -0.333027 | 1.331966 |
| H | 0.364961 | 0.534985 | -0.905927 |
| H | 0.991674 | -0.906495 | -1.680043 |
| H | -1.386069 | -1.200666 | -1.413480 |
| H | -0.565791 | -2.347954 | -0.377911 |
| H | -2.500650 | -1.428425 | 0.773252 |

| | | | |
|--|-----------|-----------|-----------|
| H | -1.040695 | -0.980850 | 1.627828 |
| H | -2.568930 | 0.897091 | 1.608078 |
| H | -1.153050 | 1.327546 | 0.674688 |
| H | -3.831892 | 0.411627 | -0.541763 |
| H | -2.421631 | 0.936429 | -1.469297 |
| H | -3.274593 | 2.087420 | -0.440086 |
| Rotational constants (GHz): | 3.2416000 | 0.8963100 | 0.8011300 |
| Vibrational harmonic frequencies (cm-1): | | | |
| 38.0151 | 49.6260 | 88.5151 | |
| 138.8567 | 182.2156 | 216.6286 | |
| 256.0574 | 285.7377 | 334.1169 | |
| 403.6458 | 467.9264 | 484.2074 | |
| 557.1671 | 722.9299 | 759.1317 | |
| 811.2100 | 839.2700 | 885.7008 | |
| 904.9073 | 950.4759 | 983.4641 | |
| 1034.4395 | 1040.7090 | 1079.5851 | |
| 1094.2859 | 1107.8315 | 1133.2796 | |
| 1178.2700 | 1200.5199 | 1252.6005 | |
| 1291.3036 | 1315.4612 | 1323.3393 | |
| 1345.6739 | 1361.9326 | 1371.1992 | |
| 1378.5401 | 1395.8239 | 1406.1391 | |
| 1419.2961 | 1431.2209 | 1491.7616 | |
| 1496.8436 | 1502.7439 | 1507.8146 | |
| 1516.1681 | 1520.1157 | 1526.4388 | |
| 2882.2264 | 2933.7708 | 3019.6077 | |
| 3022.7397 | 3030.2045 | 3032.2832 | |
| 3037.3469 | 3041.3055 | 3055.7428 | |
| 3064.1682 | 3071.9136 | 3077.1319 | |
| 3089.5099 | 3108.2789 | 3115.5251 | |
| Zero-point correction (Hartree): | 0.208828 | | |

C7H15O.ptppt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.95164087
Electronic state : 2-A
Cartesian coordinates (Angs):

| | | | |
|--|-----------|-----------|-----------|
| O | -2.673835 | -1.497418 | -0.442649 |
| C | -2.847495 | -0.368212 | 0.313843 |
| C | -1.562435 | 0.387533 | 0.671952 |
| C | -0.799261 | 0.869172 | -0.567825 |
| C | 0.529004 | 1.584753 | -0.267575 |
| C | 1.619655 | 0.729947 | 0.402238 |
| C | 2.105960 | -0.461169 | -0.434995 |
| C | 3.258889 | -1.223387 | 0.226801 |
| H | -3.523085 | 0.279469 | -0.288484 |
| H | -3.452085 | -0.609917 | 1.210368 |
| H | -1.822730 | 1.238748 | 1.316723 |
| H | -0.935082 | -0.280110 | 1.274817 |
| H | -0.630928 | 0.008335 | -1.225080 |
| H | -1.444373 | 1.557164 | -1.132522 |
| H | 0.927993 | 1.984430 | -1.209817 |
| H | 0.325283 | 2.458050 | 0.367590 |
| H | 2.477892 | 1.379769 | 0.621932 |
| H | 1.268477 | 0.366401 | 1.377663 |
| H | 1.275219 | -1.153914 | -0.618507 |
| H | 2.424238 | -0.100321 | -1.422988 |
| H | 2.961502 | -1.621064 | 1.204073 |
| H | 4.125654 | -0.571700 | 0.387054 |
| H | 3.586798 | -2.067816 | -0.388273 |
| Rotational constants (GHz): | 3.0564900 | 0.8629300 | 0.7422900 |
| Vibrational harmonic frequencies (cm-1): | | | |
| 33.1094 | 43.8745 | 78.4617 | |
| 135.0629 | 182.8952 | 211.2524 | |
| 246.9962 | 267.2165 | 293.3752 | |
| 378.7776 | 467.7844 | 482.9894 | |
| 551.5536 | 725.7769 | 768.6071 | |
| 812.9442 | 842.2873 | 884.0863 | |
| 910.7812 | 948.8232 | 988.5710 | |
| 1041.7864 | 1042.3008 | 1080.9172 | |
| 1090.2334 | 1104.3221 | 1133.7078 | |
| 1176.8339 | 1210.7377 | 1259.8187 | |
| 1301.2032 | 1312.0703 | 1326.5284 | |
| 1333.6830 | 1351.5220 | 1361.4652 | |
| 1375.2117 | 1396.7827 | 1409.0237 | |
| 1417.5723 | 1427.5642 | 1494.6221 | |
| 1497.5210 | 1504.1427 | 1508.9484 | |
| 1513.4383 | 1516.2052 | 1524.1635 | |
| 2882.2344 | 2933.6504 | 3015.1207 | |
| 3019.6059 | 3028.1555 | 3029.1149 | |
| 3031.4744 | 3038.1383 | 3047.4317 | |
| 3055.8094 | 3072.2756 | 3075.3280 | |
| 3090.4561 | 3106.0210 | 3112.1827 | |
| Zero-point correction (Hartree): | 0.208463 | | |

C7H15O.ptptm

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.95142468

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 3.425022 | -0.260808 | 1.075219 |
| C | 3.186235 | -0.097147 | -0.263981 |
| C | 1.720811 | -0.234745 | -0.694033 |
| C | 0.808052 | 0.789955 | -0.009070 |
| C | -0.681193 | 0.677863 | -0.375414 |
| C | -1.369637 | -0.598709 | 0.131600 |
| C | -2.862309 | -0.699816 | -0.226981 |
| C | -3.752958 | 0.350141 | 0.448466 |
| H | 3.563288 | 0.923541 | -0.498507 |
| H | 3.855086 | -0.760910 | -0.846785 |
| H | 1.664624 | -0.125485 | -1.786228 |
| H | 1.394594 | -1.256130 | -0.464577 |
| H | 0.932107 | 0.692965 | 1.076815 |
| H | 1.160102 | 1.798754 | -0.267402 |
| H | -1.199911 | 1.554504 | 0.031287 |
| H | -0.793978 | 0.739623 | -1.468013 |
| H | -0.855669 | -1.478275 | -0.275983 |
| H | -1.255076 | -0.659472 | 1.223655 |
| H | -2.976664 | -0.629637 | -1.317616 |
| H | -3.221121 | -1.699369 | 0.049957 |
| H | -3.492635 | 1.368468 | 0.141957 |
| H | -3.662047 | 0.299923 | 1.539891 |
| H | -4.806883 | 0.192706 | 0.196276 |

Rotational constants (GHz): 5.7650100 0.6334500 0.6314300

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 33.9063 | 48.3976 | 98.1150 |
| 128.3074 | 145.4372 | 211.8668 |
| 243.2289 | 267.5370 | 287.6246 |
| 378.8833 | 456.5983 | 474.7001 |
| 567.9074 | 737.0460 | 759.1734 |
| 797.0634 | 864.5940 | 878.3921 |
| 910.8043 | 949.8757 | 987.9864 |
| 1026.1568 | 1056.3608 | 1080.8546 |
| 1096.6458 | 1101.4399 | 1138.4939 |
| 1172.9714 | 1215.6290 | 1267.8460 |
| 1291.5775 | 1318.8458 | 1322.9615 |
| 1346.1996 | 1356.4668 | 1363.1079 |
| 1375.6593 | 1387.8226 | 1410.5631 |
| 1420.8431 | 1429.4231 | 1494.1143 |
| 1495.5546 | 1501.6454 | 1510.9414 |
| 1512.0647 | 1516.6172 | 1522.1668 |
| 2881.2244 | 2933.9249 | 3012.0693 |
| 3021.3211 | 3021.7975 | 3025.9613 |
| 3031.2498 | 3040.9991 | 3056.8230 |
| 3061.6592 | 3065.8442 | 3080.3132 |
| 3087.8851 | 3108.2356 | 3115.9437 |

Zero-point correction (Hartree): 0.208465

C7H15O.ptptp

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.95151446

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 3.515085 | -0.792342 | -0.379511 |
| C | 3.073357 | 0.498380 | -0.252307 |
| C | 1.550837 | 0.678624 | -0.267756 |
| C | 0.855613 | -0.082821 | 0.867780 |
| C | -0.677381 | 0.033222 | 0.877355 |
| C | -1.375419 | -0.643152 | -0.312777 |
| C | -2.910986 | -0.652293 | -0.224530 |
| C | -3.560228 | 0.735048 | -0.298360 |
| H | 3.495047 | 0.850870 | 0.715651 |
| H | 3.575736 | 1.140453 | -1.002693 |
| H | 1.324093 | 1.752068 | -0.202122 |
| H | 1.179275 | 0.339344 | -1.241950 |
| H | 1.148848 | -1.138500 | 0.806602 |
| H | 1.244503 | 0.287379 | 1.827046 |
| H | -1.054841 | -0.418667 | 1.805043 |
| H | -0.956587 | 1.094478 | 0.922700 |
| H | -1.078432 | -0.154702 | -1.250805 |
| H | -1.018889 | -1.679828 | -0.384217 |
| H | -3.304436 | -1.272189 | -1.040294 |
| H | -3.215647 | -1.149154 | 0.706966 |
| H | -3.271814 | 1.256614 | -1.218714 |
| H | -3.269678 | 1.369047 | 0.545663 |
| H | -4.652622 | 0.659473 | -0.289218 |

Rotational constants (GHz): 5.3563000 0.6549700 0.6453400

Vibrational harmonic frequencies (cm-1):

| | | |
|---------|---------|----------|
| 30.3206 | 46.9025 | 105.6345 |
|---------|---------|----------|

| | | |
|-----------|-----------|-----------|
| 132.0949 | 139.5489 | 212.3501 |
| 244.0849 | 274.9329 | 297.6096 |
| 364.2605 | 460.1630 | 468.4844 |
| 569.6818 | 743.2803 | 778.8574 |
| 781.1737 | 861.2709 | 873.3133 |
| 912.8147 | 951.5798 | 982.1968 |
| 1029.9019 | 1056.6688 | 1084.2923 |
| 1097.1415 | 1100.6050 | 1140.6313 |
| 1170.6208 | 1210.9748 | 1267.2272 |
| 1297.7565 | 1310.7982 | 1328.8241 |
| 1340.5738 | 1356.7237 | 1362.6728 |
| 1375.2328 | 1385.1474 | 1411.9941 |
| 1418.5872 | 1428.2260 | 1493.3411 |
| 1495.3578 | 1503.0487 | 1511.4853 |
| 1513.7958 | 1516.4407 | 1522.3033 |
| 2881.2741 | 2933.1004 | 3014.2373 |
| 3021.9460 | 3025.2500 | 3027.5730 |
| 3031.5044 | 3040.5250 | 3047.5119 |
| 3059.3916 | 3064.3266 | 3076.7622 |
| 3087.4636 | 3107.3114 | 3115.9881 |

Zero-point correction (Hartree): 0.208441

C7H15O.ptptt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.95288337

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -3.336601 | -1.020608 | -0.700510 |
| C | -3.137705 | -0.247696 | 0.413233 |
| C | -1.674627 | 0.079441 | 0.735237 |
| C | -0.978945 | 0.845109 | -0.397040 |
| C | 0.507488 | 1.150143 | -0.150612 |
| C | 1.421931 | -0.082863 | -0.130074 |
| C | 2.905813 | 0.266269 | 0.045552 |
| C | 3.817907 | -0.964529 | 0.065689 |
| H | -3.709176 | 0.687189 | 0.217351 |
| H | -3.663889 | -0.696686 | 1.278767 |
| H | -1.642162 | 0.662257 | 1.666484 |
| H | -1.153803 | -0.863876 | 0.938204 |
| H | -1.090749 | 0.268120 | -1.323711 |
| H | -1.513217 | 1.791839 | -0.560028 |
| H | 0.857820 | 1.832855 | -0.936538 |
| H | 0.616220 | 1.699614 | 0.795757 |
| H | 1.120128 | -0.763557 | 0.677258 |
| H | 1.289630 | -0.645134 | -1.065594 |
| H | 3.216997 | 0.939759 | -0.764697 |
| H | 3.035962 | 0.834043 | 0.977135 |
| H | 3.734189 | -1.534334 | -0.866749 |
| H | 3.554886 | -1.639312 | 0.888424 |
| H | 4.868798 | -0.683164 | 0.190103 |

Rotational constants (GHz): 4.7596600 0.6427900 0.6106100

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 43.5721 | 64.8477 | 86.7513 |
| 133.7991 | 137.9973 | 201.2895 |
| 239.7294 | 251.3538 | 282.4973 |
| 400.3570 | 424.3840 | 483.8511 |
| 565.3217 | 735.8018 | 768.7344 |
| 792.9750 | 871.8675 | 889.3989 |
| 921.5248 | 946.4784 | 1001.8728 |
| 1028.6744 | 1056.9077 | 1078.4677 |
| 1095.9111 | 1101.6883 | 1142.2179 |
| 1173.9861 | 1227.4469 | 1269.7744 |
| 1293.0475 | 1314.0076 | 1326.7716 |
| 1336.7469 | 1348.2629 | 1362.7247 |
| 1374.5860 | 1384.2177 | 1414.3634 |
| 1419.9130 | 1427.5630 | 1494.6974 |
| 1498.2561 | 1501.9374 | 1512.9110 |
| 1513.6791 | 1514.1633 | 1525.7585 |
| 2880.9375 | 2933.7862 | 3012.3817 |
| 3018.0166 | 3022.5283 | 3027.8145 |
| 3031.8388 | 3039.1962 | 3042.3742 |
| 3051.5324 | 3065.6806 | 3076.6976 |
| 3088.3226 | 3107.4210 | 3112.0373 |

Zero-point correction (Hartree): 0.208438

C7H15O.pttmm

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.95181971

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 2.902186 | 1.422376 | -0.206616 |
| C | 3.037297 | 0.063007 | -0.100767 |
| C | 1.840496 | -0.671120 | 0.515749 |
| C | 0.542058 | -0.459008 | -0.270130 |
| C | -0.682255 | -1.097791 | 0.398458 |

| | | | |
|--|-----------|-----------|-----------|
| C | -1.988358 | -0.966735 | -0.404863 |
| C | -2.489068 | 0.469316 | -0.642126 |
| C | -2.832615 | 1.237467 | 0.639426 |
| H | 3.207612 | -0.286648 | -1.143701 |
| H | 3.986988 | -0.182067 | 0.414236 |
| H | 2.081306 | -1.741111 | 0.582137 |
| H | 1.713441 | -0.316072 | 1.547005 |
| H | 0.393100 | 0.619882 | -0.393128 |
| H | 0.658973 | -0.871115 | -1.283710 |
| H | -0.482446 | -2.165823 | 0.561731 |
| H | -0.813674 | -0.664609 | 1.399090 |
| H | -1.854176 | -1.458527 | -1.378275 |
| H | -2.775185 | -1.531816 | 0.113572 |
| H | -1.743549 | 1.033593 | -1.216544 |
| H | -3.381262 | 0.420085 | -1.279471 |
| H | -1.952538 | 1.387551 | 1.273240 |
| H | -3.580726 | 0.700033 | 1.234204 |
| H | -3.240678 | 2.226820 | 0.408060 |
| Rotational constants (GHz): | 3.4909100 | 0.7936400 | 0.7109200 |
| Vibrational harmonic frequencies (cm-1): | | | |
| 42.7378 | 59.4146 | | 92.4111 |
| 126.3874 | 165.7488 | | 191.3654 |
| 266.4914 | 278.4453 | | 315.5090 |
| 388.0588 | 485.5413 | | 499.3372 |
| 533.6629 | 730.5853 | | 769.9598 |
| 804.5141 | 859.3496 | | 877.5631 |
| 918.8550 | 970.4125 | | 978.2358 |
| 1029.9529 | 1036.9226 | | 1088.5290 |
| 1093.8445 | 1103.2101 | | 1137.8459 |
| 1178.7613 | 1208.4897 | | 1258.3552 |
| 1293.5787 | 1306.4941 | | 1327.6419 |
| 1340.1477 | 1357.5329 | | 1365.4579 |
| 1381.2988 | 1394.9444 | | 1401.1624 |
| 1419.3532 | 1431.1899 | | 1493.8077 |
| 1494.6256 | 1505.9040 | | 1506.4724 |
| 1516.9866 | 1518.4409 | | 1527.7944 |
| 2881.5292 | 2935.8566 | | 3013.2752 |
| 3017.5394 | 3025.0825 | | 3030.5535 |
| 3036.5928 | 3041.5371 | | 3051.5163 |
| 3061.2830 | 3066.6996 | | 3071.8416 |
| 3090.9846 | 3108.8049 | | 3116.6256 |
| Zero-point correction (Hartree): | 0.208733 | | |

C7H15O.pttmp

```

-----
E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.94909002
Electronic state : 2-A
Cartesian coordinates (Angs):
O      -2.848795      1.354234      -0.425329
C      -2.950146      0.171508      0.259018
C      -1.862925     -0.863706     -0.052938
C      -0.449296     -0.352012      0.246550
C      0.646368     -1.337852     -0.180448
C      2.089078     -0.963543      0.205060
C      2.670718      0.302810     -0.460887
C      2.414582      1.617326      0.288689
H      -2.909526      0.461229      1.332995
H      -3.969453     -0.245842      0.140640
H      -2.072147     -1.777265      0.520709
H      -1.942624     -1.136849     -1.113463
H      -0.323888      0.608241     -0.265243
H      -0.358198     -0.145322      1.323232
H      0.421318     -2.321112      0.256600
H      0.595363     -1.476471     -1.270042
H      2.162934     -0.866157      1.297822
H      2.725049     -1.817726     -0.060033
H      3.756345      0.176204     -0.558762
H      2.287413      0.380666     -1.487725
H      2.827644      1.573360      1.303202
H      1.349141      1.846377      0.377291
H      2.890711      2.459606     -0.224859
Rotational constants (GHz):      3.2435700      0.8475400      0.7133700
Vibrational harmonic frequencies (cm-1):
38.2131      58.0908      77.8856
109.4362     162.2663     178.9728
222.5304     296.4749     308.6673
363.0390     464.0011     495.4030
535.8139     747.6507     763.5869
809.2243     825.8116     894.9820
920.4251     970.2243     982.0215
1037.8847    1044.5231    1080.4123
1093.7433    1106.0830    1132.4248
1188.3228    1214.4424    1252.7951
1297.0258    1311.3586    1323.1823
1337.1640    1359.2802    1365.2573

```

| | | |
|-----------|-----------|-----------|
| 1381.3095 | 1392.0281 | 1397.8253 |
| 1418.3069 | 1431.0854 | 1493.2311 |
| 1493.9459 | 1500.6774 | 1504.7698 |
| 1514.5291 | 1518.2514 | 1523.3095 |
| 2881.0200 | 2936.2573 | 3010.1883 |
| 3016.8671 | 3018.2487 | 3025.2768 |
| 3029.5472 | 3044.0964 | 3046.2568 |
| 3061.1396 | 3063.7519 | 3066.7508 |
| 3093.9844 | 3106.6320 | 3130.7753 |

Zero-point correction (Hartree): 0.208381

C7H15O.pttmt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.95304490

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -3.053660 | 1.482389 | -0.202714 |
| C | -3.170984 | 0.196388 | 0.255330 |
| C | -2.058335 | -0.762702 | -0.184424 |
| C | -0.665763 | -0.304567 | 0.262307 |
| C | 0.463559 | -1.203175 | -0.259683 |
| C | 1.870035 | -0.804444 | 0.217007 |
| C | 2.368213 | 0.548220 | -0.310925 |
| C | 3.795816 | 0.874737 | 0.140048 |
| H | -3.181807 | 0.290895 | 1.364383 |
| H | -4.178774 | -0.197551 | 0.017959 |
| H | -2.280287 | -1.763476 | 0.211217 |
| H | -2.088972 | -0.846457 | -1.278790 |
| H | -0.523257 | 0.727884 | -0.076144 |
| H | -0.628066 | -0.277290 | 1.361729 |
| H | 0.265224 | -2.238350 | 0.050565 |
| H | 0.441972 | -1.208202 | -1.359026 |
| H | 1.891343 | -0.794236 | 1.316537 |
| H | 2.580216 | -1.584303 | -0.090309 |
| H | 2.322201 | 0.544042 | -1.408800 |
| H | 1.694316 | 1.349008 | 0.017621 |
| H | 4.505236 | 0.114145 | -0.206220 |
| H | 3.865975 | 0.915924 | 1.233209 |
| H | 4.128717 | 1.842113 | -0.250176 |

Rotational constants (GHz): 4.2089900 0.6846100 0.6147900

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 52.8023 | 63.5688 | 75.7417 |
| 123.6476 | 154.0887 | 190.7775 |
| 247.7091 | 269.7373 | 292.3953 |
| 331.0808 | 482.4510 | 512.4362 |
| 533.4533 | 737.1851 | 757.6648 |
| 813.6937 | 853.5358 | 891.3176 |
| 920.1087 | 968.7119 | 991.9443 |
| 1037.0104 | 1045.3734 | 1087.7398 |
| 1091.4119 | 1095.4331 | 1135.3557 |
| 1199.4200 | 1212.3365 | 1262.8520 |
| 1301.6166 | 1307.3048 | 1330.4974 |
| 1338.5622 | 1348.9195 | 1361.5463 |
| 1365.8739 | 1391.7655 | 1412.0795 |
| 1418.4530 | 1426.8548 | 1494.2384 |
| 1497.3443 | 1500.9935 | 1508.5644 |
| 1513.8625 | 1519.7796 | 1524.1545 |
| 2880.6532 | 2935.8586 | 3010.0691 |
| 3014.5312 | 3017.3765 | 3029.1400 |
| 3030.1370 | 3037.8845 | 3046.7146 |
| 3051.4984 | 3066.6084 | 3072.4006 |
| 3092.7920 | 3106.2662 | 3111.6843 |

Zero-point correction (Hartree): 0.208446

C7H15O.pttpm

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.94905750

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -3.367766 | 0.202286 | -0.979220 |
| C | -2.938328 | 0.518831 | 0.282778 |
| C | -1.742888 | -0.293596 | 0.794803 |
| C | -0.501106 | -0.151688 | -0.091727 |
| C | 0.655895 | -1.066284 | 0.336673 |
| C | 1.931344 | -0.951897 | -0.529036 |
| C | 3.006163 | 0.021477 | -0.012231 |
| C | 2.590105 | 1.495140 | 0.062216 |
| H | -2.676548 | 1.599422 | 0.230957 |
| H | -3.792569 | 0.492086 | 0.987711 |
| H | -1.519796 | 0.021294 | 1.823682 |
| H | -2.042297 | -1.348674 | 0.850185 |
| H | -0.786907 | -0.385342 | -1.124913 |
| H | -0.176289 | 0.896798 | -0.094200 |
| H | 0.910162 | -0.872944 | 1.389036 |
| H | 0.293531 | -2.102251 | 0.306177 |

| | | | | |
|--|-----------|-----------|-----------|-----------|
| H | 2.395799 | -1.942715 | -0.607071 | |
| H | 1.650179 | -0.673758 | -1.554604 | |
| H | 3.333773 | -0.310228 | 0.982866 | |
| H | 3.887066 | -0.064052 | -0.661877 | |
| H | 1.782735 | 1.655603 | 0.784138 | |
| H | 2.243977 | 1.861294 | -0.911345 | |
| H | 3.432202 | 2.123284 | 0.372159 | |
| Rotational constants (GHz): | 4.0325600 | | 0.7318500 | 0.6920300 |
| Vibrational harmonic frequencies (cm-1): | | | | |
| 37.8431 | 66.5983 | | | 92.2075 |
| 112.8785 | 151.2947 | | | 183.6076 |
| 254.0259 | 290.9039 | | | 320.5761 |
| 359.7218 | 464.4004 | | | 492.3456 |
| 536.4198 | 736.2903 | | | 774.2117 |
| 802.1374 | 850.4428 | | | 877.7280 |
| 918.6289 | 967.0625 | | | 985.6904 |
| 1031.9760 | 1048.3641 | | | 1085.4772 |
| 1094.4295 | 1109.6970 | | | 1137.7762 |
| 1171.9904 | 1215.6350 | | | 1262.1331 |
| 1289.2433 | 1313.6747 | | | 1321.1341 |
| 1336.9697 | 1359.8037 | | | 1364.9410 |
| 1384.2947 | 1391.9490 | | | 1393.3228 |
| 1416.5303 | 1428.1828 | | | 1494.2415 |
| 1497.6883 | 1500.1983 | | | 1504.5432 |
| 1515.4372 | 1519.5192 | | | 1525.1140 |
| 2882.0075 | 2934.9884 | | | 3015.3622 |
| 3021.9685 | 3023.4255 | | | 3027.5730 |
| 3038.6691 | 3042.6148 | | | 3048.9485 |
| 3059.5988 | 3063.5514 | | | 3067.7078 |
| 3089.1974 | 3107.0171 | | | 3113.9038 |
| Zero-point correction (Hartree): | 0.208511 | | | |

C7H15O.pttpp

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.95170335

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | | |
|--|-----------|-----------|-----------|-----------|
| O | -3.423068 | -0.296999 | -0.910692 | |
| C | -2.976163 | 0.631894 | -0.007999 | |
| C | -1.765605 | 0.204934 | 0.830691 | |
| C | -0.540512 | -0.139613 | -0.023436 | |
| C | 0.640969 | -0.670811 | 0.798978 | |
| C | 1.859223 | -1.099577 | -0.037701 | |
| C | 2.571505 | 0.022589 | -0.814199 | |
| C | 3.193763 | 1.107808 | 0.072467 | |
| H | -2.724117 | 1.525618 | -0.621764 | |
| H | -3.818449 | 0.978766 | 0.622516 | |
| H | -1.527234 | 1.010850 | 1.538552 | |
| H | -2.054983 | -0.664958 | 1.434965 | |
| H | -0.838615 | -0.887140 | -0.769479 | |
| H | -0.236657 | 0.753339 | -0.587119 | |
| H | 0.941695 | 0.084922 | 1.537217 | |
| H | 0.300992 | -1.537100 | 1.382577 | |
| H | 2.588830 | -1.580773 | 0.628117 | |
| H | 1.541348 | -1.874059 | -0.749005 | |
| H | 3.360695 | -0.432472 | -1.426219 | |
| H | 1.875084 | 0.485571 | -1.524918 | |
| H | 3.900143 | 0.674124 | 0.790081 | |
| H | 2.436580 | 1.653479 | 0.645401 | |
| H | 3.740160 | 1.842490 | -0.528188 | |
| Rotational constants (GHz): | 4.3014900 | | 0.6957400 | 0.6872500 |
| Vibrational harmonic frequencies (cm-1): | | | | |
| 30.8534 | 60.3720 | | | 86.7688 |
| 122.7410 | 151.7777 | | | 197.5907 |
| 266.0896 | 279.8652 | | | 311.1791 |
| 391.8397 | 475.0245 | | | 489.8451 |
| 525.5551 | 732.0348 | | | 764.1030 |
| 813.8410 | 855.3806 | | | 873.8047 |
| 917.8254 | 964.2650 | | | 988.6040 |
| 1017.1798 | 1043.7176 | | | 1091.7799 |
| 1094.6735 | 1103.0154 | | | 1138.4039 |
| 1174.9093 | 1207.5352 | | | 1268.8269 |
| 1286.9110 | 1304.9290 | | | 1330.3367 |
| 1342.7691 | 1358.3233 | | | 1364.0058 |
| 1381.1805 | 1396.7644 | | | 1401.1271 |
| 1419.8367 | 1428.4967 | | | 1493.7726 |
| 1495.5650 | 1505.3949 | | | 1506.9098 |
| 1515.5656 | 1518.7161 | | | 1527.9287 |
| 2881.7898 | 2935.3638 | | | 3018.2488 |
| 3024.0369 | 3025.8186 | | | 3033.1103 |
| 3036.9216 | 3041.5535 | | | 3051.9620 |
| 3058.1102 | 3065.4735 | | | 3070.9535 |
| 3085.8235 | 3108.3377 | | | 3115.4288 |
| Zero-point correction (Hartree): | 0.208614 | | | |

C7H15O.pttpt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.95291228

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 3.354586 | -1.045491 | -0.703468 |
| C | 3.138532 | -0.319824 | 0.438524 |
| C | 2.012733 | 0.717880 | 0.355933 |
| C | 0.653286 | 0.097299 | 0.015763 |
| C | -0.455897 | 1.139331 | -0.182620 |
| C | -1.817802 | 0.554020 | -0.591387 |
| C | -2.501998 | -0.303322 | 0.482779 |
| C | -3.884083 | -0.806139 | 0.052293 |
| H | 2.906533 | -1.079727 | 1.218054 |
| H | 4.091191 | 0.126225 | 0.786118 |
| H | 1.961620 | 1.256783 | 1.312169 |
| H | 2.284525 | 1.460355 | -0.405968 |
| H | 0.765445 | -0.501259 | -0.897153 |
| H | 0.372278 | -0.604829 | 0.812512 |
| H | -0.575511 | 1.726495 | 0.739601 |
| H | -0.132672 | 1.851623 | -0.953780 |
| H | -2.489970 | 1.380727 | -0.859348 |
| H | -1.694380 | -0.042927 | -1.506513 |
| H | -1.869367 | -1.163621 | 0.735038 |
| H | -2.597567 | 0.285483 | 1.405839 |
| H | -3.816725 | -1.423389 | -0.850962 |
| H | -4.558150 | 0.029160 | -0.169987 |
| H | -4.352565 | -1.412637 | 0.834410 |

Rotational constants (GHz): 4.7921100 0.6377900 0.6074400

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 42.7150 | 57.2662 | 85.1860 |
| 105.9321 | 150.8322 | 201.9347 |
| 249.0025 | 266.2172 | 296.1578 |
| 328.9443 | 484.0805 | 508.5883 |
| 533.2507 | 735.3252 | 755.2621 |
| 819.2737 | 853.7212 | 880.9351 |
| 920.4138 | 969.4354 | 997.3189 |
| 1024.8414 | 1045.0094 | 1086.1276 |
| 1093.3549 | 1095.3945 | 1140.4548 |
| 1179.6648 | 1221.9345 | 1273.7723 |
| 1284.2854 | 1311.2789 | 1330.3197 |
| 1336.4245 | 1348.9717 | 1361.0908 |
| 1365.9021 | 1391.8402 | 1410.6882 |
| 1418.7792 | 1426.4501 | 1493.5138 |
| 1497.2238 | 1500.9028 | 1508.5404 |
| 1513.8199 | 1519.9020 | 1523.7392 |
| 2881.1692 | 2935.3195 | 3012.7691 |
| 3016.1668 | 3025.3333 | 3027.2055 |
| 3031.9969 | 3038.3137 | 3046.9404 |
| 3050.6656 | 3063.4987 | 3070.9358 |
| 3085.8477 | 3106.8369 | 3111.7728 |

Zero-point correction (Hartree): 0.208340

C7H15O.ptttm

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.95294815

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 3.690472 | -0.829952 | -0.218243 |
| C | 3.282110 | 0.406587 | 0.207518 |
| C | 1.867932 | 0.816302 | -0.221254 |
| C | 0.790308 | -0.149965 | 0.281785 |
| C | -0.615723 | 0.171464 | -0.239219 |
| C | -1.683592 | -0.804705 | 0.273896 |
| C | -3.093603 | -0.573053 | -0.293668 |
| C | -3.742273 | 0.750301 | 0.130896 |
| H | 3.350570 | 0.361879 | 1.317606 |
| H | 4.038063 | 1.167831 | -0.068921 |
| H | 1.672615 | 1.834947 | 0.141275 |
| H | 1.841786 | 0.865015 | -1.317845 |
| H | 1.072926 | -1.167474 | -0.016157 |
| H | 0.782108 | -0.143285 | 1.381811 |
| H | -0.879610 | 1.199263 | 0.043589 |
| H | -0.606794 | 0.151313 | -1.338676 |
| H | -1.368591 | -1.828216 | 0.029300 |
| H | -1.723195 | -0.754704 | 1.371786 |
| H | -3.053139 | -0.624913 | -1.390465 |
| H | -3.738885 | -1.402086 | 0.023911 |
| H | -3.181341 | 1.617249 | -0.233171 |
| H | -3.799755 | 0.828339 | 1.223080 |
| H | -4.761492 | 0.832875 | -0.260900 |

Rotational constants (GHz): 6.5472800 0.5957400 0.5686100

Vibrational harmonic frequencies (cm-1):

| | | |
|----------|----------|----------|
| 35.3095 | 66.3737 | 113.5415 |
| 118.9919 | 121.9248 | 170.4227 |

| | | |
|-----------|-----------|-----------|
| 222.3025 | 276.3633 | 334.8610 |
| 358.1966 | 451.3649 | 475.5602 |
| 544.2884 | 739.0526 | 762.3531 |
| 798.1026 | 861.9399 | 892.2992 |
| 920.3243 | 970.9647 | 986.3839 |
| 1022.3997 | 1053.6414 | 1087.1842 |
| 1094.4597 | 1095.2805 | 1132.2254 |
| 1196.3142 | 1208.7208 | 1263.3709 |
| 1289.9966 | 1308.6305 | 1333.0216 |
| 1336.8574 | 1345.7964 | 1363.8596 |
| 1373.5705 | 1386.1810 | 1406.1437 |
| 1418.7170 | 1428.8430 | 1493.0572 |
| 1497.0283 | 1501.7496 | 1505.6441 |
| 1515.5713 | 1521.8902 | 1523.8680 |
| 2881.2693 | 2934.8140 | 3012.2805 |
| 3013.0387 | 3022.5779 | 3025.4970 |
| 3031.0477 | 3041.0122 | 3045.2010 |
| 3057.7651 | 3062.3471 | 3069.0333 |
| 3085.1746 | 3107.6343 | 3117.0997 |

Zero-point correction (Hartree): 0.208295

C7H15O.ptttt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.95296494

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -3.545619 | -0.034400 | 1.090892 |
| C | -3.303670 | 0.081880 | -0.252121 |
| C | -1.892219 | 0.543675 | -0.633065 |
| C | -0.798418 | -0.394477 | -0.112455 |
| C | 0.624140 | 0.098030 | -0.402308 |
| C | 1.709936 | -0.849334 | 0.127009 |
| C | 3.149786 | -0.423135 | -0.203395 |
| C | 3.597886 | 0.878676 | 0.472251 |
| H | -3.502512 | -0.931531 | -0.667711 |
| H | -4.087205 | 0.709719 | -0.721259 |
| H | -1.836280 | 0.631324 | -1.726903 |
| H | -1.739613 | 1.553321 | -0.229824 |
| H | -0.936672 | -0.517916 | 0.969021 |
| H | -0.936214 | -1.391914 | -0.555559 |
| H | 0.753425 | 0.224235 | -1.487373 |
| H | 0.751605 | 1.096023 | 0.037266 |
| H | 1.602850 | -0.948046 | 1.216825 |
| H | 1.534189 | -1.851600 | -0.286979 |
| H | 3.831043 | -1.230305 | 0.094518 |
| H | 3.255350 | -0.324497 | -1.292750 |
| H | 3.507932 | 0.806628 | 1.562498 |
| H | 2.998445 | 1.734858 | 0.146358 |
| H | 4.643965 | 1.103008 | 0.239244 |

Rotational constants (GHz): 5.7791000 0.5935100 0.5927000

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 38.8310 | 69.4745 | 96.2426 |
| 121.4475 | 145.8596 | 159.3152 |
| 220.5219 | 273.1504 | 337.8780 |
| 357.7861 | 451.0917 | 478.5397 |
| 548.3873 | 738.4729 | 766.8248 |
| 794.7556 | 871.2830 | 882.0554 |
| 923.6571 | 978.8288 | 981.9082 |
| 1025.0161 | 1052.2957 | 1084.6375 |
| 1095.9459 | 1097.5408 | 1137.9052 |
| 1186.1112 | 1219.1855 | 1266.5544 |
| 1284.2316 | 1316.2217 | 1332.5621 |
| 1337.4842 | 1349.5806 | 1363.4543 |
| 1377.2352 | 1386.7064 | 1407.1368 |
| 1420.0300 | 1428.2971 | 1493.3845 |
| 1497.0732 | 1502.1880 | 1506.4646 |
| 1515.4974 | 1521.2751 | 1524.2849 |
| 2880.3569 | 2931.1452 | 3012.3579 |
| 3013.9295 | 3021.1460 | 3024.4497 |
| 3030.3539 | 3040.5351 | 3046.5742 |
| 3059.0775 | 3062.1048 | 3069.2718 |
| 3085.4388 | 3108.7378 | 3115.6580 |

Zero-point correction (Hartree): 0.208374

C7H15O.ptttt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.95428681

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 3.618474 | -1.077366 | -0.417628 |
| C | 3.407762 | 0.094743 | 0.259852 |
| C | 2.085130 | 0.805656 | -0.051133 |
| C | 0.857661 | -0.055499 | 0.264523 |
| C | -0.469322 | 0.590911 | -0.150135 |
| C | -1.695164 | -0.273024 | 0.171529 |

| | | | |
|--|-----------|-----------|-----------|
| C | -3.024529 | 0.365567 | -0.250232 |
| C | -4.243358 | -0.503166 | 0.076494 |
| H | 3.449765 | -0.187752 | 1.335668 |
| H | 4.280696 | 0.764874 | 0.132700 |
| H | 2.051638 | 1.747138 | 0.514387 |
| H | 2.084335 | 1.080207 | -1.114205 |
| H | 0.974527 | -1.021914 | -0.241744 |
| H | 0.835672 | -0.274191 | 1.342407 |
| H | -0.572584 | 1.566704 | 0.346408 |
| H | -0.446897 | 0.801824 | -1.228853 |
| H | -1.589664 | -1.249923 | -0.321718 |
| H | -1.720293 | -0.481285 | 1.250965 |
| H | -3.128592 | 1.342487 | 0.241693 |
| H | -3.000239 | 0.571540 | -1.329081 |
| H | -4.314181 | -0.698010 | 1.152817 |
| H | -4.185703 | -1.473396 | -0.430196 |
| H | -5.175356 | -0.020502 | -0.235615 |
| Rotational constants (GHz): | 7.2614000 | 0.5499800 | 0.5302900 |
| Vibrational harmonic frequencies (cm-1): | | | |
| 51.7775 | 60.1684 | | 90.9855 |
| 125.6230 | 132.5219 | | 166.3958 |
| 231.3770 | 252.2092 | | 276.1526 |
| 385.8249 | 439.3420 | | 487.2692 |
| 546.7137 | 735.9641 | | 751.2470 |
| 801.0183 | 878.5790 | | 895.9081 |
| 924.8720 | 975.1788 | | 1012.6860 |
| 1022.4720 | 1058.4949 | | 1070.1483 |
| 1094.5925 | 1096.1024 | | 1136.9072 |
| 1194.7387 | 1228.0702 | | 1263.2238 |
| 1283.8621 | 1318.7540 | | 1325.0700 |
| 1335.7002 | 1341.6961 | | 1361.5567 |
| 1365.3526 | 1385.2150 | | 1413.0212 |
| 1419.2369 | 1428.1863 | | 1493.9312 |
| 1499.6809 | 1500.2114 | | 1509.9350 |
| 1513.6745 | 1520.2622 | | 1527.4939 |
| 2881.7287 | 2935.4134 | | 3010.2952 |
| 3012.2233 | 3018.0560 | | 3025.8548 |
| 3030.4586 | 3035.2034 | | 3038.8827 |
| 3047.3322 | 3061.5291 | | 3068.5388 |
| 3083.9840 | 3106.5495 | | 3111.9008 |
| Zero-point correction (Hartree): | 0.208218 | | |

C7H15O.tpmmm

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.94638389
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | |
|--|-----------|-----------|-----------|
| O | 3.241647 | -1.097140 | 0.155911 |
| C | 1.995064 | -0.687818 | -0.230454 |
| C | 1.746822 | 0.825251 | -0.133856 |
| C | 0.358472 | 1.291604 | -0.619111 |
| C | -0.755839 | 1.329232 | 0.445043 |
| C | -1.199444 | -0.014085 | 1.052973 |
| C | -1.787678 | -1.038060 | 0.065646 |
| C | -3.075740 | -0.577055 | -0.627002 |
| H | 1.761764 | -1.071921 | -1.244738 |
| H | 1.300194 | -1.254689 | 0.424892 |
| H | 1.921145 | 1.145726 | 0.900814 |
| H | 2.523707 | 1.307984 | -0.738649 |
| H | 0.459620 | 2.309253 | -1.014536 |
| H | 0.044445 | 0.679957 | -1.476833 |
| H | -0.425004 | 1.982810 | 1.263507 |
| H | -1.629747 | 1.826610 | 0.005425 |
| H | -0.357094 | -0.472632 | 1.587788 |
| H | -1.952503 | 0.195242 | 1.825133 |
| H | -1.041173 | -1.299039 | -0.695825 |
| H | -1.990407 | -1.967054 | 0.613691 |
| H | -2.908709 | 0.300149 | -1.260590 |
| H | -3.845005 | -0.311807 | 0.107647 |
| H | -3.484355 | -1.367872 | -1.264458 |
| Rotational constants (GHz): | 3.1173100 | 0.9421500 | 0.8283700 |
| Vibrational harmonic frequencies (cm-1): | | | |
| 52.0482 | 55.6352 | | 90.6052 |
| 97.3234 | 183.4341 | | 202.5886 |
| 254.6080 | 299.1520 | | 339.5151 |
| 394.1993 | 454.7194 | | 500.7981 |
| 539.3493 | 733.1420 | | 748.3339 |
| 816.2969 | 850.7090 | | 853.4805 |
| 926.0435 | 944.9213 | | 1002.1352 |
| 1032.9622 | 1046.3968 | | 1079.4833 |
| 1084.5950 | 1108.9321 | | 1134.7155 |
| 1170.5066 | 1220.2920 | | 1245.5072 |
| 1287.7646 | 1300.5506 | | 1329.9152 |
| 1344.6471 | 1372.5463 | | 1374.5871 |
| 1383.5976 | 1391.9561 | | 1405.5960 |

| | | |
|-----------|-----------|-----------|
| 1408.5171 | 1429.9888 | 1492.8974 |
| 1499.0021 | 1502.0747 | 1508.6476 |
| 1512.1618 | 1518.4742 | 1525.2135 |
| 2903.9108 | 2923.1202 | 3020.7248 |
| 3026.5915 | 3028.3647 | 3035.9023 |
| 3042.5947 | 3042.8648 | 3053.8670 |
| 3064.8521 | 3071.2103 | 3071.8281 |
| 3087.3771 | 3110.2471 | 3116.6318 |

Zero-point correction (Hartree): 0.208796

C7H15O.tpmmp

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.94405126

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -3.452015 | -0.919484 | 0.187273 |
| C | -2.117361 | -0.618037 | 0.232712 |
| C | -1.800155 | 0.882266 | 0.141143 |
| C | -0.307140 | 1.245211 | 0.216230 |
| C | 0.549301 | 0.757132 | -0.975506 |
| C | 1.206469 | -0.636371 | -0.827432 |
| C | 2.640121 | -0.624016 | -0.266588 |
| C | 2.786891 | -0.096875 | 1.165296 |
| H | -1.627769 | -1.092249 | 1.106499 |
| H | -1.694515 | -1.156942 | -0.643127 |
| H | -2.234921 | 1.267570 | -0.789565 |
| H | -2.332670 | 1.379035 | 0.961623 |
| H | -0.243394 | 2.338516 | 0.275370 |
| H | 0.112339 | 0.872582 | 1.159138 |
| H | -0.079273 | 0.769444 | -1.875926 |
| H | 1.343480 | 1.489642 | -1.169594 |
| H | 0.584322 | -1.285576 | -0.197100 |
| H | 1.240314 | -1.119991 | -1.811821 |
| H | 3.036149 | -1.646969 | -0.309368 |
| H | 3.274265 | -0.027351 | -0.936852 |
| H | 2.166838 | -0.668331 | 1.866044 |
| H | 2.496985 | 0.955851 | 1.246820 |
| H | 3.825216 | -0.175224 | 1.504546 |

Rotational constants (GHz): 3.4925700 0.8320400 0.7995000

Vibrational harmonic frequencies (cm⁻¹):

| | | |
|-----------|-----------|-----------|
| 36.8415 | 71.9890 | 101.5891 |
| 117.5138 | 130.0993 | 227.5143 |
| 251.3241 | 296.4372 | 311.3241 |
| 377.4463 | 441.0303 | 474.0129 |
| 662.8665 | 757.1322 | 774.6040 |
| 812.5226 | 846.0263 | 875.3704 |
| 926.5267 | 953.4878 | 996.1753 |
| 1033.8133 | 1063.4681 | 1079.3205 |
| 1082.1897 | 1114.7316 | 1131.9419 |
| 1164.2495 | 1211.0890 | 1252.8215 |
| 1289.5117 | 1296.2557 | 1320.6417 |
| 1336.8231 | 1364.2889 | 1373.3536 |
| 1387.5929 | 1392.9971 | 1395.3330 |
| 1397.6674 | 1429.7787 | 1495.4378 |
| 1495.5375 | 1501.4494 | 1503.9966 |
| 1508.9904 | 1517.3573 | 1522.2217 |
| 2892.6122 | 2933.0867 | 3023.0324 |
| 3024.4921 | 3030.1388 | 3037.5798 |
| 3040.1418 | 3043.7210 | 3057.9720 |
| 3064.4721 | 3070.0970 | 3077.6213 |
| 3089.0228 | 3107.0965 | 3114.9411 |

Zero-point correction (Hartree): 0.208932

C7H15O.tpmmt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.94767732

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -2.773212 | -1.662261 | -0.300026 |
| C | -1.758761 | -0.900049 | 0.210470 |
| C | -1.884066 | 0.609715 | -0.044689 |
| C | -0.759382 | 1.467853 | 0.570481 |
| C | 0.475336 | 1.708289 | -0.320507 |
| C | 1.327767 | 0.484976 | -0.700056 |
| C | 1.998964 | -0.227725 | 0.482402 |
| C | 2.894595 | -1.392299 | 0.046476 |
| H | -1.622383 | -1.117800 | 1.289777 |
| H | -0.837533 | -1.313454 | -0.252421 |
| H | -1.952645 | 0.779612 | -1.126403 |
| H | -2.848715 | 0.918863 | 0.375122 |
| H | -1.175037 | 2.452475 | 0.815283 |
| H | -0.454176 | 1.037107 | 1.534413 |
| H | 0.139435 | 2.198682 | -1.244151 |
| H | 1.123655 | 2.435995 | 0.186749 |

| | | | | |
|--|-----------|-----------|-----------|-----------|
| H | 0.723846 | -0.235371 | -1.269768 | |
| H | 2.110574 | 0.817464 | -1.395334 | |
| H | 2.594617 | 0.501905 | 1.048039 | |
| H | 1.237701 | -0.599205 | 1.180498 | |
| H | 3.692183 | -1.048851 | -0.622155 | |
| H | 2.320433 | -2.154759 | -0.492686 | |
| H | 3.367021 | -1.879134 | 0.905784 | |
| Rotational constants (GHz): | 2.4129400 | | 1.0627100 | 0.8116200 |
| Vibrational harmonic frequencies (cm-1): | | | | |
| 36.8207 | 62.7649 | | | 82.2541 |
| 96.1931 | 171.9683 | | | 222.2120 |
| 260.1915 | 268.9815 | | | 312.2714 |
| 377.4457 | 446.8145 | | | 501.0771 |
| 535.4112 | 736.1285 | | | 767.5792 |
| 811.3433 | 849.4989 | | | 860.3163 |
| 923.0413 | 952.6456 | | | 1016.4033 |
| 1036.4112 | 1047.1563 | | | 1073.5836 |
| 1084.5140 | 1110.9416 | | | 1135.2928 |
| 1180.8148 | 1220.5251 | | | 1255.5188 |
| 1291.3018 | 1307.8010 | | | 1334.0529 |
| 1334.9482 | 1348.1667 | | | 1371.0438 |
| 1387.8873 | 1392.3421 | | | 1402.6613 |
| 1414.6918 | 1428.4925 | | | 1495.5747 |
| 1501.2154 | 1504.3865 | | | 1507.2930 |
| 1513.4532 | 1513.8534 | | | 1523.7885 |
| 2904.3894 | 2922.0626 | | | 3018.2021 |
| 3022.2296 | 3029.2189 | | | 3031.6310 |
| 3039.2100 | 3042.3595 | | | 3046.5572 |
| 3059.7130 | 3069.7718 | | | 3072.9183 |
| 3086.6983 | 3106.6819 | | | 3113.8330 |
| Zero-point correction (Hartree): | 0.208622 | | | |

C7H15O.tpmpp

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.94348911

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | | |
|--|-----------|-----------|-----------|-----------|
| O | -2.777830 | -1.546972 | -0.074774 | |
| C | -2.008814 | -0.517533 | 0.393676 | |
| C | -1.561291 | 0.496985 | -0.670597 | |
| C | -0.719718 | 1.670254 | -0.128438 | |
| C | 0.809363 | 1.483183 | -0.062031 | |
| C | 1.344588 | 0.404149 | 0.908492 | |
| C | 1.621984 | -0.978249 | 0.284978 | |
| C | 2.846975 | -1.003963 | -0.637621 | |
| H | -2.505881 | -0.013240 | 1.247232 | |
| H | 0.745458 | -1.327578 | -0.275069 | |
| H | -1.027647 | -0.034317 | -1.467828 | |
| H | -2.476460 | 0.892011 | -1.127955 | |
| H | -0.909852 | 2.545274 | -0.761645 | |
| H | -1.090365 | 1.947768 | 0.869831 | |
| H | 1.186650 | 1.288923 | -1.074849 | |
| H | 1.233844 | 2.452997 | 0.225410 | |
| H | 2.282591 | 0.759448 | 1.355153 | |
| H | 0.646341 | 0.297546 | 1.749746 | |
| H | 1.774606 | -1.705395 | 1.092972 | |
| H | -1.135331 | -1.020211 | 0.860428 | |
| H | 3.753833 | -0.716128 | -0.093367 | |
| H | 2.737159 | -0.315424 | -1.482047 | |
| H | 3.009174 | -2.004855 | -1.050575 | |
| Rotational constants (GHz): | 2.5214700 | | 1.0820500 | 0.8638000 |
| Vibrational harmonic frequencies (cm-1): | | | | |
| 42.7677 | 82.9156 | | | 98.4784 |
| 130.6513 | 136.8024 | | | 226.0617 |
| 248.0632 | 285.5525 | | | 312.9041 |
| 396.9511 | 425.6018 | | | 476.4265 |
| 580.7475 | 738.8818 | | | 797.9791 |
| 811.2526 | 827.6320 | | | 870.5142 |
| 914.8319 | 956.6219 | | | 990.5582 |
| 1035.6406 | 1061.8202 | | | 1076.5072 |
| 1085.9951 | 1121.4952 | | | 1133.1968 |
| 1165.3840 | 1214.4539 | | | 1267.9736 |
| 1281.3842 | 1301.6620 | | | 1328.8074 |
| 1338.4333 | 1367.5029 | | | 1375.7433 |
| 1383.1437 | 1394.0978 | | | 1395.8873 |
| 1406.0917 | 1429.5127 | | | 1496.4529 |
| 1496.9287 | 1500.4832 | | | 1508.9696 |
| 1511.0803 | 1519.2270 | | | 1520.5825 |
| 2909.2732 | 2927.4407 | | | 3013.3975 |
| 3022.9840 | 3029.2421 | | | 3036.7710 |
| 3043.1352 | 3043.5254 | | | 3057.9148 |
| 3066.7638 | 3070.2467 | | | 3072.6393 |
| 3087.8432 | 3112.0798 | | | 3117.1379 |

Zero-point correction (Hartree): 0.208865

C7H15O.tpmpt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.94487590

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -2.340116 | -1.929900 | -0.097417 |
| C | -1.742274 | -0.823038 | 0.439028 |
| C | -1.718184 | 0.414584 | -0.471154 |
| C | -1.027621 | 1.646474 | 0.150225 |
| C | 0.481237 | 1.825357 | -0.111823 |
| C | 1.436549 | 0.747640 | 0.447622 |
| C | 1.769903 | -0.398869 | -0.520867 |
| C | 2.724969 | -1.433474 | 0.082876 |
| H | -2.180099 | -0.584671 | 1.429746 |
| H | 0.853970 | -0.901420 | -0.855017 |
| H | -1.254641 | 0.145297 | -1.427293 |
| H | -2.763333 | 0.658330 | -0.696421 |
| H | -1.527972 | 2.546750 | -0.226145 |
| H | -1.204459 | 1.649383 | 1.236281 |
| H | 0.646858 | 1.923144 | -1.193961 |
| H | 0.762149 | 2.795060 | 0.317662 |
| H | 2.383444 | 1.227585 | 0.728403 |
| H | 1.030593 | 0.340252 | 1.385134 |
| H | -0.712517 | -1.158768 | 0.686578 |
| H | 2.219204 | 0.029079 | -1.427105 |
| H | 2.289116 | -1.908986 | 0.969354 |
| H | 3.668429 | -0.968351 | 0.391082 |
| H | 2.962713 | -2.225540 | -0.634404 |

Rotational constants (GHz): 2.1442400 1.2240500 0.8478700

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 53.4872 | 64.7732 | 88.5957 |
| 107.6876 | 149.4808 | 238.5533 |
| 253.2020 | 256.8703 | 298.9486 |
| 360.1874 | 437.4995 | 484.6143 |
| 569.5895 | 733.9664 | 782.3450 |
| 805.0902 | 842.9701 | 885.7499 |
| 910.4318 | 959.1470 | 999.9043 |
| 1035.7592 | 1058.0736 | 1083.6587 |
| 1083.9430 | 1114.6251 | 1136.8624 |
| 1170.5008 | 1223.2576 | 1267.5649 |
| 1282.3742 | 1299.8659 | 1334.6207 |
| 1336.0391 | 1343.7678 | 1371.6277 |
| 1384.1674 | 1393.4282 | 1397.7866 |
| 1407.0209 | 1429.1606 | 1496.3032 |
| 1499.9998 | 1504.4414 | 1506.1040 |
| 1509.0478 | 1513.7459 | 1524.8154 |
| 2903.2838 | 2924.8312 | 3013.0326 |
| 3015.6672 | 3022.0186 | 3034.3862 |
| 3038.8882 | 3045.7511 | 3048.3259 |
| 3064.9570 | 3068.9807 | 3073.7593 |
| 3091.7706 | 3106.0934 | 3114.9083 |

Zero-point correction (Hartree): 0.208585

C7H15O.tpmtm

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.94786291

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 3.268290 | -1.348493 | 0.238234 |
| C | 2.322651 | -0.545166 | -0.336726 |
| C | 1.814297 | 0.602518 | 0.549416 |
| C | 0.773141 | 1.522645 | -0.120798 |
| C | -0.702233 | 1.116201 | 0.048962 |
| C | -1.113275 | -0.209938 | -0.609370 |
| C | -2.628730 | -0.475971 | -0.596720 |
| C | -3.227305 | -0.661290 | 0.802748 |
| H | 2.680718 | -0.169702 | -1.317322 |
| H | 1.498231 | -1.236475 | -0.613291 |
| H | 1.415689 | 0.180103 | 1.480205 |
| H | 2.693630 | 1.192731 | 0.833580 |
| H | 0.887223 | 2.531424 | 0.293321 |
| H | 1.004965 | 1.617766 | -1.192225 |
| H | -0.933457 | 1.084066 | 1.121714 |
| H | -1.326129 | 1.917976 | -0.370404 |
| H | -0.763997 | -0.213193 | -1.651493 |
| H | -0.608184 | -1.048752 | -0.110335 |
| H | -3.141583 | 0.350529 | -1.107708 |
| H | -2.832166 | -1.374177 | -1.193491 |
| H | -3.118688 | 0.239313 | 1.415354 |
| H | -2.737832 | -1.485316 | 1.335236 |
| H | -4.296012 | -0.892337 | 0.745913 |

Rotational constants (GHz): 3.3359500 0.8034100 0.7219900

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 46.2958 | 50.1875 | 87.5469 |
| 112.3862 | 133.3058 | 203.7826 |
| 248.8208 | 289.5565 | 300.6511 |
| 367.6186 | 454.4894 | 498.9166 |
| 538.4152 | 740.9324 | 785.7876 |
| 799.4721 | 842.3221 | 880.8298 |
| 919.6896 | 954.8490 | 992.4498 |
| 1038.0486 | 1068.6323 | 1073.0990 |
| 1085.0768 | 1105.3631 | 1131.7559 |
| 1187.2633 | 1218.6688 | 1262.9775 |
| 1284.6210 | 1310.5919 | 1331.0125 |
| 1337.1484 | 1354.5492 | 1372.7057 |
| 1383.3339 | 1390.1431 | 1392.6647 |
| 1413.7487 | 1430.2134 | 1491.5711 |
| 1501.4945 | 1502.5312 | 1503.4636 |
| 1511.6520 | 1517.3525 | 1522.0069 |
| 2902.0876 | 2921.8549 | 3011.8321 |
| 3016.2619 | 3023.3287 | 3026.1556 |
| 3042.3264 | 3042.3307 | 3047.4481 |
| 3062.0522 | 3067.6812 | 3076.0297 |
| 3086.7148 | 3109.3393 | 3119.0085 |

Zero-point correction (Hartree): 0.208508

C7H15O.tpmtp

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.94768614

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -3.469150 | -1.158046 | -0.106116 |
| C | -2.380685 | -0.517392 | 0.417809 |
| C | -1.908878 | 0.719225 | -0.362742 |
| C | -0.687842 | 1.437107 | 0.249859 |
| C | 0.692546 | 0.987696 | -0.264308 |
| C | 1.071660 | -0.471979 | 0.024030 |
| C | 2.492640 | -0.858473 | -0.424502 |
| C | 3.618969 | -0.173753 | 0.359096 |
| H | -2.554636 | -0.277169 | 1.486867 |
| H | -1.587747 | -1.294529 | 0.457634 |
| H | -1.706170 | 0.425201 | -1.400076 |
| H | -2.759231 | 1.410190 | -0.401641 |
| H | -0.780342 | 2.511293 | 0.051300 |
| H | -0.717783 | 1.338755 | 1.345393 |
| H | 0.740003 | 1.158343 | -1.349455 |
| H | 1.445933 | 1.650922 | 0.178325 |
| H | 0.967785 | -0.671908 | 1.100981 |
| H | 0.362735 | -1.138087 | -0.484405 |
| H | 2.604775 | -1.945774 | -0.327568 |
| H | 2.603996 | -0.638081 | -1.495026 |
| H | 3.537404 | -0.384369 | 1.431929 |
| H | 3.606308 | 0.913667 | 0.233382 |
| H | 4.599706 | -0.528678 | 0.025831 |

Rotational constants (GHz): 4.0155800 0.7553200 0.6754400

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 44.7173 | 55.6912 | 88.8834 |
| 115.8656 | 133.6150 | 202.2469 |
| 241.8009 | 290.4222 | 294.5372 |
| 382.9518 | 458.9551 | 491.5370 |
| 543.7954 | 747.1682 | 755.6654 |
| 818.2657 | 839.6686 | 897.3888 |
| 919.6598 | 947.0926 | 1001.7934 |
| 1030.7901 | 1062.9306 | 1084.0361 |
| 1086.3257 | 1100.8330 | 1135.0412 |
| 1179.4995 | 1227.3308 | 1260.8803 |
| 1280.9066 | 1306.7236 | 1332.3269 |
| 1341.2157 | 1355.8349 | 1371.9146 |
| 1387.6323 | 1389.5309 | 1392.5218 |
| 1415.1182 | 1430.1357 | 1493.0908 |
| 1501.0001 | 1504.1149 | 1504.6133 |
| 1511.2556 | 1518.0144 | 1522.2100 |
| 2900.5139 | 2921.0987 | 3010.8897 |
| 3014.9980 | 3023.6070 | 3027.8840 |
| 3041.7326 | 3043.8257 | 3053.1533 |
| 3063.5660 | 3070.2816 | 3076.6410 |
| 3088.2136 | 3109.6031 | 3116.3369 |

Zero-point correction (Hartree): 0.208589

C7H15O.tpmtt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.94921649

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -3.076996 | -1.620049 | -0.243343 |
| C | -2.171259 | -0.778869 | 0.341532 |
| C | -1.990102 | 0.576305 | -0.359841 |

| | | | |
|---|-----------|-----------|-----------|
| C | -0.987091 | 1.526851 | 0.326008 |
| C | 0.476695 | 1.416910 | -0.137594 |
| C | 1.179596 | 0.082549 | 0.147772 |
| C | 2.672409 | 0.098946 | -0.209152 |
| C | 3.373560 | -1.236486 | 0.058077 |
| H | -2.406765 | -0.648252 | 1.417732 |
| H | -1.221643 | -1.355217 | 0.356299 |
| H | -1.702551 | 0.397848 | -1.403475 |
| H | -2.979008 | 1.048769 | -0.391152 |
| H | -1.312436 | 2.559000 | 0.150571 |
| H | -1.036323 | 1.385630 | 1.416149 |
| H | 0.523252 | 1.621463 | -1.216587 |
| H | 1.048193 | 2.221489 | 0.345239 |
| H | 1.066404 | -0.173092 | 1.211694 |
| H | 0.695350 | -0.725619 | -0.417501 |
| H | 2.786924 | 0.367861 | -1.268094 |
| H | 3.169502 | 0.895551 | 0.360925 |
| H | 2.922847 | -2.045645 | -0.527961 |
| H | 3.303632 | -1.516732 | 1.115357 |
| H | 4.435745 | -1.189898 | -0.203271 |
| Rotational constants (GHz): 2.9451800 0.8281300 0.6796300 | | | |
| Vibrational harmonic frequencies (cm-1): | | | |
| 38.7593 | 69.7741 | 81.8159 | |
| 110.2005 | 130.6566 | 179.0827 | |
| 250.9586 | 271.3384 | 294.9295 | |
| 389.9089 | 423.6112 | 485.2541 | |
| 543.6063 | 742.7443 | 775.7846 | |
| 810.2576 | 843.3818 | 898.8766 | |
| 926.2476 | 959.9080 | 998.6458 | |
| 1045.1596 | 1065.0188 | 1069.9613 | |
| 1085.6522 | 1103.7726 | 1135.0986 | |
| 1190.9153 | 1229.1085 | 1264.7888 | |
| 1283.6292 | 1313.5970 | 1325.8504 | |
| 1338.8532 | 1341.4245 | 1372.7079 | |
| 1387.2685 | 1389.6582 | 1393.0845 | |
| 1416.3214 | 1428.3433 | 1493.8757 | |
| 1500.5087 | 1502.1465 | 1504.0161 | |
| 1513.4405 | 1513.9196 | 1524.8913 | |
| 2902.4382 | 2921.8555 | 3010.9407 | |
| 3014.8649 | 3018.7964 | 3028.0078 | |
| 3039.0193 | 3040.2390 | 3042.9388 | |
| 3054.7357 | 3069.1913 | 3073.8253 | |
| 3087.3686 | 3107.4787 | 3113.4358 | |
| Zero-point correction (Hartree): 0.208416 | | | |

C7H15O.tppmm

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.94588157

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 2.687493 | -1.561809 | 0.147571 |
| C | 1.960047 | -0.551593 | -0.419402 |
| C | 1.545914 | 0.568093 | 0.546992 |
| C | 0.713156 | 1.677651 | -0.114598 |
| C | -0.676825 | 1.288151 | -0.656949 |
| C | -1.707174 | 0.835485 | 0.402931 |
| C | -1.780691 | -0.677082 | 0.689743 |
| C | -2.353206 | -1.505000 | -0.467374 |
| H | 2.459121 | -0.147600 | -1.322820 |
| H | 1.056792 | -1.066524 | -0.815776 |
| H | 1.015295 | 0.121858 | 1.394900 |
| H | 2.463446 | 1.008112 | 0.956664 |
| H | 0.585097 | 2.490649 | 0.612006 |
| H | 1.297840 | 2.107434 | -0.940286 |
| H | -1.073347 | 2.170236 | -1.174457 |
| H | -0.578419 | 0.521863 | -1.437374 |
| H | -1.506954 | 1.371097 | 1.340841 |
| H | -2.706643 | 1.160760 | 0.084695 |
| H | -0.791019 | -1.063851 | 0.960950 |
| H | -2.411444 | -0.829179 | 1.574911 |
| H | -1.743446 | -1.425520 | -1.374239 |
| H | -3.365678 | -1.172837 | -0.724792 |
| H | -2.407911 | -2.566254 | -0.203855 |
| Rotational constants (GHz): 2.3720700 1.1606700 0.8872100 | | | |
| Vibrational harmonic frequencies (cm-1): | | | |
| 35.9589 | 59.7570 | 98.4303 | |
| 130.4241 | 169.2312 | 216.5464 | |
| 242.2963 | 297.9835 | 313.7899 | |
| 404.2248 | 432.3675 | 489.6684 | |
| 670.1489 | 743.5965 | 773.5586 | |
| 808.3676 | 832.3377 | 900.1045 | |
| 921.8451 | 944.5293 | 998.5258 | |
| 1023.2822 | 1060.2315 | 1083.3478 | |
| 1088.8286 | 1112.8607 | 1125.3834 | |
| 1168.1377 | 1194.1145 | 1241.7792 | |

| | | |
|-----------|-----------|-----------|
| 1276.7408 | 1311.8058 | 1328.4782 |
| 1335.1590 | 1356.0134 | 1372.9122 |
| 1389.9448 | 1394.8541 | 1399.2392 |
| 1403.8729 | 1429.9345 | 1494.1487 |
| 1499.2476 | 1503.2928 | 1506.1416 |
| 1510.0170 | 1517.3310 | 1521.9558 |
| 2883.4030 | 2931.3454 | 3019.5959 |
| 3021.7602 | 3032.4384 | 3039.8415 |
| 3041.4616 | 3049.1742 | 3056.9801 |
| 3062.1623 | 3071.9163 | 3076.2702 |
| 3097.9985 | 3108.7079 | 3113.5367 |

Zero-point correction (Hartree): 0.208998

C7H15O.tppmp

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.94308116

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 3.252662 | -0.928654 | -0.584019 |
| C | 2.450711 | 0.110098 | -0.200833 |
| C | 1.211612 | -0.289766 | 0.615646 |
| C | 0.304053 | 0.906666 | 0.952870 |
| C | -0.535422 | 1.458706 | -0.222723 |
| C | -1.967617 | 0.910970 | -0.383590 |
| C | -2.132148 | -0.585804 | -0.728194 |
| C | -2.214124 | -1.531683 | 0.477623 |
| H | 3.033081 | 0.905647 | 0.305897 |
| H | 2.140491 | 0.576540 | -1.162908 |
| H | -1.307535 | -1.515374 | 1.089110 |
| H | 1.564014 | -0.759318 | 1.542191 |
| H | -0.364284 | 0.635831 | 1.778752 |
| H | 0.939545 | 1.711542 | 1.347836 |
| H | -0.620994 | 2.546391 | -0.107425 |
| H | 0.005620 | 1.309828 | -1.168371 |
| H | -2.539597 | 1.133241 | 0.528766 |
| H | -2.441393 | 1.500066 | -1.179267 |
| H | -3.055511 | -0.704934 | -1.308890 |
| H | -1.321223 | -0.900686 | -1.398857 |
| H | -3.053309 | -1.257461 | 1.127272 |
| H | 0.669433 | -1.061099 | 0.059319 |
| H | -2.372024 | -2.566107 | 0.153935 |

Rotational constants (GHz): 2.9192600 0.9490100 0.8368300

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 49.6833 | 85.0146 | 99.2228 |
| 120.6027 | 133.4262 | 212.6324 |
| 245.0428 | 295.8077 | 315.7522 |
| 367.4916 | 447.0160 | 477.0290 |
| 654.4190 | 736.6652 | 790.4556 |
| 816.8054 | 826.4037 | 886.5662 |
| 917.1131 | 959.6630 | 1001.4179 |
| 1023.2547 | 1067.8227 | 1085.7495 |
| 1089.3968 | 1119.3504 | 1130.4735 |
| 1163.0651 | 1210.6220 | 1237.5771 |
| 1295.6095 | 1301.3781 | 1325.4701 |
| 1336.0864 | 1359.6830 | 1378.4300 |
| 1385.7254 | 1389.5331 | 1396.7423 |
| 1405.3367 | 1429.6387 | 1494.8990 |
| 1497.7363 | 1500.8893 | 1505.7220 |
| 1510.8960 | 1515.4372 | 1523.3905 |
| 2878.3641 | 2929.3461 | 3015.9067 |
| 3018.2311 | 3025.3737 | 3029.0748 |
| 3045.2838 | 3050.7577 | 3058.9948 |
| 3062.7535 | 3065.4011 | 3073.8371 |
| 3107.1939 | 3108.3962 | 3128.4423 |

Zero-point correction (Hartree): 0.208943

C7H15O.tppmt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.94738802

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 2.702721 | -1.717867 | -0.074390 |
| C | 2.129089 | -0.523298 | -0.413310 |
| C | 1.512515 | 0.252939 | 0.760215 |
| C | 0.868591 | 1.585903 | 0.347739 |
| C | -0.356294 | 1.517832 | -0.586016 |
| C | -1.615454 | 0.837290 | -0.003865 |
| C | -1.750850 | -0.666382 | -0.292430 |
| C | -3.038697 | -1.267396 | 0.280121 |
| H | 2.821890 | 0.109789 | -1.002871 |
| H | 1.335467 | -0.807894 | -1.139281 |
| H | 0.793541 | -0.396106 | 1.271351 |
| H | 2.313344 | 0.452890 | 1.482672 |
| H | 0.577698 | 2.123936 | 1.259399 |
| H | 1.635005 | 2.210210 | -0.133073 |

| | | | | |
|--|-----------|-----------|-----------|--|
| H | -0.608144 | 2.551541 | -0.852932 | |
| H | -0.086925 | 1.032755 | -1.534914 | |
| H | -1.653110 | 1.006623 | 1.081868 | |
| H | -2.505563 | 1.334969 | -0.411052 | |
| H | -1.728636 | -0.821524 | -1.380035 | |
| H | -0.889625 | -1.213013 | 0.110065 | |
| H | -3.924344 | -0.767630 | -0.129023 | |
| H | -3.074752 | -1.160853 | 1.370351 | |
| H | -3.121019 | -2.334089 | 0.047870 | |
| Rotational constants (GHz): | 2.4706200 | 1.0355500 | 0.8057700 | |
| Vibrational harmonic frequencies (cm-1): | | | | |
| 40.0874 | 57.6089 | | 92.2259 | |
| 106.2927 | 166.6335 | | 217.1322 | |
| 246.1503 | 259.8604 | | 320.1337 | |
| 367.3547 | 444.4257 | | 503.1988 | |
| 680.0977 | 731.0790 | | 776.9260 | |
| 803.8935 | 856.2310 | | 893.7311 | |
| 930.7584 | 957.4978 | | 1014.8840 | |
| 1023.8060 | 1058.8069 | | 1082.9346 | |
| 1087.4737 | 1114.7092 | | 1125.6280 | |
| 1169.6316 | 1215.0946 | | 1245.7185 | |
| 1278.8828 | 1312.7799 | | 1329.7143 | |
| 1336.6993 | 1341.1712 | | 1359.1674 | |
| 1388.2928 | 1398.0611 | | 1399.5249 | |
| 1405.7186 | 1427.0716 | | 1495.1277 | |
| 1495.6199 | 1506.5476 | | 1507.3753 | |
| 1508.9374 | 1512.8303 | | 1524.4397 | |
| 2887.7609 | 2931.3691 | | 3017.4214 | |
| 3019.0230 | 3024.7940 | | 3030.1000 | |
| 3039.3498 | 3047.0782 | | 3052.4630 | |
| 3060.1096 | 3069.1077 | | 3075.8514 | |
| 3099.2290 | 3108.4486 | | 3114.3708 | |
| Zero-point correction (Hartree): | 0.208895 | | | |

C7H15O.tpppm

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.94590003

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | | |
|--|-----------|-----------|-----------|--|
| O | -3.694346 | -0.243160 | -0.685138 | |
| C | -2.654421 | -0.139779 | 0.196897 | |
| C | -1.468355 | 0.702853 | -0.298071 | |
| C | -0.304869 | 0.780931 | 0.704551 | |
| C | 0.468172 | -0.536531 | 0.919677 | |
| C | 1.325222 | -1.021353 | -0.272912 | |
| C | 2.798590 | -0.575404 | -0.255354 | |
| C | 3.039915 | 0.934708 | -0.365815 | |
| H | -3.000213 | 0.188682 | 1.197511 | |
| H | -2.335381 | -1.194453 | 0.352661 | |
| H | -1.137054 | 0.299886 | -1.261950 | |
| H | -1.841629 | 1.714293 | -0.498663 | |
| H | 0.386250 | 1.563763 | 0.374374 | |
| H | -0.698751 | 1.120218 | 1.673045 | |
| H | 1.114830 | -0.425409 | 1.800361 | |
| H | -0.247459 | -1.324481 | 1.189129 | |
| H | 1.313989 | -2.118152 | -0.291136 | |
| H | 0.864572 | -0.706983 | -1.219251 | |
| H | 3.269963 | -0.949310 | 0.664145 | |
| H | 3.316609 | -1.076615 | -1.083360 | |
| H | 2.650465 | 1.476645 | 0.502092 | |
| H | 2.562142 | 1.350298 | -1.260717 | |
| H | 4.110908 | 1.154343 | -0.430966 | |
| Rotational constants (GHz): | 4.5055200 | 0.7447800 | 0.7204300 | |
| Vibrational harmonic frequencies (cm-1): | | | | |
| 23.3654 | 52.5466 | | 92.7476 | |
| 117.2275 | 159.7998 | | 236.7878 | |
| 261.6871 | 298.6366 | | 301.8281 | |
| 399.0583 | 450.1614 | | 482.8949 | |
| 673.7368 | 742.1916 | | 774.3424 | |
| 804.6703 | 853.0056 | | 897.9373 | |
| 915.9465 | 942.5486 | | 1004.4056 | |
| 1028.7521 | 1058.6400 | | 1084.9760 | |
| 1089.3186 | 1106.8311 | | 1128.9506 | |
| 1173.1814 | 1199.1537 | | 1242.1167 | |
| 1266.5225 | 1317.4808 | | 1328.2073 | |
| 1334.0517 | 1358.2265 | | 1374.9377 | |
| 1390.3146 | 1390.7180 | | 1397.0721 | |
| 1400.0169 | 1429.4177 | | 1495.3806 | |
| 1500.0682 | 1503.4926 | | 1506.5923 | |
| 1509.6961 | 1517.3137 | | 1523.9912 | |
| 2883.5486 | 2929.9915 | | 3021.7999 | |
| 3023.5530 | 3027.0178 | | 3033.5222 | |
| 3040.7968 | 3050.0312 | | 3055.8324 | |
| 3062.9310 | 3069.1880 | | 3091.6295 | |
| 3094.5724 | 3107.4602 | | 3115.8728 | |

Zero-point correction (Hartree): 0.209019

C7H15O.tpppp

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.94868177

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -3.634198 | -0.724743 | -0.154613 |
| C | -2.590131 | 0.044417 | 0.280478 |
| C | -1.470644 | 0.257072 | -0.750129 |
| C | -0.314016 | 1.127409 | -0.232405 |
| C | 0.505509 | 0.529645 | 0.927578 |
| C | 1.229847 | -0.794638 | 0.621140 |
| C | 2.276780 | -0.738576 | -0.505764 |
| C | 3.454654 | 0.202597 | -0.227573 |
| H | -2.942426 | 1.005612 | 0.705512 |
| H | -2.199056 | -0.514119 | 1.159706 |
| H | -1.113194 | -0.724316 | -1.081347 |
| H | -1.916393 | 0.736038 | -1.630247 |
| H | 0.354133 | 1.352986 | -1.072292 |
| H | -0.716829 | 2.097377 | 0.090732 |
| H | 1.238584 | 1.278926 | 1.250942 |
| H | -0.147262 | 0.373662 | 1.797198 |
| H | 1.723559 | -1.135379 | 1.541540 |
| H | 0.491348 | -1.569307 | 0.377245 |
| H | 2.661652 | -1.753755 | -0.665503 |
| H | 1.795274 | -0.452502 | -1.449823 |
| H | 3.955744 | -0.059407 | 0.711718 |
| H | 3.136463 | 1.247586 | -0.150695 |
| H | 4.199985 | 0.146980 | -1.027727 |

Rotational constants (GHz): 4.7125700 0.7562400 0.7388800

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 33.2649 | 41.8572 | 93.5154 |
| 106.7272 | 176.2486 | 214.1294 |
| 264.9267 | 303.0884 | 344.2803 |
| 398.2528 | 460.7626 | 521.8806 |
| 671.4024 | 719.4435 | 752.8724 |
| 824.1003 | 838.6965 | 901.1396 |
| 923.5000 | 944.3529 | 999.6144 |
| 1024.5785 | 1049.7870 | 1080.9793 |
| 1088.2100 | 1100.4474 | 1128.2141 |
| 1172.2876 | 1199.0904 | 1233.1104 |
| 1274.0395 | 1305.6859 | 1329.4048 |
| 1342.0786 | 1359.1167 | 1375.4337 |
| 1381.5197 | 1391.6588 | 1405.8991 |
| 1407.5025 | 1428.8110 | 1489.8411 |
| 1498.2200 | 1503.0081 | 1511.4366 |
| 1512.9644 | 1518.2785 | 1526.3635 |
| 2884.8661 | 2930.7609 | 3022.2037 |
| 3026.6236 | 3031.7547 | 3037.9958 |
| 3041.1641 | 3050.5515 | 3056.8965 |
| 3064.7390 | 3073.0951 | 3076.8736 |
| 3096.3899 | 3108.8953 | 3114.6681 |

Zero-point correction (Hartree): 0.209112

C7H15O.tpppt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.94999899

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 3.356343 | -1.265194 | -0.159498 |
| C | 2.543371 | -0.173771 | -0.298037 |
| C | 1.474567 | -0.022067 | 0.795081 |
| C | 0.578386 | 1.214345 | 0.615939 |
| C | -0.306487 | 1.221195 | -0.645469 |
| C | -1.319831 | 0.069161 | -0.762694 |
| C | -2.384249 | 0.035301 | 0.343468 |
| C | -3.427459 | -1.067132 | 0.133751 |
| H | 3.130874 | 0.757126 | -0.427989 |
| H | 2.059292 | -0.329509 | -1.287717 |
| H | 0.879875 | -0.941870 | 0.828502 |
| H | 1.992419 | 0.045686 | 1.759345 |
| H | -0.053284 | 1.317220 | 1.506149 |
| H | 1.211448 | 2.112373 | 0.599267 |
| H | -0.851596 | 2.174249 | -0.675553 |
| H | 0.330746 | 1.221247 | -1.540242 |
| H | -1.824999 | 0.153410 | -1.734462 |
| H | -0.793739 | -0.895332 | -0.785983 |
| H | -1.904511 | -0.105108 | 1.320366 |
| H | -2.886451 | 1.011712 | 0.389372 |
| H | -2.958632 | -2.057623 | 0.114828 |
| H | -3.957605 | -0.935452 | -0.816420 |
| H | -4.174368 | -1.068768 | 0.934286 |

Rotational constants (GHz): 3.5424000 0.7851600 0.7268400

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 34.8050 | 74.2794 | 92.0952 |
| 102.2487 | 164.7089 | 232.7863 |
| 257.5501 | 271.8533 | 315.1679 |
| 378.3903 | 456.8457 | 525.2942 |
| 672.3305 | 722.5669 | 761.7811 |
| 815.6279 | 857.1242 | 899.9187 |
| 925.3925 | 948.6102 | 1010.0881 |
| 1029.3886 | 1050.3388 | 1079.4777 |
| 1086.9901 | 1107.8454 | 1124.7673 |
| 1178.3701 | 1202.4768 | 1246.3250 |
| 1278.6985 | 1316.5357 | 1327.8769 |
| 1336.1782 | 1346.5978 | 1362.9325 |
| 1388.9208 | 1393.1309 | 1403.8744 |
| 1415.2342 | 1428.0006 | 1492.7665 |
| 1502.5050 | 1504.8883 | 1506.4165 |
| 1513.9975 | 1515.0879 | 1524.5575 |
| 2885.5461 | 2930.4848 | 3018.6754 |
| 3022.3191 | 3028.5177 | 3032.6769 |
| 3039.6474 | 3048.2946 | 3050.4154 |
| 3056.5296 | 3071.8978 | 3077.7447 |
| 3096.4004 | 3108.0047 | 3113.4960 |

Zero-point correction (Hartree): 0.209054

C7H15O.tpptm

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.94983646

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 3.554670 | -1.099330 | -0.024231 |
| C | 2.518036 | -0.337506 | -0.489530 |
| C | 1.848125 | 0.554712 | 0.566380 |
| C | 0.681925 | 1.392837 | 0.016638 |
| C | -0.549686 | 0.602797 | -0.464367 |
| C | -1.279006 | -0.173878 | 0.641921 |
| C | -2.521997 | -0.944667 | 0.164130 |
| C | -3.677342 | -0.057443 | -0.315095 |
| H | 2.810442 | 0.240775 | -1.388776 |
| H | 1.791333 | -1.087387 | -0.873784 |
| H | 1.526490 | -0.077396 | 1.401381 |
| H | 2.615522 | 1.227621 | 0.967666 |
| H | 0.364866 | 2.099371 | 0.794740 |
| H | 1.051611 | 2.010154 | -0.813857 |
| H | -1.243978 | 1.312762 | -0.929708 |
| H | -0.263278 | -0.094487 | -1.265046 |
| H | -0.586369 | -0.887266 | 1.105956 |
| H | -1.571678 | 0.525481 | 1.438739 |
| H | -2.231648 | -1.634251 | -0.640681 |
| H | -2.878315 | -1.576333 | 0.987698 |
| H | -3.403358 | 0.536463 | -1.193065 |
| H | -3.990599 | 0.639191 | 0.471309 |
| H | -4.548729 | -0.661175 | -0.589197 |

Rotational constants (GHz): 4.3826300 0.7160000 0.6673500

Vibrational harmonic frequencies (cm⁻¹):

| | | |
|-----------|-----------|-----------|
| 36.3510 | 45.3115 | 89.1298 |
| 118.6014 | 175.3541 | 212.1564 |
| 226.8467 | 289.5400 | 303.1847 |
| 381.3440 | 463.1586 | 505.7729 |
| 671.8925 | 735.5147 | 759.3111 |
| 826.7776 | 871.0410 | 876.3665 |
| 929.4736 | 947.4647 | 1006.1104 |
| 1015.0766 | 1069.4795 | 1083.8665 |
| 1093.2363 | 1096.8279 | 1129.0450 |
| 1164.5600 | 1215.7257 | 1237.8368 |
| 1294.0243 | 1300.1742 | 1329.1603 |
| 1340.1356 | 1349.8205 | 1369.0625 |
| 1387.5855 | 1392.3903 | 1395.4464 |
| 1414.7296 | 1430.1544 | 1496.8257 |
| 1500.3284 | 1503.3104 | 1507.3475 |
| 1514.0882 | 1517.5360 | 1522.3203 |
| 2885.2878 | 2931.1166 | 3015.0347 |
| 3023.0502 | 3024.2821 | 3027.1573 |
| 3041.6735 | 3049.1972 | 3057.7245 |
| 3062.8357 | 3064.8251 | 3078.8854 |
| 3097.4836 | 3109.1817 | 3115.9159 |

Zero-point correction (Hartree): 0.208964

C7H15O.tpptp

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.94992271

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|----------|-----------|-----------|
| O | 3.176266 | 1.403868 | -0.311816 |
| C | 2.274466 | 0.616336 | 0.349749 |
| C | 1.817877 | -0.631317 | -0.421684 |
| C | 0.800363 | -1.492048 | 0.344790 |

| | | | |
|--|-----------|-----------|-----------|
| C | -0.565986 | -0.835337 | 0.614664 |
| C | -1.370428 | -0.503375 | -0.651382 |
| C | -2.798315 | 0.000400 | -0.380958 |
| C | -2.869078 | 1.352053 | 0.340100 |
| H | 2.627886 | 0.361154 | 1.368912 |
| H | 1.409915 | 1.294872 | 0.524270 |
| H | 1.419112 | -0.313506 | -1.391338 |
| H | 2.708762 | -1.233587 | -0.636745 |
| H | 0.639630 | -2.421491 | -0.216883 |
| H | 1.243408 | -1.794717 | 1.303752 |
| H | -1.157783 | -1.519759 | 1.237828 |
| H | -0.431416 | 0.070541 | 1.220271 |
| H | -0.837573 | 0.248288 | -1.249688 |
| H | -1.425573 | -1.404849 | -1.277244 |
| H | -3.327838 | 0.080381 | -1.338787 |
| H | -3.342009 | -0.754395 | 0.203792 |
| H | -2.333111 | 2.126842 | -0.220883 |
| H | -2.430612 | 1.305182 | 1.342258 |
| H | -3.906322 | 1.683830 | 0.453336 |
| Rotational constants (GHz): | 3.1011900 | 0.8433400 | 0.7316500 |
| Vibrational harmonic frequencies (cm-1): | | | |
| 40.5254 | 41.9090 | | 89.7772 |
| 126.9632 | 173.3403 | | 207.7696 |
| 236.2309 | 295.0548 | | 302.9802 |
| 371.1416 | 461.0988 | | 512.5815 |
| 664.7725 | 732.9827 | | 778.3643 |
| 808.7583 | 871.5147 | | 877.8277 |
| 920.4821 | 951.1538 | | 998.6930 |
| 1018.5141 | 1069.5676 | | 1082.5039 |
| 1090.7356 | 1098.8387 | | 1125.1819 |
| 1172.3173 | 1203.3104 | | 1242.2655 |
| 1289.2674 | 1312.0140 | | 1327.9445 |
| 1336.7089 | 1349.3393 | | 1367.4737 |
| 1385.5146 | 1391.9513 | | 1395.6184 |
| 1415.4707 | 1431.5396 | | 1493.9274 |
| 1500.0332 | 1502.5908 | | 1505.8212 |
| 1514.9729 | 1517.8569 | | 1522.7834 |
| 2883.0125 | 2929.8502 | | 3017.4295 |
| 3023.4918 | 3026.4665 | | 3029.9822 |
| 3042.4787 | 3048.3410 | | 3049.9094 |
| 3059.9689 | 3064.9787 | | 3076.2762 |
| 3098.3394 | 3108.9715 | | 3118.5046 |
| Zero-point correction (Hartree): | 0.208922 | | |

C7H15O.tpptt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.95119725

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|--|-----------|-----------|-----------|
| O | 3.314305 | -1.468773 | -0.032829 |
| C | 2.499046 | -0.446190 | -0.433841 |
| C | 1.821957 | 0.326572 | 0.708323 |
| C | 0.904463 | 1.461668 | 0.225001 |
| C | -0.354168 | 1.024739 | -0.546602 |
| C | -1.360725 | 0.208858 | 0.276272 |
| C | -2.636459 | -0.141627 | -0.501121 |
| C | -3.641701 | -0.953264 | 0.322029 |
| H | 3.018168 | 0.235090 | -1.137503 |
| H | 1.732014 | -0.951092 | -1.062435 |
| H | 1.275404 | -0.386900 | 1.334833 |
| H | 2.614069 | 0.747850 | 1.338940 |
| H | 0.595631 | 2.054247 | 1.095933 |
| H | 1.488858 | 2.143963 | -0.407812 |
| H | -0.855353 | 1.926207 | -0.923872 |
| H | -0.070120 | 0.452716 | -1.441684 |
| H | -0.894792 | -0.720561 | 0.630708 |
| H | -1.630883 | 0.774798 | 1.179688 |
| H | -3.111952 | 0.784607 | -0.851545 |
| H | -2.366038 | -0.703414 | -1.405792 |
| H | -3.959528 | -0.402242 | 1.214552 |
| H | -3.205592 | -1.900977 | 0.658133 |
| H | -4.538809 | -1.188636 | -0.259868 |
| Rotational constants (GHz): | 3.5054900 | 0.7318500 | 0.6601000 |
| Vibrational harmonic frequencies (cm-1): | | | |
| 30.7260 | 70.0090 | | 90.9695 |
| 112.9694 | 146.0412 | | 183.7481 |
| 254.1062 | 256.8043 | | 309.6590 |
| 396.8147 | 428.0851 | | 496.8678 |
| 670.4045 | 730.5292 | | 761.7028 |
| 825.3179 | 869.6311 | | 896.9429 |
| 927.9548 | 950.9344 | | 1010.9029 |
| 1027.3063 | 1062.0788 | | 1080.1646 |
| 1086.7968 | 1101.6638 | | 1126.9969 |
| 1168.7382 | 1215.3616 | | 1245.4776 |
| 1288.8708 | 1302.6447 | | 1330.5743 |

| | | |
|-----------|-----------|-----------|
| 1337.2007 | 1339.6119 | 1362.2659 |
| 1383.8329 | 1393.4602 | 1396.0025 |
| 1414.4248 | 1429.6745 | 1493.9566 |
| 1499.4853 | 1500.4881 | 1505.1757 |
| 1512.6784 | 1514.9111 | 1524.9767 |
| 2879.0500 | 2930.2151 | 3011.9290 |
| 3017.2768 | 3023.9967 | 3027.2677 |
| 3039.5508 | 3041.0785 | 3050.1212 |
| 3052.6466 | 3064.9857 | 3073.8444 |
| 3098.6269 | 3107.7619 | 3113.0502 |

Zero-point correction (Hartree): 0.208674

C7H15O.tptmm

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.94988176

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 3.988568 | -0.183182 | -0.399353 |
| C | 2.763786 | 0.321439 | -0.059024 |
| C | 1.719839 | -0.730835 | 0.345344 |
| C | 0.352751 | -0.138514 | 0.722457 |
| C | -0.415503 | 0.483016 | -0.453884 |
| C | -1.770086 | 1.105833 | -0.070082 |
| C | -2.829924 | 0.132513 | 0.476130 |
| C | -3.269636 | -0.947900 | -0.519059 |
| H | 2.854257 | 1.121361 | 0.703313 |
| H | 2.434429 | 0.858803 | -0.975776 |
| H | 1.614389 | -1.450067 | -0.476172 |
| H | 2.126000 | -1.287906 | 1.198123 |
| H | -0.251920 | -0.933608 | 1.174047 |

| | | | |
|---|-----------|-----------|-----------|
| H | 0.486777 | 0.618509 | 1.509475 |
| H | 0.194987 | 1.269025 | -0.918026 |
| H | -0.559842 | -0.278911 | -1.231620 |
| H | -1.596453 | 1.893128 | 0.676348 |
| H | -2.183363 | 1.612163 | -0.953022 |
| H | -2.464079 | -0.343323 | 1.394919 |
| H | -3.707918 | 0.718623 | 0.776225 |
| H | -2.447028 | -1.619609 | -0.786552 |
| H | -3.644894 | -0.500716 | -1.447058 |
| H | -4.071251 | -1.565317 | -0.100695 |

Rotational constants (GHz): 5.4649800 0.6595200 0.6401200

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 33.2736 | 56.5377 | 90.1943 |
| 105.4322 | 164.8248 | 230.6427 |
| 242.6685 | 262.7209 | 313.0755 |
| 365.5037 | 456.2464 | 535.9075 |
| 656.1449 | 723.3234 | 764.6627 |
| 829.4598 | 833.7359 | 886.1441 |
| 917.5101 | 978.8908 | 992.8085 |
| 1026.0857 | 1059.5908 | 1075.5698 |
| 1088.3064 | 1105.7951 | 1129.2238 |
| 1177.5648 | 1202.7344 | 1260.6597 |
| 1275.2467 | 1304.5609 | 1331.9798 |
| 1341.4921 | 1348.8228 | 1367.4648 |
| 1386.5036 | 1389.9982 | 1399.0474 |
| 1414.1163 | 1429.1987 | 1492.6293 |
| 1498.7385 | 1503.1560 | 1506.5879 |
| 1509.6936 | 1517.3734 | 1524.0246 |
| 2886.3734 | 2927.4908 | 3016.8226 |
| 3020.3996 | 3026.8114 | 3036.4206 |
| 3041.2321 | 3044.0004 | 3053.0315 |
| 3059.6937 | 3070.9789 | 3080.4715 |
| 3089.4110 | 3109.0472 | 3114.0096 |

Zero-point correction (Hartree): 0.208867

C7H15O.tptmp

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.94723679

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -3.966157 | 0.062613 | -0.412322 |
| C | -2.747094 | -0.308368 | 0.084591 |
| C | -1.674146 | 0.791241 | 0.053113 |
| C | -0.315334 | 0.352440 | 0.620468 |
| C | 0.402172 | -0.726127 | -0.208747 |
| C | 1.813386 | -1.098811 | 0.301617 |
| C | 2.982123 | -0.334179 | -0.346310 |
| C | 2.997912 | 1.181976 | -0.120591 |
| H | -2.840500 | -0.759551 | 1.092966 |
| H | -2.444343 | -1.158440 | -0.565935 |
| H | -1.564552 | 1.140218 | -0.981114 |
| H | -2.054928 | 1.641644 | 0.631442 |
| H | 0.324705 | 1.236610 | 0.708713 |
| H | -0.451200 | -0.019465 | 1.646480 |

| | | | |
|--|-----------|-----------|-----------|
| H | -0.216534 | -1.632727 | -0.219078 |
| H | 0.465851 | -0.399233 | -1.256759 |
| H | 1.851287 | -0.967894 | 1.392489 |
| H | 1.983047 | -2.168109 | 0.125155 |
| H | 3.920146 | -0.757914 | 0.035518 |
| H | 2.979427 | -0.536467 | -1.426291 |
| H | 2.982892 | 1.427305 | 0.947780 |
| H | 2.139090 | 1.674475 | -0.588053 |
| H | 3.900750 | 1.629618 | -0.549588 |
| Rotational constants (GHz): | 5.1798300 | 0.6846000 | 0.6415400 |
| Vibrational harmonic frequencies (cm-1): | | | |
| 32.5582 | 76.2699 | | 88.7700 |
| 106.8837 | 126.3643 | | 222.6158 |
| 270.9399 | 283.2467 | | 306.2593 |
| 330.6480 | 447.7221 | | 530.6461 |
| 666.1801 | 734.0957 | | 776.8146 |
| 803.4029 | 852.4401 | | 890.5674 |
| 915.3501 | 976.9578 | | 1001.3772 |
| 1032.7486 | 1064.1394 | | 1082.9807 |
| 1086.4704 | 1102.3305 | | 1121.0083 |
| 1182.6291 | 1210.1868 | | 1256.6239 |
| 1273.4498 | 1316.2712 | | 1321.6183 |
| 1343.6830 | 1347.0432 | | 1367.5806 |
| 1388.7873 | 1388.9287 | | 1394.1118 |
| 1408.2260 | 1429.4089 | | 1496.1208 |
| 1499.0840 | 1502.0887 | | 1504.0329 |
| 1514.4512 | 1517.5964 | | 1523.3264 |
| 2887.5050 | 2929.2913 | | 3016.0261 |
| 3020.5795 | 3023.6917 | | 3024.9318 |
| 3040.2124 | 3044.3206 | | 3052.0109 |
| 3061.3894 | 3067.4008 | | 3088.2163 |
| 3091.1354 | 3107.4154 | | 3114.5578 |
| Zero-point correction (Hartree): | 0.208871 | | |

C7H15O.tptmt

```

-----
E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.95109231
Electronic state : 2-A
Cartesian coordinates (Angs):
O      -4.165338      -0.187144      -0.142892
C      -2.869960      -0.336708      0.269445
C      -1.922428      0.798720      -0.147080
C      -0.472797      0.603054      0.323799
C      0.263623      -0.560842      -0.358421
C      1.715210      -0.759684      0.109985
C      2.677738      0.374764      -0.269599
C      4.123105      0.096154      0.156123
H      -2.813097      -0.537100      1.358361
H      -2.551197      -1.294475      -0.198284
H      -1.961723      0.902339      -1.238412
H      -2.320865      1.731561      0.269735
H      0.073873      1.536304      0.146110
H      -0.459524      0.450486      1.413212
H      -0.284822      -1.495762      -0.181578
H      0.251384      -0.405225      -1.446826
H      1.729131      -0.897310      1.200983
H      2.095974      -1.697897      -0.315975
H      2.639008      0.529394      -1.356867
H      2.344738      1.316845      0.183576
H      4.505267      -0.818314      -0.311994
H      4.198074      -0.034116      1.241845
H      4.789529      0.917671      -0.126259
Rotational constants (GHz):      8.0343100      0.5794300      0.5625500
Vibrational harmonic frequencies (cm-1):
33.6418      69.8670      84.3092
97.1410      134.5959      235.0940
246.5514      257.5189      287.9618
311.9736      447.2839      552.3017
659.9544      730.8561      755.7453
824.6098      854.0647      882.5155
922.6625      979.4518      1010.1049
1034.9435      1054.1014      1077.1254
1088.4379      1090.7690      1127.3942

1189.1513      1214.0780      1266.9892
1274.8992      1315.0760      1331.3917
1335.2451      1347.8079      1357.4574
1367.9482      1390.4733      1407.8045
1414.9544      1427.0013      1494.8308
1498.0417      1502.4190      1507.9306
1511.0124      1513.6259      1523.4482
2886.6161      2928.8202      3012.3956
3016.1163      3020.9787      3028.4653
3038.8547      3043.7600      3047.5159
3051.0570      3071.4288      3080.7431
    
```

3089.3462 3107.2607 3112.9782
Zero-point correction (Hartree): 0.208632

C7H15O.tptpm

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.94733454

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 3.704248 | 0.613050 | -0.471260 |
| C | 2.352195 | 0.585716 | -0.267444 |
| C | 1.851719 | -0.569524 | 0.613232 |
| C | 0.329050 | -0.576801 | 0.817729 |
| C | -0.475395 | -0.926316 | -0.446440 |
| C | -2.004607 | -1.017707 | -0.243407 |
| C | -2.800345 | 0.275881 | -0.496314 |
| C | -2.491940 | 1.447913 | 0.442386 |
| H | 1.978510 | 1.565412 | 0.093022 |
| H | 1.930562 | 0.496878 | -1.293159 |
| H | 2.185300 | -1.515446 | 0.168727 |
| H | 2.352734 | -0.486276 | 1.585192 |
| H | 0.085456 | -1.311394 | 1.596028 |
| H | 0.011715 | 0.394778 | 1.216833 |
| H | -0.265894 | -0.202659 | -1.247090 |
| H | -0.107175 | -1.892193 | -0.817251 |
| H | -2.400921 | -1.782933 | -0.922330 |
| H | -2.214368 | -1.382963 | 0.772047 |
| H | -2.635948 | 0.593818 | -1.535243 |
| H | -3.869248 | 0.037046 | -0.422089 |
| H | -1.468572 | 1.815353 | 0.315833 |
| H | -2.615591 | 1.161115 | 1.493166 |
| H | -3.164594 | 2.290086 | 0.247950 |

Rotational constants (GHz): 3.7361400 0.7662300 0.7115200

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 30.5426 | 78.5368 | 84.5925 |
| 115.6014 | 124.5860 | 241.1642 |
| 252.3460 | 286.4365 | 311.5375 |
| 329.7950 | 439.0654 | 531.2509 |
| 654.1245 | 736.5687 | 780.5908 |
| 791.1836 | 860.7260 | 874.0491 |
| 920.9347 | 974.5045 | 1006.1742 |
| 1025.5589 | 1062.7235 | 1079.4329 |
| 1087.4982 | 1110.7870 | 1132.8126 |
| 1163.8464 | 1216.7914 | 1250.1114 |
| 1292.0836 | 1307.5080 | 1324.8334 |
| 1343.7359 | 1349.5704 | 1366.6266 |
| 1386.9054 | 1391.5571 | 1394.0794 |
| 1408.5743 | 1429.7119 | 1495.8309 |
| 1498.6400 | 1503.2248 | 1503.9094 |
| 1513.5907 | 1517.2738 | 1522.7319 |
| 2883.0411 | 2926.3309 | 3017.1523 |
| 3021.4518 | 3023.8863 | 3036.7680 |
| 3041.3854 | 3044.7742 | 3049.3751 |
| 3060.6250 | 3067.4737 | 3078.2138 |
| 3090.5947 | 3108.1940 | 3116.7688 |

Zero-point correction (Hartree): 0.208840

C7H15O.tptpp

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.94996186

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -3.718410 | 0.761551 | 0.223519 |
| C | -2.369115 | 0.653110 | 0.028172 |
| C | -1.882575 | -0.748521 | -0.371185 |
| C | -0.363829 | -0.838282 | -0.585941 |
| C | 0.467797 | -0.648293 | 0.692317 |
| C | 1.974500 | -0.905856 | 0.512818 |
| C | 2.708190 | 0.037530 | -0.457118 |
| C | 2.695246 | 1.511952 | -0.036819 |
| H | -1.998875 | 1.429027 | -0.671970 |
| H | -1.933763 | 0.944385 | 1.009528 |
| H | -2.204861 | -1.460884 | 0.398222 |
| H | -2.401721 | -1.029003 | -1.295543 |
| H | -0.129861 | -1.820679 | -1.016955 |
| H | -0.063714 | -0.100820 | -1.342905 |
| H | 0.317180 | 0.362568 | 1.093680 |
| H | 0.089048 | -1.334277 | 1.462342 |
| H | 2.458798 | -0.842245 | 1.496855 |
| H | 2.115063 | -1.940868 | 0.172149 |
| H | 3.749136 | -0.300031 | -0.539635 |
| H | 2.284362 | -0.059311 | -1.464838 |
| H | 3.116193 | 1.640906 | 0.967276 |
| H | 1.681366 | 1.925934 | -0.024227 |
| H | 3.287651 | 2.123057 | -0.725595 |

Rotational constants (GHz): 3.8122500 0.7629100 0.6947300

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 36.3496 | 50.2476 | 92.1819 |
| 113.9880 | 159.9392 | 237.1873 |
| 250.4474 | 256.7170 | 315.5667 |
| 364.9437 | 451.0315 | 544.6650 |
| 659.4216 | 727.2810 | 778.1037 |
| 811.7769 | 837.2887 | 880.2705 |
| 926.1447 | 970.8079 | 1002.8520 |
| 1018.6269 | 1059.5919 | 1083.9338 |
| 1087.6951 | 1102.2060 | 1129.7604 |
| 1170.5845 | 1202.1345 | 1252.6218 |
| 1286.1627 | 1306.2902 | 1325.8983 |
| 1341.9988 | 1348.8363 | 1367.7764 |
| 1385.9726 | 1388.1278 | 1398.9230 |
| 1413.9227 | 1428.6662 | 1491.9675 |
| 1501.3572 | 1504.5629 | 1505.6858 |
| 1509.7107 | 1517.9702 | 1524.2642 |
| 2885.9073 | 2927.3950 | 3018.3794 |
| 3023.5630 | 3029.7566 | 3036.8138 |
| 3040.8862 | 3042.7230 | 3050.4015 |
| 3057.9898 | 3070.8984 | 3074.8383 |
| 3090.1024 | 3108.6200 | 3113.2761 |

Zero-point correction (Hartree): 0.208894

C7H15O.tptpt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.95122271

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 3.994671 | -0.605590 | 0.240546 |
| C | 2.635510 | -0.633318 | 0.090427 |
| C | 2.022215 | 0.645620 | -0.500097 |
| C | 0.494999 | 0.583796 | -0.655923 |
| C | -0.276215 | 0.553423 | 0.673294 |
| C | -1.804990 | 0.626674 | 0.524401 |
| C | -2.447193 | -0.594176 | -0.149862 |
| C | -3.976128 | -0.508398 | -0.203370 |
| H | 2.309026 | -1.536421 | -0.463653 |
| H | 2.256700 | -0.799018 | 1.123170 |
| H | 2.311132 | 1.494182 | 0.132111 |
| H | 2.484735 | 0.813235 | -1.480231 |
| H | 0.167312 | 1.458613 | -1.232974 |
| H | 0.231676 | -0.292151 | -1.264135 |
| H | -0.021246 | -0.355022 | 1.237677 |
| H | 0.059613 | 1.397484 | 1.291191 |
| H | -2.249281 | 0.749960 | 1.521436 |
| H | -2.070584 | 1.533233 | -0.038398 |
| H | -2.056668 | -0.708153 | -1.168871 |
| H | -2.150215 | -1.502218 | 0.393408 |
| H | -4.303877 | 0.373168 | -0.766199 |
| H | -4.403953 | -0.433669 | 0.803011 |
| H | -4.410931 | -1.390224 | -0.685132 |

Rotational constants (GHz): 5.7401700 0.6135000 0.5994200

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 35.0523 | 73.5973 | 86.0128 |
| 116.1054 | 126.2111 | 235.3762 |
| 248.1745 | 267.5023 | 288.1586 |
| 308.0495 | 441.3849 | 560.3012 |
| 659.1007 | 739.0797 | 761.7863 |
| 820.5650 | 841.7977 | 885.1010 |
| 923.0055 | 980.1866 | 1015.7342 |
| 1028.0650 | 1053.8461 | 1082.3764 |
| 1089.1877 | 1096.0207 | 1134.8132 |
| 1170.8135 | 1220.9669 | 1258.2928 |
| 1297.7925 | 1305.4071 | 1329.6045 |
| 1334.9610 | 1348.5725 | 1358.7711 |
| 1369.0278 | 1388.6353 | 1410.0121 |
| 1414.8230 | 1426.4988 | 1495.0336 |
| 1498.3632 | 1501.9369 | 1508.1648 |
| 1512.1978 | 1512.4980 | 1524.0815 |
| 2886.9220 | 2927.9621 | 3013.2886 |
| 3016.5997 | 3026.9257 | 3028.8040 |
| 3038.7603 | 3042.2505 | 3047.6615 |
| 3048.8810 | 3071.7091 | 3072.2692 |
| 3090.1571 | 3107.0680 | 3112.9286 |

Zero-point correction (Hartree): 0.208715

C7H15O.tpttm

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.95125061

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|----------|-----------|-----------|
| O | 3.754896 | 1.037646 | -0.171052 |
| C | 2.527537 | 0.628824 | 0.273084 |
| C | 2.074779 | -0.744258 | -0.246524 |

| | | | |
|---|-----------|-----------|-----------|
| C | 0.695347 | -1.179047 | 0.271487 |
| C | -0.479460 | -0.339478 | -0.251939 |
| C | -1.842216 | -0.844705 | 0.243267 |
| C | -3.053983 | -0.079565 | -0.314128 |
| C | -3.144395 | 1.384467 | 0.133194 |
| H | 2.456740 | 0.691258 | 1.377712 |
| H | 1.836870 | 1.423352 | -0.086648 |
| H | 2.084751 | -0.722425 | -1.343142 |
| H | 2.829414 | -1.479058 | 0.058783 |
| H | 0.532747 | -2.228298 | -0.006724 |
| H | 0.695259 | -1.158804 | 1.371161 |
| H | -0.348361 | 0.709097 | 0.045010 |
| H | -0.467391 | -0.348525 | -1.351579 |
| H | -1.940976 | -1.905627 | -0.024220 |
| H | -1.864699 | -0.806519 | 1.342029 |
| H | -3.035763 | -0.126162 | -1.411734 |
| H | -3.968152 | -0.602234 | -0.005172 |
| H | -2.296922 | 1.976613 | -0.227168 |
| H | -3.161983 | 1.462600 | 1.226664 |
| H | -4.056350 | 1.856133 | -0.247206 |

Rotational constants (GHz): 4.0971700 0.6836900 0.6125700

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 46.6999 | 66.6595 | 83.9446 |
| 113.5467 | 138.5652 | 176.9600 |
| 248.2303 | 276.6405 | 299.4397 |
| 346.6339 | 454.9143 | 515.5435 |
| 658.9361 | 735.2146 | 771.1546 |
| 811.1128 | 864.4296 | 884.6135 |
| 926.9769 | 979.1135 | 1001.3005 |
| 1019.4159 | 1069.7996 | 1085.0808 |
| 1088.2652 | 1090.0609 | 1128.3019 |
| 1185.3842 | 1213.7385 | 1259.6284 |
| 1280.4701 | 1313.8396 | 1323.6173 |
| 1337.6531 | 1346.0527 | 1367.4448 |
| 1384.8234 | 1389.1484 | 1391.2820 |
| 1414.9581 | 1429.8785 | 1495.5525 |
| 1497.4641 | 1501.7138 | 1503.5731 |
| 1515.1779 | 1518.8976 | 1521.6108 |
| 2887.4866 | 2928.3549 | 3013.4401 |
| 3014.9565 | 3024.9989 | 3026.3448 |
| 3040.9463 | 3042.3470 | 3046.6245 |
| 3056.8058 | 3063.3627 | 3077.3359 |
| 3089.9742 | 3109.0120 | 3116.4565 |

Zero-point correction (Hartree): 0.208707

C7H15O.tpptp

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.95125954

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 3.848634 | -0.956252 | -0.098703 |
| C | 2.660417 | -0.375476 | -0.447672 |
| C | 2.011478 | 0.483020 | 0.648283 |
| C | 0.679032 | 1.121430 | 0.227619 |
| C | -0.468729 | 0.123544 | 0.012117 |
| C | -1.797218 | 0.806758 | -0.342128 |
| C | -2.961718 | -0.158541 | -0.620184 |
| C | -3.412755 | -0.977086 | 0.595585 |
| H | 2.749261 | 0.180277 | -1.402981 |
| H | 2.005887 | -1.239156 | -0.699419 |
| H | 1.875372 | -0.137818 | 1.542345 |
| H | 2.726076 | 1.269390 | 0.919624 |
| H | 0.379292 | 1.843716 | 0.997813 |
| H | 0.828683 | 1.708672 | -0.690229 |
| H | -0.210898 | -0.581842 | -0.790829 |
| H | -0.587590 | -0.480318 | 0.921294 |
| H | -2.079908 | 1.489399 | 0.472257 |
| H | -1.642877 | 1.439017 | -1.227165 |
| H | -3.814688 | 0.421900 | -0.994108 |
| H | -2.679102 | -0.839072 | -1.435313 |
| H | -3.705937 | -0.322154 | 1.424478 |
| H | -2.620732 | -1.638595 | 0.961265 |
| H | -4.274944 | -1.605288 | 0.348874 |

Rotational constants (GHz): 4.6086800 0.6407800 0.6102500

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 39.4926 | 77.1738 | 83.4644 |
| 113.2119 | 131.2193 | 183.1713 |
| 263.0959 | 269.1253 | 300.4802 |
| 347.8423 | 458.0627 | 515.0941 |
| 653.5816 | 736.5188 | 765.0481 |
| 822.1472 | 863.7423 | 877.4636 |
| 925.9926 | 985.0559 | 995.1247 |
| 1019.5432 | 1071.6847 | 1077.4396 |
| 1087.8463 | 1092.6364 | 1134.4350 |
| 1173.6180 | 1216.1904 | 1258.7646 |

| | | |
|-----------|-----------|-----------|
| 1289.4439 | 1301.8081 | 1331.0396 |
| 1334.8038 | 1345.8215 | 1368.2951 |
| 1386.0994 | 1389.5460 | 1391.1288 |
| 1414.8220 | 1429.0024 | 1495.8022 |
| 1498.1872 | 1502.5209 | 1504.7844 |
| 1514.5970 | 1519.4197 | 1522.6024 |
| 2886.3113 | 2926.9970 | 3013.7314 |
| 3016.4242 | 3023.4856 | 3025.9198 |
| 3041.3583 | 3043.3193 | 3047.0920 |
| 3058.2043 | 3063.3825 | 3077.6496 |
| 3089.8743 | 3109.0966 | 3116.8571 |

Zero-point correction (Hartree): 0.208720

C7H15O.tpttt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.95255829

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -4.054787 | -0.805794 | -0.054364 |
| C | -2.782220 | -0.507277 | 0.348623 |
| C | -2.167449 | 0.734785 | -0.314071 |
| C | -0.739177 | 1.046611 | 0.158400 |
| C | 0.315658 | 0.012906 | -0.262480 |
| C | 1.740619 | 0.397660 | 0.156358 |
| C | 2.800815 | -0.631556 | -0.255775 |
| C | 4.221034 | -0.235726 | 0.160711 |
| H | -2.709875 | -0.458963 | 1.453848 |
| H | -2.198384 | -1.415091 | 0.079389 |
| H | -2.190908 | 0.596766 | -1.401983 |
| H | -2.821237 | 1.586857 | -0.092417 |
| H | -0.448478 | 2.028982 | -0.235664 |
| H | -0.730655 | 1.150132 | 1.253319 |
| H | 0.075028 | -0.970079 | 0.166253 |
| H | 0.279513 | -0.115613 | -1.353825 |
| H | 1.993988 | 1.374651 | -0.279605 |
| H | 1.774174 | 0.535804 | 1.246666 |
| H | 2.548770 | -1.606371 | 0.183765 |
| H | 2.764030 | -0.772122 | -1.344705 |
| H | 4.297976 | -0.121662 | 1.248097 |
| H | 4.515277 | 0.717972 | -0.292098 |
| H | 4.953388 | -0.989334 | -0.146721 |

Rotational constants (GHz): 6.5748000 0.5663100 0.5415400

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 43.5164 | 67.2636 | 81.8608 |
| 116.1340 | 130.4842 | 156.7759 |
| 244.5039 | 250.2835 | 299.9018 |
| 341.5689 | 427.4791 | 527.0762 |
| 661.1471 | 733.7645 | 753.2588 |
| 822.9744 | 866.0977 | 899.1562 |
| 923.9391 | 989.5223 | 1015.4578 |
| 1025.1624 | 1066.3350 | 1074.0285 |
| 1087.1474 | 1091.9299 | 1131.9224 |
| 1182.7264 | 1230.8722 | 1256.5260 |
| 1280.5471 | 1304.6599 | 1326.4956 |
| 1335.6438 | 1345.5117 | 1352.6902 |
| 1368.1031 | 1389.6100 | 1401.8655 |
| 1414.6070 | 1426.3561 | 1495.1304 |
| 1498.4953 | 1501.8146 | 1505.3382 |
| 1512.6098 | 1516.2375 | 1525.5860 |
| 2888.7717 | 2928.5960 | 3011.1554 |
| 3013.3698 | 3020.7944 | 3027.4688 |
| 3035.3643 | 3039.2937 | 3042.3486 |
| 3048.1876 | 3062.4714 | 3074.8631 |
| 3090.0492 | 3107.0767 | 3113.0164 |

Zero-point correction (Hartree): 0.208459

C7H15O.ttpmm

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.94714553

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -3.412402 | 1.080134 | 0.032831 |
| C | -2.671275 | -0.054454 | 0.223552 |
| C | -1.226670 | 0.003548 | -0.287521 |
| C | -0.452106 | -1.290775 | -0.000262 |
| C | 0.991512 | -1.338006 | -0.546979 |
| C | 2.091160 | -0.793704 | 0.385896 |
| C | 2.071229 | 0.709397 | 0.713912 |
| C | 2.250517 | 1.627776 | -0.499960 |
| H | -2.682402 | -0.219230 | 1.324579 |
| H | -3.213012 | -0.937567 | -0.172449 |
| H | -1.252021 | 0.185183 | -1.369768 |
| H | -0.739498 | 0.873475 | 0.163805 |
| H | -0.436379 | -1.479967 | 1.083348 |
| H | -1.017375 | -2.125534 | -0.437329 |

| | | | |
|--|-----------|-----------|-----------|
| H | 1.243215 | -2.384903 | -0.757453 |
| H | 1.029177 | -0.826870 | -1.517963 |
| H | 2.051604 | -1.357790 | 1.328111 |
| H | 3.064361 | -1.032967 | -0.065215 |
| H | 1.143754 | 0.968111 | 1.240071 |
| H | 2.879208 | 0.908005 | 1.430092 |
| H | 1.425451 | 1.532798 | -1.213384 |
| H | 3.178307 | 1.395181 | -1.035925 |
| H | 2.298618 | 2.678300 | -0.194997 |
| Rotational constants (GHz): | 3.0001700 | 0.8940700 | 0.7548000 |
| Vibrational harmonic frequencies (cm-1): | | | |
| 49.7917 | 64.0093 | | 74.6538 |
| 132.4074 | 155.7093 | | 188.2783 |
| 247.8698 | 258.6690 | | 340.9355 |
| 405.3550 | 430.2519 | | 485.3827 |
| 517.1548 | 740.6833 | | 749.4228 |
| 785.2984 | 862.2798 | | 896.0149 |
| 912.6223 | 972.8544 | | 996.6979 |
| 1029.2757 | 1051.6714 | | 1076.3577 |
| 1087.5611 | 1107.6923 | | 1132.2873 |
| 1183.7526 | 1229.8075 | | 1253.3965 |
| 1283.1357 | 1299.8451 | | 1328.4594 |
| 1334.5319 | 1368.2168 | | 1374.2723 |
| 1380.8364 | 1400.4384 | | 1402.6090 |
| 1405.5517 | 1430.6236 | | 1493.4026 |
| 1497.4025 | 1503.4393 | | 1507.3183 |
| 1513.5892 | 1517.3467 | | 1525.2341 |
| 2878.1329 | 2921.7433 | | 3011.2193 |
| 3016.1848 | 3028.5569 | | 3035.5409 |
| 3041.7774 | 3043.8284 | | 3050.4827 |
| 3054.9353 | 3067.8221 | | 3071.4355 |
| 3107.8002 | 3110.2605 | | 3116.6035 |
| Zero-point correction (Hartree): | 0.208545 | | |

C7H15O.ttpmp

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.94416479
Electronic state : 2-A
Cartesian coordinates (Angs):

| | | | |
|--|-----------|-----------|-----------|
| O | -3.418141 | 0.782139 | -0.402219 |
| C | -2.507036 | 0.089815 | 0.348787 |
| C | -1.211758 | -0.300575 | -0.372086 |
| C | -0.283660 | -1.153152 | 0.504917 |
| C | 1.048191 | -1.562094 | -0.163049 |
| C | 2.263476 | -0.634037 | 0.033324 |
| C | 2.175238 | 0.799267 | -0.536428 |
| C | 1.632515 | 1.851612 | 0.440000 |
| H | -2.304645 | 0.632056 | 1.295055 |
| H | -3.047879 | -0.821960 | 0.688824 |
| H | -1.476419 | -0.853455 | -1.281826 |
| H | 0.616968 | 1.625994 | 0.778792 |
| H | -0.076769 | -0.634052 | 1.451450 |
| H | -0.830244 | -2.064863 | 0.783176 |
| H | 1.337557 | -2.547406 | 0.223656 |
| H | 0.877384 | -1.707087 | -1.239041 |
| H | 2.501728 | -0.577524 | 1.105175 |
| H | 3.119933 | -1.138971 | -0.431401 |
| H | 3.181036 | 1.114472 | -0.841316 |
| H | 1.577197 | 0.795343 | -1.457434 |
| H | 2.266707 | 1.914224 | 1.331752 |
| H | -0.711163 | 0.616248 | -0.700683 |
| H | 1.611936 | 2.844846 | -0.021219 |
| Rotational constants (GHz): | 2.9010000 | 0.9504200 | 0.7826900 |
| Vibrational harmonic frequencies (cm-1): | | | |
| 60.4920 | 76.1648 | | 95.4551 |
| 134.5794 | 161.9269 | | 184.1073 |
| 222.2416 | 277.3473 | | 333.8874 |
| 382.7897 | 424.9302 | | 461.7167 |
| 488.7154 | 737.1320 | | 760.7102 |
| 797.9649 | 845.6765 | | 904.1705 |
| 914.5049 | 971.8223 | | 1006.5929 |
| 1032.3246 | 1060.4770 | | 1067.9806 |
| 1088.1890 | 1123.7718 | | 1136.0769 |
| 1172.2876 | 1229.4198 | | 1273.5303 |
| 1279.4257 | 1308.4242 | | 1317.9353 |
| 1333.5415 | 1365.6550 | | 1379.9911 |
| 1383.5602 | 1397.2071 | | 1402.0580 |
| 1406.9554 | 1429.9630 | | 1495.1488 |
| 1501.0529 | 1504.1538 | | 1505.5026 |
| 1512.8060 | 1517.6064 | | 1524.7343 |
| 2878.5941 | 2920.8495 | | 3015.9561 |
| 3018.5396 | 3022.1791 | | 3030.9896 |
| 3044.6534 | 3047.4157 | | 3056.0124 |
| 3059.3029 | 3065.2652 | | 3067.4005 |
| 3106.1852 | 3108.9134 | | 3123.8395 |

Zero-point correction (Hartree): 0.208586

C7H15O.ttpmt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.94860029

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 3.378430 | -1.411267 | -0.061674 |
| C | 2.814687 | -0.186558 | 0.171596 |
| C | 1.328385 | -0.061815 | -0.186815 |
| C | 0.757959 | 1.314791 | 0.176737 |
| C | -0.682036 | 1.599160 | -0.287499 |
| C | -1.786152 | 0.716908 | 0.334928 |
| C | -2.117284 | -0.570157 | -0.436761 |
| C | -3.240695 | -1.381835 | 0.216515 |
| H | 2.960426 | -0.011689 | 1.261491 |
| H | 3.420016 | 0.613870 | -0.300275 |
| H | 1.215414 | -0.245055 | -1.263181 |
| H | 0.787988 | -0.862868 | 0.328694 |
| H | 0.810874 | 1.448636 | 1.267314 |
| H | 1.411168 | 2.089154 | -0.250775 |
| H | -0.896082 | 2.648404 | -0.049021 |
| H | -0.732869 | 1.527262 | -1.383133 |
| H | -1.513836 | 0.465400 | 1.370394 |
| H | -2.708674 | 1.308187 | 0.409091 |
| H | -2.408568 | -0.302197 | -1.461614 |
| H | -1.224519 | -1.198719 | -0.532417 |
| H | -4.161984 | -0.792810 | 0.294212 |
| H | -2.965280 | -1.696244 | 1.229848 |
| H | -3.470699 | -2.284161 | -0.359444 |

Rotational constants (GHz): 3.0589900 0.8008200 0.6676300

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 42.9211 | 81.4899 | 86.8804 |
| 110.1782 | 127.2750 | 182.8578 |
| 244.3548 | 255.6415 | 294.6953 |
| 399.7375 | 426.1090 | 484.2976 |
| 538.1518 | 734.9727 | 763.7294 |
| 798.1139 | 869.6405 | 891.8216 |
| 915.8833 | 978.7233 | 1009.7719 |
| 1037.2339 | 1055.8633 | 1063.6925 |
| 1088.4304 | 1099.5492 | 1135.7586 |
| 1193.8657 | 1240.9918 | 1248.4383 |
| 1282.5445 | 1310.4571 | 1326.7750 |
| 1339.3282 | 1342.6406 | 1369.9681 |
| 1378.3573 | 1391.4923 | 1405.0680 |
| 1413.4400 | 1427.8885 | 1493.0778 |
| 1502.2650 | 1503.0014 | 1508.6965 |
| 1512.1927 | 1513.1264 | 1525.1427 |
| 2876.9070 | 2924.0568 | 3008.1328 |
| 3014.8082 | 3021.3121 | 3032.6293 |
| 3038.2896 | 3041.1575 | 3044.6289 |
| 3053.8811 | 3065.8785 | 3081.8852 |
| 3099.3103 | 3108.4059 | 3112.7268 |

Zero-point correction (Hartree): 0.208385

C7H15O.ttpm

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.94710394

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -3.487590 | 0.771442 | -0.506991 |
| C | -2.589355 | 0.177833 | 0.337712 |
| C | -1.289356 | -0.310411 | -0.311991 |
| C | -0.309897 | -0.903864 | 0.708616 |
| C | 0.950222 | -1.536392 | 0.092510 |
| C | 1.883958 | -0.626374 | -0.729773 |
| C | 2.633203 | 0.476746 | 0.047820 |
| C | 1.872978 | 1.797239 | 0.231922 |
| H | -2.367076 | 0.951269 | 1.106991 |
| H | -3.085421 | -0.625249 | 0.920026 |
| H | -1.542180 | -1.064715 | -1.068598 |
| H | -0.838685 | 0.532217 | -0.847517 |
| H | -0.028741 | -0.134843 | 1.439939 |
| H | -0.829042 | -1.682352 | 1.285813 |
| H | 1.538165 | -1.993932 | 0.899856 |
| H | 0.631610 | -2.366337 | -0.553380 |
| H | 2.631055 | -1.282915 | -1.193612 |
| H | 1.333415 | -0.174240 | -1.565749 |
| H | 2.938236 | 0.084830 | 1.028130 |
| H | 3.566310 | 0.698978 | -0.485242 |
| H | 0.963353 | 1.678256 | 0.827475 |
| H | 1.580404 | 2.218367 | -0.736821 |
| H | 2.498792 | 2.540475 | 0.737725 |

Rotational constants (GHz): 3.1090400 0.8838300 0.7620200

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 44.2378 | 62.8572 | 81.3779 |
| 115.7956 | 149.9794 | 227.8071 |
| 232.5613 | 254.9680 | 349.7251 |
| 396.0424 | 418.3992 | 484.1810 |
| 499.4253 | 739.6990 | 751.9620 |
| 807.6651 | 822.3916 | 894.5716 |
| 924.6652 | 969.0428 | 1006.5929 |
| 1025.0901 | 1059.0230 | 1066.4741 |
| 1087.1377 | 1122.7202 | 1134.9628 |
| 1172.6811 | 1233.0521 | 1255.5226 |
| 1282.8875 | 1309.6881 | 1323.9496 |
| 1337.8297 | 1365.7511 | 1377.7445 |
| 1384.6004 | 1396.5786 | 1406.7332 |
| 1413.2194 | 1428.5072 | 1492.4864 |
| 1500.4261 | 1502.9147 | 1505.1455 |
| 1512.7941 | 1521.7665 | 1523.1032 |
| 2877.5302 | 2922.1121 | 3015.0864 |
| 3022.6029 | 3025.1075 | 3030.7756 |
| 3042.7090 | 3044.2411 | 3049.6448 |
| 3061.4668 | 3064.0534 | 3070.0941 |
| 3099.5963 | 3107.4732 | 3124.6318 |

Zero-point correction (Hartree): 0.208529

C7H15O.ttppp

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.94989885

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -3.762028 | -0.703357 | 0.376392 |
| C | -2.748536 | -0.280403 | -0.440009 |
| C | -1.497989 | 0.248226 | 0.272040 |
| C | -0.384566 | 0.635935 | -0.709503 |
| C | 0.841111 | 1.297527 | -0.056159 |
| C | 1.601857 | 0.434721 | 0.968279 |
| C | 2.190388 | -0.881796 | 0.431116 |
| C | 3.250567 | -0.702009 | -0.661819 |
| H | -2.491184 | -1.168611 | -1.059878 |
| H | -3.135571 | 0.445505 | -1.183976 |
| H | -1.785490 | 1.119262 | 0.875586 |
| H | -1.155502 | -0.519995 | 0.974602 |
| H | -0.072270 | -0.253502 | -1.274270 |
| H | -0.793228 | 1.331935 | -1.455551 |
| H | 1.529797 | 1.615408 | -0.848906 |
| H | 0.516598 | 2.220042 | 0.443821 |
| H | 2.418413 | 1.040118 | 1.385072 |
| H | 0.940435 | 0.206443 | 1.813699 |
| H | 2.635424 | -1.427239 | 1.273014 |
| H | 1.384472 | -1.525719 | 0.055305 |
| H | 4.076185 | -0.072242 | -0.310218 |
| H | 2.837270 | -0.231813 | -1.560252 |
| H | 3.673880 | -1.665942 | -0.962855 |

Rotational constants (GHz): 4.1221800 0.7258600 0.7021500

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 37.9298 | 69.1970 | 87.9417 |
| 122.4635 | 145.7632 | 203.4062 |
| 236.9503 | 273.4527 | 345.8812 |
| 408.3132 | 427.5086 | 491.0449 |
| 512.0839 | 720.2666 | 751.6157 |
| 797.5207 | 848.3210 | 894.2495 |
| 922.4010 | 966.7542 | 1002.5283 |
| 1026.2741 | 1047.9153 | 1067.2984 |
| 1086.6518 | 1107.9099 | 1139.8371 |
| 1174.1984 | 1228.3266 | 1253.0107 |
| 1281.2461 | 1303.9156 | 1321.1828 |
| 1341.3089 | 1366.2174 | 1375.2451 |
| 1380.6402 | 1394.9033 | 1404.9823 |
| 1413.9533 | 1428.4649 | 1489.8128 |
| 1498.6597 | 1505.7416 | 1506.8119 |
| 1514.7170 | 1517.0543 | 1524.5779 |
| 2878.4472 | 2922.4801 | 3017.7875 |
| 3023.0882 | 3030.2070 | 3036.3075 |
| 3040.7084 | 3040.9462 | 3051.1663 |
| 3058.8257 | 3066.8988 | 3075.6766 |
| 3093.7098 | 3108.9694 | 3113.5081 |

Zero-point correction (Hartree): 0.208510

C7H15O.ttppt

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.95110565

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|----------|-----------|-----------|
| O | 3.615865 | -1.147791 | -0.332582 |
| C | 2.799910 | -0.298218 | 0.363754 |
| C | 1.499244 | 0.102267 | -0.342515 |
| C | 0.611415 | 0.999343 | 0.529283 |

| | | | |
|--|-----------|-----------|-----------|
| C | -0.643940 | 1.536792 | -0.180731 |
| C | -1.664517 | 0.479502 | -0.636624 |
| C | -2.329066 | -0.306178 | 0.502550 |
| C | -3.386055 | -1.298064 | 0.005749 |
| H | 2.572662 | -0.834466 | 1.312550 |
| H | 3.372520 | 0.588821 | 0.703538 |
| H | 1.757825 | 0.623195 | -1.273818 |
| H | 0.972910 | -0.814153 | -0.632118 |
| H | 0.322803 | 0.453725 | 1.438173 |
| H | 1.203950 | 1.858302 | 0.874224 |
| H | -1.147417 | 2.246667 | 0.489451 |
| H | -0.326310 | 2.120110 | -1.055585 |
| H | -2.448243 | 0.986155 | -1.216111 |
| H | -1.189728 | -0.223856 | -1.334062 |
| H | -1.568864 | -0.850516 | 1.077512 |
| H | -2.791542 | 0.400953 | 1.205288 |
| H | -2.945663 | -2.041640 | -0.668472 |
| H | -4.182586 | -0.785311 | -0.545556 |
| H | -3.851173 | -1.838323 | 0.836837 |
| Rotational constants (GHz): | 3.5063300 | 0.7307600 | 0.6552600 |
| Vibrational harmonic frequencies (cm-1): | | | |
| 38.4449 | 67.3764 | | 78.3417 |
| 109.8503 | 152.3965 | | 193.3295 |
| 241.3853 | 267.5133 | | 291.0974 |
| 410.7248 | 433.5663 | | 501.3282 |
| 516.0538 | 721.8369 | | 758.6591 |
| 810.3737 | 844.4365 | | 907.2818 |
| 912.6188 | 975.6435 | | 1013.5133 |
| 1025.8536 | 1046.5724 | | 1071.9941 |
| 1087.2829 | 1100.6015 | | 1145.4151 |
| 1172.0086 | 1243.5915 | | 1254.5030 |
| 1280.9881 | 1308.6729 | | 1320.8642 |
| 1335.6185 | 1346.3644 | | 1367.9567 |
| 1382.3470 | 1396.8355 | | 1406.1288 |
| 1413.0557 | 1426.7431 | | 1493.9339 |
| 1498.8115 | 1502.6873 | | 1509.4114 |
| 1513.2340 | 1514.1226 | | 1524.0582 |
| 2878.7333 | 2922.3220 | | 3016.2793 |
| 3018.3802 | 3026.6778 | | 3029.0407 |
| 3039.1452 | 3041.9634 | | 3047.3822 |
| 3049.5740 | 3064.5019 | | 3072.1051 |
| 3095.5895 | 3107.2862 | | 3112.4312 |
| Zero-point correction (Hartree): | 0.208354 | | |

C7H15O.ttpm

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.95094867

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|--|-----------|-----------|-----------|
| O | 4.073915 | -0.721027 | -0.016981 |
| C | 3.115087 | 0.233459 | 0.188709 |
| C | 1.691349 | -0.155899 | -0.226347 |
| C | 0.666462 | 0.940400 | 0.093054 |
| C | -0.762873 | 0.647847 | -0.394700 |
| C | -1.440949 | -0.543489 | 0.297879 |
| C | -2.877578 | -0.820801 | -0.178315 |
| C | -3.890240 | 0.275311 | 0.174956 |
| H | 3.152270 | 0.444360 | 1.281195 |
| H | 3.428426 | 1.194564 | -0.267436 |
| H | 1.690354 | -0.365289 | -1.304157 |
| H | 1.436415 | -1.095246 | 0.276290 |
| H | 0.648010 | 1.117033 | 1.178672 |
| H | 1.004085 | 1.883524 | -0.359066 |
| H | -1.367674 | 1.550227 | -0.243525 |
| H | -0.744573 | 0.472240 | -1.480041 |
| H | -0.841968 | -1.448182 | 0.135926 |
| H | -1.447941 | -0.372935 | 1.384607 |
| H | -2.872615 | -0.977887 | -1.265819 |
| H | -3.213973 | -1.768459 | 0.261142 |
| H | -3.649138 | 1.228559 | -0.306411 |
| H | -3.920890 | 0.449363 | 1.257048 |
| H | -4.899652 | -0.004628 | -0.143990 |
| Rotational constants (GHz): | 6.8870600 | 0.5902500 | 0.5649100 |
| Vibrational harmonic frequencies (cm-1): | | | |
| 31.1420 | 69.3093 | | 74.2679 |
| 117.7933 | 132.8628 | | 198.4953 |
| 210.4262 | 266.4858 | | 283.5320 |
| 393.8830 | 437.2967 | | 503.2142 |
| 518.3092 | 735.2117 | | 751.0369 |
| 791.2182 | 865.6940 | | 897.4727 |
| 918.7839 | 972.1197 | | 1004.3290 |
| 1022.5962 | 1061.5020 | | 1072.6947 |
| 1085.8963 | 1094.4837 | | 1132.5269 |
| 1196.3140 | 1231.7070 | | 1251.6805 |
| 1291.5485 | 1296.5312 | | 1323.5587 |

| | | |
|-----------|-----------|-----------|
| 1338.8385 | 1355.1448 | 1368.0304 |
| 1380.9211 | 1386.6739 | 1405.4501 |
| 1413.6342 | 1429.0125 | 1494.4897 |
| 1497.0123 | 1501.4418 | 1510.8200 |
| 1512.9559 | 1516.7443 | 1520.8006 |
| 2878.5855 | 2922.8237 | 3010.5474 |
| 3014.4660 | 3022.4012 | 3027.1233 |
| 3040.5672 | 3041.2798 | 3048.3943 |
| 3058.2786 | 3062.5690 | 3080.0673 |
| 3096.8215 | 3107.9588 | 3115.5885 |

Zero-point correction (Hartree): 0.208209

C7H15O.ttpptp

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.95110686

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 3.877390 | -1.009248 | 0.152484 |
| C | 3.068423 | 0.083057 | -0.005885 |
| C | 1.568367 | -0.212861 | -0.120299 |
| C | 0.724245 | 1.064165 | -0.225134 |
| C | -0.777689 | 0.820930 | -0.448476 |
| C | -1.494664 | 0.148416 | 0.732045 |
| C | -3.017029 | 0.018503 | 0.555541 |
| C | -3.446940 | -0.932956 | -0.567739 |
| H | 3.267049 | 0.716819 | 0.887624 |

| | | | |
|---|-----------|-----------|-----------|
| H | 3.430067 | 0.708160 | -0.847572 |
| H | 1.405758 | -0.840898 | -1.006016 |
| H | 1.273351 | -0.812412 | 0.748017 |
| H | 0.861831 | 1.667928 | 0.683972 |
| H | 1.107526 | 1.675753 | -1.054007 |
| H | -1.262977 | 1.785969 | -0.649158 |
| H | -0.907663 | 0.220238 | -1.358282 |
| H | -1.071195 | -0.849422 | 0.908759 |
| H | -1.292344 | 0.730769 | 1.641865 |
| H | -3.450628 | -0.330384 | 1.501415 |
| H | -3.445189 | 1.014335 | 0.375331 |
| H | -3.038410 | -1.938071 | -0.410221 |
| H | -3.107173 | -0.588338 | -1.549839 |
| H | -4.537399 | -1.021997 | -0.612070 |

Rotational constants (GHz): 4.9840700 0.6277300 0.6019400

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 41.5634 | 70.5122 | 80.0271 |
| 125.9868 | 132.1192 | 207.0233 |
| 216.8077 | 272.0576 | 296.0464 |
| 386.7723 | 438.1285 | 511.9665 |
| 526.2402 | 738.4056 | 767.0865 |
| 786.3289 | 857.7100 | 905.2282 |
| 913.2470 | 981.4208 | 1001.1469 |
| 1020.6865 | 1064.4845 | 1070.8130 |
| 1088.3163 | 1096.3982 | 1144.9363 |
| 1179.2264 | 1241.1879 | 1251.8825 |
| 1289.3595 | 1303.6880 | 1326.3520 |
| 1335.3037 | 1355.5894 | 1368.5061 |
| 1381.9653 | 1385.7211 | 1406.5896 |
| 1413.5978 | 1429.6823 | 1495.3214 |
| 1498.2179 | 1503.3104 | 1512.1431 |
| 1513.2536 | 1517.8685 | 1522.8005 |
| 2878.0097 | 2923.1609 | 3010.0764 |
| 3018.2293 | 3025.7282 | 3026.4686 |
| 3041.7330 | 3042.2414 | 3046.4755 |
| 3051.0546 | 3061.7235 | 3076.4618 |
| 3096.0032 | 3108.8307 | 3117.3811 |

Zero-point correction (Hartree): 0.208445

C7H15O.ttpptt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.95244049

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 3.889625 | -1.124828 | -0.189358 |
| C | 3.113487 | -0.073438 | 0.216666 |
| C | 1.654925 | -0.104166 | -0.254639 |
| C | 0.835727 | 1.071835 | 0.292645 |
| C | -0.607691 | 1.146327 | -0.231734 |
| C | -1.510712 | -0.016981 | 0.201692 |
| C | -2.961103 | 0.133457 | -0.275829 |
| C | -3.863286 | -1.026188 | 0.158031 |
| H | 3.158757 | -0.097742 | 1.328803 |
| H | 3.607838 | 0.886419 | -0.037233 |
| H | 1.645905 | -0.086687 | -1.352421 |
| H | 1.219496 | -1.062803 | 0.047776 |
| H | 0.818365 | 1.023949 | 1.391453 |
| H | 1.349098 | 2.010313 | 0.040412 |

| | | | |
|--|-----------|-----------|-----------|
| H | -1.056312 | 2.087883 | 0.112675 |
| H | -0.590356 | 1.203470 | -1.329455 |
| H | -1.108907 | -0.966746 | -0.175786 |
| H | -1.497317 | -0.095742 | 1.298737 |
| H | -3.370723 | 1.079198 | 0.104565 |
| H | -2.973851 | 0.217273 | -1.371143 |
| H | -3.897010 | -1.114969 | 1.250008 |
| H | -3.499710 | -1.981048 | -0.238659 |
| H | -4.890354 | -0.889216 | -0.195853 |
| Rotational constants (GHz): | 4.9749600 | 0.6017200 | 0.5580700 |
| Vibrational harmonic frequencies (cm-1): | | | |
| 57.8564 | 65.3288 | | 74.0021 |
| 117.2665 | 125.7759 | | 191.1808 |
| 212.0949 | 250.9653 | | 283.7342 |
| 394.2171 | 429.9547 | | 490.3090 |
| 503.9010 | 735.0165 | | 754.2777 |
| 793.5031 | 877.0036 | | 908.9809 |
| 920.6500 | 978.9453 | | 1014.5789 |
| 1020.2384 | 1057.8415 | | 1076.8411 |
| 1087.8872 | 1089.8021 | | 1141.2280 |
| 1195.9776 | 1248.1744 | | 1252.8991 |
| 1290.3183 | 1297.5190 | | 1326.9850 |
| 1335.2914 | 1339.4037 | | 1368.1305 |
| 1381.7992 | 1385.1697 | | 1408.5734 |
| 1416.0544 | 1427.5306 | | 1495.6441 |
| 1499.2417 | 1502.2667 | | 1512.5168 |
| 1513.5177 | 1514.0895 | | 1525.9196 |
| 2878.4788 | 2921.6864 | | 3010.4736 |
| 3014.8966 | 3018.5661 | | 3027.4758 |
| 3038.8180 | 3041.5389 | | 3044.3900 |
| 3047.7300 | 3055.3062 | | 3075.8949 |
| 3097.1245 | 3106.8018 | | 3112.5541 |
| Zero-point correction (Hartree): | 0.208184 | | |

C7H15O.tttpm

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.94848787
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | |
|--|-----------|-----------|-----------|
| O | 4.067244 | 0.359665 | -0.250384 |
| C | 2.836906 | 0.423782 | 0.345870 |
| C | 1.727313 | -0.389049 | -0.330271 |
| C | 0.366899 | -0.226312 | 0.357901 |
| C | -0.738416 | -1.079382 | -0.284452 |
| C | -2.129122 | -0.961935 | 0.378146 |
| C | -3.069243 | 0.106758 | -0.208351 |
| C | -2.601891 | 1.560404 | -0.071383 |
| H | 2.926282 | 0.179423 | 1.424108 |
| H | 2.574878 | 1.505577 | 0.351339 |
| H | 1.664091 | -0.081417 | -1.381430 |
| H | 2.024105 | -1.445887 | -0.331585 |
| H | 0.457422 | -0.506514 | 1.417575 |
| H | 0.081195 | 0.833090 | 0.351469 |
| H | -0.819374 | -0.831216 | -1.352342 |
| H | -0.414069 | -2.127695 | -0.248804 |
| H | -2.639813 | -1.929053 | 0.291432 |
| H | -2.004719 | -0.787311 | 1.456504 |
| H | -3.239392 | -0.117684 | -1.270395 |
| H | -4.047187 | 0.003943 | 0.279853 |
| H | -1.695329 | 1.755206 | -0.653242 |
| H | -2.389208 | 1.814288 | 0.973690 |
| H | -3.371514 | 2.252333 | -0.429863 |
| Rotational constants (GHz): | 4.5980200 | 0.6678700 | 0.6147800 |
| Vibrational harmonic frequencies (cm-1): | | | |
| 44.3520 | 56.5188 | | 90.4218 |
| 120.1028 | 131.7880 | | 154.1296 |
| 260.1475 | 298.8686 | | 303.0558 |
| 354.2966 | 405.4777 | | 456.3329 |
| 518.4864 | 730.5671 | | 772.1903 |
| 787.2814 | 836.8937 | | 883.6130 |
| 956.0434 | 970.5531 | | 1012.9056 |
| 1038.0044 | 1054.4499 | | 1063.7142 |
| 1087.5262 | 1107.4382 | | 1132.1356 |
| 1188.5185 | 1236.6746 | | 1264.0293 |
| 1278.1871 | 1310.4093 | | 1321.6202 |
| 1340.2408 | 1351.2991 | | 1372.4386 |
| 1388.6366 | 1392.6385 | | 1397.7810 |
| 1410.9021 | 1428.7778 | | 1495.7291 |
| 1498.9521 | 1501.6554 | | 1504.6010 |
| 1516.8501 | 1519.5385 | | 1524.3177 |
| 2881.0401 | 2921.5794 | | 3015.4280 |
| 3020.0885 | 3022.8603 | | 3024.5533 |
| 3040.1844 | 3040.4242 | | 3050.2206 |

3059.9774 3066.1151 3069.6996
3090.3737 3107.2389 3115.7704
Zero-point correction (Hartree): 0.208217

C7H15O.tttpp

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.95110670

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 4.115949 | 0.416306 | -0.159002 |
| C | 2.879012 | 0.375964 | 0.425577 |
| C | 1.757578 | -0.220171 | -0.432255 |
| C | 0.414410 | -0.284215 | 0.304497 |
| C | -0.717619 | -0.864985 | -0.554724 |
| C | -2.056319 | -1.035287 | 0.184869 |
| C | -2.729606 | 0.262549 | 0.666163 |
| C | -3.143970 | 1.214861 | -0.461650 |
| H | 3.016165 | -0.223427 | 1.353328 |
| H | 2.611320 | 1.381035 | 0.811127 |
| H | 1.658835 | 0.385706 | -1.342158 |
| H | 2.064241 | -1.222392 | -0.756351 |
| H | 0.524731 | -0.894074 | 1.213532 |
| H | 0.143089 | 0.723338 | 0.648198 |
| H | -0.856696 | -0.235233 | -1.443339 |
| H | -0.403105 | -1.847135 | -0.932267 |
| H | -2.754920 | -1.567446 | -0.475229 |
| H | -1.897934 | -1.693176 | 1.050536 |
| H | -3.619899 | -0.008907 | 1.247687 |
| H | -2.068324 | 0.789985 | 1.365706 |
| H | -3.813996 | 0.717001 | -1.172353 |
| H | -2.280764 | 1.583121 | -1.025889 |
| H | -3.671247 | 2.088872 | -0.065376 |

Rotational constants (GHz): 4.8994700 0.6356900 0.6101300

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 44.0105 | 55.8265 | 92.7365 |
| 112.7266 | 134.1890 | 180.3489 |
| 244.9150 | 273.1749 | 348.2779 |
| 358.9851 | 408.9066 | 459.0419 |
| 532.9032 | 728.9631 | 757.3784 |
| 800.4812 | 853.2525 | 865.3266 |
| 955.5585 | 976.6585 | 1006.9534 |
| 1032.7872 | 1050.6278 | 1056.8784 |
| 1087.8011 | 1102.8026 | 1144.3522 |
| 1175.9585 | 1242.6546 | 1249.1763 |
| 1286.7463 | 1300.2681 | 1325.9587 |
| 1338.6769 | 1350.1040 | 1370.6799 |
| 1385.0414 | 1396.9654 | 1399.1605 |
| 1414.7673 | 1430.9840 | 1494.0048 |
| 1498.9140 | 1504.5100 | 1505.9993 |
| 1515.9383 | 1519.5143 | 1527.6454 |
| 2880.5942 | 2920.5370 | 3010.6055 |
| 3019.3498 | 3028.3518 | 3035.1982 |
| 3040.8835 | 3042.6586 | 3044.9546 |
| 3055.2106 | 3068.4154 | 3071.8398 |
| 3088.7730 | 3109.7469 | 3116.2388 |

Zero-point correction (Hartree): 0.208299

C7H15O.tttpt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.95232766

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -4.284565 | -0.328762 | -0.155372 |
| C | -2.997511 | -0.612839 | 0.213626 |
| C | -1.947433 | 0.433058 | -0.176317 |
| C | -0.524765 | 0.025470 | 0.225257 |
| C | 0.530402 | 1.077688 | -0.144997 |
| C | 1.960517 | 0.742666 | 0.309591 |
| C | 2.588017 | -0.479336 | -0.375949 |
| C | 4.037645 | -0.724626 | 0.056008 |
| H | -2.960114 | -0.847942 | 1.297112 |
| H | -2.766962 | -1.590506 | -0.265806 |
| H | -2.006959 | 0.597312 | -1.259393 |
| H | -2.213755 | 1.385680 | 0.299291 |
| H | -0.487772 | -0.154139 | 1.309990 |
| H | -0.278745 | -0.934127 | -0.249117 |
| H | 0.521600 | 1.230239 | -1.233650 |
| H | 0.235749 | 2.039119 | 0.296669 |
| H | 2.600811 | 1.615578 | 0.123077 |
| H | 1.968655 | 0.590817 | 1.398749 |
| H | 1.992562 | -1.375863 | -0.162162 |
| H | 2.548698 | -0.340407 | -1.465339 |
| H | 4.105208 | -0.895851 | 1.136558 |
| H | 4.672431 | 0.137089 | -0.180375 |
| H | 4.463886 | -1.599398 | -0.445932 |

Rotational constants (GHz): 6.6222700 0.5623800 0.5378000
 Vibrational harmonic frequencies (cm-1):
 54.2283 69.0978 72.6773
 112.2640 135.0603 167.3469
 241.3418 263.7023 276.9840
 347.9861 379.7289 456.6050
 541.4389 733.1837 750.2206
 799.0735 853.1696 876.9091
 965.3754 968.6447 1027.7167
 1035.8562 1047.5085 1057.9994
 1085.7428 1092.4119 1141.6569
 1195.3472 1244.0939 1263.3099
 1279.9658 1309.5829 1327.6124
 1332.0208 1348.3582 1355.1973
 1373.1600 1398.2853 1410.1339
 1414.3812 1426.8946 1495.7433
 1498.1249 1501.9165 1508.4198
 1512.9374 1518.8378 1524.2924
 2881.2048 2920.3102 3010.8279
 3015.8730 3020.3888 3028.3506
 3038.6307 3040.5558 3044.2920
 3047.9945 3065.6006 3071.7712
 3088.9806 3107.0634 3112.4700
 Zero-point correction (Hartree): 0.207967

C7H15O.ttttt

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.95237972

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -4.313784 | 0.507790 | -0.106622 |
| C | -3.206497 | -0.217172 | 0.242180 |
| C | -1.862306 | 0.363118 | -0.210645 |
| C | -0.671794 | -0.522339 | 0.174932 |
| C | 0.682905 | 0.050754 | -0.261118 |
| C | 1.869118 | -0.843078 | 0.125868 |
| C | 3.239536 | -0.332728 | -0.349117 |
| C | 3.694182 | 0.976069 | 0.308606 |
| H | -3.218887 | -0.422864 | 1.332149 |
| H | -3.365000 | -1.223013 | -0.207393 |
| H | -1.895509 | 0.507720 | -1.297599 |
| H | -1.748632 | 1.360186 | 0.233906 |
| H | -0.665730 | -0.673840 | 1.264230 |
| H | -0.800944 | -1.521373 | -0.267023 |
| H | 0.680068 | 0.196592 | -1.350858 |
| H | 0.805470 | 1.049107 | 0.178611 |
| H | 1.889025 | -0.966447 | 1.218453 |
| H | 1.703203 | -1.846773 | -0.288938 |
| H | 3.989516 | -1.108838 | -0.150076 |
| H | 3.218551 | -0.205614 | -1.440308 |
| H | 3.727975 | 0.877533 | 1.400101 |
| H | 3.023635 | 1.808894 | 0.072735 |
| H | 4.696666 | 1.258661 | -0.029254 |

Rotational constants (GHz): 7.4264000 0.5425000 0.5246800
 Vibrational harmonic frequencies (cm-1):
 51.7629 56.8159 91.8444
 117.6980 130.7626 156.3766
 210.9140 278.5523 282.2608
 363.0487 378.1754 461.2493
 520.4234 735.2655 756.9432
 787.5127 860.0847 885.1439
 965.0355 973.7731 1012.8389
 1043.8289 1048.0205 1062.6955
 1088.0600 1089.8533 1138.5109
 1199.8336 1242.4697 1253.0920
 1287.5525 1307.6557 1328.5922
 1337.0279 1340.9143 1367.4671
 1385.4988 1389.3837 1406.5133
 1417.3410 1429.5333 1496.3047
 1499.1712 1502.0238 1507.2832
 1515.9592 1521.4587 1523.9705
 2881.2948 2920.8347 3008.6200
 3013.7024 3023.3598 3025.8457
 3037.1606 3041.3648 3041.8970
 3048.5483 3061.8295 3073.2354
 3088.6532 3108.1338 3116.1519
 Zero-point correction (Hartree): 0.207990

C7H15O.ttttt

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.95372608

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|----------|-----------|-----------|
| O | 4.478582 | 0.212530 | 0.017018 |
| C | 3.284929 | -0.455802 | -0.019868 |

| | | | |
|---|------------|-----------|-----------|
| C | 2.029504 | 0.423227 | -0.005802 |
| C | 0.732233 | -0.393804 | 0.001915 |
| C | -0.534374 | 0.471499 | -0.005738 |
| C | -1.832799 | -0.344848 | 0.003996 |
| C | -3.100433 | 0.519121 | -0.004116 |
| C | -4.392596 | -0.303861 | 0.006145 |
| H | 3.277360 | -1.168583 | -0.869725 |
| H | 3.298848 | -1.123049 | 0.870941 |
| H | 2.074302 | 1.078568 | 0.872842 |
| H | 2.055283 | 1.078474 | -0.885966 |
| H | 0.716561 | -1.064354 | -0.869629 |
| H | 0.717664 | -1.048375 | 0.885737 |
| H | -0.519599 | 1.142295 | 0.864841 |
| H | -0.521266 | 1.123853 | -0.890298 |
| H | -1.846855 | -1.016238 | -0.866696 |
| H | -1.845460 | -0.997646 | 0.888743 |
| H | -3.086109 | 1.189787 | 0.865819 |
| H | -3.087816 | 1.170722 | -0.888461 |
| H | -4.450426 | -0.939560 | 0.897159 |
| H | -4.451818 | -0.959418 | -0.870263 |
| H | -5.278106 | 0.340084 | -0.000383 |
| Rotational constants (GHz): | 11.7148600 | 0.4895600 | 0.4796300 |
| Vibrational harmonic frequencies (cm ⁻¹): | | | |
| 51.9349 | 78.6247 | | 80.6346 |
| 112.9779 | 144.9152 | | 164.1958 |
| 200.3591 | 245.6926 | | 270.0152 |
| 353.1191 | 422.3739 | | 466.7670 |
| 515.6365 | 736.7326 | | 745.9093 |
| 790.0420 | 872.4502 | | 902.1757 |
| 966.9151 | 986.1949 | | 1028.1844 |
| 1045.3932 | 1049.8945 | | 1065.3645 |
| 1071.3125 | 1090.1935 | | 1141.1872 |
| 1216.1962 | 1240.5315 | | 1255.4533 |
| 1289.1940 | 1304.9179 | | 1325.7141 |
| 1339.9449 | 1345.7651 | | 1354.9813 |
| 1373.2472 | 1395.4616 | | 1411.1472 |
| 1417.9770 | 1427.5779 | | 1498.3831 |
| 1500.0832 | 1503.0613 | | 1510.9243 |
| 1512.7497 | 1520.6676 | | 1528.2335 |
| 2881.2416 | 2921.6453 | | 3008.9883 |
| 3012.2812 | 3019.8708 | | 3028.5363 |
| 3034.6130 | 3039.0105 | | 3039.5764 |
| 3042.1102 | 3056.5979 | | 3072.2566 |
| 3088.5157 | 3106.7204 | | 3112.4233 |
| Zero-point correction (Hartree): | 0.208078 | | |

C7H15O.1-7Hshift.BB.a

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.93358575

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -0.726073 | -1.725750 | -0.260679 |
| H | 0.397997 | -1.230178 | 0.008393 |
| C | 1.447105 | -0.630479 | 0.419341 |
| C | -1.678995 | -0.972405 | 0.440869 |
| C | 0.970756 | 0.658778 | 1.071542 |
| C | -2.011208 | 0.393023 | -0.199502 |
| C | 0.268932 | 1.676835 | 0.147771 |
| C | -0.807791 | 1.130444 | -0.810437 |
| C | 2.383198 | -0.521123 | -0.769417 |
| H | 1.813169 | -1.345183 | 1.165052 |
| H | -2.587339 | -1.595768 | 0.467267 |
| H | -1.385447 | -0.848817 | 1.495617 |
| H | 0.314416 | 0.404995 | 1.912369 |
| H | 1.841028 | 1.155454 | 1.531504 |
| H | -2.734975 | 0.230109 | -1.007822 |
| H | -2.516769 | 1.022092 | 0.546459 |
| H | -0.170559 | 2.458995 | 0.780807 |
| H | 1.026154 | 2.183983 | -0.464212 |
| H | -1.189751 | 1.979268 | -1.391261 |
| H | -0.345424 | 0.453684 | -1.537089 |
| H | 3.333303 | -0.056903 | -0.466536 |
| H | 1.964116 | 0.090748 | -1.573492 |
| H | 2.616680 | -1.506915 | -1.182622 |
| Rotational constants (GHz): | 2.4642700 | 1.6102000 | 1.2387300 |
| Vibrational harmonic frequencies (cm ⁻¹): | | | |
| 11464.6279 | 86.9343 | | 169.6462 |
| 176.7557 | 192.3474 | | 249.4115 |
| 268.6255 | 279.0910 | | 319.3438 |
| 400.0684 | 535.6276 | | 546.9077 |
| 565.8416 | 728.4508 | | 767.0562 |
| 793.2025 | 817.7966 | | 868.9945 |
| 900.2124 | 942.2196 | | 985.5005 |
| 991.5528 | 1044.9593 | | 1064.4962 |
| 1089.7012 | 1120.0545 | | 1144.4134 |

| | | |
|-----------|-----------|-----------|
| 1155.5665 | 1202.2553 | 1215.1776 |
| 1235.5481 | 1279.4233 | 1298.7331 |
| 1312.3612 | 1353.5603 | 1366.5228 |
| 1386.2003 | 1394.5595 | 1403.3018 |
| 1413.0961 | 1421.1032 | 1448.9364 |
| 1469.6981 | 1491.8719 | 1494.6167 |
| 1497.2803 | 1504.9292 | 1505.6603 |
| 1513.8964 | 2981.3180 | 2989.3912 |
| 3007.1569 | 3017.8755 | 3027.3971 |
| 3029.8453 | 3045.5026 | 3053.2924 |
| 3069.2052 | 3071.5465 | 3077.9989 |
| 3092.5777 | 3095.9818 | 3130.0166 |

Zero-point correction (Hartree): 0.205269

C7H15O.1-7Hshift.BB.e

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.93536122

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -0.183055 | -1.740641 | -0.470859 |
| H | 0.668249 | -0.811997 | -0.532682 |
| C | 1.476000 | 0.163358 | -0.409765 |
| C | -1.081716 | -1.402687 | 0.550893 |
| C | 0.834332 | 1.125284 | 0.573606 |
| C | -2.087244 | -0.295343 | 0.173113 |
| C | -0.471861 | 1.788342 | 0.087093 |
| C | -1.491596 | 0.877953 | -0.622791 |
| H | 1.505223 | 0.555698 | -1.433565 |
| C | 2.789828 | -0.457216 | 0.021818 |
| H | -1.629071 | -2.331510 | 0.779965 |
| H | -0.548348 | -1.146658 | 1.481127 |
| H | 0.668866 | 0.603878 | 1.525639 |
| H | 1.560683 | 1.919310 | 0.811661 |
| H | -2.877249 | -0.740306 | -0.444633 |
| H | -2.574953 | 0.066040 | 1.089357 |
| H | -0.951569 | 2.282298 | 0.942477 |
| H | -0.210026 | 2.591863 | -0.614253 |
| H | -2.320893 | 1.512330 | -0.959787 |
| H | -1.040824 | 0.467274 | -1.533279 |
| H | 2.696871 | -0.945879 | 0.997822 |
| H | 3.573523 | 0.308722 | 0.111201 |
| H | 3.137505 | -1.204080 | -0.697981 |

Rotational constants (GHz): 2.5020200 1.5831500 1.1144100

Vibrational harmonic frequencies (cm-1):

| | | |
|------------|-----------|-----------|
| i1443.3093 | 70.5373 | 143.6905 |
| 187.0714 | 212.6006 | 250.9789 |
| 278.5024 | 287.4745 | 325.0491 |
| 386.5357 | 501.7895 | 559.1606 |
| 568.5748 | 745.6880 | 787.5355 |
| 809.4908 | 822.7261 | 866.7226 |
| 911.4234 | 934.7193 | 991.2663 |
| 1011.1947 | 1046.2710 | 1073.6949 |
| 1082.8331 | 1122.6094 | 1143.6336 |
| 1155.4053 | 1191.7646 | 1216.8918 |
| 1229.7013 | 1275.5532 | 1295.2794 |
| 1306.9165 | 1330.3527 | 1376.5346 |
| 1393.3597 | 1395.9145 | 1400.6473 |
| 1416.7141 | 1419.1231 | 1448.5699 |
| 1474.2018 | 1495.3167 | 1495.6763 |
| 1500.3499 | 1502.9260 | 1507.8559 |
| 1511.8911 | 2980.2090 | 2992.8593 |
| 3005.6058 | 3020.1689 | 3025.8617 |
| 3027.2144 | 3042.5282 | 3047.3437 |
| 3063.4199 | 3070.2458 | 3071.4080 |
| 3089.4107 | 3091.1783 | 3124.0758 |

Zero-point correction (Hartree): 0.205295

C7H15O.1-7Hshift.BC.e

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.93340212

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -0.314710 | -1.570374 | -0.718707 |
| H | 0.649182 | -0.877538 | -0.268848 |
| C | 1.425470 | -0.122606 | 0.367698 |
| C | -1.372072 | -1.448098 | 0.197094 |
| C | 1.139738 | 1.297277 | -0.104845 |
| C | -2.174222 | -0.144427 | 0.103108 |
| C | -0.312862 | 1.569700 | -0.544771 |
| C | -1.421411 | 1.153966 | 0.457724 |
| C | 2.833297 | -0.641549 | 0.152821 |
| H | 1.073770 | -0.300541 | 1.390617 |
| H | -2.041986 | -2.295235 | -0.024951 |
| H | -1.025323 | -1.606775 | 1.233616 |
| H | 1.409583 | 1.991812 | 0.706589 |

| | | | | |
|--|-----------|-----------|-----------|--|
| H | 1.803857 | 1.540051 | -0.944279 | |
| H | -2.572444 | -0.057929 | -0.916302 | |
| H | -3.042515 | -0.242139 | 0.770048 | |
| H | -0.397458 | 2.642893 | -0.753394 | |
| H | -0.486628 | 1.057642 | -1.497552 | |
| H | -2.166862 | 1.956334 | 0.507743 | |
| H | -1.009234 | 1.076728 | 1.473797 | |
| H | 3.558861 | -0.041572 | 0.721357 | |
| H | 3.121653 | -0.585897 | -0.902422 | |
| H | 2.935588 | -1.680418 | 0.480661 | |
| Rotational constants (GHz): | 2.5595800 | 1.4939700 | 1.0627800 | |
| Vibrational harmonic frequencies (cm-1): | | | | |
| i1336.6985 | 85.2433 | | 146.4430 | |
| 153.1964 | 197.2510 | | 202.0052 | |
| 256.4545 | 309.7541 | | 344.2999 | |
| 369.3143 | 463.4942 | | 503.2120 | |
| 574.3497 | 740.3311 | | 790.2772 | |
| 847.9479 | 858.6369 | | 875.8085 | |
| 911.3236 | 943.5601 | | 978.4085 | |
| 1013.8184 | 1053.3552 | | 1077.6317 | |
| 1097.5507 | 1116.9563 | | 1120.4180 | |
| 1153.6151 | 1211.9903 | | 1228.9147 | |
| 1240.3624 | 1278.3074 | | 1288.1464 | |
| 1305.4477 | 1341.5129 | | 1370.8935 | |
| 1384.9442 | 1392.9276 | | 1408.6538 | |
| 1412.9882 | 1419.5015 | | 1462.1662 | |
| 1477.3443 | 1487.7490 | | 1491.4846 | |
| 1499.9090 | 1503.5466 | | 1504.7605 | |
| 1506.0725 | 2960.5775 | | 2996.1891 | |
| 3000.3645 | 3017.5632 | | 3022.7798 | |
| 3027.3181 | 3041.1998 | | 3055.3043 | |
| 3065.3901 | 3069.8021 | | 3075.3555 | |
| 3088.2318 | 3091.5538 | | 3123.7307 | |
| Zero-point correction (Hartree): | 0.205121 | | | |

C7H15O.1-7Hshift.CR.a

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.93333612

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | | |
|--|-----------|-----------|-----------|--|
| O | -0.362119 | -1.861874 | -0.008075 | |
| H | 0.600563 | -1.103202 | 0.292926 | |
| C | 1.578675 | -0.346210 | 0.501704 | |
| C | -1.563428 | -1.245477 | 0.363080 | |
| C | 1.061999 | 1.064234 | 0.749699 | |
| C | -1.973783 | -0.029652 | -0.482272 | |
| C | 0.079112 | 1.646421 | -0.288933 | |
| C | -1.417743 | 1.345051 | -0.064857 | |
| C | 2.467432 | -0.552608 | -0.711446 | |
| H | 2.015598 | -0.783503 | 1.406541 | |
| H | -2.318717 | -2.037913 | 0.227109 | |
| H | -1.587574 | -0.992578 | 1.438664 | |
| H | 0.600377 | 1.115956 | 1.744203 | |
| H | 1.943958 | 1.723657 | 0.800393 | |
| H | -1.712406 | -0.246277 | -1.526070 | |
| H | -3.069567 | 0.043725 | -0.446024 | |
| H | 0.189660 | 2.737619 | -0.267914 | |
| H | 0.370494 | 1.341482 | -1.302341 | |
| H | -1.985776 | 2.100096 | -0.623621 | |
| H | -1.659077 | 1.520786 | 0.993989 | |
| H | 3.399044 | 0.022798 | -0.612039 | |
| H | 1.978915 | -0.231890 | -1.636627 | |
| H | 2.737886 | -1.606318 | -0.826440 | |
| Rotational constants (GHz): | 2.3434900 | 1.5958700 | 1.1107200 | |
| Vibrational harmonic frequencies (cm-1): | | | | |
| i1314.4996 | 46.2505 | | 86.5444 | |
| 154.2711 | 203.5776 | | 218.1687 | |
| 264.4618 | 306.5878 | | 324.9469 | |
| 414.6942 | 453.9538 | | 481.5309 | |
| 580.1017 | 724.8615 | | 778.9664 | |
| 799.5908 | 836.1734 | | 882.9929 | |
| 894.2464 | 953.8288 | | 968.8824 | |
| 1005.6668 | 1045.8130 | | 1067.9787 | |
| 1102.1175 | 1118.1473 | | 1141.5068 | |
| 1148.4876 | 1197.8865 | | 1213.1165 | |
| 1256.8515 | 1277.3079 | | 1298.8383 | |
| 1312.3002 | 1349.0193 | | 1372.2054 | |
| 1387.7835 | 1394.2267 | | 1399.0646 | |
| 1402.1499 | 1413.4068 | | 1427.6923 | |
| 1463.6983 | 1482.1018 | | 1485.5369 | |
| 1494.8385 | 1500.1558 | | 1501.3574 | |
| 1510.5170 | 2953.0177 | | 2986.7326 | |
| 2992.2136 | 3012.6639 | | 3021.8612 | |
| 3026.4316 | 3034.6467 | | 3051.5875 | |

| | | |
|-----------|-----------|-----------|
| 3059.8022 | 3071.5893 | 3075.7301 |
| 3077.4297 | 3097.8382 | 3128.8153 |

Zero-point correction (Hartree): 0.204431

C7H15O.1-7Hshift.CR.e

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.93468607

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -0.056171 | -1.823841 | -0.417104 |
| H | 0.752233 | -0.854556 | -0.415170 |
| C | 1.560860 | 0.105139 | -0.405169 |
| C | -1.155077 | -1.504110 | 0.389534 |
| C | 0.895393 | 1.292851 | 0.265281 |
| C | -2.066354 | -0.385136 | -0.142574 |
| C | -0.460780 | 1.724689 | -0.329612 |
| C | -1.720115 | 1.060366 | 0.263121 |
| H | 1.689061 | 0.264770 | -1.482970 |
| C | 2.816521 | -0.424303 | 0.259478 |
| H | -1.734341 | -2.442159 | 0.424507 |
| H | -0.860983 | -1.296210 | 1.434609 |
| H | 0.785039 | 1.101597 | 1.342041 |
| H | 1.597552 | 2.139507 | 0.192467 |
| H | -2.104423 | -0.479012 | -1.235435 |
| H | -3.084133 | -0.582623 | 0.220854 |
| H | -0.568094 | 2.804564 | -0.169197 |
| H | -0.445285 | 1.585920 | -1.419541 |
| H | -2.577860 | 1.684890 | -0.018564 |
| H | -1.664001 | 1.116850 | 1.360282 |
| H | 2.630095 | -0.694180 | 1.304711 |
| H | 3.612360 | 0.334413 | 0.253542 |
| H | 3.199460 | -1.310018 | -0.255659 |

Rotational constants (GHz): 2.4084600 1.5373800 1.0319300

Vibrational harmonic frequencies (cm-1):

| | | |
|------------|-----------|-----------|
| i1307.0126 | 55.5180 | 96.3402 |
| 130.7591 | 198.9954 | 226.3651 |
| 281.1163 | 295.5225 | 326.2465 |
| 389.0268 | 458.7900 | 472.7593 |
| 562.5123 | 733.0918 | 785.0081 |
| 809.2185 | 842.0122 | 884.1898 |
| 909.6820 | 948.8099 | 983.2534 |
| 1017.4055 | 1046.3643 | 1075.1570 |
| 1095.3680 | 1115.2591 | 1141.7897 |
| 1154.9994 | 1195.6633 | 1215.7023 |
| 1254.2543 | 1274.1452 | 1300.0700 |
| 1306.0306 | 1330.0725 | 1380.9751 |
| 1390.8138 | 1392.9219 | 1401.4193 |
| 1407.2296 | 1416.8737 | 1429.3502 |
| 1469.3571 | 1482.9480 | 1485.3530 |
| 1497.4640 | 1501.7460 | 1501.8442 |
| 1504.2979 | 2951.7852 | 2986.4270 |
| 2992.3619 | 3013.1690 | 3019.7675 |
| 3025.8904 | 3028.2624 | 3038.9029 |
| 3057.8537 | 3064.7738 | 3068.2122 |
| 3076.2157 | 3089.5547 | 3125.1187 |

Zero-point correction (Hartree): 0.204380

C7H15O.1-8Hshift.SCBd

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.91819417

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| C | -1.527719 | 0.942270 | 0.465106 |
| C | -2.242424 | -0.304628 | -0.078610 |
| O | -1.386702 | -1.328760 | -0.507872 |
| H | -0.411837 | -1.449300 | 0.254881 |
| C | 0.779046 | -1.590549 | 0.723132 |
| C | 1.669511 | -1.015985 | -0.364326 |
| C | 2.080276 | 0.465451 | -0.215135 |
| C | 1.020315 | 1.461419 | 0.298040 |
| C | -0.359211 | 1.458286 | -0.415905 |
| H | -2.284499 | 1.723144 | 0.609990 |
| H | -1.155228 | 0.703571 | 1.469128 |
| H | -2.816733 | -0.029839 | -0.980259 |
| H | -2.972710 | -0.659044 | 0.669188 |
| H | 0.821060 | -2.678398 | 0.816645 |
| H | 0.815391 | -1.103084 | 1.699587 |
| H | 1.159133 | -1.168829 | -1.323744 |
| H | 2.589144 | -1.615756 | -0.431333 |
| H | 2.451355 | 0.806526 | -1.190378 |
| H | 2.939006 | 0.527072 | 0.466808 |
| H | 1.467538 | 2.460609 | 0.230999 |
| H | 0.865684 | 1.293206 | 1.371286 |
| H | -0.303949 | 0.847301 | -1.323242 |

| | | | | |
|---|-----------|-----------|-----------|-----------|
| H | -0.588506 | 2.475331 | -0.750388 | |
| Rotational constants (GHz): | 2.4742300 | | 1.6250400 | 1.1289400 |
| Vibrational harmonic frequencies (cm ⁻¹): | | | | |
| i1643.9550 | | 85.9909 | | 97.9792 |
| 134.5527 | | 168.5721 | | 217.8622 |
| 262.3057 | | 319.1503 | | 405.5796 |
| 444.0342 | | 495.5575 | | 516.3213 |
| 632.1973 | | 703.4147 | | 744.2406 |
| 805.3471 | | 851.4092 | | 889.5048 |
| 910.7170 | | 972.3306 | | 997.0200 |
| 1003.6212 | | 1061.4814 | | 1065.2788 |
| 1085.9332 | | 1112.9693 | | 1126.3492 |
| 1146.6993 | | 1199.1220 | | 1218.2354 |
| 1237.8653 | | 1252.9633 | | 1267.8669 |
| 1296.9506 | | 1320.0125 | | 1344.9789 |
| 1367.0505 | | 1381.5490 | | 1395.3486 |
| 1399.0930 | | 1405.2438 | | 1426.7885 |
| 1471.5935 | | 1482.6479 | | 1496.2614 |
| 1499.3957 | | 1502.2665 | | 1509.8781 |
| 1522.0616 | | 2961.2319 | | 2990.7814 |
| 3011.8513 | | 3026.4373 | | 3033.6474 |
| 3038.9216 | | 3046.8977 | | 3053.6469 |
| 3063.0025 | | 3071.3110 | | 3078.5314 |
| 3089.6773 | | 3097.0641 | | 3165.4334 |
| Zero-point correction (Hartree): 0.204994 | | | | |

C7H15O.1-8Hshift.SCBc

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.91847681

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | | |
|---|-----------|-----------|-----------|-----------|
| C | 1.311028 | 1.350246 | -0.186058 | |
| C | 2.165604 | 0.108601 | 0.156006 | |
| C | 1.432510 | -1.240403 | 0.259195 | |
| O | 0.504258 | -1.492466 | -0.771717 | |
| H | -0.634935 | -1.428778 | -0.303190 | |
| C | -1.718633 | -1.257363 | 0.377407 | |
| C | -2.298389 | 0.109456 | 0.044846 | |
| C | -1.257361 | 1.114623 | -0.484699 | |
| C | -0.085819 | 1.446537 | 0.480205 | |
| H | 1.908213 | 2.232661 | 0.073176 | |
| H | 1.179106 | 1.395133 | -1.272607 | |
| H | 2.677775 | 0.262259 | 1.116639 | |
| H | 2.958951 | 0.028126 | -0.597411 | |
| H | 0.931574 | -1.313127 | 1.235515 | |
| H | 2.174757 | -2.055196 | 0.255632 | |
| H | -1.337986 | -1.368817 | 1.395929 | |
| H | -2.335365 | -2.113485 | 0.095931 | |
| H | -2.786751 | 0.518776 | 0.942474 | |
| H | -3.084719 | 0.000435 | -0.710859 | |
| H | -1.777609 | 2.038906 | -0.763239 | |
| H | -0.848937 | 0.698918 | -1.410724 | |
| H | -0.122868 | 0.794573 | 1.361646 | |
| H | -0.228914 | 2.459162 | 0.873414 | |
| Rotational constants (GHz): | 2.5243300 | | 1.6242200 | 1.1284600 |
| Vibrational harmonic frequencies (cm ⁻¹): | | | | |
| i1629.1953 | | 32.9695 | | 115.6970 |
| 145.4268 | | 163.8395 | | 210.0276 |
| 291.8868 | | 315.2623 | | 392.4448 |
| 445.8306 | | 547.0171 | | 553.1957 |
| 598.6501 | | 714.4499 | | 751.7716 |
| 793.2200 | | 828.6220 | | 916.0094 |
| 919.4664 | | 944.7816 | | 972.7423 |
| 997.8438 | | 1062.3719 | | 1066.6944 |
| 1084.8458 | | 1101.5521 | | 1125.1772 |
| 1136.4642 | | 1194.6377 | | 1225.9316 |
| 1245.9572 | | 1258.0931 | | 1273.3668 |
| 1312.8489 | | 1316.0952 | | 1344.7400 |
| 1361.6233 | | 1381.4836 | | 1398.0148 |
| 1402.8120 | | 1414.6951 | | 1439.0838 |
| 1469.2315 | | 1483.9193 | | 1496.8913 |
| 1502.3943 | | 1504.2665 | | 1516.4773 |
| 1523.0140 | | 2987.0008 | | 3006.8096 |
| 3019.1544 | | 3022.8740 | | 3041.2911 |
| 3045.2995 | | 3047.6579 | | 3065.6503 |
| 3071.8593 | | 3078.8269 | | 3084.8023 |
| 3085.6760 | | 3102.2663 | | 3160.7329 |
| Zero-point correction (Hartree): 0.205294 | | | | |

C7H15O.1-8Hshift.SCBg

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.92569914

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|----------|
| C | -1.913458 | -0.269783 | 0.440467 |
|---|-----------|-----------|----------|

| | | | |
|--|-----------|-----------|-----------|
| C | -1.268358 | -1.510712 | -0.213579 |
| C | 0.224763 | -1.397297 | -0.562159 |
| C | 1.136978 | -1.011735 | 0.619257 |
| C | 2.225602 | 0.002239 | 0.223020 |
| O | 1.750858 | 1.069046 | -0.557781 |
| H | 0.650913 | 1.431614 | -0.151986 |
| C | -0.496780 | 1.904941 | 0.230807 |
| C | -1.675312 | 1.085503 | -0.264268 |
| H | -2.993398 | -0.455645 | 0.486412 |
| H | -1.592803 | -0.182442 | 1.486746 |
| H | -1.815822 | -1.741200 | -1.137488 |
| H | -1.432567 | -2.367557 | 0.454155 |
| H | 0.346309 | -0.641644 | -1.344746 |
| H | 0.558404 | -2.345059 | -1.001677 |
| H | 1.614519 | -1.893567 | 1.063342 |
| H | 0.544453 | -0.557874 | 1.422222 |
| H | 2.977055 | -0.495337 | -0.413228 |
| H | 2.751281 | 0.352717 | 1.127212 |
| H | -0.422760 | 2.895025 | -0.227732 |
| H | -0.416640 | 1.970533 | 1.319660 |
| H | -1.607282 | 0.947505 | -1.351475 |
| H | -2.569135 | 1.711627 | -0.110439 |
| Rotational constants (GHz): | 2.3995000 | 1.6575100 | 1.1261400 |
| Vibrational harmonic frequencies (cm-1): | | | |
| i1637.7983 | 122.4076 | | 140.9691 |
| 149.7971 | 217.5649 | | 230.8566 |
| 294.2136 | 333.4278 | | 383.5106 |
| 455.4816 | 499.9391 | | 536.8337 |
| 641.3687 | 725.9124 | | 742.6801 |
| 818.8241 | 830.6162 | | 863.1146 |
| 906.7805 | 959.4043 | | 978.6558 |
| 1015.8780 | 1055.2417 | | 1066.5317 |
| 1090.3486 | 1100.5235 | | 1118.5264 |
| 1148.7306 | 1195.3402 | | 1223.0438 |
| 1244.0515 | 1253.9854 | | 1279.9228 |
| 1298.5618 | 1322.5851 | | 1346.7283 |
| 1362.4069 | 1379.5843 | | 1396.4536 |
| 1398.7994 | 1417.0088 | | 1427.5085 |
| 1468.0467 | 1480.5525 | | 1497.7375 |
| 1500.7767 | 1504.8666 | | 1514.1274 |
| 1519.9175 | 2967.5198 | | 2988.3455 |
| 2998.2944 | 3021.4705 | | 3032.7205 |
| 3047.4484 | 3051.3201 | | 3053.7979 |
| 3056.2843 | 3071.2433 | | 3074.6394 |
| 3084.7409 | 3099.6660 | | 3150.3232 |
| Zero-point correction (Hartree): | 0.205395 | | |

C7H15O.1-8Hshift.SCBh

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.92778842

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|--|-----------|-----------|-----------|
| C | 1.997878 | 0.516524 | -0.456881 |
| C | 1.915942 | -0.891240 | 0.169865 |
| C | 0.499804 | -1.345130 | 0.564584 |
| C | -0.537760 | -1.304786 | -0.579565 |
| C | -1.933990 | -0.829959 | -0.148652 |
| C | -1.934354 | 0.593369 | 0.439377 |
| O | -1.244898 | 1.539097 | -0.340865 |
| H | -0.047858 | 1.523032 | -0.055233 |
| C | 1.210374 | 1.597749 | 0.256613 |
| H | 3.056529 | 0.819735 | -0.486281 |
| H | 1.685924 | 0.486634 | -1.508354 |
| H | 2.547437 | -0.916927 | 1.067892 |
| H | 2.358704 | -1.609070 | -0.532977 |
| H | 0.162898 | -0.711187 | 1.393038 |
| H | 0.554891 | -2.357250 | 0.983687 |
| H | -0.616275 | -2.292416 | -1.048873 |
| H | -0.201321 | -0.623848 | -1.367261 |
| H | -2.369328 | -1.514107 | 0.593528 |
| H | -2.596282 | -0.850882 | -1.022818 |
| H | -1.555817 | 0.591009 | 1.473982 |
| H | -2.970079 | 0.961787 | 0.512542 |
| H | 1.223855 | 1.550848 | 1.349283 |
| H | 1.418556 | 2.610705 | -0.097283 |
| Rotational constants (GHz): | 2.5359800 | 1.6058000 | 1.1205200 |
| Vibrational harmonic frequencies (cm-1): | | | |
| i1652.6426 | 107.6962 | | 158.6888 |
| 181.0781 | 202.3449 | | 258.9319 |
| 290.7439 | 332.8385 | | 370.2146 |
| 468.9065 | 499.7410 | | 562.0988 |
| 618.5061 | 700.6981 | | 771.0685 |
| 789.4693 | 836.3133 | | 871.9712 |
| 902.9311 | 945.4713 | | 981.2000 |
| 1006.7677 | 1050.1517 | | 1053.4298 |

| | | |
|-----------|-----------|-----------|
| 1086.3355 | 1108.8469 | 1114.6863 |
| 1137.1425 | 1191.1831 | 1222.4055 |
| 1226.7835 | 1261.5474 | 1269.5410 |
| 1309.3620 | 1328.3290 | 1349.1227 |
| 1380.8253 | 1384.3469 | 1394.2467 |
| 1400.3321 | 1414.3019 | 1417.6326 |
| 1469.9423 | 1473.2060 | 1485.6564 |
| 1495.6979 | 1504.7758 | 1515.0300 |
| 1518.3127 | 2983.1266 | 2999.0244 |
| 3011.0211 | 3027.7965 | 3028.9480 |
| 3045.1067 | 3050.8145 | 3056.2136 |
| 3066.6076 | 3073.1948 | 3078.4098 |
| 3084.0195 | 3103.6620 | 3154.7143 |

Zero-point correction (Hartree): 0.205453

C7H15O.1-8Hshift.TBCa

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.92358188

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| H | 0.032386 | -1.558623 | -0.264131 |
| C | 1.267758 | -1.442797 | -0.655989 |
| C | 2.092260 | -0.458513 | 0.161009 |
| C | 1.357239 | 0.725444 | 0.826995 |
| C | 0.589511 | 1.698612 | -0.086407 |
| C | -0.649475 | 1.191761 | -0.852851 |
| C | -1.852262 | 0.693759 | -0.030157 |
| C | -1.678093 | -0.647986 | 0.707387 |
| O | -1.173897 | -1.695901 | -0.079058 |
| H | 1.117264 | -1.162584 | -1.699948 |
| H | 1.595971 | -2.482414 | -0.580507 |
| H | 2.880159 | -0.052953 | -0.493048 |
| H | 2.612803 | -1.003773 | 0.957037 |
| H | 2.118797 | 1.309489 | 1.360213 |
| H | 0.692827 | 0.339353 | 1.606059 |
| H | 1.294956 | 2.110193 | -0.822534 |
| H | 0.278594 | 2.551871 | 0.532906 |
| H | -0.372706 | 0.407648 | -1.563384 |
| H | -1.003271 | 2.028980 | -1.468496 |
| H | -2.697089 | 0.586690 | -0.721954 |
| H | -2.148502 | 1.454898 | 0.706070 |
| H | -2.672414 | -0.999553 | 1.029221 |
| H | -1.100231 | -0.523695 | 1.635039 |

Rotational constants (GHz): 2.2781400 1.7083800 1.1983200

Vibrational harmonic frequencies (cm-1):

| | | |
|------------|-----------|-----------|
| i1679.0463 | 47.1706 | 123.4570 |
| 190.7025 | 245.9161 | 260.7836 |
| 279.0043 | 352.7344 | 402.8136 |
| 447.5654 | 471.7655 | 503.5631 |
| 573.8045 | 747.2000 | 758.3863 |
| 804.0505 | 816.3757 | 841.5166 |
| 902.1193 | 953.1941 | 984.7083 |
| 1032.3353 | 1043.8665 | 1066.4699 |
| 1092.1633 | 1110.9478 | 1134.2498 |
| 1149.1598 | 1183.8702 | 1215.1577 |
| 1223.6257 | 1248.8538 | 1298.0479 |
| 1319.1559 | 1321.8196 | 1370.3284 |
| 1376.9845 | 1393.9682 | 1404.1501 |
| 1410.2774 | 1416.2599 | 1429.9033 |
| 1470.6131 | 1476.5914 | 1489.1932 |
| 1496.7728 | 1500.4069 | 1513.4536 |
| 1515.7185 | 2986.4420 | 2999.5886 |
| 3011.2635 | 3017.9711 | 3023.2462 |
| 3037.2322 | 3044.5641 | 3047.7404 |
| 3067.0259 | 3069.9105 | 3089.1213 |
| 3099.4099 | 3110.3875 | 3165.1262 |

Zero-point correction (Hartree): 0.205446

C7H15O.1-8Hshift.TBCb

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.92490978

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 1.413989 | 1.631822 | -0.155438 |
| H | 0.195155 | 1.613645 | -0.270870 |
| C | -1.097178 | 1.738598 | -0.223085 |
| C | -1.696309 | 0.664280 | 0.659620 |
| C | -1.884405 | -0.699616 | -0.027443 |
| C | -0.666407 | -1.290392 | -0.759138 |
| C | 0.518748 | -1.768878 | 0.100208 |
| C | 1.443763 | -0.702517 | 0.721214 |
| C | 1.982499 | 0.352775 | -0.272249 |
| H | -1.423130 | 1.724517 | -1.266890 |
| H | -1.146500 | 2.746885 | 0.195502 |

| | | | | |
|--|-----------|-----------|-----------|--|
| H | -2.683259 | 1.009951 | 1.006339 | |
| H | -1.094730 | 0.564080 | 1.571026 | |
| H | -2.692779 | -0.595763 | -0.764184 | |
| H | -2.245428 | -1.424025 | 0.715075 | |
| H | -0.311035 | -0.577667 | -1.514725 | |
| H | -1.024760 | -2.157301 | -1.328945 | |
| H | 1.141679 | -2.412428 | -0.536029 | |
| H | 0.142355 | -2.421166 | 0.900195 | |
| H | 2.288486 | -1.231514 | 1.180115 | |
| H | 0.952878 | -0.161470 | 1.536429 | |
| H | 1.934988 | -0.032144 | -1.306070 | |
| H | 3.049902 | 0.534320 | -0.068219 | |
| Rotational constants (GHz): | 2.2224300 | 1.7529400 | 1.1463800 | |
| Vibrational harmonic frequencies (cm-1): | | | | |
| i1660.4615 | 72.2571 | | 144.3480 | |
| 176.1795 | 214.1804 | | 232.7638 | |
| 276.8452 | 373.1128 | | 411.8296 | |
| 441.6957 | 473.7966 | | 496.6373 | |
| 597.2900 | 722.7513 | | 778.9034 | |
| 800.2410 | 823.7143 | | 879.5306 | |
| 902.3155 | 957.4774 | | 990.2742 | |
| 1016.9884 | 1041.3597 | | 1061.9971 | |
| 1076.0636 | 1109.3364 | | 1122.8577 | |
| 1151.3593 | 1182.0721 | | 1217.4311 | |
| 1220.8232 | 1252.5694 | | 1266.6281 | |
| 1314.6022 | 1326.9086 | | 1354.4583 | |
| 1378.3185 | 1396.3191 | | 1399.8329 | |
| 1406.0849 | 1413.4352 | | 1415.0181 | |
| 1471.7026 | 1481.0616 | | 1484.0956 | |
| 1497.1094 | 1502.6302 | | 1508.3685 | |
| 1512.4278 | 2963.4715 | | 2996.5561 | |
| 3003.1846 | 3017.9568 | | 3022.6676 | |
| 3033.8060 | 3046.3290 | | 3051.9496 | |
| 3054.9512 | 3066.9159 | | 3072.7070 | |
| 3080.8882 | 3100.9219 | | 3156.8516 | |
| Zero-point correction (Hartree): | 0.205074 | | | |

C7H15O.1-8Hshift.TBCC

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.92744932

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | | |
|--|-----------|-----------|-----------|--|
| C | -1.916869 | -0.799014 | -0.005132 | |
| O | -0.928279 | -1.568248 | -0.640974 | |
| H | 0.089894 | -1.582071 | 0.048563 | |
| C | 1.148944 | -1.441753 | 0.770046 | |
| C | 2.078050 | -0.502158 | 0.019946 | |
| C | 1.387371 | 0.595692 | -0.817471 | |
| C | 0.658681 | 1.710967 | -0.049195 | |
| C | -0.634594 | 1.365236 | 0.717183 | |
| C | -1.774817 | 0.727104 | -0.112042 | |
| H | -2.854922 | -1.099489 | -0.500290 | |
| H | -2.029996 | -1.087483 | 1.054498 | |
| H | 1.506629 | -2.469191 | 0.870955 | |
| H | 0.761048 | -1.067999 | 1.719178 | |
| H | 2.702954 | -1.093686 | -0.659122 | |
| H | 2.767632 | -0.029488 | 0.737516 | |
| H | 0.695614 | 0.108978 | -1.513072 | |
| H | 2.162279 | 1.074377 | -1.429903 | |
| H | 0.407082 | 2.495123 | -0.776832 | |
| H | 1.362414 | 2.176365 | 0.655723 | |
| H | -1.002581 | 2.306383 | 1.144445 | |
| H | -0.413473 | 0.729334 | 1.583092 | |
| H | -1.677117 | 0.999630 | -1.170645 | |
| H | -2.731817 | 1.148757 | 0.223674 | |
| Rotational constants (GHz): | 2.2812200 | 1.7399100 | 1.1960300 | |
| Vibrational harmonic frequencies (cm-1): | | | | |
| i1564.0412 | 90.7378 | | 140.7127 | |
| 173.5925 | 213.9572 | | 227.0913 | |
| 317.0617 | 322.0394 | | 399.2894 | |
| 465.8787 | 483.2316 | | 549.2517 | |
| 591.8414 | 720.5722 | | 779.6023 | |
| 793.4249 | 817.9022 | | 895.4881 | |
| 904.8183 | 939.6953 | | 983.7254 | |
| 1011.5287 | 1047.3675 | | 1070.3103 | |
| 1070.9026 | 1111.2860 | | 1123.4965 | |
| 1151.9220 | 1201.5129 | | 1213.1233 | |
| 1248.6921 | 1265.3940 | | 1286.5923 | |
| 1309.3333 | 1321.7985 | | 1369.6214 | |
| 1375.5747 | 1388.5729 | | 1398.4110 | |
| 1406.6955 | 1413.6547 | | 1421.2897 | |
| 1465.9619 | 1470.0258 | | 1488.4870 | |
| 1493.9712 | 1497.8633 | | 1504.4563 | |
| 1512.9838 | 2964.9860 | | 2996.8924 | |
| 3003.7351 | 3012.7308 | | 3028.1174 | |

| | | |
|-----------|-----------|-----------|
| 3035.7722 | 3042.9178 | 3049.3289 |
| 3070.4944 | 3072.3450 | 3076.0819 |
| 3091.3290 | 3098.4039 | 3165.8074 |

Zero-point correction (Hartree): 0.205399

C7H15O.1-8Hshift.TBCd

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.92887505

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| C | -1.963957 | -0.634620 | 0.134605 |
| C | -1.755619 | 0.870619 | 0.353365 |
| O | -1.028381 | 1.530668 | -0.655927 |
| H | 0.168222 | 1.533998 | -0.389438 |
| C | 1.422280 | 1.578353 | -0.076960 |
| C | 1.829160 | 0.334734 | 0.681684 |
| C | 1.777732 | -0.969295 | -0.133311 |
| C | 0.399954 | -1.321634 | -0.722816 |
| C | -0.723144 | -1.521877 | 0.331391 |
| H | -2.747349 | -0.961556 | 0.832962 |
| H | -2.367871 | -0.778773 | -0.875970 |
| H | -1.310396 | 1.053720 | 1.346577 |
| H | -2.739467 | 1.367720 | 0.376949 |
| H | 1.481671 | 2.505028 | 0.499080 |
| H | 1.883989 | 1.689531 | -1.062752 |
| H | 1.217806 | 0.243396 | 1.589181 |
| H | 2.859499 | 0.476485 | 1.046776 |
| H | 2.121348 | -1.792382 | 0.507680 |
| H | 2.504726 | -0.898571 | -0.953725 |
| H | 0.512439 | -2.237860 | -1.314403 |
| H | 0.099448 | -0.542629 | -1.429074 |
| H | -0.328780 | -1.351702 | 1.342734 |
| H | -1.046672 | -2.569429 | 0.323090 |

Rotational constants (GHz): 2.3586600 1.6911900 1.1534900

Vibrational harmonic frequencies (cm-1):

| | | |
|------------|-----------|-----------|
| i1603.4598 | 86.3437 | 110.2111 |
| 205.8920 | 223.4095 | 272.1982 |
| 312.6673 | 350.7588 | 370.9029 |
| 465.6257 | 477.0829 | 508.8637 |
| 548.6665 | 738.9651 | 759.1572 |
| 810.0308 | 860.1464 | 867.5239 |
| 897.5551 | 933.6747 | 983.2791 |
| 999.3077 | 1055.9929 | 1079.1844 |
| 1080.5213 | 1108.5921 | 1117.4123 |
| 1140.4123 | 1189.1499 | 1217.1421 |
| 1238.0743 | 1246.6677 | 1286.9993 |
| 1300.7804 | 1326.0470 | 1357.2846 |
| 1383.4661 | 1387.3634 | 1399.5992 |
| 1403.3319 | 1408.4232 | 1417.8207 |
| 1464.4656 | 1467.6086 | 1481.0407 |
| 1487.9453 | 1501.5674 | 1514.0746 |
| 1522.1949 | 2967.9160 | 2992.1747 |
| 3000.2998 | 3023.7299 | 3024.4038 |
| 3030.5713 | 3046.7328 | 3049.9742 |
| 3062.9208 | 3067.7463 | 3074.9196 |
| 3077.6359 | 3109.9961 | 3155.0421 |

Zero-point correction (Hartree): 0.205148

C7H15O.1-8Hshift.TBCe

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.92436469

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| C | 0.965178 | 1.541978 | -0.045690 |
| C | 1.690822 | 0.367542 | 0.644919 |
| C | 1.888212 | -0.910219 | -0.187892 |
| O | 0.755588 | -1.412943 | -0.846917 |
| H | -0.168035 | -1.541503 | -0.044732 |
| C | -1.167295 | -1.412853 | 0.758964 |
| C | -2.126129 | -0.454865 | 0.077324 |
| C | -1.469446 | 0.720238 | -0.677949 |
| C | -0.563604 | 1.659716 | 0.157610 |
| H | 1.406246 | 2.470128 | 0.338889 |
| H | 1.185925 | 1.530494 | -1.121538 |
| H | 1.176948 | 0.117983 | 1.581913 |
| H | 2.696938 | 0.691168 | 0.943512 |
| H | 2.371155 | -1.676903 | 0.442503 |
| H | 2.593590 | -0.686978 | -1.005932 |
| H | -0.717904 | -1.040853 | 1.681495 |
| H | -1.533150 | -2.434740 | 0.883461 |
| H | -2.816133 | -0.052725 | 0.836829 |
| H | -2.747687 | -1.011385 | -0.633948 |
| H | -2.282683 | 1.310987 | -1.116333 |
| H | -0.893377 | 0.310447 | -1.512596 |
| H | -0.790748 | 1.554384 | 1.228370 |

| | | | | |
|---|-----------|-----------|-----------|-----------|
| H | -0.832215 | 2.693824 | -0.090286 | |
| Rotational constants (GHz): | 2.3234100 | | 1.7207800 | 1.2021600 |
| Vibrational harmonic frequencies (cm-1): | | | | |
| i1564.3515 | | 91.1744 | | 149.9409 |
| 183.3222 | | 190.3215 | | 238.0248 |
| 267.1906 | | 312.9192 | | 429.1997 |
| 436.1062 | | 460.9432 | | 563.6219 |
| 612.2349 | | 716.3844 | | 754.9492 |
| 803.5772 | | 848.9780 | | 901.9228 |
| 910.3069 | | 940.9083 | | 976.2902 |
| 1004.5095 | | 1062.7107 | | 1076.8505 |
| 1084.5737 | | 1113.9622 | | 1122.2564 |
| 1153.7261 | | 1203.2044 | | 1217.6583 |
| 1256.6987 | | 1269.6844 | | 1278.2143 |
| 1304.1730 | | 1323.3457 | | 1365.4657 |
| 1374.8723 | | 1379.9816 | | 1386.1447 |
| 1403.7195 | | 1406.1978 | | 1421.4326 |
| 1469.9544 | | 1488.4050 | | 1492.2224 |
| 1496.4398 | | 1498.7833 | | 1507.5159 |
| 1511.1523 | | 2963.7087 | | 2992.1012 |
| 2998.9009 | | 3019.2888 | | 3024.9633 |
| 3033.9712 | | 3042.7989 | | 3063.2001 |
| 3067.3872 | | 3070.0490 | | 3072.4492 |
| 3092.9012 | | 3110.1836 | | 3167.7311 |
| Zero-point correction (Hartree): 0.205449 | | | | |

C7H15O.1-8Hshift.TBCf

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.92771814

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | | |
|---|-----------|-----------|-----------|-----------|
| C | 0.583667 | -1.609066 | -0.271822 | |
| C | -0.581945 | -1.304911 | 0.706570 | |
| C | -1.872988 | -0.808953 | 0.037480 | |
| C | -1.732938 | 0.551219 | -0.656124 | |
| O | -1.359235 | 1.593220 | 0.208899 | |
| H | -0.144537 | 1.557534 | 0.378484 | |
| C | 1.141824 | 1.625992 | 0.486649 | |
| C | 1.872921 | 0.668757 | -0.432796 | |
| C | 1.885500 | -0.820184 | -0.037605 | |
| H | 0.827459 | -2.676412 | -0.213305 | |
| H | 0.259174 | -1.444783 | -1.308299 | |
| H | -0.271502 | -0.559461 | 1.446387 | |
| H | -0.817572 | -2.207440 | 1.282045 | |
| H | -2.660772 | -0.724888 | 0.796105 | |
| H | -2.219534 | -1.546747 | -0.700422 | |
| H | -2.706240 | 0.852108 | -1.076150 | |
| H | -1.049027 | 0.485575 | -1.519011 | |
| H | 1.306817 | 1.449863 | 1.553439 | |
| H | 1.289449 | 2.679148 | 0.233459 | |
| H | 2.920133 | 1.011175 | -0.477426 | |
| H | 1.498653 | 0.777080 | -1.460941 | |
| H | 2.182909 | -0.910837 | 1.016732 | |
| H | 2.682229 | -1.304791 | -0.616404 | |
| Rotational constants (GHz): | 2.3264000 | | 1.6879000 | 1.1287100 |
| Vibrational harmonic frequencies (cm-1): | | | | |
| i1601.1102 | | 84.3551 | | 101.1029 |
| 196.5018 | | 220.2349 | | 278.1893 |
| 309.2360 | | 352.7012 | | 387.2268 |
| 421.9697 | | 480.5618 | | 516.1278 |
| 554.1362 | | 729.3746 | | 761.6209 |
| 806.5901 | | 844.2724 | | 865.0779 |
| 908.2265 | | 943.6137 | | 987.9068 |
| 1026.8048 | | 1051.7469 | | 1073.0287 |
| 1093.3662 | | 1105.0303 | | 1126.6201 |
| 1140.5936 | | 1182.4178 | | 1212.9520 |
| 1235.0012 | | 1241.6946 | | 1287.2184 |
| 1302.6052 | | 1324.1905 | | 1359.9611 |
| 1378.4599 | | 1390.3454 | | 1396.0732 |
| 1398.2721 | | 1414.2306 | | 1434.7598 |
| 1467.4386 | | 1469.8478 | | 1479.2115 |
| 1491.2843 | | 1502.4456 | | 1510.3333 |
| 1522.6560 | | 2977.0507 | | 2984.2973 |
| 3008.3116 | | 3021.4585 | | 3025.8934 |
| 3029.8970 | | 3037.1586 | | 3050.4849 |
| 3064.3568 | | 3068.9660 | | 3076.3751 |
| 3078.5179 | | 3095.4700 | | 3152.6611 |
| Zero-point correction (Hartree): 0.205123 | | | | |

C7H15O.1-8Hshift.TBCh

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.92733277

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|----------|----------|-----------|
| C | 2.015204 | 0.285786 | -0.250371 |
|---|----------|----------|-----------|

| | | | |
|--|-----------|-----------|-----------|
| C | 1.441658 | -0.790641 | 0.703281 |
| C | 0.482106 | -1.800291 | 0.040905 |
| C | -0.723208 | -1.258634 | -0.749499 |
| C | -1.883417 | -0.637060 | 0.045999 |
| C | -1.626517 | 0.764934 | 0.621110 |
| O | -1.136836 | 1.681362 | -0.327371 |
| H | 0.088061 | 1.616094 | -0.334505 |
| C | 1.364752 | 1.649518 | -0.147458 |
| H | 3.085440 | 0.427064 | -0.030162 |
| H | 1.979723 | -0.072470 | -1.286935 |
| H | 0.957220 | -0.300577 | 1.556142 |
| H | 2.270078 | -1.367865 | 1.131134 |
| H | 0.120978 | -2.494295 | 0.812616 |
| H | 1.078344 | -2.411068 | -0.651226 |
| H | -1.133129 | -2.099762 | -1.322559 |
| H | -0.390941 | -0.529136 | -1.497900 |
| H | -2.188020 | -1.306002 | 0.863893 |
| H | -2.744910 | -0.561794 | -0.629349 |
| H | -0.966986 | 0.722172 | 1.501140 |
| H | -2.576276 | 1.186209 | 0.988077 |
| H | 1.420164 | 2.094415 | 0.850420 |
| H | 1.671465 | 2.364439 | -0.915628 |
| Rotational constants (GHz): | 2.2168200 | 1.7773800 | 1.1511700 |
| Vibrational harmonic frequencies (cm-1): | | | |
| i1597.2025 | 87.1088 | | 136.7100 |
| 177.0230 | 210.5680 | | 231.7696 |
| 277.3259 | 373.9886 | | 384.7286 |
| 449.9781 | 502.6541 | | 527.4298 |
| 595.2967 | 720.3214 | | 777.9188 |
| 797.8360 | 807.7541 | | 856.7539 |
| 902.0107 | 955.2363 | | 988.0438 |
| 1018.4507 | 1049.0910 | | 1060.4252 |
| 1085.9609 | 1101.2145 | | 1128.4077 |
| 1148.7344 | 1194.6321 | | 1232.8882 |
| 1234.3426 | 1254.6314 | | 1282.2698 |
| 1312.9389 | 1329.0894 | | 1354.3040 |
| 1380.5981 | 1394.5529 | | 1398.6094 |
| 1405.8838 | 1414.1034 | | 1420.4653 |
| 1467.5335 | 1473.4211 | | 1486.7329 |
| 1491.5107 | 1501.2436 | | 1511.8537 |
| 1514.2916 | 2988.4061 | | 2992.5014 |
| 3014.8922 | 3016.4106 | | 3024.3210 |
| 3036.8931 | 3044.6439 | | 3053.1289 |
| 3059.9271 | 3069.2743 | | 3075.2626 |
| 3078.8914 | 3082.8288 | | 3152.4005 |
| Zero-point correction (Hartree): | 0.205259 | | |

C7H15O.1-8Hshift.TBCi

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.92712625

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|--|-----------|-----------|-----------|
| C | -1.163792 | -1.707376 | 0.017167 |
| C | -1.770838 | -0.496167 | 0.694123 |
| C | -1.808365 | 0.797753 | -0.145815 |
| C | -0.502842 | 1.257515 | -0.825544 |
| C | 0.684034 | 1.639839 | 0.082788 |
| C | 1.382915 | 0.522427 | 0.880937 |
| C | 2.014869 | -0.619141 | 0.068092 |
| O | 1.170418 | -1.280415 | -0.841382 |
| H | 0.062927 | -1.494890 | -0.349038 |
| H | -1.088064 | -2.593604 | 0.652143 |
| H | -1.598953 | -1.952283 | -0.956521 |
| H | -1.270628 | -0.317754 | 1.651729 |
| H | -2.809829 | -0.751713 | 0.961158 |
| H | -2.189438 | 1.605371 | 0.494290 |
| H | -2.557686 | 0.666655 | -0.938488 |
| H | -0.755351 | 2.148219 | -1.416401 |
| H | -0.172309 | 0.499445 | -1.539286 |
| H | 0.354747 | 2.408925 | 0.796233 |
| H | 1.440162 | 2.125791 | -0.549544 |
| H | 0.699553 | 0.088477 | 1.617682 |
| H | 2.192966 | 0.974372 | 1.469757 |
| H | 2.491559 | -1.326890 | 0.768717 |
| H | 2.821105 | -0.205899 | -0.561870 |
| Rotational constants (GHz): | 2.3217100 | 1.7134000 | 1.2381000 |
| Vibrational harmonic frequencies (cm-1): | | | |
| i1649.9982 | 77.1490 | | 156.3566 |
| 193.5922 | 252.2028 | | 263.0114 |
| 280.3610 | 348.5291 | | 400.1875 |
| 453.1512 | 485.8960 | | 546.6939 |
| 583.5235 | 743.8557 | | 768.7409 |
| 811.3397 | 827.1923 | | 873.3589 |
| 883.2646 | 934.0524 | | 976.3560 |
| 996.4486 | 1059.8090 | | 1066.9608 |

| | | |
|-----------|-----------|-----------|
| 1080.4449 | 1108.1455 | 1133.8363 |
| 1158.1391 | 1193.7375 | 1218.9500 |
| 1241.8052 | 1254.5572 | 1284.7214 |
| 1318.3207 | 1325.5675 | 1369.1875 |
| 1385.2726 | 1394.4777 | 1403.9004 |
| 1407.3281 | 1420.3030 | 1422.2680 |
| 1469.4870 | 1482.3846 | 1492.5063 |
| 1499.0820 | 1501.4066 | 1511.5382 |
| 1514.8159 | 2958.8669 | 2986.1660 |
| 2993.3917 | 3012.1712 | 3019.9757 |
| 3035.2901 | 3040.7586 | 3048.3862 |
| 3051.4532 | 3074.4017 | 3079.7445 |
| 3101.8095 | 3123.3369 | 3154.5650 |

Zero-point correction (Hartree): 0.205615

C7H15O.1-8Hshift.TCBg

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.92852084

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| C | 1.560329 | 1.012818 | 0.219786 |
| C | 0.361707 | 1.405823 | -0.686346 |
| C | -0.992585 | 1.569146 | 0.033399 |
| C | -1.517050 | 0.354058 | 0.813747 |
| C | -1.901770 | -0.877524 | -0.019193 |
| O | -0.900188 | -1.383237 | -0.866271 |
| H | 0.141684 | -1.511475 | -0.233578 |
| C | 1.258472 | -1.555769 | 0.421177 |
| C | 2.127580 | -0.399216 | -0.026829 |
| H | 2.378001 | 1.725379 | 0.060593 |
| H | 1.289601 | 1.112276 | 1.280045 |
| H | 0.251136 | 0.670008 | -1.487085 |
| H | 0.585800 | 2.362576 | -1.173649 |
| H | -1.746741 | 1.866397 | -0.708473 |
| | | | |
| H | -0.914760 | 2.410167 | 0.736438 |
| H | -2.412518 | 0.653610 | 1.375224 |
| H | -0.783366 | 0.052591 | 1.571894 |
| H | -2.724018 | -0.604373 | -0.702061 |
| H | -2.298143 | -1.657429 | 0.654451 |
| H | 1.634007 | -2.543061 | 0.139805 |
| H | 0.966023 | -1.529389 | 1.474306 |
| H | 2.362801 | -0.511076 | -1.093150 |
| H | 3.091891 | -0.486311 | 0.500960 |

Rotational constants (GHz): 2.3365000 1.7220100 1.1956700

Vibrational harmonic frequencies (cm-1):

| | | |
|------------|-----------|-----------|
| i1580.9815 | 103.1986 | 154.4068 |
| 178.1688 | 223.2265 | 238.1516 |
| 311.1907 | 314.2174 | 418.9408 |
| 433.6790 | 499.5562 | 553.8753 |
| 622.5253 | 731.5825 | 770.7261 |
| 817.4120 | 844.2772 | 872.6718 |
| 897.1949 | 931.2060 | 975.4219 |
| 1003.0190 | 1056.8431 | 1068.5776 |
| 1083.1374 | 1105.0839 | 1121.4041 |
| 1157.5209 | 1205.8404 | 1210.2892 |
| 1245.9153 | 1263.2804 | 1289.2618 |
| 1291.2333 | 1327.5784 | 1361.9571 |
| 1380.0106 | 1388.7581 | 1392.6591 |
| 1402.4497 | 1412.8787 | 1423.1607 |
| 1468.4681 | 1483.9951 | 1488.1687 |
| 1494.9620 | 1501.3607 | 1510.6609 |
| 1519.3193 | 2959.7229 | 2985.4116 |
| 2996.9372 | 3016.3824 | 3027.7243 |
| 3034.3937 | 3044.3873 | 3052.4057 |
| 3057.4129 | 3071.8320 | 3075.4080 |
| 3081.0417 | 3117.8217 | 3155.0647 |

Zero-point correction (Hartree): 0.205549

C7H15O.1-8Hshift.TCCA

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.92066077

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| H | -0.270395 | -1.589221 | -0.176113 |
| C | -1.415678 | -1.280260 | -0.708894 |
| C | -2.168987 | -0.298751 | 0.163454 |
| C | -1.299626 | 0.832877 | 0.744684 |
| C | -0.483627 | 1.639618 | -0.299582 |
| C | 1.045283 | 1.624583 | -0.112289 |
| C | 1.810036 | 0.325347 | -0.442603 |
| C | 1.665500 | -0.857472 | 0.548618 |
| O | 0.858795 | -1.929933 | 0.136067 |
| H | -1.877096 | -2.265430 | -0.808475 |
| H | -1.105099 | -0.895234 | -1.682285 |

| | | | | |
|---|-----------|-----------|-----------|--|
| H | -2.652751 | -0.832367 | 0.989865 | |
| H | -2.983906 | 0.142066 | -0.434061 | |
| H | -0.624888 | 0.395369 | 1.488172 | |
| H | -1.952946 | 1.511191 | 1.305586 | |
| H | -0.807915 | 2.686588 | -0.270233 | |
| H | -0.717976 | 1.295011 | -1.314885 | |
| H | 1.281740 | 1.920899 | 0.920076 | |
| H | 1.464489 | 2.415427 | -0.747977 | |
| H | 2.873427 | 0.591528 | -0.493149 | |
| H | 1.545264 | -0.039896 | -1.442604 | |
| H | 1.387085 | -0.481040 | 1.547680 | |
| H | 2.653205 | -1.331078 | 0.669537 | |
| Rotational constants (GHz): | 2.1742400 | 1.7491300 | 1.1326800 | |
| Vibrational harmonic frequencies (cm ⁻¹): | | | | |
| i1631.2766 | 55.0549 | | 127.5574 | |
| 153.6840 | 201.1346 | | 254.6871 | |
| 294.3568 | 313.7214 | | 397.0495 | |
| 431.4518 | 457.8387 | | 504.0408 | |
| 551.4604 | 729.5798 | | 752.1738 | |
| 793.8331 | 848.6449 | | 887.3436 | |
| 911.2548 | 942.5554 | | 997.4593 | |
| 1019.3414 | 1052.1072 | | 1071.9418 | |
| 1081.3689 | 1107.5527 | | 1121.0724 | |
| 1144.6391 | 1195.6074 | | 1208.2287 | |
| 1239.7884 | 1263.1692 | | 1287.7950 | |
| 1294.1331 | 1315.0180 | | 1357.6836 | |
| 1370.3317 | 1375.7551 | | 1390.8583 | |
| 1395.3835 | 1404.4600 | | 1408.1610 | |
| 1472.3854 | 1485.3704 | | 1490.2058 | |
| 1492.7749 | 1498.2662 | | 1513.6893 | |
| 1515.9546 | 2967.1365 | | 2988.9090 | |
| 2999.7115 | 3016.3862 | | 3034.8513 | |
| 3037.8305 | 3049.5457 | | 3060.0579 | |
| 3069.0531 | 3075.0094 | | 3081.2419 | |
| 3091.7723 | 3094.2749 | | 3165.5616 | |
| Zero-point correction (Hartree): | 0.204828 | | | |

C7H15O.1-8Hshift.TCCb

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.92750165

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | | |
|---|-----------|-----------|-----------|--|
| O | -1.039099 | -1.420679 | -0.690553 | |
| H | 0.027612 | -1.447358 | -0.082994 | |
| C | 1.151808 | -1.499333 | 0.558054 | |
| C | 2.145298 | -0.585212 | -0.127046 | |
| C | 1.874118 | 0.926637 | -0.016449 | |
| C | 0.487724 | 1.364166 | -0.534147 | |
| C | -0.636217 | 1.357619 | 0.537373 | |
| C | -1.971098 | 0.761038 | 0.058509 | |
| C | -2.008914 | -0.772750 | 0.095989 | |
| H | 1.383699 | -2.563533 | 0.465305 | |
| H | 0.901185 | -1.235733 | 1.589073 | |
| H | 2.204829 | -0.862057 | -1.188324 | |
| H | 3.145279 | -0.794643 | 0.287435 | |
| H | 2.658555 | 1.441636 | -0.584404 | |
| H | 1.998147 | 1.249989 | 1.026510 | |
| H | 0.201136 | 0.713472 | -1.366632 | |
| H | 0.564958 | 2.374859 | -0.951757 | |
| H | -0.803868 | 2.384698 | 0.882757 | |
| H | -0.307298 | 0.806817 | 1.428328 | |
| H | -2.189010 | 1.106484 | -0.960252 | |
| H | -2.790948 | 1.123365 | 0.693807 | |
| H | -2.977814 | -1.127606 | -0.291499 | |
| H | -1.959978 | -1.117944 | 1.143374 | |
| Rotational constants (GHz): | 2.5556700 | 1.5724900 | 1.1134200 | |
| Vibrational harmonic frequencies (cm ⁻¹): | | | | |
| i1611.2861 | 119.4600 | | 143.6514 | |
| 157.0825 | 183.4662 | | 287.8695 | |
| 311.7093 | 319.8053 | | 346.5452 | |
| 445.5945 | 504.0023 | | 529.0136 | |
| 605.3153 | 727.6778 | | 786.7801 | |
| 821.3485 | 837.8809 | | 883.2772 | |
| 899.1972 | 938.3255 | | 986.1814 | |
| 992.3413 | 1049.9071 | | 1068.8932 | |
| 1090.5785 | 1107.2411 | | 1114.6505 | |
| 1144.2280 | 1189.3994 | | 1220.5085 | |
| 1237.7550 | 1268.4632 | | 1277.4040 | |
| 1300.5381 | 1322.2486 | | 1352.0894 | |
| 1381.0724 | 1386.2552 | | 1393.1046 | |
| 1402.0195 | 1406.8255 | | 1419.6886 | |
| 1466.4451 | 1469.4828 | | 1478.9855 | |
| 1492.9047 | 1508.0663 | | 1515.0574 | |
| 1519.0972 | 2966.6516 | | 2988.5872 | |

| | | |
|-----------|-----------|-----------|
| 3006.1822 | 3025.3816 | 3028.5319 |
| 3036.3226 | 3043.2470 | 3048.0880 |
| 3065.5640 | 3071.6941 | 3075.6890 |
| 3080.8408 | 3098.2018 | 3155.1358 |

Zero-point correction (Hartree): 0.205262

C7H15O.1-8Hshift.TCCE

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.92442266

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| C | 0.460304 | -1.587226 | -0.299038 |
| C | 1.270292 | -0.796207 | 0.756104 |
| C | 2.145722 | 0.309420 | 0.145311 |
| O | 1.476871 | 1.105187 | -0.796826 |
| H | 0.409789 | 1.477986 | -0.323857 |
| C | -0.731046 | 1.941653 | 0.074173 |
| C | -1.695906 | 0.866103 | 0.533477 |
| C | -1.866378 | -0.351963 | -0.409975 |
| C | -1.062360 | -1.625657 | -0.071195 |
| H | 0.652631 | -1.156780 | -1.288619 |
| H | 0.824518 | -2.620730 | -0.333370 |
| H | 1.916018 | -1.466064 | 1.337335 |
| H | 0.597042 | -0.333648 | 1.486481 |
| H | 2.971874 | -0.149996 | -0.422979 |
| H | 2.607945 | 0.910420 | 0.947072 |
| H | -1.030087 | 2.435376 | -0.855414 |
| H | -0.461491 | 2.673931 | 0.839439 |
| H | -2.676001 | 1.358524 | 0.639878 |
| H | -1.437815 | 0.524005 | 1.542587 |
| H | -1.643200 | -0.046259 | -1.440797 |
| H | -2.925500 | -0.636720 | -0.405181 |
| H | -1.473335 | -2.433805 | -0.690456 |
| H | -1.271130 | -1.914476 | 0.969340 |

Rotational constants (GHz): 2.2607600 1.7187200 1.1482700

Vibrational harmonic frequencies (cm-1):

| | | |
|------------|-----------|-----------|
| i1601.1769 | 44.7894 | 139.2145 |
| 166.5841 | 205.8685 | 261.9111 |
| 298.9108 | 310.0634 | 384.3616 |
| 449.5183 | 488.0024 | 509.2398 |
| 577.0199 | 729.3456 | 769.0456 |
| 800.8383 | 862.7089 | 870.0026 |
| 899.7061 | 951.5428 | 994.7739 |
| 1009.8596 | 1060.2205 | 1075.5886 |
| 1085.9385 | 1100.5912 | 1118.6832 |
| 1145.3873 | 1197.9451 | 1227.9691 |
| 1229.8291 | 1262.0980 | 1283.1576 |
| 1301.7022 | 1317.6790 | 1351.2184 |
| 1368.2959 | 1380.6662 | 1395.7343 |
| 1400.8278 | 1409.6747 | 1429.4748 |
| 1467.8774 | 1489.2537 | 1491.4135 |
| 1496.2747 | 1498.9547 | 1504.8590 |
| 1511.4791 | 2966.7660 | 2988.9629 |
| 3000.4419 | 3014.6241 | 3031.4462 |
| 3039.2366 | 3049.3515 | 3059.5356 |
| 3064.9461 | 3072.5091 | 3076.0150 |
| 3085.6936 | 3091.5314 | 3153.3755 |

Zero-point correction (Hartree): 0.205082

5-me-pentoxy.pmm

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -311.63366618

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -1.442558 | -1.287750 | 0.489498 |
| C | -1.924369 | -0.084036 | -0.092075 |
| C | -1.046768 | 1.143807 | 0.177529 |
| C | 0.285492 | 1.239959 | -0.591010 |
| C | 1.379436 | 0.174774 | -0.303510 |
| C | 1.674533 | -0.001548 | 1.196772 |
| H | -2.080212 | -0.199242 | -1.178432 |
| H | -2.911356 | 0.081733 | 0.353869 |
| H | -1.636283 | 2.033435 | -0.084458 |
| H | -0.867013 | 1.204579 | 1.257575 |
| H | 0.077374 | 1.238969 | -1.670436 |
| H | 0.721188 | 2.222979 | -0.371455 |
| C | 1.126939 | -1.135988 | -0.980707 |
| H | 2.300609 | 0.583348 | -0.764644 |
| H | 0.824902 | -0.463445 | 1.707231 |
| H | 1.880565 | 0.962732 | 1.673375 |
| H | 2.549968 | -0.642401 | 1.346535 |
| H | 0.726014 | -1.158887 | -1.991525 |
| H | -0.643933 | -1.547567 | -0.004760 |
| H | 1.627062 | -2.036041 | -0.630850 |

Rotational constants (GHz): 3.2539600 1.9643800 1.6905700

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 97.7856 | 117.1868 | 182.5332 |
| 245.7691 | 271.4921 | 283.1386 |
| 307.9490 | 371.4887 | 387.1615 |
| 464.2386 | 521.9452 | 552.9783 |
| 654.1490 | 739.6388 | 844.2027 |
| 868.4014 | 900.5669 | 939.7288 |
| 966.1328 | 1032.9239 | 1041.1990 |
| 1051.8100 | 1102.5501 | 1151.6093 |
| 1184.4488 | 1218.4188 | 1249.2848 |
| 1279.6479 | 1322.5342 | 1348.1405 |
| 1388.5224 | 1402.0618 | 1410.6115 |
| 1422.7898 | 1434.8435 | 1474.6011 |
| 1486.7357 | 1498.5851 | 1511.0322 |
| 1517.0007 | 1532.1170 | 2907.1853 |
| 2974.6436 | 3019.6235 | 3031.0212 |
| 3046.9627 | 3060.8970 | 3077.9359 |
| 3084.1390 | 3112.8398 | 3135.4465 |
| 3135.8947 | 3236.4224 | 3604.8167 |

Zero-point correction (Hartree): 0.180444

5-me-pentoxo.pmp

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -311.63353901

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -1.973044 | 1.090057 | -0.402751 |
| C | -2.091365 | -0.150183 | 0.275524 |
| C | -1.095582 | -1.221858 | -0.186338 |
| C | 0.364366 | -1.079786 | 0.283121 |
| C | 1.176021 | 0.110773 | -0.280797 |
| C | 0.840810 | 1.419295 | 0.367771 |
| H | -2.016770 | -0.021369 | 1.369552 |
| H | -3.108610 | -0.500324 | 0.067711 |
| H | -1.465253 | -2.192189 | 0.173161 |
| H | -1.129348 | -1.264510 | -1.283024 |
| H | 0.394530 | -1.038959 | 1.382407 |
| H | 0.889566 | -2.002544 | 0.005419 |
| C | 2.696756 | -0.160501 | -0.130549 |
| H | 0.967706 | 0.192292 | -1.357412 |
| H | 0.698142 | 1.464592 | 1.445901 |
| H | -1.116124 | 1.479123 | -0.147820 |
| H | 1.088787 | 2.353282 | -0.130920 |
| H | 2.979093 | -1.070638 | -0.671918 |
| H | 2.965841 | -0.294647 | 0.922988 |
| H | 3.290753 | 0.668994 | -0.526420 |

Rotational constants (GHz): 4.2858600 1.6167900 1.2857100

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 61.4690 | 111.4572 | 172.1023 |
| 226.7645 | 262.8872 | 280.2634 |
| 297.0902 | 351.0632 | 414.7260 |
| 423.9409 | 486.2794 | 514.8060 |
| 685.0694 | 758.3341 | 854.7088 |
| 864.9672 | 916.9712 | 931.8325 |
| 972.8639 | 1010.1215 | 1040.1617 |
| 1057.4536 | 1111.0797 | 1148.0034 |
| 1155.0039 | 1224.1378 | 1262.8707 |
| 1295.4679 | 1317.1544 | 1369.1099 |
| 1393.4937 | 1396.7995 | 1408.0726 |
| 1413.0953 | 1439.3224 | 1472.9435 |
| 1485.3519 | 1497.8537 | 1506.8940 |
| 1512.4808 | 1518.4391 | 2968.8142 |
| 3010.7209 | 3022.6249 | 3024.9004 |
| 3037.4737 | 3058.6222 | 3071.1582 |
| 3078.7509 | 3109.9001 | 3119.7655 |
| 3131.6804 | 3233.3262 | 3583.7949 |

Zero-point correction (Hartree): 0.180145

5-me-pentoxo.pmt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -311.63752378

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 1.795453 | 1.146979 | -0.674964 |
| C | 2.116905 | -0.141839 | -0.339152 |
| C | 1.229143 | -0.779953 | 0.740548 |
| C | -0.196332 | -1.085418 | 0.251691 |
| C | -1.037376 | 0.124830 | -0.202081 |
| C | -2.379499 | -0.353161 | -0.777298 |
| H | 2.202840 | -0.791162 | -1.232377 |
| H | 3.154443 | -0.057229 | 0.054083 |
| H | 1.703602 | -1.715772 | 1.063863 |
| H | 1.209812 | -0.115621 | 1.611446 |
| H | -0.133387 | -1.801013 | -0.580750 |
| H | -0.734956 | -1.606785 | 1.056017 |

| | | | |
|--|-----------|-----------|-----------|
| C | -1.256075 | 1.146979 | 0.922700 |
| H | -0.489262 | 0.635985 | -1.008451 |
| H | -2.976063 | -0.861277 | -0.009170 |
| H | -2.235205 | -1.056610 | -1.604932 |
| H | -2.971360 | 0.488365 | -1.152693 |
| | | | |
| H | -0.313722 | 1.597864 | 1.244374 |
| H | -1.732017 | 0.679496 | 1.794164 |
| H | -1.908944 | 1.959297 | 0.585690 |
| Rotational constants (GHz): | 3.8988900 | 1.5603900 | 1.4331400 |
| Vibrational harmonic frequencies (cm-1): | | | |
| 64.1861 | 101.7838 | 119.7999 | |
| 218.8664 | 241.6082 | 256.0727 | |
| 316.4897 | 363.7446 | 403.6464 | |
| 438.6676 | 493.6763 | 751.3970 | |
| 804.5606 | 834.9952 | 899.9024 | |
| 932.5337 | 935.0615 | 968.9666 | |
| 983.3304 | 1027.2078 | 1085.6521 | |
| 1099.6079 | 1124.2053 | 1172.8478 | |
| 1196.2087 | 1213.7354 | 1281.5469 | |
| 1326.5782 | 1343.2624 | 1362.0874 | |
| 1381.6082 | 1399.1887 | 1406.1298 | |
| 1413.4146 | 1432.8223 | 1483.9537 | |
| 1492.9870 | 1504.0241 | 1509.5718 | |
| 1517.4775 | 1528.9019 | 2881.9505 | |
| 2940.2341 | 2997.4591 | 3012.4946 | |
| 3031.7206 | 3037.5903 | 3040.3855 | |
| 3051.4911 | 3095.2652 | 3097.8043 | |
| 3102.5613 | 3111.2164 | 3130.6763 | |
| Zero-point correction (Hartree): | 0.179891 | | |

5-me-pentoxy.ppm

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -311.63354639
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | |
|--|-----------|-----------|-----------|
| O | 2.712658 | 0.351358 | 0.472712 |
| C | 1.924009 | 0.091670 | -0.614202 |
| C | 0.814287 | -0.950257 | -0.385097 |
| C | -0.124223 | -0.628041 | 0.795557 |
| C | -1.414055 | 0.165009 | 0.480749 |
| C | -1.154956 | 1.541726 | -0.150733 |
| H | 1.483415 | 1.080112 | -0.866584 |
| H | 2.541974 | -0.159443 | -1.498320 |
| H | 0.258034 | -1.077121 | -1.322598 |
| H | 1.312444 | -1.909239 | -0.199396 |
| H | -0.425831 | -1.569124 | 1.271702 |
| H | 0.464039 | -0.088556 | 1.548574 |
| C | -2.405028 | -0.647436 | -0.367972 |
| H | -1.895656 | 0.344301 | 1.452965 |
| H | -0.747060 | 1.451323 | -1.165069 |
| H | -0.453666 | 2.134955 | 0.446382 |
| H | -2.086344 | 2.112667 | -0.233727 |
| H | -2.635095 | -1.610302 | 0.101288 |
| H | -2.009969 | -0.852048 | -1.370001 |
| H | -3.347751 | -0.104416 | -0.496728 |
| Rotational constants (GHz): | 4.5295600 | 1.4114200 | 1.2762600 |
| Vibrational harmonic frequencies (cm-1): | | | |
| 49.6190 | 92.0444 | 157.6253 | |
| 223.4215 | 235.9357 | 266.2698 | |
| 295.8209 | 372.2669 | 375.3119 | |
| 473.7582 | 552.8615 | 670.2468 | |
| 757.9370 | 839.6976 | 891.5241 | |
| 909.8612 | 939.9873 | 970.7341 | |
| 995.7643 | 1016.0892 | 1083.0194 | |
| 1104.8151 | 1132.5272 | 1167.5606 | |
| 1210.3345 | 1227.9034 | 1293.4897 | |
| 1323.2589 | 1360.1457 | 1368.1081 | |
| 1376.7189 | 1384.1599 | 1411.8273 | |
| 1415.5941 | 1434.6739 | 1494.7258 | |
| 1500.7227 | 1504.4418 | 1511.5269 | |
| 1523.3421 | 1524.8209 | 2902.7582 | |
| 2940.5028 | 3012.9288 | 3031.2515 | |
| 3036.6608 | 3038.3080 | 3046.0110 | |
| 3075.7392 | 3081.2315 | 3095.6097 | |
| 3104.6367 | 3107.6887 | 3110.0783 | |
| Zero-point correction (Hartree): | 0.180030 | | |

5-me-pentoxy.ppp

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -311.63676277
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -2.551903 | -0.965762 | -0.316347 |
| C | -2.067114 | 0.306900 | -0.455905 |

| | | | |
|--|-----------|-----------|-----------|
| C | -1.115513 | 0.770593 | 0.658564 |
| C | 0.101832 | -0.145806 | 0.853688 |
| C | 1.163386 | -0.122473 | -0.266589 |
| C | 1.853161 | 1.244436 | -0.395281 |
| H | -1.536863 | 0.288436 | -1.433899 |
| H | -2.892938 | 1.026595 | -0.616965 |
| H | -0.811797 | 1.803870 | 0.448456 |
| H | -1.690874 | 0.805413 | 1.591909 |
| H | 0.593371 | 0.111547 | 1.801999 |
| H | -0.272380 | -1.170469 | 0.967936 |
| C | 2.202681 | -1.229059 | -0.031542 |
| H | 0.664580 | -0.340796 | -1.223002 |
| H | 2.363337 | 1.511371 | 0.538581 |
| H | 1.146965 | 2.047950 | -0.628053 |
| H | 2.605853 | 1.230484 | -1.191010 |
| H | 1.730672 | -2.216237 | 0.014974 |
| H | 2.734804 | -1.069619 | 0.914457 |
| H | 2.949900 | -1.249992 | -0.832213 |
| Rotational constants (GHz): | 4.2924000 | 1.3676800 | 1.2131500 |
| Vibrational harmonic frequencies (cm-1): | | | |
| 30.2759 | 74.6910 | 165.7788 | |
| 208.2263 | 235.2299 | 255.2297 | |
| 305.0614 | 371.6822 | 412.7151 | |
| 441.5043 | 523.2208 | 627.4280 | |
| 767.7580 | 825.5426 | 901.6594 | |
| 913.7916 | 932.3703 | 970.3834 | |
| 985.4194 | 1040.6464 | 1082.8111 | |
| 1098.2484 | 1125.5953 | 1182.9709 | |
| 1196.0231 | 1232.4169 | 1288.8981 | |
| 1324.3741 | 1345.1408 | 1370.8407 | |
| 1371.8676 | 1395.9734 | 1408.4418 | |
| 1416.1701 | 1435.7168 | 1489.7516 | |
| 1496.5212 | 1503.9642 | 1510.1380 | |
| 1519.4427 | 1525.8200 | 2885.7798 | |
| 2942.2891 | 3006.7377 | 3028.5299 | |
| 3033.1735 | 3037.7558 | 3045.4048 | |
| 3074.0342 | 3084.0761 | 3099.6476 | |
| 3105.7747 | 3111.3385 | 3113.2875 | |
| Zero-point correction (Hartree): | 0.179696 | | |

5-me-pentoxy.ppt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -311.63482962
Electronic state : 2-A
Cartesian coordinates (Angs):

| | | | |
|--|-----------|-----------|-----------|
| O | 2.521572 | -0.038231 | 1.047281 |
| C | 2.086687 | 0.376428 | -0.181551 |
| C | 1.092315 | -0.572307 | -0.874612 |
| C | -0.168153 | -0.889273 | -0.046723 |
| C | -1.408877 | -0.016866 | -0.329364 |
| C | -2.603772 | -0.514995 | 0.497668 |
| H | 1.608856 | 1.358560 | 0.024060 |
| H | 2.941055 | 0.625461 | -0.840547 |
| H | 0.825195 | -0.148895 | -1.852634 |
| H | 1.635806 | -1.501128 | -1.084461 |
| H | -0.452169 | -1.933779 | -0.223678 |
| H | 0.095265 | -0.830479 | 1.018352 |
| C | -1.175772 | 1.481788 | -0.083906 |
| H | -1.662100 | -0.142467 | -1.393435 |
| H | -2.407437 | -0.407253 | 1.571401 |
| H | -2.811610 | -1.572916 | 0.303394 |
| H | -3.511688 | 0.053159 | 0.267809 |
| H | -0.407960 | 1.894593 | -0.747165 |
| H | -0.866785 | 1.669469 | 0.951915 |
| H | -2.093575 | 2.052872 | -0.262327 |
| Rotational constants (GHz): | 4.5593000 | 1.3187300 | 1.2433800 |
| Vibrational harmonic frequencies (cm-1): | | | |
| 67.8777 | 79.6854 | 150.3475 | |
| 235.5169 | 247.9849 | 265.7048 | |
| 286.1910 | 369.1299 | 409.3975 | |
| 442.7317 | 502.0584 | 687.4296 | |
| 777.4444 | 850.9661 | 899.1549 | |
| 912.2914 | 933.0618 | 969.7898 | |
| 980.6198 | 1048.2355 | 1090.6997 | |
| 1109.0973 | 1125.9788 | 1175.6591 | |
| 1200.7784 | 1235.7268 | 1295.1813 | |
| 1318.2336 | 1338.0908 | 1373.8633 | |
| 1381.1699 | 1387.1222 | 1404.2013 | |
| 1416.3987 | 1434.7290 | 1495.8643 | |
| 1500.1874 | 1505.4941 | 1514.2334 | |
| 1520.6830 | 1525.7428 | 2899.1218 | |
| 2941.4056 | 3001.7088 | 3031.1209 | |
| 3032.1154 | 3033.9959 | 3038.3121 | |
| 3070.0544 | 3079.1780 | 3099.6388 | |
| 3104.4772 | 3105.4228 | 3110.7170 | |

Zero-point correction (Hartree): 0.180003

5-me-pentoxo.ptm

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -311.63652601

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -2.859385 | 0.688562 | 0.247000 |
| C | -2.312319 | -0.468697 | -0.240765 |
| C | -0.810223 | -0.410996 | -0.547894 |
| C | 0.021779 | -0.073967 | 0.696663 |
| C | 1.535268 | 0.137573 | 0.471715 |
| C | 2.231360 | -1.118463 | -0.075643 |
| H | -2.516858 | -1.232279 | 0.542939 |
| H | -2.900569 | -0.824138 | -1.109698 |
| H | -0.508860 | -1.376235 | -0.974399 |
| H | -0.655233 | 0.341071 | -1.330715 |
| H | -0.402866 | 0.831058 | 1.148356 |
| H | -0.112233 | -0.877756 | 1.435444 |
| C | 1.835802 | 1.363812 | -0.404751 |
| H | 1.962111 | 0.338399 | 1.465001 |
| H | 1.901617 | -1.351263 | -1.094647 |
| H | 2.026657 | -1.994754 | 0.550038 |
| H | 3.317472 | -0.980065 | -0.109622 |
| H | 1.357102 | 2.265345 | -0.007001 |
| H | 1.482820 | 1.225001 | -1.432960 |
| H | 2.913925 | 1.551547 | -0.454690 |

Rotational constants (GHz): 5.0079800 1.2286000 1.1146200

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 48.1205 | 93.4081 | 149.2436 |
| 199.3296 | 240.3523 | 254.2218 |
| 259.8839 | 364.5458 | 377.7796 |
| 473.7271 | 521.2449 | 575.0134 |
| 778.2215 | 793.9240 | 899.1750 |
| 926.4777 | 941.7314 | 969.6572 |
| 990.2720 | 1020.9503 | 1074.4127 |
| 1094.5131 | 1135.5274 | 1191.3436 |
| 1210.3981 | 1238.5313 | 1308.5365 |
| 1327.7676 | 1361.3647 | 1364.5444 |
| 1375.0615 | 1381.0526 | 1415.6194 |
| 1417.5523 | 1436.7192 | 1493.2642 |
| 1500.0337 | 1507.7743 | 1511.6569 |
| 1522.1552 | 1524.7274 | 2881.1228 |
| 2934.5623 | 3009.0482 | 3022.0256 |
| 3035.1653 | 3039.0399 | 3044.3026 |
| 3067.9653 | 3089.2998 | 3103.9463 |
| 3106.0253 | 3109.7090 | 3110.8458 |

Zero-point correction (Hartree): 0.179572

5-me-pentoxo.ptp

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -311.63777732

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -2.757281 | -0.179083 | 0.974273 |
| C | -2.447196 | -0.091146 | -0.357374 |
| C | -1.037400 | 0.423164 | -0.673251 |
| C | 0.059285 | -0.467987 | -0.078959 |
| C | 1.504207 | 0.009990 | -0.323112 |
| C | 1.805326 | 1.349616 | 0.366733 |
| H | -2.581269 | -1.123416 | -0.751452 |
| H | -3.229175 | 0.490645 | -0.884403 |
| H | -0.925905 | 0.491578 | -1.764449 |
| H | -0.957370 | 1.445380 | -0.285331 |
| H | -0.116760 | -0.563003 | 1.000776 |
| H | -0.049851 | -1.479959 | -0.495823 |
| C | 2.504732 | -1.063705 | 0.131041 |
| H | 1.632761 | 0.150888 | -1.407462 |
| H | 1.665232 | 1.267795 | 1.451662 |
| H | 1.159133 | 2.156528 | 0.007680 |
| H | 2.841697 | 1.656319 | 0.188253 |
| H | 2.334446 | -2.014524 | -0.385949 |
| H | 2.414656 | -1.250468 | 1.208165 |
| H | 3.536933 | -0.754698 | -0.066317 |

Rotational constants (GHz): 5.0942300 1.1427800 1.0795500

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 48.5520 | 89.2719 | 139.9803 |
| 187.7623 | 230.3314 | 255.8587 |
| 279.5766 | 373.7267 | 397.9287 |
| 440.5987 | 462.4109 | 531.9931 |
| 779.2780 | 826.0361 | 895.8857 |
| 931.3665 | 947.5125 | 962.8489 |
| 973.8411 | 1033.5481 | 1092.2344 |
| 1095.0319 | 1145.2394 | 1189.9346 |

| | | |
|-----------|-----------|-----------|
| 1199.8507 | 1244.0381 | 1304.8903 |
| 1325.0204 | 1355.5621 | 1362.7710 |
| 1376.5101 | 1383.9827 | 1414.6382 |
| 1417.1434 | 1436.0203 | 1491.2710 |
| 1502.8736 | 1504.5622 | 1513.0306 |
| 1518.9639 | 1525.6708 | 2882.0738 |
| 2933.3332 | 3002.7769 | 3013.6515 |
| 3031.6256 | 3033.7816 | 3039.7646 |
| 3061.6730 | 3086.2184 | 3100.3185 |
| 3105.9083 | 3110.1770 | 3117.9319 |

Zero-point correction (Hartree): 0.179307

5-me-pentoxy.ptt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -311.63808357

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 2.881407 | -0.864103 | -0.202341 |
| C | 2.432547 | 0.355915 | 0.229457 |
| C | 1.013597 | 0.732675 | -0.217161 |
| C | -0.037542 | -0.277040 | 0.257979 |
| C | -1.447204 | -0.084964 | -0.332532 |
| C | -2.360928 | -1.251170 | 0.072672 |
| H | 2.482418 | 0.297633 | 1.339937 |
| H | 3.170719 | 1.141821 | -0.024200 |
| H | 0.793749 | 1.741821 | 0.153300 |
| H | 1.004300 | 0.791838 | -1.313775 |
| H | 0.324611 | -1.279672 | -0.000673 |
| H | -0.102474 | -0.246445 | 1.356597 |
| C | -2.075853 | 1.258800 | 0.067842 |
| H | -1.350863 | -0.099058 | -1.428872 |
| H | -2.490995 | -1.286303 | 1.161436 |
| H | -1.943307 | -2.213390 | -0.242877 |
| H | -3.355367 | -1.152576 | -0.375998 |
| H | -1.481187 | 2.111582 | -0.274693 |
| H | -2.171686 | 1.334758 | 1.158407 |
| H | -3.078876 | 1.365514 | -0.359401 |

Rotational constants (GHz): 5.2583900 1.1700200 1.0134100

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 54.1099 | 95.4306 | 149.2438 |
| 177.8513 | 230.2027 | 256.9880 |
| 270.6347 | 366.2393 | 417.6595 |
| 440.4894 | 500.2726 | 541.6561 |
| 777.5327 | 831.6344 | 908.0835 |
| 925.1457 | 932.8123 | 969.1318 |
| 993.4215 | 1021.7413 | 1090.7931 |
| 1094.8827 | 1136.8072 | 1198.2154 |
| 1205.8296 | 1237.7483 | 1293.7121 |
| 1327.6686 | 1353.3506 | 1364.3238 |
| 1373.4503 | 1382.4106 | 1414.4195 |
| 1415.7034 | 1434.4901 | 1491.6519 |
| 1501.8775 | 1505.1953 | 1513.7606 |
| 1518.6743 | 1524.6581 | 2880.9853 |
| 2937.1264 | 3002.4956 | 3013.1074 |
| 3032.3871 | 3036.0627 | 3037.6723 |
| 3064.6848 | 3084.0440 | 3098.2616 |
| 3104.3166 | 3111.3032 | 3115.8384 |

Zero-point correction (Hartree): 0.179424

5-me-pentoxy.tpm

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -311.63271746

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 3.031435 | 0.177710 | -0.594987 |
| C | 1.922760 | 0.264038 | 0.200600 |
| C | 0.868087 | -0.830453 | -0.025841 |
| C | -0.364704 | -0.722716 | 0.897716 |
| C | -1.580589 | 0.074662 | 0.365762 |
| C | -1.257183 | 1.538046 | 0.027459 |
| H | 2.216462 | 0.327229 | 1.268488 |
| H | 1.504920 | 1.271479 | -0.010723 |
| H | 0.579423 | -0.823602 | -1.082825 |
| H | 1.367830 | -1.791282 | 0.143779 |
| H | -0.715490 | -1.734527 | 1.134804 |
| H | -0.052980 | -0.289116 | 1.859378 |
| C | -2.255351 | -0.625675 | -0.824095 |
| H | -2.310303 | 0.087132 | 1.188253 |
| H | -0.591822 | 1.614170 | -0.840567 |
| H | -0.779543 | 2.052684 | 0.869000 |
| H | -2.170257 | 2.089715 | -0.221473 |
| H | -2.538408 | -1.653740 | -0.572825 |
| H | -1.595978 | -0.666230 | -1.698495 |
| H | -3.163457 | -0.093002 | -1.126504 |

Rotational constants (GHz): 4.4800500 1.2887000 1.1919700
 Vibrational harmonic frequencies (cm-1):
 60.9897 87.2347 111.0591
 225.3068 245.7941 263.9986
 288.2289 353.6858 375.0955
 441.0444 546.8444 569.2609
 757.5339 841.2006 854.4540
 933.1458 949.9046 970.7259
 1005.0880 1024.8828 1084.2585
 1097.3186 1137.8571 1171.5185
 1212.5919 1248.4058 1292.2806
 1330.4207 1357.0625 1371.1246
 1373.8615 1389.1032 1398.9147
 1416.5484 1435.9898 1498.1153
 1500.8116 1503.6716 1512.0512
 1523.4162 1525.5913 2904.5778
 2923.5055 3008.9093 3022.8650
 3033.6125 3040.6161 3050.2649
 3067.4878 3095.6672 3100.7454
 3105.5221 3110.0979 3110.8657
 Zero-point correction (Hartree): 0.179659

5-me-pentoxy.tpp

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -311.63619359
 Electronic state : 2-A
 Cartesian coordinates (Angs):
 O -3.204294 0.254775 -0.370027
 C -1.932501 -0.239571 -0.466937
 C -1.092239 -0.117520 0.813596
 C 0.326039 -0.693902 0.680306
 C 1.272737 0.026000 -0.303805
 C 1.537827 1.484468 0.099464
 H -1.929423 -1.275519 -0.861550
 H -1.476851 0.362149 -1.284461
 H -1.069767 0.934986 1.116262
 H -1.622592 -0.654540 1.609216
 H 0.796994 -0.696849 1.672952
 H 0.250208 -1.749821 0.383440
 C 2.593951 -0.748216 -0.427157
 H 0.802188 0.030810 -1.298754
 H 1.999272 1.534265 1.093518
 H 0.621027 2.081540 0.129106
 H 2.221304 1.967239 -0.607228
 H 2.425106 -1.779328 -0.756527
 H 3.113498 -0.788677 0.538108
 H 3.268505 -0.272012 -1.146670

Rotational constants (GHz): 5.1335100 1.1598200 1.0953800
 Vibrational harmonic frequencies (cm-1):
 47.0644 91.0526 111.7692
 214.3236 240.0211 265.9031
 295.4028 331.6369 396.2881
 418.1442 534.9106 661.0455
 768.9197 830.3922 897.7575
 930.6358 958.8684 969.3768
 979.8965 1057.0897 1080.1217
 1086.1639 1135.9508 1184.8089
 1197.4165 1236.9130 1286.4080
 1330.0253 1342.7994 1361.7946
 1378.4284 1391.0076 1401.6975
 1415.1562 1435.2989 1490.5392
 1499.0918 1506.0818 1509.4540
 1519.0044 1525.8379 2883.9785
 2928.4321 3003.9515 3016.6742
 3033.7677 3038.8847 3048.5920
 3059.5056 3097.3729 3100.8350
 3106.0243 3111.7280 3116.0279
 Zero-point correction (Hartree): 0.179657

5-me-pentoxy.tpt

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -311.63403567
 Electronic state : 2-A
 Cartesian coordinates (Angs):
 O 3.230564 0.303313 -0.078904
 C 1.974760 0.115494 0.427922
 C 1.044041 -0.756283 -0.429607
 C -0.370086 -0.946041 0.158906
 C -1.458017 0.019874 -0.356845
 C -2.825714 -0.359544 0.230253
 H 2.030905 -0.259966 1.470198
 H 1.564191 1.141094 0.547840
 H 0.993032 -0.329025 -1.438700
 H 1.533442 -1.731271 -0.536534
 H -0.706750 -1.967285 -0.056101

| | | | | |
|--|-----------|-----------|-----------|--|
| H | -0.324444 | -0.879034 | 1.257154 | |
| C | -1.144247 | 1.497642 | -0.079893 | |
| H | -1.513925 | -0.108561 | -1.448375 | |
| H | -2.828932 | -0.246759 | 1.321471 | |
| H | -3.084209 | -1.399790 | 0.003854 | |
| H | -3.620831 | 0.278392 | -0.170394 | |
| H | -0.230640 | 1.826318 | -0.585742 | |
| H | -1.023694 | 1.681112 | 0.995342 | |
| H | -1.957082 | 2.141422 | -0.433197 | |
| Rotational constants (GHz): | 5.6927500 | 1.1688700 | 1.0457500 | |
| Vibrational harmonic frequencies (cm-1): | | | | |
| 62.2230 | 82.7770 | | 96.0741 | |
| 226.3995 | 241.9104 | | 272.7710 | |
| 283.1422 | 327.2642 | | 392.6025 | |
| 415.1891 | 500.9189 | | 560.5422 | |
| 757.9720 | 852.8130 | | 863.0161 | |
| 930.8065 | 937.4026 | | 969.6149 | |
| 1004.1129 | 1058.1137 | | 1083.3050 | |
| 1087.0932 | 1141.5042 | | 1189.2923 | |
| 1203.2497 | 1251.0891 | | 1292.5501 | |
| 1331.7744 | 1336.7848 | | 1371.9258 | |
| 1380.4577 | 1387.5850 | | 1393.6132 | |
| 1415.6631 | 1434.3605 | | 1496.4591 | |
| 1501.9854 | 1504.5182 | | 1511.6283 | |
| 1519.1289 | 1526.0164 | | 2900.9046 | |
| 2922.3802 | 3002.5574 | | 3013.8006 | |
| 3031.7061 | 3037.0660 | | 3044.7207 | |
| 3066.5904 | 3088.3020 | | 3098.1746 | |
| 3103.9528 | 3110.3932 | | 3113.0925 | |
| Zero-point correction (Hartree): | 0.179359 | | | |

5-me-pentoxy.ttp

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -311.63738871
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | | |
|--|-----------|-----------|-----------|--|
| O | -3.478660 | 0.257822 | -0.100760 | |
| C | -2.328814 | -0.423789 | 0.192340 | |
| C | -1.025058 | 0.256016 | -0.243488 | |
| C | 0.217103 | -0.538494 | 0.178664 | |
| C | 1.558847 | 0.015332 | -0.340470 | |
| C | 1.862680 | 1.420293 | 0.201712 | |
| H | -2.344959 | -0.550440 | 1.298200 | |
| H | -2.396109 | -1.464670 | -0.184540 | |
| H | -1.043950 | 0.370434 | -1.335230 | |
| H | -1.012655 | 1.266733 | 0.178622 | |
| H | 0.258667 | -0.597424 | 1.277131 | |
| H | 0.110943 | -1.574711 | -0.174010 | |
| C | 2.703710 | -0.952490 | -0.006054 | |
| H | 1.486156 | 0.084450 | -1.436482 | |
| H | 1.920676 | 1.411315 | 1.297450 | |
| H | 1.097873 | 2.147846 | -0.086117 | |
| H | 2.823437 | 1.786044 | -0.176392 | |
| H | 2.520054 | -1.949593 | -0.421309 | |
| H | 2.820781 | -1.060719 | 1.079319 | |
| H | 3.657558 | -0.593050 | -0.406794 | |
| Rotational constants (GHz): | 6.3989600 | 1.0104100 | 0.9174300 | |
| Vibrational harmonic frequencies (cm-1): | | | | |
| 68.0488 | 80.2268 | | 130.1292 | |
| 145.6995 | 226.0334 | | 250.9438 | |
| 294.3925 | 321.4393 | | 411.6763 | |
| 431.3454 | 464.1804 | | 527.3524 | |
| 761.3492 | 823.3587 | | 910.8303 | |
| 932.8206 | 954.8079 | | 969.0703 | |
| 1018.3736 | 1048.0169 | | 1055.3785 | |
| 1088.3861 | 1150.2269 | | 1197.3521 | |
| 1213.6129 | 1258.8769 | | 1280.8683 | |
| 1324.4943 | 1346.4105 | | 1369.6988 | |
| 1378.2048 | 1386.2557 | | 1408.6303 | |
| 1416.9559 | 1436.0369 | | 1491.9309 | |
| 1502.1633 | 1508.0996 | | 1512.5278 | |
| 1519.2283 | 1524.3227 | | 2879.9671 | |
| 2922.3197 | 3002.4658 | | 3009.3867 | |
| 3032.6236 | 3038.4231 | | 3039.5669 | |
| 3045.4989 | 3097.0838 | | 3099.1900 | |
| 3104.4784 | 3110.2726 | | 3119.7883 | |
| Zero-point correction (Hartree): | 0.179157 | | | |

5-me-pentoxy.ttt

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -311.63738876
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | | |
|---|----------|-----------|-----------|--|
| O | 3.478611 | 0.258031 | -0.100876 | |
| C | 2.328936 | -0.423930 | 0.192053 | |

| | | | |
|---|-----------|-----------|-----------|
| C | 1.025189 | 0.255875 | -0.243453 |
| C | -0.217027 | -0.538119 | 0.179225 |
| C | -1.558748 | 0.015307 | -0.340397 |
| C | -2.703432 | -0.952736 | -0.006310 |
| H | 2.395784 | -1.465167 | -0.183843 |
| H | 2.345513 | -0.549354 | 1.298083 |
| H | 1.013206 | 1.266765 | 0.178272 |
| H | 1.043709 | 0.369802 | -1.335276 |
| H | -0.110784 | -1.574590 | -0.172678 |
| H | -0.258672 | -0.596104 | 1.277755 |
| C | -1.863293 | 1.420171 | 0.201618 |
| H | -1.485637 | 0.084426 | -1.436380 |
| H | -2.820077 | -1.061708 | 1.079037 |
| H | -2.519837 | -1.949517 | -0.422380 |
| H | -3.657403 | -0.592951 | -0.406445 |
| H | -1.098134 | 2.147798 | -0.085062 |
| H | -1.922763 | 1.411002 | 1.297265 |
| H | -2.823547 | 1.785942 | -0.177753 |

Rotational constants (GHz): 6.3991800 1.0103800 0.9174100

| | | | |
|--|-----------|-----------|--|
| Vibrational harmonic frequencies (cm-1): | | | |
| 67.8922 | 80.0058 | 130.0619 | |
| 145.8114 | 226.0837 | 251.0161 | |
| 294.3729 | 321.5200 | 412.0941 | |
| 431.3610 | 470.3399 | 529.8219 | |
| 761.6597 | 823.4485 | 911.4498 | |
| 932.8207 | 954.9204 | 969.1124 | |
| 1018.3284 | 1048.2236 | 1055.6019 | |
| 1088.4507 | 1150.2199 | 1197.4031 | |
| 1213.5917 | 1258.4571 | 1280.9545 | |
| 1324.5531 | 1346.5464 | 1369.9057 | |
| 1378.1080 | 1385.7088 | 1408.6655 | |
| 1416.9428 | 1436.0286 | 1491.9251 | |
| 1502.1523 | 1508.0922 | 1512.5378 | |
| 1519.2283 | 1524.3278 | 2879.5954 | |
| 2922.6122 | 3002.3682 | 3009.3718 | |
| 3032.6067 | 3038.4388 | 3039.4856 | |
| 3045.3430 | 3097.0088 | 3099.1700 | |
| 3104.4835 | 3110.2674 | 3119.8368 | |

Zero-point correction (Hartree): 0.179179

5-me-pentoxy-1-5Hshift

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -311.62680175

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| C | -0.909997 | -0.022929 | -0.019429 |
| C | -0.003628 | 1.046710 | -0.638857 |
| C | 1.411820 | 1.006939 | -0.036679 |
| C | 1.969807 | -0.422956 | -0.155153 |
| O | 1.135124 | -1.352745 | 0.475840 |
| C | -1.478706 | 0.339847 | 1.345686 |
| C | -1.934018 | -0.624149 | -0.969641 |
| H | -0.446110 | 2.044148 | -0.499023 |
| H | 0.068208 | 0.882579 | -1.721726 |
| H | 1.384175 | 1.291839 | 1.021486 |
| H | 2.074278 | 1.714168 | -0.549496 |

| | | | |
|---|-----------|-----------|-----------|
| H | 2.949680 | -0.474522 | 0.346793 |
| H | 2.133889 | -0.665824 | -1.221441 |
| H | -0.056019 | -0.907271 | 0.222114 |
| H | -2.233484 | 1.133566 | 1.247368 |
| H | -0.703198 | 0.698598 | 2.028233 |
| H | -1.965629 | -0.521061 | 1.814856 |
| H | -1.462891 | -1.008513 | -1.879949 |
| H | -2.668500 | 0.136512 | -1.273156 |
| H | -2.487060 | -1.443024 | -0.498342 |

Rotational constants (GHz): 3.5717600 1.8101200 1.7055400

| | | | |
|--|-----------|-----------|--|
| Vibrational harmonic frequencies (cm-1): | | | |
| i1256.6761 | 102.6029 | 140.4995 | |
| 183.4110 | 204.8174 | 273.8841 | |
| 297.9533 | 361.7271 | 386.7256 | |
| 468.0047 | 492.3648 | 592.1227 | |
| 769.3164 | 855.6022 | 897.6660 | |
| 920.1838 | 939.6265 | 954.7697 | |
| 985.7985 | 1021.3554 | 1043.7022 | |
| 1083.1235 | 1142.8560 | 1166.3899 | |
| 1189.5350 | 1215.0486 | 1244.2906 | |
| 1257.6960 | 1292.8377 | 1354.6544 | |
| 1373.3488 | 1386.0508 | 1409.9967 | |
| 1426.5439 | 1481.0044 | 1490.6080 | |
| 1492.6394 | 1498.1238 | 1503.9279 | |
| 1506.9359 | 1513.1322 | 1566.5115 | |
| 2944.3563 | 3001.6946 | 3011.7319 | |
| 3014.2615 | 3021.9060 | 3050.6624 | |
| 3063.4403 | 3087.7012 | 3094.3827 | |

3097.3702 3121.0383 3127.5490
 Zero-point correction (Hartree): 0.175700

C7H15O.pmmm

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.94833175

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 2.120558 | 1.147662 | -0.602592 |
| C | 2.507635 | -0.000861 | 0.037359 |
| C | 1.413519 | -0.668088 | 0.889808 |
| C | 0.320461 | -1.346167 | 0.041945 |
| C | -0.457253 | -0.446717 | -0.940450 |
| C | -1.638384 | 0.394045 | -0.397346 |
| C | -2.788230 | -0.481673 | 0.125769 |
| H | 2.983752 | -0.725679 | -0.650738 |
| H | 3.317481 | 0.340572 | 0.719262 |
| H | 1.892723 | -1.427245 | 1.521954 |
| H | 0.992012 | 0.088035 | 1.557382 |
| H | 0.803063 | -2.143970 | -0.539174 |
| H | -0.376770 | -1.858360 | 0.716958 |
| H | 0.250191 | 0.232446 | -1.438387 |
| H | -0.857514 | -1.090991 | -1.734943 |
| C | -1.235192 | 1.451424 | 0.643514 |
| H | -2.023903 | 0.939338 | -1.271209 |
| H | -2.495931 | -1.041330 | 1.021938 |
| H | -3.116676 | -1.206387 | -0.627774 |
| H | -3.653525 | 0.132961 | 0.397406 |
| H | -0.354476 | 2.014477 | 0.320569 |
| H | -1.004733 | 0.994551 | 1.612892 |
| H | -2.055501 | 2.158511 | 0.811013 |

Rotational constants (GHz): 3.2215700 1.1612600 1.0317200

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 55.2705 | 79.9365 | 122.9226 |
| 153.9053 | 227.4972 | 233.7039 |
| 284.6860 | 304.6176 | 340.6114 |
| 375.2114 | 396.5894 | 459.5656 |
| 556.5129 | 722.7287 | 797.6579 |
| 817.4440 | 856.1733 | 886.6647 |
| 934.0255 | 955.5825 | 969.1496 |
| 983.5193 | 1023.8795 | 1037.2621 |
| 1091.0295 | 1110.8548 | 1135.3420 |
| 1152.3202 | 1188.2274 | 1217.4020 |
| 1245.0351 | 1310.9021 | 1335.6560 |
| 1354.7531 | 1365.8812 | 1379.8928 |
| 1393.0039 | 1409.8080 | 1414.9610 |
| 1417.9828 | 1437.1065 | 1485.4781 |
| 1491.4069 | 1499.6705 | 1503.3583 |
| 1513.2291 | 1521.8847 | 1529.9458 |
| 2883.9592 | 2947.2512 | 3000.8261 |
| 3015.6324 | 3023.9447 | 3034.1379 |
| 3039.2410 | 3043.7506 | 3050.3748 |
| 3067.7559 | 3096.7424 | 3103.8485 |
| 3106.5690 | 3121.5551 | 3126.3398 |

Zero-point correction (Hartree): 0.209004

C7H15O.pmp

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.94930436

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -1.666147 | -1.526720 | -0.514756 |
| C | -2.437770 | -0.430873 | -0.227449 |
| C | -1.748835 | 0.629477 | 0.649503 |
| C | -0.670750 | 1.428221 | -0.107117 |
| C | 0.485093 | 0.625641 | -0.738793 |
| C | 1.692757 | 0.287916 | 0.161734 |
| C | 1.342249 | -0.595354 | 1.369803 |
| H | -2.885633 | 0.018744 | -1.134420 |
| H | -3.290228 | -0.855125 | 0.347549 |
| H | -2.516973 | 1.326541 | 1.009551 |
| H | -1.335571 | 0.125088 | 1.526962 |
| H | -1.178128 | 1.984710 | -0.907069 |
| H | -0.260819 | 2.191909 | 0.568391 |
| H | 0.092823 | -0.308976 | -1.168529 |
| H | 0.866120 | 1.204472 | -1.590500 |
| C | 2.794566 | -0.376216 | -0.679868 |
| H | 2.093134 | 1.239850 | 0.544046 |
| H | 0.801671 | -1.494308 | 1.053234 |
| H | 0.717231 | -0.067650 | 2.096412 |
| H | 2.251056 | -0.910830 | 1.894482 |
| H | 3.086828 | 0.251752 | -1.528986 |
| H | 2.452838 | -1.338504 | -1.080168 |
| H | 3.690961 | -0.566790 | -0.079786 |

Rotational constants (GHz): 3.0144800 1.1284400 1.0523500

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 53.7996 | 61.1190 | 119.5331 |
| 154.5607 | 228.7314 | 248.3213 |
| 270.2204 | 278.8484 | 343.1980 |
| 378.7280 | 411.6626 | 443.6790 |
| 497.4906 | 744.3666 | 803.6923 |
| 818.3429 | 862.9854 | 897.8954 |
| 936.3964 | 939.5026 | 972.0481 |
| 977.5080 | 1010.9716 | 1058.6343 |
| 1101.8257 | 1115.4242 | 1127.8667 |
| 1154.1305 | 1193.3778 | 1205.5793 |
| 1251.8316 | 1314.0586 | 1333.1008 |
| 1335.9423 | 1367.3002 | 1379.9968 |
| 1392.9186 | 1401.7263 | 1416.2950 |
| 1418.0784 | 1435.3539 | 1484.0344 |
| 1488.0932 | 1498.5855 | 1507.0883 |
| 1509.0918 | 1518.4655 | 1529.6650 |
| 2883.9857 | 2948.0053 | 2992.6300 |
| 3003.1109 | 3018.0007 | 3033.4766 |
| 3041.6408 | 3044.0304 | 3051.5851 |
| 3055.5361 | 3102.0527 | 3105.3135 |
| 3109.5720 | 3117.2503 | 3123.8629 |

Zero-point correction (Hartree): 0.208731

C7H15O.pmmt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.95206336

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -1.806271 | 1.530218 | -0.272474 |
| C | -2.487084 | 0.345830 | -0.171754 |
| C | -1.647393 | -0.918493 | -0.413302 |
| C | -0.641587 | -1.202024 | 0.715632 |
| C | 0.423606 | -0.116792 | 0.946283 |
| C | 1.371415 | 0.185441 | -0.231913 |
| C | 2.325337 | 1.329350 | 0.144265 |
| H | -3.061300 | 0.279264 | 0.773091 |
| H | -3.257959 | 0.421025 | -0.970852 |
| H | -2.332080 | -1.771613 | -0.506827 |
| H | -1.134994 | -0.813752 | -1.376370 |
| H | -1.199572 | -1.343070 | 1.651881 |
| H | -0.156417 | -2.164960 | 0.513650 |
| H | -0.076147 | 0.820433 | 1.229014 |
| H | 1.027731 | -0.410125 | 1.817484 |
| C | 2.162576 | -1.049788 | -0.687589 |
| H | 0.758564 | 0.534694 | -1.073253 |
| H | 2.968233 | 1.044303 | 0.986738 |
| H | 1.771548 | 2.228205 | 0.435707 |
| H | 2.978027 | 1.594711 | -0.694629 |
| H | 1.510281 | -1.851842 | -1.048156 |
| H | 2.764596 | -1.455624 | 0.135435 |
| H | 2.848442 | -0.794538 | -1.502849 |

Rotational constants (GHz): 2.9289000 1.1929900 0.9976700

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 49.2366 | 64.2152 | 109.5869 |
| 161.3315 | 209.1005 | 237.2134 |
| 261.1912 | 310.8309 | 348.0125 |
| 377.5983 | 421.7314 | 452.0788 |
| 510.1589 | 738.3681 | 776.2839 |
| 826.0238 | 850.7560 | 894.0814 |
| 933.6881 | 957.7287 | 961.9889 |
| 978.0269 | 1005.0003 | 1061.1685 |
| 1102.0506 | 1108.0290 | 1121.9385 |
| 1167.6457 | 1194.0617 | 1199.8991 |
| 1247.1861 | 1305.7527 | 1336.0144 |
| 1345.2866 | 1370.6704 | 1373.0156 |
| 1395.1740 | 1403.2588 | 1409.6219 |
| 1416.9966 | 1436.2204 | 1486.7490 |
| 1491.0818 | 1498.1983 | 1506.4690 |
| 1509.6988 | 1519.4189 | 1527.0698 |
| 2880.5715 | 2939.8714 | 3007.3702 |
| 3025.3735 | 3030.9446 | 3033.6629 |
| 3037.5376 | 3040.0590 | 3049.5509 |
| 3069.8688 | 3092.4791 | 3096.2475 |
| 3103.7157 | 3110.5305 | 3112.3679 |

Zero-point correction (Hartree): 0.208673

C7H15O.pmpm

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.94123328

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -2.121260 | 1.397568 | 0.255786 |
| C | -2.540962 | 0.039104 | 0.268273 |
| C | -1.540243 | -0.896987 | -0.413075 |

| | | | |
|--|-----------|-----------|-----------|
| C | -0.265082 | -1.153164 | 0.429386 |
| C | 1.048019 | -1.220991 | -0.382692 |
| C | 1.865384 | 0.100848 | -0.409080 |
| C | 1.070650 | 1.276484 | -0.884023 |
| H | -2.731376 | -0.307465 | 1.299123 |
| H | -3.500729 | 0.017050 | -0.259989 |
| H | -2.029241 | -1.853522 | -0.636390 |
| H | -1.282178 | -0.451347 | -1.380831 |
| H | -0.166274 | -0.372204 | 1.195418 |
| H | -0.399609 | -2.083898 | 0.991831 |
| H | 1.702080 | -2.002585 | 0.022584 |
| H | 0.821271 | -1.523322 | -1.413026 |
| C | 2.548906 | 0.385294 | 0.940395 |
| H | 2.677296 | -0.068481 | -1.142669 |
| H | -1.167943 | 1.421031 | 0.424105 |
| H | 0.442798 | 1.200748 | -1.766397 |
| H | 1.303613 | 2.277953 | -0.532438 |
| H | 3.198545 | -0.445585 | 1.234309 |
| H | 1.817338 | 0.538434 | 1.741271 |
| H | 3.164455 | 1.289127 | 0.881706 |
| Rotational constants (GHz): | 2.9677100 | 1.1540400 | 0.9894800 |
| Vibrational harmonic frequencies (cm-1): | | | |
| 35.3699 | 48.2547 | | 104.3570 |
| 167.9170 | 187.2702 | | 215.6501 |
| 247.9686 | 262.9745 | | 289.6792 |
| 316.6573 | 382.3880 | | 392.9372 |
| 476.6206 | 534.8233 | | 625.3732 |
| 728.7228 | 803.3006 | | 826.8492 |
| 899.5431 | 919.7703 | | 951.1656 |
| 984.0661 | 989.5223 | | 1048.1289 |
| 1068.6909 | 1085.5496 | | 1100.8714 |
| 1150.3984 | 1170.9325 | | 1209.0725 |
| 1223.0494 | 1257.8091 | | 1282.9743 |
| 1324.5565 | 1339.3006 | | 1356.2923 |
| 1375.1184 | 1381.8905 | | 1401.7723 |
| 1423.2407 | 1440.0308 | | 1477.1751 |
| 1498.1218 | 1502.6335 | | 1508.3548 |
| 1513.4605 | 1520.5035 | | 1532.3260 |
| 2919.8108 | 2968.4209 | | 3032.1641 |
| 3034.9589 | 3040.7808 | | 3043.9337 |
| 3068.2499 | 3073.1000 | | 3077.7649 |
| 3090.2187 | 3111.7497 | | 3116.8221 |
| 3150.1590 | 3251.1364 | | 3766.1325 |
| Zero-point correction (Hartree): | 0.208062 | | |

C7H15O.pmpp

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.94854079

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|--|-----------|-----------|-----------|
| O | -2.659280 | -1.176974 | -0.631391 |
| C | -2.771498 | 0.005981 | 0.051911 |
| C | -1.461609 | 0.548859 | 0.635323 |
| C | -0.407125 | 0.828802 | -0.444573 |
| C | 0.982501 | 1.232039 | 0.101418 |
| C | 2.029980 | 0.100774 | 0.237910 |
| C | 2.481121 | -0.434919 | -1.130310 |
| H | -3.185681 | 0.721539 | -0.693749 |
| H | -3.570531 | -0.069737 | 0.815104 |
| H | -1.680737 | 1.466640 | 1.198298 |
| H | -1.085147 | -0.178942 | 1.362881 |
| H | -0.329141 | -0.056598 | -1.085770 |
| H | -0.787435 | 1.630878 | -1.091555 |
| H | 1.414013 | 1.998885 | -0.554270 |
| H | 0.855530 | 1.716333 | 1.079567 |
| C | 1.572554 | -1.048166 | 1.149886 |
| H | 2.910402 | 0.561135 | 0.709842 |
| H | 3.281017 | -1.174780 | -1.016356 |
| H | 2.860132 | 0.370929 | -1.768808 |
| H | 1.659374 | -0.924877 | -1.664668 |
| H | 0.720418 | -1.585976 | 0.719674 |
| H | 1.277485 | -0.683620 | 2.140316 |
| H | 2.378987 | -1.776235 | 1.291227 |
| Rotational constants (GHz): | 3.2189600 | 0.9459200 | 0.9099800 |
| Vibrational harmonic frequencies (cm-1): | | | |
| 42.7236 | 64.0286 | | 106.9358 |
| 153.4740 | 224.1070 | | 242.3576 |
| 252.5950 | 289.5531 | | 314.0509 |
| 374.9987 | 384.5236 | | 494.9173 |
| 527.7413 | 581.6342 | | 745.0794 |
| 792.0272 | 838.4659 | | 908.1402 |
| 929.6774 | 947.5743 | | 974.4567 |
| 982.3925 | 1017.5919 | | 1059.3039 |
| 1087.0962 | 1108.4234 | | 1140.1343 |
| 1170.9431 | 1207.5811 | | 1218.9821 |

| | | |
|-----------|-----------|-----------|
| 1279.2659 | 1311.9620 | 1328.9763 |
| 1358.0531 | 1363.7447 | 1366.5527 |
| 1378.7900 | 1395.6396 | 1412.8942 |
| 1418.5993 | 1438.2658 | 1495.6614 |
| 1499.4611 | 1502.4175 | 1511.5572 |
| 1515.2034 | 1526.8821 | 1527.7447 |
| 2879.1454 | 2938.5377 | 3008.6809 |
| 3023.0634 | 3030.2148 | 3035.5110 |
| 3036.4342 | 3041.7015 | 3062.1075 |
| 3080.3001 | 3096.7704 | 3104.3191 |
| 3107.8359 | 3108.3494 | 3113.6217 |

Zero-point correction (Hartree): 0.208406

C7H15O.pmp1

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.94979986

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 1.629627 | 1.956516 | -0.321078 |
| C | -2.206044 | 1.015489 | 0.891287 |
| C | -2.497826 | 0.031685 | -0.248348 |
| C | -1.413991 | -1.033655 | -0.492659 |
| C | -0.029059 | -0.466266 | -0.880257 |
| C | 0.974485 | -0.336876 | 0.282787 |
| C | 1.608907 | -1.680947 | 0.664426 |
| H | -2.053634 | 0.490303 | 1.841930 |
| H | -3.041597 | 1.709940 | 1.029671 |
| H | -3.448677 | -0.479049 | -0.047101 |
| H | -2.648909 | 0.596839 | -1.178249 |
| H | -1.322192 | -1.668842 | 0.399423 |
| H | -1.769183 | -1.696523 | -1.291084 |
| H | 0.429064 | -1.098885 | -1.653472 |
| H | -0.160978 | 0.523391 | -1.334715 |
| C | 2.072064 | 0.688393 | -0.058731 |
| H | 0.447634 | 0.057721 | 1.161256 |
| H | 2.190539 | -2.091658 | -0.170529 |
| H | 0.846550 | -2.420572 | 0.927628 |
| H | 2.281563 | -1.581556 | 1.523911 |
| H | -1.312215 | 1.615202 | 0.691138 |
| H | 2.600500 | 0.375456 | -0.988478 |
| H | 2.873298 | 0.709169 | 0.706274 |

Rotational constants (GHz): 2.4581400 1.2356300 0.9791600

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 42.8440 | 68.0869 | 127.0135 |
| 144.2240 | 227.5078 | 253.1949 |
| 258.3196 | 263.3395 | 298.7631 |
| 371.3913 | 402.2650 | 461.6380 |
| 525.7378 | 608.7475 | 774.5908 |
| 793.4438 | 824.8549 | 897.6306 |
| 906.4213 | 927.8758 | 989.2270 |
| 1018.7895 | 1060.8717 | 1079.7374 |
| 1082.4248 | 1101.4493 | 1142.3501 |
| 1173.2860 | 1180.6158 | 1257.8498 |
| 1275.5164 | 1313.5310 | 1318.2582 |
| 1330.0033 | 1361.2083 | 1372.5501 |
| 1390.2997 | 1393.4460 | 1404.0201 |
| 1427.1120 | 1431.6771 | 1498.9175 |
| 1501.6716 | 1509.5632 | 1513.9639 |
| 1517.6452 | 1521.4380 | 1525.4802 |
| 2868.4303 | 2933.5627 | 3017.5828 |
| 3024.9644 | 3026.9372 | 3034.6337 |
| 3037.7197 | 3047.4357 | 3059.4443 |
| 3069.5377 | 3071.8430 | 3100.4316 |
| 3104.2335 | 3117.2709 | 3117.8517 |

Zero-point correction (Hartree): 0.208458

C7H15O.pmtm

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.95124110

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -2.521664 | 1.038945 | -0.753259 |
| C | -2.673236 | 0.204000 | 0.321118 |
| C | -1.814749 | -1.072568 | 0.282770 |
| C | -0.318333 | -0.803473 | 0.513099 |
| C | 0.342567 | 0.013465 | -0.606647 |
| C | 1.839223 | 0.349897 | -0.411837 |
| C | 2.089804 | 1.260785 | 0.800498 |
| H | -2.560725 | 0.735235 | 1.286406 |
| H | -3.744379 | -0.092819 | 0.271759 |
| H | -2.186267 | -1.755499 | 1.057787 |
| H | -1.970251 | -1.563360 | -0.685783 |
| H | -0.199164 | -0.291150 | 1.477485 |
| H | 0.190216 | -1.769882 | 0.617999 |
| H | 0.226267 | -0.532906 | -1.552753 |

| | | | |
|--|-----------|-----------|-----------|
| H | -0.210550 | 0.953798 | -0.740823 |
| C | 2.724778 | -0.905103 | -0.353533 |
| H | 2.137504 | 0.915157 | -1.306518 |
| H | 1.871502 | 0.749391 | 1.744820 |
| H | 1.468871 | 2.162603 | 0.757482 |
| H | 3.137472 | 1.578724 | 0.839138 |
| H | 2.556230 | -1.553195 | -1.220907 |
| H | 2.530354 | -1.496533 | 0.548327 |
| H | 3.785896 | -0.633142 | -0.341158 |
| Rotational constants (GHz): | 3.5913700 | 0.9438300 | 0.8671700 |
| Vibrational harmonic frequencies (cm-1): | | | |
| 43.0855 | 83.5675 | 118.4244 | |
| 120.8730 | 200.7027 | 236.3349 | |
| 254.1721 | 280.5942 | 331.9537 | |
| 368.8172 | 385.3323 | 459.8222 | |
| 554.6581 | 755.7606 | 777.3917 | |
| 812.8507 | 862.8225 | 893.5762 | |
| 935.2570 | 967.9888 | 974.6860 | |
| 979.1499 | 1011.4308 | 1037.5856 | |
| 1095.0763 | 1099.4053 | 1124.9794 | |
| 1157.3038 | 1204.1647 | 1210.4459 | |
| 1257.8422 | 1316.5399 | 1329.0313 | |
| 1343.9148 | 1366.9833 | 1373.0298 | |
| 1383.8078 | 1411.7035 | 1416.7726 | |
| 1418.1186 | 1438.0097 | 1484.2989 | |
| 1486.9984 | 1500.8166 | 1505.9744 | |
| 1511.5558 | 1521.3400 | 1524.2260 | |
| 2882.2990 | 2941.8645 | 3007.9704 | |
| 3021.5805 | 3029.9378 | 3035.2030 | |
| 3036.7011 | 3041.2445 | 3047.5165 | |
| 3074.5786 | 3087.2526 | 3103.8606 | |
| 3106.8203 | 3108.8524 | 3109.5302 | |
| Zero-point correction (Hartree): | 0.208599 | | |

C7H15O.pmtp

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.95273194
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | |
|--|-----------|-----------|-----------|
| O | -2.393778 | 1.413949 | -0.177126 |
| C | -2.755058 | 0.182095 | 0.299048 |
| C | -1.966202 | -1.001686 | -0.287867 |
| C | -0.513030 | -1.070336 | 0.209745 |
| C | 0.360750 | 0.107862 | -0.239721 |
| C | 1.788947 | 0.120288 | 0.342506 |
| C | 2.622189 | -1.088296 | -0.112346 |
| H | -2.770245 | 0.146654 | 1.405922 |
| H | -3.818426 | 0.083439 | -0.012987 |
| H | -2.489194 | -1.927626 | -0.015519 |
| H | -1.991385 | -0.923593 | -1.381650 |
| H | -0.514693 | -1.125952 | 1.308548 |
| H | -0.077961 | -2.014371 | -0.140060 |
| H | 0.418526 | 0.119266 | -1.338025 |
| H | -0.137206 | 1.047676 | 0.037728 |
| C | 2.502486 | 1.431819 | -0.018226 |
| H | 1.701303 | 0.076496 | 1.439028 |
| H | 2.718882 | -1.104915 | -1.205192 |
| H | 2.176943 | -2.038723 | 0.197581 |
| H | 3.632980 | -1.046953 | 0.308098 |
| H | 1.941634 | 2.302861 | 0.337433 |
| H | 2.613941 | 1.530130 | -1.105066 |
| H | 3.504628 | 1.473546 | 0.422332 |
| Rotational constants (GHz): | 3.5451500 | 0.9492900 | 0.7910100 |
| Vibrational harmonic frequencies (cm-1): | | | |
| 38.7785 | 80.0725 | 110.3418 | |
| 122.8724 | 181.6285 | 229.9919 | |
| 255.0144 | 282.8010 | 336.9143 | |
| 373.3617 | 421.0194 | 443.2738 | |
| 477.4798 | 754.8745 | 804.5963 | |
| 813.9510 | 873.0774 | 888.7268 | |
| 931.7347 | 960.3969 | 967.3583 | |
| 986.9396 | 1007.8198 | 1051.9200 | |
| 1092.4537 | 1102.2143 | 1126.8404 | |
| 1158.0295 | 1197.3949 | 1219.0259 | |
| 1253.2759 | 1300.9058 | 1326.7340 | |
| 1336.7205 | 1366.5612 | 1374.8450 | |
| 1378.2062 | 1407.8393 | 1413.8561 | |
| 1415.5301 | 1434.7538 | 1483.6443 | |
| 1485.1777 | 1502.1936 | 1505.4050 | |
| 1508.5432 | 1518.4796 | 1524.2722 | |
| 2882.2404 | 2940.9639 | 3002.9647 | |
| 3007.5001 | 3017.1438 | 3032.7781 | |
| 3035.9003 | 3038.1366 | 3043.8034 | |
| 3073.6338 | 3086.6482 | 3098.8094 | |

3104.9537 3110.5859 3115.5273
Zero-point correction (Hartree): 0.208269

C7H15O.pmtt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.95269326

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -2.217296 | 1.435262 | 0.513390 |
| C | -2.656832 | 0.139719 | 0.457489 |
| C | -2.036703 | -0.715383 | -0.660676 |
| C | -0.560074 | -1.061531 | -0.409985 |
| C | 0.378263 | 0.152486 | -0.424864 |
| C | 1.873624 | -0.177408 | -0.239127 |
| C | 2.730745 | 1.074654 | -0.478093 |
| H | -2.587590 | -0.367690 | 1.439630 |
| H | -3.746983 | 0.243599 | 0.260246 |
| H | -2.620215 | -1.641410 | -0.745212 |
| H | -2.145678 | -0.174092 | -1.608546 |
| H | -0.481325 | -1.590585 | 0.549154 |
| H | -0.234695 | -1.776776 | -1.177896 |
| H | 0.249188 | 0.680822 | -1.379150 |
| H | 0.071502 | 0.869021 | 0.351470 |
| C | 2.178765 | -0.780359 | 1.140916 |
| H | 2.147790 | -0.922833 | -1.001744 |
| H | 2.494727 | 1.855354 | 0.255292 |
| H | 2.557975 | 1.493794 | -1.475370 |
| H | 3.798995 | 0.848461 | -0.389194 |
| H | 1.645517 | -1.720894 | 1.310910 |
| H | 1.893276 | -0.085077 | 1.940206 |
| H | 3.249160 | -0.986852 | 1.249127 |

Rotational constants (GHz): 3.3626900 0.9299000 0.8643300

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 42.9665 | 73.7736 | 112.6304 |
| 131.9557 | 185.9794 | 231.6361 |
| 258.8076 | 288.6343 | 335.0960 |
| 376.6670 | 415.5216 | 440.8595 |
| 487.4118 | 758.6265 | 801.4772 |
| 814.9594 | 855.4267 | 904.1011 |
| 931.1244 | 955.8490 | 969.7217 |
| 984.1627 | 1004.8719 | 1058.7755 |
| 1093.5625 | 1104.1159 | 1127.6425 |
| 1165.3653 | 1195.4639 | 1209.6005 |
| 1258.8286 | 1309.3192 | 1327.5911 |
| 1336.7576 | 1368.0807 | 1373.3344 |
| 1377.4788 | 1406.1972 | 1413.2056 |
| 1415.3562 | 1433.9645 | 1484.0404 |
| 1487.5964 | 1503.2053 | 1506.1443 |
| 1509.5241 | 1518.3387 | 1525.4387 |
| 2881.6417 | 2940.0460 | 2999.1349 |
| 3010.6838 | 3025.3974 | 3033.1719 |
| 3036.0984 | 3038.7190 | 3046.4360 |
| 3068.4827 | 3086.6854 | 3099.4972 |
| 3105.2457 | 3109.0769 | 3114.6217 |

Zero-point correction (Hartree): 0.208375

C7H15O.ppm

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.94390985

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 2.680200 | -0.821061 | -0.704109 |
| C | 2.011277 | -0.619689 | 0.471782 |
| C | 1.396221 | 0.781008 | 0.638378 |
| C | 0.463465 | 1.205239 | -0.520118 |
| C | -1.046670 | 1.299981 | -0.217268 |
| C | -1.869558 | 0.005178 | -0.001472 |
| C | -1.718153 | -0.993030 | -1.159311 |
| H | -0.636429 | -1.111847 | 1.439886 |
| H | 2.632564 | -0.902629 | 1.343093 |
| H | 0.878564 | 0.821616 | 1.604469 |
| H | 2.233709 | 1.484329 | 0.715706 |
| H | 0.773478 | 2.198481 | -0.864366 |
| H | 0.645172 | 0.543933 | -1.375715 |
| H | -1.192084 | 1.953367 | 0.654772 |
| H | -1.505481 | 1.829799 | -1.063009 |
| C | -1.636819 | -0.674667 | 1.357585 |
| H | -2.919368 | 0.333993 | -0.000640 |
| H | -0.708407 | -1.415894 | -1.206499 |
| H | -1.920076 | -0.517307 | -2.125480 |
| H | -2.416817 | -1.829185 | -1.046695 |
| H | -1.758177 | 0.033488 | 2.184755 |
| H | 1.207532 | -1.389019 | 0.445970 |
| H | -2.354364 | -1.488761 | 1.509169 |

Rotational constants (GHz): 2.6889900 1.1442000 1.0898500

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 28.0149 | 83.4231 | 123.7563 |
| 142.4791 | 215.9061 | 245.6600 |
| 250.0293 | 281.5865 | 336.3997 |
| 367.3207 | 392.7002 | 477.4510 |
| 550.7906 | 697.8597 | 738.6397 |
| 825.4311 | 843.5713 | 897.6875 |
| 930.5471 | 944.8827 | 968.1964 |
| 988.7689 | 1029.8962 | 1041.9884 |
| 1098.8019 | 1117.9240 | 1138.3244 |
| 1152.8723 | 1208.4328 | 1214.0243 |
| 1277.1992 | 1293.2289 | 1316.2356 |
| 1351.3575 | 1375.3505 | 1382.5217 |
| 1384.7225 | 1401.0229 | 1409.8430 |
| 1418.5160 | 1437.8141 | 1491.6450 |
| 1495.7241 | 1503.0892 | 1506.4286 |
| 1516.9412 | 1520.9130 | 1526.4023 |
| 2880.9491 | 2946.0528 | 3003.3763 |
| 3020.2905 | 3038.1053 | 3042.1960 |
| 3043.9284 | 3048.4644 | 3057.7222 |
| 3081.3679 | 3086.6912 | 3105.2995 |
| 3107.9499 | 3109.5514 | 3116.4197 |

Zero-point correction (Hartree): 0.208750

C7H15O.pmp

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.94575077
Electronic state : 2-A
Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 2.650115 | -0.552677 | -1.161356 |
| C | 2.087859 | -0.776852 | 0.065695 |
| C | 1.638568 | 0.490282 | 0.815403 |
| C | 0.655560 | 1.380692 | 0.030900 |
| C | -0.854760 | 1.141234 | 0.225437 |
| C | -1.442419 | -0.214706 | -0.243878 |
| C | -1.425595 | -1.283119 | 0.862917 |
| H | -0.427860 | -1.446595 | 1.280963 |
| H | 2.745179 | -1.411016 | 0.691796 |
| H | 1.223960 | 0.201048 | 1.790108 |
| H | 2.548252 | 1.063731 | 1.031313 |
| H | 0.849709 | 2.425265 | 0.302894 |
| H | 0.909102 | 1.301796 | -1.034336 |
| H | -1.116103 | 1.294919 | 1.282798 |
| H | -1.366623 | 1.943074 | -0.322347 |
| C | -2.880019 | -0.031923 | -0.758090 |
| H | -0.836761 | -0.575896 | -1.088131 |
| H | -2.076667 | -0.981907 | 1.692700 |
| H | 1.217277 | -1.430223 | -0.157704 |
| H | -1.790770 | -2.246473 | 0.489935 |
| H | -2.914819 | 0.658666 | -1.607440 |
| H | -3.526027 | 0.376062 | 0.029221 |
| H | -3.313929 | -0.984687 | -1.081225 |

Rotational constants (GHz): 3.0407200 1.0406300 0.9639200

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 40.1978 | 88.5511 | 116.8006 |
| 139.2056 | 225.0336 | 232.3334 |
| 253.5753 | 277.8403 | 337.9244 |
| 366.2674 | 416.6305 | 471.7754 |
| 501.4095 | 681.4470 | 754.0728 |
| 833.3385 | 857.2099 | 884.2646 |
| 921.7361 | 943.6824 | 962.0935 |
| 966.8030 | 1035.4946 | 1060.1002 |
| 1101.3415 | 1117.5618 | 1132.1660 |
| 1162.3659 | 1195.2194 | 1220.5487 |
| 1286.3776 | 1292.6102 | 1324.3413 |
| 1348.8349 | 1369.2698 | 1370.3172 |
| 1385.9761 | 1398.2055 | 1412.5837 |
| 1415.9231 | 1435.7030 | 1490.1291 |
| 1497.6742 | 1504.5230 | 1506.0610 |
| 1510.7234 | 1518.7557 | 1524.1166 |
| 2900.4261 | 2941.3855 | 3009.8951 |
| 3017.9110 | 3032.7075 | 3034.4297 |
| 3038.5917 | 3040.4861 | 3056.9854 |
| 3075.8475 | 3077.9554 | 3098.1044 |
| 3104.8330 | 3110.8716 | 3119.6925 |

Zero-point correction (Hartree): 0.208565

C7H15O.ppm

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.94986129
Electronic state : 2-A
Cartesian coordinates (Angs):

| | | | |
|---|----------|----------|-----------|
| O | 2.315905 | 1.299381 | 0.247133 |
| C | 2.042966 | 0.412594 | -0.757299 |

| | | | |
|---|-----------|-----------|-----------|
| C | 1.716701 | -1.022945 | -0.307135 |
| C | 0.643047 | -1.147536 | 0.788666 |
| C | -0.827035 | -1.125679 | 0.328648 |
| C | -1.392560 | 0.183609 | -0.261653 |
| C | -2.861782 | -0.017943 | -0.665768 |
| H | 1.171531 | 0.865254 | -1.278347 |
| H | 2.843480 | 0.422554 | -1.522371 |
| H | 1.438655 | -1.609553 | -1.193735 |
| H | 2.652004 | -1.459187 | 0.065466 |
| H | 0.802841 | -2.102954 | 1.303304 |
| H | 0.825478 | -0.371729 | 1.540616 |
| H | -0.975407 | -1.930085 | -0.406160 |
| H | -1.450744 | -1.394710 | 1.193741 |
| C | -1.253409 | 1.373249 | 0.699691 |
| H | -0.838934 | 0.420312 | -1.183012 |
| H | -3.479517 | -0.242966 | 0.212353 |
| H | -2.973936 | -0.848079 | -1.372099 |
| H | -3.271640 | 0.881893 | -1.137006 |
| H | -0.208293 | 1.599779 | 0.931502 |
| H | -1.767764 | 1.166280 | 1.646533 |
| H | -1.702564 | 2.276048 | 0.271256 |
| Rotational constants (GHz): | 2.9468300 | 1.1598900 | 0.9933100 |
| Vibrational harmonic frequencies (cm ⁻¹): | | | |
| 50.7885 | 82.1679 | | 118.3664 |
| 159.9864 | 222.9645 | | 241.6309 |
| 252.4520 | 303.7868 | | 333.2505 |
| 386.9062 | 424.4282 | | 466.8476 |
| 520.6143 | 658.3916 | | 752.5685 |
| 812.9812 | 872.8145 | | 876.5530 |
| 919.5625 | 939.6639 | | 972.9636 |
| 976.4065 | 1026.9322 | | 1061.5332 |
| 1100.4673 | 1116.0460 | | 1127.3387 |
| 1178.9900 | 1197.4256 | | 1214.6400 |
| 1284.4412 | 1304.3367 | | 1314.8713 |
| 1351.9596 | 1366.1546 | | 1378.0553 |
| 1389.4637 | 1405.6225 | | 1412.2592 |
| 1417.6903 | 1438.1064 | | 1488.1933 |
| 1494.7908 | 1501.8640 | | 1508.8145 |
| 1510.2633 | 1519.3059 | | 1532.5250 |
| 2892.4749 | 2939.7239 | | 3000.7231 |
| 3009.9498 | 3029.1502 | | 3032.5005 |
| 3037.6033 | 3042.8198 | | 3050.5384 |
| 3071.9995 | 3091.1504 | | 3098.2333 |
| 3103.4214 | 3109.8705 | | 3120.9318 |
| Zero-point correction (Hartree): | 0.208724 | | |

C7H15O.pppm

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.94746430

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -3.330913 | -0.629532 | -0.138897 |
| C | -2.556685 | 0.491543 | -0.272597 |
| C | -1.357011 | 0.571818 | 0.686172 |
| C | -0.391044 | -0.617239 | 0.547527 |
| C | 0.516631 | -0.586958 | -0.705016 |
| C | 1.935259 | 0.006085 | -0.523472 |
| C | 1.930958 | 1.459715 | -0.026187 |
| H | -2.201384 | 0.447501 | -1.326647 |
| H | -3.176436 | 1.407964 | -0.237249 |
| H | -0.844310 | 1.526442 | 0.518419 |
| H | -1.754539 | 0.606575 | 1.708123 |
| H | 0.223564 | -0.687617 | 1.452231 |
| H | -1.004200 | -1.525285 | 0.533774 |
| H | 0.635061 | -1.609412 | -1.085110 |
| H | 0.012034 | -0.033840 | -1.510010 |
| C | 2.821453 | -0.875845 | 0.370867 |
| H | 2.391024 | 0.006953 | -1.524399 |
| H | 1.525708 | 1.536225 | 0.989183 |
| H | 1.332326 | 2.107221 | -0.676890 |
| H | 2.948516 | 1.864925 | -0.000906 |
| H | 2.865860 | -1.904700 | -0.002985 |
| H | 2.451049 | -0.912536 | 1.401679 |
| H | 3.845659 | -0.488875 | 0.408202 |
| Rotational constants (GHz): | 4.2048400 | 0.8803400 | 0.8180100 |
| Vibrational harmonic frequencies (cm ⁻¹): | | | |
| 43.3706 | 73.1913 | | 98.7948 |
| 154.9823 | 203.0987 | | 222.1765 |
| 267.7398 | 293.6907 | | 335.8428 |
| 376.5543 | 396.3345 | | 490.4123 |
| 543.1553 | 654.0817 | | 747.5496 |
| 811.7651 | 852.2182 | | 893.2291 |
| 933.9333 | 936.1807 | | 967.9521 |
| 976.4261 | 1027.7242 | | 1042.5048 |
| 1093.8850 | 1103.2301 | | 1138.0633 |

| | | |
|-----------|-----------|-----------|
| 1171.0735 | 1191.7503 | 1215.8216 |
| 1258.3862 | 1312.1649 | 1315.6469 |
| 1359.6144 | 1364.3777 | 1375.5208 |
| 1381.5609 | 1403.2383 | 1406.6290 |
| 1415.4708 | 1434.9332 | 1492.9813 |
| 1496.3808 | 1501.1787 | 1506.5663 |
| 1509.9898 | 1523.0524 | 1524.7633 |
| 2881.2319 | 2945.6834 | 3007.9483 |
| 3023.3388 | 3034.3613 | 3040.6407 |
| 3045.2675 | 3051.1048 | 3064.3048 |
| 3086.4030 | 3093.5029 | 3103.5617 |
| 3104.8256 | 3109.5216 | 3110.2214 |

Zero-point correction (Hartree): 0.208546

C7H15O.pppp

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.95123391

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -3.185432 | -0.649154 | 0.376737 |
| C | -2.342233 | -0.402979 | -0.673076 |
| C | -1.451013 | 0.839665 | -0.519589 |
| C | -0.592397 | 0.834522 | 0.754817 |
| C | 0.511110 | -0.237764 | 0.815514 |
| C | 1.605257 | -0.171567 | -0.270866 |
| C | 2.381061 | 1.153987 | -0.241494 |
| H | -1.716090 | -1.320645 | -0.737440 |
| H | -2.897237 | -0.395036 | -1.631175 |
| H | -0.830387 | 0.932649 | -1.420030 |
| H | -2.105726 | 1.719829 | -0.506519 |
| H | -0.148057 | 1.828273 | 0.883931 |
| H | -1.264814 | 0.688500 | 1.608087 |
| H | 0.997854 | -0.171568 | 1.798904 |
| H | 0.050719 | -1.234994 | 0.786175 |
| C | 2.565982 | -1.361979 | -0.128518 |
| H | 1.121977 | -0.256090 | -1.255561 |
| H | 2.865722 | 1.298784 | 0.732113 |
| H | 1.732409 | 2.016941 | -0.421313 |
| H | 3.164776 | 1.166215 | -1.006717 |
| H | 2.031723 | -2.316992 | -0.183989 |
| H | 3.087619 | -1.329580 | 0.835892 |
| H | 3.326358 | -1.356366 | -0.916988 |

Rotational constants (GHz): 3.6786000 0.9187700 0.8464700

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 31.2193 | 47.0283 | 100.6804 |
| 167.3880 | 211.0831 | 233.9360 |
| 264.6856 | 296.3761 | 349.0624 |
| 382.7793 | 425.3199 | 463.7353 |
| 540.4612 | 622.3775 | 736.7036 |
| 801.8516 | 854.9588 | 889.8708 |
| 930.9656 | 936.0682 | 967.6638 |
| 981.2110 | 1018.9365 | 1063.4391 |
| 1084.1445 | 1105.8452 | 1130.2033 |
| 1181.9446 | 1194.5697 | 1212.7438 |
| 1263.4673 | 1312.3098 | 1314.7494 |
| 1346.1191 | 1369.9884 | 1373.7381 |
| 1387.1802 | 1402.2127 | 1411.9011 |
| 1414.5470 | 1433.9824 | 1492.7370 |
| 1496.7260 | 1499.6849 | 1508.2908 |
| 1510.6468 | 1519.3613 | 1526.6870 |
| 2884.3729 | 2940.9778 | 3009.1885 |
| 3019.1029 | 3032.4858 | 3037.7433 |
| 3039.9750 | 3046.9901 | 3058.1314 |
| 3079.1469 | 3090.1989 | 3099.1911 |
| 3104.6931 | 3109.3919 | 3115.5611 |

Zero-point correction (Hartree): 0.208404

C7H15O.pppt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.94902279

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -3.329388 | -0.729494 | -0.085950 |
| C | -2.480153 | 0.135329 | -0.722283 |
| C | -1.490903 | 0.870742 | 0.197140 |
| C | -0.586674 | -0.084258 | 0.993926 |
| C | 0.553407 | -0.748733 | 0.188025 |
| C | 1.933614 | -0.065803 | 0.290611 |
| C | 2.997322 | -0.895685 | -0.443551 |
| H | -1.924935 | -0.511836 | -1.437749 |
| H | -3.040152 | 0.834786 | -1.372059 |
| H | -0.902023 | 1.564349 | -0.415177 |
| H | -2.078593 | 1.486500 | 0.889218 |
| H | -0.158843 | 0.449977 | 1.851682 |
| H | -1.238140 | -0.857437 | 1.416520 |

| | | | |
|--|-----------|-----------|-----------|
| H | 0.672338 | -1.784866 | 0.528512 |
| H | 0.275429 | -0.821701 | -0.874606 |
| C | 1.936902 | 1.383555 | -0.218170 |
| H | 2.203494 | -0.043290 | 1.357598 |
| H | 2.779424 | -0.949713 | -1.517490 |
| H | 3.039266 | -1.921707 | -0.061829 |
| H | 3.993761 | -0.454764 | -0.330900 |
| H | 1.248409 | 2.019732 | 0.346430 |
| H | 1.648459 | 1.430641 | -1.276012 |
| H | 2.936129 | 1.824392 | -0.130721 |
| Rotational constants (GHz): | 4.1209400 | 0.8499300 | 0.7945800 |
| Vibrational harmonic frequencies (cm-1): | | | |
| 48.3912 | 69.9394 | | 84.6244 |
| 155.9348 | 223.7846 | | 241.9817 |
| 252.2832 | 278.9008 | | 356.4205 |
| 375.2092 | 405.9905 | | 464.1117 |
| 503.2666 | 662.3078 | | 767.0430 |
| 815.3146 | 866.6855 | | 893.4717 |
| 932.8585 | 940.3127 | | 961.9398 |
| 970.7810 | 1037.6406 | | 1056.2810 |
| 1091.3418 | 1113.3688 | | 1134.1096 |
| 1175.6690 | 1194.9608 | | 1216.1068 |
| 1258.3452 | 1311.7564 | | 1318.4151 |
| 1338.9725 | 1371.7638 | | 1377.7618 |
| 1379.9259 | 1397.1385 | | 1405.7859 |
| 1415.3199 | 1434.0360 | | 1493.4105 |
| 1495.6156 | 1504.3815 | | 1505.4207 |
| 1512.4741 | 1519.9816 | | 1524.6383 |
| 2882.0884 | 2946.5234 | | 3001.0814 |
| 3012.1815 | 3031.3293 | | 3036.3989 |
| 3038.6654 | 3046.8629 | | 3060.4676 |
| 3081.7198 | 3090.2936 | | 3096.5576 |
| 3102.7107 | 3110.1196 | | 3116.4918 |
| Zero-point correction (Hartree): | 0.208474 | | |

C7H15O.pptm

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.95105947

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|--|-----------|-----------|-----------|
| O | -2.846596 | 1.139019 | -0.357532 |
| C | -2.687412 | 0.007599 | 0.396634 |
| C | -1.767109 | -1.060219 | -0.215909 |
| C | -0.348763 | -0.555644 | -0.523766 |
| C | 0.517412 | -0.341601 | 0.727682 |
| C | 1.960156 | 0.156527 | 0.478290 |
| C | 2.803671 | -0.851224 | -0.318735 |
| H | -2.264528 | 0.378967 | 1.356347 |
| H | -3.669899 | -0.412618 | 0.686478 |
| H | -1.732634 | -1.922358 | 0.464465 |
| H | -2.240007 | -1.412404 | -1.140880 |
| H | 0.140366 | -1.276744 | -1.188733 |
| H | -0.441189 | 0.378462 | -1.089469 |
| H | 0.024061 | 0.378139 | 1.395770 |
| H | 0.568576 | -1.287328 | 1.286504 |
| C | 1.997755 | 1.547644 | -0.173895 |
| H | 2.422828 | 0.250598 | 1.471586 |
| H | 2.445123 | -0.954784 | -1.348877 |
| H | 2.783560 | -1.844687 | 0.143650 |
| H | 3.849323 | -0.528766 | -0.370040 |
| H | 1.410766 | 2.274005 | 0.399253 |
| H | 1.596754 | 1.526642 | -1.193094 |
| H | 3.025415 | 1.922233 | -0.234515 |
| Rotational constants (GHz): | 3.6937300 | 0.9079600 | 0.8088800 |
| Vibrational harmonic frequencies (cm-1): | | | |
| 28.8906 | 61.2359 | | 102.6785 |
| 163.3702 | 218.5446 | | 229.9097 |
| 237.2193 | 253.4078 | | 339.2341 |
| 366.8993 | 395.1617 | | 501.8866 |
| 553.8918 | 636.2638 | | 754.8318 |
| 790.7498 | 858.5979 | | 874.1883 |
| 932.4539 | 966.0774 | | 971.8993 |
| 982.0498 | 1014.8145 | | 1049.2156 |
| 1096.9390 | 1103.3525 | | 1127.1352 |
| 1168.8084 | 1210.6311 | | 1219.2715 |
| 1276.5738 | 1308.8821 | | 1339.7314 |
| 1341.7959 | 1367.1419 | | 1373.6313 |
| 1381.5838 | 1400.1970 | | 1415.1169 |
| 1418.5453 | 1437.7477 | | 1492.4623 |
| 1494.5053 | 1499.7068 | | 1510.4738 |
| 1512.3941 | 1520.7824 | | 1525.5899 |
| 2887.2912 | 2941.9197 | | 3005.1064 |
| 3019.2417 | 3031.2209 | | 3036.5481 |
| 3041.7725 | 3045.3728 | | 3052.6786 |
| 3076.4741 | 3096.1627 | | 3105.6948 |

3107.5467 3108.9328 3114.3360
Zero-point correction (Hartree): 0.208445

C7H15O.pptp

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.95265306

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 2.819875 | 1.148196 | -0.552714 |
| C | 2.636606 | -0.207946 | -0.592218 |
| C | 1.928148 | -0.807004 | 0.633327 |
| C | 0.550686 | -0.190750 | 0.917175 |
| C | -0.532135 | -0.573742 | -0.102903 |
| C | -1.953932 | -0.091475 | 0.250136 |
| C | -2.060664 | 1.440641 | 0.291734 |
| H | 2.028420 | -0.372867 | -1.509146 |
| H | 3.589926 | -0.726728 | -0.811248 |
| H | 1.844137 | -1.893185 | 0.489718 |
| H | 2.582333 | -0.657406 | 1.501078 |
| H | 0.222982 | -0.505558 | 1.916709 |
| H | 0.670930 | 0.897524 | 0.956644 |
| H | -0.271334 | -0.181680 | -1.096914 |
| H | -0.550921 | -1.668661 | -0.203195 |
| C | -2.980479 | -0.676380 | -0.731332 |
| H | -2.192462 | -0.474428 | 1.254242 |
| H | -1.804767 | 1.875064 | -0.682781 |
| H | -1.392320 | 1.881207 | 1.037354 |
| H | -3.081189 | 1.754928 | 0.536337 |
| H | -2.948658 | -1.771532 | -0.740297 |
| H | -2.785845 | -0.329577 | -1.753865 |
| H | -3.999602 | -0.372735 | -0.468438 |

Rotational constants (GHz): 3.6765400 0.8471400 0.7989500

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 32.1773 | 58.4306 | 108.6548 |
| 144.0730 | 213.1461 | 231.0780 |
| 242.5702 | 259.2687 | 343.3528 |
| 378.5686 | 439.5787 | 441.2846 |
| 518.5544 | 624.9233 | 762.0116 |
| 811.5794 | 863.7831 | 879.5989 |
| 934.0548 | 947.4984 | 969.8232 |
| 980.1178 | 1035.4393 | 1049.8986 |
| 1100.6681 | 1105.8357 | 1128.8692 |
| 1173.4718 | 1198.6891 | 1226.9918 |
| 1274.8112 | 1305.7566 | 1323.4724 |
| 1339.9906 | 1368.7211 | 1374.3274 |
| 1379.3819 | 1397.5824 | 1410.9907 |
| 1417.6982 | 1435.9485 | 1490.9542 |
| 1495.0233 | 1503.3782 | 1507.0823 |
| 1511.1093 | 1519.2528 | 1525.1899 |
| 2888.3140 | 2942.0013 | 3003.2186 |
| 3008.5156 | 3030.3137 | 3032.8291 |
| 3037.1857 | 3039.0423 | 3046.4624 |
| 3075.0371 | 3093.2519 | 3098.7037 |
| 3104.2008 | 3110.1459 | 3120.8777 |

Zero-point correction (Hartree): 0.208258

C7H15O.pptt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.95250995

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 3.012583 | -0.688661 | -0.973452 |
| C | 2.722171 | -0.430278 | 0.339106 |
| C | 1.879065 | 0.831410 | 0.584430 |
| C | 0.530993 | 0.831629 | -0.152084 |
| C | -0.508275 | -0.130278 | 0.442157 |
| C | -1.841992 | -0.206348 | -0.328867 |
| C | -2.722291 | -1.335634 | 0.227331 |
| H | 2.171721 | -1.335788 | 0.678334 |
| H | 3.643065 | -0.436182 | 0.953781 |
| H | 1.728885 | 0.945053 | 1.667005 |
| H | 2.474215 | 1.694327 | 0.261385 |
| H | 0.132567 | 1.852411 | -0.148018 |
| H | 0.716342 | 0.573604 | -1.202636 |
| H | -0.084880 | -1.143399 | 0.484952 |
| H | -0.715353 | 0.154769 | 1.484963 |
| C | -2.606323 | 1.126700 | -0.314565 |
| H | -1.605189 | -0.449305 | -1.375712 |
| H | -2.984934 | -1.147372 | 1.275797 |
| H | -2.209754 | -2.302937 | 0.181759 |
| H | -3.657300 | -1.425070 | -0.336257 |
| H | -2.032676 | 1.937790 | -0.773239 |
| H | -2.846632 | 1.426449 | 0.713363 |
| H | -3.550830 | 1.041721 | -0.862919 |

Rotational constants (GHz): 3.8762000 0.8194000 0.7570300

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 33.8217 | 61.4230 | 105.5670 |
| 148.7036 | 202.1216 | 233.3626 |
| 237.5495 | 257.2626 | 345.9229 |
| 378.3889 | 438.5190 | 443.0636 |
| 510.0838 | 631.0517 | 751.5516 |
| 829.5085 | 857.7576 | 875.9451 |
| 932.9374 | 955.7640 | 967.4984 |
| 978.7056 | 1041.1274 | 1044.2325 |
| 1100.3112 | 1106.8740 | 1129.0115 |
| 1172.7928 | 1198.9903 | 1227.2036 |
| 1276.1665 | 1300.2005 | 1329.8751 |
| 1339.1519 | 1367.8069 | 1372.5657 |
| 1381.3163 | 1399.4664 | 1411.6075 |
| 1416.4924 | 1434.4446 | 1492.1724 |
| 1494.2878 | 1503.4665 | 1508.1715 |
| 1511.8803 | 1519.2511 | 1524.7253 |
| 2884.9905 | 2942.2996 | 3004.2354 |
| 3011.9967 | 3031.4061 | 3032.0186 |
| 3037.4699 | 3043.7784 | 3044.2176 |
| 3076.9305 | 3088.3405 | 3097.7020 |
| 3103.5184 | 3109.6249 | 3117.7639 |

Zero-point correction (Hartree): 0.208239

C7H15O.ptmm

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.94839879

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 3.463529 | -0.308404 | -0.259004 |
| C | 2.643877 | 0.415960 | 0.565061 |
| C | 1.203105 | 0.599456 | 0.065966 |
| C | 0.489939 | -0.742473 | -0.148709 |
| C | -0.821201 | -0.712285 | -0.956919 |
| C | -2.091685 | -0.102445 | -0.313965 |
| C | -2.422484 | -0.730736 | 1.048355 |
| H | 2.645052 | -0.149345 | 1.524358 |
| H | 3.119470 | 1.381042 | 0.827312 |
| H | 0.672299 | 1.231199 | 0.787426 |
| H | 1.236905 | 1.161257 | -0.876682 |
| H | 1.193178 | -1.391398 | -0.684977 |
| H | 0.320933 | -1.224405 | 0.823898 |
| H | -0.634406 | -0.203341 | -1.912970 |
| H | -1.060807 | -1.752354 | -1.216283 |
| C | -2.083248 | 1.432774 | -0.226631 |
| H | -2.911987 | -0.367983 | -0.997111 |
| H | -1.679272 | -0.462083 | 1.807821 |
| H | -2.456528 | -1.824476 | 0.988540 |
| H | -3.396975 | -0.386290 | 1.411505 |
| H | -1.819739 | 1.886910 | -1.188269 |
| H | -1.373057 | 1.799631 | 0.521012 |
| H | -3.073120 | 1.807355 | 0.057501 |

Rotational constants (GHz): 3.9451800 0.8492600 0.8133200

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 25.7301 | 54.0281 | 111.3846 |
| 151.7330 | 229.6419 | 234.7288 |
| 256.1987 | 267.1261 | 337.7147 |
| 371.5684 | 387.5914 | 498.9651 |
| 568.4997 | 588.9796 | 745.0712 |
| 775.7698 | 843.0110 | 913.6279 |
| 931.4949 | 941.5570 | 968.1802 |
| 980.6865 | 1042.2902 | 1048.7937 |
| 1083.5400 | 1096.0130 | 1140.2138 |
| 1189.2375 | 1209.9882 | 1222.4430 |
| 1272.3965 | 1323.8348 | 1328.5114 |
| 1357.9922 | 1367.9177 | 1373.7722 |
| 1382.5579 | 1403.3854 | 1417.7381 |
| 1420.1084 | 1438.6540 | 1489.0857 |
| 1497.4646 | 1501.4495 | 1507.1212 |
| 1516.1761 | 1522.4329 | 1527.5113 |
| 2878.2909 | 2939.8309 | 3004.5137 |
| 3023.1280 | 3028.6507 | 3036.1968 |
| 3041.8472 | 3045.2537 | 3058.1650 |
| 3068.0933 | 3091.7688 | 3103.3651 |
| 3105.7898 | 3108.0476 | 3119.8926 |

Zero-point correction (Hartree): 0.208491

C7H15O.ptmp

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.94976175

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -3.584171 | -0.600504 | -0.082694 |
| C | -2.849336 | 0.554773 | -0.029710 |
| C | -1.415397 | 0.401206 | 0.493260 |

| | | | |
|---|-----------|-----------|-----------|
| C | -0.584443 | -0.578584 | -0.347271 |
| C | 0.825942 | -0.889806 | 0.199541 |
| C | 1.984475 | -0.039713 | -0.364048 |
| C | 1.830755 | 1.465104 | -0.097643 |
| H | -2.838557 | 0.930511 | -1.077523 |
| H | -3.411351 | 1.334741 | 0.520704 |
| H | -0.952377 | 1.394322 | 0.531764 |
| H | -1.465877 | 0.041553 | 1.529363 |
| H | -1.162113 | -1.507340 | -0.413050 |
| H | -0.505450 | -0.202534 | -1.378125 |
| H | 0.821089 | -0.806758 | 1.296393 |
| H | 1.059759 | -1.940247 | -0.015406 |
| C | 3.327963 | -0.545913 | 0.182971 |
| H | 1.991856 | -0.184613 | -1.455268 |
| H | 1.764501 | 1.670287 | 0.978105 |
| H | 0.936835 | 1.878216 | -0.574679 |
| H | 2.692796 | 2.018544 | -0.486468 |
| H | 3.473704 | -1.609884 | -0.033622 |
| H | 3.380297 | -0.418777 | 1.271415 |
| H | 4.168498 | 0.003610 | -0.254656 |

Rotational constants (GHz): 5.0976000 0.7634000 0.7013700

| | | | |
|--|-----------|-----------|--|
| Vibrational harmonic frequencies (cm-1): | | | |
| 39.4288 | 70.2882 | 84.3134 | |
| 142.8757 | 215.9144 | 235.2912 | |
| 261.4266 | 272.2650 | 288.8640 | |
| 377.2323 | 408.3508 | 460.7108 | |
| 512.2977 | 567.7584 | 740.0918 | |
| 801.7343 | 848.7664 | 916.1593 | |
| 930.1235 | 941.3631 | 962.2908 | |
| 970.9767 | 1043.5492 | 1068.5211 | |
| 1080.4890 | 1097.7619 | 1139.5027 | |
| 1195.2331 | 1200.8536 | 1227.3855 | |
| 1263.5208 | 1321.3588 | 1331.6861 | |
| 1342.1957 | 1363.9882 | 1370.1254 | |
| 1381.1344 | 1393.9625 | 1413.7373 | |
| 1415.1593 | 1433.6203 | 1493.5645 | |
| 1496.8536 | 1503.1766 | 1509.5487 | |
| 1513.5682 | 1518.7762 | 1525.0657 | |
| 2880.6171 | 2936.2416 | 3002.4968 | |
| 3014.5011 | 3018.8602 | 3032.3418 | |
| 3037.1837 | 3043.7739 | 3057.8018 | |
| 3074.8147 | 3093.4147 | 3098.0324 | |
| 3103.5610 | 3110.0414 | 3116.0375 | |

Zero-point correction (Hartree): 0.208025

C7H15O.ptmt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.95256192

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 3.578626 | -0.434352 | 0.289945 |
| C | 2.817931 | 0.455362 | -0.421547 |
| C | 1.356275 | 0.044449 | -0.641537 |
| C | 0.601503 | -0.168544 | 0.676435 |
| C | -0.799953 | -0.780799 | 0.521957 |
| C | -1.826769 | 0.039333 | -0.286597 |
| C | -3.136449 | -0.749724 | -0.435176 |
| H | 2.866651 | 1.400611 | 0.164482 |
| H | 3.325965 | 0.711183 | -1.372068 |
| H | 0.871338 | 0.812983 | -1.257159 |
| H | 1.344886 | -0.881999 | -1.231214 |
| H | 1.208095 | -0.831360 | 1.304723 |
| H | 0.539288 | 0.786106 | 1.216680 |
| H | -0.699036 | -1.769942 | 0.053412 |
| H | -1.214818 | -0.963255 | 1.523660 |
| C | -2.096727 | 1.418126 | 0.334967 |
| H | -1.421286 | 0.197680 | -1.296537 |
| H | -3.595287 | -0.933571 | 0.544241 |
| H | -2.966114 | -1.722613 | -0.909259 |
| H | -3.864432 | -0.202726 | -1.044144 |
| H | -1.194224 | 2.036014 | 0.380407 |
| H | -2.480966 | 1.316306 | 1.357705 |
| H | -2.843933 | 1.970186 | -0.245502 |

Rotational constants (GHz): 4.7911300 0.7621200 0.7303700

| | | | |
|--|-----------|-----------|--|
| Vibrational harmonic frequencies (cm-1): | | | |
| 51.5524 | 55.5019 | 101.5198 | |
| 148.5678 | 222.4962 | 241.9683 | |
| 247.1028 | 271.0811 | 313.3099 | |
| 377.7324 | 423.2175 | 467.4650 | |
| 528.0767 | 573.6089 | 744.4773 | |
| 809.5775 | 840.8719 | 913.0992 | |
| 931.8847 | 937.0560 | 963.4011 | |
| 978.7793 | 1030.0072 | 1066.7836 | |
| 1089.9924 | 1098.7542 | 1143.4836 | |

| | | |
|-----------|-----------|-----------|
| 1190.7806 | 1200.6747 | 1226.5464 |
| 1274.8868 | 1318.4217 | 1327.2278 |
| 1349.3736 | 1366.0353 | 1369.5151 |
| 1380.5345 | 1403.6120 | 1415.5524 |
| 1417.9470 | 1434.6655 | 1490.3964 |
| 1498.5848 | 1501.1919 | 1509.9997 |
| 1513.4222 | 1520.3660 | 1527.3421 |
| 2880.9237 | 2936.6039 | 3012.2536 |
| 3017.4918 | 3028.0020 | 3032.1748 |
| 3035.4757 | 3038.0897 | 3056.0346 |
| 3067.5995 | 3086.6950 | 3098.1595 |
| 3104.0972 | 3109.2210 | 3112.8747 |

Zero-point correction (Hartree): 0.208280

C7H15O.ptpm

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.94854087

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -2.660723 | -1.176063 | -0.632082 |
| C | -2.771870 | 0.006346 | 0.052338 |
| C | -1.461419 | 0.547869 | 0.635721 |
| C | -0.407187 | 0.828105 | -0.444327 |
| C | 0.982398 | 1.231834 | 0.101438 |
| C | 2.030306 | 0.100969 | 0.237756 |
| C | 1.573399 | -1.048185 | 1.149726 |
| H | -3.186102 | 0.722908 | -0.692311 |
| H | -3.570580 | -0.069736 | 0.815851 |
| H | -1.679735 | 1.465301 | 1.199584 |
| H | -1.085120 | -0.180813 | 1.362485 |
| H | -0.329023 | -0.057270 | -1.085541 |
| H | -0.787860 | 1.630044 | -1.091268 |
| H | 1.413522 | 1.998808 | -0.554354 |
| H | 0.855425 | 1.716104 | 1.079598 |
| C | 2.481540 | -0.434478 | -1.130525 |
| H | 2.910592 | 0.561617 | 0.709657 |
| H | 0.721596 | -1.586470 | 0.719441 |
| H | 1.278006 | -0.683740 | 2.140097 |
| H | 2.380208 | -1.775807 | 1.291192 |
| H | 2.860220 | 0.371544 | -1.769001 |
| H | 1.659920 | -0.924677 | -1.664858 |
| H | 3.281708 | -1.174060 | -1.016679 |

Rotational constants (GHz): 3.2201400 0.9454900 0.9097300

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 42.7555 | 64.0311 | 106.9267 |
| 153.3519 | 224.0857 | 242.3355 |
| 252.5961 | 289.5448 | 314.0399 |
| 374.9883 | 384.5139 | 494.8347 |
| 526.5716 | 581.2983 | 745.1325 |
| 791.9952 | 838.4088 | 908.1343 |
| 929.6420 | 947.5546 | 974.4548 |
| 982.3500 | 1017.5787 | 1059.3123 |
| 1087.0779 | 1108.4289 | 1140.1821 |
| 1170.9296 | 1207.6107 | 1219.0108 |
| 1279.2819 | 1312.0367 | 1329.0029 |
| 1358.0747 | 1363.8111 | 1366.4902 |
| 1378.8028 | 1395.6449 | 1412.8871 |
| 1418.5783 | 1438.2455 | 1495.6603 |
| 1499.4587 | 1502.4194 | 1511.5518 |
| 1515.1941 | 1526.8829 | 1527.7285 |
| 2879.2568 | 2938.4117 | 3008.6927 |
| 3023.0619 | 3030.2145 | 3035.4958 |
| 3036.4302 | 3041.6996 | 3062.1164 |
| 3080.2893 | 3096.7746 | 3104.3394 |
| 3107.8285 | 3108.3494 | 3113.6058 |

Zero-point correction (Hartree): 0.208402

C7H15O.ptpp

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.95241374

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -3.094661 | 1.021090 | 0.082306 |
| C | -2.866871 | -0.263830 | -0.335926 |
| C | -1.393213 | -0.639989 | -0.528915 |
| C | -0.580095 | -0.506147 | 0.764539 |
| C | 0.916729 | -0.827944 | 0.624134 |
| C | 1.735980 | 0.085910 | -0.311540 |
| C | 1.691919 | 1.559060 | 0.121752 |
| H | -3.332711 | -0.906906 | 0.443876 |
| H | -3.472379 | -0.473288 | -1.239931 |
| H | -1.338449 | -1.668880 | -0.911418 |
| H | -0.980007 | 0.006584 | -1.312398 |
| H | -0.719729 | 0.507554 | 1.156682 |
| H | -1.008412 | -1.181119 | 1.519108 |

| | | | | |
|---|-----------|-----------|-----------|-----------|
| H | 1.374432 | -0.793743 | 1.623288 | |
| H | 1.025088 | -1.866356 | 0.279461 | |
| C | 3.187365 | -0.410630 | -0.394565 | |
| H | 1.307567 | 0.018781 | -1.322063 | |
| H | 2.079391 | 1.677725 | 1.141537 | |
| H | 0.676081 | 1.965515 | 0.102855 | |
| H | 2.307014 | 2.179181 | -0.539458 | |
| H | 3.236672 | -1.451375 | -0.733706 | |
| H | 3.675116 | -0.357848 | 0.586765 | |
| H | 3.776736 | 0.196874 | -1.089919 | |
| Rotational constants (GHz): | 4.0694800 | | 0.8448500 | 0.7768500 |
| Vibrational harmonic frequencies (cm ⁻¹): | | | | |
| 42.0338 | 50.9609 | | | 118.9279 |
| 139.5586 | 220.2806 | | | 245.6621 |
| 250.6307 | 276.3368 | | | 305.4086 |
| 377.7160 | 421.4619 | | | 451.9469 |
| 456.2261 | 573.1680 | | | 745.1818 |
| 814.1779 | 826.0770 | | | 912.1987 |
| 927.5635 | 936.7134 | | | 964.9515 |
| 971.5360 | 1038.0926 | | | 1059.9524 |
| 1095.8185 | 1102.2917 | | | 1142.3407 |
| 1182.9726 | 1198.1959 | | | 1225.0971 |
| 1291.3338 | 1313.4423 | | | 1326.4952 |
| 1350.4357 | 1362.0597 | | | 1371.4741 |
| 1381.0294 | 1402.1449 | | | 1416.7353 |
| 1417.5786 | 1436.2225 | | | 1490.7133 |
| 1497.3844 | 1501.9024 | | | 1509.5000 |
| 1513.8748 | 1520.3355 | | | 1528.8020 |
| 2882.7880 | 2933.4229 | | | 3008.9656 |
| 3016.2416 | 3025.9866 | | | 3031.3609 |
| 3031.9119 | 3037.6593 | | | 3048.9386 |
| 3075.2830 | 3091.2009 | | | 3098.0555 |
| 3103.5390 | 3108.8739 | | | 3117.2341 |
| Zero-point correction (Hartree): | 0.208034 | | | |

C7H15O.ptpt

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.94993012
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | | |
|---|-----------|-----------|-----------|-----------|
| O | 2.944466 | 0.937130 | -0.654167 | |
| C | 2.876949 | -0.094060 | 0.246497 | |
| C | 1.464506 | -0.443279 | 0.729579 | |
| C | 0.543919 | -0.892449 | -0.414047 | |
| C | -0.944650 | -1.039172 | -0.027316 | |
| C | -1.842109 | 0.172731 | -0.357518 | |
| C | -3.305141 | -0.135464 | -0.006476 | |
| H | 3.328838 | -0.961829 | -0.284599 | |
| H | 3.573974 | 0.090620 | 1.087146 | |
| H | 1.535851 | -1.232837 | 1.490172 | |
| H | 1.050791 | 0.436630 | 1.234603 | |
| H | 0.645337 | -0.180175 | -1.242617 | |
| H | 0.918771 | -1.851621 | -0.795859 | |
| H | -1.364388 | -1.909862 | -0.546805 | |
| H | -1.027989 | -1.266665 | 1.045912 | |
| C | -1.386287 | 1.474084 | 0.319377 | |
| H | -1.783763 | 0.328734 | -1.445531 | |
| H | -3.423682 | -0.294752 | 1.072525 | |
| H | -3.658550 | -1.038933 | -0.515817 | |
| H | -3.965587 | 0.690333 | -0.292606 | |
| H | -0.378107 | 1.766366 | 0.010469 | |
| H | -1.390952 | 1.372644 | 1.412111 | |
| H | -2.059391 | 2.299959 | 0.063657 | |
| Rotational constants (GHz): | 4.1393800 | | 0.8596800 | 0.7845900 |
| Vibrational harmonic frequencies (cm ⁻¹): | | | | |
| 32.6226 | 69.5586 | | | 93.9020 |
| 161.6498 | 232.3011 | | | 236.7742 |
| 245.3928 | 290.4938 | | | 306.0078 |
| 373.8945 | 403.4175 | | | 443.8875 |
| 513.0763 | 575.3619 | | | 737.2905 |
| 810.8123 | 849.1498 | | | 916.8868 |
| 924.0725 | 932.5368 | | | 969.8650 |
| 982.2517 | 1038.9397 | | | 1064.1693 |
| 1090.1951 | 1106.7009 | | | 1143.6135 |
| 1175.4141 | 1200.5014 | | | 1227.9078 |
| 1275.5069 | 1314.1182 | | | 1328.7364 |
| 1340.6434 | 1365.3964 | | | 1369.4037 |
| 1381.5344 | 1392.8246 | | | 1412.2279 |
| 1415.1529 | 1434.0241 | | | 1495.3571 |
| 1497.1584 | 1505.1060 | | | 1509.6949 |
| 1515.9259 | 1521.1096 | | | 1526.9370 |
| 2880.0185 | 2938.5330 | | | 3003.8044 |
| 3015.3316 | 3026.2264 | | | 3030.9273 |
| 3035.6713 | 3037.2586 | | | 3060.7809 |

3069.6177 3095.1933 3096.5928
3102.1675 3108.7470 3118.4981
Zero-point correction (Hartree): 0.208154

C7H15O.pttm

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.95222148

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -3.104921 | 1.111214 | 0.403172 |
| C | -2.951148 | -0.243995 | 0.272061 |
| C | -1.730580 | -0.692154 | -0.540665 |
| C | -0.406311 | -0.193739 | 0.049244 |
| C | 0.805855 | -0.556539 | -0.820323 |
| C | 2.183967 | -0.084038 | -0.303964 |
| C | 2.289358 | 1.447117 | -0.224106 |
| H | -2.878236 | -0.622424 | 1.316341 |
| H | -3.890451 | -0.695436 | -0.103608 |
| H | -1.735667 | -1.789082 | -0.605201 |
| H | -1.845208 | -0.319524 | -1.567187 |
| H | -0.478151 | 0.892723 | 0.172827 |
| H | -0.285406 | -0.613248 | 1.057437 |
| H | 0.837944 | -1.648165 | -0.947244 |
| H | 0.651867 | -0.140302 | -1.825911 |
| C | 2.569682 | -0.735889 | 1.033465 |
| H | 2.917585 | -0.421036 | -1.050829 |
| H | 1.624313 | 1.859106 | 0.542912 |
| H | 2.026249 | 1.915728 | -1.179085 |
| H | 3.309531 | 1.755505 | 0.029190 |
| H | 2.507598 | -1.828771 | 0.978436 |
| H | 1.916435 | -0.404895 | 1.848702 |
| H | 3.596024 | -0.474473 | 1.313581 |

Rotational constants (GHz): 3.8065700 0.7984200 0.7557200

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 39.2995 | 70.2964 | 115.9485 |
| 128.2858 | 171.9082 | 239.9044 |
| 251.8348 | 275.1970 | 307.0659 |
| 369.9940 | 383.3815 | 496.4844 |
| 528.1601 | 556.7383 | 751.8981 |
| 794.7250 | 840.9718 | 911.1100 |
| 931.1358 | 960.4517 | 969.1240 |
| 978.1902 | 1020.9282 | 1042.1691 |
| 1094.4921 | 1096.0604 | 1142.8296 |
| 1190.4710 | 1210.0191 | 1222.9419 |
| 1282.5752 | 1312.9971 | 1336.4203 |
| 1353.0889 | 1363.3076 | 1367.3826 |
| 1381.1760 | 1397.1184 | 1416.1940 |
| 1419.8443 | 1436.8772 | 1494.7001 |
| 1496.8628 | 1500.2458 | 1511.4244 |
| 1520.0463 | 1521.8180 | 1525.9652 |
| 2881.4905 | 2935.8707 | 3006.0519 |
| 3020.0282 | 3026.2347 | 3031.9056 |
| 3035.8914 | 3041.4519 | 3048.6698 |
| 3066.1058 | 3091.8444 | 3105.1917 |
| 3105.7729 | 3108.2329 | 3111.6354 |

Zero-point correction (Hartree): 0.208102

C7H15O.pttp

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.95364771

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 3.377842 | 0.330434 | 0.996081 |
| C | 3.093623 | 0.075764 | -0.319851 |
| C | 1.763521 | -0.641692 | -0.579405 |
| C | 0.553355 | 0.139777 | -0.055274 |
| C | -0.771094 | -0.616524 | -0.220379 |
| C | -2.007742 | 0.088075 | 0.372650 |
| C | -2.317164 | 1.421427 | -0.325494 |
| H | 3.093982 | 1.075521 | -0.809112 |
| H | 3.947749 | -0.446126 | -0.794621 |
| H | 1.667423 | -0.821411 | -1.659163 |
| H | 1.805516 | -1.629272 | -0.101576 |
| H | 0.722563 | 0.366586 | 1.004996 |
| H | 0.504283 | 1.106776 | -0.573794 |
| H | -0.951359 | -0.813048 | -1.288226 |
| H | -0.671210 | -1.602817 | 0.254375 |
| C | -3.230758 | -0.840013 | 0.323237 |
| H | -1.791028 | 0.303012 | 1.430046 |
| H | -2.513630 | 1.265199 | -1.393820 |
| H | -1.492349 | 2.135255 | -0.238776 |
| H | -3.206011 | 1.892668 | 0.107961 |
| H | -3.042923 | -1.779142 | 0.855164 |
| H | -3.490272 | -1.090796 | -0.712839 |
| H | -4.107916 | -0.366755 | 0.777835 |

Rotational constants (GHz): 4.7245200 0.7057400 0.6779200
Vibrational harmonic frequencies (cm⁻¹):
40.4030 71.0841 112.1624
128.8070 160.7560 227.9599
252.6294 265.9921 299.4310
383.0424 432.7940 442.7981
480.4565 544.2780 750.4976
821.7567 840.2162 913.5077
934.9240 953.1202 966.1558
977.4432 1032.0492 1058.5502
1093.5761 1098.2422 1147.2336
1189.5002 1199.6024 1231.8442
1281.6520 1304.7798 1335.5203

1341.7124 1363.0065 1368.0051
1378.0474 1395.5911 1415.5565
1419.5887 1436.3994 1493.6528
1494.3221 1503.2754 1510.0305
1519.2104 1519.7692 1525.7811
2881.5036 2935.5941 3003.9505
3010.6814 3026.3658 3031.6488
3033.3096 3038.0585 3043.7495
3063.2812 3085.0364 3098.0984
3103.8413 3109.3788 3118.4431
Zero-point correction (Hartree): 0.207859

C7H15O.pttt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.95373849

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -3.303438 | 1.030610 | -0.225084 |
| C | -3.096604 | -0.254068 | 0.204100 |
| C | -1.760676 | -0.880353 | -0.213629 |
| C | -0.548740 | -0.088616 | 0.290258 |
| C | 0.788206 | -0.647958 | -0.212598 |
| C | 2.043412 | 0.058406 | 0.337593 |
| C | 3.312309 | -0.702675 | -0.075142 |
| H | -3.164511 | -0.196077 | 1.313655 |
| H | -3.960097 | -0.888713 | -0.076618 |
| H | -1.726875 | -1.914725 | 0.155562 |
| H | -1.736640 | -0.939965 | -1.309722 |
| H | -0.673690 | 0.954134 | -0.021806 |
| H | -0.550786 | -0.084935 | 1.390515 |
| H | 0.845712 | -1.714185 | 0.049218 |
| H | 0.809143 | -0.606043 | -1.311922 |
| C | 2.130147 | 1.528598 | -0.100151 |
| H | 1.981754 | 0.036159 | 1.436543 |
| H | 3.422352 | -0.717385 | -1.166575 |
| H | 3.285651 | -1.742401 | 0.269490 |
| H | 4.210791 | -0.234260 | 0.341108 |
| H | 1.270825 | 2.113236 | 0.241447 |
| H | 2.173285 | 1.606930 | -1.193741 |
| H | 3.032270 | 2.003345 | 0.300926 |

Rotational constants (GHz): 4.6873600 0.7376200 0.6664900
Vibrational harmonic frequencies (cm⁻¹):
44.6781 67.5063 114.1734
132.4857 159.8921 227.1721
245.2488 270.6854 297.0641
385.0108 430.2103 442.8089
486.9447 545.4897 753.1851
810.2536 853.2056 913.0844
932.4888 948.2641 968.9796
979.7825 1028.0583 1059.5385
1093.6987 1096.5360 1145.1068
1197.1864 1202.1270 1225.8626
1276.9741 1312.0734 1336.4414
1338.4402 1363.8058 1366.6757
1379.2722 1395.6854 1415.1988
1419.0798 1436.6474 1493.9336
1494.3061 1503.2628 1509.3466
1518.9742 1519.5764 1525.5997
2881.0223 2936.1205 3002.0402
3008.1700 3016.7350 3029.9100
3032.9028 3038.6808 3045.2342
3066.9280 3092.5002 3098.6644
3104.1051 3109.4716 3120.4705
Zero-point correction (Hartree): 0.207871

C7H15O.tpmmm

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.94766311

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|----------|----------|----------|
| O | 3.700448 | 0.607363 | 0.160893 |
|---|----------|----------|----------|

| | | | |
|--|-----------|-----------|-----------|
| C | 2.647945 | -0.223429 | 0.435313 |
| C | 1.394576 | -0.013563 | -0.421662 |
| C | 0.249343 | -0.957186 | -0.026713 |
| C | -1.038814 | -0.798773 | -0.868079 |
| C | -2.127897 | 0.154054 | -0.318319 |
| C | -2.783848 | -0.392763 | 0.959827 |
| H | 2.983748 | -1.280525 | 0.423244 |
| H | -0.901535 | 1.656553 | 0.700073 |
| | | | |
| H | 1.093822 | 1.035590 | -0.338526 |
| H | 1.662152 | -0.179052 | -1.473223 |
| H | 0.609678 | -1.989999 | -0.125127 |
| H | 0.020474 | -0.830370 | 1.040321 |
| H | -0.761247 | -0.472264 | -1.879444 |
| H | -1.503779 | -1.785135 | -0.991288 |
| C | -1.639365 | 1.595300 | -0.108100 |
| H | -2.910145 | 0.187404 | -1.090609 |
| H | -2.072098 | -0.444099 | 1.791853 |
| H | -3.185380 | -1.400062 | 0.802910 |
| H | -3.610580 | 0.250287 | 1.280907 |
| H | -1.178690 | 2.002351 | -1.014795 |
| H | 2.411745 | -0.042585 | 1.508095 |
| H | -2.473376 | 2.251165 | 0.164865 |
| Rotational constants (GHz): | 3.9543400 | 0.8012900 | 0.7559200 |
| Vibrational harmonic frequencies (cm-1): | | | |
| 38.2588 | 61.5551 | | 84.3756 |
| 132.6373 | 183.1211 | | 234.6152 |
| 238.4042 | 278.1219 | | 323.1462 |
| 375.3833 | 387.0566 | | 409.9343 |
| 480.4337 | 549.2612 | | 733.9396 |
| 778.0889 | 856.5877 | | 906.6376 |
| 931.0652 | 956.4215 | | 971.5177 |
| 995.2170 | 1030.4524 | | 1045.4355 |
| 1087.8251 | 1099.7684 | | 1143.3543 |
| 1169.4483 | 1211.3495 | | 1250.9719 |
| 1261.7171 | 1305.0092 | | 1321.1801 |
| 1359.4810 | 1366.1432 | | 1374.6463 |
| 1381.5951 | 1394.2620 | | 1406.8034 |
| 1416.1427 | 1436.0194 | | 1496.4121 |
| 1499.2918 | 1500.8805 | | 1507.4114 |
| 1515.8126 | 1523.3948 | | 1525.1703 |
| 2878.6822 | 2921.4021 | | 3010.0500 |
| 3020.5703 | 3028.9605 | | 3034.8811 |
| 3040.9242 | 3045.6089 | | 3056.8590 |
| 3064.6006 | 3101.1118 | | 3106.1121 |
| 3108.5092 | 3110.2012 | | 3111.0215 |
| Zero-point correction (Hartree): | 0.207713 | | |

C7H15O.tpm

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.94501489
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | |
|--|-----------|-----------|-----------|
| O | 3.130012 | -1.062601 | -0.116056 |
| C | 2.069703 | -0.311446 | -0.542160 |
| C | 1.585354 | 0.758858 | 0.448348 |
| C | 0.379540 | 1.584703 | -0.046881 |
| C | -1.033700 | 1.094220 | 0.326617 |
| C | -1.498057 | -0.271940 | -0.239439 |
| C | -1.161263 | -1.446303 | 0.695482 |
| H | 2.278650 | 0.129343 | -1.538201 |
| H | -0.097724 | -1.501347 | 0.943694 |
| H | 1.368826 | 0.283498 | 1.412016 |
| H | 2.435443 | 1.428780 | 0.624588 |
| H | 0.477936 | 2.603025 | 0.347938 |
| H | 0.441561 | 1.692791 | -1.140259 |
| H | -1.132822 | 1.078174 | 1.421409 |
| H | -1.732028 | 1.866679 | -0.020743 |
| C | -3.009434 | -0.255646 | -0.522440 |
| H | -0.989032 | -0.434201 | -1.201856 |
| H | -1.708680 | -1.347695 | 1.640826 |
| H | 1.272205 | -1.055742 | -0.752815 |
| H | -1.448605 | -2.403855 | 0.247237 |
| H | -3.270728 | 0.517168 | -1.253357 |
| H | -3.575181 | -0.051008 | 0.394908 |
| H | -3.352778 | -1.219478 | -0.914093 |
| Rotational constants (GHz): | 3.1492500 | 1.0139300 | 0.8545500 |
| Vibrational harmonic frequencies (cm-1): | | | |
| 51.2287 | 68.5430 | | 105.7982 |
| 143.9138 | 213.2309 | | 236.9087 |
| 256.9176 | 272.2035 | | 313.4791 |
| 368.2379 | 411.5654 | | 453.3563 |
| 490.7174 | 559.7258 | | 751.8967 |
| 815.0546 | 870.8708 | | 878.0764 |
| 928.9587 | 938.9518 | | 967.8668 |

| | | |
|-----------|-----------|-----------|
| 996.5417 | 1020.9679 | 1071.2324 |
| 1085.3638 | 1110.6284 | 1144.4818 |
| 1178.5514 | 1196.6767 | 1232.4046 |
| 1288.5225 | 1291.1417 | 1337.1096 |
| 1344.1524 | 1366.5137 | 1374.1811 |
| 1383.0817 | 1393.6488 | 1406.5371 |
| 1417.0610 | 1438.2665 | 1493.5677 |
| 1498.3517 | 1502.2389 | 1505.8227 |
| 1511.0101 | 1520.3617 | 1524.2082 |
| 2906.4236 | 2924.9004 | 3002.3361 |
| 3012.4408 | 3020.5399 | 3033.0887 |
| 3041.5987 | 3045.2773 | 3059.8771 |
| 3067.7226 | 3090.2214 | 3098.6808 |
| 3105.5217 | 3110.7320 | 3127.0168 |

Zero-point correction (Hartree): 0.208171

C7H15O.tpmt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.94834449

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -3.173014 | -1.030956 | -0.516296 |
| C | -2.052688 | -0.580790 | 0.126321 |
| C | -1.645413 | 0.862100 | -0.209231 |
| C | -0.416760 | 1.391113 | 0.558924 |
| C | 0.957523 | 1.132953 | -0.088680 |
| C | 1.450817 | -0.324768 | -0.196239 |
| C | 2.779011 | -0.373389 | -0.967914 |
| H | -2.151156 | -0.729705 | 1.221269 |
| H | -1.258773 | -1.302619 | -0.161548 |
| H | -1.487051 | 0.940998 | -1.292006 |
| H | -2.513366 | 1.492041 | 0.019552 |
| H | -0.522518 | 2.477904 | 0.658819 |
| H | -0.432074 | 1.005632 | 1.587900 |
| H | 0.945916 | 1.569289 | -1.097314 |
| H | 1.711658 | 1.701766 | 0.474470 |
| C | 1.603118 | -0.997527 | 1.176159 |
| H | 0.717320 | -0.898685 | -0.781476 |
| H | 3.559952 | 0.183615 | -0.435681 |
| H | 2.678165 | 0.067662 | -1.965627 |
| H | 3.131408 | -1.403182 | -1.090194 |
| H | 0.657794 | -1.042260 | 1.726148 |
| H | 2.321419 | -0.449255 | 1.798230 |
| H | 1.971780 | -2.023699 | 1.071782 |

Rotational constants (GHz): 3.0178100 0.9667600 0.8798100

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 47.2888 | 63.6249 | 87.9923 |
| 124.2501 | 202.2781 | 229.3469 |
| 248.2803 | 290.8381 | 314.1138 |
| 374.6398 | 413.8018 | 451.0145 |
| 489.6363 | 538.4275 | 740.4601 |
| 826.3852 | 848.9814 | 874.5193 |
| 927.2797 | 944.4047 | 965.6485 |
| 988.9663 | 1034.9143 | 1071.7558 |
| 1084.9646 | 1089.1126 | 1145.0500 |
| 1191.3126 | 1194.5708 | 1225.2734 |
| 1288.4116 | 1296.1854 | 1334.0770 |
| 1347.4291 | 1368.9549 | 1372.3337 |
| 1389.5286 | 1394.2127 | 1406.4138 |
| 1414.5453 | 1434.9634 | 1490.5359 |
| 1499.4055 | 1501.2335 | 1506.0087 |
| 1509.5083 | 1518.9940 | 1524.6483 |
| 2901.6575 | 2921.5902 | 3007.6304 |
| 3015.0006 | 3025.1510 | 3033.8687 |
| 3039.3333 | 3041.9828 | 3053.8262 |
| 3069.9128 | 3086.4205 | 3100.2297 |
| 3105.9352 | 3111.0586 | 3113.9799 |

Zero-point correction (Hartree): 0.207892

C7H15O.tppm

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.94616183

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 3.225581 | 0.792068 | -0.283327 |
| C | 2.225244 | 0.075465 | 0.314531 |
| C | 1.248138 | -0.601176 | -0.658405 |
| C | 0.149483 | -1.426036 | 0.033477 |
| C | -0.821519 | -0.694629 | 0.983842 |
| C | -1.833554 | 0.320351 | 0.390817 |
| C | -1.236451 | 1.705434 | 0.089840 |
| H | 2.627150 | -0.642253 | 1.057477 |
| H | 1.689910 | 0.832766 | 0.928533 |
| H | 0.825591 | 0.164663 | -1.315776 |
| H | 1.834155 | -1.268580 | -1.302433 |

| | | | | |
|---|-----------|-----------|-----------|--|
| H | -0.428158 | -1.947129 | -0.738962 | |
| H | 0.637023 | -2.220892 | 0.615431 | |
| H | -1.405215 | -1.476019 | 1.488577 | |
| H | -0.256253 | -0.195084 | 1.782905 | |
| C | -2.586090 | -0.236167 | -0.827648 | |
| H | -2.579625 | 0.475866 | 1.183855 | |
| H | -0.530515 | 1.683537 | -0.746210 | |
| H | -0.711854 | 2.110841 | 0.962642 | |
| H | -2.027705 | 2.415575 | -0.175324 | |
| H | -3.030821 | -1.214645 | -0.613373 | |
| H | -1.924451 | -0.353409 | -1.693268 | |
| H | -3.395395 | 0.438773 | -1.126182 | |
| Rotational constants (GHz): | 3.1775500 | 1.0253500 | 0.9113100 | |
| Vibrational harmonic frequencies (cm ⁻¹): | | | | |
| 34.6993 | 76.1356 | | 101.8996 | |
| 171.1947 | 200.5293 | | 247.6038 | |
| 266.9819 | 305.5279 | | 326.9886 | |
| 368.1519 | 380.2102 | | 466.6384 | |
| 562.9677 | 672.6615 | | 732.8221 | |
| 784.8004 | 861.5574 | | 905.3640 | |
| 928.1286 | 941.4791 | | 972.1107 | |
| 1000.4714 | 1020.6188 | | 1063.8853 | |
| 1085.4494 | 1117.0556 | | 1128.9433 | |
| 1166.6667 | 1212.2221 | | 1217.5866 | |
| 1261.1405 | 1321.7497 | | 1326.0482 | |
| 1356.9589 | 1363.1917 | | 1384.2869 | |
| 1389.4410 | 1400.6504 | | 1409.3756 | |
| 1418.5459 | 1438.0953 | | 1492.6005 | |
| 1497.1531 | 1502.3576 | | 1506.0029 | |
| 1517.3808 | 1523.8454 | | 1528.7327 | |
| 2891.3588 | 2931.8485 | | 3006.0527 | |
| 3020.4451 | 3029.5797 | | 3037.1188 | |
| 3042.5306 | 3050.5825 | | 3054.1246 | |
| 3075.9656 | 3102.5766 | | 3103.3300 | |
| 3106.6998 | 3109.2075 | | 3121.3149 | |
| Zero-point correction (Hartree): | 0.208775 | | | |

C7H15O.tppp

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.95064033
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | | |
|---|-----------|-----------|-----------|--|
| O | 3.325979 | 0.836434 | -0.649342 | |
| C | 2.341730 | 0.433936 | 0.211186 | |
| C | 1.501349 | -0.754998 | -0.279296 | |
| C | 0.402858 | -1.183607 | 0.707732 | |
| C | -0.705370 | -0.146742 | 0.970602 | |
| C | -1.538989 | 0.295554 | -0.250008 | |
| C | -2.274426 | -0.878163 | -0.914162 | |
| H | 2.739428 | 0.260769 | 1.231214 | |
| H | 1.700287 | 1.336569 | 0.319552 | |
| H | 1.079909 | -0.500935 | -1.258459 | |
| H | 2.183299 | -1.597438 | -0.446370 | |
| H | -0.045941 | -2.115781 | 0.345317 | |
| H | 0.870575 | -1.438415 | 1.668880 | |
| H | -1.389625 | -0.560262 | 1.725196 | |
| H | -0.266835 | 0.747945 | 1.434489 | |
| C | -2.532776 | 1.393751 | 0.158591 | |
| H | -0.856927 | 0.729897 | -0.995445 | |
| H | -2.950364 | -1.367689 | -0.201868 | |
| H | -1.584290 | -1.637760 | -1.294230 | |
| H | -2.879024 | -0.531858 | -1.759280 | |
| H | -2.019737 | 2.255303 | 0.600480 | |
| H | -3.248387 | 1.018021 | 0.900387 | |
| H | -3.106466 | 1.751781 | -0.702995 | |
| Rotational constants (GHz): | 3.3006900 | 0.8960700 | 0.8332400 | |
| Vibrational harmonic frequencies (cm ⁻¹): | | | | |
| 43.1849 | 59.8954 | | 97.1088 | |
| 177.1005 | 188.1443 | | 230.6045 | |
| 256.1822 | 300.5239 | | 321.6539 | |
| 375.3343 | 420.9293 | | 449.8528 | |
| 515.9108 | 664.1053 | | 736.3400 | |
| 819.6967 | 867.7703 | | 902.9843 | |
| 932.7662 | 937.2217 | | 969.9220 | |
| 982.5392 | 1021.4854 | | 1081.4933 | |
| 1087.3036 | 1092.6379 | | 1131.0172 | |
| 1182.7843 | 1195.9947 | | 1215.0524 | |
| 1258.6256 | 1309.8913 | | 1325.4834 | |
| 1342.8725 | 1363.1373 | | 1373.2271 | |
| 1391.5823 | 1398.2123 | | 1405.0158 | |
| 1416.5898 | 1436.5121 | | 1493.2908 | |
| 1498.6366 | 1505.7921 | | 1508.8314 | |
| 1510.3254 | 1518.8423 | | 1526.5783 | |
| 2885.1350 | 2930.6272 | | 3009.8057 | |

| | | |
|-----------|-----------|-----------|
| 3016.6112 | 3030.5533 | 3032.3076 |
| 3039.0297 | 3048.4181 | 3052.3893 |
| 3076.3263 | 3095.8849 | 3098.8908 |
| 3104.8277 | 3109.7098 | 3116.4317 |

Zero-point correction (Hartree): 0.208425

C7H15O.tppt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.94749216

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -3.267610 | 0.951530 | -0.096592 |
| C | -2.253188 | 0.118376 | -0.481113 |
| C | -1.502266 | -0.560570 | 0.674458 |
| C | -0.367869 | -1.489219 | 0.212898 |
| C | 0.822793 | -0.852420 | -0.532294 |
| C | 1.708203 | 0.122844 | 0.284406 |
| C | 3.173443 | 0.034644 | -0.173012 |
| H | -2.593697 | -0.618608 | -1.235495 |
| H | -1.562915 | 0.785133 | -1.043713 |
| H | -1.135770 | 0.212068 | 1.358346 |
| H | -2.232568 | -1.149987 | 1.242333 |
| H | 0.020232 | -2.020534 | 1.091702 |
| H | -0.798678 | -2.265884 | -0.434829 |
| H | 1.450981 | -1.682435 | -0.880220 |
| H | 0.479115 | -0.348703 | -1.447257 |
| C | 1.228096 | 1.582098 | 0.203692 |
| H | 1.670191 | -0.190932 | 1.338435 |
| H | 3.268414 | 0.300760 | -1.233188 |
| H | 3.571060 | -0.978320 | -0.048040 |
| H | 3.811107 | 0.719030 | 0.397211 |
| H | 0.199505 | 1.708494 | 0.552283 |
| H | 1.276556 | 1.946018 | -0.830344 |
| H | 1.862067 | 2.237139 | 0.811304 |

Rotational constants (GHz): 3.5715100 0.9421500 0.8169600

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 36.7776 | 58.4944 | 116.3098 |
| 172.5811 | 208.6721 | 232.5548 |
| 255.5163 | 302.9688 | 311.7532 |
| 370.6339 | 413.2814 | 462.3011 |
| 508.6752 | 683.9440 | 762.7248 |
| 806.5013 | 872.1226 | 909.0216 |
| 933.0341 | 941.6195 | 967.0222 |
| 991.0157 | 1018.6838 | 1085.8180 |
| 1090.6776 | 1106.6357 | 1128.8475 |
| 1174.9823 | 1195.4912 | 1224.5522 |
| 1255.0676 | 1317.2329 | 1322.5965 |
| 1344.2224 | 1365.2454 | 1368.4985 |
| 1391.3775 | 1397.2668 | 1405.3566 |
| 1416.1448 | 1436.3210 | 1496.4468 |
| 1498.1795 | 1503.4315 | 1508.1812 |
| 1514.5611 | 1522.2085 | 1524.0131 |
| 2888.7711 | 2931.6264 | 3007.9132 |
| 3018.5502 | 3024.0023 | 3032.5776 |
| 3039.7997 | 3050.1574 | 3055.9207 |
| 3066.2110 | 3097.6586 | 3100.6022 |
| 3104.0724 | 3110.5588 | 3128.2352 |

Zero-point correction (Hartree): 0.208649

C7H15O.tptm

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.95034219

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 3.869235 | 0.200840 | -0.257197 |
| C | 2.543764 | 0.461483 | -0.044269 |
| C | 1.704612 | -0.753508 | 0.380591 |
| C | 0.219820 | -0.431023 | 0.615031 |
| C | -0.547194 | -0.060835 | -0.665229 |
| C | -2.063733 | 0.194136 | -0.501294 |
| C | -2.828053 | -1.058849 | -0.045135 |
| H | 2.405608 | 1.315592 | 0.649026 |
| H | 2.188647 | 0.849183 | -1.024707 |
| H | 1.813850 | -1.535639 | -0.380689 |
| H | 2.142858 | -1.151619 | 1.303709 |
| H | -0.249209 | -1.303868 | 1.083756 |
| H | 0.142476 | 0.383035 | 1.348455 |
| H | -0.101018 | 0.838198 | -1.112751 |
| H | -0.407515 | -0.865778 | -1.400718 |
| C | -2.365585 | 1.391029 | 0.414396 |
| H | -2.435314 | 0.451475 | -1.503722 |
| H | -2.558794 | -1.350473 | 0.976102 |
| H | -2.623790 | -1.912376 | -0.701266 |
| H | -3.908705 | -0.880365 | -0.057166 |
| H | -1.836872 | 2.292023 | 0.083184 |

| | | | | |
|---|-----------|----------|-----------|-----------|
| H | -2.070506 | 1.192407 | 1.450795 | |
| H | -3.437386 | 1.616893 | 0.419025 | |
| Rotational constants (GHz): | 4.6717100 | | 0.7474300 | 0.7042900 |
| Vibrational harmonic frequencies (cm-1): | | | | |
| 27.1210 | 84.3720 | | | 91.5856 |
| 126.0922 | 199.0355 | | | 239.9760 |
| 246.3641 | 252.1593 | | | 306.1336 |
| 366.9394 | 379.3195 | | | 468.9236 |
| 575.7606 | 662.1396 | | | 754.2906 |
| 787.2533 | 860.9574 | | | 898.8307 |
| 933.8433 | 968.1886 | | | 974.6355 |
| 989.0482 | 1020.2955 | | | 1063.1158 |
| 1086.0127 | 1091.7776 | | | 1135.2400 |
| 1180.7555 | 1210.1118 | | | 1226.3979 |
| 1272.8356 | 1312.0838 | | | 1335.6062 |
| 1343.1441 | 1365.1556 | | | 1371.9714 |
| 1382.2822 | 1389.4633 | | | 1416.6723 |
| 1417.0322 | 1437.7649 | | | 1493.8316 |
| 1499.6246 | 1500.8112 | | | 1511.2905 |
| 1512.3129 | 1521.3695 | | | 1524.7251 |
| 2886.9201 | 2927.3253 | | | 3007.8972 |
| 3022.0218 | 3032.3671 | | | 3036.5747 |
| 3042.0427 | 3043.7987 | | | 3049.0446 |
| 3081.5889 | 3089.9452 | | | 3105.5966 |
| 3106.9640 | 3109.2445 | | | 3111.7309 |
| Zero-point correction (Hartree): 0.208379 | | | | |

C7H15O.tptp

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.95194824

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | | |
|---|-----------|-----------|-----------|-----------|
| O | 3.812119 | -0.492662 | -0.468792 | |
| C | 2.508454 | -0.087996 | -0.556312 | |
| C | 1.853110 | 0.279690 | 0.783572 | |
| C | 0.390819 | 0.733597 | 0.654468 | |
| C | -0.576552 | -0.375322 | 0.211927 | |
| C | -2.069610 | 0.008389 | 0.255117 | |
| C | -2.414639 | 1.143693 | -0.720973 | |
| H | 2.386465 | 0.719390 | -1.306264 | |
| H | 1.989298 | -0.959913 | -1.012272 | |
| H | 1.930222 | -0.582730 | 1.457083 | |
| H | 2.448107 | 1.083322 | 1.233942 | |
| H | 0.060819 | 1.122973 | 1.626559 | |
| H | 0.338318 | 1.580889 | -0.042056 | |
| H | -0.333103 | -0.707309 | -0.808301 | |
| H | -0.422810 | -1.250217 | 0.859431 | |
| C | -2.949596 | -1.220899 | -0.016219 | |
| H | -2.289791 | 0.360832 | 1.274425 | |
| H | -2.188077 | 0.851864 | -1.754269 | |
| H | -1.857842 | 2.060152 | -0.503278 | |
| H | -3.481226 | 1.388616 | -0.674070 | |
| H | -2.745373 | -2.025970 | 0.698186 | |
| H | -2.770205 | -1.616484 | -1.023636 | |
| H | -4.013658 | -0.971027 | 0.055369 | |
| Rotational constants (GHz): | 4.3950900 | | 0.7200900 | 0.6947700 |
| Vibrational harmonic frequencies (cm-1): | | | | |
| 38.8984 | 81.0244 | | | 87.3458 |
| 124.6210 | 197.0649 | | | 229.5909 |
| 251.0204 | 256.4248 | | | 300.3254 |
| 378.8382 | 401.2496 | | | 444.9014 |
| 522.7534 | 654.5917 | | | 759.9479 |
| 810.9359 | 870.7930 | | | 893.2651 |
| 933.7933 | 963.3310 | | | 968.4596 |
| 992.1169 | 1023.8021 | | | 1073.0061 |
| 1087.1318 | 1095.1628 | | | 1142.0120 |
| 1179.1405 | 1199.8647 | | | 1231.7291 |
| 1270.2705 | 1310.0604 | | | 1322.4362 |
| 1342.7378 | 1367.2388 | | | 1370.2569 |
| 1378.7139 | 1389.5217 | | | 1409.6753 |
| 1416.4750 | 1435.3375 | | | 1491.5977 |
| 1502.6062 | 1503.9018 | | | 1507.5006 |
| 1512.1595 | 1519.5658 | | | 1524.7885 |
| 2886.2773 | 2927.9968 | | | 3004.0740 |
| 3011.0562 | 3029.8175 | | | 3032.8550 |
| 3037.8335 | 3041.4325 | | | 3045.8775 |
| 3071.5732 | 3090.0350 | | | 3098.6428 |
| 3104.3302 | 3110.5380 | | | 3117.1601 |
| Zero-point correction (Hartree): 0.208173 | | | | |

C7H15O.tppt

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.95179560

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|--|-----------|-----------|-----------|
| O | 3.878683 | 0.537299 | -0.186814 |
| C | 2.598226 | 0.427571 | 0.280840 |
| C | 1.817187 | -0.784804 | -0.249028 |
| C | 0.379871 | -0.882361 | 0.287090 |
| C | -0.560262 | 0.220856 | -0.222445 |
| C | -2.001837 | 0.155050 | 0.323130 |
| C | -2.788539 | 1.409348 | -0.086501 |
| H | 2.565993 | 0.482406 | 1.387686 |
| H | 2.112563 | 1.371909 | -0.050652 |
| H | 1.817299 | -0.746942 | -1.345263 |
| H | 2.374936 | -1.686043 | 0.032628 |
| H | -0.021132 | -1.863959 | 0.010621 |
| H | 0.399303 | -0.864187 | 1.386865 |
| H | -0.145189 | 1.204322 | 0.038057 |
| H | -0.592537 | 0.188939 | -1.321871 |
| C | -2.744199 | -1.113629 | -0.124419 |
| H | -1.940322 | 0.141027 | 1.422065 |
| H | -2.875727 | 1.477400 | -1.177916 |
| H | -2.297904 | 2.323719 | 0.265058 |
| H | -3.803312 | 1.394193 | 0.325558 |
| H | -2.246327 | -2.027143 | 0.214463 |
| H | -2.815258 | -1.157316 | -1.218425 |
| H | -3.764531 | -1.128900 | 0.273632 |
| Rotational constants (GHz): | 4.6431400 | 0.7265100 | 0.6577200 |
| Vibrational harmonic frequencies (cm-1): | | | |
| 38.5232 | 80.8555 | | 86.1471 |
| 123.5299 | 189.6989 | | 231.8787 |
| 245.5171 | 256.2641 | | 300.3781 |
| 379.4916 | 407.3391 | | 443.9992 |
| 518.5045 | 663.6316 | | 749.8246 |
| 824.7020 | 862.6690 | | 905.4801 |
| 933.9049 | 954.7363 | | 969.9064 |
| 1002.7071 | 1021.1049 | | 1069.7301 |
| 1088.6697 | 1093.9050 | | 1136.9695 |
| 1188.9561 | 1198.0105 | | 1230.0669 |
| 1269.5071 | 1302.0546 | | 1325.7634 |
| 1342.8857 | 1363.9344 | | 1370.8956 |
| 1379.6415 | 1390.0838 | | 1407.9336 |
| 1417.2305 | 1435.7670 | | 1491.1734 |
| 1501.0109 | 1503.3046 | | 1507.7787 |
| 1512.3131 | 1519.0268 | | 1525.0884 |
| 2884.6417 | 2927.6929 | | 3004.2513 |
| 3011.1597 | 3020.8996 | | 3033.1510 |
| 3039.0382 | 3044.1590 | | 3048.2792 |
| 3083.3061 | 3089.5551 | | 3099.6951 |
| 3105.0802 | 3110.0865 | | 3118.2718 |
| Zero-point correction (Hartree): | 0.208183 | | |

C7H15O.ttpm

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.94760101
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | |
|--|-----------|-----------|-----------|
| O | -3.579272 | 0.758787 | 0.290012 |
| C | -2.674372 | -0.264044 | 0.210331 |
| C | -1.259192 | 0.135168 | -0.228708 |
| C | -0.292921 | -1.057546 | -0.206848 |
| C | 1.073679 | -0.855301 | -0.890958 |
| C | 2.128252 | 0.056749 | -0.215169 |
| C | 1.837717 | 1.561947 | -0.335374 |
| H | -2.646951 | -0.692910 | 1.237774 |
| H | -3.076505 | -1.094117 | -0.405332 |
| H | -1.317486 | 0.553667 | -1.241729 |
| H | -0.919197 | 0.943402 | 0.425619 |
| H | -0.145227 | -1.388976 | 0.829820 |
| H | -0.783173 | -1.900778 | -0.714800 |
| H | 1.529102 | -1.849325 | -0.995087 |
| H | 0.905434 | -0.495764 | -1.915802 |
| C | 2.402139 | -0.338945 | 1.243752 |
| H | 3.057551 | -0.123460 | -0.775461 |
| H | 0.987974 | 1.870483 | 0.281028 |
| H | 1.619164 | 1.845758 | -1.370707 |
| H | 2.704217 | 2.146610 | -0.006565 |
| H | 2.632725 | -1.406540 | 1.334431 |
| H | 1.541513 | -0.127673 | 1.888689 |
| H | 3.253222 | 0.221152 | 1.645867 |
| Rotational constants (GHz): | 3.5626600 | 0.8357700 | 0.7889500 |
| Vibrational harmonic frequencies (cm-1): | | | |
| 25.1526 | 72.1748 | | 93.7369 |
| 121.6707 | 197.9618 | | 237.3510 |
| 257.7222 | 271.1359 | | 348.0154 |
| 370.1833 | 388.1179 | | 435.5314 |
| 551.5258 | 565.2394 | | 739.2364 |
| 772.1676 | 854.0919 | | 901.9743 |
| 934.0476 | 964.6586 | | 978.8045 |

| | | |
|-----------|-----------|-----------|
| 995.8276 | 1030.6985 | 1054.8420 |
| 1084.5827 | 1089.4689 | 1144.0656 |
| 1186.5583 | 1213.1812 | 1250.7382 |
| 1265.7939 | 1313.5649 | 1325.5493 |
| 1359.2131 | 1370.7435 | 1374.4541 |
| 1383.5344 | 1401.0843 | 1412.8120 |
| 1417.9641 | 1438.1366 | 1490.0607 |
| 1498.1938 | 1501.0228 | 1508.7366 |
| 1517.3395 | 1520.9844 | 1529.0135 |
| 2875.1033 | 2923.5668 | 3004.3535 |
| 3013.2652 | 3024.6762 | 3037.0931 |
| 3043.8374 | 3046.8171 | 3051.8487 |
| 3062.2547 | 3104.8313 | 3105.7705 |
| 3109.1524 | 3110.1392 | 3125.9312 |

Zero-point correction (Hartree): 0.208218

C7H15O.ttpp

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.95186667
Electronic state : 2-A
Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -3.735971 | 0.332229 | -0.784714 |
| C | -2.834422 | 0.058134 | 0.207588 |
| C | -1.401416 | -0.226672 | -0.257473 |
| C | -0.439086 | -0.456442 | 0.915128 |
| C | 0.980811 | -0.882235 | 0.504842 |
| C | 1.786161 | 0.125956 | -0.341086 |
| C | 2.003787 | 1.460574 | 0.387934 |
| H | -2.853197 | 0.956141 | 0.865341 |
| H | -3.221348 | -0.747362 | 0.864415 |
| H | -1.417869 | -1.111527 | -0.907319 |
| H | -1.073470 | 0.612955 | -0.880770 |
| H | -0.394841 | 0.449978 | 1.534085 |
| H | -0.853900 | -1.238549 | 1.566480 |
| H | 1.555537 | -1.106233 | 1.414954 |
| H | 0.913924 | -1.828200 | -0.050458 |
| C | 3.132222 | -0.488483 | -0.754316 |
| H | 1.221249 | 0.331638 | -1.261482 |
| H | 2.543516 | 1.306749 | 1.330792 |
| H | 1.060183 | 1.963041 | 0.623323 |
| H | 2.597031 | 2.148315 | -0.224279 |
| H | 2.992486 | -1.423162 | -1.308474 |
| H | 3.746992 | -0.712822 | 0.126139 |
| H | 3.703140 | 0.196227 | -1.390746 |

Rotational constants (GHz): 4.3219400 0.7314400 0.7169200
Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 38.3866 | 78.3924 | 84.7915 |
| 121.6411 | 199.7789 | 224.5463 |
| 241.3046 | 264.3970 | 305.3677 |
| 384.2520 | 416.2975 | 437.6700 |
| 508.0966 | 523.0265 | 735.2578 |
| 800.9135 | 848.6246 | 909.6370 |
| 930.6482 | 965.4442 | 971.1965 |
| 994.6534 | 1020.7977 | 1071.9888 |
| 1078.0533 | 1090.7729 | 1153.7502 |
| 1185.3258 | 1200.0825 | 1254.2216 |
| 1264.7682 | 1311.4819 | 1315.6128 |
| 1349.4374 | 1366.1581 | 1376.0197 |
| 1384.6716 | 1403.9908 | 1409.7462 |
| 1415.1241 | 1435.3865 | 1489.3695 |
| 1498.0403 | 1503.3333 | 1508.4470 |
| 1512.4894 | 1518.7811 | 1525.6276 |
| 2878.6236 | 2923.1458 | 3011.5010 |
| 3020.8297 | 3022.5287 | 3032.1228 |
| 3038.1155 | 3041.9058 | 3047.5959 |
| 3061.0280 | 3093.6286 | 3098.6549 |
| 3105.1779 | 3109.9676 | 3113.5539 |

Zero-point correction (Hartree): 0.207829

C7H15O.ttppt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.94911699
Electronic state : 2-A
Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -3.794296 | 0.614658 | -0.331990 |
| C | -2.826989 | -0.129219 | 0.288108 |
| C | -1.443222 | -0.099318 | -0.370595 |
| C | -0.406911 | -0.931304 | 0.398700 |
| C | 1.005640 | -0.955714 | -0.228865 |
| C | 2.019096 | 0.061030 | 0.338709 |
| C | 3.400075 | -0.156303 | -0.297993 |
| H | -2.770543 | 0.279493 | 1.322071 |
| H | -3.186264 | -1.166970 | 0.444483 |
| H | -1.539675 | -0.487411 | -1.392727 |
| H | -1.127721 | 0.944918 | -0.463644 |

| | | | | |
|---|-----------|-----------|-----------|--|
| H | -0.339230 | -0.572024 | 1.436081 | |
| H | -0.783121 | -1.960692 | 0.469121 | |
| H | 1.435481 | -1.955996 | -0.092234 | |
| H | 0.925221 | -0.813133 | -1.316307 | |
| C | 1.577701 | 1.523233 | 0.176731 | |
| H | 2.111668 | -0.141149 | 1.416931 | |
| H | 3.367766 | 0.038318 | -1.377096 | |
| H | 3.750105 | -1.184793 | -0.156470 | |
| H | 4.148251 | 0.515331 | 0.136708 | |
| H | 0.646457 | 1.734486 | 0.711069 | |
| H | 1.423038 | 1.773284 | -0.880111 | |
| H | 2.340586 | 2.204649 | 0.569283 | |
| Rotational constants (GHz): | 4.8862200 | 0.7364500 | 0.6804600 | |
| Vibrational harmonic frequencies (cm ⁻¹): | | | | |
| 55.0449 | 63.9715 | 75.7741 | | |
| 133.8747 | 188.2761 | 232.3328 | | |
| 246.8424 | 272.9372 | 291.7727 | | |
| 382.9252 | 387.2754 | 408.2866 | | |
| 474.4082 | 516.0994 | 732.0980 | | |
| 794.6945 | 869.0741 | 910.1461 | | |
| 934.0764 | 950.9665 | 970.0709 | | |
| 1005.9857 | 1024.6995 | 1071.8523 | | |
| 1087.6346 | 1091.7662 | 1147.0394 | | |
| 1189.3541 | 1202.7653 | 1251.1956 | | |
| 1263.1705 | 1305.0295 | 1324.0395 | | |
| 1341.2524 | 1367.0676 | 1381.0574 | | |
| 1383.4755 | 1393.4336 | 1405.5641 | | |
| 1416.5392 | 1434.5672 | 1495.9682 | | |
| 1498.5925 | 1503.8774 | 1511.3363 | | |
| 1515.6140 | 1519.5807 | 1525.0306 | | |
| 2879.5291 | 2920.9197 | 3002.4060 | | |
| 3014.9246 | 3018.8520 | 3033.1591 | | |
| 3038.6748 | 3044.5331 | 3053.4072 | | |
| 3062.9843 | 3099.1546 | 3103.6242 | | |
| 3105.5293 | 3110.3354 | 3117.8034 | | |
| Zero-point correction (Hartree): | 0.207665 | | | |

C7H15O.tttm

```

-----
E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.95155499
Electronic state : 2-A
Cartesian coordinates (Angs):
O      4.079287    -0.023507    -0.036387
C      2.806906    0.050502    -0.535440
C      1.681249    -0.024741    0.501751
C      0.284562    0.014704    -0.131121
C     -0.839566    -0.029728    0.914797
C     -2.285974    -0.011300    0.369729
C     -2.610300    1.277495    -0.402240
H      2.708265    0.944176    -1.185177
H      2.728271    -0.795686    -1.254321
H      1.810646    -0.943229    1.087521
H      1.800297    0.811692    1.202491
H      0.191395    0.924390    -0.739534
H      0.182265    -0.829126    -0.827054
H     -0.711455    -0.931813    1.529250
H     -0.714673    0.821506    1.598691
C     -2.616431    -1.256459    -0.468386
H     -2.940354    -0.033079    1.253277
H     -2.036592    1.345992    -1.333263
H     -2.386017    2.168767    0.194660
H     -3.671536    1.314680    -0.671056
H     -2.399650    -2.178363    0.082937
H     -2.040701    -1.281677    -1.400438
H     -3.677132    -1.273012    -0.741439
Rotational constants (GHz): 4.9385100 0.6745700 0.6570200
Vibrational harmonic frequencies (cm-1):
51.7720 63.6929 108.3529
128.5460 132.9689 228.7678
238.0870 249.2176 336.0387
367.6718 381.4192 402.4245
468.2925 578.0158 740.4252
793.7466 815.0779 932.9214
952.4357 960.1096 976.0690
997.9561 1037.0294 1055.2799
1059.6494 1089.3617 1146.7466
1200.8659 1211.2151 1248.6790
1268.1332 1311.4245 1335.8877
1338.1724 1366.8010 1376.8981
1381.6898 1398.6314 1415.0677
1418.8616 1438.5055 1493.9934
1500.2604 1500.6038 1511.9382
1518.1031 1522.2418 1525.2253
2881.0481 2919.9590 3008.5167
3021.8068 3025.3454 3035.8263
    
```

| | | |
|-----------|-----------|-----------|
| 3041.1231 | 3042.0746 | 3044.7631 |
| 3064.2631 | 3089.4026 | 3105.4463 |
| 3106.6747 | 3108.5685 | 3111.0874 |

Zero-point correction (Hartree): 0.207726

C7H15O.tttt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.95303905

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -4.180147 | -0.197298 | 0.144550 |
| C | -2.979104 | 0.368672 | -0.187912 |
| C | -1.734587 | -0.434900 | 0.204923 |
| C | -0.428811 | 0.234162 | -0.241385 |
| C | 0.820695 | -0.556040 | 0.171129 |
| C | 2.160142 | 0.017199 | -0.332898 |
| C | 2.461930 | 1.407571 | 0.247565 |
| H | -3.018970 | 0.504447 | -1.291925 |
| H | -2.933709 | 1.409217 | 0.193723 |
| H | -1.736454 | -0.564447 | 1.294841 |
| H | -1.818748 | -1.438940 | -0.228901 |
| H | -0.435818 | 0.354326 | -1.334942 |
| H | -0.385148 | 1.249219 | 0.175084 |
| H | 0.855717 | -0.632605 | 1.268084 |
| H | 0.720022 | -1.585570 | -0.199751 |
| C | 3.308560 | -0.955473 | -0.025143 |
| H | 2.088698 | 0.116334 | -1.426965 |
| H | 2.521092 | 1.368062 | 1.342537 |
| H | 1.695764 | 2.142150 | -0.018639 |
| H | 3.421456 | 1.786076 | -0.121245 |
| H | 3.129634 | -1.940015 | -0.471113 |
| H | 3.422367 | -1.096761 | 1.056750 |
| H | 4.262329 | -0.580265 | -0.411619 |

Rotational constants (GHz): 5.9657600 0.6322300 0.5941300

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 56.5669 | 61.0076 | 99.6583 |
| 134.1916 | 137.2481 | 222.6618 |
| 246.9907 | 250.2242 | 277.4754 |
| 382.9085 | 399.2430 | 424.1294 |
| 457.6346 | 524.3707 | 741.7389 |
| 807.3657 | 833.8616 | 931.5663 |
| 939.1450 | 960.8322 | 971.3769 |
| 1012.7952 | 1044.2668 | 1056.5944 |
| 1066.7536 | 1089.0115 | 1151.7218 |
| 1196.6414 | 1211.8759 | 1246.8408 |
| 1266.6667 | 1311.1350 | 1326.8073 |
| 1337.6357 | 1364.0886 | 1374.9361 |
| 1381.7698 | 1400.0706 | 1413.0208 |
| 1417.3052 | 1436.0337 | 1492.0668 |
| 1499.9085 | 1502.0693 | 1508.7146 |
| 1518.3046 | 1519.1900 | 1524.7543 |
| 2881.4732 | 2921.4979 | 3003.2047 |
| 3009.7478 | 3017.6842 | 3032.4865 |
| 3037.9166 | 3041.8322 | 3042.8437 |
| 3062.3526 | 3089.2612 | 3098.6871 |
| 3104.4582 | 3109.5050 | 3116.5807 |

Zero-point correction (Hartree): 0.207543

C7H15O-1-6Hshift.a

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.94250665

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 0.739846 | -1.671238 | -0.292243 |
| H | -0.317282 | -0.919708 | -0.122466 |
| C | -1.149612 | -0.020430 | -0.002156 |
| C | 1.812519 | -0.981936 | 0.289451 |
| C | -0.418696 | 1.231820 | -0.493092 |
| C | 2.046760 | 0.426394 | -0.276975 |
| C | 0.981909 | 1.469824 | 0.105353 |
| C | -1.536163 | -0.000935 | 1.471399 |
| C | -2.290494 | -0.449055 | -0.915666 |
| H | 1.726720 | -0.933557 | 1.390829 |
| H | 2.695280 | -1.606886 | 0.075711 |
| H | -0.325793 | 1.178829 | -1.585770 |
| H | -1.051172 | 2.108632 | -0.282705 |
| H | 3.022391 | 0.777781 | 0.084395 |
| H | 2.119917 | 0.350895 | -1.369819 |
| H | 1.328468 | 2.454898 | -0.230700 |
| H | 0.918059 | 1.535069 | 1.199980 |
| H | -1.965995 | -0.959197 | 1.779483 |
| H | -2.292034 | 0.776475 | 1.655602 |
| H | -0.684591 | 0.209949 | 2.124883 |
| H | -3.078477 | 0.318156 | -0.931097 |
| H | -2.746381 | -1.384385 | -0.575763 |

```

H      -1.945222   -0.591143   -1.944495
Rotational constants (GHz):  2.6043100   1.4701000   1.2444100
Vibrational harmonic frequencies (cm-1):
i1034.1119           82.2121           111.2014
 190.0576           200.2668           223.7078
 248.9840           329.7613           336.1386
 380.4386           391.4020           448.1756
 501.6471           611.6503           759.0146
 800.7266           844.6424           898.9852
 933.2178           940.4262           965.5760
 985.4501           992.8104           1064.3189
1068.2761           1094.5286           1142.3693
1172.6949           1190.2041           1224.6696
1246.2507           1273.8488           1282.4454
1313.5569           1378.5919           1384.6520
1396.9226           1404.6275           1406.7992
1425.7702           1429.4230           1478.1903
1479.0533           1485.8457           1493.7721
1498.0825           1503.1297           1507.6612
1520.5554           2947.4648           2999.8095
3000.3062           3015.4393           3021.3958
3029.3533           3033.2199           3055.4510
3068.5055           3078.1311           3091.0374
3096.0896           3123.1264           3127.1562
Zero-point correction (Hartree): 0.204418
  
```

C7H15O-1-6Hshift.b

```

-----
E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.93858884
Electronic state : 2-A
Cartesian coordinates (Angs):
O      0.773352   -1.374968   0.879041
H     -0.317148   -0.776804   0.483361
C     -1.151421   -0.020704  -0.035742
C      1.699228   -1.061359  -0.126115
C     -0.305779   1.059781  -0.725799
C      2.141039   0.414665  -0.132605
C      0.982326   1.419691   0.044207
C     -1.964040   0.491229   1.147667
C     -1.956302  -0.890361  -0.990177
H      2.570797  -1.710652   0.052622
H      1.314591  -1.347165  -1.120890
H     -0.047172   0.737620  -1.742813
H     -0.925409   1.961180  -0.843219
H      2.872457   0.581707   0.666840
H      2.661646   0.606911  -1.080893
H      1.330506   2.411994  -0.264502
H      0.743295   1.500760   1.110429
H     -2.430589  -0.332776   1.696737
H     -2.767646   1.154766   0.796450
H     -1.349605   1.059293   1.852241
H     -2.704406  -0.284272  -1.522143
H     -2.491783  -1.683310  -0.458537
H     -1.316657  -1.357159  -1.746631
Rotational constants (GHz):  2.6697000   1.4641000   1.2624100
Vibrational harmonic frequencies (cm-1):
i1131.7555           84.1916           109.8077
 197.8920           205.7171           215.1904
 252.1208           269.4487           340.8266
 383.9735           388.7601           427.5326
 565.7688           596.3032           746.1388
 807.5005           812.3872           894.1191
 932.4326           942.9433           974.9146
 979.1759           1002.7331          1053.4415
1062.0235           1110.9202          1132.7174
1165.6729           1198.6476          1228.5601
1248.8401           1263.5859          1275.2185
1307.3984           1361.2583          1382.0572
1389.1917           1407.3772          1411.3893
1426.4373           1452.9466          1475.7350
1485.1116           1493.2063          1493.7906
1503.8845           1504.6784          1510.8398
1515.9341           2958.3955          3010.4260
3012.3367           3014.6503          3021.7712
3030.4672           3048.3901          3060.3742
3075.4253           3086.9686          3092.0270
3095.8554           3119.5330          3126.2788
Zero-point correction (Hartree): 0.204451
  
```

C7H15O-1-6Hshift.c

```

-----
E(UB+HF-LYP/6-31G(d,p)) (Hartree): -350.93755866
Electronic state : 2-A
Cartesian coordinates (Angs):
C      0.350871   -0.903644   -0.909945
  
```

| | | | |
|---|-----------|-----------|-----------|
| C | -0.963637 | -1.480270 | -0.339369 |
| C | -1.907022 | -0.469155 | 0.358693 |
| C | -1.837735 | 0.972081 | -0.175399 |
| O | -0.744357 | 1.695521 | 0.326450 |
| H | 0.300272 | 0.919310 | 0.258188 |
| C | 1.128038 | 0.026922 | 0.017871 |
| H | 0.129346 | -0.349781 | -1.831154 |
| H | 0.998570 | -1.740099 | -1.215644 |
| H | -1.496407 | -1.955009 | -1.172373 |
| H | -0.738041 | -2.289384 | 0.365276 |
| H | -2.936826 | -0.836745 | 0.274069 |
| H | -1.685763 | -0.410708 | 1.430621 |
| H | -1.875583 | 0.980346 | -1.279759 |
| H | -2.726683 | 1.522615 | 0.172880 |
| C | 1.519387 | -0.569978 | 1.362721 |
| C | 2.272000 | 0.753793 | -0.676343 |
| H | 1.983980 | 0.181611 | 2.008815 |
| H | 2.249354 | -1.380635 | 1.221031 |
| H | 0.662683 | -0.989554 | 1.897371 |
| H | 3.052031 | 0.040842 | -0.980967 |
| H | 2.738379 | 1.489919 | -0.013875 |
| H | 1.928136 | 1.274610 | -1.575448 |
| Rotational constants (GHz): | 2.5732100 | 1.5182800 | 1.2692800 |
| Vibrational harmonic frequencies (cm ⁻¹): | | | |
| i1158.4978 | 96.1963 | | 110.3937 |
| 165.9703 | 199.7263 | | 222.5779 |
| 233.7141 | 277.5104 | | 331.0269 |
| 361.7770 | 389.1395 | | 436.0554 |
| 561.0488 | 595.6189 | | 728.4671 |
| 800.8188 | 824.4652 | | 909.1425 |
| | | | |
| 936.5519 | 951.8840 | | 959.3037 |
| 984.2547 | 989.4047 | | 1059.0382 |
| 1075.4835 | 1104.6898 | | 1140.6405 |
| 1149.0590 | 1212.0247 | | 1238.6784 |
| 1240.6945 | 1243.4384 | | 1291.9033 |
| 1302.6846 | 1360.5075 | | 1386.7704 |
| 1391.9932 | 1396.6283 | | 1408.1658 |
| 1426.0501 | 1447.8022 | | 1481.6103 |
| 1487.8366 | 1492.5898 | | 1496.1610 |
| 1501.6891 | 1507.3201 | | 1510.8657 |
| 1519.4467 | 2952.9192 | | 3001.1581 |
| 3003.8906 | 3015.1028 | | 3020.9907 |
| 3038.6601 | 3050.0850 | | 3050.7168 |
| 3073.5118 | 3090.7998 | | 3093.4984 |
| 3095.2296 | 3123.2498 | | 3128.9858 |
| Zero-point correction (Hartree): | 0.204301 | | |

C4H7O2.hcm

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -307.04379113
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -2.070832 | 0.260605 | 0.636511 |
| C | -1.027992 | 0.022522 | -0.038667 |
| C | 0.107719 | 0.992756 | -0.198858 |
| C | 1.450155 | 0.317393 | -0.524889 |
| C | 2.013785 | -0.508028 | 0.636220 |
| H | 2.975620 | -0.954094 | 0.365909 |
| O | -1.080363 | -1.115572 | -0.578885 |
| H | -0.184463 | 1.678818 | -1.005328 |
| H | 0.163237 | 1.594640 | 0.715625 |
| H | 1.322884 | -0.319052 | -1.407562 |
| H | 2.162435 | 1.100787 | -0.806808 |
| H | 2.172182 | 0.113314 | 1.524882 |
| H | 1.335671 | -1.322529 | 0.909440 |
| Rotational constants (GHz): | 6.7890000 | 2.2702600 | 2.0907600 |
| Vibrational harmonic frequencies (cm ⁻¹): | | | |
| 40.1226 | 105.7050 | | 189.0024 |
| 272.5394 | 344.6160 | | 471.1330 |
| 534.5418 | 606.2528 | | 772.5972 |
| 863.5375 | 887.9790 | | 922.2370 |
| 1053.2427 | 1099.3983 | | 1107.3415 |
| 1181.9499 | 1246.8360 | | 1294.1479 |
| 1362.9967 | 1383.2180 | | 1429.9405 |
| 1465.5361 | 1500.8588 | | 1515.1986 |
| 1522.6579 | 1599.7343 | | 3045.0429 |
| 3047.9607 | 3057.7540 | | 3088.0775 |
| 3096.8817 | 3119.8387 | | 3127.9473 |
| Zero-point correction (Hartree): | 0.105609 | | |

C4H7O2.hct

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -307.04385566
 Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -2.243710 | -0.760782 | -0.073256 |
| C | -1.201718 | -0.047506 | 0.015498 |
| C | 0.190221 | -0.606560 | 0.077450 |
| C | 1.287351 | 0.451439 | -0.102606 |
| C | 2.691589 | -0.148212 | 0.016463 |
| H | 3.457434 | 0.621378 | -0.117976 |
| O | -1.486204 | 1.178984 | 0.058475 |
| H | 0.288753 | -1.109647 | 1.049322 |
| H | 0.261276 | -1.398119 | -0.678730 |
| H | 1.167182 | 0.932893 | -1.079725 |
| H | 1.152034 | 1.240851 | 0.644797 |
| H | 2.847515 | -0.605487 | 0.999972 |
| H | 2.860462 | -0.922453 | -0.740248 |

Rotational constants (GHz): 9.9159800 1.8362800 1.5992000

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 25.0210 | 93.5211 | 167.1367 |
| 241.8232 | 333.9496 | 446.2869 |
| 535.1795 | 621.3723 | 749.2296 |
| 882.1415 | 886.5928 | 940.3438 |
| 1047.5259 | 1111.9599 | 1123.1784 |
| 1171.4240 | 1256.3134 | 1306.9627 |
| 1332.4236 | 1399.2220 | 1430.4960 |
| 1465.9702 | 1505.4818 | 1513.0383 |
| 1521.7071 | 1600.8400 | 3041.6209 |
| 3043.8624 | 3059.7309 | 3078.5582 |
| 3094.7359 | 3116.8290 | 3123.4787 |

Zero-point correction (Hartree): 0.105406

C4H7O2.1-5Hshift

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -307.02254333
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| C | -1.831375 | -0.649315 | 0.124641 |
| C | -1.394905 | 0.730279 | -0.328651 |
| C | -0.026554 | 1.063867 | 0.281823 |
| C | 1.009368 | -0.031857 | 0.019775 |
| O | 0.548097 | -1.288280 | -0.030417 |
| H | -2.085123 | -0.738826 | 1.183724 |
| H | -2.524360 | -1.189715 | -0.521650 |
| H | -2.137759 | 1.485612 | -0.037053 |
| H | -1.328593 | 0.757945 | -1.421857 |
| H | -0.116081 | 1.162859 | 1.372414 |
| H | 0.388359 | 2.002315 | -0.092065 |
| O | 2.199327 | 0.175461 | -0.108719 |
| H | -0.715033 | -1.255483 | 0.044039 |

Rotational constants (GHz): 7.0136900 2.7562800 2.1157500

Vibrational harmonic frequencies (cm-1):

| | | |
|------------|-----------|-----------|
| 11462.1067 | 103.0679 | 223.2445 |
| 394.4103 | 445.8866 | 471.3027 |
| 510.7727 | 609.3802 | 712.2326 |
| 822.8111 | 871.4458 | 894.6599 |
| 912.5003 | 1036.5067 | 1105.0837 |
| 1115.3730 | 1196.3863 | 1201.7255 |
| 1247.3488 | 1302.5788 | 1339.1325 |
| 1369.8695 | 1465.2841 | 1483.2050 |
| 1500.2635 | 1531.6971 | 1780.1387 |
| 3031.6657 | 3044.6178 | 3087.1861 |
| 3097.6446 | 3134.8456 | 3182.2720 |

Zero-point correction (Hartree): 0.100751

C4H7O2.phomch

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -306.99770396
 Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 2.146845 | -0.769285 | -0.304294 |
| C | 0.930043 | -0.755578 | 0.364654 |
| C | 0.147064 | 0.532762 | 0.090577 |
| C | -1.366071 | 0.525209 | 0.159294 |
| C | -2.102317 | -0.785934 | -0.223031 |
| H | -3.174638 | -0.614478 | -0.124573 |
| O | 0.743861 | 1.578684 | -0.144659 |
| H | 0.317958 | -1.607329 | 0.038334 |
| H | 1.096159 | -0.794744 | 1.453257 |
| H | -1.630480 | 0.781238 | 1.193096 |
| H | -1.693270 | 1.334870 | -0.496941 |
| H | -1.877846 | -1.063876 | -1.255650 |
| H | -1.815846 | -1.609631 | 0.435129 |

Rotational constants (GHz): 5.6232025 2.5051444 1.8602969

C4H7O2.phomhh

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -307.00673936

Electronic state : 2-A
Cartesian coordinates (Angs):
O 2.264805 -0.436705 -0.451086
C 1.208268 -0.670424 0.328020
C 0.079129 0.445896 0.208145
C -1.297092 -0.041908 0.643183
C -2.112875 -0.527345 -0.569277
H -3.107409 -0.850251 -0.248975
O 0.299359 1.556353 -0.192576
H 0.721587 -1.657036 0.200344
H 1.462707 -0.549322 1.405315
H -1.194810 -0.847271 1.379146
H -1.800797 0.804177 1.120187
H -2.230848 0.277846 -1.299259
H -1.628314 -1.372641 -1.067887
Rotational constants (GHz): 6.1345447 2.2805614 1.9518528

C4H7O2.phopch

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -307.00624946
Electronic state : 2-A
Cartesian coordinates (Angs):
O -2.293331 -0.574472 0.086350
C -0.981871 -0.811470 -0.014003
C -0.112773 0.521488 0.045195
C 1.311268 0.311325 0.545373
C 2.120943 -0.666188 -0.323543
H 3.142627 -0.744679 0.058371
O -0.554641 1.584023 -0.300082
H -0.569391 -1.539564 0.710399
H -0.727859 -1.163619 -1.038463
H 1.783693 1.296923 0.566834
H 1.260197 -0.063564 1.575371
H 1.691902 -1.672710 -0.320645
H 2.177202 -0.320128 -1.360140
Rotational constants (GHz): 5.9764400 2.3997500 1.8742400
Vibrational harmonic frequencies (cm-1):
62.8509 96.1450 205.6306
217.7665 293.3347 383.1478
480.8414 598.9434 623.4174
776.6102 863.8412 924.0930
949.2390 1033.5787 1084.6781
1163.6520 1193.9806 1282.5032
1294.6061 1335.9010 1427.0317
1480.8567 1485.0836 1516.0550
1516.7215 1861.0600 2877.7976
2948.7202 3052.6477 3057.2120
3116.0962 3132.2386 3136.2560
Zero-point correction (Hartree): 0.103594

C4H7O2.phopch

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -307.00880002
Electronic state : 2-A
Cartesian coordinates (Angs):
O -2.491142 0.061759 -0.268410
C -1.445380 -0.611249 0.224757
C -0.074820 0.177245 0.050543
C 1.130430 -0.737418 -0.108044
C 2.463541 0.002746 -0.022927
H 3.295540 -0.691288 -0.171270
O -0.021565 1.377540 0.066562
H -1.499121 -0.655079 1.335042
H -1.317125 -1.643142 -0.153634
H 1.054646 -1.533059 0.646150
H 1.018460 -1.247446 -1.075301
H 2.521915 0.784488 -0.783951
H 2.584709 0.483193 0.951773
Rotational constants (GHz): 8.8752500 2.0284600 1.7295800
Vibrational harmonic frequencies (cm-1):
49.0291 98.7649 197.9961
215.5097 298.5868 355.0753
461.2193 531.1533 700.6369
758.9011 863.2043 931.2595
972.5877 1026.3721 1087.8534
1122.4407 1187.8705 1281.2498
1290.5129 1364.2214 1427.7969
1461.6528 1479.6266 1506.4259
1512.2367 1862.8870 2880.5850
2952.0903 3032.5966 3062.9285
3065.1565 3137.3297 3146.6611
Zero-point correction (Hartree): 0.103252

C4H7O2.pohmhh

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -307.01450240
Electronic state : 2-A
Cartesian coordinates (Angs):
O 1.128218 -1.524271 -0.090615
C 1.483946 -0.245804 0.036442
C 0.204626 0.717736 0.099079
C -1.051820 0.111579 0.680894
C -1.821137 -0.658928 -0.410153
H -2.710905 -1.123265 0.024194
O 0.312405 1.839793 -0.320593
H 1.908927 -0.029175 1.042870
H 2.154178 0.168214 -0.735413
H -0.773906 -0.575757 1.485327
H -1.659915 0.926757 1.082925
H -2.138523 0.012609 -1.212916
H -1.198522 -1.451056 -0.834892
Rotational constants (GHz): 4.0749100 3.4992600 2.1499800
Vibrational harmonic frequencies (cm-1):
84.3762 107.6927 195.2417
224.4852 296.2869 419.5200
480.5639 591.8656 671.3208
797.6990 848.3821 925.7601
993.5236 1081.0080 1089.4430
1167.1142 1229.7782 1279.3858
1287.0543 1331.5441 1416.4235
1479.1189 1489.9448 1507.3493
1522.2376 1853.3486 2864.5328
2998.9604 3057.9874 3074.0415
3127.8875 3136.4879 3147.0391
Zero-point correction (Hartree): 0.104289

C4H7O2.pohpch

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -307.01431884
Electronic state : 2-A
Cartesian coordinates (Angs):
O 1.040230 -1.579774 -0.387575
C 1.266742 -0.499909 0.361821
C 0.294580 0.705945 -0.051386
C -1.068289 0.314523 -0.575441
C -1.882100 -0.525536 0.423548
H -2.862959 -0.754281 -0.002147
O 0.693158 1.831866 0.089696
H 0.937826 -0.642123 1.415795
H 2.290972 -0.091824 0.354261
H -1.590806 1.235045 -0.849296
H -0.890308 -0.277885 -1.481877
H -1.374656 -1.469638 0.632823
H -2.042768 0.013831 1.362216
Rotational constants (GHz): 3.9123400 3.5389300 2.1329700
Vibrational harmonic frequencies (cm-1):
88.7691 117.3002 214.8309
218.6104 287.4066 462.0480
475.3283 572.5535 624.1995
800.0475 858.4310 910.3891
1003.5483 1067.5619 1106.7412
1176.4256 1224.8289 1280.7267
1284.4695 1341.2446 1418.1511
1471.4389 1489.4652 1512.4283
1526.6625 1853.7316 2868.4762
3002.5582 3052.5453 3060.9200
3121.6073 3131.2732 3155.0107
Zero-point correction (Hartree): 0.104294

C4H7O2.pohphc

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -307.01583016
Electronic state : 2-A
Cartesian coordinates (Angs):
O 1.993310 -0.975856 -0.227117
C 1.637608 0.235634 0.209412
C 0.073174 0.488419 0.013823
C -0.798566 -0.743468 0.054199
C -2.293993 -0.441009 -0.009374
H -2.868763 -1.371215 0.002718
O -0.312235 1.618103 -0.141786
H 1.695835 0.306045 1.318740
H 2.160987 1.100473 -0.232032
H -0.473613 -1.364843 -0.791995
H -0.514657 -1.323839 0.941386
H -2.605506 0.147070 0.877163
H -2.552228 0.130875 -0.885604
Rotational constants (GHz): 6.1219000 2.4687200 1.8437500
Vibrational harmonic frequencies (cm-1):
76.3355 99.3758 188.5431

| | | |
|-----------|-----------|-----------|
| 197.4874 | 290.6650 | 414.4461 |
| 484.6836 | 536.8231 | 712.4276 |
| 753.2939 | 821.3140 | 916.9506 |
| 996.2807 | 1075.0050 | 1097.5670 |
| 1142.0778 | 1218.8421 | 1271.2125 |
| 1280.1612 | 1371.6681 | 1429.0694 |
| 1446.9451 | 1486.3879 | 1507.2492 |
| 1512.9891 | 1851.0142 | 2872.1447 |
| 2997.5167 | 3045.1667 | 3063.6583 |
| 3076.2130 | 3135.8913 | 3141.5897 |

Zero-point correction (Hartree): 0.103682

C4H7O2.1-5Hshift

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -306.99284210

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| C | -1.539332 | -0.931136 | -0.292930 |
| C | -0.208961 | -1.245957 | 0.340184 |
| C | 0.843442 | -0.168218 | 0.025263 |
| C | 0.317928 | 1.296802 | -0.021616 |
| O | -1.053784 | 1.435822 | 0.127637 |
| H | -1.615070 | -1.143333 | -1.360563 |
| H | -2.425478 | -1.229865 | 0.266002 |
| H | 0.217166 | -2.203071 | 0.021682 |
| H | -0.305331 | -1.268876 | 1.433978 |
| O | 2.010787 | -0.407212 | -0.167469 |
| H | 0.701860 | 1.720222 | -0.965422 |
| H | 0.832441 | 1.809353 | 0.806728 |
| H | -1.540072 | 0.377743 | -0.189159 |

Rotational constants (GHz): 4.6676500 3.5237500 2.1581200

Vibrational harmonic frequencies (cm-1):

| | | |
|------------|-----------|-----------|
| 11559.6425 | 83.2101 | 121.8934 |
| 353.9977 | 450.9727 | 472.0527 |
| 503.0381 | 562.5659 | 631.8685 |
| 712.0149 | 804.2287 | 924.7477 |
| 993.5497 | 1057.9986 | 1100.1722 |
| 1125.6212 | 1150.1678 | 1186.6981 |
| 1227.8488 | 1246.7707 | 1297.5737 |
| 1325.7332 | 1451.4780 | 1479.3027 |
| 1491.1485 | 1556.9819 | 1836.2087 |
| 2977.2748 | 3021.8935 | 3042.9628 |
| 3099.8318 | 3109.0862 | 3194.9108 |

Zero-point correction (Hartree): 0.099314

C4H7O2.mphc

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -307.01386108

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -2.037398 | -0.018106 | 0.924248 |
| C | -1.627477 | -0.037652 | -0.378863 |
| C | -0.264502 | -0.706847 | -0.598707 |
| C | 0.892662 | 0.168359 | -0.111775 |
| C | 2.131624 | -0.543835 | 0.386334 |
| H | 2.473307 | -1.287070 | -0.343505 |
| O | 0.813320 | 1.381637 | -0.153188 |
| H | -2.410734 | -0.452239 | -1.039455 |
| H | -1.533714 | 1.032129 | -0.664870 |
| H | -0.242807 | -1.692631 | -0.122288 |
| H | -0.103878 | -0.874425 | -1.674178 |
| H | 2.925381 | 0.176647 | 0.587650 |
| H | 1.891223 | -1.090811 | 1.306231 |

Rotational constants (GHz): 6.6350200 2.2074500 2.0325000

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 44.8883 | 94.0119 | 140.4186 |
| 235.8531 | 343.1627 | 450.4686 |
| 478.5705 | 582.5971 | 688.7442 |
| 791.7838 | 875.0568 | 939.5904 |
| 983.3851 | 1053.7479 | 1092.4562 |
| 1154.8385 | 1199.8273 | 1212.0915 |
| 1326.0774 | 1378.0358 | 1382.2593 |
| 1400.7490 | 1463.1288 | 1474.7244 |
| 1487.5159 | 1816.6802 | 2903.4105 |
| 2965.1935 | 3030.7564 | 3044.2036 |
| 3098.8033 | 3104.7954 | 3167.7654 |

Zero-point correction (Hartree): 0.103442

C4H7O2.pmhh

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -307.01330321

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|----------|-----------|-----------|
| O | 1.835362 | 0.852104 | -0.482912 |
| C | 1.570533 | -0.416179 | -0.047571 |

| | | | | |
|--|-----------|-----------|-----------|--|
| C | 0.318433 | -0.575961 | 0.840357 | |
| C | -0.944388 | -0.208245 | 0.060530 | |
| C | -1.411306 | 1.227036 | 0.157002 | |
| H | -0.582698 | 1.887109 | -0.125189 | |
| O | -1.494737 | -1.035518 | -0.642108 | |
| H | 1.462202 | -1.036491 | -0.962793 | |
| H | 2.468742 | -0.831162 | 0.449384 | |
| H | 0.238205 | -1.623811 | 1.146369 | |
| H | 0.436358 | 0.047785 | 1.732713 | |
| H | -2.270675 | 1.391100 | -0.494520 | |
| H | -1.676765 | 1.472878 | 1.192289 | |
| Rotational constants (GHz): | 5.5676500 | 2.5365100 | 2.1278000 | |
| Vibrational harmonic frequencies (cm-1): | | | | |
| 32.0121 | 122.9173 | | 174.1566 | |
| 204.8870 | 356.1573 | | 429.7301 | |
| 506.2014 | 515.7944 | | 626.5662 | |
| 773.8552 | 884.1994 | | 916.0417 | |
| 1007.8001 | 1048.6890 | | 1080.7835 | |
| 1139.0090 | 1190.8403 | | 1252.2462 | |
| 1316.3401 | 1356.6734 | | 1389.2893 | |
| 1397.5958 | 1475.5765 | | 1485.9559 | |
| 1487.8241 | 1816.2140 | | 2905.8659 | |
| 2944.1210 | 3043.2999 | | 3064.6108 | |
| 3107.1087 | 3122.5424 | | 3168.0140 | |
| Zero-point correction (Hartree): | 0.103299 | | | |

C4H7O2.ppch

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -307.01081468
Electronic state : 2-A
Cartesian coordinates (Angs):

| | | | | |
|--|-----------|-----------|-----------|--|
| O | -1.823255 | 0.395909 | -0.887040 | |
| C | -1.599942 | -0.127999 | 0.358524 | |
| C | -0.277970 | -0.893260 | 0.519204 | |
| C | 0.971012 | -0.161463 | 0.021461 | |
| C | 1.080481 | 1.326248 | 0.297810 | |
| H | 0.834738 | 1.561955 | 1.339935 | |
| O | 1.848486 | -0.770840 | -0.556976 | |
| H | -1.624266 | 0.757999 | 1.029908 | |
| H | -2.458098 | -0.738626 | 0.695338 | |
| H | -0.130615 | -1.122112 | 1.584982 | |
| H | -0.323456 | -1.849081 | -0.010132 | |
| H | 2.091400 | 1.664593 | 0.067490 | |
| H | 0.366958 | 1.863562 | -0.337386 | |
| Rotational constants (GHz): | 5.8404200 | 2.4243600 | 2.1352800 | |
| Vibrational harmonic frequencies (cm-1): | | | | |
| 53.2891 | 119.3019 | | 179.8564 | |
| 225.1718 | 348.7320 | | 460.5667 | |
| 509.7039 | 551.9998 | | 647.8988 | |
| 755.5698 | 856.0594 | | 942.2382 | |
| 988.8594 | 1048.3702 | | 1082.6653 | |
| 1141.2517 | 1218.0115 | | 1240.2942 | |
| 1302.2566 | 1372.9671 | | 1384.7575 | |
| 1394.8567 | 1467.4741 | | 1481.5543 | |
| 1491.8555 | 1823.0099 | | 2894.4124 | |
| 2959.8679 | 3032.8906 | | 3045.3226 | |
| 3109.7645 | 3119.1593 | | 3167.9980 | |
| Zero-point correction (Hartree): | 0.103470 | | | |

C4H7O2.tphc

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -307.01491815
Electronic state : 2-A
Cartesian coordinates (Angs):

| | | | | |
|--|-----------|-----------|-----------|--|
| O | -2.703375 | -0.275409 | -0.138283 | |
| C | -1.505472 | 0.250198 | 0.240889 | |
| C | -0.288962 | -0.634537 | -0.066489 | |
| C | 1.018590 | 0.147933 | -0.038224 | |
| C | 2.300770 | -0.655344 | 0.053117 | |
| H | 2.307465 | -1.467514 | -0.682236 | |
| O | 1.023083 | 1.364362 | -0.099151 | |
| H | -1.392004 | 1.195539 | -0.334905 | |
| H | -1.512000 | 0.585367 | 1.294564 | |
| H | -0.238086 | -1.490842 | 0.616842 | |
| H | -0.406365 | -1.059034 | -1.073395 | |
| H | 3.161161 | -0.002592 | -0.100264 | |
| H | 2.372612 | -1.122054 | 1.043111 | |
| Rotational constants (GHz): | 8.9702300 | 1.8741200 | 1.6112800 | |
| Vibrational harmonic frequencies (cm-1): | | | | |
| 72.4523 | 82.4388 | | 127.6225 | |
| 193.5075 | 348.9518 | | 415.1401 | |
| 481.8733 | 590.0991 | | 703.9214 | |
| 818.0795 | 883.4908 | | 949.8326 | |
| 1004.8548 | 1043.1919 | | 1102.7898 | |
| 1141.6457 | 1179.0762 | | 1210.4323 | |

| | | |
|-----------|-----------|-----------|
| 1338.0335 | 1355.5203 | 1379.0841 |
| 1399.2396 | 1464.9022 | 1475.5363 |
| 1489.3537 | 1805.6984 | 2889.0780 |
| 2960.8366 | 3041.0679 | 3047.9748 |
| 3085.3881 | 3108.9976 | 3167.5685 |

Zero-point correction (Hartree): 0.103332

C4H7O2.1-5Hshift

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -306.99068299
Electronic state : 2-A
Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| C | 0.594682 | 1.378408 | 0.171577 |
| C | 0.975984 | -0.071020 | 0.084778 |
| C | -0.134461 | -1.016473 | 0.516525 |
| C | -1.394581 | -0.651528 | -0.301363 |
| O | -1.739529 | 0.703344 | -0.123962 |
| H | 0.539159 | 1.773032 | 1.189005 |
| H | 1.123582 | 2.033047 | -0.520877 |
| O | 2.042193 | -0.440626 | -0.375992 |
| H | -0.353421 | -0.867054 | 1.581191 |
| H | 0.173910 | -2.051568 | 0.352933 |
| H | -2.255081 | -1.237727 | 0.049540 |
| H | -1.231625 | -0.898237 | -1.362649 |
| H | -0.667574 | 1.310441 | -0.118615 |

Rotational constants (GHz): 6.2514500 2.8563700 2.1889000
Vibrational harmonic frequencies (cm-1):

| | | |
|------------|-----------|-----------|
| i1703.3095 | 96.2564 | 215.9101 |
| 393.2016 | 418.6242 | 456.4917 |
| 499.3067 | 582.3017 | 674.4111 |
| 772.0424 | 875.4258 | 909.5038 |
| 957.9591 | 1041.9506 | 1076.8453 |
| 1109.6478 | 1158.0214 | 1181.7080 |
| 1214.2847 | 1244.2015 | 1321.1469 |
| 1383.7497 | 1437.3126 | 1474.1346 |
| 1508.6711 | 1533.5470 | 1785.7158 |
| 2992.6518 | 3045.7840 | 3059.8159 |
| 3102.4843 | 3139.0596 | 3196.8230 |

Zero-point correction (Hartree): 0.099918

C4H7O2.pmc

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -307.00176929
Electronic state : 2-A
Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 1.248120 | -1.228182 | 0.398651 |
| C | 1.690623 | -0.048424 | -0.132577 |
| C | 0.586017 | 0.950581 | -0.524437 |
| C | -0.533480 | 0.991059 | 0.517263 |
| C | -1.531260 | -0.142670 | 0.361735 |
| H | 2.294691 | 0.387099 | 0.696570 |
| H | 2.414605 | -0.208425 | -0.952368 |
| H | 1.035676 | 1.940277 | -0.661318 |
| H | 0.155051 | 0.647335 | -1.483993 |
| H | -0.145461 | 0.982542 | 1.543716 |
| H | -1.116817 | 1.919876 | 0.425721 |
| O | -1.719694 | -0.747798 | -0.669793 |
| H | -2.136545 | -0.364141 | 1.268903 |

Rotational constants (GHz): 5.5557400 2.7087500 2.2425400
Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 82.0298 | 94.9362 | 116.9683 |
| 276.2681 | 281.1100 | 500.3431 |
| 626.9963 | 744.6872 | 782.4939 |
| 842.4566 | 909.4621 | 990.9341 |
| 1021.0391 | 1057.3526 | 1106.3886 |
| 1157.0220 | 1214.2858 | 1255.2777 |
| 1307.8103 | 1363.6055 | 1384.3629 |
| 1401.4799 | 1425.8838 | 1464.1080 |
| 1493.2713 | 1834.2471 | 2864.7291 |
| 2903.4946 | 2965.6001 | 3024.5372 |
| 3062.8202 | 3073.2971 | 3112.4985 |

Zero-point correction (Hartree): 0.104207

C4H7O2.pmt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -307.00194409
Electronic state : 2-A
Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -1.113605 | -1.404542 | 0.129747 |
| C | -1.701145 | -0.226424 | -0.246667 |
| C | -0.961167 | 1.028991 | 0.234147 |
| C | 0.504184 | 1.061495 | -0.217210 |
| C | 1.358782 | -0.053498 | 0.362981 |
| H | -1.693705 | -0.263483 | -1.359027 |
| H | -2.773500 | -0.207978 | 0.023111 |

| | | | | |
|--|-----------|-----------|-----------|--|
| H | -1.488911 | 1.917811 | -0.131016 | |
| H | -1.014769 | 1.063325 | 1.329999 | |
| H | 0.603196 | 1.034994 | -1.307797 | |
| H | 0.958762 | 2.003583 | 0.123766 | |
| O | 2.245519 | -0.610107 | -0.243282 | |
| H | 1.149690 | -0.294448 | 1.429741 | |
| Rotational constants (GHz): | 5.8474800 | 2.5261000 | 1.9281000 | |
| Vibrational harmonic frequencies (cm-1): | | | | |
| 78.9892 | 113.8203 | | 162.3728 | |
| 293.4458 | 324.7451 | | 454.2572 | |
| 542.3869 | 727.8886 | | 739.8563 | |
| 847.6855 | 916.9666 | | 1012.3696 | |
| 1016.0448 | 1065.7744 | | 1098.5335 | |
| 1163.7225 | 1206.0237 | | 1246.4922 | |
| 1324.4880 | 1346.3914 | | 1378.3484 | |
| 1396.0859 | 1428.6625 | | 1467.5780 | |
| 1495.6345 | 1836.6825 | | 2884.4401 | |
| 2895.5378 | 2959.5307 | | 3026.8624 | |
| 3046.2431 | 3086.2627 | | 3101.5717 | |
| Zero-point correction (Hartree): | 0.104080 | | | |

C4H7O2.ppc

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -307.00564575
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | | |
|--|-----------|-----------|-----------|--|
| O | 1.949251 | -0.382202 | -0.844548 | |
| C | 1.378297 | -0.440886 | 0.393423 | |
| C | 0.483524 | 0.757949 | 0.754900 | |
| C | -0.588714 | 1.026619 | -0.301464 | |
| C | -1.670735 | -0.024242 | -0.371054 | |
| H | 0.742754 | -1.353830 | 0.367122 | |
| H | 2.129851 | -0.644717 | 1.179240 | |
| H | 0.017677 | 0.564320 | 1.727664 | |
| H | 1.113528 | 1.647522 | 0.865780 | |
| H | -1.082479 | 1.996120 | -0.145446 | |
| H | -0.128031 | 1.089436 | -1.298244 | |
| O | -1.689049 | -1.043820 | 0.287434 | |
| H | -2.489145 | 0.192682 | -1.094034 | |
| Rotational constants (GHz): | 6.0118100 | 2.3408900 | 2.1423500 | |
| Vibrational harmonic frequencies (cm-1): | | | | |
| 75.1088 | 138.7977 | | 199.8538 | |
| 233.3783 | 311.6379 | | 486.5984 | |
| 636.1556 | 712.1899 | | 780.9388 | |
| 839.5701 | 905.9926 | | 958.5718 | |
| 1018.3472 | 1085.9491 | | 1106.4416 | |
| 1150.4305 | 1211.8894 | | 1275.2747 | |
| 1309.6936 | 1374.3590 | | 1384.2788 | |
| 1398.5122 | 1427.4345 | | 1453.3461 | |
| 1490.7096 | 1822.9587 | | 2888.5623 | |
| 2900.9908 | 2955.3876 | | 3031.9188 | |
| 3055.6775 | 3066.0318 | | 3103.1240 | |
| Zero-point correction (Hartree): | 0.104318 | | | |

C4H7O2.ptc

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -307.00367983
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | | |
|--|------------|-----------|-----------|--|
| O | 2.378862 | -0.552701 | -0.545218 | |
| C | 1.858655 | 0.429934 | 0.255494 | |
| C | 0.349543 | 0.660909 | 0.113142 | |
| C | -0.455839 | -0.617621 | 0.333077 | |
| C | -1.931364 | -0.477547 | 0.045361 | |
| H | 2.105666 | 0.102203 | 1.290441 | |
| H | 2.431468 | 1.369066 | 0.133960 | |
| H | 0.034130 | 1.438935 | 0.817981 | |
| H | 0.139195 | 1.052650 | -0.887636 | |
| H | -0.062681 | -1.425772 | -0.300822 | |
| H | -0.355363 | -0.991946 | 1.364057 | |
| O | -2.465171 | 0.538122 | -0.344508 | |
| H | -2.527923 | -1.402556 | 0.217380 | |
| Rotational constants (GHz): | 10.4796100 | 1.6348400 | 1.5345800 | |
| Vibrational harmonic frequencies (cm-1): | | | | |
| 51.8942 | 138.8957 | | 185.7818 | |
| 193.8431 | 268.4339 | | 494.4715 | |
| 598.1245 | 684.7909 | | 701.3939 | |
| 859.6868 | 882.9524 | | 947.2910 | |
| 1010.3280 | 1086.1542 | | 1099.1222 | |
| 1165.6840 | 1216.8991 | | 1299.1301 | |
| 1311.4343 | 1362.9815 | | 1368.9755 | |
| 1410.7777 | 1428.7526 | | 1466.1478 | |
| 1496.9777 | 1832.1674 | | 2879.4394 | |
| 2891.5932 | 2949.0202 | | 3016.2015 | |
| 3052.6722 | 3064.1445 | | 3107.1704 | |

Zero-point correction (Hartree): 0.103710

C4H7O2.ptt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -307.00185674

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -2.411042 | -0.813300 | 0.179589 |
| C | -1.957121 | 0.412659 | -0.223248 |
| C | -0.521712 | 0.748746 | 0.208523 |
| C | 0.486383 | -0.307288 | -0.272246 |
| C | 1.844662 | -0.137844 | 0.366080 |
| H | -2.030479 | 0.392282 | -1.333080 |
| H | -2.671469 | 1.203752 | 0.074945 |
| H | -0.255148 | 1.741655 | -0.173770 |
| H | -0.499270 | 0.813991 | 1.304053 |
| H | 0.096338 | -1.294074 | 0.016884 |
| H | 0.607309 | -0.290714 | -1.360108 |
| O | 2.887217 | -0.030216 | -0.240246 |
| H | 1.830052 | -0.116400 | 1.481691 |

Rotational constants (GHz): 12.5337900 1.4551800 1.3945900

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 66.1483 | 81.7358 | 154.6699 |
| 218.2006 | 324.4158 | 502.4915 |
| 518.4344 | 617.6852 | 780.3491 |
| 834.7424 | 938.3471 | 984.5507 |
| 1039.3958 | 1091.6573 | 1092.0470 |
| 1172.5482 | 1213.6470 | 1284.0412 |
| 1308.8654 | 1358.5310 | 1365.5745 |
| 1400.8483 | 1434.0321 | 1479.8667 |
| 1501.1538 | 1837.5904 | 2871.8132 |
| 2889.7108 | 2949.0702 | 3030.9820 |
| 3043.1673 | 3083.5004 | 3111.3783 |

Zero-point correction (Hartree): 0.103842

C4H7O2.tpc

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -307.00327780

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -2.561117 | -0.414765 | -0.073761 |
| C | -1.289486 | -0.221546 | 0.377718 |
| C | -0.464319 | 0.789663 | -0.436319 |
| C | 0.925624 | 1.055211 | 0.147350 |
| C | 1.866439 | -0.127726 | 0.130606 |
| H | -1.280720 | 0.015441 | 1.461551 |
| H | -0.803347 | -1.218431 | 0.309696 |
| H | -0.375562 | 0.418892 | -1.462593 |
| H | -1.020390 | 1.732540 | -0.480900 |
| H | 1.429521 | 1.874045 | -0.386332 |
| H | 0.866455 | 1.402743 | 1.191538 |
| O | 1.568122 | -1.246709 | -0.230591 |
| H | 2.898455 | 0.092955 | 0.485723 |

Rotational constants (GHz): 7.1139900 2.0584900 1.7254800

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 101.3115 | 105.2517 | 151.8328 |
| 235.5417 | 285.0304 | 438.4911 |
| 639.0403 | 684.9665 | 731.6541 |
| 860.8460 | 912.2124 | 949.1602 |
| 1045.3237 | 1078.3775 | 1103.7914 |
| 1158.5710 | 1220.6629 | 1276.8631 |
| 1326.0153 | 1372.7530 | 1383.4388 |
| 1391.6306 | 1427.4400 | 1455.0734 |
| 1495.3649 | 1826.4245 | 2897.4535 |
| 2899.7997 | 2925.2024 | 3012.8169 |
| 3047.0658 | 3065.0688 | 3111.8072 |

Zero-point correction (Hartree): 0.103922

C4H7O2.tpt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -307.00012486

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 2.645274 | -0.530986 | 0.183950 |
| C | 1.358220 | -0.409447 | -0.259760 |
| C | 0.646271 | 0.884117 | 0.160522 |
| C | -0.815792 | 0.949730 | -0.325019 |
| C | -1.695302 | -0.047415 | 0.397426 |
| H | 1.328788 | -0.551238 | -1.359233 |
| H | 0.819169 | -1.304503 | 0.120067 |
| H | 0.690762 | 0.970004 | 1.253347 |
| H | 1.203178 | 1.736529 | -0.242560 |
| H | -1.213234 | 1.953299 | -0.121800 |
| H | -0.891668 | 0.763964 | -1.401614 |

| | | | | |
|--|-----------|-----------|-----------|-----------|
| O | -2.287987 | -0.961069 | -0.132479 | |
| H | -1.755676 | 0.106479 | 1.501012 | |
| Rotational constants (GHz): | 7.8145600 | | 1.7549400 | 1.5459000 |
| Vibrational harmonic frequencies (cm-1): | | | | |
| 36.1980 | | 94.8471 | | 121.1354 |
| 252.7977 | | 320.0765 | | 412.4851 |
| 464.3060 | | 530.8525 | | 787.3820 |
| 810.2285 | | 934.4363 | | 1001.9759 |
| 1023.6582 | | 1083.7172 | | 1096.7786 |
| 1169.5407 | | 1216.7243 | | 1281.0970 |
| 1327.6550 | | 1345.1715 | | 1369.9812 |
| 1410.0486 | | 1431.3753 | | 1480.1282 |
| 1502.4516 | | 1835.3059 | | 2873.5577 |
| 2897.2944 | | 2927.0801 | | 3039.6227 |
| 3053.6421 | | 3099.6009 | | 3108.5758 |

Zero-point correction (Hartree): 0.103292

C4H7O2.ttc

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -307.00184728
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | | |
|---|-----------|-----------|-----------|--|
| O | 2.821912 | -0.546941 | 0.006328 | |
| C | 1.797456 | 0.359983 | -0.018499 | |
| C | 0.388478 | -0.240697 | 0.005765 | |
| C | -0.704454 | 0.827026 | 0.006965 | |
| C | -2.111655 | 0.271752 | 0.002687 | |
| H | 1.961383 | 1.024439 | 0.858404 | |
| H | 1.939385 | 1.043669 | -0.881146 | |
| H | 0.263704 | -0.895508 | -0.862987 | |
| H | 0.287476 | -0.881125 | 0.887895 | |
| H | -0.622540 | 1.493761 | 0.880194 | |
| H | -0.619908 | 1.497348 | -0.863367 | |
| O | -2.386111 | -0.907382 | -0.007567 | |
| H | -2.914857 | 1.043614 | 0.009422 | |

Rotational constants (GHz): 11.7413800 1.4852800 1.3509800
 Vibrational harmonic frequencies (cm-1):

| | | | | |
|-----------|--|-----------|--|-----------|
| 65.1286 | | 106.7057 | | 144.9201 |
| 181.2514 | | 293.2216 | | 318.1019 |
| 452.2767 | | 672.0703 | | 697.3631 |
| 818.9413 | | 902.9777 | | 980.0130 |
| 1032.3176 | | 1078.6483 | | 1094.4569 |
| 1166.4534 | | 1260.2445 | | 1273.6120 |
| 1310.8781 | | 1360.3964 | | 1390.1743 |
| 1414.5824 | | 1426.5338 | | 1463.3875 |
| 1501.1504 | | 1836.1229 | | 2887.4851 |
| 2891.9374 | | 2915.8223 | | 3006.8699 |
| 3032.3063 | | 3072.2878 | | 3116.5107 |

Zero-point correction (Hartree): 0.102894

C4H7O2.ttt

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -307.00028638
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | | |
|---|-----------|-----------|-----------|--|
| O | -2.973763 | -0.376438 | -0.140460 | |
| C | -1.854092 | 0.394746 | -0.001955 | |
| C | -0.527759 | -0.376031 | 0.025150 | |
| C | 0.688111 | 0.558153 | 0.153994 | |
| C | 1.980347 | -0.213609 | 0.307769 | |
| H | -1.873269 | 1.108663 | -0.854026 | |
| H | -1.961041 | 1.052536 | 0.884934 | |
| H | -0.553757 | -1.079837 | 0.866456 | |
| H | -0.451629 | -0.976093 | -0.888413 | |
| H | 0.785363 | 1.222996 | -0.710263 | |
| H | 0.569999 | 1.184111 | 1.052373 | |
| O | 2.945805 | -0.093113 | -0.411889 | |
| H | 1.988353 | -0.935526 | 1.157980 | |

Rotational constants (GHz): 17.4468900 1.2607400 1.2355600
 Vibrational harmonic frequencies (cm-1):

| | | | | |
|-----------|--|-----------|--|-----------|
| 57.8881 | | 91.5644 | | 122.9913 |
| 184.8234 | | 342.0735 | | 407.5651 |
| 454.4287 | | 541.8800 | | 760.6137 |
| 838.4639 | | 965.8688 | | 992.4069 |
| 1031.0212 | | 1087.1191 | | 1101.4584 |
| 1168.7518 | | 1251.8728 | | 1267.9000 |
| 1311.0618 | | 1348.3082 | | 1375.6720 |
| 1403.5305 | | 1433.6497 | | 1477.3671 |
| 1508.5751 | | 1839.2475 | | 2878.2805 |
| 2894.5462 | | 2922.6323 | | 3012.6969 |
| 3050.1458 | | 3093.9528 | | 3110.4723 |

Zero-point correction (Hartree): 0.103267

1butanal40.1-5Hshift

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -306.99785746
 Cartesian coordinates (Angs):
 C 1.188546 -0.240507 0.054109
 C 0.496190 1.107990 0.190246
 C -0.943836 1.032730 -0.329901
 C -1.675049 -0.207672 0.235198
 O -1.036985 -1.392012 -0.126079
 H 1.101312 1.870632 -0.310171
 H 0.496576 1.338668 1.266175
 H -0.942398 0.972388 -1.423721
 H -1.491567 1.937347 -0.045113
 H -2.688966 -0.237215 -0.196375
 H -1.788556 -0.100824 1.330688
 H 0.346139 -1.100168 0.070644
 O 2.358529 -0.462497 -0.072676
 Rotational constants (GHz): 6.1172063 2.6082214 1.9462376
 Vibrational harmonic frequencies (cm-1):
 i539.3557 91.4340 225.5753
 283.5158 410.8697 475.9617
 506.0695 709.9788 772.8648
 847.4385 913.5012 948.9797
 995.1537 1037.0730 1088.2842
 1160.7945 1182.0277 1219.5918
 1269.1080 1324.2805 1361.0217
 1381.9835 1451.8052 1490.7153
 1500.5726 1856.3331 1887.3431
 2939.0952 2999.8999 3027.4219
 3061.5153 3104.6937 3112.4582
 Zero-point correction (Hartree): 0.101691

C4H7O2.ppc.M052X

E(UM052X+HF-M052X/6-31G(d,p)) (Hartree): -306.95352066
 Electronic state : 2-A
 Cartesian coordinates (Angs):
 O 1.964428 -0.279423 -0.846967
 C 1.348832 -0.498172 0.361033
 C 0.463929 0.662097 0.820864
 C -0.559845 1.036767 -0.243018
 C -1.649491 0.010682 -0.400651
 H 0.716468 -1.387793 0.194050
 H 2.081927 -0.787230 1.126617
 H -0.042828 0.372633 1.743630
 H 1.095638 1.524931 1.040154
 H -1.042378 1.996008 -0.028315
 H -0.067462 1.154339 -1.214531
 O -1.706077 -1.019811 0.229065
 H -2.428722 0.252739 -1.147758
 Rotational constants (GHz): 6.1736000 2.3487900 2.1789300
 Vibrational harmonic frequencies (cm-1):
 79.4155 150.4438 211.6111
 254.3300 327.2269 484.7379
 654.0893 726.3907 795.2429
 875.0024 936.1718 983.9605
 1034.2109 1105.8589 1129.4202
 1173.0466 1232.2422 1304.9090
 1352.0806 1391.8870 1423.9818
 1430.2147 1445.8419 1476.0281
 1510.6598 1876.4550 3012.5093
 3037.0257 3061.4091 3089.4317
 3110.3385 3127.6264 3159.4045
 Zero-point correction (Hartree): 0.106990

1butanal40.1-5Hshift.M052X

E(UM052X+HF-M052X/6-31G(d,p)) (Hartree): -306.93734097
 Electronic state : 2-A
 Cartesian coordinates (Angs):
 C 1.177410 -0.244768 0.057672
 C 0.496200 1.101562 0.193213
 C -0.931333 1.025380 -0.342695
 C -1.659480 -0.192384 0.249309
 O -1.047309 -1.383203 -0.134010
 H 1.109454 1.853507 -0.304070
 H 0.480746 1.329921 1.265251
 H -0.920853 0.928056 -1.429952
 H -1.477081 1.934418 -0.085267
 H -2.679232 -0.221857 -0.155070
 H -1.730479 -0.091569 1.342300
 H 0.359534 -1.106896 0.080116
 O 2.342450 -0.462337 -0.073277
 Rotational constants (GHz): 6.1690000 2.6372200 1.9718200
 Vibrational harmonic frequencies (cm-1):
 i1081.4596 84.9600 216.8148
 285.3115 408.2526 472.7390

| | | |
|-----------|-----------|-----------|
| 503.0518 | 660.9723 | 766.7202 |
| 869.7078 | 928.5696 | 951.9840 |
| 1024.3691 | 1071.3368 | 1101.8609 |
| 1169.9341 | 1199.8184 | 1234.1093 |
| 1285.2759 | 1345.8503 | 1377.3555 |
| 1401.2433 | 1471.0288 | 1506.7492 |
| 1518.7049 | 1872.5062 | 1955.3713 |
| 3032.6347 | 3075.5928 | 3083.8206 |
| 3116.2394 | 3157.8376 | 3170.1081 |

Zero-point correction (Hartree): 0.103248

C4H7O2.ppc.CBSAPNO

E(MP2/6-311G(d,p)) (Hartree): -306.22322591
E(MP3/6-311G(d,p)) (Hartree): -306.26376904
E(PMP2/6-311G(d,p)) (Hartree): -306.22521057
E(PMP3/6-311G(d,p)) (Hartree): -306.26496311
E(PUHF/6-311G(d,p)) (Hartree): -305.30286127
E(QCI,CC/6-311G(d,p)) (Hartree): -306.28171763
E(UHF/6-311G(d,p)) (Hartree): -305.29956114
Electronic state : 2-A
Cartesian coordinates (Angs):
O 2.061669 -0.230676 -0.825929
C 1.379845 -0.525489 0.341295
C 0.479364 0.611215 0.815004
C -0.578204 1.020655 -0.206414
C -1.694262 0.025679 -0.395424
H 0.797009 -1.416609 0.117929

H 2.096677 -0.800539 1.111877
H 0.000787 0.308611 1.741216
H 1.100169 1.473928 1.041100
H -1.047159 1.961592 0.078902
H -0.126852 1.201186 -1.179624
O -1.797904 -0.999152 0.188077
H -2.451200 0.318097 -1.135347
Rotational constants (GHz): 6.4490400 2.2106300 2.0636100
Vibrational harmonic frequencies (cm-1):
74.1221 143.4092 197.2100
249.1803 339.4478 508.2216
702.9337 778.5247 829.4222
903.0032 971.9255 1045.2218
1096.5024 1166.1182 1194.3561
1263.6768 1320.8222 1404.0517
1489.8077 1508.7439 1526.8578
1540.2796 1574.0112 1576.2265
1600.3804 1998.9749 3090.5182
3160.5989 3161.8841 3180.6286
3196.1824 3204.4907 3224.3500
Zero-point correction (Hartree): 0.112136

C4H7O2.ppc.CBSAPNO

E(CBS-APNO) excl. ZPE (Hartree): -306.98945100
E(CBS-APNO) inc. ZPE scaled by 0.9251 (Hartree): -306.88571400
E(MP2/6-311++G(2df,p)) (Hartree): -306.38558277
E(MP2/6-311G(d,p)) (Hartree): -306.22563503
E(MP2/CBSB5) (Hartree): -306.48310260
E(MP2/CBSB6) (Hartree): -306.62925014
E(MP3/6-311++G(2df,p)) (Hartree): -306.42552609
E(MP3/6-311G(d,p)) (Hartree): -306.26491107
E(PMP2/6-311++G(2df,p)) (Hartree): -306.38800607
E(PMP2/6-311G(d,p)) (Hartree): -306.22769184
E(PMP2/CBSB5) (Hartree): -306.48557632
E(PMP2/CBSB6) (Hartree): -306.63159554
E(PMP3/6-311++G(2df,p)) (Hartree): -306.42700070
E(PMP3/6-311G(d,p)) (Hartree): -306.26615702
E(PUHF/6-311++G(2df,p)) (Hartree): -305.32321195
E(PUHF/6-311G(d,p)) (Hartree): -305.30036781
E(PUHF/CBSB5) (Hartree): -305.35737187
E(PUHF/CBSB6) (Hartree): -305.34475901
E(QCI,CC/6-311G(d,p)) (Hartree): -306.28406463
E(QCISD(T)/6-311++G(2df,p)) (Hartree): -306.48302502
E(QCISD/6-311++G(2df,p)) (Hartree): -306.43978513
E(UHF/6-311++G(2df,p)) (Hartree): -305.31924109
E(UHF/6-311G(d,p)) (Hartree): -305.29697643
E(UHF/CBSB5) (Hartree): -305.35332235
E(UHF/CBSB5A) (Hartree): -305.34592689
E(UHF/CBSB6) (Hartree): -305.34094207
Electronic state : 2-A
Cartesian coordinates (Angs):
O 1.979217 -0.313188 -0.848910
C 1.369835 -0.486061 0.375014
C 0.478880 0.690026 0.796395
C -0.572561 1.036433 -0.258250

| | | | |
|---|-----------|-----------|-----------|
| C | -1.668301 | -0.001783 | -0.395872 |
| H | 0.751600 | -1.396002 | 0.254741 |
| H | 2.116743 | -0.728350 | 1.149278 |
| H | -0.008692 | 0.437624 | 1.745691 |
| H | 1.115388 | 1.566173 | 0.971195 |
| H | -1.063159 | 1.994596 | -0.033966 |
| H | -0.101113 | 1.158027 | -1.243033 |
| O | -1.730258 | -1.024385 | 0.249130 |
| H | -2.449557 | 0.236833 | -1.149398 |

Rotational constants (GHz): 6.1146456 2.3022682 2.1301592

1butanal40.1-5Hshift.CBSAPNO

 E(MP2/6-311G(d,p)) (Hartree): -306.20782649
 E(MP3/6-311G(d,p)) (Hartree): -306.23880346
 E(PMP2/6-311G(d,p)) (Hartree): -306.21429646
 E(PMP3/6-311G(d,p)) (Hartree): -306.24276935
 E(PUHF/6-311G(d,p)) (Hartree): -305.25646671
 E(QCI,CC/6-311G(d,p)) (Hartree): -306.26606546
 E(UHF/6-311G(d,p)) (Hartree): -305.24722408
 Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| C | 1.174995 | -0.220447 | 0.048802 |
| C | 0.480968 | 1.133260 | 0.179159 |
| C | -0.959141 | 1.024943 | -0.333341 |
| C | -1.645228 | -0.220414 | 0.256735 |
| O | -0.994862 | -1.401170 | -0.140534 |
| H | 1.077532 | 1.887093 | -0.345904 |
| H | 0.485566 | 1.373293 | 1.252194 |
| H | -0.958235 | 0.935991 | -1.426292 |
| H | -1.522442 | 1.925354 | -0.061624 |
| H | -2.675434 | -0.278047 | -0.120609 |
| H | -1.690216 | -0.125390 | 1.356400 |
| H | 0.256681 | -1.088901 | 0.032206 |
| O | 2.334485 | -0.465510 | -0.058779 |

Rotational constants (GHz): 6.0357000 2.6748400 1.9770700
 Vibrational harmonic frequencies (cm-1):

| | | |
|------------|-----------|-----------|
| i2671.1744 | 202.7612 | 272.8548 |
| 367.0305 | 416.9254 | 481.1276 |
| 537.5300 | 639.1437 | 830.9151 |
| 907.2749 | 980.5428 | 1043.8484 |
| 1057.4046 | 1122.5350 | 1137.3666 |
| 1252.0911 | 1315.4722 | 1334.0810 |
| 1392.5940 | 1458.8862 | 1499.5609 |
| 1534.4809 | 1583.1693 | 1614.5579 |
| 1639.0688 | 1702.1362 | 1906.0173 |
| 3016.0398 | 3072.2623 | 3083.0176 |
| 3098.4411 | 3130.7344 | 3140.8801 |

Zero-point correction (Hartree): 0.106552

1butanal40.1-5Hshift.CBSAPNO

 E(CBS-APNO) excl. ZPE (Hartree): -306.98055500
 E(CBS-APNO) inc. ZPE scaled by 0.9251 (Hartree): -306.88198400
 E(MP2/6-311++G(2df,p)) (Hartree): -306.36661957
 E(MP2/6-311G(d,p)) (Hartree): -306.20442483
 E(MP2/CBSB5) (Hartree): -306.46468981
 E(MP2/CBSB6) (Hartree): -306.61093364
 E(MP3/6-311++G(2df,p)) (Hartree): -306.40051551
 E(MP3/6-311G(d,p)) (Hartree): -306.23829574
 E(PMP2/6-311++G(2df,p)) (Hartree): -306.37192325
 E(PMP2/6-311G(d,p)) (Hartree): -306.20948070
 E(PMP2/CBSB5) (Hartree): -306.47003376
 E(PMP2/CBSB6) (Hartree): -306.61615326
 E(PMP3/6-311++G(2df,p)) (Hartree): -306.40389834
 E(PMP3/6-311G(d,p)) (Hartree): -306.24152906
 E(PUHF/6-311++G(2df,p)) (Hartree): -305.28345193
 E(PUHF/6-311G(d,p)) (Hartree): -305.25979721
 E(PUHF/CBSB5) (Hartree): -305.31794321
 E(PUHF/CBSB6) (Hartree): -305.30525401
 E(QCI,CC/6-311G(d,p)) (Hartree): -306.26532361
 E(QCISD(T)/6-311++G(2df,p)) (Hartree): -306.47067058
 E(QCISD/6-311++G(2df,p)) (Hartree): -306.42253152
 E(UHF/6-311++G(2df,p)) (Hartree): -305.27578835
 E(UHF/6-311G(d,p)) (Hartree): -305.25253125
 E(UHF/CBSB5) (Hartree): -305.31022764
 E(UHF/CBSB5A) (Hartree): -305.30281921
 E(UHF/CBSB6) (Hartree): -305.29771806

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| C | 1.173494 | -0.230961 | 0.045441 |
| C | 0.488058 | 1.126253 | 0.178078 |
| C | -0.952923 | 1.027147 | -0.332920 |
| C | -1.648743 | -0.212185 | 0.259882 |
| O | -1.014671 | -1.397500 | -0.142545 |
| H | 1.085504 | 1.878529 | -0.347651 |

| | | | |
|-----------------------------|-----------|-----------|-----------|
| H | 0.493825 | 1.370206 | 1.250384 |
| H | -0.955834 | 0.936701 | -1.425748 |
| H | -1.513615 | 1.929086 | -0.060975 |
| H | -2.679606 | -0.261677 | -0.119129 |
| H | -1.691432 | -0.121038 | 1.359407 |
| H | 0.304071 | -1.086619 | 0.032625 |
| O | 2.339392 | -0.465839 | -0.056429 |
| Rotational constants (GHz): | 6.0580089 | 2.6592027 | 1.9711083 |

C5H9O2.chmt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.35972148

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|-----------------------------|-----------|-----------|-----------|
| O | -1.423338 | -1.174433 | -0.630167 |
| C | -1.559564 | -0.078262 | -0.022192 |
| C | -0.618843 | 1.087176 | -0.139737 |
| C | 0.807862 | 0.687527 | -0.548569 |
| C | 1.567865 | -0.083930 | 0.538805 |
| C | 2.994103 | -0.449239 | 0.116976 |
| H | 3.514187 | -0.996363 | 0.909407 |
| O | -2.611189 | -0.069009 | 0.680779 |
| H | -1.058942 | 1.762394 | -0.885954 |
| H | -0.636785 | 1.627340 | 0.813972 |
| H | 0.762649 | 0.086158 | -1.464370 |
| H | 1.357645 | 1.601303 | -0.804427 |
| H | 1.598256 | 0.520342 | 1.455706 |
| H | 1.014970 | -0.998073 | 0.787714 |
| H | 2.992493 | -1.081690 | -0.777710 |
| H | 3.583210 | 0.446494 | -0.110935 |
| Rotational constants (GHz): | 5.8643200 | 1.2951300 | 1.2115000 |

| | | |
|--|-----------|-----------|
| Vibrational harmonic frequencies (cm-1): | | |
| 33.8801 | 79.8692 | 96.5627 |
| 215.1566 | 244.0161 | 263.0193 |
| 358.1538 | 505.7647 | 536.6919 |
| 610.3219 | 748.4858 | 831.5164 |
| 840.0076 | 918.2006 | 950.6104 |
| 1017.1403 | 1064.4753 | 1108.8782 |
| 1122.1239 | 1183.9391 | 1234.5844 |
| 1270.9613 | 1335.4175 | 1340.1268 |
| 1366.3377 | 1412.2901 | 1428.8543 |
| 1465.0789 | 1497.4054 | 1507.3518 |
| 1512.8538 | 1522.1877 | 1599.4031 |
| 3030.3014 | 3041.0781 | 3044.1045 |
| 3050.5999 | 3067.3211 | 3087.4632 |
| 3096.0113 | 3111.4837 | 3118.5419 |

Zero-point correction (Hartree): 0.134112

C5H9O2.chpm

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.35792591

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|-----------------------------|-----------|-----------|-----------|
| O | -1.468655 | -0.321481 | 1.183490 |
| C | -1.299600 | 0.048441 | -0.011084 |
| C | -0.344119 | 1.125537 | -0.435285 |
| C | 0.993681 | 1.110758 | 0.331599 |
| C | 2.009948 | 0.073332 | -0.172500 |
| C | 1.564293 | -1.389245 | -0.053095 |
| H | 2.373067 | -2.063986 | -0.351128 |
| O | -2.063972 | -0.576812 | -0.800379 |
| H | -0.199473 | 1.047803 | -1.518700 |
| H | -0.865797 | 2.074366 | -0.251787 |
| H | 1.437873 | 2.109155 | 0.252146 |
| H | 0.787274 | 0.948552 | 1.396400 |
| H | 2.255463 | 0.295848 | -1.220083 |
| H | 2.940435 | 0.212791 | 0.391689 |
| H | 1.280403 | -1.637626 | 0.974871 |
| H | 0.706559 | -1.613504 | -0.696104 |
| Rotational constants (GHz): | 4.0456100 | 1.7889800 | 1.5848300 |

| | | |
|--|-----------|-----------|
| Vibrational harmonic frequencies (cm-1): | | |
| 43.7405 | 78.2642 | 106.7440 |
| 220.6539 | 259.3288 | 309.8724 |
| 391.1426 | 474.7818 | 538.3065 |
| 628.4960 | 779.6248 | 797.1499 |
| 858.3966 | 926.6269 | 937.9494 |
| 987.7759 | 1086.0669 | 1096.3946 |
| 1111.4414 | 1179.8326 | 1235.7208 |
| 1260.5122 | 1314.7329 | 1358.8549 |
| 1385.4447 | 1393.5725 | 1435.7862 |
| 1467.7730 | 1498.2877 | 1501.7815 |
| 1515.1888 | 1525.0168 | 1598.3929 |
| 3028.7512 | 3044.0991 | 3048.2021 |
| 3050.6740 | 3069.0696 | 3090.9489 |
| 3098.0368 | 3116.9347 | 3122.2156 |

Zero-point correction (Hartree): 0.134349

C5H9O2.chpp

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.35843070

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -1.694918 | -0.794588 | -0.848017 |
| C | -1.431474 | 0.085653 | 0.015766 |
| C | -0.337789 | -0.022203 | 1.039539 |
| C | 0.825485 | -0.928629 | 0.599885 |
| C | 1.664283 | -0.379629 | -0.566879 |
| C | 2.441822 | 0.901019 | -0.241527 |
| H | 3.057968 | 1.209454 | -1.091891 |
| O | -2.227402 | 1.065247 | -0.067738 |
| H | -0.010801 | 0.992926 | 1.287174 |
| H | -0.806275 | -0.423453 | 1.948358 |
| H | 1.471982 | -1.094432 | 1.470247 |
| H | 0.418185 | -1.907617 | 0.324165 |
| H | 2.372442 | -1.160197 | -0.870206 |
| H | 1.013227 | -0.211634 | -1.433795 |
| H | 1.778637 | 1.739879 | -0.004117 |
| H | 3.109228 | 0.752536 | 0.615405 |

Rotational constants (GHz): 4.6730200 1.4849100 1.4128800

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 35.3201 | 47.8234 | 129.4594 |
| 199.1080 | 243.0257 | 315.5707 |
| 403.8191 | 482.8134 | 533.7655 |
| 608.4696 | 752.1277 | 820.7407 |
| 839.4241 | 921.0411 | 944.6334 |
| 990.7665 | 1070.5517 | 1112.9005 |
| 1118.9744 | 1173.3612 | 1221.1926 |
| 1262.0017 | 1322.7922 | 1354.2543 |
| 1391.4089 | 1394.2968 | 1431.2173 |
| 1467.1510 | 1497.1513 | 1504.9958 |
| 1517.3395 | 1521.9130 | 1599.2498 |
| 3041.1989 | 3044.2065 | 3044.7966 |
| 3053.3239 | 3077.5794 | 3090.3829 |
| 3105.3566 | 3111.7324 | 3117.5580 |

Zero-point correction (Hartree): 0.134218

C5H9O2.chtp

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.35853560

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -2.026557 | 1.022458 | -0.513010 |
| C | -1.670985 | -0.093316 | -0.046811 |
| C | -0.248541 | -0.501282 | 0.202751 |
| C | 0.714913 | 0.690312 | 0.313928 |
| C | 2.177316 | 0.276061 | 0.544739 |
| C | 2.819131 | -0.476000 | -0.626973 |
| H | 3.873660 | -0.687325 | -0.423847 |
| O | -2.667620 | -0.842557 | 0.168422 |
| H | -0.235749 | -1.121880 | 1.106964 |
| H | 0.034973 | -1.163466 | -0.625764 |
| H | 0.642462 | 1.297016 | -0.596490 |
| H | 0.386248 | 1.334356 | 1.137633 |
| H | 2.758339 | 1.183930 | 0.747046 |
| H | 2.242729 | -0.334392 | 1.455637 |
| H | 2.329398 | -1.436334 | -0.821089 |
| H | 2.770347 | 0.114233 | -1.549192 |

Rotational constants (GHz): 6.7706100 1.1604700 1.0924200

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 23.1498 | 66.2433 | 122.7370 |
| 158.1082 | 240.8408 | 291.3673 |
| 423.2722 | 440.6346 | 544.3821 |
| 625.7149 | 750.8392 | 793.8350 |
| 886.0065 | 909.5200 | 952.2283 |
| 994.9586 | 1079.3085 | 1118.2673 |
| 1120.1553 | 1174.7363 | 1225.9362 |
| 1284.8340 | 1323.3644 | 1333.3307 |
| 1387.2142 | 1401.3551 | 1433.6439 |
| 1467.9763 | 1501.6967 | 1505.0976 |
| 1518.1321 | 1521.3581 | 1599.7568 |
| 3032.4001 | 3042.9740 | 3047.0678 |
| 3053.1963 | 3072.2048 | 3081.4017 |
| 3099.9544 | 3112.5632 | 3117.6797 |

Zero-point correction (Hartree): 0.134137

C5H9O2.hcttp

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.35857933

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -2.579890 | -0.997679 | -0.008163 |
| C | -1.676399 | -0.112045 | 0.016695 |
| C | -0.234159 | -0.398132 | 0.320279 |
| C | 0.710926 | 0.737753 | -0.099454 |
| C | 2.168383 | 0.512600 | 0.333806 |
| C | 2.849618 | -0.691065 | -0.327845 |
| H | 3.899132 | -0.760812 | -0.024994 |
| O | -2.146207 | 1.031910 | -0.225701 |
| H | -0.168425 | -0.573924 | 1.403495 |
| H | 0.017038 | -1.351046 | -0.157723 |
| H | 0.664627 | 0.861429 | -1.188625 |
| H | 0.344570 | 1.676421 | 0.330357 |
| H | 2.737350 | 1.419995 | 0.098006 |
| H | 2.209059 | 0.405005 | 1.426333 |
| H | 2.370834 | -1.638104 | -0.056379 |
| H | 2.824381 | -0.607475 | -1.420439 |

Rotational constants (GHz): 6.7894600 1.1840300 1.0607700

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 20.0676 | 67.7097 | 116.9177 |
| 159.8111 | 233.7510 | 290.5937 |
| 427.9595 | 440.7266 | 541.4042 |
| 622.2748 | 750.7571 | 799.4506 |
| 881.8472 | 909.0618 | 951.2630 |
| 995.1078 | 1076.9126 | 1115.0973 |
| 1131.5550 | 1164.9942 | 1228.2483 |
| 1286.2092 | 1315.4798 | 1335.4853 |
| 1386.8278 | 1401.3482 | 1432.4861 |
| 1468.0035 | 1501.2156 | 1505.0840 |
| 1517.2088 | 1521.1907 | 1599.0400 |
| 3031.6321 | 3038.0956 | 3043.2542 |
| 3049.5556 | 3072.2569 | 3086.4276 |
| 3103.1537 | 3111.8151 | 3117.0787 |

Zero-point correction (Hartree): 0.134066

C5H9O2.hctt

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.35975088
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -2.895356 | -0.563474 | -0.178408 |
| C | -1.785886 | 0.014203 | 0.011988 |
| C | -0.473893 | -0.707548 | 0.116827 |
| C | 0.744306 | 0.204321 | -0.084264 |
| C | 2.071893 | -0.539180 | 0.110290 |
| C | 3.292631 | 0.362230 | -0.096663 |
| H | 4.224697 | -0.193207 | 0.047172 |
| O | -1.928660 | 1.261743 | 0.120265 |
| H | -0.447884 | -1.173644 | 1.111844 |
| H | -0.491372 | -1.533603 | -0.604058 |
| H | 0.708619 | 0.640759 | -1.090047 |
| H | 0.684846 | 1.046075 | 0.615684 |
| H | 2.100563 | -0.971384 | 1.119727 |
| H | 2.118872 | -1.387781 | -0.585558 |
| H | 3.308132 | 0.782648 | -1.108374 |
| H | 3.291345 | 1.199834 | 0.609683 |

Rotational constants (GHz): 8.4217100 1.0562200 0.9659600

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 7.5136 | 78.7776 | 113.6642 |
| 123.1470 | 245.0012 | 281.8082 |
| 340.0728 | 476.0788 | 549.6237 |
| 620.1802 | 736.7558 | 800.9062 |
| 899.4441 | 917.5157 | 940.6752 |
| 1027.8897 | 1066.9244 | 1114.6189 |
| 1129.3364 | 1171.8345 | 1239.8337 |
| 1280.4547 | 1315.6861 | 1338.6810 |
| 1363.2251 | 1411.7561 | 1427.8658 |
| 1466.2117 | 1500.9448 | 1509.7224 |
| 1512.4520 | 1524.2639 | 1599.6281 |
| 3025.3950 | 3038.4048 | 3042.7216 |
| 3050.6123 | 3055.0589 | 3079.8591 |
| 3097.3763 | 3112.5216 | 3118.5326 |

Zero-point correction (Hartree): 0.133849

C5H9O2.1-5Hshift.m

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.34257144
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| C | -1.487774 | -0.174679 | -0.547341 |
| C | -0.738212 | 1.155850 | -0.510168 |
| C | 0.495567 | 1.058318 | 0.398720 |
| C | 1.380780 | -0.144038 | 0.064353 |
| O | 0.759837 | -1.237180 | -0.385044 |

| | | | | |
|--|-----------|-----------|-----------|-----------|
| C | -2.330680 | -0.542510 | 0.656462 | |
| H | -1.993588 | -0.369117 | -1.498107 | |
| H | -1.403218 | 1.959739 | -0.164970 | |
| H | -0.420233 | 1.421111 | -1.524216 | |
| H | 0.192976 | 0.947161 | 1.448258 | |
| H | 1.125226 | 1.949490 | 0.346992 | |
| O | 2.587041 | -0.161701 | 0.220399 | |
| H | -0.511595 | -0.942984 | -0.563658 | |
| H | -3.201739 | 0.124825 | 0.721182 | |
| H | -1.774448 | -0.449639 | 1.594171 | |
| H | -2.706489 | -1.567186 | 0.585356 | |
| Rotational constants (GHz): | 5.0397200 | | 1.7096200 | 1.4831400 |
| Vibrational harmonic frequencies (cm-1): | | | | |
| i1185.6481 | 78.8167 | | | 162.1743 |
| 187.9049 | 212.6481 | | | 339.4441 |
| 431.5324 | 460.4473 | | | 513.2323 |
| 607.0319 | 734.5938 | | | 805.9688 |
| 835.8063 | 846.3931 | | | 911.7071 |
| 970.3060 | 989.9981 | | | 1069.9730 |
| 1110.1706 | 1152.8651 | | | 1179.4796 |
| 1203.3439 | 1237.4852 | | | 1309.5391 |
| 1338.2941 | 1361.7841 | | | 1379.1649 |
| 1423.2106 | 1479.1311 | | | 1490.0735 |
| 1500.3662 | 1506.0630 | | | 1563.2550 |
| 1764.4400 | 3025.9197 | | | 3032.0937 |
| 3052.1925 | 3087.0551 | | | 3097.3637 |
| 3103.3547 | 3130.0326 | | | 3134.0091 |
| Zero-point correction (Hartree): | 0.129442 | | | |

C5H9O2.1-5Hshift.p

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.34398115
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | | |
|--|-----------|-----------|-----------|-----------|
| C | -1.437384 | -0.024846 | 0.413769 | |
| C | -0.701574 | 1.135384 | -0.243317 | |
| C | 0.764431 | 1.151016 | 0.207007 | |
| C | 1.455182 | -0.197555 | -0.005195 | |
| O | 0.693693 | -1.284922 | 0.136534 | |
| H | -1.527335 | 0.092034 | 1.500210 | |
| C | -2.700008 | -0.530844 | -0.245135 | |
| H | -1.190752 | 2.088128 | 0.003161 | |
| H | -0.752737 | 1.028344 | -1.333868 | |
| H | 0.825632 | 1.375202 | 1.280887 | |
| H | 1.358630 | 1.906985 | -0.311142 | |
| O | 2.638263 | -0.321067 | -0.259011 | |
| H | -0.546655 | -0.890742 | 0.326223 | |
| H | -2.529638 | -0.783386 | -1.296565 | |
| H | -3.478232 | 0.245707 | -0.215395 | |
| H | -3.098440 | -1.413289 | 0.263526 | |
| Rotational constants (GHz): | 5.5772100 | | 1.5930600 | 1.3240600 |
| Vibrational harmonic frequencies (cm-1): | | | | |
| i1194.1170 | 78.7767 | | | 173.7128 |
| 188.3767 | 214.4487 | | | 336.2597 |
| 392.2558 | 435.7454 | | | 503.3254 |
| 614.6637 | 715.2147 | | | 788.5014 |
| 829.1752 | 843.3911 | | | 909.4704 |
| 961.3129 | 1012.3644 | | | 1077.5655 |
| 1111.0152 | 1130.2480 | | | 1195.3823 |
| 1223.9701 | 1266.4831 | | | 1311.7082 |
| 1327.9912 | 1342.9853 | | | 1395.9152 |
| 1417.3225 | 1480.1040 | | | 1491.3024 |
| 1496.8301 | 1501.7855 | | | 1573.4043 |
| 1767.1592 | 3020.2212 | | | 3028.4733 |
| 3043.6120 | 3068.4992 | | | 3083.5842 |
| 3095.6158 | 3131.6962 | | | 3132.2158 |
| Zero-point correction (Hartree): | 0.129200 | | | |

C5H9O2.1-6Hshift.b

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.33963387
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | | |
|---|-----------|-----------|-----------|--|
| O | -0.805606 | -1.311349 | -0.015517 | |
| H | 0.438352 | -1.328278 | 0.057958 | |
| C | 1.709942 | -1.190494 | -0.045503 | |
| C | -1.340772 | -0.094408 | 0.033456 | |
| C | 1.975712 | 0.272731 | 0.215023 | |
| C | -0.464298 | 1.126531 | 0.281918 | |
| C | 0.913483 | 1.200162 | -0.404971 | |
| H | 1.869645 | -1.513149 | -1.077324 | |
| H | 2.119562 | -1.899478 | 0.676440 | |
| O | -2.550740 | -0.007572 | -0.081445 | |
| H | 2.034682 | 0.462441 | 1.293765 | |
| H | 2.960464 | 0.535441 | -0.200297 | |

| | | | | |
|--|-----------|-----------|-----------|--|
| H | -1.079524 | 1.979716 | -0.016774 | |
| H | -0.332499 | 1.207350 | 1.370464 | |
| H | 1.264785 | 2.235207 | -0.331815 | |
| H | 0.810890 | 0.984985 | -1.476251 | |
| Rotational constants (GHz): | 4.6483600 | 1.9025200 | 1.4357800 | |
| Vibrational harmonic frequencies (cm-1): | | | | |
| i1434.0055 | 84.6458 | | 111.9766 | |
| 274.4090 | 314.8017 | | 383.2593 | |
| 419.5203 | 464.4660 | | 513.9866 | |
| 619.7334 | 696.2778 | | 806.3826 | |
| 824.8789 | 862.9290 | | 929.5711 | |
| 948.3145 | 994.6657 | | 1079.7818 | |
| 1092.2493 | 1124.3990 | | 1203.2886 | |
| 1236.1867 | 1250.0800 | | 1267.9316 | |
| 1329.1316 | 1361.8126 | | 1370.2056 | |
| 1387.5564 | 1394.1118 | | 1469.1615 | |
| 1474.6997 | 1491.1286 | | 1506.0554 | |
| 1761.9225 | 3010.2057 | | 3034.8490 | |
| 3046.2330 | 3069.2107 | | 3091.0776 | |
| 3092.5104 | 3114.3258 | | 3173.7024 | |
| Zero-point correction (Hartree): | 0.129130 | | | |

C5H9O2.1-6Hshift.c

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.33582628
Electronic state : 2-A
Cartesian coordinates (Angs):

| | | | | |
|--|-----------|-----------|-----------|--|
| C | -1.735646 | 0.126194 | -0.592769 | |
| C | -0.894630 | 1.335940 | -0.125609 | |
| C | 0.407114 | 0.984732 | 0.637198 | |
| C | 1.274258 | -0.109077 | 0.030733 | |
| O | 0.771685 | -1.347194 | -0.016228 | |
| H | -0.439415 | -1.356341 | 0.317745 | |
| C | -1.684950 | -1.051273 | 0.352386 | |
| H | -1.389297 | -0.211053 | -1.576528 | |
| H | -2.778346 | 0.447305 | -0.733275 | |
| H | -0.648357 | 1.950438 | -0.997712 | |
| H | -1.494481 | 1.969199 | 0.537904 | |
| H | 1.035365 | 1.874530 | 0.716970 | |
| H | 0.156573 | 0.667657 | 1.656951 | |
| O | 2.407519 | 0.065159 | -0.375962 | |
| H | -2.172397 | -1.962489 | 0.000380 | |
| H | -1.900148 | -0.842048 | 1.403455 | |
| Rotational constants (GHz): | 4.3283600 | 2.0416300 | 1.5849600 | |
| Vibrational harmonic frequencies (cm-1): | | | | |
| i1490.6746 | 94.5150 | | 174.7072 | |
| 209.1569 | 308.1383 | | 386.0382 | |
| 467.1450 | 492.3066 | | 552.9680 | |
| 628.6030 | 745.4257 | | 784.2433 | |
| 814.0154 | 849.9231 | | 923.7550 | |
| 973.3085 | 977.3186 | | 1078.8058 | |
| 1104.0545 | 1124.3922 | | 1211.0591 | |
| 1234.6837 | 1252.4040 | | 1275.3889 | |
| 1316.9355 | 1359.8482 | | 1378.6441 | |
| 1399.2171 | 1423.7907 | | 1470.4026 | |
| 1486.5636 | 1495.4107 | | 1514.6992 | |
| 1775.5881 | 3018.2459 | | 3053.3994 | |
| 3057.9216 | 3072.5283 | | 3089.5315 | |
| 3101.2959 | 3132.0413 | | 3172.8426 | |
| Zero-point correction (Hartree): | 0.129813 | | | |

C5H9O2.phhmchp

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.32432941
Electronic state : 2-A
Cartesian coordinates (Angs):

| | | | | |
|--|-----------|-----------|-----------|--|
| O | -0.324801 | 1.740924 | -0.544434 | |
| C | -1.057230 | 1.141334 | 0.397847 | |
| C | -1.078993 | -0.442333 | 0.100136 | |
| C | 0.219338 | -1.231251 | 0.174985 | |
| C | 1.470277 | -0.646391 | -0.518280 | |
| C | 2.315876 | 0.289411 | 0.349751 | |
| H | 3.228518 | 0.579653 | -0.180403 | |
| O | -2.147497 | -0.946790 | -0.121649 | |
| H | -0.592699 | 1.177429 | 1.406409 | |
| H | -2.115760 | 1.441069 | 0.452502 | |
| H | 0.424921 | -1.373636 | 1.246682 | |
| H | -0.029156 | -2.216507 | -0.229715 | |
| H | 2.084565 | -1.501128 | -0.825805 | |
| H | 1.175279 | -0.130529 | -1.437726 | |
| H | 1.770506 | 1.205395 | 0.586022 | |
| H | 2.616600 | -0.199440 | 1.284068 | |
| Rotational constants (GHz): | 3.6113100 | 2.0619400 | 1.4693900 | |
| Vibrational harmonic frequencies (cm-1): | | | | |

| | | |
|-----------|-----------|-----------|
| 40.9618 | 52.1095 | 148.9335 |
| 181.4860 | 243.2363 | 289.9613 |
| 342.5652 | 402.2748 | 480.7595 |
| 592.2758 | 660.8050 | 760.8661 |
| 839.7142 | 887.9920 | 924.0460 |
| 999.4078 | 1070.9325 | 1089.9567 |
| 1121.8755 | 1157.6636 | 1227.9306 |
| 1250.4205 | 1297.8010 | 1312.3412 |
| 1358.3044 | 1380.2307 | 1427.2571 |
| 1467.6444 | 1492.3012 | 1506.6832 |
| 1517.5417 | 1531.7771 | 1843.8462 |
| 2885.9580 | 3011.4002 | 3024.1451 |
| 3045.4106 | 3049.3634 | 3095.2531 |
| 3109.6595 | 3113.6878 | 3149.1824 |

Zero-point correction (Hartree): 0.133013

C5H9O2.phhpchm

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.32754742
Electronic state : 2-A
Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 1.201445 | 1.661946 | 0.540245 |
| C | 1.482985 | 0.717207 | -0.359174 |
| C | 0.767165 | -0.675612 | -0.006484 |
| C | -0.437698 | -0.627636 | 0.908659 |
| C | -1.781834 | -0.488294 | 0.153193 |
| C | -1.966735 | 0.827119 | -0.611091 |
| H | -2.992875 | 0.911793 | -0.982047 |
| O | 1.214736 | -1.678938 | -0.497836 |
| H | 1.011122 | 0.922307 | -1.344050 |
| H | 2.549563 | 0.480460 | -0.515103 |
| H | -0.440601 | -1.566681 | 1.470786 |
| H | -0.306171 | 0.213695 | 1.596104 |
| H | -1.895860 | -1.341301 | -0.526151 |
| H | -2.573671 | -0.585327 | 0.905010 |
| H | -1.759537 | 1.691602 | 0.026498 |
| H | -1.304714 | 0.892679 | -1.480937 |

Rotational constants (GHz): 3.1014700 2.1591700 1.5516000
Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 32.2653 | 72.3147 | 112.5831 |
| 201.8722 | 236.4834 | 275.1324 |
| 358.0960 | 454.0474 | 475.2637 |
| 587.2747 | 620.4793 | 752.1375 |
| 854.5723 | 869.3149 | 907.5402 |
| 947.4035 | 1057.7980 | 1077.0609 |
| 1118.2417 | 1160.2386 | 1216.2699 |
| 1259.0176 | 1280.9643 | 1286.7219 |
| 1354.2757 | 1379.7323 | 1437.3930 |
| 1473.7495 | 1484.7134 | 1501.2122 |
| 1511.5118 | 1522.6874 | 1849.8064 |
| 2890.2662 | 2990.4693 | 3048.5365 |
| 3052.4258 | 3064.1887 | 3085.7446 |
| 3117.9145 | 3126.9677 | 3133.2801 |

Zero-point correction (Hartree): 0.132676

C5H9O2.phomcht

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.32224763
Electronic state : 2-A
Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 2.765783 | -0.800610 | 0.119960 |
| C | 1.440433 | -0.879390 | -0.031849 |
| C | 0.731702 | 0.545508 | 0.047359 |
| C | -0.715067 | 0.493165 | 0.518688 |
| C | -1.632117 | -0.312282 | -0.423905 |
| C | -3.090381 | -0.302080 | 0.046274 |
| H | -3.725812 | -0.872863 | -0.637709 |
| O | 1.300985 | 1.554701 | -0.270745 |
| H | 1.184264 | -1.164145 | -1.076483 |
| H | 0.919296 | -1.576617 | 0.651502 |
| H | -0.740088 | 0.048059 | 1.521906 |
| H | -1.059830 | 1.528515 | 0.597190 |
| H | -1.567058 | 0.109678 | -1.434265 |
| H | -1.280574 | -1.348951 | -0.493344 |
| H | -3.188766 | -0.745042 | 1.043400 |
| H | -3.482995 | 0.719110 | 0.094684 |

Rotational constants (GHz): 5.5090000 1.2915100 1.1151900
Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 52.9385 | 69.0486 | 97.4676 |
| 165.7509 | 248.6038 | 272.8877 |
| 311.2422 | 395.8568 | 479.8729 |
| 595.4368 | 664.1422 | 753.2836 |
| 821.6749 | 892.8285 | 911.2222 |
| 954.6525 | 1028.2935 | 1050.2904 |
| 1106.6843 | 1166.5129 | 1193.9048 |

| | | |
|-----------|-----------|-----------|
| 1261.1445 | 1292.5809 | 1296.7001 |
| 1332.9855 | 1385.0803 | 1427.9225 |
| 1479.7659 | 1482.7999 | 1505.8838 |
| 1512.0941 | 1521.0177 | 1860.1749 |
| 2877.8893 | 2949.6668 | 3039.1249 |
| 3045.3187 | 3049.3071 | 3076.6350 |
| 3113.3073 | 3121.0639 | 3123.7628 |

Zero-point correction (Hartree): 0.132104

C5H9O2.phomhmm

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.32250433

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 2.505082 | -0.021041 | -0.895791 |
| C | 1.707846 | -0.649701 | -0.032308 |
| C | 0.508940 | 0.267089 | 0.488164 |
| C | -0.697682 | -0.533738 | 0.953826 |
| C | -1.698880 | -0.787577 | -0.198895 |
| C | -2.368739 | 0.484672 | -0.726200 |
| H | -3.061275 | 0.245835 | -1.539149 |
| O | 0.572359 | 1.466705 | 0.500830 |
| H | 1.276931 | -1.607929 | -0.381149 |
| H | 2.219993 | -0.833641 | 0.939126 |
| H | -0.361857 | -1.491371 | 1.368141 |
| H | -1.181816 | 0.041666 | 1.749408 |
| H | -1.186440 | -1.309545 | -1.016823 |
| H | -2.460977 | -1.481243 | 0.175013 |
| H | -2.938179 | 0.985653 | 0.064057 |
| H | -1.634822 | 1.200790 | -1.106466 |

Rotational constants (GHz): 4.4423300 1.5087500 1.4292400

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 30.7203 | 86.2643 | 109.2424 |
| 186.6502 | 236.4861 | 274.7878 |
| 361.7203 | 385.4939 | 499.5617 |
| 572.4228 | 636.6364 | 788.4920 |
| 843.9187 | 854.1407 | 917.0847 |
| 964.1798 | 993.6215 | 1062.8334 |
| 1101.0956 | 1147.2306 | 1195.1948 |
| 1245.6276 | 1283.7580 | 1301.2384 |
| 1350.2810 | 1380.0814 | 1435.9750 |
| 1485.6825 | 1487.0463 | 1502.7627 |
| 1512.5370 | 1518.6120 | 1861.0254 |
| 2869.7612 | 2945.5434 | 3043.1240 |
| 3051.9318 | 3053.6129 | 3080.6691 |
| 3113.1525 | 3121.2395 | 3134.2355 |

Zero-point correction (Hartree): 0.132192

C5H9O2.phomhht

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.32291883

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 2.721241 | -0.716539 | -0.470487 |
| C | 1.655181 | -0.776525 | 0.327679 |
| C | 0.705943 | 0.497187 | 0.206263 |
| C | -0.718931 | 0.231857 | 0.670376 |
| C | -1.631402 | -0.127038 | -0.522379 |
| C | -3.079861 | -0.372245 | -0.089850 |
| H | -3.708347 | -0.613909 | -0.952502 |
| O | 1.085302 | 1.554539 | -0.218896 |
| H | 1.021530 | -1.678732 | 0.222240 |
| H | 1.942569 | -0.681055 | 1.399236 |
| H | -0.733187 | -0.577628 | 1.409890 |
| H | -1.079693 | 1.147837 | 1.149508 |
| H | -1.588361 | 0.690415 | -1.250621 |
| H | -1.239375 | -1.018261 | -1.028110 |
| H | -3.149155 | -1.205738 | 0.617799 |
| H | -3.503918 | 0.513658 | 0.395093 |

Rotational constants (GHz): 5.4750200 1.2702000 1.1441500

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 29.6993 | 86.7691 | 98.4940 |
| 190.3878 | 242.2853 | 257.8111 |
| 305.2676 | 388.8630 | 493.5451 |
| 563.8134 | 673.3056 | 759.8765 |
| 834.4973 | 881.2762 | 907.6621 |
| 961.5117 | 1017.1864 | 1044.3548 |
| 1105.2226 | 1154.8852 | 1193.4036 |
| 1261.1019 | 1296.0697 | 1302.3347 |
| 1333.3488 | 1383.2379 | 1427.3230 |
| 1483.2040 | 1489.8985 | 1506.9713 |
| 1511.0997 | 1521.2777 | 1863.6351 |
| 2869.4296 | 2940.5760 | 3043.9249 |
| 3044.8802 | 3054.1725 | 3085.6164 |
| 3109.7949 | 3121.0936 | 3122.0127 |

Zero-point correction (Hartree): 0.132045

C5H9O2.phopchp

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.32179807

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -2.671988 | -0.547529 | -0.290302 |
| C | -1.379728 | -0.810018 | -0.074773 |
| C | -0.529046 | 0.510428 | 0.203273 |
| C | 0.714065 | 0.275750 | 1.051927 |
| C | 1.747516 | -0.649229 | 0.373293 |
| C | 2.336714 | -0.063647 | -0.914278 |
| H | 3.073897 | -0.744375 | -1.350677 |
| O | -0.847262 | 1.576016 | -0.251413 |
| H | -1.165709 | -1.546588 | 0.722621 |
| H | -0.891618 | -1.161975 | -1.010583 |
| H | 1.151695 | 1.258603 | 1.251006 |
| H | 0.401107 | -0.161389 | 2.007948 |
| H | 2.550844 | -0.835780 | 1.095151 |
| H | 1.295352 | -1.628209 | 0.170733 |
| H | 1.565681 | 0.120673 | -1.670275 |
| H | 2.835610 | 0.891435 | -0.718859 |

Rotational constants (GHz): 4.4721400 1.5197000 1.3936100

Vibrational harmonic frequencies (cm-1):
45.2567 65.9006 111.0364

| | | |
|-----------|-----------|-----------|
| 167.8615 | 237.5585 | 289.9899 |
| 375.0431 | 389.4109 | 475.4868 |
| 600.8360 | 616.0385 | 795.6304 |
| 804.0569 | 879.0028 | 919.5086 |
| 943.7944 | 998.6663 | 1066.6193 |
| 1093.7490 | 1166.4509 | 1188.6738 |
| 1244.6555 | 1283.0025 | 1292.4759 |
| 1353.7439 | 1380.5320 | 1436.5422 |
| 1479.5456 | 1482.7932 | 1504.6065 |
| 1512.9074 | 1518.5214 | 1859.6993 |
| 2875.6045 | 2951.2673 | 3045.1565 |
| 3048.4279 | 3053.6744 | 3080.7164 |
| 3115.4873 | 3119.4228 | 3124.7875 |

Zero-point correction (Hartree): 0.132120

C5H9O2.phopcht

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.32224751

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -2.765960 | -0.800534 | 0.119631 |
| C | -1.440330 | -0.879082 | -0.031603 |
| C | -0.731592 | 0.545242 | 0.047548 |
| C | 0.715067 | 0.492952 | 0.518891 |
| C | 1.632299 | -0.311299 | -0.424431 |
| C | 3.090343 | -0.302538 | 0.046411 |
| H | 3.725837 | -0.872224 | -0.638421 |
| O | -1.300959 | 1.554454 | -0.270605 |
| H | -0.919656 | -1.576889 | 0.651554 |
| H | -1.184779 | -1.164465 | -1.076221 |
| H | 1.059622 | 1.528279 | 0.598544 |
| H | 0.740120 | 0.046725 | 1.521655 |
| H | 1.280323 | -1.347713 | -0.495748 |
| H | 1.567871 | 0.112303 | -1.434155 |
| H | 3.483256 | 0.718433 | 0.096966 |
| H | 3.188049 | -0.747467 | 1.042723 |

Rotational constants (GHz): 5.5104000 1.2914300 1.1152300

Vibrational harmonic frequencies (cm-1):
52.9076 68.9191 97.4627
165.6933 248.6145 272.9495
311.2401 395.8005 479.8837
594.7176 664.6245 753.3632
822.0713 892.4845 911.4881
954.0147 1028.4569 1050.4395
1106.7316 1166.7802 1193.5971
1261.1981 1292.2436 1296.7722
1333.0201 1385.1815 1427.8878
1479.3039 1482.8657 1505.9059
1512.0793 1521.0152 1859.9021
2877.9482 2949.4686 3038.9286
3045.2615 3049.0906 3076.4896
3113.2954 3121.0499 3123.7857

Zero-point correction (Hartree): 0.132099

C5H9O2.phopchm

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.32436778

Electronic state : 2-A
Cartesian coordinates (Angs):
O 2.944519 0.165374 0.015965
C 1.859748 -0.488739 0.443377
C 0.508389 0.113214 -0.143501
C -0.596224 -0.924036 -0.290103
C -1.986492 -0.322599 -0.523983
C -2.564802 0.381831 0.707550
H -3.564192 0.774849 0.497088
O 0.397942 1.275609 -0.428372
H 1.862430 -1.583220 0.279973
H 1.690685 -0.302339 1.527225
H -0.299960 -1.567655 -1.131147
H -0.581003 -1.577031 0.593954
H -1.925419 0.383540 -1.358668
H -2.658348 -1.129924 -0.838507
H -2.651799 -0.306954 1.556105
H -1.935800 1.222852 1.013194
Rotational constants (GHz): 6.3214900 1.3199400 1.2308100
Vibrational harmonic frequencies (cm-1):
42.8943 84.3302 127.7829
178.0848 251.9827 301.9244
314.9208 393.5602 468.6511
520.7695 685.3798 788.7646
821.7829 877.5986 896.3831
946.4638 1012.8361 1062.5000
1090.8289 1140.3863 1183.7538
1249.9750 1292.9926 1301.5220
1373.8400 1389.3960 1428.8419
1456.7112 1479.9161 1496.6846
1513.2537 1524.0137 1860.0636
2878.5502 2951.6926 3027.0732
3045.7153 3052.1434 3062.3628
3096.2345 3116.7501 3132.5594
Zero-point correction (Hartree): 0.131956

C5H9O2.phophcp

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.32405977
Electronic state : 2-A
Cartesian coordinates (Angs):
O 2.814850 -0.395838 0.491996
C 1.975855 0.540837 0.037434
C 0.517374 -0.043204 -0.239012
C -0.591254 0.966638 0.016528
C -1.993323 0.475520 -0.362793
C -2.555448 -0.580279 0.595120
H -3.564660 -0.878531 0.294455
O 0.352708 -1.161372 -0.647369
H 1.887011 1.449721 0.661771
H 2.253349 0.851761 -0.993709
H -0.543384 1.250019 1.077552
H -0.322313 1.879149 -0.535708
H -2.660993 1.345081 -0.386415
H -1.964446 0.072446 -1.381221
H -1.928927 -1.475608 0.603439
H -2.615324 -0.193424 1.619148
Rotational constants (GHz): 6.0723700 1.3407700 1.2323500
Vibrational harmonic frequencies (cm-1):
38.2594 73.4468 124.7428
185.9502 257.9530 295.5856
307.0006 406.3218 458.0038
537.4156 688.8670 797.0433
819.8066 858.5019 912.3185
965.9300 1008.8404 1064.0695
1102.6542 1127.4204 1189.6657
1249.1922 1293.6340 1305.0760
1374.6233 1384.0415 1427.5535
1455.2628 1484.6545 1496.5747
1512.5745 1526.2324 1860.8024
2882.1779 2954.7559 3025.1362
3047.2356 3048.5413 3060.3071
3090.8920 3115.1449 3142.0335
Zero-point correction (Hartree): 0.132034

C5H9O2.phophct

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.32465405
Electronic state : 2-A
Cartesian coordinates (Angs):
O 3.039220 -0.202744 -0.314136
C 1.930122 -0.712368 0.231374
C 0.671251 0.248781 0.060937
C -0.647948 -0.500410 -0.037290
C -1.877008 0.407339 0.051219

| | | | | |
|--|-----------|-----------|-----------|--|
| C | -3.188732 | -0.370630 | -0.086120 | |
| H | -4.050190 | 0.300686 | -0.017235 | |
| O | 0.781091 | 1.445070 | 0.036284 | |
| H | 1.651729 | -1.728824 | -0.105941 | |
| H | 2.007274 | -0.724550 | 1.341060 | |
| H | -0.634120 | -1.053231 | -0.988355 | |
| H | -0.661050 | -1.275396 | 0.742932 | |
| H | -1.855699 | 0.946080 | 1.005433 | |
| H | -1.805795 | 1.174083 | -0.727190 | |
| H | -3.247872 | -0.888240 | -1.050303 | |
| H | -3.292870 | -1.125486 | 0.701690 | |
| Rotational constants (GHz): | 7.5410100 | 1.1564400 | 1.0394300 | |
| Vibrational harmonic frequencies (cm-1): | | | | |
| 45.2526 | 72.8473 | | 110.7844 | |
| 156.3414 | 244.9812 | | 282.9863 | |
| 314.7400 | 375.8640 | | 462.3955 | |
| 533.8877 | 731.0074 | | 758.4355 | |
| 823.6939 | 871.3100 | | 916.0919 | |
| 953.8096 | 1021.5670 | | 1052.5225 | |
| 1106.3216 | 1138.4427 | | 1190.3173 | |
| 1253.8655 | 1295.0662 | | 1314.4657 | |
| 1329.3197 | 1397.5529 | | 1430.0291 | |
| 1460.3564 | 1482.7001 | | 1502.2763 | |
| 1513.5437 | 1520.0522 | | 1862.2363 | |
| 2880.2522 | 2952.4371 | | 3022.3406 | |
| 3041.1109 | 3051.8507 | | 3062.0677 | |
| 3092.7969 | 3115.8213 | | 3119.7223 | |
| Zero-point correction (Hartree): | 0.131823 | | | |

C5H9O2.pohmchp

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.31794282
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | | |
|--|-----------|-----------|-----------|--|
| O | -0.042006 | 1.819300 | -0.445146 | |
| C | -0.999641 | 1.131153 | 0.339250 | |
| C | -1.086168 | -0.379211 | 0.073459 | |
| C | 0.148648 | -1.276880 | 0.204070 | |
| C | 1.478347 | -0.823943 | -0.439684 | |
| C | 2.255620 | 0.186996 | 0.336470 | |
| H | 3.058015 | 0.741302 | -0.142585 | |
| O | -2.169148 | -0.882547 | -0.162957 | |
| H | -0.831449 | 1.277619 | 1.420691 | |
| H | -1.981231 | 1.544670 | 0.096806 | |
| H | 0.312391 | -1.428500 | 1.282448 | |
| H | -0.156416 | -2.245085 | -0.201444 | |
| H | 2.103610 | -1.728139 | -0.552067 | |
| H | 1.304807 | -0.466639 | -1.461456 | |
| H | 0.840437 | 1.624506 | -0.082663 | |
| H | 2.258233 | 0.157546 | 1.423704 | |
| Rotational constants (GHz): | 3.4737500 | 2.1747100 | 1.4731600 | |
| Vibrational harmonic frequencies (cm-1): | | | | |
| 39.4979 | 74.8837 | | 171.0361 | |
| 208.2966 | 264.6169 | | 271.4857 | |
| 368.8088 | 408.6274 | | 486.1323 | |
| 530.6756 | 607.7226 | | 632.0851 | |
| 749.7751 | 821.3359 | | 899.0955 | |
| 917.2342 | 964.3178 | | 1074.1513 | |
| 1096.3093 | 1106.7820 | | 1167.9589 | |
| 1201.0788 | 1253.2326 | | 1289.8983 | |
| 1352.2477 | 1378.3405 | | 1384.1241 | |
| 1416.7890 | 1465.0525 | | 1471.9659 | |
| 1484.1403 | 1493.7586 | | 1803.9395 | |
| 2953.0900 | 2971.4320 | | 3015.8664 | |
| 3073.4744 | 3115.0289 | | 3127.2920 | |
| 3141.9397 | 3244.2141 | | 3623.6428 | |
| Zero-point correction (Hartree): | 0.132410 | | | |

C5H9O2.pohmhhm

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.33036755
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | | |
|---|-----------|-----------|-----------|--|
| O | 1.607133 | -1.424636 | -0.342840 | |
| C | 1.878446 | -0.123562 | -0.245988 | |
| C | 0.584180 | 0.713663 | 0.202248 | |
| C | -0.410049 | -0.026523 | 1.064641 | |
| C | -1.390529 | -0.845200 | 0.189212 | |
| C | -2.350784 | 0.016139 | -0.635243 | |
| H | -3.012035 | -0.614209 | -1.237842 | |
| O | 0.480887 | 1.850492 | -0.177961 | |
| H | 2.538076 | 0.105211 | 0.621646 | |
| H | 2.277417 | 0.374724 | -1.145419 | |
| H | 0.137938 | -0.707925 | 1.721773 | |
| H | -0.953775 | 0.711700 | 1.662394 | |

| | | | | |
|--|-----------|-----------|-----------|--|
| H | -0.808556 | -1.508538 | -0.461223 | |
| H | -1.956994 | -1.499538 | 0.861867 | |
| H | -2.978858 | 0.639791 | 0.010322 | |
| H | -1.814960 | 0.684831 | -1.316326 | |
| Rotational constants (GHz): | 3.5301800 | 1.9784900 | 1.5302200 | |
| Vibrational harmonic frequencies (cm-1): | | | | |
| 61.2002 | 101.1867 | | 115.7387 | |
| 175.2365 | 240.9098 | | 315.7396 | |
| 361.8238 | 423.7744 | | 482.8481 | |
| 592.4311 | 665.8305 | | 789.5202 | |
| 816.8499 | 889.0124 | | 922.6957 | |
| 959.2997 | 1049.5675 | | 1095.5212 | |
| 1106.2500 | 1160.7208 | | 1228.7824 | |
| 1249.8168 | 1279.6887 | | 1283.0426 | |
| 1349.8440 | 1378.1150 | | 1436.1199 | |
| 1479.0390 | 1493.2281 | | 1506.9027 | |
| 1515.0436 | 1519.9411 | | 1849.4852 | |
| 2865.1477 | 2997.7946 | | 3048.2808 | |
| 3051.4290 | 3068.3669 | | 3088.2171 | |
| 3119.1441 | 3125.6278 | | 3132.1216 | |
| Zero-point correction (Hartree): | 0.133025 | | | |

C5H9O2.pohmhht

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.33069156
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | | |
|--|-----------|-----------|-----------|--|
| O | -1.096155 | 1.768766 | -0.109518 | |
| C | -1.840909 | 0.676670 | 0.063035 | |
| C | -0.937123 | -0.646785 | 0.107299 | |
| C | 0.463431 | -0.472907 | 0.643052 | |
| C | 1.418053 | -0.033425 | -0.490407 | |
| C | 2.840463 | 0.208825 | 0.023149 | |
| H | 3.501358 | 0.511889 | -0.794789 | |
| O | -1.411795 | -1.677040 | -0.293473 | |
| H | -2.273128 | 0.622711 | 1.088007 | |
| H | -2.638159 | 0.490710 | -0.675999 | |
| H | 0.456036 | 0.293043 | 1.424894 | |
| H | 0.785536 | -1.430292 | 1.064088 | |
| H | 1.423086 | -0.805951 | -1.268198 | |
| H | 1.026687 | 0.883413 | -0.945223 | |
| H | 2.857730 | 1.002114 | 0.778148 | |
| H | 3.260964 | -0.695710 | 0.476226 | |
| Rotational constants (GHz): | 3.7953200 | 1.7363900 | 1.3047000 | |
| Vibrational harmonic frequencies (cm-1): | | | | |
| 65.9095 | 94.7367 | | 105.7904 | |
| 171.2792 | 243.3359 | | 269.5834 | |
| 337.1821 | 421.6635 | | 491.2812 | |
| 587.2992 | 685.7267 | | 763.7388 | |
| 833.0650 | 904.3138 | | 912.0239 | |
| 974.0677 | 1042.0267 | | 1095.5977 | |
| 1106.2987 | 1169.9956 | | 1229.5246 | |
| 1264.0089 | 1279.6599 | | 1297.2553 | |
| 1334.2486 | 1381.5420 | | 1425.7943 | |
| 1478.3511 | 1491.0141 | | 1507.4249 | |
| 1511.7167 | 1519.6859 | | 1851.9312 | |
| 2865.0620 | 2999.0511 | | 3044.2384 | |
| 3050.0130 | 3067.8011 | | 3089.5259 | |
| 3116.2048 | 3121.7104 | | 3131.7271 | |
| Zero-point correction (Hartree): | 0.132891 | | | |

C5H9O2.pohpchk

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.32754766
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | | |
|--|-----------|-----------|-----------|--|
| O | 1.194340 | 1.664740 | 0.541223 | |
| C | 1.479575 | 0.721743 | -0.358847 | |
| C | 0.769772 | -0.674214 | -0.006672 | |
| C | -0.436442 | -0.631587 | 0.906923 | |
| C | -1.780197 | -0.493120 | 0.150538 | |
| C | -1.968638 | 0.824660 | -0.608808 | |
| H | -2.994863 | 0.907555 | -0.979942 | |
| O | 1.222757 | -1.675601 | -0.497037 | |
| H | 1.006394 | 0.925428 | -1.343396 | |
| H | 2.547077 | 0.489669 | -0.515411 | |
| H | -0.437856 | -1.572246 | 1.466328 | |
| H | -0.307637 | 0.208045 | 1.596994 | |
| H | -1.891067 | -1.343845 | -0.532198 | |
| H | -2.572434 | -0.595528 | 0.901221 | |
| H | -1.764386 | 1.687320 | 0.032163 | |
| H | -1.306421 | 0.895587 | -1.478056 | |
| Rotational constants (GHz): | 3.1010500 | 2.1605200 | 1.5512000 | |
| Vibrational harmonic frequencies (cm-1): | | | | |
| 33.0260 | 73.1702 | | 113.1615 | |

| | | |
|-----------|-----------|-----------|
| 202.2605 | 236.7287 | 275.4350 |
| 358.0338 | 454.2332 | 475.3064 |
| 587.5544 | 620.4108 | 752.1439 |
| 854.5750 | 869.5448 | 907.5101 |
| 947.4858 | 1057.8810 | 1077.1526 |
| 1118.1859 | 1160.3082 | 1216.3527 |
| 1259.1530 | 1280.9305 | 1286.8921 |
| 1354.3113 | 1379.8717 | 1437.5781 |
| 1473.6824 | 1484.6515 | 1501.1670 |
| 1511.5295 | 1522.8444 | 1849.7499 |
| 2890.2021 | 2990.5770 | 3048.4957 |
| 3052.5724 | 3064.1304 | 3085.6962 |
| 3118.0356 | 3126.9366 | 3133.4258 |

Zero-point correction (Hartree): 0.132687

C5H9O2.pohpchp

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.32984111

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -1.726169 | -1.444909 | 0.064921 |
| C | -1.561259 | -0.319540 | -0.630833 |
| C | -0.616476 | 0.714020 | 0.155916 |
| C | 0.435826 | 0.101427 | 1.050636 |
| C | 1.455872 | -0.769546 | 0.286705 |
| C | 2.304488 | 0.015053 | -0.718710 |
| H | 3.026999 | -0.641163 | -1.213522 |
| O | -0.790699 | 1.890507 | -0.022341 |
| H | -0.942376 | -0.473046 | -1.543191 |
| H | -2.472330 | 0.240008 | -0.900779 |
| H | 0.932337 | 0.917777 | 1.584017 |
| H | -0.102373 | -0.527617 | 1.770245 |
| H | 2.108582 | -1.238157 | 1.032002 |
| H | 0.918817 | -1.586242 | -0.206275 |
| H | 1.690760 | 0.477673 | -1.499948 |
| H | 2.863821 | 0.817495 | -0.225483 |

Rotational constants (GHz): 3.3415000 1.9789800 1.5415000

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 60.7565 | 104.5545 | 111.9601 |
| 183.7348 | 233.5142 | 301.0694 |
| 365.1803 | 466.8219 | 478.7347 |
| 567.3104 | 618.4751 | 783.3599 |
| 846.4778 | 880.0418 | 909.3548 |
| 946.6437 | 1053.9959 | 1087.0908 |
| 1108.6446 | 1179.2494 | 1220.0329 |
| 1246.2251 | 1281.6204 | 1283.1025 |
| 1357.7720 | 1378.5592 | 1437.0589 |
| 1465.6273 | 1492.2442 | 1509.9209 |
| 1515.5705 | 1520.5096 | 1852.9833 |
| 2869.3816 | 3000.3659 | 3044.3289 |
| 3052.4500 | 3061.3772 | 3095.2682 |
| 3114.3161 | 3120.9379 | 3125.4341 |

Zero-point correction (Hartree): 0.132890

C5H9O2.pohpcht

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.33031701

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -1.192538 | 1.750066 | -0.377291 |
| C | -1.668838 | 0.732837 | 0.341657 |
| C | -0.955336 | -0.646465 | -0.058704 |
| C | 0.471276 | -0.543025 | -0.542582 |
| C | 1.427701 | 0.071766 | 0.499788 |
| C | 2.869303 | 0.125946 | -0.015217 |
| H | 3.534259 | 0.564984 | 0.734890 |
| O | -1.581644 | -1.666119 | 0.064263 |
| H | -1.358165 | 0.789949 | 1.409103 |
| H | -2.754815 | 0.548909 | 0.290127 |
| H | 0.795324 | -1.546285 | -0.835317 |
| H | 0.453709 | 0.101188 | -1.431416 |
| H | 1.081896 | 1.082177 | 0.738762 |
| H | 1.388477 | -0.519071 | 1.423443 |
| H | 3.246999 | -0.874696 | -0.252176 |
| H | 2.941139 | 0.734917 | -0.922844 |

Rotational constants (GHz): 3.7643800 1.7028100 1.2867200

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 76.9938 | 85.5020 | 123.3496 |
| 173.6155 | 243.0238 | 253.8606 |
| 330.5794 | 463.4504 | 482.8220 |
| 573.5884 | 629.5216 | 760.6317 |
| 869.3490 | 883.4925 | 913.2278 |
| 959.7530 | 1045.7018 | 1100.5765 |
| 1115.0534 | 1176.4125 | 1224.7819 |
| 1264.4045 | 1281.5972 | 1300.4147 |

| | | |
|-----------|-----------|-----------|
| 1335.9822 | 1387.0685 | 1428.8020 |
| 1465.7839 | 1488.5808 | 1509.8942 |
| 1512.5330 | 1520.7604 | 1852.1840 |
| 2869.4007 | 3001.5005 | 3040.9607 |
| 3044.9544 | 3052.1220 | 3096.2340 |
| 3113.8447 | 3121.8452 | 3126.6591 |

Zero-point correction (Hartree): 0.132819

C5H9O2.pohphcm

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.33127905

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 2.482263 | -0.931598 | 0.048815 |
| C | 2.013836 | 0.275748 | 0.373940 |
| C | 0.510718 | 0.472368 | -0.131981 |
| C | -0.315774 | -0.788693 | -0.223305 |
| C | -1.801179 | -0.557742 | -0.514463 |
| C | -2.569263 | 0.062453 | 0.657985 |
| H | -3.628937 | 0.179987 | 0.411244 |
| O | 0.139570 | 1.584767 | -0.405282 |
| H | 1.847791 | 0.372268 | 1.470513 |
| H | 2.588294 | 1.148355 | 0.019879 |
| H | 0.168279 | -1.389376 | -1.006852 |
| H | -0.156856 | -1.364062 | 0.697991 |
| H | -1.895394 | 0.083309 | -1.397917 |
| H | -2.248149 | -1.523614 | -0.777439 |
| H | -2.504945 | -0.568292 | 1.552307 |
| H | -2.174767 | 1.051268 | 0.908954 |

Rotational constants (GHz): 5.0029700 1.5043800 1.2933700

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 51.2279 | 97.1445 | 122.3641 |
| 176.8367 | 227.3722 | 283.0731 |
| 369.3687 | 422.6117 | 492.0945 |
| 532.5685 | 697.9805 | 781.2436 |
| 827.4634 | 838.8381 | 910.6345 |
| 934.6565 | 1058.9194 | 1083.2282 |
| 1103.1689 | 1151.4647 | 1216.8435 |
| 1243.0966 | 1279.9192 | 1300.3810 |
| 1374.9621 | 1391.8420 | 1425.6474 |
| 1441.1093 | 1486.9026 | 1497.9843 |
| 1513.0856 | 1524.7945 | 1847.5479 |
| 2870.1081 | 2997.1996 | 3038.0610 |
| 3046.2536 | 3053.3727 | 3073.4696 |
| 3092.4853 | 3116.1805 | 3132.2135 |

Zero-point correction (Hartree): 0.132420

C5H9O2.pohphcp

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.33098225

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 2.337167 | -0.999007 | -0.474361 |
| C | 2.094613 | 0.222223 | 0.007707 |
| C | 0.524582 | 0.494590 | 0.153055 |
| C | -0.326089 | -0.724077 | 0.423657 |
| C | -1.823216 | -0.441171 | 0.581950 |
| C | -2.518893 | -0.045888 | -0.725313 |
| H | -3.589483 | 0.113359 | -0.563052 |
| O | 0.133967 | 1.630336 | 0.069620 |
| H | 2.392792 | 0.310680 | 1.076442 |
| H | 2.514171 | 1.074449 | -0.553156 |
| H | -0.118777 | -1.431553 | -0.390933 |
| H | 0.094675 | -1.205916 | 1.317172 |
| H | -2.293991 | -1.343287 | 0.990331 |
| H | -1.962560 | 0.348625 | 1.328838 |
| H | -2.100910 | 0.879324 | -1.130865 |
| H | -2.410965 | -0.830374 | -1.483182 |

Rotational constants (GHz): 4.8095600 1.5243000 1.3161500

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 49.6956 | 98.8263 | 121.8033 |
| 175.1161 | 228.0364 | 284.5864 |
| 364.0168 | 415.1942 | 482.9780 |
| 546.4864 | 693.6625 | 777.8563 |
| 803.9238 | 860.9241 | 900.8072 |
| 947.6837 | 1054.5630 | 1083.8255 |
| 1123.2482 | 1136.2047 | 1216.6061 |
| 1244.9174 | 1281.3093 | 1304.2793 |
| 1378.4023 | 1385.3733 | 1428.0573 |
| 1442.0794 | 1487.6155 | 1497.2189 |
| 1513.2642 | 1525.7816 | 1848.7174 |
| 2871.7396 | 2996.2565 | 3039.1546 |
| 3048.0485 | 3049.9982 | 3070.3062 |
| 3088.4855 | 3115.7222 | 3137.2036 |

Zero-point correction (Hartree): 0.132407

C5H9O2.pohphct

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.33159527

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 2.150459 | -1.399556 | -0.230448 |
| C | 2.166517 | -0.140967 | 0.215325 |
| C | 0.747913 | 0.566666 | 0.013342 |
| C | -0.450898 | -0.348922 | 0.050112 |
| C | -1.795781 | 0.378052 | 0.009162 |
| C | -2.980079 | -0.593021 | 0.003194 |
| H | -3.930638 | -0.051615 | -0.025182 |
| O | 0.719299 | 1.759951 | -0.143195 |
| H | 2.232606 | -0.098036 | 1.325721 |
| H | 2.925834 | 0.533604 | -0.215060 |
| H | -0.328572 | -1.036364 | -0.799745 |
| H | -0.354793 | -0.993214 | 0.934464 |
| H | -1.867730 | 1.052335 | 0.870432 |
| H | -1.828464 | 1.020170 | -0.877841 |
| H | -2.948346 | -1.255783 | -0.868882 |
| H | -2.983990 | -1.225110 | 0.898420 |

Rotational constants (GHz): 4.6786100 1.4251500 1.1325200

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 65.0610 | 91.1965 | 102.8269 |
| 141.8868 | 248.1574 | 262.4359 |
| 339.8952 | 416.5110 | 490.2552 |
| 534.0532 | 724.6517 | 746.1801 |
| 819.9640 | 858.3165 | 919.4257 |
| 942.4990 | 1052.1026 | 1087.2416 |
| 1120.9538 | 1149.0635 | 1219.0704 |
| 1249.9529 | 1279.4075 | 1315.9667 |
| 1328.1789 | 1403.3423 | 1432.5296 |
| 1445.3034 | 1486.7415 | 1503.1411 |
| 1514.6860 | 1520.7853 | 1849.6287 |
| 2870.7305 | 2997.0438 | 3034.2011 |
| 3042.5497 | 3057.8300 | 3064.3975 |
| 3090.6570 | 3114.6375 | 3120.1911 |

Zero-point correction (Hartree): 0.132256

C5H9O2.1-5Hshift.m

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.31278492

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| C | -1.410267 | 0.053885 | 0.489059 |
| C | -0.241837 | -0.830262 | 0.871185 |
| C | 1.001533 | -0.520396 | 0.024393 |
| C | 1.254958 | 0.987968 | -0.270112 |
| O | 0.246487 | 1.844970 | 0.140469 |
| C | -2.168859 | -0.321402 | -0.766666 |
| H | -2.049476 | 0.330460 | 1.331197 |
| H | -0.448039 | -1.900757 | 0.761083 |
| H | 0.043481 | -0.645999 | 1.915508 |
| O | 1.761721 | -1.362225 | -0.390276 |
| H | 1.471367 | 1.048828 | -1.350159 |
| H | 2.187795 | 1.224490 | 0.268597 |
| H | -0.773641 | 1.145469 | 0.267294 |
| H | -2.710745 | -1.267561 | -0.626471 |
| H | -1.496310 | -0.459194 | -1.620862 |
| H | -2.903268 | 0.443555 | -1.034883 |

Rotational constants (GHz): 3.3022100 2.2198000 1.6239900

Vibrational harmonic frequencies (cm-1):

| | | |
|------------|-----------|-----------|
| 11466.4796 | 74.9106 | 95.6688 |
| 145.6723 | 198.1752 | 335.1433 |
| 427.4094 | 472.0128 | 499.0288 |
| 549.3552 | 627.7191 | 710.2761 |
| 817.7828 | 838.4797 | 922.9471 |
| 966.1382 | 1041.6710 | 1096.7329 |
| 1104.1260 | 1138.0200 | 1160.6543 |
| 1188.7330 | 1230.3359 | 1241.4323 |
| 1286.9753 | 1321.6778 | 1367.8647 |
| 1425.1035 | 1455.0750 | 1491.0666 |
| 1498.0580 | 1503.2034 | 1572.2425 |
| 1834.7137 | 2973.6888 | 3010.4615 |
| 3021.9026 | 3040.7121 | 3086.0789 |
| 3096.6661 | 3111.6466 | 3128.0556 |

Zero-point correction (Hartree): 0.127823

C5H9O2.1-5Hshift.p

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.31278022

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|----------|-----------|----------|
| C | 1.271834 | -0.225815 | 0.474480 |
|---|----------|-----------|----------|

| | | | |
|--|-----------|-----------|-----------|
| C | 0.215513 | -1.027314 | -0.256910 |
| C | -1.189412 | -0.450615 | -0.042167 |
| C | -1.285620 | 1.102418 | -0.030469 |
| O | -0.067137 | 1.763210 | -0.078717 |
| H | 1.259106 | -0.391138 | 1.556791 |
| C | 2.662533 | -0.188198 | -0.122104 |
| H | 0.181345 | -2.081757 | 0.037391 |
| H | 0.407304 | -0.986670 | -1.338987 |
| O | -2.180245 | -1.127100 | 0.100896 |
| H | -1.891725 | 1.359160 | 0.854952 |
| H | -1.879485 | 1.356383 | -0.923932 |
| H | 0.775887 | 0.947246 | 0.335448 |
| H | 2.634753 | 0.141417 | -1.166185 |
| H | 3.124472 | -1.185570 | -0.102447 |
| H | 3.318315 | 0.489188 | 0.432557 |
| Rotational constants (GHz): | 4.0858900 | 1.8948900 | 1.3754700 |
| Vibrational harmonic frequencies (cm-1): | | | |
| i1464.7275 | 82.7791 | | 92.5723 |
| 156.2481 | 202.9239 | | 319.3522 |
| 379.7839 | 479.8250 | | 487.2140 |
| 548.0463 | 615.9244 | | 756.0441 |
| 780.3483 | 847.5361 | | 926.2406 |
| 964.1804 | 1048.2645 | | 1106.6678 |
| 1109.7391 | 1133.1687 | | 1160.3078 |
| 1220.7281 | 1236.1323 | | 1259.5687 |
| 1271.2152 | 1321.8961 | | 1376.3923 |
| 1421.5673 | 1456.3142 | | 1489.9112 |
| 1496.9780 | 1501.7822 | | 1568.6401 |
| 1832.9087 | 2975.2128 | | 3014.0502 |
| 3021.5071 | 3029.9231 | | 3084.1690 |
| 3092.2975 | 3100.5190 | | 3127.9424 |
| Zero-point correction (Hartree): | 0.127798 | | |

C5H9O2.1-6Hshift.a

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.30377154
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | |
|--|-----------|-----------|-----------|
| O | 0.182141 | 1.761571 | -0.394407 |
| H | 1.224146 | 1.173912 | -0.099196 |
| C | 2.057911 | 0.240122 | 0.151780 |
| C | -0.854872 | 1.185888 | 0.362125 |
| C | 1.382634 | -1.021242 | -0.340474 |
| C | -1.099591 | -0.304436 | 0.068923 |
| C | 0.025060 | -1.304011 | 0.338529 |
| H | 2.214996 | 0.293329 | 1.232812 |
| H | 2.944796 | 0.544693 | -0.407747 |
| H | -0.705488 | 1.317448 | 1.449438 |
| H | -1.771133 | 1.721731 | 0.084166 |
| H | 1.246553 | -0.965637 | -1.426661 |
| H | 2.042428 | -1.882285 | -0.159121 |
| O | -2.192448 | -0.682307 | -0.308777 |
| H | -0.355969 | -2.283379 | 0.037614 |
| H | 0.175271 | -1.331841 | 1.428874 |
| Rotational constants (GHz): | 3.5339100 | 2.3432800 | 1.5524500 |
| Vibrational harmonic frequencies (cm-1): | | | |
| i1501.1764 | 57.0699 | | 124.2195 |
| 214.4664 | 288.1733 | | 359.9186 |
| 406.9169 | 488.4657 | | 551.5844 |
| 588.0154 | 646.1838 | | 767.1791 |
| 836.3564 | 878.0342 | | 900.0319 |
| 969.2120 | 1042.5339 | | 1060.1120 |
| 1093.0803 | 1115.3839 | | 1193.8534 |
| 1215.2049 | 1239.8377 | | 1267.3062 |
| 1289.3176 | 1354.3374 | | 1371.4731 |
| 1381.0405 | 1450.7469 | | 1461.2585 |
| 1464.7686 | 1482.2258 | | 1494.2372 |
| 1809.6930 | 2955.1864 | | 3015.4545 |
| 3019.6576 | 3071.7444 | | 3077.1349 |
| 3086.3545 | 3118.5195 | | 3166.4584 |
| Zero-point correction (Hartree): | 0.128427 | | |

C5H9O2.1-6Hshift.c

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.30606981
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| C | -1.241864 | -1.135285 | 0.327959 |
| C | 0.014815 | -1.136219 | -0.580395 |
| C | 1.126192 | -0.246914 | -0.039939 |
| C | 0.796440 | 1.223647 | 0.264064 |
| O | -0.323817 | 1.748011 | -0.391739 |
| H | -1.304223 | 1.086628 | -0.036538 |

| | | | | |
|--|-----------|-----------|-----------|--|
| C | -2.101075 | 0.103948 | 0.161380 | |
| H | -0.934928 | -1.251954 | 1.374023 | |
| H | -1.841690 | -2.024244 | 0.088974 | |
| H | 0.431769 | -2.142018 | -0.670504 | |
| H | -0.263607 | -0.786203 | -1.582958 | |
| O | 2.239072 | -0.674435 | 0.200675 | |
| H | 0.745360 | 1.332652 | 1.362350 | |
| H | 1.659463 | 1.822944 | -0.059278 | |
| H | -2.708607 | 0.384966 | 1.023848 | |
| H | -2.672621 | 0.133565 | -0.769828 | |
| Rotational constants (GHz): | 3.5845100 | 2.3155900 | 1.5628800 | |
| Vibrational harmonic frequencies (cm-1): | | | | |
| i1533.0316 | 55.8303 | | 158.4468 | |
| 207.8209 | 282.3588 | | 359.2974 | |
| 441.3882 | 481.3429 | | 531.1412 | |
| 547.1582 | 641.3104 | | 714.9981 | |
| 837.8046 | 890.3677 | | 915.6134 | |
| 970.8697 | 1047.3815 | | 1072.1448 | |
| 1092.2309 | 1108.5017 | | 1183.3965 | |
| 1223.0475 | 1236.0811 | | 1250.5471 | |
| 1285.6751 | 1346.8084 | | 1354.7234 | |
| 1368.9900 | 1438.5617 | | 1442.0469 | |
| 1468.6457 | 1480.1323 | | 1502.7850 | |
| 1812.4643 | 2966.3398 | | 3028.8465 | |
| 3048.9956 | 3049.5656 | | 3076.0648 | |
| 3088.7293 | 3129.0348 | | 3170.2666 | |
| Zero-point correction (Hartree): | 0.128279 | | | |

C5H9O2.pmchmch

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.32106701
Electronic state : 2-A
Cartesian coordinates (Angs):

| | | | | |
|--|-----------|-----------|-----------|--|
| O | -2.219347 | 0.309116 | -0.104736 | |
| C | -1.522627 | -0.821163 | 0.388200 | |
| C | -0.241391 | -1.165350 | -0.393800 | |
| C | 1.050885 | -0.451504 | 0.002964 | |
| C | 0.998368 | 0.995525 | 0.513692 | |
| C | 0.291002 | 1.969154 | -0.372566 | |
| H | -0.029504 | 2.926545 | 0.027707 | |
| O | 2.118861 | -1.028006 | -0.074801 | |
| H | -1.296173 | -0.724860 | 1.463559 | |
| H | -2.220118 | -1.658795 | 0.290940 | |
| H | -0.020158 | -2.235083 | -0.324693 | |
| H | -0.435997 | -0.954326 | -1.454849 | |
| H | 0.536728 | 0.994253 | 1.512386 | |
| H | 2.047700 | 1.293270 | 0.667321 | |
| H | 0.368712 | 1.887408 | -1.452677 | |
| H | -1.604728 | 1.062740 | -0.124338 | |
| Rotational constants (GHz): | 3.4491600 | 2.1228800 | 1.4510000 | |
| Vibrational harmonic frequencies (cm-1): | | | | |
| 36.7611 | 94.6646 | | 156.6146 | |
| 193.5594 | 218.1511 | | 256.3791 | |
| 374.3829 | 424.4018 | | 481.0343 | |
| 495.5989 | 582.5220 | | 621.2463 | |
| 698.8468 | 835.0544 | | 887.7507 | |
| 948.7318 | 996.1079 | | 1051.4729 | |
| 1095.6384 | 1105.2921 | | 1141.0388 | |
| 1210.6154 | 1221.6650 | | 1267.8635 | |
| 1337.6260 | 1352.1866 | | 1393.7586 | |
| 1437.5846 | 1451.8218 | | 1456.8655 | |
| 1480.4021 | 1528.2138 | | 1806.7086 | |
| 2979.3480 | 2995.7667 | | 3038.8334 | |
| 3040.4060 | 3092.1053 | | 3107.8144 | |
| 3152.6895 | 3255.7643 | | 3645.9787 | |
| Zero-point correction (Hartree): | 0.132018 | | | |

C5H9O2.pmchmch

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.33053196
Electronic state : 2-A
Cartesian coordinates (Angs):

| | | | | |
|---|-----------|-----------|-----------|--|
| O | -1.920304 | -1.291948 | -0.476249 | |
| C | -2.085219 | 0.027112 | -0.156967 | |
| C | -1.026785 | 0.616741 | 0.797371 | |
| C | 0.356314 | 0.576762 | 0.147157 | |
| C | 1.261374 | -0.579213 | 0.527538 | |
| C | 2.598710 | -0.587246 | -0.206826 | |
| H | 3.203704 | -1.446042 | 0.098142 | |
| O | 0.666732 | 1.415113 | -0.679859 | |
| H | -2.056694 | 0.574618 | -1.123384 | |
| H | -3.111378 | 0.198411 | 0.220607 | |
| H | -1.280561 | 1.662703 | 0.998587 | |
| H | -1.047692 | 0.060402 | 1.740300 | |

| | | | |
|---|-----------|-----------|-----------|
| H | 1.400115 | -0.554362 | 1.618423 |
| H | 0.682028 | -1.494304 | 0.335128 |
| H | 2.448192 | -0.637025 | -1.288448 |
| H | 3.164502 | 0.325348 | -0.000136 |
| Rotational constants (GHz): | 4.3577100 | 1.6220100 | 1.3962000 |
| Vibrational harmonic frequencies (cm ⁻¹): | | | |
| 29.2816 | 85.0917 | | 117.6018 |
| 184.1006 | 217.8568 | | 252.2320 |
| 384.4898 | 429.3239 | | 534.9737 |
| 545.2212 | 638.5279 | | 757.4635 |
| 828.7479 | 897.0815 | | 936.9888 |
| 1004.6344 | 1054.1315 | | 1073.2085 |
| 1097.3123 | 1128.9108 | | 1162.8807 |
| 1231.5933 | 1284.4406 | | 1315.9267 |
| 1361.2358 | 1377.9120 | | 1398.3836 |
| 1429.6436 | 1467.5723 | | 1486.2335 |
| 1507.5336 | 1512.1964 | | 1808.4050 |
| 2905.0188 | 2949.2868 | | 3023.1335 |
| 3053.2807 | 3062.0902 | | 3064.6265 |
| 3120.0000 | 3133.7133 | | 3138.9870 |
| Zero-point correction (Hartree): | 0.132114 | | |

C5H9O2.pmchmhh

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.32697550
Electronic state : 2-A
Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -1.815253 | -1.122918 | -0.466823 |
| C | -1.878259 | 0.171970 | -0.036533 |
| C | -0.680016 | 0.682309 | 0.787136 |
| C | 0.604355 | 0.799041 | -0.035644 |
| C | 1.231209 | -0.476441 | -0.584218 |
| C | 1.505681 | -1.562686 | 0.468181 |
| H | 2.054706 | -2.393010 | 0.014536 |
| O | 1.089368 | 1.892915 | -0.261663 |
| H | -2.091487 | 0.836177 | -0.897669 |
| H | -2.804004 | 0.242299 | 0.573539 |
| H | -0.904729 | 1.678410 | 1.179387 |
| H | -0.528190 | -0.000351 | 1.630759 |
| H | 0.549060 | -0.889737 | -1.339998 |
| H | 2.150070 | -0.175372 | -1.095107 |
| H | 2.110297 | -1.177889 | 1.296283 |
| H | 0.573536 | -1.965665 | 0.872626 |
| Rotational constants (GHz): | 3.0627600 | 2.2058100 | 1.5072900 |
| Vibrational harmonic frequencies (cm ⁻¹): | | | |
| 48.2433 | 66.1714 | | 134.2463 |
| 188.5988 | 238.6650 | | 273.1114 |
| 375.8901 | 415.2796 | | 506.1121 |
| 518.3809 | 658.8273 | | 721.3996 |
| 814.2321 | 892.8627 | | 927.2102 |
| 998.3829 | 1056.7431 | | 1081.5075 |
| 1091.1969 | 1139.3709 | | 1188.5453 |
| 1259.1882 | 1291.2731 | | 1331.5056 |
| 1348.5753 | 1355.5458 | | 1382.5552 |
| 1422.9154 | 1475.4028 | | 1481.2441 |
| 1514.7011 | 1526.9677 | | 1804.5659 |
| 2901.8863 | 2934.5332 | | 3036.1136 |
| 3053.9496 | 3066.4466 | | 3110.4344 |
| 3122.6046 | 3125.0684 | | 3141.1940 |
| Zero-point correction (Hartree): | 0.132183 | | |

C5H9O2.pmchpch

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.32441017
Electronic state : 2-A
Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 1.748897 | 1.136368 | -0.006512 |
| C | 1.770854 | -0.244749 | -0.319594 |
| C | 0.760844 | -1.086373 | 0.495774 |
| C | -0.682600 | -0.768551 | 0.140436 |
| C | -1.294028 | 0.534320 | 0.692775 |
| C | -1.317843 | 1.586279 | -0.369211 |
| H | -1.219199 | 2.635836 | -0.111765 |
| O | -1.330763 | -1.475932 | -0.606770 |
| H | 1.606023 | -0.423876 | -1.392562 |
| H | 2.779938 | -0.595300 | -0.081667 |
| H | 0.928870 | -2.145543 | 0.277342 |
| H | 0.942322 | -0.903625 | 1.560948 |
| H | -2.323103 | 0.283299 | 0.999130 |
| H | -0.752747 | 0.886731 | 1.574857 |
| H | 0.951129 | 1.522830 | -0.401798 |
| H | -1.681663 | 1.330603 | -1.359309 |
| Rotational constants (GHz): | 3.2598000 | 2.2856000 | 1.5750900 |
| Vibrational harmonic frequencies (cm ⁻¹): | | | |
| 56.1932 | 73.8010 | | 150.5174 |

| | | |
|-----------|-----------|-----------|
| 192.0216 | 243.2089 | 264.2071 |
| 342.3478 | 464.9340 | 485.6533 |
| 526.4965 | 595.9703 | 667.0668 |
| 768.1256 | 813.0443 | 895.3550 |
| 934.9701 | 1019.4509 | 1043.0993 |
| 1066.6747 | 1106.3633 | 1147.9565 |
| 1180.7462 | 1222.0400 | 1256.3141 |
| 1338.6591 | 1349.0013 | 1406.4426 |
| 1424.8961 | 1459.1131 | 1469.0171 |
| 1480.9814 | 1520.2106 | 1809.5171 |
| 2983.8898 | 3012.7370 | 3057.4071 |
| 3098.4796 | 3109.3204 | 3121.9727 |
| 3159.4270 | 3269.5455 | 3706.3847 |

Zero-point correction (Hartree): 0.132803

C5H9O2.pmchphc

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.33053209
Electronic state : 2-A
Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -1.920769 | -1.290867 | -0.478015 |
| C | -2.085706 | 0.027486 | -0.155887 |
| C | -1.026450 | 0.614878 | 0.798925 |
| C | 0.355996 | 0.575732 | 0.147267 |
| C | 1.263036 | -0.578552 | 0.528022 |
| C | 2.599854 | -0.585272 | -0.207288 |
| H | 3.205912 | -1.443472 | 0.097245 |
| O | 0.664309 | 1.413389 | -0.681224 |
| H | -2.057340 | 0.577080 | -1.121108 |
| H | -3.111632 | 0.198049 | 0.222647 |
| H | -1.279681 | 1.660514 | 1.002614 |
| H | -1.046726 | 0.056719 | 1.740794 |
| H | 1.402412 | -0.552837 | 1.618793 |
| H | 0.684841 | -1.494568 | 0.336469 |
| H | 2.448579 | -0.635159 | -1.288793 |
| H | 3.164932 | 0.327858 | -0.000981 |

Rotational constants (GHz): 4.3619600 1.6207800 1.3964800
Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 28.9495 | 85.0149 | 117.4502 |
| 184.1716 | 217.7516 | 252.3659 |
| 384.6702 | 429.0981 | 534.7901 |
| 545.8529 | 638.8460 | 757.4569 |
| 828.8076 | 897.1026 | 937.1364 |
| 1004.6235 | 1054.1596 | 1073.1864 |
| 1097.2559 | 1128.8807 | 1162.9663 |
| 1231.2753 | 1284.4838 | 1315.8150 |
| 1361.4101 | 1377.8013 | 1398.3369 |
| 1429.6563 | 1467.4904 | 1486.2737 |
| 1507.5350 | 1512.1939 | 1808.4533 |
| 2905.1343 | 2949.3622 | 3023.1366 |
| 3053.2292 | 3062.0973 | 3064.5577 |
| 3119.8444 | 3133.6935 | 3139.0296 |

Zero-point correction (Hartree): 0.132114

C5H9O2.pmchphh

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.33053211
Electronic state : 2-A
Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -1.921145 | -1.290681 | -0.478222 |
| C | -2.085833 | 0.027644 | -0.155771 |
| C | -1.026388 | 0.614567 | 0.799073 |
| C | 0.356019 | 0.575555 | 0.147273 |
| C | 1.263362 | -0.578447 | 0.528142 |
| C | 2.600023 | -0.585124 | -0.207471 |
| H | 3.206401 | -1.442991 | 0.097357 |
| O | 0.664149 | 1.413206 | -0.681296 |
| H | -2.057546 | 0.577494 | -1.120845 |
| H | -3.111670 | 0.198210 | 0.222981 |
| H | -1.279462 | 1.660180 | 1.003100 |
| H | -1.046621 | 0.056111 | 1.740761 |
| H | 1.403002 | -0.552348 | 1.618873 |
| H | 0.685382 | -1.494711 | 0.337113 |
| H | 2.448525 | -0.635598 | -1.288918 |
| H | 3.164860 | 0.328283 | -0.001745 |

Rotational constants (GHz): 4.3625800 1.6204600 1.3964000
Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 28.8389 | 85.0045 | 117.4103 |
| 184.1603 | 217.7228 | 252.3805 |
| 384.6828 | 429.0667 | 534.7440 |
| 545.6274 | 638.7750 | 757.4563 |
| 828.7890 | 897.1195 | 937.1443 |
| 1004.6140 | 1054.1458 | 1073.1559 |
| 1097.2369 | 1128.8700 | 1162.9732 |
| 1231.2797 | 1284.4858 | 1315.8607 |

| | | |
|-----------|-----------|-----------|
| 1361.4030 | 1377.8133 | 1398.3392 |
| 1429.6524 | 1467.4787 | 1486.2460 |
| 1507.5286 | 1512.1952 | 1808.4355 |
| 2905.1786 | 2949.4270 | 3023.1238 |
| 3053.1914 | 3062.1064 | 3064.5541 |
| 3119.8461 | 3133.7143 | 3139.0277 |

Zero-point correction (Hartree): 0.132113

C5H9O2.pmhcmch

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.32818376

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 2.548785 | -0.190788 | 0.832865 |
| C | 1.995280 | -0.370643 | -0.402735 |
| C | 0.502129 | -0.727412 | -0.377252 |
| C | -0.372026 | 0.491584 | -0.070757 |
| C | -1.699186 | 0.254862 | 0.630681 |
| C | -2.630664 | -0.716952 | -0.114785 |
| H | -3.571414 | -0.832880 | 0.430853 |
| O | -0.010562 | 1.606832 | -0.399885 |
| H | 2.100167 | 0.613932 | -0.907924 |
| H | 2.586912 | -1.080412 | -1.009140 |
| H | 0.196444 | -1.107752 | -1.362784 |
| H | 0.319049 | -1.535216 | 0.339262 |
| H | -1.478031 | -0.148029 | 1.629098 |
| H | -2.176649 | 1.229595 | 0.761979 |
| H | -2.869911 | -0.344980 | -1.116196 |
| H | -2.185538 | -1.711247 | -0.219908 |

Rotational constants (GHz): 5.0207600 1.4497300 1.3020500

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 49.1262 | 62.3179 | 92.0141 |
| 202.3257 | 228.0849 | 257.9356 |
| 379.6140 | 452.8919 | 528.8971 |
| 607.6503 | 681.1337 | 790.9402 |
| 826.9186 | 892.2172 | 944.6077 |
| 984.9881 | 1047.8304 | 1075.6494 |
| 1095.2327 | 1159.4151 | 1199.9532 |
| 1204.6968 | 1284.0630 | 1322.2405 |
| 1344.7935 | 1380.1509 | 1384.9377 |
| 1426.0067 | 1461.8654 | 1484.8532 |
| 1516.5857 | 1519.8279 | 1807.4885 |
| 2899.5299 | 2965.4086 | 3034.1755 |
| 3036.0418 | 3053.5715 | 3097.4707 |
| 3111.1135 | 3127.7982 | 3132.0543 |

Zero-point correction (Hartree): 0.132486

C5H9O2.pmhcmhc

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.33089875

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 2.453380 | 0.152719 | 1.055922 |
| C | 2.167357 | 0.021732 | -0.273606 |
| C | 0.882695 | -0.765926 | -0.565952 |
| C | -0.375228 | 0.051777 | -0.266610 |
| C | -1.602284 | -0.714916 | 0.194353 |
| C | -2.862443 | 0.139855 | 0.302276 |
| H | -3.703894 | -0.455112 | 0.668755 |
| O | -0.379425 | 1.259849 | -0.417307 |
| H | 2.019680 | 1.061806 | -0.636882 |
| H | 3.036057 | -0.367138 | -0.835475 |
| H | 0.845332 | -1.028428 | -1.633480 |
| H | 0.881738 | -1.709953 | -0.010713 |
| H | -1.747068 | -1.568023 | -0.484046 |
| H | -1.344702 | -1.166924 | 1.163939 |
| H | -2.704226 | 0.977585 | 0.985841 |
| H | -3.135133 | 0.560521 | -0.669619 |

Rotational constants (GHz): 5.9825600 1.3276900 1.2771500

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 38.4297 | 81.1197 | 102.3356 |
| 194.5062 | 206.0949 | 280.4902 |
| 360.1086 | 461.8403 | 473.0888 |
| 605.3102 | 712.6454 | 740.1697 |
| 841.5848 | 890.8825 | 961.3136 |
| 1001.5135 | 1046.7968 | 1078.7594 |
| 1093.9779 | 1132.3822 | 1169.4115 |
| 1204.5365 | 1286.9532 | 1321.1015 |
| 1365.6335 | 1381.2678 | 1398.2696 |
| 1429.1114 | 1462.4197 | 1465.6515 |
| 1507.5295 | 1513.3073 | 1809.1093 |
| 2900.6654 | 2965.4402 | 3022.1377 |
| 3033.2804 | 3051.2817 | 3063.3528 |
| 3098.3653 | 3133.9824 | 3143.6937 |

Zero-point correction (Hartree): 0.132202

C5H9O2.pmhcmhh

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.32818395
Electronic state : 2-A
Cartesian coordinates (Angs):
O 2.549459 -0.190668 0.832250
C 1.994976 -0.371190 -0.402813
C 0.501776 -0.727608 -0.375946
C -0.372082 0.491919 -0.070762
C -1.700003 0.256105 0.629597
C -2.630387 -0.717761 -0.114523
H -3.571621 -0.832774 0.430474
O -0.009806 1.606914 -0.399844
H 2.099722 0.613043 -0.908691
H 2.585988 -1.081487 -1.009207
H 0.195348 -1.109541 -1.360634
H 0.318973 -1.534232 0.341980
H -1.479702 -0.144388 1.629177
H -2.177950 1.230950 0.758282
H -2.868839 -0.348197 -1.117018
H -2.184822 -1.712135 -0.216926
Rotational constants (GHz): 5.0210500 1.4497500 1.3017300
Vibrational harmonic frequencies (cm-1):
49.3894 62.5167 91.9246
202.3936 228.3688 258.0929
379.6335 452.9942 528.9050
607.3659 681.0597 790.7963
826.9269 892.1817 944.6363
984.9892 1047.9207 1075.6875
1095.2715 1159.4740 1199.9209
1204.7317 1284.0639 1322.3142
1344.8000 1380.1276 1384.9400
1426.0262 1461.8184 1484.7947
1516.6328 1519.8345 1807.4883
2899.5460 2965.3887 3034.1531
3036.0012 3053.5986 3097.3893
3111.1259 3127.7751 3132.0990
Zero-point correction (Hartree): 0.132487

C5H9O2.pmhcpch

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.32858538
Electronic state : 2-A
Cartesian coordinates (Angs):
O 1.881941 1.211185 -0.522197
C 1.977466 0.021400 0.144003
C 0.724552 -0.343565 0.953093
C -0.434692 -0.745291 0.036943
C -1.814565 -0.205968 0.364878
C -1.965148 1.230100 -0.178035
H -2.935414 1.646418 0.107106
O -0.230024 -1.454090 -0.931930
H 2.105328 -0.745079 -0.650850
H 2.901009 -0.025328 0.749211
H 0.940743 -1.210210 1.593817
H 0.449669 0.483895 1.614609
H -2.557721 -0.863644 -0.094408
H -1.966081 -0.209334 1.451456
H -1.182624 1.891876 0.206089
H -1.895926 1.234587 -1.269305
Rotational constants (GHz): 3.7282400 1.8132100 1.5224600
Vibrational harmonic frequencies (cm-1):
34.4063 62.1723 107.5235
195.9195 230.0378 248.7385
363.0497 460.1785 568.7565
600.4548 681.0270 801.0408
843.4526 896.3913 946.5184
988.4401 1043.9552 1074.3536
1088.3835 1152.0772 1192.0378
1204.3489 1282.1447 1318.3603
1340.4757 1381.0176 1385.3672
1424.9367 1471.3031 1492.4724
1510.5102 1519.8187 1808.5281
2901.1305 2967.0462 3039.6093
3048.8510 3056.9556 3105.5205
3113.9758 3132.8083 3138.9307
Zero-point correction (Hartree): 0.132642

C5H9O2.pmhcpch

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.33089875
Electronic state : 2-A
Cartesian coordinates (Angs):
O 2.453852 0.153091 1.055552

| | | | | |
|--|-----------|-----------|-----------|--|
| C | 2.167333 | 0.021620 | -0.273841 | |
| C | 0.882611 | -0.766192 | -0.565440 | |
| C | -0.375273 | 0.051687 | -0.266398 | |
| C | -1.602458 | -0.714848 | 0.194523 | |
| C | -2.862587 | 0.140028 | 0.302021 | |
| H | -3.704055 | -0.454701 | 0.668845 | |
| O | -0.379354 | 1.259733 | -0.417290 | |
| H | 2.019578 | 1.061544 | -0.637490 | |
| H | 3.035867 | -0.367475 | -0.835809 | |
| H | 0.845023 | -1.029414 | -1.632785 | |
| H | 0.881735 | -1.709862 | -0.009590 | |
| H | -1.747169 | -1.568082 | -0.483732 | |
| H | -1.345101 | -1.166669 | 1.164251 | |
| H | -2.704309 | 0.978122 | 0.985125 | |
| H | -3.135306 | 0.560181 | -0.670091 | |
| Rotational constants (GHz): | 5.9839000 | 1.3275800 | 1.2769700 | |
| Vibrational harmonic frequencies (cm-1): | | | | |
| 38.4855 | 81.1129 | | 102.3143 | |
| 194.5341 | 206.1047 | | 280.5124 | |
| 360.0942 | 461.8866 | | 473.0417 | |
| 605.2273 | 712.5270 | | 740.1568 | |
| 841.5283 | 890.8446 | | 961.3211 | |
| 1001.5169 | 1046.7692 | | 1078.7584 | |
| 1093.9412 | 1132.3792 | | 1169.4030 | |
| 1204.5474 | 1286.9572 | | 1321.1688 | |
| 1365.6306 | 1381.2430 | | 1398.2556 | |
| 1429.1176 | 1462.4082 | | 1465.6498 | |
| 1507.5380 | 1513.3160 | | 1809.1140 | |
| 2900.7434 | 2965.4427 | | 3022.1610 | |
| 3033.2584 | 3051.2997 | | 3063.3501 | |
| 3098.3472 | 3133.9709 | | 3143.6977 | |
| Zero-point correction (Hartree): | 0.132201 | | | |

C5H9O2.pmhcpqh

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.32858534

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | | |
|--|-----------|-----------|-----------|--|
| O | 1.881467 | 1.211462 | -0.522254 | |
| C | 1.977326 | 0.021706 | 0.143779 | |
| C | 0.724571 | -0.343727 | 0.953198 | |
| C | -0.434649 | -0.745553 | 0.037022 | |
| C | -1.814490 | -0.205892 | 0.364439 | |
| C | -1.964744 | 1.230499 | -0.177866 | |
| H | -2.935440 | 1.646322 | 0.106517 | |
| O | -0.229975 | -1.454811 | -0.931498 | |
| H | 2.104808 | -0.744695 | -0.651280 | |
| H | 2.900918 | -0.025154 | 0.748867 | |
| H | 0.941434 | -1.210474 | 1.593525 | |
| H | 0.449685 | 0.483442 | 1.615066 | |
| H | -2.557472 | -0.863268 | -0.095543 | |
| H | -1.966730 | -0.209529 | 1.450931 | |
| H | -1.182842 | 1.892240 | 0.207556 | |
| H | -1.894378 | 1.235711 | -1.269062 | |
| Rotational constants (GHz): | 3.7269100 | 1.8137200 | 1.5224600 | |
| Vibrational harmonic frequencies (cm-1): | | | | |
| 34.4697 | 62.1144 | | 107.4934 | |
| 195.9171 | 230.0237 | | 248.7947 | |
| 363.0822 | 460.1219 | | 568.7027 | |
| 600.6196 | 681.3721 | | 801.0638 | |
| 843.5471 | 896.3645 | | 946.4824 | |
| 988.3613 | 1043.9719 | | 1074.2707 | |
| 1088.5712 | 1152.0638 | | 1191.9705 | |
| 1204.2636 | 1282.1863 | | 1318.0996 | |
| 1340.4401 | 1381.1225 | | 1385.2884 | |
| 1424.8989 | 1471.3514 | | 1492.4353 | |
| 1510.5001 | 1519.8058 | | 1808.5767 | |
| 2900.6618 | 2967.2101 | | 3039.7558 | |
| 3048.7481 | 3056.9812 | | 3105.6323 | |
| 3114.0060 | 3132.8640 | | 3138.9307 | |
| Zero-point correction (Hartree): | 0.132642 | | | |

C5H9O2.pmhmqh

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.32697511

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | | |
|---|-----------|-----------|-----------|--|
| O | -1.812359 | -1.124457 | -0.470712 | |
| C | -1.878187 | 0.168517 | -0.035165 | |
| C | -0.680381 | 0.678506 | 0.789498 | |
| C | 0.602630 | 0.800150 | -0.034620 | |
| C | 1.234457 | -0.472931 | -0.583121 | |
| C | 1.507977 | -1.561118 | 0.467410 | |
| H | 2.060739 | -2.388863 | 0.013580 | |
| O | 1.082025 | 1.896027 | -0.262916 | |

| | | | | |
|--|-----------|-----------|-----------|-----------|
| H | -2.093576 | 0.835661 | -0.893476 | |
| H | -2.803600 | 0.234182 | 0.575938 | |
| H | -0.906845 | 1.673067 | 1.184638 | |
| H | -0.526839 | -0.006365 | 1.630962 | |
| H | 0.555559 | -0.885771 | -1.342121 | |
| H | 2.154102 | -0.168671 | -1.090715 | |
| H | 2.108689 | -1.177000 | 1.298672 | |
| H | 0.575458 | -1.967539 | 0.867532 | |
| Rotational constants (GHz): | 3.0603200 | | 2.2070000 | 1.5080500 |
| Vibrational harmonic frequencies (cm-1): | | | | |
| 48.2814 | | 66.4723 | | 133.8858 |
| 188.6862 | | 239.0013 | | 273.7269 |
| 376.1248 | | 414.8504 | | 506.1455 |
| 518.1305 | | 658.4793 | | 721.3582 |
| 814.1758 | | 892.8964 | | 927.1301 |
| 998.4506 | | 1056.9811 | | 1081.4847 |
| 1091.2543 | | 1139.3378 | | 1188.4205 |
| 1259.3618 | | 1291.1320 | | 1331.5268 |
| 1348.6353 | | 1355.4928 | | 1382.5659 |
| 1422.9882 | | 1475.4116 | | 1481.2854 |
| 1514.7514 | | 1527.0915 | | 1804.5361 |
| 2901.8661 | | 2934.6255 | | 3035.9230 |
| 3053.9175 | | 3066.7119 | | 3110.3330 |
| 3122.5374 | | 3125.2139 | | 3141.1801 |
| Zero-point correction (Hartree): | 0.132185 | | | |

C5H9O2.pmhmmhc

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.33053150
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | | |
|--|-----------|-----------|-----------|-----------|
| O | -1.919698 | -1.294267 | -0.472180 | |
| C | -2.083997 | 0.026506 | -0.159813 | |
| C | -1.027551 | 0.620713 | 0.793962 | |
| C | 0.357044 | 0.578990 | 0.147036 | |
| C | 1.258031 | -0.580518 | 0.526842 | |
| C | 2.596075 | -0.591693 | -0.206252 | |
| H | 3.198454 | -1.452358 | 0.098655 | |
| O | 0.672141 | 1.418777 | -0.676699 | |
| H | -2.055528 | 0.570069 | -1.128365 | |
| H | -3.110771 | 0.198817 | 0.215910 | |
| H | -1.282261 | 1.667337 | 0.990397 | |
| H | -1.049987 | 0.068055 | 1.739032 | |
| H | 1.395931 | -0.557049 | 1.617885 | |
| H | 0.676282 | -1.493792 | 0.333383 | |
| H | 2.446577 | -0.640360 | -1.288083 | |
| H | 3.164156 | 0.319210 | 0.001567 | |
| Rotational constants (GHz): | 4.3484600 | | 1.6245600 | 1.3955100 |
| Vibrational harmonic frequencies (cm-1): | | | | |
| 29.5558 | | 85.2212 | | 117.8624 |
| 183.9621 | | 217.9918 | | 252.0371 |
| 383.9370 | | 429.9064 | | 534.3628 |
| 540.0672 | | 636.9409 | | 757.4042 |
| 828.3477 | | 896.8160 | | 936.5038 |
| 1004.5726 | | 1053.9303 | | 1073.2113 |
| 1097.4747 | | 1128.9672 | | 1162.6075 |
| 1232.3942 | | 1284.3193 | | 1316.5940 |
| 1360.5330 | | 1378.2321 | | 1398.4908 |
| 1429.6419 | | 1467.7386 | | 1486.1678 |
| 1507.5433 | | 1512.2048 | | 1808.5498 |
| 2905.6687 | | 2948.2663 | | 3023.2587 |
| 3053.5386 | | 3062.0454 | | 3064.6410 |
| 3120.1063 | | 3133.6787 | | 3138.8849 |
| Zero-point correction (Hartree): | 0.132098 | | | |

C5H9O2.pmhmmhh

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.32749401
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | | |
|---|-----------|-----------|-----------|--|
| O | -2.018920 | -1.045399 | -0.714623 | |
| C | -2.010085 | -0.095118 | 0.268179 | |
| C | -0.651399 | 0.125359 | 0.964164 | |
| C | 0.373804 | 0.648576 | -0.043476 | |
| C | 1.348175 | -0.349821 | -0.642427 | |
| C | 2.421770 | -0.814796 | 0.358774 | |
| H | 3.097174 | -1.531575 | -0.117026 | |
| O | 0.353309 | 1.820332 | -0.374613 | |
| H | -2.330069 | 0.848707 | -0.222815 | |
| H | -2.811779 | -0.304280 | 1.002107 | |
| H | -0.777579 | 0.878238 | 1.749132 | |
| H | -0.332912 | -0.814623 | 1.425517 | |
| H | 0.765082 | -1.212121 | -0.990893 | |
| H | 1.817055 | 0.126516 | -1.507958 | |
| H | 3.021760 | 0.029966 | 0.711067 | |

```

H          1.982562   -1.305491   1.233478
Rotational constants (GHz):  3.8063300   1.7057000   1.4505300
Vibrational harmonic frequencies (cm-1):
  19.1590           65.6749           109.9348
 188.7272          208.9301           252.6915
 373.9466          451.5797           512.6365
 521.8736          713.8338           765.9328
 812.2928          895.6586           924.5628

 991.8403          1046.4413          1070.2446
1093.8385          1137.0381          1189.2883
1245.2469          1280.6965          1317.2573
1348.7234          1362.0915          1391.3098
1423.9326          1484.8477          1492.3709
1513.0481          1520.0334          1809.2453
2905.7470          2948.3451          3047.9144
3051.7165          3067.4654          3109.9882
3121.9412          3128.2255          3130.6787
Zero-point correction (Hartree): 0.132241
  
```

C5H9O2.pmhphch

```

-----
E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.32858539
Electronic state : 2-A
Cartesian coordinates (Angs):
O          1.881641   1.211436   -0.521963
C          1.977391   0.021471   0.143767
C          0.724665   -0.343930   0.953020
C         -0.434746   -0.745422   0.036928
C         -1.814458   -0.205796   0.364984
C         -1.964785   1.230311   -0.178012
H         -2.934742   1.647011   0.107630
O         -0.230283   -1.454332   -0.931908
H          2.105005   -0.744720   -0.651439
H          2.901094   -0.025596   0.748724
H          0.941114   -1.210825   1.593306
H          0.449877   0.483234   1.614946
H         -2.557816   -0.863311   -0.094180
H         -1.965832   -0.208935   1.451573
H         -1.181780   1.891803   0.205609
H         -1.896183   1.234704   -1.269323
Rotational constants (GHz):  3.7275200   1.8135300   1.5225100
Vibrational harmonic frequencies (cm-1):
  34.3858           62.1806           107.5168
 195.8798          229.9996           248.7730
 363.0800          460.1498           568.7327
 600.5780          681.2352           801.0857
 843.5144          896.4075           946.4824
 988.4000          1043.9715          1074.3380
1088.5024          1152.0703          1192.0144
1204.3202          1282.1200          1318.2803
1340.4290          1381.0596          1385.3456
1424.9254          1471.3365          1492.4525
1510.4896          1519.8249          1808.5249
2900.8826          2966.9480          3039.6664
3048.9224          3056.9552          3105.5380
3114.0673          3132.8252          3138.9345
Zero-point correction (Hartree): 0.132642
  
```

C5H9O2.pmhphc

```

-----
E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.33053132
Electronic state : 2-A
Cartesian coordinates (Angs):
O         -1.918822   -1.294974   -0.471192
C         -2.083909   0.025992   -0.160207
C         -1.027861   0.622026   0.792900
C          0.357130   0.579570   0.146905
C          1.256913   -0.580881   0.526462
C          2.595434   -0.592689   -0.205713
H          3.196419   -1.454632   0.098317
O          0.673430   1.419690   -0.676053
H         -2.055072   0.568196   -1.129587
H         -3.110754   0.198651   0.215045
H         -1.282930   1.668930   0.987289
H         -1.050549   0.071055   1.738963
H          1.394134   -0.558185   1.617603
H          0.674487   -1.493524   0.331986
H          2.446571   -0.639441   -1.287708
H          3.164588   0.317123   0.003959
Rotational constants (GHz):  4.3461600   1.6254600   1.3954600
Vibrational harmonic frequencies (cm-1):
  29.6975           85.2032           118.0033
 183.9687          218.0706           251.9324
 383.8341          429.9877           534.9909
  
```

| | | |
|-----------|-----------|-----------|
| 541.2851 | 637.1705 | 757.4525 |
| 828.4380 | 896.9377 | 936.4667 |
| 1004.6302 | 1054.0063 | 1073.3675 |
| 1097.4912 | 1129.0238 | 1162.6695 |
| 1232.4838 | 1284.3116 | 1316.3486 |
| 1360.6607 | 1378.2077 | 1398.5045 |
| 1429.6154 | 1467.7908 | 1486.1862 |
| 1507.5405 | 1512.2029 | 1808.4850 |
| 2905.0470 | 2948.6203 | 3023.2236 |
| 3053.4966 | 3062.0538 | 3064.6270 |
| 3120.1304 | 3133.6887 | 3138.9312 |

Zero-point correction (Hartree): 0.132104

C5H9O2.pmhphh

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.32858540

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 1.881927 | 1.211358 | -0.521911 |
| C | 1.977501 | 0.021355 | 0.143844 |
| C | 0.724683 | -0.343836 | 0.953013 |
| C | -0.434704 | -0.745277 | 0.036909 |
| C | -1.814491 | -0.205940 | 0.365133 |
| C | -1.965212 | 1.230041 | -0.178055 |
| H | -2.935332 | 1.646470 | 0.107426 |
| O | -0.230183 | -1.453868 | -0.932139 |
| H | 2.105066 | -0.744828 | -0.651365 |
| H | 2.901152 | -0.025777 | 0.748856 |
| H | 0.941001 | -1.210678 | 1.593426 |
| H | 0.449935 | 0.483413 | 1.614851 |
| H | -2.557766 | -0.863689 | -0.093841 |
| H | -1.965726 | -0.209005 | 1.451747 |
| H | -1.182469 | 1.891832 | 0.205591 |
| H | -1.896478 | 1.234285 | -1.269355 |

Rotational constants (GHz): 3.7283100 1.8131600 1.5224600

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 34.3888 | 62.1975 | 107.5126 |
| 195.9270 | 229.9983 | 248.7905 |
| 363.0488 | 460.1615 | 568.7697 |
| 600.5239 | 681.2398 | 801.1032 |
| 843.5220 | 896.4140 | 946.5032 |
| 988.4114 | 1043.9744 | 1074.3431 |
| 1088.4460 | 1152.0823 | 1191.9995 |
| 1204.3384 | 1282.1364 | 1318.2988 |
| 1340.4484 | 1381.0559 | 1385.3595 |
| 1424.9207 | 1471.3187 | 1492.4699 |
| 1510.5010 | 1519.8222 | 1808.5640 |
| 2900.9687 | 2967.0518 | 3039.6141 |
| 3048.8821 | 3056.9613 | 3105.5198 |
| 3114.0287 | 3132.8207 | 3138.9522 |

Zero-point correction (Hartree): 0.132643

C5H9O2.ppchmch

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.33089874

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 2.452861 | 0.152366 | 1.056372 |
| C | 2.167361 | 0.021899 | -0.273335 |
| C | 0.882810 | -0.765691 | -0.566469 |
| C | -0.375194 | 0.051842 | -0.266918 |
| C | -1.602133 | -0.714999 | 0.194106 |
| C | -2.862272 | 0.139726 | 0.302663 |
| H | -3.703597 | -0.455347 | 0.669254 |
| O | -0.379481 | 1.259933 | -0.417442 |
| H | 2.019872 | 1.062072 | -0.636351 |
| H | 3.036285 | -0.366832 | -0.834947 |
| H | 0.845783 | -1.027579 | -1.634150 |
| H | 0.881782 | -1.710010 | -0.011729 |
| H | -1.747109 | -1.567850 | -0.484593 |
| H | -1.344316 | -1.167432 | 1.163424 |
| H | -2.703882 | 0.977283 | 0.986407 |
| H | -3.135284 | 0.560646 | -0.669034 |

Rotational constants (GHz): 5.9808300 1.3277900 1.2773400

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 38.4102 | 81.1498 | 102.3622 |
| 194.5122 | 206.0862 | 280.4649 |
| 360.1355 | 461.7814 | 473.1378 |
| 605.2324 | 712.4935 | 740.1843 |
| 841.5258 | 890.8679 | 961.2820 |
| 1001.5022 | 1046.7967 | 1078.7376 |
| 1093.9192 | 1132.3719 | 1169.3971 |
| 1204.5017 | 1286.9435 | 1321.0885 |
| 1365.6330 | 1381.2488 | 1398.2624 |
| 1429.1180 | 1462.4255 | 1465.6554 |

| | | |
|-----------|-----------|-----------|
| 1507.5317 | 1513.3081 | 1809.1173 |
| 2900.8216 | 2965.4766 | 3022.1445 |
| 3033.3498 | 3051.2274 | 3063.3486 |
| 3098.3933 | 3133.9809 | 3143.6647 |

Zero-point correction (Hartree): 0.132201

C5H9O2.ppchmhc

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.32770696

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 2.032759 | -0.896957 | -0.873150 |
| C | 2.007521 | -0.297870 | 0.358203 |
| C | 1.036335 | 0.884356 | 0.493064 |
| C | -0.398677 | 0.630003 | 0.022457 |
| C | -1.018244 | -0.728468 | 0.317626 |
| C | -2.513805 | -0.792262 | 0.015277 |
| H | -2.903430 | -1.797078 | 0.202350 |
| O | -1.016866 | 1.509098 | -0.545894 |
| H | 1.724241 | -1.119434 | 1.051423 |
| H | 3.025605 | -0.015615 | 0.684959 |
| H | 0.991957 | 1.183476 | 1.550645 |
| H | 1.408679 | 1.747822 | -0.065537 |
| H | -0.466075 | -1.463909 | -0.284095 |
| H | -0.808717 | -0.990836 | 1.365101 |
| H | -3.071099 | -0.084675 | 0.635564 |
| H | -2.707080 | -0.531435 | -1.027823 |

Rotational constants (GHz): 4.2079900 1.6517400 1.3796500

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 48.0397 | 82.9438 | 119.0111 |
| 191.6587 | 200.0484 | 266.2958 |
| 363.7273 | 459.4336 | 540.9682 |
| 559.5929 | 664.8335 | 749.0838 |
| 772.0231 | 887.3183 | 961.7101 |
| 1000.1810 | 1041.4227 | 1085.3520 |
| 1090.1909 | 1134.6450 | 1193.1542 |
| 1221.0318 | 1289.9342 | 1304.0250 |
| 1371.6928 | 1376.0359 | 1395.9048 |
| 1427.3638 | 1467.4174 | 1472.7329 |
| 1506.5534 | 1512.1389 | 1815.6060 |
| 2895.6194 | 2958.6036 | 3022.3620 |
| 3033.3430 | 3058.3411 | 3063.0819 |
| 3116.3253 | 3132.8715 | 3145.6326 |

Zero-point correction (Hartree): 0.132130

C5H9O2.ppchmhh

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.32770694

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 2.032604 | -0.896821 | -0.873310 |
| C | 2.007524 | -0.297984 | 0.358167 |
| C | 1.036366 | 0.884232 | 0.493331 |
| C | -0.398570 | 0.629942 | 0.022499 |
| C | -1.018336 | -0.728468 | 0.317667 |
| C | -2.513901 | -0.792030 | 0.015261 |
| H | -2.903684 | -1.796820 | 0.202145 |
| O | -1.016608 | 1.509021 | -0.546043 |
| H | 1.724292 | -1.119682 | 1.051247 |
| H | 3.025644 | -0.015820 | 0.684888 |
| H | 0.991924 | 1.183055 | 1.550995 |
| H | 1.408749 | 1.747840 | -0.065023 |
| H | -0.466277 | -1.463996 | -0.284041 |
| H | -0.808900 | -0.990875 | 1.365143 |
| H | -3.071101 | -0.084496 | 0.635704 |
| H | -2.707117 | -0.530957 | -1.027786 |

Rotational constants (GHz): 4.2081700 1.6517200 1.3797400

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 48.0585 | 82.9080 | 119.0081 |
| 191.6362 | 200.1002 | 266.3055 |
| 363.7474 | 459.4162 | 540.9713 |
| 559.6438 | 664.9081 | 749.0744 |
| 772.0372 | 887.3297 | 961.7105 |
| 1000.1628 | 1041.4188 | 1085.3443 |
| 1090.1878 | 1134.6361 | 1193.1568 |
| 1221.0250 | 1289.9196 | 1304.0036 |
| 1371.6893 | 1376.0188 | 1395.8925 |
| 1427.3615 | 1467.4312 | 1472.7316 |
| 1506.5590 | 1512.1392 | 1815.5975 |
| 2895.6180 | 2958.6149 | 3022.4169 |
| 3033.3325 | 3058.3833 | 3063.0744 |
| 3116.3305 | 3132.8376 | 3145.6502 |

Zero-point correction (Hartree): 0.132130

C5H9O2.ppchpch

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.32474265
 Electronic state : 2-A
 Cartesian coordinates (Angs):
 O 2.095799 -0.367824 -0.930276
 C 1.687774 -0.587775 0.358014
 C 0.702113 0.449672 0.918533
 C -0.474333 0.791748 -0.000769
 C -1.225558 -0.345072 -0.682457
 C -1.857449 -1.348963 0.297696
 H -2.418431 -2.112027 -0.249552
 O -0.806707 1.950985 -0.155111
 H 1.218515 -1.595055 0.321182
 H 2.551914 -0.722464 1.034840
 H 0.304408 0.079572 1.874030
 H 1.220551 1.389151 1.128561
 H -1.995564 0.118775 -1.304368
 H -0.528664 -0.863632 -1.353346
 H -1.108164 -1.867752 0.905543
 H -2.552584 -0.849506 0.980103
 Rotational constants (GHz): 3.2059400 1.9827200 1.5542900
 Vibrational harmonic frequencies (cm-1):
 56.3544 82.8594 116.0556
 203.5531 217.1439 264.4116
 375.9892 498.2214 543.4728
 574.3752 661.9538 727.4589
 813.5449 890.9877 967.6351
 974.6641 1039.9872 1080.9211
 1087.4255 1145.2895 1215.4183
 1226.4039 1289.5534 1298.6315
 1347.5118 1374.5974 1390.0267
 1426.2060 1471.2693 1498.1465
 1514.3895 1519.1249 1814.7589
 2894.1410 2958.4953 3040.0857
 3048.9541 3053.6584 3107.3672
 3119.9499 3126.9537 3128.7154
 Zero-point correction (Hartree): 0.132559

C5H9O2.ppchphc

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.32770693
 Electronic state : 2-A
 Cartesian coordinates (Angs):
 O 2.033558 -0.897550 -0.872560
 C 2.007465 -0.297398 0.358237
 C 1.036254 0.884889 0.491999
 C -0.399028 0.630132 0.022273
 C -1.018078 -0.728456 0.317939
 C -2.513543 -0.793067 0.014982
 H -2.902848 -1.797868 0.202782
 O -1.017853 1.509243 -0.545345
 H 1.724911 -1.118240 1.052550
 H 3.025584 -0.014618 0.684635
 H 0.992246 1.185204 1.549270
 H 1.408229 1.747798 -0.067680
 H -0.465338 -1.464309 -0.282630
 H -0.808985 -0.989702 1.365837
 H -3.071374 -0.085117 0.634346
 H -2.706482 -0.533295 -1.028454
 Rotational constants (GHz): 4.2074200 1.6516100 1.3792200
 Vibrational harmonic frequencies (cm-1):
 47.9273 82.9938 118.8823
 191.7251 199.9224 266.3247
 363.7313 459.4602 541.0107
 558.5423 662.0649 749.0865
 771.6656 887.1746 961.6865
 1000.0201 1040.9491 1085.3336
 1090.3200 1134.5576 1193.1555
 1221.2364 1290.1007 1304.5609
 1371.4446 1376.1172 1395.9685
 1427.3486 1467.3528 1472.6790
 1506.5378 1512.1157 1815.6292
 2895.9564 2957.9543 3022.1809
 3033.2611 3058.6516 3063.1294
 3116.4359 3132.9839 3145.5726
 Zero-point correction (Hartree): 0.132119

C5H9O2.ppchphh

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.32474264
 Electronic state : 2-A
 Cartesian coordinates (Angs):
 O 2.098365 -0.364352 -0.929533
 C 1.685235 -0.594387 0.355405

| | | | |
|--|-----------|-----------|-----------|
| C | 0.701089 | 0.441622 | 0.921454 |
| C | -0.472416 | 0.792434 | 0.001805 |
| C | -1.229494 | -0.338813 | -0.682733 |
| C | -1.861606 | -1.346397 | 0.293311 |
| H | -2.419445 | -2.109423 | -0.257182 |
| O | -0.797160 | 1.953915 | -0.151751 |
| H | 1.212040 | -1.599351 | 0.307211 |
| H | 2.546190 | -0.738401 | 1.034293 |
| H | 0.301025 | 0.065762 | 1.873703 |
| H | 1.221511 | 1.378394 | 1.138487 |
| H | -1.999631 | 0.130503 | -1.300388 |
| H | -0.535795 | -0.855670 | -1.358389 |
| H | -1.112790 | -1.864933 | 0.901935 |
| H | -2.559591 | -0.850144 | 0.975148 |
| Rotational constants (GHz): | 3.2061400 | 1.9820500 | 1.5537400 |
| Vibrational harmonic frequencies (cm-1): | | | |
| 55.9538 | 83.1100 | | 115.4354 |
| 203.6154 | 216.6209 | | 264.7439 |
| 376.3591 | 498.3770 | | 542.6450 |
| 575.2522 | 664.3183 | | 728.2389 |
| 813.4799 | 890.8651 | | 967.7844 |
| 975.1533 | 1040.6448 | | 1080.8408 |
| 1087.1837 | 1145.2767 | | 1215.0575 |
| 1226.6407 | 1289.3513 | | 1298.2150 |
| 1347.6297 | 1374.9658 | | 1389.8801 |
| 1426.2305 | 1471.1657 | | 1497.9654 |
| 1514.2996 | 1519.1290 | | 1814.8889 |
| 2894.3210 | 2958.9575 | | 3039.8274 |
| 3048.9927 | 3052.9531 | | 3107.3402 |
| 3120.0831 | 3126.9285 | | 3128.5964 |
| Zero-point correction (Hartree): | 0.132565 | | |

C5H9O2.pphcmch

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.32818379

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|--|-----------|-----------|-----------|
| O | 2.546836 | -0.189821 | 0.834164 |
| C | 1.995476 | -0.371274 | -0.402189 |
| C | 0.502204 | -0.727610 | -0.378826 |
| C | -0.371687 | 0.491355 | -0.071352 |
| C | -1.698199 | 0.254571 | 0.631254 |
| C | -2.630669 | -0.716288 | -0.114251 |
| H | -3.570861 | -0.832647 | 0.432257 |
| O | -0.010444 | 1.606585 | -0.400753 |
| H | 2.101621 | 0.612512 | -0.908595 |
| H | 2.587952 | -1.082150 | -1.006473 |
| H | 0.197535 | -1.106128 | -1.365375 |
| H | 0.318083 | -1.536556 | 0.336117 |
| H | -1.476260 | -0.149270 | 1.629107 |
| H | -2.175230 | 1.229348 | 0.763787 |
| H | -2.870897 | -0.343191 | -1.115006 |
| H | -2.185824 | -1.710546 | -0.220925 |
| Rotational constants (GHz): | 5.0188600 | 1.4502400 | 1.3027700 |
| Vibrational harmonic frequencies (cm-1): | | | |
| 48.8923 | 62.3684 | | 92.2548 |
| 202.3038 | 227.8652 | | 257.6582 |
| 379.7039 | 452.7700 | | 528.9286 |
| 607.7625 | 681.0359 | | 791.0054 |
| 826.7736 | 892.2956 | | 944.5224 |
| 984.9079 | 1047.7575 | | 1075.6285 |
| 1095.1304 | 1159.3706 | | 1200.0475 |
| 1204.7423 | 1284.0458 | | 1322.1651 |
| 1344.7835 | 1380.1172 | | 1385.0062 |
| 1425.9925 | 1461.9574 | | 1484.8746 |
| 1516.5560 | 1519.8279 | | 1807.5328 |
| 2899.7822 | 2965.4408 | | 3034.1884 |
| 3036.0691 | 3053.5657 | | 3097.5319 |
| 3111.1188 | 3127.8083 | | 3132.0391 |
| Zero-point correction (Hartree): | 0.132485 | | |

C5H9O2.pphcmh

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.33089875

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 2.453262 | 0.153384 | 1.055839 |
| C | 2.167388 | 0.021493 | -0.273666 |
| C | 0.882700 | -0.766247 | -0.565564 |
| C | -0.375196 | 0.051655 | -0.266584 |
| C | -1.602315 | -0.714843 | 0.194591 |
| C | -2.862423 | 0.140046 | 0.302165 |
| C | -3.703964 | -0.454762 | 0.668697 |
| O | -0.379349 | 1.259653 | -0.417736 |
| H | 2.019833 | 1.061322 | -0.637636 |

| | | | | |
|---|-----------|-----------|-----------|-----------|
| H | 3.036110 | -0.367916 | -0.835112 | |
| H | 0.845245 | -1.029264 | -1.632970 | |
| H | 0.881684 | -1.710037 | -0.009913 | |
| H | -1.747119 | -1.568132 | -0.483563 | |
| H | -1.344821 | -1.166564 | 1.164333 | |
| H | -2.704220 | 0.977927 | 0.985547 | |
| H | -3.134980 | 0.560503 | -0.669859 | |
| Rotational constants (GHz): | 5.9826500 | | 1.3277300 | 1.2771700 |
| Vibrational harmonic frequencies (cm ⁻¹): | | | | |
| 38.4490 | 81.1119 | | | 102.3581 |
| 194.4961 | 206.0981 | | | 280.4785 |
| 360.1099 | 461.8452 | | | 473.0791 |
| 605.2788 | 712.6040 | | | 740.1800 |
| 841.5577 | 890.8973 | | | 961.3035 |
| 1001.5118 | 1046.7591 | | | 1078.7565 |
| 1093.9194 | 1132.3740 | | | 1169.4141 |
| 1204.5557 | 1286.9495 | | | 1321.0894 |
| 1365.6307 | 1381.2642 | | | 1398.2577 |
| 1429.1155 | 1462.4293 | | | 1465.6619 |
| 1507.5344 | 1513.3054 | | | 1809.1967 |
| 2900.8332 | 2965.5403 | | | 3022.1583 |
| 3033.2146 | 3051.3221 | | | 3063.3515 |
| 3098.3121 | 3133.9737 | | | 3143.7014 |
| Zero-point correction (Hartree): | 0.132202 | | | |

C5H9O2.pphcmhh

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.33089873
Electronic state : 2-A
Cartesian coordinates (Angs):

| | | | | |
|---|-----------|-----------|-----------|-----------|
| O | 2.453049 | 0.152605 | 1.056161 | |
| C | 2.167395 | 0.021727 | -0.273437 | |
| C | 0.882772 | -0.765768 | -0.566219 | |
| C | -0.375186 | 0.051811 | -0.266745 | |
| C | -1.602199 | -0.714899 | 0.194261 | |
| C | -2.862395 | 0.139747 | 0.302430 | |
| H | -3.703915 | -0.455468 | 0.668360 | |
| O | -0.379444 | 1.259878 | -0.417420 | |
| H | 2.020091 | 1.061872 | -0.636651 | |
| H | 3.036211 | -0.367180 | -0.835157 | |
| H | 0.845525 | -1.027965 | -1.633815 | |
| H | 0.881808 | -1.709955 | -0.011226 | |
| H | -1.746946 | -1.567892 | -0.484306 | |
| H | -1.344634 | -1.167119 | 1.163740 | |
| H | -2.704396 | 0.977042 | 0.986600 | |
| H | -3.134906 | 0.561088 | -0.669221 | |
| Rotational constants (GHz): | 5.9818200 | | 1.3277300 | 1.2772500 |
| Vibrational harmonic frequencies (cm ⁻¹): | | | | |
| 38.3591 | 81.0519 | | | 102.3255 |
| 194.4541 | 206.0848 | | | 280.4450 |
| 360.1050 | 461.8140 | | | 473.0978 |
| 605.3274 | 712.6722 | | | 740.1926 |
| 841.6124 | 890.9136 | | | 961.3273 |
| 1001.5375 | 1046.8275 | | | 1078.7929 |
| 1094.0185 | 1132.4021 | | | 1169.4059 |
| 1204.5972 | 1286.9764 | | | 1321.1785 |
| 1365.6846 | 1381.2622 | | | 1398.3210 |
| 1429.1389 | 1462.4265 | | | 1465.6582 |
| 1507.5234 | 1513.3103 | | | 1809.1581 |
| 2900.6884 | 2965.1812 | | | 3022.1652 |
| 3033.3575 | 3051.2424 | | | 3063.3215 |
| 3098.2656 | 3133.9769 | | | 3143.5802 |
| Zero-point correction (Hartree): | 0.132202 | | | |

C5H9O2.pphcpch

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.32735441
Electronic state : 2-A
Cartesian coordinates (Angs):

| | | | | |
|---|-----------|-----------|-----------|--|
| O | 2.447605 | -0.012032 | 0.813867 | |
| C | 1.983829 | -0.459609 | -0.392130 | |
| C | 0.487731 | -0.786938 | -0.406548 | |
| C | -0.358467 | 0.469388 | -0.205140 | |
| C | -1.867078 | 0.345448 | -0.385411 | |
| C | -2.526920 | -0.693663 | 0.537473 | |
| H | -3.611725 | -0.687087 | 0.397409 | |
| O | 0.162496 | 1.530022 | 0.083013 | |
| H | 2.254331 | 0.225633 | -1.214325 | |
| H | 2.557379 | -1.390900 | -0.585950 | |
| H | 0.194335 | -1.285189 | -1.340735 | |
| H | 0.261129 | -1.489261 | 0.405632 | |
| H | -2.289550 | 1.339261 | -0.214712 | |
| H | -2.061933 | 0.076069 | -1.433033 | |
| H | -2.174148 | -1.708634 | 0.331079 | |
| H | -2.325204 | -0.471563 | 1.590137 | |


```

Rotational constants (GHz):    5.201000    1.4883400    1.3332400
Vibrational harmonic frequencies (cm-1):
  20.3248                54.1882                100.0472
 205.3911                221.6386                259.5618
 369.3310                445.0052                515.3870
 635.3903                711.8454                781.7458
 862.2583                883.4868                959.5636
 987.7239                1045.2274               1073.9078
1101.6615                1162.4529               1193.1671
1212.3561                1286.2890               1341.5072
1361.6583                1376.6546               1393.3956
1426.6967                1448.5366               1485.6324
1516.0344                1518.6941               1806.9156
2906.1602                2981.8382               3032.7835
3041.0307                3054.0246               3083.8611
3111.0744                3127.6850               3132.5098
Zero-point correction (Hartree): 0.132668
  
```

C5H9O2.pphcphc

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.33089865

Electronic state : 2-A

Cartesian coordinates (Angs):

```

O      2.453424      0.153463      1.055843
C      2.167471      0.021406     -0.273839
C      0.882864     -0.766216     -0.565396
C     -0.375280      0.051765     -0.266649
C     -1.602379     -0.714772      0.194386
C     -2.862592      0.139907      0.302275
H     -3.704108     -0.455180      0.668410
O     -0.379509      1.259750     -0.417758
H      2.020436      1.061296     -0.637874
H      3.036353     -0.368168     -0.834935
H      0.845158     -1.030196     -1.632550
H      0.881877     -1.709587     -0.009043
H     -1.747129     -1.568020     -0.483871
H     -1.344747     -1.166716      1.163986
H     -2.704623      0.977472      0.986098
H     -3.135050      0.560864     -0.669564
  
```

```

Rotational constants (GHz):    5.9826100    1.3275800    1.2770200
Vibrational harmonic frequencies (cm-1):
  38.5106                81.1697                102.5139
 194.4724                206.0373                280.4579
 360.0730                461.8987                472.9838
 605.1335                712.4361                740.1527
 841.3762                890.8579                961.3107
1001.5015                1046.6715               1078.8148
1093.5330                1132.3330               1169.4022
1204.7026                1287.0101               1321.4495
1365.6941                1381.1743               1398.2342
1429.1212                1462.4187               1465.6832
1507.5143                1513.3116               1809.2818
2900.8485                2965.5025               3022.1031
3033.2907                3051.1642               3063.3491
3098.3119                3133.9749               3143.6741
Zero-point correction (Hartree): 0.132201
  
```

C5H9O2.pphcphh

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.32858540

Electronic state : 2-A

Cartesian coordinates (Angs):

```

O      1.881512      1.211616     -0.521737
C      1.977394      0.021451      0.143675
C      0.724811     -0.344293      0.952949
C     -0.434725     -0.745447      0.036890
C     -1.814371     -0.205781      0.365196
C     -1.964827      1.230238     -0.177938
H     -2.934758      1.646948      0.107778
O     -0.230396     -1.454003     -0.932215
H      2.105052     -0.744473     -0.651752
H      2.901138     -0.025595      0.748559
H      0.941405     -1.211417      1.592874
H      0.450069      0.482594      1.615248
H     -2.557820     -0.863353     -0.093754
H     -1.965535     -0.208881      1.451816
H     -1.181797      1.891814      0.205482
H     -1.896372      1.234453     -1.269258
  
```

```

Rotational constants (GHz):    3.7275800    1.8135400    1.5225700
Vibrational harmonic frequencies (cm-1):
  34.3540                62.0980                107.4934
 195.8721                229.9370                248.7519
 363.0864                460.1436                568.7252
 600.5555                681.1367                801.0839
 843.4866                896.4158                946.4918
  
```

| | | |
|-----------|-----------|-----------|
| 988.4254 | 1043.9879 | 1074.3534 |
| 1088.4641 | 1152.0887 | 1192.0254 |
| 1204.3335 | 1282.1389 | 1318.3295 |
| 1340.4569 | 1381.0343 | 1385.3686 |
| 1424.9237 | 1471.3544 | 1492.4735 |
| 1510.4895 | 1519.8240 | 1808.6022 |
| 2901.0754 | 2967.0193 | 3039.6701 |
| 3048.9053 | 3056.9641 | 3105.5027 |
| 3114.0202 | 3132.8232 | 3138.9375 |

Zero-point correction (Hartree): 0.132642

C5H9O2.pphmch

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.33089875

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 2.453536 | 0.153038 | 1.055789 |
| C | 2.167353 | 0.021670 | -0.273667 |
| C | 0.882678 | -0.766137 | -0.565641 |
| C | -0.375250 | 0.051689 | -0.266587 |
| C | -1.602378 | -0.714887 | 0.194405 |
| C | -2.862463 | 0.140003 | 0.302262 |
| H | -3.703920 | -0.454792 | 0.669001 |
| O | -0.379398 | 1.259732 | -0.417495 |
| H | 2.019553 | 1.061617 | -0.637248 |
| H | 3.035990 | -0.367382 | -0.835503 |
| H | 0.845313 | -1.029071 | -1.633062 |
| H | 0.881725 | -1.709948 | -0.010032 |
| H | -1.747206 | -1.567995 | -0.483987 |
| H | -1.344879 | -1.166951 | 1.163984 |
| H | -2.704079 | 0.977907 | 0.985574 |
| H | -3.135240 | 0.560425 | -0.669714 |

Rotational constants (GHz): 5.9829000 1.3276500 1.2770900

Vibrational harmonic frequencies (cm-1):

| | | |
|----------|----------|----------|
| 38.4497 | 81.1041 | 102.3286 |
| 194.5313 | 206.0984 | 280.5080 |
| 360.1089 | 461.8373 | 473.0759 |
| 605.2730 | 712.5819 | 740.1645 |

| | | |
|-----------|-----------|-----------|
| 841.5535 | 890.8601 | 961.3051 |
| 1001.5157 | 1046.7793 | 1078.7408 |
| 1093.9762 | 1132.3795 | 1169.4094 |
| 1204.5105 | 1286.9448 | 1321.0790 |
| 1365.6236 | 1381.2735 | 1398.2524 |
| 1429.1122 | 1462.4179 | 1465.6582 |
| 1507.5332 | 1513.3087 | 1809.1148 |
| 2900.6841 | 2965.4630 | 3022.1534 |
| 3033.2865 | 3051.2653 | 3063.3627 |
| 3098.3537 | 3133.9912 | 3143.7115 |

Zero-point correction (Hartree): 0.132201

C5H9O2.pphmhc

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.32770699

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 2.033011 | -0.897784 | -0.872317 |
| C | 2.007514 | -0.297339 | 0.358382 |
| C | 1.036367 | 0.885066 | 0.491687 |
| C | -0.398952 | 0.630218 | 0.022237 |
| C | -1.017747 | -0.728617 | 0.317333 |
| C | -2.513377 | -0.793071 | 0.015490 |
| H | -2.902338 | -1.798251 | 0.201993 |
| O | -1.017997 | 1.509348 | -0.545147 |
| H | 1.724083 | -1.118116 | 1.052467 |
| H | 3.025546 | -0.014739 | 0.685009 |
| H | 0.992454 | 1.186049 | 1.548761 |
| H | 1.408525 | 1.747603 | -0.068479 |
| H | -0.465390 | -1.463694 | -0.284652 |
| H | -0.807760 | -0.991032 | 1.364710 |
| H | -3.070875 | -0.086262 | 0.636481 |
| H | -2.707186 | -0.531613 | -1.027353 |

Rotational constants (GHz): 4.2074000 1.6519900 1.3793300

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 47.9853 | 83.0449 | 119.1157 |
| 191.7914 | 200.0505 | 266.3309 |
| 363.6514 | 459.4977 | 540.9869 |
| 559.3832 | 664.5653 | 749.0588 |
| 771.9346 | 887.2964 | 961.7054 |
| 1000.1924 | 1041.4147 | 1085.3648 |
| 1090.1663 | 1134.6633 | 1193.1086 |
| 1221.0596 | 1289.9316 | 1304.1099 |
| 1371.6952 | 1376.0508 | 1395.8898 |
| 1427.3679 | 1467.3564 | 1472.7099 |
| 1506.5479 | 1512.1423 | 1815.5386 |

| | | |
|-----------|-----------|-----------|
| 2895.6560 | 2958.5846 | 3022.3380 |
| 3033.3445 | 3058.3631 | 3063.0806 |
| 3116.2657 | 3132.8684 | 3145.6252 |

Zero-point correction (Hartree): 0.132129

C5H9O2.pphmhh

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.32770694

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 2.032870 | -0.896760 | -0.873274 |
| C | 2.007506 | -0.297971 | 0.358214 |
| C | 1.036312 | 0.884249 | 0.493241 |
| C | -0.398649 | 0.629962 | 0.022486 |
| C | -1.018334 | -0.728471 | 0.317636 |
| C | -2.513890 | -0.792162 | 0.015215 |
| H | -2.903594 | -1.796951 | 0.202269 |
| O | -1.016734 | 1.509078 | -0.545950 |
| H | 1.724026 | -1.119704 | 1.051156 |
| H | 3.025531 | -0.015832 | 0.685245 |
| H | 0.991909 | 1.183159 | 1.550879 |
| H | 1.408700 | 1.747801 | -0.065197 |
| H | -0.466206 | -1.463983 | -0.284032 |
| H | -0.808877 | -0.990826 | 1.365130 |
| H | -3.071164 | -0.084538 | 0.635478 |
| H | -2.707086 | -0.531312 | -1.027892 |

Rotational constants (GHz): 4.2081300 1.6516500 1.3796600

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 48.0433 | 82.9288 | 118.9840 |
| 191.6535 | 200.0452 | 266.2994 |
| 363.7346 | 459.4227 | 540.9655 |
| 559.6791 | 665.0879 | 749.0809 |
| 772.0562 | 887.3163 | 961.7158 |
| 1000.1790 | 1041.4675 | 1085.3502 |
| 1090.1771 | 1134.6469 | 1193.1618 |
| 1220.9982 | 1289.9074 | 1303.9633 |
| 1371.7180 | 1376.0190 | 1395.8986 |
| 1427.3580 | 1467.4186 | 1472.7350 |
| 1506.5523 | 1512.1380 | 1815.5936 |
| 2895.5868 | 2958.6323 | 3022.3631 |
| 3033.3532 | 3058.3557 | 3063.0880 |
| 3116.3357 | 3132.8775 | 3145.6478 |

Zero-point correction (Hartree): 0.132130

C5H9O2.pphhphc

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.32770697

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 2.032835 | -0.897034 | -0.873068 |
| C | 2.007531 | -0.297840 | 0.358241 |
| C | 1.036356 | 0.884448 | 0.492827 |
| C | -0.398727 | 0.630064 | 0.022488 |
| C | -1.018206 | -0.728458 | 0.317680 |
| C | -2.513727 | -0.792401 | 0.015227 |
| H | -2.903531 | -1.796939 | 0.203443 |
| O | -1.017049 | 1.509137 | -0.545754 |
| H | 1.723993 | -1.119300 | 1.051458 |
| H | 3.025551 | -0.015581 | 0.685142 |
| H | 0.992134 | 1.183912 | 1.550320 |
| H | 1.408699 | 1.747711 | -0.066097 |
| H | -0.465892 | -1.463829 | -0.284013 |
| H | -0.808710 | -0.990880 | 1.365143 |
| H | -3.070985 | -0.083989 | 0.634601 |
| H | -2.706917 | -0.532804 | -1.028199 |

Rotational constants (GHz): 4.2079000 1.6517500 1.3795900

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 48.0269 | 82.9420 | 119.0280 |
| 191.6771 | 199.9958 | 266.2771 |
| 363.6994 | 459.4381 | 540.9615 |
| 559.6444 | 665.0592 | 749.0718 |
| 772.0429 | 887.3083 | 961.7136 |
| 1000.1964 | 1041.4790 | 1085.3430 |
| 1090.1410 | 1134.6581 | 1193.1436 |
| 1220.9910 | 1289.8922 | 1303.9363 |
| 1371.7343 | 1376.0207 | 1395.8861 |
| 1427.3827 | 1467.4105 | 1472.7463 |
| 1506.5475 | 1512.1281 | 1815.5955 |
| 2895.7336 | 2958.7651 | 3022.3739 |
| 3033.3154 | 3058.2783 | 3063.0689 |
| 3116.2900 | 3132.8649 | 3145.5903 |

Zero-point correction (Hartree): 0.132130

C5H9O2.pphhphh

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.32770691
Electronic state : 2-A
Cartesian coordinates (Angs):
O 2.032697 -0.896458 -0.873537
C 2.007440 -0.298213 0.358204
C 1.036280 0.884062 0.493702
C -0.398538 0.629942 0.022516
C -1.018382 -0.728453 0.317519
C -2.513974 -0.791956 0.015290
H -2.903784 -1.796679 0.202467
O -1.016396 1.509067 -0.546154
H 1.723810 -1.120143 1.050806
H 3.025476 -0.016275 0.685380
H 0.991775 1.182368 1.551497
H 1.408828 1.747831 -0.064283
H -0.466408 -1.463881 -0.284414
H -0.808760 -0.991023 1.364928
H -3.071027 -0.084180 0.635572
H -2.707277 -0.531180 -1.027813
Rotational constants (GHz): 4.2081700 1.6516800 1.3798000
Vibrational harmonic frequencies (cm-1):
48.0377 82.9229 118.9709
191.6201 200.0178 266.2668
363.7290 459.4062 540.9500
559.7438 665.1818 749.0863
772.0924 887.3173 961.6915
1000.2046 1041.5040 1085.3373
1090.1705 1134.6411 1193.1612
1220.9203 1289.8804 1303.8355
1371.7409 1376.0083 1395.8965
1427.3442 1467.4184 1472.7512
1506.5496 1512.1356 1815.6097
2895.8239 2958.6376 3022.3159
3033.4180 3058.2704 3063.0977
3116.3978 3132.9041 3145.6653
Zero-point correction (Hartree): 0.132131

C5H9O2.tpchmch

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.32952849
Electronic state : 2-A
Cartesian coordinates (Angs):
O 3.089112 -0.515770 0.017885
C 1.904842 0.026626 -0.380005
C 0.678905 -0.458982 0.405638
C -0.519792 0.466381 0.241710
C -1.888283 -0.083747 0.615378
C -2.552667 -0.767149 -0.595959
H -3.540271 -1.149911 -0.323627
O -0.384332 1.600408 -0.183998
H 2.000780 1.122712 -0.213252
H 1.750823 -0.059680 -1.471598
H 0.411303 -1.486219 0.129617
H 0.932136 -0.491849 1.474792
H -1.793763 -0.799731 1.440343
H -2.503946 0.755784 0.951019
H -2.676155 -0.056371 -1.418009
H -1.957174 -1.610613 -0.960952
Rotational constants (GHz): 5.5946400 1.2837300 1.1604500
Vibrational harmonic frequencies (cm-1):
51.1865 72.0922 82.6729
180.6860 229.3917 241.3251
359.0395 423.1558 560.9097
586.3350 715.4190 803.3475
843.7052 922.6261 954.3752
1009.6020 1039.0198 1068.7505
1103.6157 1134.9967 1171.0982
1206.7492 1285.9713 1324.7556
1350.5243 1360.4822 1380.5998
1422.5107 1462.9878 1494.0298
1513.8609 1521.3095 1799.2042
2887.6808 2959.9496 3040.1083
3053.0676 3055.6029 3083.4953
3111.0415 3128.8546 3137.4803
Zero-point correction (Hartree): 0.132438

C5H9O2.tpchmhc

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.33179766
Electronic state : 2-A
Cartesian coordinates (Angs):
O -3.252776 -0.205968 -0.151937
C -2.040082 0.262513 0.253190
C -0.851250 -0.645568 -0.094587
C 0.479919 0.094860 -0.025560

| | | | |
|---|-----------|-----------|-----------|
| C | 1.736251 | -0.752885 | 0.099818 |
| C | 3.032996 | 0.042326 | -0.032635 |
| H | 3.901177 | -0.610396 | 0.095446 |
| O | 0.521656 | 1.311278 | -0.084499 |
| H | -1.893214 | 1.228352 | -0.279632 |
| H | -2.038370 | 0.548076 | 1.321561 |
| H | -0.832653 | -1.536966 | 0.543554 |
| H | -0.978857 | -1.010533 | -1.123227 |
| H | 1.683011 | -1.262303 | 1.073593 |
| H | 1.678634 | -1.560463 | -0.643465 |
| H | 3.101938 | 0.518274 | -1.014686 |
| H | 3.080288 | 0.836004 | 0.716995 |
| Rotational constants (GHz): | 8.4936300 | 1.1516600 | 1.0479700 |
| Vibrational harmonic frequencies (cm ⁻¹): | | | |
| 48.2778 | 77.8840 | | 86.0192 |
| 162.1038 | 206.3582 | | 281.7931 |
| 338.7749 | 427.5023 | | 475.9764 |
| 646.7963 | 705.8027 | | 758.6644 |
| 835.0461 | 918.4503 | | 976.3735 |
| 1012.0128 | 1045.5404 | | 1066.4718 |
| 1102.7905 | 1130.9625 | | 1154.1847 |
| 1195.1898 | 1287.2847 | | 1329.5457 |
| 1350.4894 | 1378.1528 | | 1389.8185 |
| 1428.2685 | 1461.9766 | | 1468.9840 |
| 1507.7157 | 1512.6092 | | 1799.5133 |
| 2887.9367 | 2959.1937 | | 3023.7611 |
| 3043.5827 | 3054.5556 | | 3063.7184 |
| 3088.4707 | 3135.1356 | | 3143.3206 |
| Zero-point correction (Hartree): | 0.132059 | | |

C5H9O2.tpchmhh

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.33179763
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -3.252949 | -0.206707 | -0.151222 |
| C | -2.040153 | 0.263127 | 0.252294 |
| C | -0.851283 | -0.645225 | -0.094440 |
| C | 0.479985 | 0.094936 | -0.025457 |
| C | 1.736199 | -0.753055 | 0.099660 |
| C | 3.033027 | 0.042080 | -0.032505 |
| H | 3.901162 | -0.610770 | 0.095261 |
| O | 0.522000 | 1.311368 | -0.084343 |
| H | -1.894295 | 1.228151 | -0.282158 |
| H | -2.038041 | 0.550528 | 1.320155 |
| H | -0.833267 | -1.536111 | 0.544446 |
| H | -0.978494 | -1.010956 | -1.122850 |
| H | 1.682959 | -1.262879 | 1.073203 |
| H | 1.678533 | -1.560318 | -0.643961 |
| H | 3.101962 | 0.518446 | -1.014349 |
| H | 3.080422 | 0.835441 | 0.717457 |
| Rotational constants (GHz): | 8.4938200 | 1.1516000 | 1.0478700 |
| Vibrational harmonic frequencies (cm ⁻¹): | | | |
| 48.2322 | 77.5310 | | 86.0024 |
| 161.9845 | 206.3450 | | 281.7915 |
| 338.7536 | 427.4698 | | 475.9574 |
| 646.7589 | 705.5383 | | 758.5001 |
| 835.0587 | 918.0907 | | 976.4296 |
| 1012.0236 | 1045.4119 | | 1066.5133 |
| 1102.5498 | 1130.9531 | | 1154.1662 |
| 1195.3947 | 1287.2806 | | 1329.4975 |
| 1350.6291 | 1378.0293 | | 1389.8361 |
| 1428.2667 | 1461.9570 | | 1468.9770 |
| 1507.7126 | 1512.6038 | | 1799.4029 |
| 2888.5197 | 2959.3447 | | 3023.8655 |
| 3043.5979 | 3054.5918 | | 3063.7121 |
| 3088.4325 | 3135.1380 | | 3143.3094 |
| Zero-point correction (Hartree): | 0.132057 | | |

C5H9O2.tpchpch

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.32930660
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -2.978662 | -0.743808 | -0.145110 |
| C | -1.973399 | 0.122328 | 0.158936 |
| C | -0.565966 | -0.492706 | 0.135539 |
| C | 0.521348 | 0.573203 | 0.043749 |
| C | 1.936816 | 0.184449 | 0.444581 |
| C | 2.487637 | -1.040104 | -0.305859 |
| H | 3.513652 | -1.246861 | 0.011410 |
| O | 0.254986 | 1.697639 | -0.344378 |
| H | -2.006417 | 0.915102 | -0.621387 |
| H | -2.164296 | 0.671684 | 1.099480 |
| H | -0.401697 | -1.139906 | 1.005308 |

| | | | | |
|--|-----------|-----------|-----------|--|
| H | -0.485930 | -1.142513 | -0.746407 | |
| H | 2.569658 | 1.061112 | 0.281991 | |
| H | 1.930135 | -0.025233 | 1.523731 | |
| H | 1.894360 | -1.938985 | -0.113095 | |
| H | 2.501324 | -0.868065 | -1.386802 | |
| Rotational constants (GHz): | 5.0606900 | 1.3598100 | 1.1383900 | |
| Vibrational harmonic frequencies (cm-1): | | | | |
| 56.1800 | 68.2020 | | 87.3829 | |
| 167.0390 | 224.3187 | | 259.1016 | |
| 371.3830 | 421.7577 | | 534.7471 | |
| 606.3236 | 713.2142 | | 789.0128 | |
| 819.7628 | 918.4909 | | 955.4525 | |
| 1012.7400 | 1045.3758 | | 1066.2014 | |
| 1104.9950 | 1145.8196 | | 1178.7984 | |
| 1205.2982 | 1284.6676 | | 1336.4265 | |
| 1345.8831 | 1356.7586 | | 1380.2617 | |
| 1426.8689 | 1466.2880 | | 1484.1775 | |
| 1516.3736 | 1519.0853 | | 1796.5254 | |
| 2886.6256 | 2959.6775 | | 3032.1672 | |
| 3046.2747 | 3054.8071 | | 3088.6695 | |
| 3111.1280 | 3128.4253 | | 3133.2562 | |
| Zero-point correction (Hartree): | 0.132375 | | | |

C5H9O2.tpchphc

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.33179767
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | | |
|--|-----------|-----------|-----------|--|
| O | -3.252786 | -0.205903 | -0.152235 | |
| C | -2.040139 | 0.262538 | 0.253094 | |
| C | -0.851263 | -0.645663 | -0.094044 | |
| C | 0.479929 | 0.094794 | -0.025442 | |
| C | 1.736330 | -0.752901 | 0.099517 | |
| C | 3.033012 | 0.042444 | -0.032660 | |
| H | 3.901244 | -0.610402 | 0.094429 | |
| O | 0.521633 | 1.311218 | -0.084427 | |
| H | -1.893048 | 1.228318 | -0.279807 | |
| H | -2.038834 | 0.548376 | 1.321401 | |
| H | -0.832630 | -1.536691 | 0.544591 | |
| H | -0.978817 | -1.011196 | -1.122497 | |
| H | 1.683221 | -1.262809 | 1.073043 | |
| H | 1.678718 | -1.560137 | -0.644144 | |
| H | 3.101531 | 0.519377 | -1.014258 | |
| H | 3.080629 | 0.835380 | 0.717740 | |
| Rotational constants (GHz): | 8.4939800 | 1.1516300 | 1.0479400 | |
| Vibrational harmonic frequencies (cm-1): | | | | |
| 48.2611 | 77.7167 | | 85.9880 | |
| 162.0777 | 206.3071 | | 281.8063 | |
| 338.7969 | 427.5168 | | 475.9594 | |
| 646.7640 | 705.7124 | | 758.6209 | |
| 835.0869 | 918.2718 | | 976.4119 | |
| 1012.0374 | 1045.4970 | | 1066.5410 | |
| 1102.7790 | 1130.9870 | | 1154.1861 | |
| 1195.2933 | 1287.3063 | | 1329.5443 | |
| 1350.5807 | 1378.1155 | | 1389.8234 | |
| 1428.2705 | 1461.9605 | | 1468.9757 | |
| 1507.7048 | 1512.5994 | | 1799.4800 | |
| 2887.7864 | 2959.1000 | | 3023.7578 | |
| 3043.5472 | 3054.5252 | | 3063.7177 | |
| 3088.5320 | 3135.1583 | | 3143.2889 | |
| Zero-point correction (Hartree): | 0.132057 | | | |

C5H9O2.tpchphh

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.32930657
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | | |
|-----------------------------|-----------|-----------|-----------|--|
| O | -2.978713 | -0.743557 | -0.145071 | |
| C | -1.973211 | 0.122429 | 0.158926 | |
| C | -0.565976 | -0.492802 | 0.135487 | |
| C | 0.521527 | 0.573077 | 0.043765 | |
| C | 1.936809 | 0.184364 | 0.444986 | |
| C | 2.487430 | -1.039871 | -0.306065 | |
| H | 3.513523 | -1.247037 | 0.010703 | |
| O | 0.255086 | 1.697410 | -0.344559 | |
| H | -2.006202 | 0.915421 | -0.621129 | |
| H | -2.164250 | 0.671471 | 1.099636 | |
| H | -0.401602 | -1.140177 | 1.005126 | |
| H | -0.486135 | -1.142602 | -0.746492 | |
| H | 2.569769 | 1.061056 | 0.283107 | |
| H | 1.929561 | -0.025940 | 1.523996 | |
| H | 1.894044 | -1.938744 | -0.113526 | |
| H | 2.500833 | -0.867462 | -1.386968 | |
| Rotational constants (GHz): | 5.0615000 | 1.3598600 | 1.1385100 | |

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 56.2658 | 68.1552 | 87.4027 |
| 167.0901 | 224.4161 | 259.1548 |
| 371.3799 | 421.8019 | 534.7787 |
| 606.3981 | 712.9478 | 789.0595 |
| 819.7604 | 918.2138 | 955.4269 |
| 1012.8773 | 1045.2927 | 1066.2819 |
| 1104.8409 | 1145.8425 | 1178.8803 |
| 1205.3712 | 1284.6206 | 1336.3651 |
| 1345.9111 | 1356.8389 | 1380.2058 |
| 1426.9544 | 1466.3570 | 1484.2028 |
| 1516.3993 | 1519.1124 | 1796.6264 |
| 2886.9517 | 2959.5774 | 3032.2833 |
| 3046.2012 | 3054.7268 | 3088.5162 |
| 3111.2037 | 3128.3205 | 3133.2133 |

Zero-point correction (Hartree): 0.132376

C5H9O2.tphcmch

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.32952854

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 3.088971 | -0.515812 | 0.018331 |
| C | 1.904743 | 0.026232 | -0.380179 |
| C | 0.678757 | -0.458796 | 0.405733 |
| C | -0.519836 | 0.466670 | 0.241462 |
| C | -1.888439 | -0.083048 | 0.615205 |
| C | -2.552348 | -0.767898 | -0.595584 |
| H | -3.540070 | -1.150322 | -0.323192 |
| O | -0.384105 | 1.600585 | -0.184438 |
| H | 2.000514 | 1.122454 | -0.214260 |
| H | 1.750934 | -0.060963 | -1.471735 |
| H | 0.411068 | -1.486201 | 0.130499 |
| H | 0.932121 | -0.490913 | 1.474900 |
| H | -1.794253 | -0.798086 | 1.441033 |
| H | -2.504239 | 0.756854 | 0.949666 |
| H | -2.675506 | -0.058134 | -1.418557 |
| H | -1.956746 | -1.611833 | -0.959312 |

Rotational constants (GHz): 5.5933700 1.2838700 1.1604900

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 51.3293 | 72.0504 | 82.6702 |
| 180.6953 | 229.4279 | 241.2751 |
| 359.0779 | 423.1796 | 560.9869 |
| 586.2872 | 715.4297 | 803.3610 |
| 843.7094 | 922.6433 | 954.3587 |
| 1009.5937 | 1039.0100 | 1068.7696 |
| 1103.5972 | 1134.9704 | 1171.1474 |
| 1206.7251 | 1285.9660 | 1324.7720 |
| 1350.5003 | 1360.4889 | 1380.6134 |
| 1422.5552 | 1463.0112 | 1494.0517 |
| 1513.8717 | 1521.3211 | 1799.2387 |
| 2887.7134 | 2959.9206 | 3040.0107 |
| 3053.0680 | 3055.5867 | 3083.5794 |
| 3111.0364 | 3128.8399 | 3137.4791 |

Zero-point correction (Hartree): 0.132439

C5H9O2.tphcmhc

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.33179765

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -3.252725 | -0.205996 | -0.152684 |
| C | -2.040244 | 0.262571 | 0.253091 |
| C | -0.851255 | -0.645632 | -0.093652 |
| C | 0.479936 | 0.094875 | -0.025152 |
| C | 1.736344 | -0.752903 | 0.099588 |
| C | 3.033020 | 0.042375 | -0.033024 |
| H | 3.901276 | -0.610306 | 0.094771 |
| O | 0.521653 | 1.311291 | -0.084209 |
| H | -1.893027 | 1.228249 | -0.279949 |
| H | -2.039287 | 0.548474 | 1.321356 |
| H | -0.832632 | -1.536507 | 0.545201 |
| H | -0.978654 | -1.011478 | -1.122019 |
| H | 1.683495 | -1.262803 | 1.073107 |
| H | 1.678427 | -1.560120 | -0.644081 |
| H | 3.101727 | 0.518447 | -1.015030 |
| H | 3.080449 | 0.835969 | 0.716688 |

Rotational constants (GHz): 8.4934100 1.1516300 1.0479300

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 48.2727 | 77.7196 | 85.9946 |
| 162.0825 | 206.3224 | 281.8212 |
| 338.7819 | 427.5144 | 475.9459 |
| 646.7477 | 705.7716 | 758.6834 |
| 835.0713 | 918.3830 | 976.3765 |
| 1012.0326 | 1045.5250 | 1066.5123 |

| | | |
|-----------|-----------|-----------|
| 1102.7373 | 1130.9740 | 1154.1655 |
| 1195.2335 | 1287.3020 | 1329.5368 |
| 1350.5145 | 1378.1453 | 1389.7948 |
| 1428.2822 | 1461.9608 | 1468.9812 |
| 1507.7166 | 1512.6084 | 1799.4857 |
| 2887.8506 | 2959.3383 | 3023.8700 |
| 3043.5177 | 3054.5341 | 3063.7126 |
| 3088.4959 | 3135.1243 | 3143.3102 |

Zero-point correction (Hartree): 0.132058

C5H9O2.tphcmhh

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.32952856

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 3.088763 | -0.516259 | 0.018220 |
| C | 1.904612 | 0.026069 | -0.380073 |
| C | 0.678676 | -0.458301 | 0.406363 |
| C | -0.519891 | 0.467084 | 0.241326 |
| C | -1.888608 | -0.082485 | 0.614923 |
| C | -2.551874 | -0.768838 | -0.595350 |
| H | -3.539632 | -1.151133 | -0.322908 |
| O | -0.384011 | 1.600813 | -0.185026 |
| H | 2.000831 | 1.122308 | -0.214507 |
| H | 1.750396 | -0.061358 | -1.471559 |
| H | 0.411031 | -1.485963 | 0.132066 |
| H | 0.932096 | -0.489433 | 1.475541 |
| H | -1.794668 | -0.796581 | 1.441606 |
| H | -2.504694 | 0.757686 | 0.948180 |
| H | -2.674866 | -0.060054 | -1.419197 |
| H | -1.955991 | -1.613080 | -0.957902 |

Rotational constants (GHz): 5.5911100 1.2840600 1.1605400

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 51.4540 | 72.0558 | 82.7175 |
| 180.6861 | 229.4448 | 241.2289 |
| 359.0996 | 423.1730 | 561.0601 |
| 586.2138 | 715.4269 | 803.3684 |
| 843.6676 | 922.6646 | 954.3583 |
| 1009.5834 | 1039.0203 | 1068.7540 |
| 1103.6130 | 1134.9762 | 1171.1788 |
| 1206.7539 | 1285.9792 | 1324.7846 |
| 1350.4960 | 1360.4746 | 1380.6139 |
| 1422.6033 | 1463.0303 | 1494.0653 |
| 1513.8759 | 1521.3378 | 1799.2259 |
| 2887.6922 | 2959.8627 | 3040.0425 |
| 3053.0655 | 3055.5416 | 3083.6254 |
| 3111.0158 | 3128.8375 | 3137.4527 |

Zero-point correction (Hartree): 0.132439

C5H9O2.tphcpch

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.32930661

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -2.978661 | -0.743799 | -0.144768 |
| C | -1.973252 | 0.122338 | 0.158934 |
| C | -0.565889 | -0.492774 | 0.135026 |
| C | 0.521392 | 0.573263 | 0.043619 |
| C | 1.936801 | 0.184522 | 0.444554 |
| C | 2.487494 | -1.040197 | -0.305646 |
| H | 3.513573 | -1.246911 | 0.011442 |
| O | 0.254923 | 1.697708 | -0.344273 |
| H | -2.006474 | 0.915047 | -0.621413 |
| H | -2.163762 | 0.671634 | 1.099587 |
| H | -0.401474 | -1.140394 | 1.004464 |
| H | -0.485973 | -1.142172 | -0.747227 |
| H | 2.569717 | 1.061127 | 0.281969 |
| H | 1.929846 | -0.025029 | 1.523740 |
| H | 1.894204 | -1.938993 | -0.112504 |
| H | 2.500961 | -0.868505 | -1.386654 |

Rotational constants (GHz): 5.0606000 1.3599300 1.1384300

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 56.1801 | 68.2154 | 87.4227 |
| 166.9968 | 224.3870 | 259.1028 |
| 371.3582 | 421.7507 | 534.7129 |
| 606.3363 | 713.2416 | 789.0266 |
| 819.7217 | 918.5460 | 955.4485 |
| 1012.7725 | 1045.3931 | 1066.2262 |
| 1104.9422 | 1145.8218 | 1178.7744 |
| 1205.2812 | 1284.6674 | 1336.3890 |
| 1345.8644 | 1356.7538 | 1380.2834 |
| 1426.9010 | 1466.3130 | 1484.1670 |
| 1516.3740 | 1519.0981 | 1796.7607 |
| 2886.8411 | 2959.7418 | 3032.0609 |
| 3046.2822 | 3054.7718 | 3088.6326 |

3111.1386 3128.3882 3133.2369
Zero-point correction (Hartree): 0.132376

C5H9O2.tphcphc

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.33179765

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -3.252714 | -0.206046 | -0.152855 |
| C | -2.040279 | 0.262707 | 0.252836 |
| C | -0.851260 | -0.645689 | -0.093340 |
| C | 0.479928 | 0.094822 | -0.025025 |
| C | 1.736373 | -0.752929 | 0.099632 |
| C | 3.032999 | 0.042442 | -0.033341 |
| H | 3.901308 | -0.610226 | 0.094169 |
| O | 0.521668 | 1.311233 | -0.083957 |
| H | -1.893042 | 1.228180 | -0.280537 |
| H | -2.039436 | 0.549122 | 1.320974 |
| H | -0.832703 | -1.536188 | 0.546053 |
| H | -0.978582 | -1.012189 | -1.121472 |
| H | 1.683751 | -1.262455 | 1.073371 |
| H | 1.678493 | -1.560415 | -0.643716 |
| H | 3.101397 | 0.518585 | -1.015333 |
| H | 3.080621 | 0.835976 | 0.716417 |

Rotational constants (GHz): 8.4936200 1.1516300 1.0479300

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 48.2868 | 77.6745 | 85.9541 |
| 162.0627 | 206.3159 | 281.8494 |
| 338.7834 | 427.5203 | 475.8902 |
| 646.7264 | 705.7255 | 758.6345 |
| 835.0704 | 918.2964 | 976.3435 |
| 1011.9943 | 1045.4876 | 1066.4830 |
| 1102.7175 | 1130.9467 | 1154.1382 |
| 1195.2393 | 1287.2777 | 1329.5238 |
| 1350.5380 | 1378.1088 | 1389.7711 |
| 1428.2643 | 1461.9476 | 1468.9629 |
| 1507.7140 | 1512.6042 | 1799.5411 |
| 2887.9883 | 2959.2533 | 3023.8570 |
| 3043.5783 | 3054.6551 | 3063.7186 |
| 3088.4561 | 3135.1312 | 3143.3318 |

Zero-point correction (Hartree): 0.132057

C5H9O2.tphcphh

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.32930662

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -2.978620 | -0.743849 | -0.144955 |
| C | -1.973300 | 0.122427 | 0.158670 |
| C | -0.565941 | -0.492666 | 0.135666 |
| C | 0.521417 | 0.573255 | 0.043820 |
| C | 1.936878 | 0.184462 | 0.444555 |
| C | 2.487390 | -1.040207 | -0.305918 |
| H | 3.513679 | -1.246716 | 0.010614 |
| O | 0.255016 | 1.697631 | -0.344334 |
| H | -2.006334 | 0.914813 | -0.622010 |
| H | -2.164205 | 0.672205 | 1.098973 |
| H | -0.401818 | -1.139575 | 1.005696 |
| H | -0.485700 | -1.142830 | -0.745992 |
| H | 2.569793 | 1.061054 | 0.281906 |
| H | 1.930146 | -0.025203 | 1.523712 |
| H | 1.894363 | -1.939094 | -0.112406 |
| H | 2.500235 | -0.868538 | -1.386937 |

Rotational constants (GHz): 5.0605400 1.3599100 1.1384400

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 56.1626 | 68.2051 | 87.3812 |
| 167.0109 | 224.3871 | 259.1051 |
| 371.3759 | 421.7584 | 534.7458 |
| 606.2698 | 713.1660 | 789.0392 |
| 819.7479 | 918.4333 | 955.4318 |
| 1012.7975 | 1045.3595 | 1066.2115 |
| 1104.9342 | 1145.8237 | 1178.7975 |
| 1205.3161 | 1284.6641 | 1336.4038 |
| 1345.9017 | 1356.7807 | 1380.2573 |
| 1426.8794 | 1466.3050 | 1484.1709 |
| 1516.3723 | 1519.0901 | 1796.7382 |
| 2886.8633 | 2959.6374 | 3032.1277 |
| 3046.2825 | 3054.7831 | 3088.5903 |
| 3111.1618 | 3128.4031 | 3133.2639 |

Zero-point correction (Hartree): 0.132376

C5H9O2.tphhmch

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.32952855

Electronic state : 2-A
Cartesian coordinates (Angs):
O 3.088978 -0.515424 0.018252
C 1.904469 0.025742 -0.380578
C 0.678873 -0.458548 0.406432
C -0.519841 0.466702 0.241617
C -1.888448 -0.083124 0.615191
C -2.552137 -0.767892 -0.595760
H -3.539738 -1.150706 -0.323478
O -0.384161 1.600520 -0.184552
H 1.999940 1.122204 -0.216029
H 1.750264 -0.062927 -1.471959
H 0.411162 -1.486306 0.132573
H 0.932745 -0.489281 1.475518
H -1.794284 -0.798232 1.440960
H -2.504353 0.756695 0.949667
H -2.675508 -0.057951 -1.418549
H -1.956266 -1.611542 -0.959712
Rotational constants (GHz): 5.5930700 1.2839100 1.1606000
Vibrational harmonic frequencies (cm-1):
51.3048 72.0806 82.7038
180.7571 229.3812 241.3314
359.0769 423.1585 561.0995
586.2466 715.5542 803.3789
843.6977 922.7662 954.3793
1009.5683 1038.9969 1068.7765
1103.6252 1134.9592 1171.1034
1206.6274 1285.9563 1324.7770
1350.4331 1360.4765 1380.6342
1422.5561 1463.0239 1494.0573
1513.8741 1521.3226 1799.2382
2887.6250 2959.9270 3040.0250
3053.0636 3055.5900 3083.6494
3111.0331 3128.8310 3137.4822
Zero-point correction (Hartree): 0.132439

C5H9O2.tphmhc

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.33179758
Electronic state : 2-A
Cartesian coordinates (Angs):
O -3.252702 -0.205845 -0.151946
C -2.040029 0.262311 0.253543
C -0.851143 -0.645578 -0.094514
C 0.479867 0.095002 -0.026059
C 1.736230 -0.752959 0.099253
C 3.032939 0.042341 -0.031939
H 3.901111 -0.610401 0.096165
O 0.521610 1.311351 -0.084908
H -1.893194 1.228632 -0.278488
H -2.038663 0.547097 1.322139
H -0.832102 -1.536706 0.544017
H -0.979240 -1.010863 -1.122949
H 1.682634 -1.263269 1.072490
H 1.678818 -1.559758 -0.644918
H 3.102376 0.519011 -1.013605
H 3.079814 0.835504 0.718284
Rotational constants (GHz): 8.4930500 1.1517000 1.0480000
Vibrational harmonic frequencies (cm-1):
48.0632 77.7523 85.8119
162.1130 206.4074 281.7335
338.8168 427.5240 475.9153
646.6751 705.7096 758.6127
835.1167 918.2565 976.4812
1012.0660 1045.4984 1066.5014
1102.8459 1131.0635 1154.1941
1195.2807 1287.3229 1329.6625
1350.6071 1378.1082 1389.7516
1428.3188 1461.9443 1468.9684
1507.7305 1512.6131 1799.9256
2887.6354 2958.9995 3023.9679
3043.7365 3054.5694 3063.6517
3088.4401 3135.0903 3143.1890
Zero-point correction (Hartree): 0.132058

C5H9O2.tphmhh

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.32952860
Electronic state : 2-A
Cartesian coordinates (Angs):
O 3.088526 -0.516022 0.018980
C 1.904213 0.024991 -0.380597
C 0.678405 -0.457881 0.406952
C -0.519931 0.467679 0.240999
C -1.888850 -0.081309 0.614617

| | | | |
|--|-----------|-----------|-----------|
| C | -2.551137 | -0.770156 | -0.594788 |
| H | -3.538950 | -1.152232 | -0.322246 |
| O | -0.383605 | 1.601156 | -0.185870 |
| H | 1.999989 | 1.121644 | -0.217489 |
| H | 1.750060 | -0.065053 | -1.471881 |
| H | 0.410394 | -1.485908 | 0.134441 |
| H | 0.932223 | -0.487256 | 1.476094 |
| H | -1.795365 | -0.793776 | 1.442758 |
| H | -2.505286 | 0.759425 | 0.945779 |
| H | -2.673843 | -0.062962 | -1.420043 |
| H | -1.954786 | -1.614899 | -0.955388 |
| Rotational constants (GHz): | 5.5884800 | 1.2843700 | 1.1606900 |
| Vibrational harmonic frequencies (cm-1): | | | |
| 51.6810 | 71.9972 | | 82.7101 |
| 180.7415 | 229.4953 | | 241.1745 |
| 359.1804 | 423.2203 | | 561.2153 |
| 586.1184 | 715.5402 | | 803.4079 |
| 843.6829 | 922.7678 | | 954.3590 |
| 1009.5625 | 1039.0127 | | 1068.7738 |
| 1103.6473 | 1134.9505 | | 1171.2195 |
| 1206.6683 | 1285.9625 | | 1324.8347 |
| 1350.4460 | 1360.4683 | | 1380.6343 |
| 1422.6630 | 1463.0628 | | 1494.0797 |
| 1513.8878 | 1521.3543 | | 1799.2468 |
| 2887.6064 | 2959.8362 | | 3040.0151 |
| 3053.0830 | 3055.5469 | | 3083.7205 |
| 3111.0572 | 3128.8652 | | 3137.4524 |
| Zero-point correction (Hartree): | 0.132441 | | |

C5H9O2.tphhpch

```
-----
E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.32930658
Electronic state : 2-A
Cartesian coordinates (Angs):
O      -2.978865      -0.743459      -0.145322
C      -1.973491       0.122614       0.158699
C      -0.566226      -0.492773       0.136083
C       0.521415       0.572915       0.044180
C       1.936590       0.183862       0.445597
C       2.487886      -1.039320      -0.306732
H       3.513943      -1.246291       0.010250
O       0.255486       1.697085      -0.344850
H      -2.005990       0.914950      -0.622062
H      -2.164562       0.672368       1.098966
H      -0.402326      -1.139528       1.006252
H      -0.486029      -1.143050      -0.745488
H       2.569505       1.060827       0.284960
H       1.929065      -0.027822       1.524346
H       1.894815      -1.938651      -0.115403
H       2.501566      -0.865587      -1.387410
Rotational constants (GHz): 5.0626300 1.3595700 1.1384700
Vibrational harmonic frequencies (cm-1):
56.1440      68.0433      87.4413
167.0934     224.3374     259.0730
371.3095     421.7640     534.7669
606.4651     713.3002     789.2490
819.7318     918.5752     955.4227
1012.7223    1045.4379    1066.1603
1104.9465    1145.8222    1178.7895
1205.2592    1284.6826    1336.4142
1345.8527    1356.7487    1380.2901
1426.8720    1466.3362    1484.2831
1516.3811    1519.1015    1796.8144
2886.8055    2959.7732    3032.1970
3046.3425    3054.7934    3088.7116
3111.1615    3128.4166    3133.2727
Zero-point correction (Hartree): 0.132378
```

C5H9O2.tphhpch

```
-----
E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.33179763
Electronic state : 2-A
Cartesian coordinates (Angs):
O      -3.252987      -0.206141      -0.150871
C      -2.039937       0.262821       0.252695
C      -0.851361      -0.645504      -0.094890
C       0.479965       0.094671      -0.025941
C       1.736299      -0.753002       0.099412
C       3.033006       0.042448      -0.031832
H       3.901169      -0.610363      -0.095877
O       0.521766       1.311126      -0.084830
H      -1.893755       1.228273      -0.281004
H      -2.037532       0.549602       1.320757
H      -0.832893      -1.536699       0.543543
H      -0.979019      -1.010794      -1.123399
```

| | | | |
|--|-----------|-----------|-----------|
| H | 1.682727 | -1.263382 | 1.072651 |
| H | 1.679066 | -1.559853 | -0.644720 |
| H | 3.102170 | 0.519378 | -1.013382 |
| H | 3.080000 | 0.835366 | 0.718624 |
| Rotational constants (GHz): | 8.4950400 | 1.1516200 | 1.0479200 |
| Vibrational harmonic frequencies (cm-1): | | | |
| 48.2044 | 77.5821 | | 86.0032 |
| 162.0480 | 206.3555 | | 281.8203 |
| 338.8102 | 427.5097 | | 475.9812 |
| 646.8017 | 705.5496 | | 758.5422 |
| 835.0733 | 918.0931 | | 976.5253 |
| 1012.0589 | 1045.4232 | | 1066.6256 |
| 1102.7121 | 1131.0019 | | 1154.1997 |
| 1195.4574 | 1287.3125 | | 1329.5203 |
| 1350.7284 | 1378.0167 | | 1389.8591 |
| 1428.2440 | 1461.9571 | | 1469.0002 |
| 1507.7043 | 1512.5949 | | 1799.3284 |
| 2888.0202 | 2958.9987 | | 3023.7777 |
| 3043.6345 | 3054.4456 | | 3063.7367 |
| 3088.4600 | 3135.1989 | | 3143.3139 |
| Zero-point correction (Hartree): | 0.132057 | | |

C5H9O2.tphhphh

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.32930662
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | |
|--|-----------|-----------|-----------|
| O | -2.978652 | -0.743917 | -0.144735 |
| C | -1.973255 | 0.122376 | 0.158605 |
| C | -0.565911 | -0.492661 | 0.135358 |
| C | 0.521436 | 0.573307 | 0.043681 |
| C | 1.936867 | 0.184532 | 0.444400 |
| C | 2.487410 | -1.040336 | -0.305715 |
| C | 3.513447 | -1.247176 | 0.011398 |
| O | 0.254963 | 1.697770 | -0.344173 |
| H | -2.006557 | 0.914807 | -0.622016 |
| H | -2.164012 | 0.672162 | 1.098943 |
| H | -0.401638 | -1.139657 | 1.005305 |
| H | -0.485684 | -1.142735 | -0.746370 |
| H | 2.569803 | 1.061073 | 0.281634 |
| H | 1.930028 | -0.024904 | 1.523630 |
| H | 1.893951 | -1.939003 | -0.112515 |
| H | 2.500884 | -0.868698 | -1.386729 |
| Rotational constants (GHz): | 5.0602600 | 1.3599400 | 1.1384100 |
| Vibrational harmonic frequencies (cm-1): | | | |
| 56.1768 | 68.2134 | | 87.3457 |
| 166.9817 | 224.3553 | | 259.1060 |
| 371.3974 | 421.7811 | | 534.7377 |
| 606.2414 | 713.0605 | | 789.0046 |
| 819.7528 | 918.3298 | | 955.4286 |
| 1012.8671 | 1045.3591 | | 1066.2546 |
| 1104.9164 | 1145.8435 | | 1178.8328 |
| 1205.3820 | 1284.6939 | | 1336.4033 |
| 1345.9551 | 1356.8276 | | 1380.2304 |
| 1426.8706 | 1466.3108 | | 1484.1591 |
| 1516.3666 | 1519.0949 | | 1796.7448 |
| 2886.8928 | 2959.5460 | | 3031.8941 |
| 3046.2464 | 3054.8012 | | 3088.5225 |
| 3111.2177 | 3128.4407 | | 3133.2948 |
| Zero-point correction (Hartree): | 0.132375 | | |

C5H9O2.1-5Hshift.m

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.30981885
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | |
|--|-----------|-----------|-----------|
| C | -0.936493 | -0.499554 | -0.529906 |
| C | -0.450091 | 0.853258 | -0.053008 |
| C | 0.854204 | 0.813680 | 0.728991 |
| C | 1.876239 | -0.021157 | -0.073580 |
| O | 1.378153 | -1.310385 | -0.339400 |
| C | -1.746065 | -1.309711 | 0.469757 |
| O | -1.041850 | 1.880629 | -0.332534 |
| H | -1.398531 | -0.432754 | -1.518771 |
| H | 0.683476 | 0.319308 | 1.693831 |
| H | 1.203287 | 1.832925 | 0.911246 |
| H | 2.795796 | -0.156451 | 0.513418 |
| H | 2.150633 | 0.514688 | -0.997077 |
| H | 0.171095 | -1.114693 | -0.649896 |
| H | -2.694159 | -0.801390 | 0.688085 |
| H | -1.206893 | -1.443063 | 1.411912 |
| H | -1.981898 | -2.299617 | 0.069201 |
| Rotational constants (GHz): | 3.1484100 | 2.4409500 | 1.6045600 |
| Vibrational harmonic frequencies (cm-1): | | | |

| | | |
|------------|-----------|-----------|
| i1553.2095 | 60.5859 | 133.4308 |
| 189.2915 | 200.1490 | 263.6243 |
| 420.1507 | 439.7819 | 502.4701 |
| 602.1836 | 721.9289 | 734.0531 |
| 832.7134 | 869.7513 | 915.4096 |
| 1002.2449 | 1027.7651 | 1051.5356 |
| 1106.4265 | 1127.6375 | 1168.1957 |
| 1201.0503 | 1221.8998 | 1241.9019 |
| 1318.0082 | 1324.4007 | 1386.6430 |
| 1412.4037 | 1466.2295 | 1494.2270 |
| 1503.0430 | 1509.6222 | 1552.1935 |
| 1797.1485 | 2984.9915 | 3036.9462 |
| 3038.3896 | 3054.3794 | 3106.5639 |
| 3113.0314 | 3133.4829 | 3137.2451 |

Zero-point correction (Hartree): 0.128496

C5H9O2.1-5Hshift.p

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.31255628

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| C | -0.880050 | -0.548889 | 0.480030 |
| C | -0.327417 | 0.817329 | 0.161753 |
| C | 1.170804 | 0.942361 | 0.394032 |
| C | 1.858825 | -0.185186 | -0.410397 |
| O | 1.357704 | -1.447028 | -0.044511 |
| H | -0.849998 | -0.753733 | 1.556504 |
| C | -2.172311 | -0.938799 | -0.198035 |
| O | -1.009140 | 1.700672 | -0.330731 |
| H | 1.394854 | 0.800244 | 1.458517 |
| H | 1.512326 | 1.932000 | 0.081933 |
| H | 2.935377 | -0.200315 | -0.187424 |
| H | 1.744471 | 0.009045 | -1.489324 |
| H | 0.108194 | -1.263407 | 0.125339 |
| H | -2.093844 | -0.855356 | -1.285352 |
| H | -2.972664 | -0.258717 | 0.119364 |
| H | -2.466337 | -1.959815 | 0.058085 |

Rotational constants (GHz): 3.5960100 2.2325000 1.5250800

Vibrational harmonic frequencies (cm-1):

| | | |
|------------|-----------|-----------|
| i1559.3030 | 81.4726 | 141.3499 |
| 170.5644 | 220.7315 | 271.7756 |
| 400.3574 | 450.5600 | 519.2425 |
| 579.8694 | 637.9142 | 772.1101 |
| 822.2927 | 865.4014 | 912.0149 |
| 994.9032 | 1041.1863 | 1058.8670 |
| 1093.2860 | 1128.0268 | 1151.8207 |
| 1200.2485 | 1235.9368 | 1243.4344 |
| 1318.6828 | 1351.7035 | 1384.2802 |
| 1413.5992 | 1472.3125 | 1487.6498 |
| 1497.6401 | 1507.7586 | 1548.6914 |
| 1785.6476 | 2986.0024 | 3037.5461 |
| 3044.2458 | 3058.1099 | 3084.1588 |
| 3113.1241 | 3137.6822 | 3143.0936 |

Zero-point correction (Hartree): 0.128410

C5H9O2.1-6Hshift.a

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.30917181

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 2.008084 | 0.280855 | 0.101941 |
| H | 1.204662 | 1.165554 | -0.137240 |
| C | 0.110996 | 1.825922 | -0.318768 |
| C | 1.423161 | -0.926583 | -0.312810 |
| C | -0.954485 | 1.094980 | 0.481918 |
| C | 0.121906 | -1.286899 | 0.439444 |
| C | -1.058611 | -0.383296 | 0.099419 |
| H | -0.036132 | 1.807771 | -1.400946 |
| H | 0.357956 | 2.824071 | 0.047396 |
| H | 1.247118 | -0.951923 | -1.400610 |
| H | 2.176989 | -1.697043 | -0.097113 |
| H | -0.723532 | 1.174722 | 1.551426 |
| H | -1.938992 | 1.547045 | 0.309717 |
| H | -0.174395 | -2.310038 | 0.190898 |
| H | 0.328704 | -1.228355 | 1.515544 |
| O | -2.045606 | -0.815423 | -0.466227 |

Rotational constants (GHz): 3.4885000 2.3675200 1.5880400

Vibrational harmonic frequencies (cm-1):

| | | |
|------------|-----------|-----------|
| i1566.3352 | 73.2708 | 117.7305 |
| 223.4890 | 286.3095 | 366.6403 |
| 447.8832 | 505.2807 | 539.9617 |
| 586.5850 | 676.3014 | 762.7170 |
| 797.2159 | 899.0248 | 912.0895 |
| 999.5114 | 1009.8598 | 1042.1285 |
| 1088.3854 | 1114.4330 | 1164.1674 |

| | | |
|-----------|-----------|-----------|
| 1210.3655 | 1239.3232 | 1260.1569 |
| 1268.3750 | 1339.3946 | 1344.1544 |
| 1395.6503 | 1459.2735 | 1462.3193 |
| 1473.3145 | 1478.9425 | 1489.1025 |
| 1810.3302 | 2987.7309 | 3038.5967 |
| 3041.2433 | 3054.6244 | 3088.1246 |
| 3095.5509 | 3121.9243 | 3175.9236 |

Zero-point correction (Hartree): 0.128597

C5H9O2.1-6Hshift.b

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.30792699

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 2.054798 | 0.070457 | -0.296063 |
| H | 1.312545 | 1.028568 | -0.326398 |
| C | 0.282839 | 1.818243 | -0.287376 |
| C | 1.388064 | -0.947390 | 0.407524 |
| C | -0.784541 | 1.105773 | 0.521049 |
| C | 0.016928 | -1.308432 | -0.181195 |
| C | -1.118268 | -0.296886 | 0.011646 |
| H | 0.045020 | 1.952840 | -1.344686 |
| H | 0.666044 | 2.733388 | 0.167364 |
| H | 2.046342 | -1.824681 | 0.328669 |
| H | 1.302305 | -0.721061 | 1.484299 |
| H | -0.456504 | 1.018819 | 1.566587 |
| H | -1.723049 | 1.674051 | 0.526117 |
| H | 0.132871 | -1.463674 | -1.261809 |
| H | -0.343281 | -2.258663 | 0.229482 |
| O | -2.266352 | -0.616387 | -0.228877 |

Rotational constants (GHz): 3.6705700 2.2433500 1.5414800

Vibrational harmonic frequencies (cm-1):

| | | |
|------------|-----------|-----------|
| i1574.9497 | 30.4440 | 151.6598 |
| 260.0664 | 306.2405 | 362.1395 |
| 420.3214 | 483.0853 | 526.2187 |
| 549.2363 | 609.0922 | 703.7802 |
| 825.8335 | 876.8357 | 936.0113 |
| 996.5329 | 1005.7644 | 1073.9217 |
| 1087.2946 | 1111.0959 | 1163.5667 |
| 1217.1459 | 1229.1186 | 1241.7174 |
| 1266.0977 | 1338.4516 | 1351.2932 |
| 1401.8280 | 1441.6356 | 1460.5200 |
| 1468.9426 | 1481.7668 | 1497.2140 |
| 1811.7869 | 2973.6003 | 3027.4369 |
| 3033.8557 | 3052.2044 | 3075.5235 |
| 3095.5865 | 3097.3288 | 3176.8731 |

Zero-point correction (Hartree): 0.128076

C5H9O2.1-6Hshift.c

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.30792698

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| C | -0.784494 | 1.105862 | 0.520921 |
| C | -1.118316 | -0.296810 | 0.011619 |
| C | 0.016857 | -1.308330 | -0.181466 |
| C | 1.387941 | -0.947537 | 0.407537 |
| O | 2.054904 | 0.070344 | -0.295780 |
| H | 1.312686 | 1.028485 | -0.326254 |
| C | 0.283012 | 1.818204 | -0.287444 |
| H | -0.456550 | 1.018933 | 1.566492 |
| H | -1.722957 | 1.674216 | 0.525907 |
| O | -2.266452 | -0.616336 | -0.228625 |
| H | -0.343443 | -2.258708 | 0.228781 |
| H | 0.132949 | -1.463147 | -1.262129 |
| H | 1.302033 | -0.721378 | 1.484336 |
| H | 2.046130 | -1.824892 | 0.328639 |
| H | 0.666199 | 2.733376 | 0.167259 |
| H | 0.045335 | 1.952718 | -1.344796 |

Rotational constants (GHz): 3.6707000 2.2432900 1.5414300

Vibrational harmonic frequencies (cm-1):

| | | |
|------------|-----------|-----------|
| i1574.9443 | 30.4754 | 151.6635 |
| 260.0675 | 306.2195 | 362.1642 |
| 420.3264 | 483.0918 | 526.2014 |
| 549.2368 | 609.0929 | 703.7755 |
| 825.8288 | 876.8512 | 936.0131 |
| 996.5351 | 1005.7684 | 1073.9298 |
| 1087.2925 | 1111.1027 | 1163.5729 |
| 1217.1392 | 1229.1143 | 1241.7136 |
| 1266.1070 | 1338.4641 | 1351.2877 |
| 1401.8180 | 1441.6495 | 1460.5187 |
| 1468.9434 | 1481.7703 | 1497.2258 |
| 1811.7853 | 2973.5988 | 3027.4303 |
| 3033.8482 | 3052.1870 | 3075.5145 |
| 3095.5854 | 3097.3434 | 3176.8692 |

Zero-point correction (Hartree): 0.128077

C5H9O2.pmm

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.32873614

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -1.350798 | -1.420122 | -0.199770 |
| C | -1.949072 | -0.188152 | -0.211006 |
| C | -1.171091 | 0.928898 | 0.494156 |
| C | 0.182571 | 1.242261 | -0.165033 |
| C | 1.216515 | 0.113612 | -0.167840 |
| C | 1.536706 | -0.557426 | 1.156302 |
| H | 1.581961 | 0.162391 | 1.980828 |
| O | 1.788659 | -0.196775 | -1.195110 |
| H | -2.087626 | 0.056114 | -1.287156 |
| H | -2.984224 | -0.273244 | 0.173704 |
| H | -1.788564 | 1.835995 | 0.493636 |
| H | -1.033886 | 0.649637 | 1.545643 |
| H | 0.045348 | 1.549750 | -1.206847 |
| H | 0.640847 | 2.089087 | 0.365573 |
| H | 0.744946 | -1.278643 | 1.383669 |
| H | 2.484525 | -1.091077 | 1.070524 |

Rotational constants (GHz): 3.7294800 1.8531300 1.7063200

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 65.1419 | 89.3817 | 129.0305 |
| 153.8328 | 231.0106 | 300.4744 |
| 399.5297 | 474.5699 | 513.3367 |
| 547.4274 | 574.2711 | 733.1963 |
| 839.3207 | 875.3375 | 941.7593 |
| 996.3036 | 1026.9312 | 1047.6897 |
| 1096.7785 | 1137.3307 | 1220.4829 |
| 1229.2549 | 1263.0184 | 1356.5913 |
| 1363.8147 | 1365.1963 | 1392.1869 |
| 1395.7309 | 1477.3327 | 1479.5914 |
| 1492.6746 | 1499.7110 | 1815.7385 |
| 2893.2602 | 2940.3022 | 3029.7515 |
| 3046.9652 | 3053.6152 | 3083.8457 |
| 3104.5271 | 3123.5840 | 3163.6369 |

Zero-point correction (Hartree): 0.132050

C5H9O2.pmt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.33077899

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 1.237846 | 1.427496 | 0.273257 |
| C | 2.005872 | 0.333894 | -0.022479 |
| C | 1.247766 | -1.004030 | -0.069843 |
| C | -0.101979 | -0.862683 | -0.779269 |
| C | -1.158877 | -0.215399 | 0.122104 |
| C | -2.132002 | 0.738773 | -0.536676 |
| H | -2.557182 | 0.304556 | -1.448871 |
| O | -1.217449 | -0.487249 | 1.306247 |
| H | 2.391088 | 0.568511 | -1.041841 |
| H | 2.909051 | 0.281063 | 0.612539 |
| H | 1.879506 | -1.751792 | -0.562709 |
| H | 1.059879 | -1.349293 | 0.952006 |
| H | -0.006829 | -0.309271 | -1.720792 |
| H | -0.490623 | -1.857119 | -1.038842 |
| H | -2.928126 | 1.005864 | 0.159578 |
| H | -1.584621 | 1.642182 | -0.830117 |

Rotational constants (GHz): 3.9826600 1.8564300 1.6754800

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 56.2066 | 90.4853 | 111.2944 |
| 162.4000 | 270.9300 | 278.3050 |
| 366.9352 | 485.5400 | 515.7614 |
| 593.9109 | 741.2675 | 785.7093 |
| 851.2787 | 878.5441 | 958.6189 |
| 1001.6082 | 1038.2327 | 1048.7426 |
| 1103.9051 | 1145.2632 | 1196.0256 |
| 1201.9770 | 1255.6685 | 1304.6614 |
| 1368.4842 | 1384.6552 | 1389.7850 |
| 1400.8859 | 1474.0337 | 1476.9960 |
| 1490.5459 | 1495.2202 | 1817.7246 |
| 2862.6851 | 2965.8953 | 3036.4030 |
| 3046.2628 | 3060.4731 | 3083.3838 |
| 3110.2489 | 3111.5710 | 3166.2091 |

Zero-point correction (Hartree): 0.132555

C5H9O2.ppt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.33376949

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | | |
|--|-----------|-----------|-----------|-----------|
| O | 2.218067 | -0.068188 | 1.167063 | |
| C | 1.914541 | 0.434458 | -0.063747 | |
| C | 1.056153 | -0.485163 | -0.950207 | |
| C | -0.224116 | -0.944754 | -0.251072 | |
| C | -1.258441 | 0.157336 | -0.060573 | |
| C | -2.601711 | -0.261096 | 0.509245 | |
| H | -3.109174 | -0.943216 | -0.183160 | |
| O | -1.024164 | 1.319126 | -0.347162 | |
| H | 1.323130 | 1.353938 | 0.144936 | |
| H | 2.817277 | 0.792286 | -0.594056 | |
| H | 0.814082 | 0.051428 | -1.874316 | |
| H | 1.651670 | -1.362647 | -1.227065 | |
| H | -0.699863 | -1.772507 | -0.793301 | |
| H | 0.026626 | -1.345366 | 0.740942 | |
| H | -2.468640 | -0.804950 | 1.451175 | |
| H | -3.224895 | 0.618842 | 0.673772 | |
| Rotational constants (GHz): | 4.8976100 | | 1.4803000 | 1.4435500 |
| Vibrational harmonic frequencies (cm-1): | | | | |
| 43.8247 | 77.5171 | | | 106.6353 |
| 182.4868 | 227.2246 | | | 287.7997 |
| 399.6905 | 457.7150 | | | 497.9353 |
| 610.2649 | 708.3928 | | | 783.4585 |
| 837.1709 | 890.6066 | | | 947.3311 |
| 978.1337 | 1024.9216 | | | 1081.8082 |
| 1109.3474 | 1142.5424 | | | 1192.5891 |
| 1205.1284 | 1273.5512 | | | 1309.0108 |
| 1377.7626 | 1386.2995 | | | 1396.2854 |
| 1406.1815 | 1456.6784 | | | 1476.9705 |
| 1488.1772 | 1489.8881 | | | 1804.1540 |
| 2883.0954 | 2953.0440 | | | 3037.1574 |
| 3049.1398 | 3055.2652 | | | 3073.1843 |
| 3101.7147 | 3110.0193 | | | 3167.3766 |
| Zero-point correction (Hartree): | 0.132333 | | | |

C5H9O2.ptp

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.32847072
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | | |
|--|-----------|-----------|-----------|-----------|
| O | 2.726376 | 0.358611 | -0.774405 | |
| C | 2.305644 | -0.205644 | 0.399413 | |
| C | 0.830318 | 0.040755 | 0.746901 | |
| C | -0.108526 | -0.479486 | -0.354595 | |
| C | -1.583365 | -0.173611 | -0.122742 | |
| C | -1.986232 | 1.287091 | 0.010866 | |
| H | -1.486580 | 1.913855 | -0.735328 | |
| O | -2.408189 | -1.065199 | -0.050102 | |
| H | 2.496137 | -1.294834 | 0.278126 | |
| H | 2.978968 | 0.090053 | 1.227065 | |
| H | 0.604809 | -0.443122 | 1.705684 | |
| H | 0.691810 | 1.118477 | 0.891993 | |
| H | 0.202938 | -0.022026 | -1.303337 | |
| H | -0.016523 | -1.565317 | -0.457596 | |
| H | -3.069286 | 1.374046 | -0.087175 | |
| H | -1.694807 | 1.666942 | 0.997565 | |
| Rotational constants (GHz): | 5.8881400 | | 1.2001000 | 1.1236000 |
| Vibrational harmonic frequencies (cm-1): | | | | |
| 41.1737 | 64.7190 | | | 120.0088 |
| 143.4881 | 189.2720 | | | 262.5172 |
| 395.4204 | 496.9431 | | | 524.6098 |
| 573.4160 | 594.3467 | | | 778.3362 |
| 799.7262 | 890.1934 | | | 945.4449 |
| 991.4829 | 1017.9968 | | | 1087.1969 |
| 1091.0060 | 1138.2263 | | | 1204.4075 |
| 1249.9954 | 1296.7671 | | | 1315.4407 |
| 1360.9666 | 1365.0023 | | | 1398.8152 |
| 1401.4258 | 1477.8394 | | | 1481.8954 |
| 1496.9140 | 1504.1213 | | | 1815.2330 |
| 2890.5538 | 2944.9529 | | | 3039.2153 |
| 3048.4198 | 3049.0182 | | | 3086.7447 |
| 3110.9396 | 3112.3431 | | | 3164.6981 |
| Zero-point correction (Hartree): | 0.132045 | | | |

C5H9O2.ptt

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.33140090
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | | |
|---|-----------|-----------|-----------|--|
| O | 2.700778 | -0.785499 | -0.594108 | |
| C | 2.361462 | 0.186186 | 0.310953 | |
| C | 0.935059 | 0.733364 | 0.182049 | |
| C | -0.118277 | -0.369851 | 0.255247 | |
| C | -1.534111 | 0.108993 | -0.039940 | |
| C | -2.635902 | -0.932091 | 0.064491 | |
| H | -2.695290 | -1.322606 | 1.087293 | |

| | | | |
|--|-----------|-----------|-----------|
| O | -1.772245 | 1.262754 | -0.344922 |
| H | 2.502147 | -0.301534 | 1.302100 |
| H | 3.115350 | 0.996540 | 0.307758 |
| H | 0.763263 | 1.481720 | 0.964465 |
| H | 0.837675 | 1.263156 | -0.771060 |
| H | 0.134637 | -1.167070 | -0.457279 |
| H | -0.118426 | -0.856679 | 1.241990 |
| H | -3.592486 | -0.485554 | -0.210094 |
| H | -2.424517 | -1.785616 | -0.589728 |
| Rotational constants (GHz): | 6.1184700 | 1.2122000 | 1.0835000 |
| Vibrational harmonic frequencies (cm-1): | | | |
| 31.9020 | 72.7533 | | 107.6005 |
| 139.6010 | 177.9738 | | 267.8523 |
| 387.3411 | 473.4902 | | 497.3675 |
| 587.4703 | 601.5221 | | 756.0564 |
| 839.1423 | 889.6234 | | 927.2116 |
| 970.0810 | 1010.0719 | | 1083.6281 |
| 1099.4276 | 1154.2243 | | 1181.0936 |
| 1217.8036 | 1303.5416 | | 1314.6751 |
| 1365.4521 | 1368.4380 | | 1397.1350 |
| 1414.0603 | 1468.5480 | | 1479.4877 |
| 1490.8158 | 1497.0660 | | 1815.2367 |
| 2876.7714 | 2947.3687 | | 3022.4044 |
| 3047.3570 | 3059.0413 | | 3065.6306 |
| 3107.8393 | 3109.6407 | | 3166.2229 |
| Zero-point correction (Hartree): | 0.131655 | | |

C5H9O2.tpt

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.33139347
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | |
|--|-----------|-----------|-----------|
| O | -3.078724 | -0.358084 | 0.024904 |
| C | -1.782380 | -0.195739 | 0.409246 |
| C | -0.973650 | 0.792586 | -0.448475 |
| C | 0.454978 | 1.017243 | 0.056216 |
| C | 1.371198 | -0.197153 | -0.045840 |
| C | 2.848300 | 0.045476 | 0.206388 |
| H | 3.002589 | 0.622580 | 1.124738 |
| O | 0.947169 | -1.306897 | -0.317633 |
| H | -1.707008 | 0.039763 | 1.491097 |
| H | -1.320826 | -1.202292 | 0.312368 |
| H | -0.955990 | 0.423344 | -1.479038 |
| H | -1.502633 | 1.752277 | -0.458540 |
| H | 0.929310 | 1.849818 | -0.480077 |
| H | 0.450190 | 1.330992 | 1.112064 |
| H | 3.375527 | -0.907285 | 0.269645 |
| H | 3.270611 | 0.636171 | -0.615636 |
| Rotational constants (GHz): | 6.6302100 | 1.2878000 | 1.1497000 |
| Vibrational harmonic frequencies (cm-1): | | | |
| 42.9144 | 104.5933 | | 111.9464 |
| 127.2986 | 228.7202 | | 268.9745 |
| 341.5080 | 463.5426 | | 487.6126 |
| 617.9853 | 687.1168 | | 762.7700 |
| 803.4341 | 921.4513 | | 960.1904 |
| 974.6025 | 1047.9450 | | 1073.8920 |
| 1106.4867 | 1149.6043 | | 1194.0782 |
| 1209.4217 | 1279.0944 | | 1326.9251 |
| 1370.2985 | 1385.3949 | | 1393.1690 |
| 1403.2809 | 1459.1316 | | 1476.5820 |
| 1489.9953 | 1495.4605 | | 1807.0783 |
| 2893.1999 | 2922.0943 | | 3015.3035 |
| 3047.2718 | 3055.0671 | | 3065.7033 |
| 3108.9930 | 3109.5860 | | 3167.6677 |
| Zero-point correction (Hartree): | 0.132037 | | |

C5H9O2.ttt

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.32957805
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 3.381285 | 0.265269 | 0.033780 |
| C | 2.237515 | -0.482144 | -0.045961 |
| C | 0.928406 | 0.309943 | 0.030417 |
| C | -0.303402 | -0.593515 | -0.015488 |
| C | -1.625671 | 0.169494 | -0.007991 |
| C | -2.891459 | -0.670259 | 0.026625 |
| H | -2.936723 | -1.248926 | 0.956901 |
| O | -1.663850 | 1.384487 | -0.028559 |
| H | 2.276224 | -1.131249 | -0.944938 |
| H | 2.307513 | -1.208188 | 0.794699 |
| H | 0.924209 | 0.907138 | 0.947849 |
| H | 0.891303 | 1.024086 | -0.798351 |

| | | | | |
|--|-----------|-----------|-----------|--|
| H | -0.293427 | -1.228492 | -0.914815 | |
| H | -0.311951 | -1.300066 | 0.827877 | |
| H | -3.765793 | -0.021373 | -0.038649 | |
| H | -2.903161 | -1.392092 | -0.797949 | |
| Rotational constants (GHz): | 8.0239500 | 1.0510900 | 0.9512600 | |
| Vibrational harmonic frequencies (cm-1): | | | | |
| 32.5796 | 75.1889 | | 97.5659 | |
| 127.3370 | 135.9531 | | 299.6564 | |
| 324.7302 | 420.7920 | | 474.2969 | |
| 502.5626 | 597.5206 | | 737.8234 | |
| 826.0787 | 875.4819 | | 945.3167 | |
| 1001.6536 | 1033.0638 | | 1076.4456 | |
| 1093.6090 | 1152.9472 | | 1181.0452 | |
| 1255.5497 | 1283.8007 | | 1314.4012 | |
| 1364.4764 | 1386.8481 | | 1399.1248 | |
| 1410.0081 | 1466.8211 | | 1479.0179 | |
| 1490.8127 | 1502.8070 | | 1819.0930 | |
| 2880.9522 | 2918.7313 | | 3013.4169 | |
| 3042.3666 | 3047.2229 | | 3074.8230 | |
| 3107.8971 | 3119.4987 | | 3166.6381 | |
| Zero-point correction (Hartree): | 0.131122 | | | |

C5H9O2.1-6Hshift.a

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.31206742
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | | |
|--|-----------|-----------|-----------|--|
| O | -1.493159 | 1.186046 | -0.459543 | |
| H | -0.351305 | 1.435820 | -0.049786 | |
| C | 0.816699 | 1.358517 | 0.469673 | |
| C | -1.887594 | -0.036716 | 0.104532 | |
| C | 1.281572 | -0.006206 | 0.070745 | |
| C | -0.964584 | -1.215507 | -0.230466 | |
| C | 0.405990 | -1.181776 | 0.489220 | |
| H | 0.613786 | 1.483456 | 1.536577 | |
| H | 1.406901 | 2.167576 | 0.039667 | |
| H | -2.030481 | 0.039586 | 1.197208 | |
| H | -2.883542 | -0.226499 | -0.326707 | |
| O | 2.295117 | -0.159245 | -0.590022 | |
| H | -1.471532 | -2.147378 | 0.048779 | |
| H | -0.811827 | -1.244238 | -1.315429 | |
| H | 0.962593 | -2.097134 | 0.269792 | |
| H | 0.237239 | -1.135469 | 1.574195 | |
| Rotational constants (GHz): | 4.0848400 | 2.0549500 | 1.5655800 | |
| Vibrational harmonic frequencies (cm-1): | | | | |
| i1566.9604 | 81.5679 | | 124.4243 | |
| 261.7780 | 307.3168 | | 388.9118 | |
| 449.6500 | 485.6919 | | 527.3011 | |
| 572.1074 | 671.3436 | | 751.8346 | |
| 847.4597 | 861.2865 | | 938.8215 | |
| 965.1471 | 1007.3894 | | 1029.7795 | |
| 1088.5013 | 1112.5571 | | 1167.5666 | |
| 1184.7433 | 1221.2661 | | 1249.3577 | |
| 1285.6192 | 1349.9965 | | 1375.1552 | |
| 1401.6952 | 1440.4462 | | 1453.1293 | |
| 1469.9394 | 1486.1742 | | 1491.5387 | |
| 1784.4691 | 2962.2296 | | 3014.0390 | |
| 3033.0398 | 3048.7916 | | 3096.0819 | |
| 3096.9174 | 3117.2219 | | 3195.1570 | |
| Zero-point correction (Hartree): | 0.128483 | | | |

C5H9O2.1-6Hshift.b

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.30794987
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | | |
|--|-----------|-----------|-----------|--|
| O | -1.548220 | 1.158445 | 0.157436 | |
| H | -0.360049 | 1.490143 | 0.209765 | |
| C | 0.926668 | 1.417740 | 0.302989 | |
| C | -1.573001 | 0.000986 | -0.640993 | |
| C | 1.210406 | -0.032333 | 0.049791 | |
| C | -1.016505 | -1.256827 | 0.050704 | |
| C | 0.322127 | -1.011507 | 0.803995 | |
| H | 1.068317 | 1.727749 | 1.342026 | |
| H | 1.377132 | 2.098292 | -0.419737 | |
| H | -2.631376 | -0.152070 | -0.900926 | |
| H | -1.048145 | 0.171469 | -1.595274 | |
| O | 2.052887 | -0.385038 | -0.759070 | |
| H | -1.745695 | -1.644899 | 0.769603 | |
| H | -0.871601 | -2.028171 | -0.714214 | |
| H | 0.856473 | -1.956838 | 0.928533 | |
| H | 0.099449 | -0.601284 | 1.794381 | |
| Rotational constants (GHz): | 3.7888500 | 2.2226300 | 1.7252800 | |
| Vibrational harmonic frequencies (cm-1): | | | | |
| i1635.2585 | 84.7040 | | 129.7400 | |

| | | |
|-----------|-----------|-----------|
| 236.5556 | 308.6532 | 373.2553 |
| 457.2424 | 480.3927 | 523.6849 |
| 599.4796 | 682.6478 | 765.5996 |
| 804.1354 | 854.4030 | 937.3814 |
| 980.5493 | 1018.1419 | 1046.6275 |
| 1088.1354 | 1107.0966 | 1169.3778 |
| 1197.1340 | 1233.5526 | 1248.0778 |
| 1279.3554 | 1339.1382 | 1376.1525 |
| 1407.8028 | 1428.9078 | 1447.2643 |
| 1470.5041 | 1489.2240 | 1505.0974 |
| 1783.8712 | 2986.2091 | 3030.4062 |
| 3056.9751 | 3068.3243 | 3094.5982 |
| 3102.7820 | 3131.3616 | 3192.0121 |

Zero-point correction (Hartree): 0.128754

C5H9O2.1-6Hshift.c

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.30892216

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| C | -1.271740 | 0.007503 | 0.010869 |
| C | -0.446171 | 1.277316 | 0.220397 |
| C | 1.070747 | 1.089667 | 0.438360 |
| C | 1.722242 | 0.109881 | -0.553144 |
| O | 1.575226 | -1.239878 | -0.186375 |
| H | 0.394390 | -1.418547 | 0.143304 |
| C | -0.780981 | -1.258183 | 0.630838 |
| O | -2.290527 | 0.026419 | -0.660509 |
| H | -0.639695 | 1.910455 | -0.651525 |
| H | -0.875277 | 1.808234 | 1.082353 |
| H | 1.549372 | 2.071628 | 0.347511 |
| H | 1.285335 | 0.729373 | 1.450972 |
| H | 1.358989 | 0.304056 | -1.576979 |
| H | 2.811216 | 0.273922 | -0.560664 |
| H | -1.369184 | -2.133991 | 0.357433 |
| H | -0.557317 | -1.194558 | 1.698743 |

Rotational constants (GHz): 4.0165800 2.0364800 1.5941500

Vibrational harmonic frequencies (cm-1):

| | | |
|------------|-----------|-----------|
| i1595.9875 | 64.9181 | 121.7321 |
| 266.9368 | 322.1366 | 385.1817 |
| 419.6723 | 483.3379 | 494.4520 |
| 557.3848 | 648.3163 | 749.4565 |
| 825.8741 | 849.2017 | 951.3533 |
| 971.0435 | 1020.6569 | 1045.3917 |
| 1080.8790 | 1112.7920 | 1160.3992 |
| 1199.7776 | 1220.1219 | 1249.9312 |
| 1264.2298 | 1358.3680 | 1371.2668 |
| 1396.8643 | 1424.7815 | 1452.8726 |
| 1464.5887 | 1490.2469 | 1496.0346 |
| 1777.1784 | 2972.8881 | 3018.4152 |
| 3033.3804 | 3055.5231 | 3088.9533 |
| 3097.8229 | 3107.1498 | 3195.7440 |

Zero-point correction (Hartree): 0.128186

C5H9O2.pmmc

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.31908590

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 1.717276 | -1.346628 | -0.036680 |
| C | 2.060879 | -0.029811 | -0.193953 |
| C | 0.900362 | 0.918614 | -0.531249 |
| C | -0.088571 | 1.107156 | 0.631948 |
| C | -0.855652 | -0.160141 | 1.023129 |
| C | -1.883371 | -0.610071 | 0.009707 |
| H | 2.662032 | 0.341365 | 0.659438 |
| H | 2.767821 | -0.045837 | -1.053562 |
| H | 1.325635 | 1.893977 | -0.799999 |
| H | 0.370930 | 0.540649 | -1.410691 |
| H | 0.452154 | 1.481081 | 1.511020 |
| H | -0.811365 | 1.881176 | 0.352349 |
| H | -0.181305 | -1.010276 | 1.203205 |
| H | -1.395072 | -0.016547 | 1.972259 |
| O | -2.166128 | -0.010659 | -1.005646 |
| H | -2.401899 | -1.561772 | 0.267096 |

Rotational constants (GHz): 4.1831100 1.6337400 1.5234700

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 31.1410 | 105.5272 | 131.5705 |
| 182.5282 | 220.8438 | 324.0297 |
| 344.7335 | 458.1407 | 657.4552 |
| 706.7043 | 756.4465 | 824.9709 |
| 852.1626 | 901.6437 | 956.5252 |
| 988.7425 | 1052.0767 | 1075.3366 |
| 1100.0681 | 1152.0306 | 1169.2359 |

| | | |
|-----------|-----------|-----------|
| 1223.9190 | 1301.1515 | 1328.9159 |
| 1361.9983 | 1385.4002 | 1396.3872 |
| 1403.4268 | 1427.2763 | 1456.4643 |
| 1490.8088 | 1494.7617 | 1829.0993 |
| 2879.3573 | 2892.6601 | 2935.9501 |
| 3013.6417 | 3038.0772 | 3046.3097 |
| 3049.8193 | 3093.3555 | 3118.7518 |

Zero-point correction (Hartree): 0.132497

C5H9O2.pmmt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.31512420

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 1.574058 | -1.442142 | 0.387843 |
| C | 2.109114 | -0.290618 | -0.121790 |
| C | 1.116698 | 0.695090 | -0.755707 |
| C | 0.165630 | 1.345097 | 0.264728 |
| C | -0.908066 | 0.394411 | 0.825182 |
| C | -1.983407 | 0.070562 | -0.191527 |
| H | 2.755418 | 0.211439 | 0.626084 |
| H | 2.820384 | -0.647179 | -0.899628 |
| H | 1.695750 | 1.479687 | -1.259432 |
| H | 0.545875 | 0.169302 | -1.531022 |
| H | 0.753074 | 1.757002 | 1.094920 |
| H | -0.331124 | 2.203971 | -0.206439 |
| H | -0.483825 | -0.543822 | 1.193156 |
| H | -1.416658 | 0.890050 | 1.666208 |
| O | -2.446938 | -1.028480 | -0.393790 |
| H | -2.355663 | 0.957283 | -0.761590 |

Rotational constants (GHz): 4.0269900 1.5742100 1.3249200

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 33.5014 | 53.4988 | 116.4491 |
| 158.4520 | 252.3540 | 334.0582 |
| 373.4493 | 460.9833 | 516.6794 |
| 680.2327 | 738.0837 | 823.2957 |
| 848.0634 | 930.2317 | 959.6471 |
| 1041.0342 | 1060.2629 | 1072.8016 |
| 1105.1482 | 1162.4567 | 1197.6457 |
| 1225.7081 | 1291.3482 | 1344.3354 |
| 1352.2222 | 1373.6904 | 1389.3177 |
| 1398.4924 | 1434.7233 | 1465.5897 |
| 1486.7550 | 1504.5293 | 1840.7296 |
| 2849.6540 | 2884.8766 | 2929.9434 |
| 3019.1971 | 3031.8701 | 3041.3341 |
| 3068.7026 | 3087.7691 | 3117.7703 |

Zero-point correction (Hartree): 0.132263

C5H9O2.pmpc

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.31882249

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -0.989740 | -1.394321 | 0.734210 |
| C | -1.560107 | -0.670050 | -0.280243 |
| C | -1.444163 | 0.856126 | -0.135089 |
| C | -0.030681 | 1.440420 | -0.296208 |
| C | 1.021098 | 0.877421 | 0.670198 |
| C | 1.673286 | -0.409057 | 0.211268 |
| H | -1.012613 | -1.004117 | -1.187812 |
| H | -2.608091 | -0.983779 | -0.445546 |
| H | -2.105106 | 1.315986 | -0.881344 |
| H | -1.850822 | 1.129794 | 0.847431 |
| H | 0.320801 | 1.272927 | -1.320728 |
| H | -0.095493 | 2.525371 | -0.157931 |
| H | 1.848135 | 1.592999 | 0.803509 |
| H | 0.613760 | 0.709003 | 1.674647 |
| O | 1.566346 | -0.884294 | -0.899811 |
| H | 2.319982 | -0.898419 | 0.973030 |

Rotational constants (GHz): 3.3850800 2.3033400 1.7348900

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 97.5906 | 115.6137 | 122.9768 |
| 178.5531 | 235.2797 | 307.6289 |
| 356.0272 | 482.8801 | 653.1751 |
| 690.4042 | 741.4435 | 793.8692 |
| 877.2877 | 898.9095 | 978.6828 |
| 995.1300 | 1057.5451 | 1074.8599 |
| 1112.6948 | 1157.6413 | 1196.8246 |
| 1254.2332 | 1283.1506 | 1338.5294 |
| 1376.2083 | 1383.7677 | 1390.7950 |
| 1407.6713 | 1427.2664 | 1457.9379 |
| 1490.1883 | 1498.1387 | 1825.4092 |
| 2902.7939 | 2906.5288 | 2952.1427 |
| 3012.5611 | 3033.9624 | 3053.7449 |
| 3073.7214 | 3077.3192 | 3097.8795 |

Zero-point correction (Hartree): 0.132974

C5H9O2.pmp

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.31454148

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -1.096040 | -1.570917 | 0.421854 |
| C | -1.780205 | -0.662109 | -0.352702 |
| C | -1.599987 | 0.809918 | 0.042792 |
| C | -0.225953 | 1.422107 | -0.284290 |
| C | 0.982350 | 0.889430 | 0.529457 |
| C | 1.509600 | -0.439859 | 0.037359 |
| H | -1.587790 | -0.818582 | -1.431393 |
| H | -2.845743 | -0.945010 | -0.216230 |
| H | -2.367802 | 1.396338 | -0.478885 |
| H | -1.803235 | 0.903377 | 1.116930 |
| H | -0.018806 | 1.315190 | -1.357637 |
| H | -0.286024 | 2.500654 | -0.100101 |
| H | 1.810899 | 1.603087 | 0.492095 |
| H | 0.683609 | 0.762988 | 1.579337 |
| O | 2.637865 | -0.623689 | -0.359189 |
| H | 0.765461 | -1.278125 | 0.058874 |

Rotational constants (GHz): 3.8640900 1.7950000 1.3494100

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 55.0417 | 77.3591 | 125.7749 |
| 179.7927 | 284.1599 | 307.8185 |
| 384.3390 | 474.0317 | 496.8517 |
| 768.6878 | 774.9508 | 839.2155 |
| 893.4942 | 916.7405 | 975.4543 |
| 1038.2235 | 1073.5119 | 1096.5992 |
| 1104.9518 | 1167.6368 | 1209.3792 |
| 1259.9671 | 1278.9497 | 1347.0759 |
| 1364.8547 | 1384.0546 | 1385.1767 |
| 1395.9398 | 1404.8329 | 1473.0788 |
| 1486.0213 | 1504.2399 | 1834.3192 |
| 2765.3406 | 2903.9697 | 2949.4158 |
| 3033.5470 | 3035.9658 | 3039.3088 |
| 3078.4418 | 3085.7080 | 3111.9092 |

Zero-point correction (Hartree): 0.132968

C5H9O2.pmtc

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.31913122

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -2.101056 | -1.273019 | -0.080988 |
| C | -2.225614 | 0.047982 | -0.420118 |
| C | -1.335813 | 1.018779 | 0.370814 |
| C | 0.156739 | 0.886493 | 0.033678 |
| C | 0.773914 | -0.449882 | 0.450025 |
| C | 2.236485 | -0.585582 | 0.097716 |
| H | -2.124047 | 0.199793 | -1.512728 |
| H | -3.293249 | 0.275402 | -0.203268 |
| H | -1.664765 | 2.042232 | 0.149911 |
| H | -1.503982 | 0.849570 | 1.441577 |
| H | 0.307767 | 1.030522 | -1.043364 |
| H | 0.710955 | 1.698064 | 0.518082 |
| H | 0.677529 | -0.617518 | 1.533745 |
| H | 0.245845 | -1.304509 | -0.000409 |
| O | 2.889469 | 0.256457 | -0.480014 |
| H | 2.702371 | -1.547799 | 0.411781 |

Rotational constants (GHz): 5.8051700 1.2629900 1.1222200

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 43.3758 | 91.1366 | 124.7666 |
| 182.4181 | 193.5689 | 292.4656 |
| 341.4253 | 462.4379 | 666.7411 |
| 680.8182 | 757.7239 | 816.8021 |
| 852.7678 | 917.3683 | 947.1885 |
| 1007.2826 | 1040.3568 | 1079.7947 |
| 1100.2292 | 1157.7466 | 1180.8672 |
| 1240.0760 | 1311.8633 | 1325.4835 |
| 1339.5855 | 1372.9090 | 1395.6266 |
| 1407.0397 | 1424.8675 | 1459.5129 |
| 1486.7298 | 1499.8655 | 1830.3187 |
| 2882.0182 | 2888.9679 | 2938.8934 |
| 3014.5762 | 3037.8239 | 3040.4302 |
| 3051.6283 | 3084.3970 | 3094.7461 |

Zero-point correction (Hartree): 0.132281

C5H9O2.pmtt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.31662340

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|--|-----------|-----------|-----------|
| O | 1.968171 | -1.397901 | -0.115693 |
| C | 2.308120 | -0.133847 | 0.285256 |
| C | 1.469120 | 0.996429 | -0.332470 |
| C | 0.019096 | 1.020588 | 0.177261 |
| C | -0.813130 | -0.201627 | -0.252897 |
| C | -2.183670 | -0.201068 | 0.384889 |
| H | 2.356454 | -0.047511 | 1.388505 |
| H | 3.360804 | -0.022477 | -0.057296 |
| H | 1.950376 | 1.953102 | -0.092945 |
| H | 1.485393 | 0.887375 | -1.423216 |
| H | 0.024761 | 1.094189 | 1.274399 |
| H | -0.469172 | 1.932498 | -0.187360 |
| H | -0.931367 | -0.244462 | -1.339749 |
| H | -0.299426 | -1.123009 | 0.061387 |
| O | -3.230716 | -0.247496 | -0.221289 |
| H | -2.174680 | -0.149379 | 1.499899 |
| Rotational constants (GHz): | 5.9805000 | 1.1790200 | 1.0501500 |
| Vibrational harmonic frequencies (cm-1): | | | |
| 54.7455 | 69.5938 | | 100.1658 |
| 122.1448 | 238.0770 | | 306.7262 |
| 359.2561 | 474.5239 | | 512.3274 |
| 747.1375 | 799.5415 | | 806.8934 |
| 891.6084 | 924.7195 | | 978.2054 |
| 1038.6405 | 1056.2103 | | 1073.8229 |
| 1098.0318 | 1151.9526 | | 1181.5872 |
| 1236.0223 | 1297.3127 | | 1317.2741 |
| 1334.3424 | 1373.9641 | | 1391.5212 |
| 1406.2563 | 1433.0512 | | 1468.5032 |
| 1485.4321 | 1504.9383 | | 1837.2546 |
| 2866.8940 | 2884.4163 | | 2940.3005 |
| 3011.2607 | 3023.4099 | | 3042.9437 |
| 3072.0951 | 3093.2545 | | 3114.2711 |
| Zero-point correction (Hartree): | 0.132409 | | |

C5H9O2.ppmc

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.31769037
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | |
|--|-----------|-----------|-----------|
| O | 2.396626 | -0.449624 | -0.728517 |
| C | 1.666598 | -0.487252 | 0.421617 |
| C | 0.867522 | 0.797787 | 0.712133 |
| C | -0.120327 | 1.170039 | -0.415109 |
| C | -1.597071 | 0.879593 | -0.120243 |
| C | -2.002216 | -0.565928 | 0.030956 |
| H | 0.938747 | -1.312512 | 0.255309 |
| H | 2.278200 | -0.797944 | 1.290117 |
| H | 0.347425 | 0.677019 | 1.671505 |
| H | 1.589296 | 1.609993 | 0.855318 |
| H | -0.040976 | 2.240451 | -0.632411 |
| H | 0.187294 | 0.655507 | -1.332469 |
| H | -1.927550 | 1.393082 | 0.797103 |
| H | -2.241906 | 1.294800 | -0.910397 |
| O | -1.262138 | -1.526678 | -0.017440 |
| H | -3.093482 | -0.715424 | 0.197453 |
| Rotational constants (GHz): | 4.1032300 | 1.7200500 | 1.3984900 |
| Vibrational harmonic frequencies (cm-1): | | | |
| 56.9247 | 98.6059 | | 157.0084 |
| 166.0436 | 208.3227 | | 291.5940 |
| 373.7958 | 479.9043 | | 645.0603 |
| 725.0893 | 757.6934 | | 822.8140 |
| 870.7433 | 915.0647 | | 975.0680 |
| 1005.3891 | 1073.8297 | | 1089.5860 |
| 1122.5841 | 1159.1448 | | 1190.3431 |
| 1267.5713 | 1278.3521 | | 1310.7267 |
| 1364.7230 | 1386.6506 | | 1392.0643 |
| 1405.0273 | 1432.4580 | | 1453.8323 |
| 1498.4017 | 1511.2998 | | 1826.1411 |
| 2884.1334 | 2894.3342 | | 2951.0494 |
| 3008.9274 | 3034.2808 | | 3040.2003 |
| 3059.5112 | 3084.5564 | | 3098.0094 |
| Zero-point correction (Hartree): | 0.132969 | | |

C5H9O2.ppmr

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.31639658
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -1.365093 | -1.319725 | 0.781987 |
| C | -1.456113 | -0.742886 | -0.454216 |
| C | -1.403190 | 0.797682 | -0.453575 |
| C | -0.286329 | 1.405073 | 0.407620 |
| C | 1.150220 | 1.093343 | -0.071535 |
| C | 1.636323 | -0.284589 | 0.322031 |

| | | | | |
|--|-----------|-----------|-----------|--|
| H | -0.572509 | -1.149373 | -0.993972 | |
| H | -2.327847 | -1.116364 | -1.022863 | |
| H | -1.314067 | 1.140620 | -1.492752 | |
| H | -2.367616 | 1.169392 | -0.085924 | |
| H | -0.416656 | 2.492469 | 0.421151 | |
| H | -0.407705 | 1.063899 | 1.442319 | |
| H | 1.245073 | 1.200353 | -1.157478 | |
| H | 1.836037 | 1.811464 | 0.400412 | |
| O | 1.964903 | -1.150261 | -0.461103 | |
| H | 1.681351 | -0.464318 | 1.420081 | |
| Rotational constants (GHz): | 3.3492700 | 2.0848100 | 1.5282400 | |
| Vibrational harmonic frequencies (cm-1): | | | | |
| 38.1533 | 70.5011 | | 86.8368 | |
| 210.6678 | 236.7091 | | 312.9017 | |
| 390.5593 | 484.3355 | | 543.6307 | |
| 728.5552 | 757.0254 | | 835.9096 | |
| 900.1775 | 915.6595 | | 977.0116 | |
| 1035.6490 | 1056.8349 | | 1088.4624 | |
| 1113.0604 | 1159.9660 | | 1196.2286 | |
| 1229.5189 | 1285.5621 | | 1297.5050 | |
| 1355.0958 | 1384.9159 | | 1394.0784 | |
| 1409.3444 | 1430.3239 | | 1479.2373 | |
| 1496.7048 | 1501.4784 | | 1826.7615 | |
| 2891.4360 | 2899.6472 | | 2959.0213 | |
| 3028.0170 | 3038.2090 | | 3055.7838 | |
| 3080.1239 | 3094.3596 | | 3103.7713 | |
| Zero-point correction (Hartree): | 0.132999 | | | |

C5H9O2.pppc

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.31797364
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | | |
|--|-----------|-----------|-----------|--|
| O | 2.769109 | 0.472713 | -0.131741 | |
| C | 1.864929 | -0.453054 | -0.581741 | |
| C | 0.759666 | -0.829903 | -0.415945 | |
| C | -0.032007 | 0.373785 | 0.949460 | |
| C | -0.958087 | 1.044396 | -0.071352 | |
| C | -2.165086 | 0.228175 | -0.476752 | |
| H | 1.429595 | 0.017423 | -1.491959 | |
| H | 2.382547 | -1.348340 | -0.976408 | |
| H | 0.085616 | -1.557025 | -0.049603 | |
| H | 1.235371 | -1.341934 | 1.260976 | |
| H | -0.637285 | 0.048628 | 1.801842 | |
| H | 0.680889 | 1.116435 | 1.322858 | |
| H | -1.347465 | 1.996065 | 0.322132 | |
| H | -0.431101 | 1.332854 | -0.993552 | |
| O | -2.442782 | -0.868367 | -0.040971 | |
| H | -2.825269 | 0.720737 | -1.227939 | |
| Rotational constants (GHz): | 5.7668000 | 1.3055500 | 1.2334700 | |
| Vibrational harmonic frequencies (cm-1): | | | | |
| 34.6234 | 80.4757 | | 142.7380 | |
| 171.7693 | 237.1170 | | 287.6518 | |
| 376.0055 | 506.0071 | | 617.2365 | |
| 651.4699 | 725.1309 | | 799.6461 | |
| 833.8781 | 907.8523 | | 952.8933 | |
| 1006.6337 | 1044.4439 | | 1078.0156 | |
| 1118.6330 | 1147.9540 | | 1192.2105 | |
| 1238.2028 | 1316.0624 | | 1324.8289 | |
| 1369.0503 | 1373.6595 | | 1396.9627 | |
| 1407.5986 | 1429.3497 | | 1459.5672 | |
| 1491.5165 | 1503.0370 | | 1830.9920 | |
| 2880.9830 | 2883.6028 | | 2945.6889 | |
| 3019.2190 | 3041.4644 | | 3054.7999 | |
| 3066.6866 | 3101.1944 | | 3110.7880 | |
| Zero-point correction (Hartree): | 0.132493 | | | |

C5H9O2.pppt

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.31726210
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | | |
|---|-----------|-----------|-----------|--|
| O | 2.205388 | -0.325647 | -0.893203 | |
| C | 1.514727 | -0.768145 | -0.198182 | |
| C | 0.843713 | 0.329715 | 1.043441 | |
| C | 0.057617 | 1.362880 | 0.221783 | |
| C | -0.996865 | 0.765776 | -0.748307 | |
| C | -1.968731 | -0.138444 | -0.030650 | |
| H | 0.717404 | -1.421076 | -0.225264 | |
| H | 2.122280 | -1.448096 | 0.824472 | |
| H | 0.194606 | -0.163400 | 1.777031 | |
| H | 1.616532 | 0.857474 | 1.615459 | |
| H | -0.430069 | 2.066223 | 0.907452 | |
| H | 0.757007 | 1.945437 | -0.385208 | |
| H | -1.543953 | 1.587126 | -1.225406 | |

| | | | | |
|---|-----------|-----------|-----------|--|
| H | -0.493101 | 0.187203 | -1.527554 | |
| O | -1.803555 | -1.334344 | 0.107253 | |
| H | -2.858133 | 0.358337 | 0.419927 | |
| Rotational constants (GHz): | 3.9271100 | 1.7471600 | 1.5426500 | |
| Vibrational harmonic frequencies (cm ⁻¹): | | | | |
| 57.5033 | 75.4889 | | 108.1666 | |
| 194.5616 | 223.0474 | | 286.1685 | |
| 396.5106 | 513.9724 | | 554.2811 | |
| 710.1158 | 779.2540 | | 839.7018 | |
| 882.3439 | 933.2896 | | 979.6346 | |
| 1021.7374 | 1052.9936 | | 1094.9741 | |
| 1113.0911 | 1153.7301 | | 1196.5429 | |
| 1233.8411 | 1273.9774 | | 1306.6827 | |
| 1346.8131 | 1380.5497 | | 1388.9893 | |
| 1410.0575 | 1429.8725 | | 1490.6895 | |
| 1501.2534 | 1502.0605 | | 1816.9192 | |
| 2866.4336 | 2893.3613 | | 2954.5589 | |
| 3045.4027 | 3054.9592 | | 3060.4930 | |
| 3085.9298 | 3108.6406 | | 3124.0230 | |
| Zero-point correction (Hartree): | 0.133142 | | | |

C5H9O2.pptc

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.31768050
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 2.391162 | -1.173825 | -0.361908 |
| C | 2.248227 | -0.033820 | 0.382431 |
| C | 1.290473 | 1.016384 | -0.202383 |
| C | -0.114039 | 0.480437 | -0.508847 |
| C | -0.935280 | 0.130685 | 0.734383 |
| C | -2.362682 | -0.271881 | 0.436135 |
| | | | |
| H | 1.878176 | -0.395833 | 1.367518 |
| H | 3.237098 | 0.402645 | 0.622099 |
| H | 1.240593 | 1.866334 | 0.492385 |
| H | 1.737592 | 1.398336 | -1.127947 |
| H | -0.668139 | 1.219293 | -1.096407 |
| H | -0.023554 | -0.406944 | -1.143452 |
| H | -0.486944 | -0.691245 | 1.312556 |
| H | -0.983247 | 0.977201 | 1.438530 |
| O | -2.857361 | -0.294480 | -0.669076 |
| H | -2.962175 | -0.554184 | 1.332282 |

| | | | |
|---|-----------|-----------|-----------|
| Rotational constants (GHz): | 6.0244800 | 1.1370400 | 1.1022000 |
| Vibrational harmonic frequencies (cm ⁻¹): | | | |
| 38.2474 | 62.2324 | | 158.1250 |
| 169.1277 | 213.2952 | | 233.1606 |
| 373.8122 | 512.5658 | | 599.6133 |
| 669.9708 | 689.5287 | | 807.7064 |
| 865.2989 | 901.8542 | | 932.0430 |
| 1022.0765 | 1046.9130 | | 1094.9831 |
| 1107.1253 | 1152.9489 | | 1192.3774 |
| 1275.3831 | 1299.8951 | | 1338.4365 |
| 1343.2727 | 1371.1210 | | 1396.8008 |
| 1412.1841 | 1428.1967 | | 1464.0193 |
| 1494.1204 | 1502.9523 | | 1834.8003 |
| 2884.5559 | 2886.2275 | | 2942.8020 |
| 3007.6430 | 3032.3206 | | 3039.9710 |
| 3070.1911 | 3082.8203 | | 3114.8971 |
| Zero-point correction (Hartree): | 0.132283 | | |

C5H9O2.pptt

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.31627220
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 2.510576 | -1.122122 | -0.304035 |
| C | 2.255940 | -0.052436 | 0.511293 |
| C | 1.364149 | 1.038508 | -0.102186 |
| C | 0.025244 | 0.516048 | -0.641480 |
| C | -0.958018 | 0.062852 | 0.455791 |
| C | -2.242496 | -0.478450 | -0.131006 |
| H | 1.768041 | -0.500971 | 1.405136 |
| H | 3.197273 | 0.368098 | 0.913750 |
| H | 1.200585 | 1.823008 | 0.648482 |
| H | 1.921067 | 1.504407 | -0.923975 |
| H | -0.449080 | 1.302424 | -1.239903 |
| H | 0.230879 | -0.319699 | -1.321042 |
| H | -0.507465 | -0.749085 | 1.045798 |
| H | -1.208869 | 0.880965 | 1.138710 |
| O | -3.350334 | -0.067405 | 0.133708 |
| H | -2.103282 | -1.312060 | -0.858811 |

| | | | |
|---|-----------|-----------|-----------|
| Rotational constants (GHz): | 6.9156400 | 1.0455100 | 0.9907600 |
| Vibrational harmonic frequencies (cm ⁻¹): | | | |
| 45.6115 | 60.4576 | | 69.2076 |

| | | |
|-----------|-----------|-----------|
| 179.3784 | 217.4083 | 275.1756 |
| 390.0667 | 506.7546 | 523.9839 |
| 625.2035 | 748.5932 | 821.4093 |
| 876.0490 | 897.4337 | 1006.2549 |
| 1027.7720 | 1048.1479 | 1097.1591 |
| 1111.9850 | 1155.2691 | 1192.3634 |
| 1262.8141 | 1295.7030 | 1323.3521 |
| 1344.2180 | 1370.5460 | 1390.8391 |
| 1406.4703 | 1432.8557 | 1477.7165 |
| 1492.6423 | 1506.9911 | 1836.9685 |
| 2878.4516 | 2885.4553 | 2948.3159 |
| 3022.5656 | 3040.0688 | 3050.1382 |
| 3083.2038 | 3089.0717 | 3109.6974 |

Zero-point correction (Hartree): 0.132416

C5H9O2.ptmc

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.31974131

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 2.978794 | 0.420280 | -0.133735 |
| C | 2.154450 | -0.664255 | 0.013851 |
| C | 0.740467 | -0.351733 | 0.517871 |
| C | 0.000936 | 0.630635 | -0.398351 |
| C | -1.363591 | 1.069579 | 0.137659 |
| C | -2.428830 | -0.003970 | 0.126756 |
| H | 2.106098 | -1.119607 | -1.000707 |
| H | 2.651062 | -1.441630 | 0.626199 |
| H | 0.178021 | -1.287812 | 0.601645 |
| H | 0.821708 | 0.069770 | 1.528971 |
| H | 0.633587 | 1.512551 | -0.543471 |
| H | -0.139422 | 0.170523 | -1.384259 |
| H | -1.291961 | 1.453546 | 1.166908 |
| H | -1.767537 | 1.911460 | -0.445682 |
| O | -2.278743 | -1.128397 | -0.301121 |
| H | -3.412553 | 0.314602 | 0.542527 |

Rotational constants (GHz): 6.5784500 1.1877300 1.0721700

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 53.4978 | 94.8459 | 136.0217 |
| 160.2387 | 235.7317 | 252.5068 |
| 348.1712 | 513.5852 | 576.9395 |
| 659.6353 | 713.2430 | 801.5332 |
| 861.3560 | 901.2725 | 956.6051 |
| 1020.5113 | 1033.3304 | 1086.5570 |
| 1108.3187 | 1161.4547 | 1219.8972 |
| 1245.5210 | 1320.9242 | 1328.5972 |
| 1362.4976 | 1367.6556 | 1386.8982 |
| 1416.6902 | 1429.1063 | 1455.7731 |
| 1496.1741 | 1508.1696 | 1830.2700 |
| 2882.6250 | 2887.1564 | 2942.8422 |
| 3015.2363 | 3036.6334 | 3040.0081 |
| 3055.7000 | 3090.5946 | 3108.8927 |

Zero-point correction (Hartree): 0.132369

C5H9O2.ptmt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.31722546

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -3.065537 | 0.351150 | -0.238608 |
| C | -2.259951 | -0.661366 | 0.211310 |
| C | -0.786031 | -0.557200 | -0.199694 |
| C | -0.142219 | 0.756282 | 0.260445 |
| C | 1.298685 | 0.946164 | -0.248415 |
| C | 2.261486 | -0.045661 | 0.365381 |
| H | -2.357365 | -0.633218 | 1.319509 |
| H | -2.697177 | -1.641013 | -0.062881 |
| H | -0.244472 | -1.423317 | 0.203631 |
| H | -0.723563 | -0.634694 | -1.292604 |
| H | -0.761986 | 1.588212 | -0.088925 |
| H | -0.149897 | 0.806494 | 1.359073 |
| H | 1.358284 | 0.861234 | -1.338076 |
| H | 1.646868 | 1.950834 | 0.033121 |
| O | 2.996100 | -0.781524 | -0.255050 |
| H | 2.252986 | -0.060848 | 1.482257 |

Rotational constants (GHz): 7.5494200 1.0443000 0.9719700

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 50.1627 | 53.1826 | 111.4956 |
| 154.8222 | 235.3222 | 267.0349 |
| 391.5740 | 489.8552 | 514.1188 |
| 568.1827 | 756.2772 | 783.3305 |
| 890.8478 | 920.6009 | 980.9103 |
| 1022.8078 | 1042.1373 | 1091.7171 |
| 1103.4225 | 1169.2457 | 1215.4963 |
| 1234.7830 | 1313.7431 | 1330.9194 |

| | | |
|-----------|-----------|-----------|
| 1352.0827 | 1364.5092 | 1373.9673 |
| 1416.6978 | 1432.3962 | 1475.3060 |
| 1494.7546 | 1511.8097 | 1837.9863 |
| 2859.7595 | 2884.8611 | 2942.9878 |
| 3022.0906 | 3028.3819 | 3037.8835 |
| 3075.9102 | 3099.9683 | 3109.9795 |

Zero-point correction (Hartree): 0.132164

C5H9O2.ptpc

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.31839866

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 2.521320 | 0.767631 | -0.658128 |
| C | 2.261770 | -0.078858 | 0.386556 |
| C | 0.777971 | -0.283691 | 0.719713 |
| C | -0.033967 | -0.762926 | -0.489331 |
| C | -1.517385 | -0.995508 | -0.190023 |
| C | -2.327347 | 0.252940 | 0.080273 |
| H | 2.719133 | -1.044786 | 0.072912 |
| H | 2.847846 | 0.214227 | 1.279007 |
| H | 0.706253 | -1.006804 | 1.544530 |
| H | 0.366042 | 0.663195 | 1.083097 |
| H | 0.066245 | -0.022723 | -1.289070 |

| | | | |
|---|-----------|-----------|-----------|
| H | 0.395201 | -1.699519 | -0.869408 |
| H | -2.013346 | -1.508392 | -1.028531 |
| H | -1.659483 | -1.669323 | 0.669469 |
| O | -1.895211 | 1.384739 | 0.057022 |
| H | -3.403018 | 0.063427 | 0.303720 |

Rotational constants (GHz): 5.1254300 1.3195500 1.1848200

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 53.6561 | 91.9420 | 148.0363 |
| 152.6147 | 238.6164 | 248.7005 |
| 335.1258 | 515.1201 | 613.4077 |
| 659.7691 | 714.1327 | 813.3650 |
| 858.7286 | 890.6660 | 957.6627 |
| 998.5717 | 1059.4328 | 1097.9428 |
| 1108.3999 | 1157.4817 | 1205.4266 |
| 1271.0893 | 1304.6356 | 1335.2777 |
| 1364.5708 | 1370.3658 | 1386.9936 |
| 1418.9220 | 1430.8233 | 1456.9713 |
| 1495.0595 | 1507.0555 | 1833.2406 |
| 2873.7171 | 2882.7817 | 2943.5333 |
| 3012.1290 | 3031.0414 | 3035.2704 |
| 3042.4174 | 3100.5875 | 3113.9379 |

Zero-point correction (Hartree): 0.132428

C5H9O2.ptpt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.31723488

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -2.657881 | -0.569318 | -0.834567 |
| C | -2.336394 | -0.179139 | 0.438688 |
| C | -0.835038 | -0.061102 | 0.728337 |
| C | -0.132425 | 0.923426 | -0.213991 |
| C | 1.394349 | 0.976517 | -0.019571 |
| C | 2.073467 | -0.308391 | -0.440849 |
| H | -2.834906 | 0.807374 | 0.568821 |
| H | -2.849738 | -0.829041 | 1.173587 |
| H | -0.697572 | 0.244809 | 1.773973 |
| H | -0.386124 | -1.058415 | 0.636651 |
| H | -0.366028 | 0.643127 | -1.248607 |
| H | -0.543432 | 1.930227 | -0.067769 |
| H | 1.806149 | 1.778449 | -0.649874 |
| H | 1.668579 | 1.190116 | 1.018568 |
| O | 2.832616 | -0.952149 | 0.248878 |
| H | 1.821441 | -0.642768 | -1.475522 |

Rotational constants (GHz): 5.7092400 1.1198900 1.0712100

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 44.7764 | 62.3476 | 114.0158 |
| 154.0428 | 230.8894 | 285.4245 |
| 369.4259 | 484.9271 | 515.0016 |
| 571.5646 | 760.8889 | 777.9337 |
| 883.5202 | 919.9088 | 979.1925 |
| 1027.9713 | 1041.6399 | 1094.1734 |
| 1116.8397 | 1160.3523 | 1195.9814 |
| 1255.0025 | 1307.3276 | 1332.0280 |
| 1352.2936 | 1363.1681 | 1374.4858 |
| 1416.4573 | 1433.6190 | 1476.3670 |
| 1494.7175 | 1511.3259 | 1837.0473 |
| 2870.9075 | 2884.3564 | 2943.3002 |
| 3025.0661 | 3036.1785 | 3043.7570 |
| 3069.3795 | 3088.7755 | 3107.2284 |

Zero-point correction (Hartree): 0.132165

C5H9O2.pttc

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.31896813

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 2.683407 | -0.998285 | -0.524349 |
| C | 2.470490 | 0.031430 | 0.353262 |
| C | 1.215957 | 0.872188 | 0.084679 |
| C | -0.069667 | 0.041407 | 0.142222 |
| C | -1.316251 | 0.837953 | -0.241049 |
| C | -2.607587 | 0.058914 | -0.135331 |
| H | 2.406169 | -0.450520 | 1.353928 |
| H | 3.381418 | 0.657699 | 0.423510 |
| H | 1.179593 | 1.693127 | 0.814231 |
| H | 1.321017 | 1.337464 | -0.904363 |
| H | 0.033339 | -0.820953 | -0.524515 |
| H | -0.205048 | -0.371176 | 1.149571 |
| H | -1.431205 | 1.736818 | 0.385758 |
| H | -1.248595 | 1.223694 | -1.270045 |
| O | -2.692912 | -1.087059 | 0.247888 |
| H | -3.518291 | 0.625245 | -0.439086 |

Rotational constants (GHz): 6.4490300 1.0608000 0.9633200

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 50.4064 | 86.8785 | 117.2643 |
| 161.2376 | 183.0345 | 283.6570 |
| 316.9470 | 493.8758 | 543.7156 |
| 674.8468 | 694.1307 | 778.9137 |
| 892.5889 | 907.1995 | 941.0673 |
| 1003.2401 | 1066.8545 | 1094.3505 |
| 1106.5328 | 1165.9907 | 1204.8363 |
| 1276.6333 | 1301.3836 | 1327.7155 |
| 1360.4388 | 1364.5672 | 1385.5070 |
| 1418.7658 | 1427.0818 | 1463.1944 |
| 1493.2344 | 1513.6056 | 1834.2165 |
| 2885.0275 | 2887.9867 | 2938.2903 |
| 3009.1233 | 3027.9561 | 3036.1461 |

3054.2815 3067.9875 3107.2381

Zero-point correction (Hartree): 0.132015

C5H9O2.pttt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.31741612

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 2.869600 | -1.009748 | -0.223389 |
| C | 2.577198 | 0.206151 | 0.335388 |
| C | 1.254807 | 0.834900 | -0.122153 |
| C | 0.048394 | -0.065292 | 0.164088 |
| C | -1.271357 | 0.504843 | -0.385029 |
| C | -2.430009 | -0.444438 | -0.176410 |
| H | 2.557323 | 0.018698 | 1.432053 |
| H | 3.431524 | 0.898269 | 0.204522 |
| H | 1.135463 | 1.808497 | 0.371451 |
| H | 1.321128 | 1.034827 | -1.199508 |
| H | 0.242109 | -1.051906 | -0.274244 |
| H | -0.045703 | -0.218306 | 1.247752 |
| H | -1.523842 | 1.465141 | 0.075606 |
| H | -1.167909 | 0.665458 | -1.469037 |
| O | -3.464285 | -0.161280 | 0.386109 |
| H | -2.266821 | -1.469443 | -0.585657 |

Rotational constants (GHz): 8.8630600 0.9056400 0.8637700

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 52.2692 | 69.1741 | 98.6710 |
| 149.5399 | 181.8242 | 296.4798 |
| 352.7088 | 483.9718 | 516.4306 |
| 564.4426 | 752.1097 | 813.4695 |
| 888.9692 | 909.3871 | 998.6997 |
| 1024.5476 | 1057.8854 | 1093.3637 |
| 1114.8558 | 1165.8667 | 1205.7566 |
| 1263.8816 | 1298.4221 | 1332.0005 |
| 1345.8617 | 1363.9764 | 1375.3870 |
| 1415.0259 | 1432.1068 | 1477.8068 |
| 1495.2695 | 1517.8644 | 1837.3715 |
| 2874.6083 | 2886.4155 | 2943.2216 |
| 3017.8374 | 3031.0340 | 3039.0690 |
| 3068.2758 | 3086.6891 | 3110.4785 |

Zero-point correction (Hartree): 0.132141

C5H9O2.tpmc

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.31680674

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -2.765911 | -0.631089 | -0.361878 |
| C | -1.600210 | -0.333018 | 0.277297 |
| C | -0.936199 | 0.980294 | -0.173134 |
| C | 0.435388 | 1.270561 | 0.471490 |
| C | 1.660149 | 0.762407 | -0.302870 |
| C | 1.941343 | -0.719806 | -0.257513 |
| H | -1.726531 | -0.363192 | 1.378660 |
| H | -0.923730 | -1.192367 | 0.081577 |
| H | -0.856568 | 0.971535 | -1.267215 |
| H | -1.627972 | 1.793992 | 0.074550 |
| H | 0.551023 | 2.354785 | 0.575043 |
| H | 0.462888 | 0.864509 | 1.490658 |
| H | 1.607152 | 1.049502 | -1.364538 |
| H | 2.577993 | 1.247924 | 0.064427 |
| O | 1.274840 | -1.551905 | 0.321964 |
| H | 2.861489 | -1.025366 | -0.805461 |

Rotational constants (GHz): 4.0756600 1.6109500 1.2591100

Vibrational harmonic frequencies (cm⁻¹):

| | | |
|-----------|-----------|-----------|
| 33.3843 | 88.8534 | 126.5246 |
| 153.6150 | 212.6414 | 281.8722 |
| 344.3962 | 475.1030 | 650.1123 |
| 672.4155 | 718.1090 | 790.9803 |
| 888.0880 | 905.5114 | 977.4402 |
| 1016.0381 | 1072.1861 | 1097.9028 |
| 1099.1507 | 1159.3944 | 1212.0124 |
| 1273.5666 | 1283.7807 | 1339.5662 |
| 1368.8823 | 1381.6670 | 1387.3775 |
| 1393.6042 | 1430.7311 | 1453.6944 |
| 1497.2063 | 1504.5627 | 1826.7242 |
| 2897.4996 | 2904.8113 | 2926.9198 |
| 3012.9683 | 3036.2571 | 3044.6578 |
| 3050.0340 | 3086.6212 | 3088.9916 |

Zero-point correction (Hartree): 0.132512

C5H9O2.tpmt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.31457062

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -2.691426 | -0.887622 | -0.117334 |
| C | -1.435369 | -0.476918 | 0.230967 |
| C | -1.112895 | 0.971413 | -0.175375 |
| C | 0.262876 | 1.490233 | 0.271948 |
| C | 1.474243 | 0.784792 | -0.388575 |
| C | 1.848037 | -0.508511 | 0.299088 |
| H | -1.237746 | -0.657355 | 1.307054 |
| H | -0.759498 | -1.189412 | -0.289300 |
| H | -1.210085 | 1.056006 | -1.264322 |
| H | -1.887887 | 1.615517 | 0.257127 |
| H | 0.318954 | 2.557836 | 0.034802 |
| H | 0.351956 | 1.423351 | 1.365949 |
| H | 1.282562 | 0.580409 | -1.446842 |
| H | 2.347821 | 1.447151 | -0.318310 |
| O | 1.732398 | -1.614493 | -0.183725 |
| H | 2.244804 | -0.382638 | 1.333994 |

Rotational constants (GHz): 3.6939500 1.6518100 1.2237200

Vibrational harmonic frequencies (cm⁻¹):

| | | |
|-----------|-----------|-----------|
| 44.6556 | 77.7644 | 116.9264 |
| 129.0213 | 239.0942 | 306.2521 |
| 360.5544 | 473.7326 | 507.8010 |
| 689.0519 | 771.8771 | 828.7097 |
| 877.6093 | 946.8521 | 997.2655 |
| 1027.6201 | 1067.7316 | 1084.1070 |
| 1093.6592 | 1169.7239 | 1218.1466 |
| 1239.3135 | 1294.7254 | 1325.9784 |
| 1353.5909 | 1375.5771 | 1385.9394 |
| 1396.8726 | 1431.7848 | 1482.5817 |
| 1500.1337 | 1504.7862 | 1829.6601 |
| 2878.1419 | 2901.2847 | 2929.7851 |
| 3025.9617 | 3036.5111 | 3047.4964 |
| 3085.7103 | 3092.9774 | 3110.4317 |

Zero-point correction (Hartree): 0.132720

C5H9O2.tppc

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.31633743

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 2.951518 | -0.739048 | -0.311821 |
| C | 1.932187 | 0.173736 | -0.326539 |
| C | 0.842199 | -0.057269 | 0.730496 |
| C | -0.297041 | 0.974194 | 0.681058 |
| C | -1.214282 | 0.864361 | -0.543178 |

| | | | |
|--|-----------|-----------|-----------|
| C | -2.138041 | -0.334893 | -0.533792 |
| H | 2.322349 | 1.211018 | -0.294209 |
| H | 1.508842 | 0.077726 | -1.351304 |
| H | 0.444917 | -1.071088 | 0.623717 |
| H | 1.321527 | -0.010828 | 1.715258 |
| H | -0.912556 | 0.858627 | 1.578842 |
| H | 0.123545 | 1.987465 | 0.718343 |
| H | -1.863237 | 1.749934 | -0.626949 |
| H | -0.657484 | 0.846854 | -1.492001 |
| O | -2.235641 | -1.126776 | 0.377892 |
| H | -2.765049 | -0.443883 | -1.448533 |
| Rotational constants (GHz): | 5.0891300 | 1.2463100 | 1.1733800 |
| Vibrational harmonic frequencies (cm-1): | | | |
| 46.6697 | 84.0579 | | 115.0583 |
| 176.3259 | 209.3370 | | 291.0932 |
| 342.9659 | 461.8343 | | 631.5979 |
| 654.6190 | 712.7817 | | 799.5410 |
| 862.8694 | 912.3291 | | 958.7618 |
| 996.0188 | 1070.3673 | | 1087.7222 |
| 1102.0441 | 1146.1098 | | 1204.5350 |
| 1238.9114 | 1310.5987 | | 1328.9676 |
| 1362.4519 | 1382.2175 | | 1391.3570 |
| 1393.9457 | 1428.8763 | | 1460.4153 |
| 1493.0678 | 1509.1017 | | 1833.0371 |
| 2880.6961 | 2888.5534 | | 2926.3714 |
| 3017.6062 | 3040.4548 | | 3046.4997 |
| 3060.8428 | 3099.1866 | | 3117.4929 |
| Zero-point correction (Hartree): | 0.132310 | | |

C5H9O2.tppt

```
-----
E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.31523205
Electronic state : 2-A
Cartesian coordinates (Angs):
O      -2.714038      -0.791870      -0.007940
C      -1.577107      -0.171158      0.426696
C      -0.865518      0.670952      -0.645721
C      0.326980      1.484137      -0.116978
C      1.404815      0.654848      0.627307
C      1.926974      -0.475065      -0.228395
H      -1.760463      0.406565      1.355132
H      -0.913173      -1.007691      0.738562
H      -0.552435      -0.000218      -1.453361
H      -1.597856      1.361201      -1.080035
H      0.793207      2.016587      -0.954942
H      -0.028566      2.258387      0.574019
H      2.237060      1.316858      0.897401
H      0.997762      0.223309      1.546701
O      1.573422      -1.630048      -0.114472
H      2.652527      -0.181943      -1.021635
Rotational constants (GHz):      3.8754100      1.6274900      1.2870500
Vibrational harmonic frequencies (cm-1):
53.8686      77.7456      128.7120
165.8146      214.1945      297.7761
376.3937      494.0552      509.1020
697.2696      783.4457      820.6434
900.5944      943.4060      981.3481
1025.2252      1072.5939      1086.9837
1102.5814      1160.3068      1201.9978
1241.5949      1299.2856      1312.1706
1353.2450      1376.0632      1386.7118
1401.1637      1429.7546      1491.1300
1502.4085      1507.6694      1824.6460
2885.1080      2890.7168      2928.9018
3041.6831      3050.9186      3056.1364
3078.9119      3101.2179      3115.3929
Zero-point correction (Hartree): 0.132974
```

C5H9O2.tptc

```
-----
E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.31699715
Electronic state : 2-A
Cartesian coordinates (Angs):
O      3.388463      -0.298302      -0.071445
C      2.062583      -0.271577      -0.407764
C      1.202503      0.693873      0.421390
C      -0.281809      0.699776      0.029238
C      -1.023932      -0.596290      0.365117
C      -2.504613      -0.553826      0.057588
H      1.931272      -0.103870      -1.495695
H      1.727705      -1.322082      -0.257711
H      1.323156      0.444114      1.482906
H      1.614387      1.701224      0.289821
H      -0.787691      1.529061      0.534083
H      -0.387400      0.904844      -1.043374
```

| | | | | |
|--|-----------|-----------|-----------|-----------|
| H | -0.613921 | -1.466070 | -0.170855 | |
| H | -0.920853 | -0.852201 | 1.431441 | |
| O | -3.083214 | 0.401335 | -0.411331 | |
| H | -3.057036 | -1.491017 | 0.298181 | |
| Rotational constants (GHz): | 9.2981500 | | 0.9494200 | 0.9135500 |
| Vibrational harmonic frequencies (cm-1): | | | | |
| 37.6295 | | 85.6114 | | 109.3057 |
| 172.7918 | | 195.9268 | | 251.3289 |
| 323.1658 | | 482.1759 | | 616.0325 |
| 667.7435 | | 704.2682 | | 809.5226 |
| 849.9805 | | 912.6436 | | 956.7952 |
| 1021.3811 | | 1066.0876 | | 1084.3562 |
| 1099.0447 | | 1160.2165 | | 1208.8662 |
| 1268.1251 | | 1301.8534 | | 1330.9196 |
| 1342.3133 | | 1372.5863 | | 1388.8802 |
| 1406.4111 | | 1427.1927 | | 1464.2000 |
| 1500.1893 | | 1504.7546 | | 1833.8808 |
| 2883.1447 | | 2890.1395 | | 2929.3682 |
| 3012.2448 | | 3037.5095 | | 3046.7216 |
| 3054.5820 | | 3091.5378 | | 3100.3390 |
| Zero-point correction (Hartree): | 0.132138 | | | |

C5H9O2.tptt

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.31521255
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | | |
|--|-----------|-----------|-----------|-----------|
| O | 3.347362 | -0.565069 | 0.130025 | |
| C | 2.028570 | -0.509512 | -0.228200 | |
| C | 1.333521 | 0.825106 | 0.079471 | |
| C | -0.143769 | 0.867629 | -0.337754 | |
| C | -1.051199 | -0.084159 | 0.467399 | |
| C | -2.513556 | 0.120560 | 0.137154 | |
| H | 1.893234 | -0.806801 | -1.287511 | |
| H | 1.555977 | -1.338926 | 0.342257 | |
| H | 1.435144 | 1.034079 | 1.151395 | |
| H | 1.880296 | 1.615659 | -0.447800 | |
| H | -0.512651 | 1.894520 | -0.221427 | |
| H | -0.232925 | 0.632191 | -1.406800 | |
| H | -0.812069 | -1.137557 | 0.293874 | |
| H | -0.921940 | 0.122743 | 1.540781 | |
| O | -3.263864 | -0.747636 | -0.247922 | |
| H | -2.874442 | 1.167985 | 0.269997 | |
| Rotational constants (GHz): | 8.2210900 | | 0.9262700 | 0.8729600 |
| Vibrational harmonic frequencies (cm-1): | | | | |
| 58.1046 | | 65.9402 | | 94.1596 |
| 112.4867 | | 254.9432 | | 266.0880 |
| 324.7297 | | 496.6770 | | 523.8242 |
| 616.1529 | | 758.2557 | | 801.7970 |
| 886.8432 | | 919.6752 | | 999.5597 |
| 1037.4984 | | 1065.3059 | | 1086.0358 |
| 1110.6591 | | 1159.4783 | | 1215.5949 |
| 1265.4125 | | 1289.0714 | | 1319.8151 |
| 1346.7524 | | 1375.3477 | | 1391.4080 |
| 1394.2741 | | 1433.2426 | | 1477.4303 |
| 1499.6458 | | 1508.7212 | | 1838.7270 |
| 2873.7523 | | 2892.1703 | | 2930.3408 |
| 3018.3176 | | 3034.5387 | | 3047.1748 |
| 3071.1740 | | 3094.1320 | | 3110.4002 |
| Zero-point correction (Hartree): | 0.132283 | | | |

C5H9O2.ttpc

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.31826564
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | | |
|--|-----------|-----------|-----------|-----------|
| O | 3.151997 | -0.596009 | -0.332702 | |
| C | 2.165092 | 0.075394 | 0.336081 | |
| C | 0.803284 | 0.120504 | -0.365297 | |
| C | -0.243742 | 0.898010 | 0.442582 | |
| C | -1.616121 | 0.960003 | -0.233733 | |
| C | -2.383970 | -0.343845 | -0.223514 | |
| H | 2.076500 | -0.433943 | 1.321114 | |
| H | 2.523303 | 1.090357 | 0.606583 | |
| H | 0.938071 | 0.584970 | -1.350995 | |
| H | 0.462461 | -0.905463 | -0.534038 | |
| H | -0.362109 | 0.434765 | 1.429800 | |
| H | 0.111235 | 1.922200 | 0.614788 | |
| H | -2.266857 | 1.703235 | 0.252602 | |
| H | -1.540311 | 1.295339 | -1.279048 | |
| O | -2.018420 | -1.358910 | 0.328430 | |
| H | -3.358167 | -0.312499 | -0.763334 | |
| Rotational constants (GHz): | 5.7785100 | | 1.1529900 | 1.0358800 |
| Vibrational harmonic frequencies (cm-1): | | | | |
| 70.7784 | | 80.5161 | | 127.2887 |

| | | |
|-----------|-----------|-----------|
| 141.7616 | 209.0801 | 251.9456 |
| 374.2623 | 404.7998 | 467.5880 |
| 663.4447 | 712.4194 | 777.8418 |
| 861.1400 | 941.8140 | 957.6805 |
| 1013.0628 | 1063.7568 | 1085.2277 |
| 1105.5559 | 1157.3237 | 1232.5454 |
| 1266.8671 | 1302.5030 | 1324.1237 |
| 1364.0885 | 1386.0514 | 1392.2302 |
| 1411.2958 | 1428.9364 | 1457.5743 |
| 1494.7905 | 1510.6070 | 1831.8259 |
| 2887.5772 | 2890.3271 | 2915.6910 |
| 3015.9924 | 3036.2088 | 3043.5096 |
| 3047.8719 | 3079.3793 | 3114.7632 |

Zero-point correction (Hartree): 0.131911

C5H9O2.ttpt

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.31585418

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 3.187070 | -0.862261 | -0.086753 |
| C | 2.310307 | 0.149990 | 0.192974 |
| C | 0.862178 | -0.087332 | -0.249785 |
| C | -0.065986 | 1.076125 | 0.121276 |
| C | -1.520861 | 0.868362 | -0.337919 |
| C | -2.210691 | -0.255173 | 0.405779 |
| H | 2.364950 | 0.300470 | 1.293695 |
| H | 2.710271 | 1.103114 | -0.210680 |
| H | 0.850011 | -0.242403 | -1.335772 |
| H | 0.510392 | -1.023829 | 0.200375 |
| H | -0.050438 | 1.230473 | 1.210146 |
| H | 0.312438 | 2.006489 | -0.320198 |
| H | -2.094996 | 1.784331 | -0.133914 |
| H | -1.584671 | 0.665404 | -1.411523 |
| O | -2.831074 | -1.155200 | -0.113628 |
| H | -2.115605 | -0.196187 | 1.516967 |

Rotational constants (GHz): 6.0699500 1.0309400 0.9283100

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 50.1688 | 78.2442 | 91.3573 |
| 140.5657 | 186.4961 | 284.6266 |
| 335.2681 | 404.3537 | 458.9104 |
| 527.5744 | 744.1575 | 773.7429 |
| 884.0624 | 953.2009 | 995.5715 |
| 1019.9857 | 1058.8738 | 1085.9912 |
| 1106.1473 | 1167.5075 | 1221.5198 |
| 1262.2807 | 1299.3117 | 1315.2648 |
| 1356.0753 | 1362.7710 | 1395.8342 |
| 1414.8228 | 1432.1021 | 1472.8056 |
| 1498.2033 | 1511.0962 | 1839.6553 |
| 2862.3165 | 2888.3158 | 2918.6712 |
| 3019.4603 | 3027.4080 | 3046.5441 |
| 3062.9672 | 3092.6799 | 3110.2013 |

Zero-point correction (Hartree): 0.131580

C5H9O2.tttc

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.31861675

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -3.570263 | 0.012770 | -0.010571 |
| C | -2.308061 | -0.514925 | 0.013833 |
| C | -1.163797 | 0.504614 | 0.002450 |
| C | 0.216928 | -0.159403 | 0.000267 |
| C | 1.365367 | 0.849302 | 0.002271 |
| C | 2.740577 | 0.221804 | -0.000999 |
| H | -2.224866 | -1.212628 | 0.872770 |
| H | -2.240548 | -1.193261 | -0.864784 |
| H | -1.283238 | 1.147695 | -0.878619 |
| H | -1.272432 | 1.154671 | 0.880215 |
| H | 0.321788 | -0.816928 | 0.872138 |
| H | 0.320751 | -0.812698 | -0.874971 |
| H | 1.311532 | 1.523398 | -0.866836 |
| H | 1.313174 | 1.517845 | 0.875779 |
| O | 2.953159 | -0.970986 | -0.004793 |
| H | 3.584581 | 0.949282 | 0.000287 |

Rotational constants (GHz): 10.2493300 0.8821300 0.8286200

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 54.3158 | 94.2058 | 110.3543 |
| 122.2450 | 186.2364 | 233.9995 |
| 277.3843 | 352.8134 | 466.3016 |
| 672.4348 | 711.1208 | 758.9888 |
| 886.4601 | 894.8424 | 1003.7359 |
| 1017.3429 | 1056.8874 | 1088.4123 |
| 1099.1251 | 1166.4912 | 1249.8791 |
| 1258.2670 | 1305.5165 | 1329.3148 |

| | | |
|-----------|-----------|-----------|
| 1338.3133 | 1369.6429 | 1410.4202 |
| 1416.6585 | 1426.6376 | 1463.4251 |
| 1496.7442 | 1512.1596 | 1833.0579 |
| 2889.0667 | 2891.5823 | 2917.8981 |
| 3013.3087 | 3036.7571 | 3038.1269 |
| 3047.9399 | 3071.1661 | 3093.3359 |

Zero-point correction (Hartree): 0.131366

C5H9O2.tttt

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.31511803

Point group : CS

Electronic state : 2-A"

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 3.590862 | -0.821891 | 0.000000 |
| C | 2.527844 | 0.039971 | 0.000000 |
| C | 1.143629 | -0.616966 | 0.000000 |
| C | 0.000000 | 0.402481 | 0.000000 |
| C | -1.386711 | -0.247239 | 0.000000 |
| C | -2.531290 | 0.752967 | 0.000000 |
| H | 2.650812 | 0.721564 | 0.868532 |
| H | 2.650812 | 0.721564 | -0.868532 |
| H | 1.069183 | -1.269315 | -0.879124 |
| H | 1.069183 | -1.269315 | 0.879124 |
| H | 0.092357 | 1.058614 | 0.877478 |
| H | 0.092357 | 1.058614 | -0.877478 |
| H | -1.518596 | -0.898145 | -0.874721 |
| H | -1.518596 | -0.898145 | 0.874721 |
| O | -3.700687 | 0.441844 | 0.000000 |
| H | -2.229745 | 1.827660 | 0.000000 |

Rotational constants (GHz): 16.9813000 0.7590100 0.7396600

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------------|-----------------|-----------------|
| i214.4356 (A") | i77.2131 (A") | 64.3745 (A") |
| 106.9229 (A') | 115.5730 (A") | 143.8791 (A") |
| 277.6815 (A') | 313.5946 (A') | 487.3367 (A') |
| 565.0544 (A') | 663.8187 (A") | 756.6627 (A") |
| 877.9508 (A") | 1001.0875 (A") | 1002.4221 (A') |
| 1015.6285 (A') | 1062.6924 (A') | 1087.5989 (A') |
| 1106.6376 (A') | 1164.7887 (A") | 1244.5721 (A') |
| 1253.7402 (A") | 1308.4462 (A") | 1317.5414 (A') |
| 1337.9018 (A") | 1362.3640 (A') | 1408.2312 (A') |
| 1422.7751 (A') | 1436.0818 (A') | 1459.8108 (A') |
| 1499.2798 (A') | 1514.5521 (A') | 1836.9968 (A') |
| 2869.0686 (A') | 2897.3045 (A') | 2910.8534 (A") |
| 3014.9047 (A') | 3039.1990 (A') | 3044.3197 (A') |
| 3044.6226 (A") | 3077.5168 (A") | 3089.8591 (A") |

Zero-point correction (Hartree): 0.130319

C5H9O2.1-6Hshift.a

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.31354453

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 0.821828 | -1.608666 | -0.395149 |
| H | -0.548132 | -1.141255 | -0.153700 |
| C | -1.416642 | -0.345353 | -0.048837 |
| C | 1.665773 | -0.768782 | 0.327882 |
| C | -0.955096 | 1.042134 | -0.433345 |
| C | 1.620445 | 0.707249 | -0.098535 |
| C | 0.341223 | 1.467316 | 0.298026 |
| O | -2.515703 | -0.656669 | 0.324026 |
| H | 1.510509 | -0.854797 | 1.419688 |
| H | 2.680914 | -1.161778 | 0.137518 |
| H | -0.768240 | 1.021161 | -1.516335 |
| H | -1.772271 | 1.744130 | -0.239916 |
| H | 2.474990 | 1.221735 | 0.360009 |
| H | 1.763798 | 0.757198 | -1.185411 |
| H | 0.488498 | 2.533937 | 0.093727 |
| H | 0.186720 | 1.386965 | 1.382254 |

Rotational constants (GHz): 3.7105200 1.9978500 1.4212800

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| i286.8135 | 67.2418 | 148.4692 |
| 192.0305 | 326.4497 | 343.0740 |
| 421.9340 | 492.4520 | 506.3781 |
| 767.5870 | 789.7418 | 872.2748 |
| 894.7683 | 941.9241 | 980.2950 |
| 1014.2684 | 1071.1953 | 1088.7734 |
| 1132.1701 | 1141.2733 | 1204.8265 |
| 1247.6216 | 1264.1089 | 1283.3199 |
| 1345.4897 | 1374.9757 | 1390.5668 |
| 1402.2457 | 1455.5977 | 1464.7653 |
| 1486.6521 | 1505.9884 | 1823.5319 |
| 1870.5584 | 2942.3116 | 2975.9836 |
| 3033.6296 | 3035.8358 | 3039.6241 |

3078.6395 3085.8773 3109.6274
Zero-point correction (Hartree): 0.131255

C5H9O2.1-6Hshift.b

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.31119389
Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -0.740104 | -1.546836 | -0.527294 |
| H | 0.604250 | -1.039460 | -0.357620 |
| C | 1.429650 | -0.243637 | -0.018002 |
| C | -1.457293 | -0.871652 | 0.459106 |
| C | 0.825739 | 1.127696 | 0.256881 |
| C | -1.719413 | 0.615073 | 0.141088 |
| C | -0.508826 | 1.337819 | -0.479653 |
| O | 2.588263 | -0.539590 | 0.077557 |
| H | -2.416414 | -1.407408 | 0.561636 |
| H | -0.970354 | -0.971994 | 1.446343 |
| H | 0.696282 | 1.209352 | 1.346070 |
| H | 1.576436 | 1.874966 | -0.023210 |
| H | -2.559996 | 0.701385 | -0.556834 |
| H | -2.024312 | 1.119842 | 1.068114 |
| H | -0.719253 | 2.411554 | -0.527309 |
| H | -0.391047 | 1.001384 | -1.515810 |

Rotational constants (GHz): 3.8652100 1.9962300 1.4628500

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| i393.6840 | 62.5234 | 169.3940 |
| 241.5318 | 295.7404 | 334.2589 |
| 378.1602 | 509.9666 | 550.2004 |
| 753.0038 | 765.2155 | 828.6434 |
| 897.6309 | 907.8725 | 985.1783 |
| 1008.7348 | 1043.8227 | 1078.8313 |
| 1111.5609 | 1143.5584 | 1202.1183 |
| 1226.0500 | 1261.8021 | 1287.5229 |
| 1339.0310 | 1374.9203 | 1385.9956 |
| 1410.5016 | 1452.9038 | 1464.0920 |
| 1494.0692 | 1506.3888 | 1749.1045 |
| 1873.9756 | 2948.2812 | 2991.5101 |
| 3032.3904 | 3033.3845 | 3057.8280 |
| 3083.8165 | 3095.7778 | 3100.3684 |

Zero-point correction (Hartree): 0.130853

C5H9O2.1-6Hshift.c

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -346.30845723
Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| C | 0.906547 | 0.882877 | 0.671245 |
| C | -0.266636 | 1.564689 | -0.080719 |
| C | -1.363212 | 0.631094 | -0.639949 |
| C | -1.748443 | -0.555917 | 0.268426 |
| O | -0.901276 | -1.655342 | 0.131027 |
| H | 0.462065 | -1.177992 | -0.023448 |
| C | 1.358514 | -0.398100 | 0.012148 |
| H | 0.566120 | 0.586308 | 1.672458 |
| H | 1.755350 | 1.563547 | 0.782698 |
| H | -0.715190 | 2.282793 | 0.615457 |
| H | 0.140167 | 2.155487 | -0.908653 |
| H | -2.251446 | 1.241174 | -0.841066 |
| H | -1.053324 | 0.202165 | -1.599915 |
| H | -1.846935 | -0.219161 | 1.317910 |
| H | -2.745004 | -0.917923 | -0.039356 |
| O | 2.447225 | -0.652690 | -0.426402 |

Rotational constants (GHz): 3.6055100 2.0552600 1.4957400

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| i357.6819 | 83.7101 | 142.0015 |
| 174.5874 | 261.6573 | 356.4889 |
| 422.4411 | 494.3954 | 540.6971 |
| 746.0595 | 787.9975 | 850.7921 |
| 921.1166 | 928.3130 | 965.1708 |
| 1003.7606 | 1070.0619 | 1090.0339 |
| 1106.2713 | 1131.9742 | 1204.4864 |
| 1232.4271 | 1235.7117 | 1297.9677 |
| 1318.7064 | 1372.9013 | 1385.6810 |
| 1388.5782 | 1473.6911 | 1489.2384 |
| 1495.1378 | 1510.5483 | 1816.3047 |
| 1875.1441 | 2936.0093 | 2979.2624 |
| 3040.7020 | 3047.6457 | 3054.2064 |
| 3085.5896 | 3100.8936 | 3119.7319 |

Zero-point correction (Hartree): 0.131081

C5H9O2.pttc.M052X

E(UM052X+HF-M052X/6-31G(d,p)) (Hartree): -346.25948732
Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 2.630271 | -1.000257 | -0.528842 |
| C | 2.443269 | 0.031891 | 0.362694 |
| C | 1.205721 | 0.878357 | 0.081815 |
| C | -0.069573 | 0.042747 | 0.139661 |
| C | -1.304676 | 0.846938 | -0.241710 |
| C | -2.580824 | 0.054260 | -0.134002 |
| H | 2.357945 | -0.457698 | 1.349154 |
| H | 3.360404 | 0.636188 | 0.417688 |
| H | 1.161256 | 1.697590 | 0.806805 |
| H | 1.312944 | 1.331891 | -0.908168 |
| H | 0.030604 | -0.813172 | -0.530045 |
| H | -0.206386 | -0.366572 | 1.144124 |
| H | -1.417306 | 1.735960 | 0.392000 |
| H | -1.233757 | 1.228072 | -1.267473 |
| O | -2.633608 | -1.088205 | 0.250997 |
| H | -3.502506 | 0.590283 | -0.432081 |

Rotational constants (GHz): 6.4102500 1.0929100 0.9893200

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 53.9777 | 86.5960 | 122.9998 |
| 167.1344 | 189.6183 | 296.3387 |
| 323.0791 | 508.8274 | 674.1713 |
| 687.2568 | 724.4903 | 795.8738 |
| 918.2402 | 931.1310 | 968.2668 |
| 1042.5412 | 1088.8351 | 1115.2414 |
| 1129.6465 | 1187.2851 | 1224.8570 |
| 1292.6234 | 1314.3581 | 1337.7898 |
| 1393.7008 | 1400.8621 | 1423.0372 |
| 1445.2974 | 1446.3161 | 1481.1926 |
| 1511.0494 | 1528.5104 | 1887.5127 |
| 2999.3374 | 3014.3914 | 3055.0318 |
| 3064.7073 | 3081.9684 | 3096.1276 |
| 3109.4425 | 3129.0621 | 3159.9980 |

Zero-point correction (Hartree): 0.135343

C5H9O2.1-6Hshift.a.M052X

E(UM052X+HF-M052X/6-31G(d,p)) (Hartree): -346.24578096

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -0.815303 | -1.571649 | 0.466388 |
| H | 0.547775 | -1.168941 | 0.192000 |
| C | 1.389397 | -0.352122 | 0.062086 |
| C | -1.603741 | -0.769439 | -0.361797 |
| C | 0.919441 | 1.004398 | 0.514211 |
| C | -1.611758 | 0.705992 | 0.033603 |
| C | -0.316667 | 1.459091 | -0.288819 |
| O | 2.460928 | -0.621607 | -0.394207 |
| H | -1.330852 | -0.886953 | -1.420584 |
| H | -2.616873 | -1.181794 | -0.253846 |
| H | 0.651973 | 0.921753 | 1.572182 |
| H | 1.746760 | 1.705813 | 0.402684 |
| H | -2.435013 | 1.200120 | -0.490091 |
| H | -1.821854 | 0.768384 | 1.105213 |
| H | -0.466108 | 2.520607 | -0.081782 |
| H | -0.100840 | 1.379533 | -1.358928 |

Rotational constants (GHz): 3.7380100 2.0573300 1.4810100

Vibrational harmonic frequencies (cm-1):

| | | |
|------------|-----------|-----------|
| i1130.9597 | 55.2879 | 123.7034 |
| 188.3290 | 322.2189 | 344.8225 |
| 421.9432 | 491.3273 | 505.1848 |
| 636.5327 | 796.2231 | 841.5654 |
| 880.1457 | 912.6441 | 964.5187 |
| 1021.5457 | 1068.5886 | 1101.5244 |
| 1124.1477 | 1150.1154 | 1213.1534 |
| 1246.6644 | 1281.9104 | 1293.3925 |
| 1361.5822 | 1388.0705 | 1407.8963 |
| 1425.9907 | 1478.8720 | 1484.3962 |
| 1502.9916 | 1523.3757 | 1715.3925 |
| 1937.3104 | 3027.0656 | 3064.7712 |
| 3084.5973 | 3092.9148 | 3094.5677 |
| 3135.4434 | 3142.9601 | 3165.4465 |

Zero-point correction (Hartree): 0.132177

C6H11O2.pmmmt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -385.63187476

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -1.494423 | -1.149726 | -1.082052 |
| C | -2.129630 | -0.668694 | 0.032571 |
| C | -1.227194 | 0.042142 | 1.054026 |
| C | -0.695304 | 1.395550 | 0.550587 |

| | | | | |
|--|-----------|-----------|-----------|--|
| C | 0.232731 | 1.350990 | -0.676210 | |
| C | 1.643795 | 0.786771 | -0.411322 | |
| C | 1.711045 | -0.711299 | -0.197126 | |
| H | -3.011033 | -0.052491 | -0.231025 | |
| H | -2.549470 | -1.584064 | 0.506346 | |
| H | -1.815920 | 0.211030 | 1.964839 | |
| H | -0.406934 | -0.628574 | 1.330381 | |
| H | -1.555130 | 2.036082 | 0.310463 | |
| H | -0.169683 | 1.893522 | 1.376050 | |
| H | -0.241238 | 0.780232 | -1.486575 | |
| H | 0.346427 | 2.373513 | -1.054937 | |
| H | 2.264330 | 0.989654 | -1.297791 | |
| H | 2.123709 | 1.278264 | 0.441979 | |
| O | 2.324919 | -1.244619 | 0.703714 | |
| H | 1.158306 | -1.315169 | -0.948190 | |
| Rotational constants (GHz): | 2.5713500 | 1.3760000 | 1.1672100 | |
| Vibrational harmonic frequencies (cm-1): | | | | |
| 32.6732 | 73.6869 | | 104.0392 | |
| 122.6685 | 159.3633 | | 264.8699 | |
| 301.7856 | 351.8244 | | 408.1135 | |
| 468.1001 | 526.3160 | | 731.2524 | |
| 770.6730 | 794.9188 | | 838.9637 | |
| 869.8880 | 940.9983 | | 965.7579 | |
| 1002.6798 | 1049.7269 | | 1070.4231 | |
| 1090.7439 | 1111.9723 | | 1151.6920 | |
| 1165.4279 | 1207.4290 | | 1256.1181 | |
| 1303.6173 | 1331.0634 | | 1358.9328 | |
| 1366.4383 | 1391.4164 | | 1402.0891 | |
| 1406.6455 | 1437.1291 | | 1468.4623 | |
| 1493.6437 | 1496.9517 | | 1500.0182 | |
| 1823.4154 | 2881.3236 | | 2933.3620 | |
| 2944.4391 | 3015.4764 | | 3024.2112 | |
| 3026.6376 | 3047.2268 | | 3064.4912 | |
| 3074.3375 | 3098.1226 | | 3104.6316 | |
| Zero-point correction (Hartree): | 0.161354 | | | |

C6H11O2.pmmpt

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -385.63187540
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | | |
|--|-----------|-----------|-----------|--|
| O | -1.473787 | -1.160790 | -1.077686 | |
| C | -2.120303 | -0.677480 | 0.029393 | |
| C | -1.231195 | 0.049900 | 1.050627 | |
| C | -0.705792 | 1.402453 | 0.538362 | |
| C | 0.234769 | 1.353628 | -0.678694 | |
| C | 1.643693 | 0.791834 | -0.396576 | |
| C | 1.713164 | -0.708595 | -0.200221 | |
| H | -3.005996 | -0.072001 | -0.244644 | |
| H | -2.534739 | -1.593128 | 0.507402 | |
| H | -1.828160 | 0.222864 | 1.955310 | |
| H | -0.407647 | -0.611435 | 1.339376 | |
| H | -1.568273 | 2.033596 | 0.283240 | |
| H | -0.192258 | 1.913172 | 1.363637 | |
| H | -0.230114 | 0.778787 | -1.491402 | |
| H | 0.350672 | 2.374807 | -1.060354 | |
| H | 2.278480 | 1.008051 | -1.269648 | |
| H | 2.106558 | 1.274380 | 0.471112 | |
| O | 2.303707 | -1.251019 | 0.710668 | |
| H | 1.186094 | -1.305060 | -0.975227 | |
| Rotational constants (GHz): | 2.5595000 | 1.3871100 | 1.1708100 | |
| Vibrational harmonic frequencies (cm-1): | | | | |
| 18.4024 | 72.4710 | | 103.9858 | |
| 122.5543 | 157.3323 | | 264.1253 | |
| 303.3330 | 350.9038 | | 407.5495 | |
| 468.5129 | 525.4747 | | 730.9414 | |
| 770.0494 | 793.7574 | | 838.6981 | |
| 870.4534 | 941.2515 | | 965.5345 | |
| 1002.9476 | 1048.8822 | | 1070.4090 | |
| 1090.4827 | 1111.6986 | | 1152.2015 | |
| 1165.5504 | 1207.4218 | | 1255.9193 | |
| 1303.8022 | 1331.8267 | | 1358.3203 | |
| 1366.7290 | 1391.3536 | | 1401.7326 | |
| 1406.6901 | 1436.7698 | | 1468.7402 | |
| 1493.4914 | 1497.2172 | | 1499.4958 | |
| 1823.6258 | 2881.1984 | | 2933.2967 | |
| 2944.1374 | 3015.7133 | | 3023.8888 | |
| 3026.6818 | 3047.0713 | | 3064.1099 | |
| 3074.3561 | 3098.1693 | | 3104.8317 | |
| Zero-point correction (Hartree): | 0.161304 | | | |

C6H11O2.pmmtc

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -385.63397807
 Electronic state : 2-A

```

Cartesian coordinates (Angs):
O      -1.471525   -1.674734   -0.127261
C      -2.399304   -0.666616   -0.165643
C      -1.965296    0.651363    0.491355
C      -0.884771    1.404904   -0.304275
C      0.422196    0.637109   -0.555006
C      1.154264    0.202232    0.715503
C      2.550088   -0.322104    0.470263
H      -2.784085   -0.509815   -1.192153
H      -3.263926   -1.085469    0.395926
H      -2.847999    1.295682    0.594070
H      -1.616233    0.428453    1.506367
H      -1.304984    1.701809   -1.274789
H      -0.658803    2.340912    0.224537
H      0.226952   -0.254292   -1.163970
H      1.092948    1.261841   -1.155106
H      0.600000   -0.586260    1.243091
H      1.245612    1.029273    1.438406
O      3.092404   -0.374107   -0.612178
H      3.080439   -0.672742    1.385953
Rotational constants (GHz):      3.6073800      1.0318800      0.9097800
Vibrational harmonic frequencies (cm-1):
 42.5092      76.5744      111.7214
152.3430      175.6436      208.5470
233.9959      339.5397      412.3068
493.5263      671.2351      686.1917
747.4399      782.3284      844.6573
877.4461      913.1708      947.0652
989.9196     1046.4491     1068.2912
1099.3667     1109.7357     1157.8589
1185.7208     1205.8045     1289.4965
1303.0186     1337.4577     1342.3412
1373.1717     1391.2578     1400.4019
1413.0124     1429.5755     1461.0854
1490.1367     1497.1085     1502.6532
1832.4911     2882.1369     2882.5660
2943.3471     3007.6339     3023.7723
3040.3866     3046.3499     3059.5825
3062.7627     3090.0081     3093.0954
Zero-point correction (Hartree): 0.161236

```

C6H11O2.pmmtt

```

-----
E(UB+HF-LYP/6-31G(d,p)) (Hartree): -385.63240604
Electronic state : 2-A
Cartesian coordinates (Angs):
O      1.556932   -1.655132    0.169967
C      2.474346   -0.648981    0.013050
C      1.936102    0.635048   -0.633590
C      0.966993    1.415434    0.271142
C      -0.289468    0.653001    0.724785
C      -1.197110    0.187982   -0.429461
C      -2.438289   -0.506832    0.079541
H      3.013001   -0.441590    0.958206
H      3.243805   -1.096768   -0.654500
H      2.787540    1.281508   -0.882366
H      1.455616    0.369278   -1.582195
H      1.510108    1.747553    1.166388
H      0.662601    2.329787   -0.254521
H      0.002509   -0.222480    1.320482
H      -0.862246    1.304918    1.396590
H      -0.646639   -0.540911   -1.039584
H      -1.504317    1.022228   -1.068764
O      -3.574237   -0.195441   -0.204821
H      -2.238986   -1.362854    0.766290
Rotational constants (GHz):      3.8410000      0.9518300      0.8334100
Vibrational harmonic frequencies (cm-1):
 49.5332      55.1763      87.7366
116.1796      171.2754      209.3322
280.1238      338.8670      425.7527
491.0338      514.2187      731.6308
747.4354      817.3796      845.2224
864.4763      946.3521      975.4061
1006.1090     1060.2755     1074.3648
1097.9679     1106.2461     1162.4308
1183.2194     1207.1413     1278.5711
1301.6490     1330.7915     1342.7070
1369.7697     1388.9174     1397.6631
1406.1273     1432.7332     1474.2826
1489.0283     1498.5892     1503.9036
1835.1554     2877.3015     2884.1643
2942.5587     3023.6085     3028.1504
3038.7885     3044.6394     3062.2998
3071.9153     3091.6612     3109.2224
Zero-point correction (Hartree): 0.161269

```

C6H11O2.pmpcc

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -385.63153855
Electronic state : 2-A
Cartesian coordinates (Angs):
O -1.416470 -1.612628 0.445314
C -2.057395 -0.695772 -0.343593
C -1.796310 0.792566 -0.074047
C -0.413867 1.330161 -0.512636
C 0.696018 1.338967 0.556541
C 1.204762 -0.026868 1.028252
C 1.962182 -0.818803 -0.009239
H -1.890114 -0.949026 -1.410314
H -3.137950 -0.920081 -0.197378
H -2.573448 1.344028 -0.619453
H -1.969387 0.992802 0.991398
H -0.060843 0.784310 -1.394664
H -0.546532 2.368955 -0.837734
H 1.545590 1.902525 0.153935
H 0.338815 1.897325 1.431555
H 1.883131 0.086497 1.888224
H 0.387121 -0.666800 1.387397
O 2.181097 -0.456735 -1.146794
H 2.334256 -1.807139 0.347203
Rotational constants (GHz): 2.6680600 1.3871600 1.1583700
Vibrational harmonic frequencies (cm-1):
29.1692 39.4135 120.5633
149.0758 176.6514 231.9270
288.4394 321.6294 408.3036
426.2794 536.0268 650.5401
729.5997 739.7301 828.6708
862.8283 928.9427 948.2361
999.0193 1022.5549 1078.2949
1102.5662 1112.9047 1152.3783
1224.7279 1238.5269 1270.6571
1321.3206 1357.3551 1372.4663
1381.3525 1389.3788 1398.1004
1408.3590 1431.8998 1464.2950
1485.7821 1498.3504 1511.8900
1825.2352 2878.1606 2886.3626
2925.0282 3016.5710 3030.6297
3038.0997 3048.4881 3060.9106
3074.2823 3084.4582 3096.7592
Zero-point correction (Hartree): 0.160846

C6H11O2.pmppt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -385.63027860
Electronic state : 2-A
Cartesian coordinates (Angs):
O -1.528843 -1.284890 1.021392
C -1.729718 -0.825466 -0.251471
C -1.706678 0.710915 -0.421064
C -0.343282 1.388411 -0.654963
C 0.638775 1.457919 0.528615
C 1.292420 0.120698 0.969488
C 2.047544 -0.529001 -0.163752
H -0.891910 -1.277813 -0.829702
H -2.650698 -1.260217 -0.682605
H -2.341389 0.942252 -1.286513
H -2.206519 1.152864 0.450521
H 0.146364 0.914853 -1.514771
H -0.545547 2.423197 -0.959894
H 1.433902 2.169821 0.270344
H 0.127781 1.877517 1.403877
H 1.987655 0.325002 1.792219
H 0.515342 -0.561316 1.323646
O 1.541510 -1.261733 -0.992291
H 3.129324 -0.274037 -0.241059
Rotational constants (GHz): 2.4371500 1.5475300 1.2725700
Vibrational harmonic frequencies (cm-1):
62.2939 79.3166 102.7641
134.3557 190.8414 234.0350
305.9422 332.5141 428.5497
454.5383 539.9162 730.0164
767.1420 820.8598 856.7897
865.1594 936.8801 970.6959
1009.9971 1043.9993 1087.2579
1090.8119 1119.2598 1163.6713
1200.2804 1236.6579 1249.6581
1305.1216 1338.7132 1352.4622
1385.4307 1391.9975 1397.9601
1412.6056 1434.6206 1483.6349
1498.5981 1502.8835 1516.8732

| | | |
|-----------|-----------|-----------|
| 1811.9613 | 2871.0271 | 2890.0767 |
| 2953.0922 | 3027.6015 | 3032.6986 |
| 3041.1571 | 3055.8526 | 3068.9401 |
| 3073.7059 | 3085.5774 | 3129.2690 |

Zero-point correction (Hartree): 0.161923

C6H11O2.pmpctc

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -385.63172557

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 1.612728 | -1.685454 | -0.244622 |
| C | 2.405270 | -0.630134 | 0.120639 |
| C | 2.002639 | 0.761066 | -0.391119 |
| C | 0.826414 | 1.444710 | 0.336099 |
| C | -0.596308 | 1.012432 | -0.059897 |
| C | -1.035920 | -0.364855 | 0.439687 |
| C | -2.482390 | -0.685836 | 0.148462 |
| H | 2.581447 | -0.626976 | 1.214818 |
| H | 3.396759 | -0.899569 | -0.308137 |
| H | 2.886301 | 1.404269 | -0.286068 |
| H | 1.793221 | 0.688181 | -1.465723 |
| H | 0.959599 | 1.335940 | 1.422875 |
| H | 0.905407 | 2.520373 | 0.137017 |
| H | -1.305424 | 1.755277 | 0.322520 |
| H | -0.699636 | 1.046219 | -1.151206 |
| H | -0.894667 | -0.465157 | 1.527814 |
| H | -0.431082 | -1.172091 | 0.000267 |
| O | -3.248734 | 0.043959 | -0.442975 |
| H | -2.822108 | -1.678808 | 0.523370 |

Rotational constants (GHz): 3.5580800 1.0313900 0.8535500

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 38.1428 | 48.4312 | 102.2130 |
| 148.2826 | 183.3045 | 191.5303 |
| 267.1036 | 320.4903 | 416.9535 |
| 451.7906 | 662.5960 | 687.7821 |
| 706.4268 | 773.5120 | 840.8270 |
| 871.6303 | 947.0021 | 956.0371 |
| 960.2148 | 1061.7123 | 1063.8008 |
| 1104.0593 | 1108.8762 | 1164.3020 |
| 1205.9907 | 1251.8671 | 1269.1996 |
| 1325.5746 | 1336.3627 | 1357.1962 |
| 1373.6961 | 1391.5023 | 1398.7543 |
| 1412.7876 | 1427.6877 | 1463.3535 |
| 1482.1320 | 1499.3617 | 1502.0213 |
| 1829.1850 | 2877.3829 | 2886.3294 |
| 2932.9798 | 3007.3212 | 3016.2223 |
| 3032.6266 | 3035.9637 | 3049.9736 |
| 3069.2499 | 3080.9188 | 3091.7306 |

Zero-point correction (Hartree): 0.161031

C6H11O2.pmtmc

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -385.63412210

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -2.183593 | -0.998237 | 1.016090 |
| C | -2.358553 | -0.577766 | -0.275771 |
| C | -1.831493 | 0.830315 | -0.590866 |
| C | -0.297731 | 0.910436 | -0.639843 |
| C | 0.388375 | 0.613206 | 0.701212 |
| C | 1.915367 | 0.717618 | 0.639217 |
| C | 2.603901 | -0.383727 | -0.135569 |
| H | -1.982701 | -1.326620 | -0.999677 |
| H | -3.463601 | -0.590895 | -0.407002 |
| H | -2.239776 | 1.142769 | -1.560893 |
| H | -2.226996 | 1.521632 | 0.163994 |
| H | 0.075758 | 0.210806 | -1.396812 |
| H | -0.011358 | 1.916999 | -0.975218 |
| H | 0.015081 | 1.308339 | 1.462875 |
| H | 0.115474 | -0.391397 | 1.043899 |
| H | 2.241139 | 1.676056 | 0.205254 |
| H | 2.355910 | 0.705553 | 1.648088 |
| O | 2.044642 | -1.320009 | -0.664629 |
| H | 3.713479 | -0.287758 | -0.186474 |

Rotational constants (GHz): 3.3697100 1.0391800 0.9674500

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 39.6483 | 75.0998 | 115.1573 |
| 125.8767 | 158.4695 | 244.4512 |
| 263.7744 | 309.3259 | 387.6624 |
| 473.8843 | 654.6680 | 707.4293 |
| 732.1192 | 802.8975 | 828.9683 |
| 862.4816 | 919.2371 | 949.4013 |
| 1014.2558 | 1019.8927 | 1073.5795 |
| 1094.8042 | 1103.8756 | 1156.6793 |

| | | |
|-----------|-----------|-----------|
| 1186.2265 | 1221.8077 | 1280.2012 |
| 1322.3371 | 1341.8421 | 1352.9882 |
| 1374.1231 | 1384.5592 | 1396.5927 |
| 1416.3908 | 1430.2688 | 1456.6154 |
| 1484.0959 | 1487.9102 | 1508.9459 |
| 1831.5018 | 2881.2526 | 2882.3425 |
| 2945.1574 | 3011.9790 | 3024.3458 |
| 3036.8389 | 3037.7686 | 3050.9964 |
| 3071.8580 | 3082.9277 | 3097.6041 |

Zero-point correction (Hartree): 0.161096

C6H11O2.pmtmt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -385.63253849

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -2.392033 | -1.346099 | 0.171271 |
| C | -2.496351 | -0.255003 | -0.649437 |
| C | -1.880376 | 1.043107 | -0.103701 |
| C | -0.344933 | 1.014290 | -0.053963 |
| C | 0.234134 | 0.007879 | 0.950224 |
| C | 1.775457 | -0.006668 | 0.968794 |
| C | 2.359469 | -0.562658 | -0.310620 |
| H | -2.138060 | -0.475552 | -1.674096 |
| H | -3.594837 | -0.113856 | -0.757654 |
| H | -2.206324 | 1.871995 | -0.744905 |
| H | -2.289779 | 1.227335 | 0.897214 |
| H | 0.043172 | 0.801537 | -1.060595 |
| H | 0.019619 | 2.018636 | 0.198415 |
| H | -0.132941 | 0.242949 | 1.956098 |
| H | -0.137811 | -1.001864 | 0.729409 |
| H | 2.191227 | 0.992298 | 1.136193 |
| H | 2.115566 | -0.657782 | 1.787336 |
| O | 3.176238 | -0.001329 | -1.006965 |
| H | 1.972127 | -1.571945 | -0.589653 |

Rotational constants (GHz): 3.7747700 0.8739800 0.8537300

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 33.0243 | 53.0175 | 87.4203 |
| 121.6833 | 139.8609 | 244.3496 |
| 299.5284 | 315.3462 | 403.5944 |
| 470.5518 | 533.2185 | 737.2829 |
| 769.7396 | 788.1502 | 841.5358 |
| 889.5222 | 937.3322 | 974.3171 |
| 1012.3318 | 1040.5930 | 1067.6482 |
| 1090.7337 | 1104.5011 | 1160.5027 |
| 1173.6374 | 1208.4116 | 1267.1073 |
| 1314.1635 | 1329.4911 | 1349.2350 |
| 1355.9626 | 1376.0753 | 1400.6962 |
| 1415.0423 | 1430.9687 | 1475.4233 |
| 1486.3746 | 1494.2195 | 1509.9367 |
| 1835.5460 | 2865.5463 | 2882.6345 |
| 2939.7655 | 3020.4586 | 3026.8632 |
| 3031.7183 | 3040.0196 | 3059.6474 |
| 3082.2044 | 3088.5798 | 3105.8840 |

Zero-point correction (Hartree): 0.161024

C6H11O2.pmtpc

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -385.63412214

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -2.183481 | -0.997854 | 1.016291 |
| C | -2.358644 | -0.578023 | -0.275761 |
| C | -1.831653 | 0.830196 | -0.591079 |
| C | -0.297852 | 0.910117 | -0.639980 |
| C | 0.388116 | 0.612604 | 0.700986 |
| C | 1.915087 | 0.717525 | 0.639545 |
| C | 2.604264 | -0.383366 | -0.135194 |
| H | -1.982938 | -1.326810 | -0.999691 |
| H | -3.463790 | -0.590540 | -0.406293 |
| H | -2.239918 | 1.142408 | -1.561152 |
| H | -2.227201 | 1.521480 | 0.163801 |
| H | 0.075543 | 0.210502 | -1.397012 |
| H | -0.011360 | 1.916707 | -0.975227 |
| H | 0.014507 | 1.307320 | 1.462912 |
| H | 0.115457 | -0.392238 | 1.043302 |
| H | 2.240400 | 1.676322 | 0.205945 |
| H | 2.355145 | 0.705594 | 1.648628 |
| O | 2.045276 | -1.319321 | -0.665195 |
| H | 3.713878 | -0.287662 | -0.185075 |

Rotational constants (GHz): 3.3706000 1.0390200 0.9674700

Vibrational harmonic frequencies (cm-1):

| | | |
|----------|----------|----------|
| 39.7108 | 75.1884 | 115.2302 |
| 125.9378 | 158.4889 | 244.5618 |
| 263.7663 | 309.3592 | 387.5969 |

| | | |
|-----------|-----------|-----------|
| 474.0625 | 654.6789 | 707.7498 |
| 733.7159 | 803.0127 | 829.2907 |
| 862.6843 | 919.0822 | 949.3756 |
| 1014.4745 | 1019.8694 | 1073.8846 |
| 1094.6128 | 1103.8190 | 1156.6989 |
| 1185.4899 | 1221.7827 | 1280.2038 |
| 1322.2323 | 1341.4839 | 1352.9452 |
| 1374.1503 | 1384.6467 | 1396.7341 |
| 1416.4379 | 1430.2389 | 1456.6137 |
| 1484.0551 | 1487.9138 | 1508.9437 |
| 1831.3228 | 2881.1733 | 2882.6466 |
| 2945.9522 | 3011.8006 | 3024.2588 |
| 3036.6615 | 3037.8330 | 3050.7544 |
| 3071.8534 | 3082.8582 | 3097.4182 |

Zero-point correction (Hartree): 0.161101

C6H11O2.pmtpt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -385.63253879

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -2.386405 | -1.344478 | 0.206890 |
| C | -2.494707 | -0.275569 | -0.642004 |
| C | -1.881793 | 1.038248 | -0.131722 |
| C | -0.346261 | 1.014520 | -0.081668 |
| C | 0.235338 | 0.040576 | 0.952605 |
| C | 1.776684 | 0.027160 | 0.968027 |
| C | 2.357153 | -0.572680 | -0.293106 |
| H | -2.137084 | -0.522271 | -1.660952 |
| H | -3.593733 | -0.140575 | -0.752909 |
| H | -2.209994 | 1.848703 | -0.794950 |
| H | -2.291398 | 1.248441 | 0.863985 |
| H | 0.042111 | 0.771918 | -1.081442 |
| H | 0.016213 | 2.026891 | 0.139745 |
| H | -0.129789 | 0.307074 | 1.951314 |
| H | -0.136510 | -0.975754 | 0.764392 |
| H | 2.192543 | 1.031374 | 1.100061 |
| H | 2.119068 | -0.595438 | 1.807539 |
| O | 3.171548 | -0.035872 | -1.011146 |
| H | 1.968943 | -1.591096 | -0.535520 |

Rotational constants (GHz): 3.7633800 0.8751500 0.8548700

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 33.0160 | 53.4761 | 86.9669 |
| 121.9471 | 139.2464 | 243.9856 |
| 299.9693 | 315.4288 | 403.1560 |
| 470.4166 | 533.0520 | 737.1324 |
| 769.2503 | 787.4424 | 840.8851 |
| 890.0168 | 937.1950 | 974.1345 |
| 1012.4728 | 1040.6379 | 1067.2734 |
| 1090.9405 | 1104.5100 | 1160.7079 |
| 1173.9022 | 1208.1323 | 1266.9739 |
| 1313.8280 | 1329.5415 | 1349.1906 |
| 1355.5703 | 1375.9352 | 1400.3374 |
| 1415.2612 | 1431.9233 | 1474.9739 |
| 1486.2588 | 1494.3729 | 1510.0758 |
| 1835.9957 | 2865.3948 | 2882.3738 |
| 2939.3336 | 3020.5376 | 3026.8822 |
| 3031.8985 | 3040.0848 | 3059.5879 |
| 3082.2289 | 3088.5548 | 3105.6761 |

Zero-point correction (Hartree): 0.161017

C6H11O2.pmttc

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -385.63412219

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -2.183708 | -0.997696 | 1.016222 |
| C | -2.358907 | -0.578023 | -0.275882 |
| C | -1.831739 | 0.830132 | -0.591321 |
| C | -0.297950 | 0.909920 | -0.639923 |
| C | 0.387867 | 0.612178 | 0.701113 |
| C | 1.914827 | 0.717465 | 0.639907 |
| C | 2.604460 | -0.382681 | -0.135545 |
| H | -1.983388 | -1.326871 | -0.999846 |
| H | -3.464078 | -0.590256 | -0.406283 |
| H | -2.239738 | 1.142204 | -1.561548 |
| H | -2.227407 | 1.521557 | 0.163359 |
| H | 0.075538 | 0.210379 | -1.396981 |
| H | -0.011354 | 1.916524 | -0.975041 |
| H | 0.013920 | 1.306489 | 1.463203 |
| H | 0.115520 | -0.392901 | 1.042972 |
| H | 2.240370 | 1.676610 | 0.207384 |
| H | 2.354695 | 0.704369 | 1.649054 |
| O | 2.046290 | -1.319396 | -0.664973 |
| H | 3.713924 | -0.285311 | -0.186364 |


```

Rotational constants (GHz):    3.370990    1.0387800    0.9673300
Vibrational harmonic frequencies (cm-1):
  39.6879          75.1409          115.2475
 125.8374         158.3736         244.3459
 263.7071         309.3032         387.5353
 474.0992         654.7502         707.5025
 734.0791         803.0120         829.3759
 862.6825         918.9949         949.3534
1014.4925         1019.8771        1073.9044
1094.5323         1103.7939        1156.6841
1185.3114         1221.7817        1280.1740
1322.1695         1341.4002        1352.9288
1374.1793         1384.5990        1396.7854
1416.4214         1430.2819        1456.5315
1484.0346         1487.8736        1508.9272
1831.5560         2881.1075        2882.2809
2945.9716         3012.0783        3024.2598
3036.8758         3037.8570        3050.9275
3071.8504         3082.9200        3097.4799
Zero-point correction (Hartree): 0.161100
    
```

C6H11O2.pmttt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -385.63253901

Electronic state : 2-A

Cartesian coordinates (Angs):

```

O      -2.388322      -1.344908      0.197754
C      -2.495289      -0.270212     -0.643985
C      -1.881511      1.039587     -0.124479
C      -0.345997      1.014440     -0.074679
C       0.234973      0.032067      0.951947
C       1.776279      0.018459      0.968215
C       2.357871     -0.570015     -0.297767
H      -2.137314     -0.510292     -1.664383
H      -3.594140     -0.133528     -0.754511
H      -2.209200      1.854956     -0.781911
H      -2.290908      1.242964      0.872726
H       0.042134      0.779359     -1.076344
H       0.017168      2.024815      0.154578
H      -0.130710      0.290448      1.952586
H      -0.136837     -0.982682     0.755271
H       2.192087      1.021430      1.109557
H       2.118132     -0.611603      1.802390
O       3.173612     -0.027088     -1.009663
H       1.969312     -1.585858     -0.550203
    
```

```

Rotational constants (GHz):    3.7671900    0.8746700    0.8543900
    
```

```

Vibrational harmonic frequencies (cm-1):
  33.0033          53.3953          87.1421
 121.8459         139.5325         244.1111
 299.8918         315.5240         403.3037
 470.4627         533.1819         737.1664
 769.3386         787.5282         841.0275
 889.9587         937.2435         974.2044
1012.4681         1040.6643        1067.3830
1090.9273         1104.4983        1160.6939
1173.9130         1208.2308        1267.0521
1313.9594         1329.5717        1349.2080
1355.7238         1375.9777        1400.4132
1415.2476         1431.6362        1475.0973
1486.3067         1494.3771        1510.0966
1835.8853         2865.3135        2882.4067
2939.4071         3020.4708        3026.7255
3031.8233         3040.0828        3059.6190
3082.2379         3088.5734        3105.6640
    
```

Zero-point correction (Hartree): 0.161020

C6H11O2.ppmmc

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -385.63044696

Electronic state : 2-A

Cartesian coordinates (Angs):

```

O       1.799286      -1.487505     -0.556993
C       2.311572     -0.465519      0.195907
C       1.870486      0.951126     -0.217345
C       0.358169      1.151881     -0.401409
C      -0.504151      0.830108      0.841383
C      -1.130181     -0.570573      0.821489
C      -2.313325     -0.694286     -0.113196
H       1.924278     -0.680929      1.217370
H       3.410958     -0.532818      0.292075
H       2.254588      1.645555      0.542636
H       2.383587      1.205285     -1.153200
H       0.199786      2.196878     -0.689695
H       0.013695      0.553425     -1.250383
H       0.094755      0.948749      1.753894
    
```

| | | | | |
|--|-----------|-----------|-----------|--|
| H | -1.319671 | 1.556499 | 0.912798 | |
| H | -0.407844 | -1.342769 | 0.523086 | |
| H | -1.488617 | -0.870924 | 1.818440 | |
| O | -2.782397 | 0.215008 | -0.763137 | |
| H | -2.756049 | -1.715395 | -0.166957 | |
| Rotational constants (GHz): | 3.3947400 | 1.1213300 | 0.9980000 | |
| Vibrational harmonic frequencies (cm-1): | | | | |
| 51.5243 | 79.3296 | | 93.4292 | |
| 158.5476 | 174.6316 | | 198.5213 | |
| 255.5972 | 353.2144 | | 384.5086 | |
| 513.7019 | 642.9167 | | 690.3031 | |
| 736.0138 | 793.0219 | | 838.1127 | |
| 891.5696 | 924.5075 | | 946.5689 | |
| 998.0061 | 1026.9327 | | 1073.8480 | |
| 1092.6985 | 1111.2775 | | 1148.1656 | |
| 1177.3570 | 1225.0139 | | 1247.5174 | |
| 1293.5819 | 1312.1436 | | 1363.5537 | |
| 1391.7046 | 1394.4718 | | 1398.6151 | |
| 1411.1511 | 1427.6464 | | 1456.3124 | |
| 1494.3452 | 1500.6698 | | 1505.4690 | |
| 1830.3427 | 2877.0154 | | 2889.1761 | |
| 2959.9989 | 3016.5860 | | 3030.7590 | |
| 3039.3784 | 3059.2295 | | 3062.4034 | |
| 3075.3342 | 3098.6261 | | 3106.4561 | |
| Zero-point correction (Hartree): | 0.161344 | | | |

C6H11O2.ppmmt

```
-----
E(UB+HF-LYP/6-31G(d,p)) (Hartree): -385.63017318
Electronic state : 2-A
Cartesian coordinates (Angs):
O      -2.418808      1.586676      -0.180174
C      -2.573517      0.407604      0.497928
C      -2.053971     -0.838353     -0.237376
C      -0.576546     -0.743565     -0.644682
C      0.404766      -0.887386     0.529611
C      1.893678      -0.847886     0.122225
C      2.379279      0.524392     -0.293317
H      -2.016385      0.563246     1.448167
H      -3.622535      0.281442     0.828006
H      -2.225223     -1.718831     0.397079
H      -2.670113     -0.975839     -1.133979
H      -0.358037     -1.526448     -1.382173
H      -0.430756      0.214923     -1.156229
H      0.221736      -0.109211     1.282376
H      0.217280      -1.844047     1.033495
H      2.539015     -1.189191     0.937227
H      2.049365     -1.526994     -0.730173
O      3.381763      1.049868     0.139752
H      1.749876      1.049773     -1.046755
Rotational constants (GHz):      3.6669300      0.8509300      0.7452900
Vibrational harmonic frequencies (cm-1):
      25.3956      36.5379      58.0378
      121.3001      167.8482      232.0896
      254.6856      321.9450      406.5822
      499.1767      540.3083      625.9997
      750.9604      787.9756      840.2062
      862.2951      932.4484      965.6003
      1030.2441      1052.9044      1068.4986
      1098.8951      1109.9469      1154.7678
      1179.2550      1237.9370      1293.2101
      1302.9011      1338.9175      1349.7044
      1353.6844      1371.3344      1397.1471
      1412.1417      1440.9209      1474.3462
      1496.3126      1501.6338      1513.7739
      1832.0586      2887.5133      2897.1837
      2945.6716      3018.2333      3029.5901
      3035.6089      3043.2050      3065.4467
      3080.5133      3094.2143      3109.1443
Zero-point correction (Hartree): 0.160944
```

C6H11O2.ppmpc

```
-----
E(UB+HF-LYP/6-31G(d,p)) (Hartree): -385.63107890
Electronic state : 2-A
Cartesian coordinates (Angs):
O      -1.223470      -1.402526      1.072085
C      -1.373911     -1.151537     -0.261962
C      -1.828121      0.272330     -0.629853
C      -1.085358      1.412812      0.084087
C      0.438392      1.489585     -0.154030
C      1.308077      0.624681      0.785993
C      2.095142     -0.479118      0.121593
```

| | | | | |
|--|-----------|-----------|-----------|--|
| H | -0.356445 | -1.322835 | -0.682746 | |
| H | -2.004308 | -1.916487 | -0.753660 | |
| H | -1.727436 | 0.381801 | -1.717940 | |
| H | -2.899578 | 0.359135 | -0.408191 | |
| H | -1.536503 | 2.353022 | -0.255601 | |
| H | -1.284993 | 1.352661 | 1.160420 | |
| H | 0.663267 | 1.217949 | -1.191983 | |
| H | 0.749232 | 2.532787 | -0.035616 | |
| H | 2.024247 | 1.230608 | 1.356901 | |
| H | 0.691874 | 0.122521 | 1.548316 | |
| O | 1.907344 | -0.895970 | -1.003940 | |
| H | 2.884315 | -0.935712 | 0.759973 | |
| Rotational constants (GHz): | 2.5031400 | 1.5404600 | 1.2292600 | |
| Vibrational harmonic frequencies (cm-1): | | | | |
| 60.0544 | 63.5761 | | 105.5461 | |
| 140.7012 | 189.4613 | | 221.4083 | |
| 272.5421 | 318.7682 | | 402.6777 | |
| 531.7532 | 650.9116 | | 694.3540 | |
| 728.3377 | 768.7968 | | 845.4119 | |
| 905.4751 | 932.2319 | | 945.9588 | |
| 1029.8518 | 1047.6704 | | 1082.2852 | |
| 1092.3881 | 1121.7329 | | 1159.7233 | |
| 1200.1211 | 1241.5252 | | 1258.3795 | |
| 1297.2321 | 1318.8795 | | 1364.1839 | |
| 1383.4424 | 1393.3010 | | 1397.4032 | |
| 1412.0599 | 1427.0465 | | 1459.9527 | |
| 1492.9304 | 1502.3060 | | 1504.6272 | |
| 1816.4604 | 2867.4549 | | 2904.2892 | |
| 2950.6970 | 3019.5997 | | 3032.0288 | |
| 3043.3073 | 3050.7463 | | 3061.4887 | |
| 3071.8693 | 3086.6768 | | 3096.0868 | |
| Zero-point correction (Hartree): | 0.161672 | | | |

C6H11O2.ppmpt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -385.63008744
Electronic state : 2-A
Cartesian coordinates (Angs):

| | | | | |
|--|-----------|-----------|-----------|--|
| O | 2.387697 | -0.663060 | -0.919142 | |
| C | 1.593737 | -0.884346 | 0.166668 | |
| C | 1.195877 | 0.382103 | 0.954470 | |
| C | 0.623385 | 1.521100 | 0.087209 | |
| C | -0.906956 | 1.604819 | -0.054643 | |
| C | -1.597758 | 0.395939 | -0.733468 | |
| C | -1.913402 | -0.720658 | 0.230874 | |
| H | 0.690247 | -1.389902 | -0.243578 | |
| H | 2.030606 | -1.650515 | 0.836349 | |
| H | 0.500968 | 0.098009 | 1.756259 | |
| H | 2.101663 | 0.742278 | 1.456464 | |
| H | 0.953926 | 2.480037 | 0.503513 | |
| H | 1.083968 | 1.451500 | -0.905902 | |
| H | -1.362316 | 1.770117 | 0.932661 | |
| H | -1.140656 | 2.499492 | -0.642421 | |
| H | -2.564736 | 0.730453 | -1.135946 | |
| H | -1.004530 | 0.005170 | -1.565612 | |
| O | -1.467644 | -1.848542 | 0.176025 | |
| H | -2.618871 | -0.437562 | 1.046487 | |
| Rotational constants (GHz): | 2.4246900 | 1.4976900 | 1.1113400 | |
| Vibrational harmonic frequencies (cm-1): | | | | |
| 56.9673 | 91.2136 | | 106.3513 | |
| 122.1489 | 175.9464 | | 269.1432 | |
| 278.8436 | 328.8439 | | 430.1064 | |
| 505.0523 | 512.6383 | | 724.4171 | |
| 764.6457 | 818.9889 | | 837.2167 | |
| 893.8175 | 920.3885 | | 979.3270 | |
| 1021.5319 | 1039.2487 | | 1081.6394 | |
| 1113.0209 | 1118.0624 | | 1165.7441 | |
| 1186.3054 | 1237.8137 | | 1269.9542 | |
| 1299.5873 | 1328.4310 | | 1348.6382 | |
| 1369.5561 | 1384.2715 | | 1392.4708 | |
| 1412.6124 | 1429.8054 | | 1483.7339 | |
| 1496.1385 | 1504.3548 | | 1508.0270 | |
| 1821.1845 | 2871.9747 | | 2885.5067 | |
| 2940.5982 | 3021.7785 | | 3029.4720 | |
| 3035.8600 | 3043.8134 | | 3075.5581 | |
| 3080.5477 | 3085.2183 | | 3115.0082 | |
| Zero-point correction (Hartree): | 0.161781 | | | |

C6H11O2.ppmct

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -385.63040504
Electronic state : 2-A
Cartesian coordinates (Angs):

| | | | | |
|---|----------|-----------|-----------|--|
| O | 2.800136 | -0.986940 | -0.721696 | |
| C | 2.288951 | -0.641903 | 0.499633 | |

| | | | |
|--|-----------|-----------|-----------|
| C | 1.765272 | 0.800622 | 0.609962 |
| C | 0.732918 | 1.198130 | -0.462319 |
| C | -0.742777 | 0.914132 | -0.135641 |
| C | -1.131342 | -0.562876 | -0.033530 |
| C | -2.622816 | -0.800264 | 0.066411 |
| H | 1.472672 | -1.377168 | 0.667592 |
| H | 3.015131 | -0.872540 | 1.303495 |
| H | 1.359949 | 0.953495 | 1.619792 |
| H | 2.637289 | 1.460602 | 0.528790 |
| H | 0.823197 | 2.275450 | -0.643241 |
| H | 1.014471 | 0.711271 | -1.405037 |
| H | -1.018436 | 1.418536 | 0.798899 |
| H | -1.369112 | 1.372275 | -0.908999 |
| H | -0.679665 | -1.057308 | 0.839914 |
| H | -0.770920 | -1.136544 | -0.902043 |
| O | -3.463666 | 0.071515 | 0.056978 |
| H | -2.917568 | -1.871715 | 0.151485 |
| Rotational constants (GHz): | 4.3059000 | 0.8534700 | 0.7757200 |
| Vibrational harmonic frequencies (cm-1): | | | |
| 28.1965 | 50.5079 | | 98.1481 |
| 146.5373 | 184.9220 | | 193.9826 |
| 272.9829 | 281.7025 | | 423.8625 |
| 496.5785 | 623.6601 | | 677.3422 |
| 686.8215 | 798.1327 | | 827.6797 |
| 874.3660 | 898.9843 | | 939.7750 |
| 992.9374 | 1046.1693 | | 1069.0326 |
| 1103.6319 | 1117.6666 | | 1150.7469 |
| 1184.7186 | 1253.2554 | | 1284.8229 |
| 1321.3710 | 1324.1570 | | 1348.4653 |
| 1364.9329 | 1384.2005 | | 1406.3425 |
| 1411.2908 | 1428.8691 | | 1465.6584 |
| 1492.5241 | 1502.8349 | | 1508.3955 |
| 1833.7860 | 2885.7288 | | 2900.0561 |
| 2938.8118 | 3011.4033 | | 3032.5452 |
| 3038.0803 | 3042.3117 | | 3049.4738 |
| 3076.9872 | 3082.7210 | | 3094.1947 |
| Zero-point correction (Hartree): | 0.160958 | | |

C6H11O2.ppmtt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -385.62908548

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|--|-----------|-----------|-----------|
| O | 2.687440 | -1.085316 | -0.807113 |
| C | 2.129309 | -0.888644 | 0.426082 |
| C | 1.799093 | 0.574805 | 0.769835 |
| C | 0.930023 | 1.300825 | -0.274015 |
| C | -0.593002 | 1.192901 | -0.087267 |
| C | -1.187562 | -0.220495 | -0.250226 |
| C | -2.699565 | -0.188219 | -0.292157 |
| H | 1.209161 | -1.511373 | 0.408976 |
| H | 2.747931 | -1.359943 | 1.214275 |
| H | 1.330645 | 0.609012 | 1.762904 |
| H | 2.755786 | 1.101997 | 0.865327 |
| H | 1.184313 | 2.367017 | -0.256429 |
| H | 1.214540 | 0.938158 | -1.269899 |
| H | -0.868058 | 1.581518 | 0.902124 |
| H | -1.073560 | 1.856857 | -0.818737 |
| H | -0.894258 | -0.894360 | 0.560121 |
| H | -0.839269 | -0.650461 | -1.201646 |
| O | -3.426424 | -0.807240 | 0.452336 |
| H | -3.125143 | 0.474990 | -1.082309 |
| Rotational constants (GHz): | 3.6655500 | 0.8602800 | 0.7761900 |
| Vibrational harmonic frequencies (cm-1): | | | |
| 30.8750 | 66.4601 | | 78.1818 |
| 100.7034 | 156.2513 | | 233.8707 |
| 277.2134 | 310.4059 | | 430.0744 |
| 494.3220 | 527.8911 | | 641.5489 |
| 760.6394 | 799.2379 | | 833.9419 |
| 870.6012 | 928.8613 | | 958.4327 |
| 1016.4622 | 1060.3558 | | 1073.1981 |
| 1104.4786 | 1122.1947 | | 1153.8655 |
| 1185.1523 | 1250.5535 | | 1275.1701 |
| 1309.9358 | 1323.7981 | | 1344.5624 |
| 1365.5705 | 1384.2700 | | 1398.3165 |
| 1411.5220 | 1431.4796 | | 1477.2591 |
| 1493.7487 | 1502.5509 | | 1507.8639 |
| 1837.3214 | 2872.1219 | | 2900.9840 |
| 2942.3957 | 3018.7907 | | 3027.4721 |
| 3035.6855 | 3042.4493 | | 3064.1126 |
| 3080.2163 | 3084.7018 | | 3111.1037 |
| Zero-point correction (Hartree): | 0.161087 | | |

C6H11O2.pppmc

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -385.63440692
Electronic state : 2-A
Cartesian coordinates (Angs):
O 2.681810 -0.369586 -0.732337
C 1.742324 -0.834336 0.140999
C 1.079457 0.237087 1.024556
C 0.523009 1.431269 0.235632
C -0.659306 1.148321 -0.710212
C -1.953569 0.687563 -0.023713
C -2.110254 -0.800998 0.178332
H 0.962920 -1.305456 -0.498936
H 2.131436 -1.676822 0.744939
H 0.300113 -0.248358 1.625264
H 1.828624 0.607315 1.735776
H 0.225756 2.215782 0.944487
H 1.343371 1.845856 -0.360457
H -0.873152 2.071930 -1.259616
H -0.376068 0.404843 -1.462901
H -2.095801 1.171711 0.954660
H -2.838268 0.989854 -0.606535
O -1.344663 -1.654775 -0.219308
H -3.036074 -1.095200 0.722924
Rotational constants (GHz): 2.9346800 1.3367800 1.0851000
Vibrational harmonic frequencies (cm-1):
61.9915 72.3517 118.6963
148.6017 198.3797 205.8426
283.9955 334.2807 427.4902
534.2671 648.7036 688.0087
714.0909 797.3137 820.8534
877.0982 912.2293 969.8219
1009.3145 1033.4438 1077.1580
1102.1375 1122.6084 1142.1796
1187.5120 1244.3453 1261.0130
1303.8881 1332.5727 1371.8569
1377.5600 1384.4668 1402.0091
1413.2737 1429.5048 1452.9387
1495.1331 1498.7138 1503.7193
1823.6621 2884.1795 2896.8430
2942.6413 3010.9996 3031.3890
3037.4715 3044.1467 3059.4504
3076.3194 3092.5818 3101.7562
Zero-point correction (Hartree): 0.161661

C6H11O2.pppmt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -385.63005554
Electronic state : 2-A
Cartesian coordinates (Angs):
O 2.954877 -0.265411 -0.593848
C 1.829466 -0.947097 -0.214405
C 1.028714 -0.305367 0.929512
C 0.638694 1.158546 0.670955
C -0.393165 1.415813 -0.442200
C -1.809551 0.864216 -0.170547
C -1.965201 -0.613164 -0.449652
H 1.218533 -0.999069 -1.143195
H 2.066314 -2.007390 -0.002575
H 0.150516 -0.927805 1.138047
H 1.650191 -0.346550 1.832385
H 0.258629 1.591937 1.604627

H 1.554614 1.707395 0.423896
H -0.472110 2.499237 -0.584094
H -0.029593 1.023246 -1.402255
H -2.139678 1.065432 0.853793
H -2.513707 1.368550 -0.849949
O -2.471980 -1.419762 0.298501
H -1.580620 -0.931284 -1.449880
Rotational constants (GHz): 3.0738700 1.1208800 0.9551800
Vibrational harmonic frequencies (cm-1):
22.0907 65.0323 79.8139
108.2107 197.8832 216.9981
314.5316 338.8798 424.3026
501.9741 536.7791 597.6702
735.7653 766.7696 827.3850
882.9168 924.2125 967.2051
1016.1362 1057.4341 1065.5894
1086.8569 1119.6517 1151.6419
1185.7958 1237.9961 1254.1615
1314.0971 1335.9411 1353.6131
1368.9691 1378.2886 1400.5534
1415.9780 1427.7858 1470.1598
1496.2349 1503.5825 1506.7845
1833.2628 2849.0649 2883.0623
2946.4892 3017.4291 3030.6137

3041.9735 3053.1909 3081.1035
3085.1804 3096.6603 3105.5704
Zero-point correction (Hartree): 0.161019

C6H11O2.ppppc

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -385.63440689

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 2.682089 | -0.369998 | -0.732173 |
| C | 1.742345 | -0.834448 | 0.141077 |
| C | 1.079613 | 0.237247 | 1.024407 |
| C | 0.523292 | 1.431342 | 0.235258 |
| C | -0.659282 | 1.148319 | -0.710198 |
| C | -1.953412 | 0.687709 | -0.023347 |
| C | -2.110907 | -0.800887 | 0.177778 |
| H | 0.962971 | -1.305485 | -0.498932 |
| H | 2.131203 | -1.676927 | 0.745182 |
| H | 0.300237 | -0.247993 | 1.625233 |
| H | 1.828877 | 0.607516 | 1.735503 |
| H | 0.226378 | 2.216150 | 0.943920 |
| H | 1.343629 | 1.845543 | -0.361141 |
| H | -0.873216 | 2.071846 | -1.259702 |
| H | -0.376236 | 0.404742 | -1.462879 |
| H | -2.094594 | 1.170974 | 0.955658 |
| H | -2.838408 | 0.991254 | -0.605048 |
| O | -1.344980 | -1.654806 | -0.218908 |
| H | -3.037610 | -1.094878 | 0.720999 |

Rotational constants (GHz): 2.9347700 1.3365700 1.0848800

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 62.0015 | 72.3260 | 118.5798 |
| 148.6752 | 198.3804 | 205.8176 |
| 283.9357 | 334.2355 | 427.5099 |
| 534.2353 | 648.8063 | 687.8986 |
| 714.0309 | 797.3717 | 820.7881 |
| 877.1188 | 912.2809 | 969.7991 |
| 1009.3559 | 1033.4659 | 1077.1790 |
| 1102.1044 | 1122.6081 | 1142.1513 |
| 1187.5344 | 1244.3626 | 1261.0223 |
| 1303.9138 | 1332.5632 | 1371.8653 |
| 1377.5504 | 1384.4617 | 1402.0054 |
| 1413.2684 | 1429.5029 | 1452.9398 |
| 1495.1196 | 1498.7095 | 1503.7289 |
| 1823.6656 | 2884.3245 | 2896.7483 |
| 2942.6973 | 3010.9764 | 3031.4258 |
| 3037.2108 | 3044.1623 | 3059.4266 |
| 3076.3468 | 3092.5578 | 3101.6654 |

Zero-point correction (Hartree): 0.161660

C6H11O2.ppppt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -385.63440705

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 2.680569 | -0.369011 | -0.733714 |
| C | 1.742579 | -0.834497 | 0.140848 |
| C | 1.079630 | 0.236363 | 1.025055 |
| C | 0.523104 | 1.430969 | 0.236846 |
| C | -0.658595 | 1.148425 | -0.709889 |
| C | -1.953505 | 0.687773 | -0.024564 |
| C | -2.110566 | -0.800706 | 0.177747 |
| H | 0.962846 | -1.306431 | -0.498082 |
| H | 2.133238 | -1.676502 | 0.744461 |
| H | 0.300293 | -0.249512 | 1.625406 |
| H | 1.828737 | 0.606231 | 1.736531 |
| H | 0.225133 | 2.214735 | 0.946225 |
| H | 1.343572 | 1.846429 | -0.358470 |
| H | -0.871902 | 2.072274 | -1.259110 |
| H | -0.374940 | 0.405198 | -1.462669 |
| H | -2.096702 | 1.172196 | 0.953533 |
| H | -2.837647 | 0.989936 | -0.608321 |
| O | -1.344471 | -1.654728 | -0.218377 |
| H | -3.037296 | -1.094609 | 0.720969 |

Rotational constants (GHz): 2.9344200 1.3369500 1.0853400

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 61.9094 | 72.3568 | 118.8429 |
| 148.6094 | 198.4164 | 205.7995 |
| 283.9056 | 334.2947 | 427.4115 |
| 534.4660 | 648.7136 | 687.9993 |
| 713.9995 | 797.3851 | 820.8142 |
| 877.0456 | 912.2637 | 969.8079 |
| 1009.3393 | 1033.4385 | 1077.1963 |
| 1102.1901 | 1122.6499 | 1142.2225 |
| 1187.5635 | 1244.3431 | 1261.0923 |
| 1303.7812 | 1332.6125 | 1371.9214 |

| | | |
|-----------|-----------|-----------|
| 1377.5957 | 1384.5139 | 1402.0298 |
| 1413.3042 | 1429.5322 | 1452.9505 |
| 1495.1408 | 1498.7225 | 1503.6938 |
| 1823.6994 | 2884.1726 | 2896.7376 |
| 2942.6337 | 3010.9209 | 3031.3803 |
| 3037.4302 | 3044.1732 | 3059.4089 |
| 3076.3585 | 3092.6628 | 3101.7477 |

Zero-point correction (Hartree): 0.161662

C6H11O2.ppptc

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -385.63254402

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -3.115033 | -0.970981 | 0.339089 |
| C | -2.341028 | -0.509615 | -0.691469 |
| C | -1.655268 | 0.841664 | -0.433200 |
| C | -0.749109 | 0.840120 | 0.808274 |
| C | 0.569971 | 0.061647 | 0.666592 |
| C | 1.576996 | 0.704837 | -0.289428 |
| C | 2.880938 | -0.049772 | -0.415025 |
| H | -1.582237 | -1.309149 | -0.841637 |
| H | -2.912369 | -0.507020 | -1.639681 |
| H | -1.101703 | 1.130795 | -1.336386 |
| H | -2.442861 | 1.593927 | -0.304836 |
| H | -0.524581 | 1.877036 | 1.090141 |
| H | -1.326657 | 0.414214 | 1.636631 |
| H | 1.039989 | -0.029648 | 1.651845 |
| H | 0.382020 | -0.969760 | 0.345046 |
| H | 1.823084 | 1.732754 | 0.020397 |
| H | 1.175390 | 0.812774 | -1.308748 |
| O | 3.133013 | -1.092260 | 0.148491 |
| H | 3.631085 | 0.426726 | -1.087871 |

Rotational constants (GHz): 4.3631700 0.7997500 0.7599800

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 30.4126 | 37.9495 | 93.8668 |
| 169.5992 | 173.8614 | 210.5885 |
| 222.6891 | 330.8837 | 424.7169 |
| 511.9162 | 631.3123 | 664.4670 |
| 690.3553 | 771.4557 | 846.5028 |
| 879.1501 | 889.2601 | 949.8383 |
| 994.6408 | 1054.9103 | 1063.7276 |
| 1092.0244 | 1110.3531 | 1157.7155 |
| 1187.5209 | 1224.7135 | 1293.9362 |
| 1311.1911 | 1331.8569 | 1343.1931 |
| 1370.5860 | 1383.9649 | 1405.6492 |
| 1412.0615 | 1427.5942 | 1463.8160 |
| 1495.5191 | 1500.9529 | 1504.7690 |
| 1833.1073 | 2883.9118 | 2887.2137 |
| 2944.2969 | 3012.1773 | 3034.6227 |
| 3036.8062 | 3043.2213 | 3056.2173 |
| 3078.9360 | 3089.0970 | 3094.6097 |

Zero-point correction (Hartree): 0.160961

C6H11O2.ppptt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -385.63106791

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 3.078255 | -0.697059 | -0.787048 |
| C | 2.259990 | -0.901700 | 0.291314 |
| C | 1.645797 | 0.371450 | 0.894833 |
| C | 0.872373 | 1.225765 | -0.121345 |
| C | -0.430959 | 0.609284 | -0.657904 |
| C | -1.517067 | 0.394265 | 0.415463 |
| C | -2.828269 | -0.042774 | -0.197452 |
| H | 1.463009 | -1.575259 | -0.094582 |
| H | 2.769370 | -1.514726 | 1.059400 |
| H | 1.011004 | 0.085262 | 1.743202 |
| H | 2.463156 | 0.971325 | 1.312913 |
| H | 0.642804 | 2.198145 | 0.333136 |
| H | 1.539850 | 1.425126 | -0.967187 |
| H | -0.829351 | 1.271040 | -1.438045 |
| H | -0.223405 | -0.346062 | -1.156353 |
| H | -1.225845 | -0.352930 | 1.159093 |
| H | -1.693950 | 1.346369 | 0.938654 |
| O | -3.414362 | -1.066244 | 0.077143 |
| H | -3.238976 | 0.660389 | -0.960446 |

Rotational constants (GHz): 4.1988700 0.7843200 0.7422000

Vibrational harmonic frequencies (cm-1):

| | | |
|----------|----------|----------|
| 27.3488 | 63.8972 | 69.9217 |
| 98.0390 | 176.7137 | 224.8332 |
| 279.8945 | 339.1247 | 433.6777 |
| 506.1510 | 540.3528 | 628.3363 |

| | | |
|-----------|-----------|-----------|
| 747.4047 | 781.4637 | 839.2597 |
| 876.2387 | 940.2999 | 957.6729 |
| 1029.1674 | 1056.5431 | 1063.7874 |
| 1094.1436 | 1117.3268 | 1163.6910 |
| 1186.0391 | 1231.3152 | 1286.3163 |
| 1297.0433 | 1331.6197 | 1342.7857 |
| 1370.0128 | 1382.1631 | 1399.4703 |
| 1413.4506 | 1434.0454 | 1480.0749 |
| 1495.8954 | 1499.7654 | 1511.7554 |
| 1837.1925 | 2872.7356 | 2886.3903 |
| 2946.1467 | 3019.1450 | 3037.0220 |
| 3037.9650 | 3046.4761 | 3072.5012 |
| 3081.5388 | 3093.2109 | 3118.7528 |

Zero-point correction (Hartree): 0.161217

C6H11O2.pptmc

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -385.63397460

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 3.092081 | -0.756814 | -0.580670 |
| C | 2.703283 | 0.098737 | 0.414935 |
| C | 1.558220 | 1.055611 | 0.046688 |
| C | 0.294494 | 0.350621 | -0.465089 |
| C | -0.468116 | -0.433178 | 0.614001 |
| C | -1.736580 | -1.110255 | 0.085213 |
| C | -2.879731 | -0.168340 | -0.221488 |
| H | 2.393030 | -0.576085 | 1.243673 |
| H | 3.574282 | 0.640931 | 0.830937 |
| H | 1.325636 | 1.675481 | 0.923271 |
| H | 1.930175 | 1.739157 | -0.726187 |
| H | -0.378389 | 1.099149 | -0.894863 |
| H | 0.585000 | -0.328447 | -1.276719 |
| H | 0.177886 | -1.206112 | 1.047531 |
| H | -0.746055 | 0.245076 | 1.429689 |
| H | -2.130555 | -1.843017 | 0.806681 |
| H | -1.534239 | -1.695869 | -0.824356 |
| O | -2.872793 | 1.025666 | -0.012957 |
| H | -3.780496 | -0.660251 | -0.656200 |

Rotational constants (GHz): 5.0346400 0.8225600 0.7629700

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 34.8409 | 63.7081 | 94.3859 |
| 140.0447 | 186.5290 | 222.5693 |
| 253.3250 | 306.4371 | 409.8035 |
| 519.2954 | 632.4233 | 660.2492 |
| 705.1366 | 766.7755 | 856.0030 |
| 872.0264 | 876.8550 | 971.9122 |
| 1004.8868 | 1032.4006 | 1069.5665 |
| 1097.6558 | 1113.8400 | 1153.2716 |
| 1178.2295 | 1245.5589 | 1279.9998 |
| 1309.8855 | 1342.2218 | 1348.9895 |
| 1373.4335 | 1386.8182 | 1399.9414 |
| 1414.2448 | 1429.1244 | 1456.5711 |
| 1492.8603 | 1495.6262 | 1507.3968 |
| 1831.2350 | 2884.0938 | 2885.3208 |
| 2942.9541 | 3014.8626 | 3035.4239 |
| 3039.1878 | 3045.3292 | 3051.8461 |
| 3079.1348 | 3082.5044 | 3108.2714 |

Zero-point correction (Hartree): 0.161078

C6H11O2.pptmt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -385.63012172

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 3.140214 | -0.834557 | -0.623453 |
| C | 2.822203 | -0.013833 | 0.424883 |
| C | 1.765075 | 1.058563 | 0.115762 |
| C | 0.447118 | 0.489712 | -0.430818 |
| C | -0.403644 | -0.233584 | 0.625367 |
| C | -1.693082 | -0.888101 | 0.075969 |
| C | -2.719053 | 0.115248 | -0.402408 |
| H | 2.457066 | -0.708353 | 1.213645 |
| H | 3.735397 | 0.427059 | 0.868656 |
| H | 1.586066 | 1.648381 | 1.025056 |
| H | 2.196034 | 1.747037 | -0.620932 |
| H | -0.129199 | 1.310015 | -0.874029 |
| H | 0.686462 | -0.201445 | -1.248587 |
| H | 0.187237 | -1.028911 | 1.095893 |
| H | -0.669715 | 0.464587 | 1.429966 |
| H | -1.429417 | -1.538877 | -0.770366 |
| H | -2.169468 | -1.501776 | 0.846278 |
| O | -3.808632 | 0.269366 | 0.105687 |
| H | -2.414830 | 0.735788 | -1.275979 |


```

Rotational constants (GHz):    6.0641300    0.7008700    0.6782100
Vibrational harmonic frequencies (cm-1):
  30.2735          30.7871          61.0584
 113.4751         176.7707         223.7356
 242.1457         339.0916         424.2097
 497.0170         530.3735         626.5107
 735.0979         823.2978         844.0588
 860.5035         941.4525         950.0416
1030.0354         1048.7994        1066.8511
1098.5148         1113.4416        1154.9548
1173.7432         1251.3708        1273.4284
1314.4603         1335.2969        1347.6300
1353.2817         1370.6724        1399.7382
1410.8635         1441.2697        1480.7050
1495.2810         1499.2367        1511.6144
1832.9515         2887.2769        2891.3917
2946.2436         3028.0230        3032.4472
3037.0915         3047.2131        3067.4558
3081.6008         3093.0237        3112.7323
Zero-point correction (Hartree): 0.161018

```

C6H11O2.pptpc

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -385.63298678

Electronic state : 2-A

Cartesian coordinates (Angs):

```

O      -2.390391    1.406902    -0.284672
C      -2.364951    0.283850    0.497990
C      -1.810906   -0.970357   -0.196051
C      -0.346421   -0.827147   -0.635507
C       0.662000   -1.003260    0.510345
C       2.116560   -0.808664    0.072231
C       2.518414    0.633284   -0.151391
H      -1.729261    0.565689    1.365595
H      -3.360869    0.101081    0.946254
H      -1.931858   -1.831927    0.475464
H      -2.442771   -1.166681   -1.070441
H      -0.127733   -1.569106   -1.414577
H      -0.221719    0.160138   -1.094482
H       0.449240   -0.289586    1.314822
H       0.549379   -2.007079    0.938749
H       2.817452   -1.206059    0.823101
H       2.344020   -1.368630   -0.847246
O       1.822932    1.592438    0.101945
H       3.545617    0.771210   -0.561119

```

```

Rotational constants (GHz):    3.2085500    1.0904100    0.8848000

```

```

Vibrational harmonic frequencies (cm-1):
  29.4469          59.0994          94.9042
 151.7533         162.1278         238.4820
 260.0514         296.1454         417.3897
 496.7866         638.8060         663.7575
 700.7085         787.3759         835.2751
 871.5002         887.0009         972.4986
1000.7831         1057.7322        1065.8236
1095.2172         1102.1994        1157.1485
1180.9204         1233.7717        1291.9315
1318.9606         1340.8628        1352.8036
1371.3407         1384.6649        1396.4504
1413.0693         1428.5943        1458.5240
1494.0983         1494.5032        1510.7067
1833.3181         2886.9026        2894.9230
2941.3567         3014.1188        3029.2592
3036.9548         3039.5552        3047.7208
3077.7552         3081.5639        3099.0428
Zero-point correction (Hartree): 0.161057

```

C6H11O2.pptpt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -385.63017362

Electronic state : 2-A

Cartesian coordinates (Angs):

```

O      -2.416473    1.587895    -0.181704
C      -2.572833    0.410083    0.498184
C      -2.056185   -0.837940   -0.235669
C      -0.579065   -0.746281   -0.644734
C       0.403632   -0.890356    0.528353
C       1.891600   -0.846175   -0.118852
C       2.376133    0.530207   -0.284705
H      -2.014645    0.566139    1.447755
H      -3.621781    0.286354    0.829431
H      -2.228267   -1.717105    0.400376
H      -2.673545   -0.975804   -1.131375
H      -0.362620   -1.530399   -1.381517
H      -0.432051    0.211283   -1.157722
H       0.219427   -0.114123    1.282904

```

| | | | | |
|--|-----------|-----------|-----------|-----------|
| H | 0.218605 | -1.848327 | 1.030588 | |
| H | 2.539514 | -1.195480 | 0.928431 | |
| H | 2.046588 | -1.516795 | -0.740416 | |
| O | 3.390905 | 1.042805 | 0.134888 | |
| H | 1.733617 | 1.071434 | -1.015603 | |
| Rotational constants (GHz): | 3.6702000 | | 0.8503500 | 0.7446000 |
| Vibrational harmonic frequencies (cm-1): | | | | |
| 27.9635 | | 37.0664 | | 57.7584 |
| 121.1805 | | 168.1020 | | 231.6979 |
| 255.3534 | | 321.0177 | | 405.2371 |
| 499.2147 | | 541.0801 | | 626.1934 |
| 750.5833 | | 785.7871 | | 840.1873 |
| 862.0396 | | 933.2780 | | 965.1927 |
| 1030.5899 | | 1053.1039 | | 1068.4954 |
| 1098.8922 | | 1109.7659 | | 1154.7480 |
| 1179.3576 | | 1237.6535 | | 1293.1304 |
| 1302.9077 | | 1338.7003 | | 1349.7259 |
| 1353.6859 | | 1371.2952 | | 1397.0946 |
| 1412.1308 | | 1441.2371 | | 1473.7641 |
| 1496.3372 | | 1501.6007 | | 1513.6890 |
| 1832.1852 | | 2887.3014 | | 2896.9141 |
| 2945.6031 | | 3017.9279 | | 3029.4983 |
| 3035.6051 | | 3043.2334 | | 3065.3321 |
| 3080.5319 | | 3094.1398 | | 3108.8010 |
| Zero-point correction (Hartree): | 0.160939 | | | |

C6H11O2.ppttc

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -385.63437841

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | | |
|--|-----------|-----------|-----------|-----------|
| O | -2.882531 | -0.767785 | 1.033765 | |
| C | -2.549365 | -0.707936 | -0.292612 | |
| C | -1.948073 | 0.629498 | -0.753718 | |
| C | -0.702810 | 1.052167 | 0.038831 | |
| C | 0.546833 | 0.214725 | -0.263607 | |
| C | 1.769345 | 0.666125 | 0.535761 | |
| C | 3.018892 | -0.140648 | 0.268839 | |
| H | -1.813516 | -1.531554 | -0.426420 | |
| H | -3.403906 | -1.014601 | -0.926015 | |
| H | -1.718678 | 0.559193 | -1.825685 | |
| H | -2.724427 | 1.397245 | -0.650424 | |
| H | -0.487722 | 2.107551 | -0.173291 | |
| H | -0.942138 | 0.992842 | 1.108077 | |
| H | 0.365942 | -0.844812 | -0.048393 | |
| H | 0.782003 | 0.264276 | -1.333862 | |
| H | 2.013609 | 1.721877 | 0.338676 | |
| H | 1.578798 | 0.623193 | 1.619601 | |
| O | 3.085669 | -1.075255 | -0.499683 | |
| H | 3.916007 | 0.185525 | 0.844112 | |
| Rotational constants (GHz): | 4.2689400 | | 0.7658700 | 0.7343200 |
| Vibrational harmonic frequencies (cm-1): | | | | |
| 35.1959 | | 68.7331 | | 90.6387 |
| 118.6730 | | 173.3819 | | 203.5640 |
| 258.2731 | | 297.1078 | | 403.0074 |
| 514.7482 | | 637.6327 | | 672.7006 |
| 693.4860 | | 762.9304 | | 850.6651 |
| 885.6577 | | 904.4039 | | 937.2894 |
| 1028.6070 | | 1042.9018 | | 1068.1503 |
| 1099.2272 | | 1112.7586 | | 1157.2584 |
| 1179.9447 | | 1259.5953 | | 1279.6549 |
| 1313.9738 | | 1330.0848 | | 1340.1578 |
| 1371.0098 | | 1379.4467 | | 1403.0964 |
| 1416.6191 | | 1426.9207 | | 1462.6161 |
| 1494.6196 | | 1497.6397 | | 1512.1616 |
| 1832.1639 | | 2886.3460 | | 2888.3931 |
| 2945.0137 | | 3011.2441 | | 3031.8958 |
| 3036.4059 | | 3037.3005 | | 3050.6448 |
| 3069.8096 | | 3080.3901 | | 3094.9219 |
| Zero-point correction (Hartree): | 0.160950 | | | |

C6H11O2.ppttt

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -385.63199992

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | | |
|---|-----------|-----------|-----------|--|
| O | 2.893482 | -1.269642 | -0.555202 | |
| C | 2.671523 | -0.495900 | 0.552002 | |
| C | 2.082452 | 0.895023 | 0.266849 | |
| C | 0.765496 | 0.857758 | -0.521712 | |
| C | -0.444524 | 0.379552 | 0.293623 | |
| C | -1.742295 | 0.352883 | -0.535760 | |
| C | -2.948569 | 0.000727 | 0.304536 | |
| H | 1.971813 | -1.098561 | 1.172182 | |
| H | 3.584864 | -0.434752 | 1.174552 | |

| | | | | |
|--|-----------|-----------|-----------|--|
| H | 1.949547 | 1.423700 | 1.220767 | |
| H | 2.829428 | 1.462066 | -0.301517 | |
| H | 0.553064 | 1.860851 | -0.912850 | |
| H | 0.905692 | 0.206136 | -1.392474 | |
| H | -0.261779 | -0.626310 | 0.692988 | |
| H | -0.580707 | 1.037197 | 1.163745 | |
| H | -1.915850 | 1.354404 | -0.958549 | |
| H | -1.675878 | -0.357073 | -1.365707 | |
| O | -3.714462 | -0.908405 | 0.074435 | |
| H | -3.096851 | 0.656444 | 1.195769 | |
| Rotational constants (GHz): | 4.6820400 | 0.7015700 | 0.6603900 | |
| Vibrational harmonic frequencies (cm-1): | | | | |
| 42.0223 | 47.7977 | | 82.3091 | |
| 98.5981 | 144.7472 | | 206.5939 | |
| 253.4380 | 353.5310 | | 385.1622 | |
| 498.2322 | 536.5498 | | 619.1463 | |
| 742.7265 | 783.9188 | | 863.5058 | |
| 868.5760 | 918.8598 | | 1003.6064 | |
| 1023.0306 | 1046.5261 | | 1067.0221 | |
| 1099.1400 | 1117.5511 | | 1155.6459 | |
| 1179.7867 | 1251.7670 | | 1274.9936 | |
| 1305.2738 | 1334.0873 | | 1343.8633 | |
| 1361.6122 | 1371.2671 | | 1398.0270 | |
| 1411.5158 | 1434.0683 | | 1476.8226 | |
| 1493.5561 | 1498.6961 | | 1514.4226 | |
| 1838.0860 | 2866.0971 | | 2888.7058 | |
| 2944.9002 | 3017.0696 | | 3023.7640 | |
| 3033.8386 | 3040.9789 | | 3062.6467 | |
| 3079.9978 | 3090.0492 | | 3113.3949 | |
| Zero-point correction (Hartree): | 0.160856 | | | |

C6H11O2.ptmmc

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -385.63351176

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | | |
|--|-----------|-----------|-----------|--|
| O | 3.388632 | -0.138923 | -0.514810 | |
| C | 2.580364 | -0.516937 | 0.523997 | |
| C | 1.264174 | 0.262535 | 0.648847 | |
| C | 0.386104 | 0.125148 | -0.601372 | |
| C | -0.834496 | 1.059074 | -0.638640 | |
| C | -1.861240 | 0.842327 | 0.479134 | |
| C | -2.623859 | -0.461520 | 0.409920 | |
| H | 2.370323 | -1.594625 | 0.342499 | |
| H | 3.155659 | -0.517083 | 1.470454 | |
| H | 0.741656 | -0.093392 | 1.546891 | |
| H | 1.507618 | 1.319144 | 0.825181 | |
| H | 1.014356 | 0.340104 | -1.473505 | |
| H | 0.049188 | -0.912615 | -0.706998 | |
| H | -0.492726 | 2.101055 | -0.597467 | |
| H | -1.342631 | 0.932975 | -1.600970 | |
| H | -1.411111 | 0.911013 | 1.480180 | |
| H | -2.621940 | 1.638762 | 0.467400 | |
| O | -2.527121 | -1.281046 | -0.477997 | |
| H | -3.328769 | -0.629351 | 1.257472 | |
| Rotational constants (GHz): | 4.3915100 | 0.8336100 | 0.8008000 | |
| Vibrational harmonic frequencies (cm-1): | | | | |
| 46.7644 | 49.9343 | | 105.8639 | |
| 137.7861 | 196.2431 | | 206.8737 | |
| 253.6673 | 301.0456 | | 420.7746 | |
| 509.0159 | 558.0963 | | 653.5899 | |
| 716.8267 | 766.4618 | | 832.7668 | |
| 863.2748 | 917.3802 | | 950.4772 | |
| 997.3367 | 1028.0995 | | 1087.6762 | |
| 1091.7073 | 1110.5855 | | 1153.9050 | |
| 1202.7157 | 1233.1040 | | 1281.9615 | |
| 1324.9344 | 1335.1873 | | 1364.1690 | |
| 1367.9352 | 1388.2453 | | 1397.4441 | |
| 1417.9104 | 1430.7210 | | 1459.3070 | |
| 1491.1766 | 1497.4826 | | 1518.1082 | |
| 1831.3513 | 2879.6002 | | 2884.4895 | |
| 2938.1983 | 3016.0176 | | 3026.9926 | |
| 3042.9400 | 3048.4091 | | 3053.6350 | |
| 3064.7067 | 3091.5275 | | 3101.6005 | |
| Zero-point correction (Hartree): | 0.160943 | | | |

Rotational constants (GHz): 4.3915100 0.8336100 0.8008000

Vibrational harmonic frequencies (cm-1):

C6H11O2.ptmmt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -385.63257596

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | | |
|---|----------|-----------|-----------|--|
| O | 3.363762 | 0.098437 | -0.300271 | |
| C | 2.421564 | -0.784487 | 0.156638 | |
| C | 1.093476 | -0.157772 | 0.601552 | |

| | | | | |
|--|-----------|-----------|-----------|--|
| C | 0.418639 | 0.632345 | -0.525879 | |
| C | -0.792953 | 1.469728 | -0.086753 | |
| C | -1.926923 | 0.661646 | 0.588553 | |
| C | -2.462529 | -0.414076 | -0.325842 | |
| H | 2.249131 | -1.478818 | -0.696059 | |
| H | 2.856315 | -1.435309 | 0.939718 | |
| H | 0.436379 | -0.958536 | 0.962032 | |
| H | 1.293379 | 0.502963 | 1.455856 | |
| H | 1.164866 | 1.300038 | -0.971508 | |
| H | 0.117266 | -0.066379 | -1.318857 | |
| H | -0.468097 | 2.247240 | 0.615348 | |
| H | -1.198680 | 1.996864 | -0.959895 | |
| H | -1.584240 | 0.189197 | 1.513218 | |
| H | -2.749338 | 1.346608 | 0.835729 | |
| O | -2.316698 | -1.604795 | -0.149448 | |
| H | -3.001130 | -0.037307 | -1.227449 | |
| Rotational constants (GHz): | 3.8016800 | 0.9279200 | 0.8136900 | |
| Vibrational harmonic frequencies (cm-1): | | | | |
| 37.0979 | 53.6437 | | 73.1865 | |
| 133.6996 | 182.9106 | | 224.8860 | |
| 251.8997 | 340.3522 | | 453.3351 | |
| 504.8376 | 523.5054 | | 574.7219 | |
| 752.7616 | 798.5136 | | 844.6966 | |
| 885.8333 | 939.8912 | | 965.3216 | |
| 1007.4567 | 1054.2755 | | 1066.5969 | |
| 1090.8187 | 1113.2597 | | 1162.1368 | |
| 1197.3342 | 1233.2910 | | 1271.7782 | |
| 1317.6507 | 1331.9484 | | 1352.0283 | |
| 1365.5771 | 1371.0708 | | 1390.8332 | |
| 1422.7442 | 1432.1044 | | 1486.8970 | |
| 1499.0926 | 1504.1093 | | 1515.2492 | |
| 1830.1460 | 2873.6667 | | 2882.5362 | |
| 2943.3229 | 3025.8432 | | 3035.5642 | |
| 3038.6715 | 3043.9875 | | 3075.2969 | |
| 3078.4027 | 3094.7135 | | 3122.3555 | |
| Zero-point correction (Hartree): | 0.161230 | | | |

C6H11O2.ptmpc

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -385.63274366
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | | |
|--|-----------|-----------|-----------|--|
| O | -3.294940 | -0.034100 | -0.456782 | |
| C | -2.448955 | -0.590971 | 0.465864 | |
| C | -0.952311 | -0.445055 | 0.161036 | |
| C | -0.530215 | 1.022437 | 0.021707 | |
| C | 0.904513 | 1.260204 | -0.476532 | |
| C | 2.011802 | 0.753702 | 0.459032 | |
| C | 2.432702 | -0.685706 | 0.258375 | |
| H | -2.699303 | -0.071751 | 1.418758 | |
| H | -2.732020 | -1.644052 | 0.658054 | |
| H | -0.390341 | -0.948268 | 0.958382 | |
| H | -0.723747 | -0.989389 | -0.762085 | |
| H | -1.226444 | 1.503802 | -0.674841 | |
| H | -0.664713 | 1.531913 | 0.988264 | |
| H | 1.036969 | 0.789714 | -1.457353 | |
| H | 1.039764 | 2.337874 | -0.622507 | |
| H | 2.933588 | 1.343858 | 0.334212 | |
| H | 1.746682 | 0.882706 | 1.519416 | |
| O | 2.044123 | -1.412366 | -0.630232 | |
| H | 3.180891 | -1.052341 | 0.998926 | |
| Rotational constants (GHz): | 3.8474200 | 0.9575900 | 0.8431700 | |
| Vibrational harmonic frequencies (cm-1): | | | | |
| 51.7535 | 69.6380 | | 95.6275 | |
| 140.4012 | 160.6083 | | 207.4417 | |
| 265.9750 | 290.1511 | | 425.0877 | |
| 515.3222 | 561.2317 | | 654.5752 | |
| 706.3454 | 779.5793 | | 806.5818 | |
| 878.2819 | 925.5679 | | 976.8468 | |
| 995.0487 | 1013.8650 | | 1076.7685 | |
| 1092.8339 | 1110.6033 | | 1157.8076 | |
| 1204.5681 | 1250.8374 | | 1264.2497 | |
| 1328.0305 | 1332.5775 | | 1366.5390 | |
| 1370.4489 | 1376.1649 | | 1397.0669 | |
| 1421.7561 | 1429.1278 | | 1457.3832 | |
| 1489.0219 | 1496.0979 | | 1512.7836 | |
| 1831.6115 | 2875.5040 | | 2883.8376 | |
| 2941.8268 | 3009.1620 | | 3011.4563 | |
| 3038.4785 | 3044.8176 | | 3054.5779 | |
| 3078.0787 | 3095.3487 | | 3099.9438 | |
| Zero-point correction (Hartree): | 0.160882 | | | |

C6H11O2.ptmpt

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -385.63177599

Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 3.375737 | 0.007996 | 0.248133 |
| C | 2.394487 | -0.824853 | -0.220136 |
| C | 0.961461 | -0.440770 | 0.173159 |
| C | 0.589052 | 0.969190 | -0.303340 |
| C | -0.747621 | 1.514029 | 0.223697 |
| C | -2.005451 | 0.781574 | -0.290830 |
| C | -2.276747 | -0.542037 | 0.387626 |
| H | 2.507685 | -0.803360 | -1.327097 |
| H | 2.629243 | -1.873800 | 0.045346 |
| H | 0.278375 | -1.195469 | -0.233830 |
| H | 0.881465 | -0.497777 | 1.267132 |
| H | 1.391368 | 1.648224 | 0.008110 |
| H | 0.576616 | 0.990438 | -1.402631 |
| H | -0.743946 | 1.500083 | 1.323037 |
| H | -0.829304 | 2.568701 | -0.062122 |
| H | -2.883459 | 1.410928 | -0.079404 |
| H | -1.969357 | 0.619316 | -1.373126 |
| O | -2.508303 | -1.584818 | -0.184322 |
| H | -2.269248 | -0.495509 | 1.503032 |

Rotational constants (GHz): 3.6277500 0.9392600 0.7887900
 Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 44.7463 | 65.1279 | 78.9997 |
| 108.4108 | 153.3310 | 229.7111 |
| 283.0116 | 316.6927 | 424.7695 |
| 503.1578 | 527.5543 | 573.4147 |
| 750.3984 | 773.2322 | 820.5368 |
| 915.5806 | 942.0496 | 949.6776 |
| 1010.6490 | 1055.6973 | 1068.9009 |
| 1093.0877 | 1109.9611 | 1167.8896 |
| 1205.0184 | 1241.2508 | 1260.8032 |
| 1326.2633 | 1332.9276 | 1355.4932 |
| 1364.0072 | 1372.7721 | 1391.9505 |
| 1422.2523 | 1431.0349 | 1470.8331 |
| 1496.4224 | 1502.7723 | 1513.1954 |
| 1832.2071 | 2866.3436 | 2883.9842 |
| 2943.4576 | 3017.2891 | 3021.6311 |
| 3029.2891 | 3040.3179 | 3075.6256 |
| 3079.8004 | 3096.1041 | 3103.3318 |

Zero-point correction (Hartree): 0.160937

C6H11O2.ptmtc

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -385.63379541
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 3.602845 | -0.683269 | -0.174414 |
| C | 2.976695 | 0.527446 | -0.040921 |
| C | 1.476737 | 0.531416 | -0.364686 |
| C | 0.684249 | -0.442962 | 0.515903 |
| C | -0.787341 | -0.620577 | 0.116458 |
| C | -1.640669 | 0.638703 | 0.283582 |
| C | -3.106297 | 0.439806 | -0.029172 |
| H | 3.141849 | 0.817355 | 1.020846 |
| H | 3.526601 | 1.301417 | -0.611245 |
| H | 1.105338 | 1.559211 | -0.257824 |
| H | 1.352237 | 0.260739 | -1.421637 |
| H | 1.185112 | -1.416668 | 0.469962 |
| H | 0.743931 | -0.115887 | 1.564682 |
| H | -0.851815 | -0.959689 | -0.924509 |
| H | -1.232578 | -1.422556 | 0.715253 |
| H | -1.288786 | 1.465740 | -0.351441 |
| H | -1.579690 | 1.031451 | 1.311349 |
| O | -3.601204 | -0.606204 | -0.387679 |
| H | -3.735579 | 1.351684 | 0.094319 |

Rotational constants (GHz): 7.4989900 0.6521300 0.6271500
 Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 38.5753 | 53.0763 | 90.8674 |
| 151.4921 | 176.2922 | 194.8558 |
| 242.1308 | 258.1400 | 424.1393 |
| 509.0913 | 553.5024 | 667.8734 |
| 703.0753 | 764.5007 | 837.1602 |
| 871.2285 | 915.6667 | 952.0614 |
| 989.3430 | 1044.8878 | 1080.1567 |
| 1097.7902 | 1100.4658 | 1164.7515 |
| 1216.3893 | 1231.3930 | 1304.5741 |
| 1309.9877 | 1336.5800 | 1344.0129 |
| 1365.2314 | 1372.8799 | 1407.8841 |
| 1417.3471 | 1427.9256 | 1463.8227 |
| 1493.5587 | 1502.3944 | 1512.4920 |
| 1833.8016 | 2881.9107 | 2883.0680 |
| 2939.0186 | 3009.5655 | 3015.7522 |
| 3032.1230 | 3039.9794 | 3054.6943 |
| 3068.7245 | 3088.8614 | 3096.4502 |

Zero-point correction (Hartree): 0.160683

C6H11O2.ptmtt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -385.63226054

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -3.686389 | 0.337527 | -0.400885 |
| C | -2.943141 | -0.639142 | 0.207118 |
| C | -1.444023 | -0.623702 | -0.119272 |
| C | -0.780902 | 0.708314 | 0.252455 |
| C | 0.674808 | 0.852631 | -0.214305 |
| C | 1.650410 | -0.137955 | 0.450983 |
| C | 3.088836 | 0.154922 | 0.088565 |
| H | -3.102650 | -0.481505 | 1.297196 |
| H | -3.398278 | -1.630952 | 0.018569 |
| H | -0.967651 | -1.465004 | 0.400274 |
| H | -1.323693 | -0.809927 | -1.194688 |
| H | -1.378060 | 1.514607 | -0.188606 |
| H | -0.828038 | 0.848593 | 1.342398 |
| H | 0.723228 | 0.728953 | -1.304052 |
| H | 1.011889 | 1.876729 | -0.006350 |
| H | 1.436671 | -1.175953 | 0.181677 |
| H | 1.562020 | -0.044104 | 1.544626 |
| O | 3.858053 | -0.644108 | -0.397327 |
| H | 3.415330 | 1.200798 | 0.301393 |

Rotational constants (GHz): 7.4545800 0.6255100 0.6032200

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 42.1805 | 63.3530 | 76.3895 |
| 94.0532 | 150.1764 | 236.7654 |
| 259.3901 | 276.1826 | 433.0176 |
| 504.3300 | 522.5425 | 562.8827 |
| 753.9170 | 768.3165 | 843.6093 |
| 881.3819 | 941.9399 | 966.2760 |
| 1021.4560 | 1053.2215 | 1075.4075 |
| 1095.1061 | 1110.6565 | 1166.8038 |
| 1215.6862 | 1231.5323 | 1286.1119 |
| 1304.1254 | 1333.0685 | 1345.5797 |
| 1363.7404 | 1373.5418 | 1396.4377 |
| 1419.2744 | 1434.8123 | 1476.7497 |
| 1493.7755 | 1507.2224 | 1512.1330 |
| 1837.8144 | 2869.7369 | 2883.6778 |
| 2940.8204 | 3013.2811 | 3018.5677 |
| 3031.4775 | 3036.7763 | 3069.3899 |
| 3071.4249 | 3090.4560 | 3118.2672 |

Zero-point correction (Hartree): 0.160781

C6H11O2.ptpmc

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -385.63289650

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 3.038830 | -0.055350 | 0.887576 |
| C | 2.492486 | -0.596124 | -0.247461 |
| C | 0.973302 | -0.444034 | -0.384393 |
| C | 0.537466 | 1.025736 | -0.390740 |
| C | -0.976005 | 1.272897 | -0.505131 |
| C | -1.810679 | 0.733013 | 0.665381 |
| C | -2.305514 | -0.688489 | 0.512215 |
| H | 3.012841 | -0.084961 | -1.088205 |
| H | 2.814536 | -1.651276 | -0.348563 |
| H | 0.640764 | -0.948700 | -1.299751 |
| H | 0.504839 | -0.982790 | 0.447504 |
| H | 0.921400 | 1.502497 | 0.520449 |
| H | 1.031094 | 1.535721 | -1.230018 |
| H | -1.138599 | 2.354054 | -0.579494 |
| H | -1.356036 | 0.831231 | -1.433377 |
| H | -1.271272 | 0.800960 | 1.622030 |
| H | -2.716760 | 1.340426 | 0.817609 |
| O | -2.171096 | -1.373660 | -0.478546 |
| H | -2.851020 | -1.083077 | 1.400356 |

Rotational constants (GHz): 3.4970000 0.9866800 0.8902700

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 44.0918 | 67.8611 | 96.5904 |
| 132.3633 | 158.2981 | 205.2546 |
| 278.0579 | 288.5529 | 402.0673 |
| 443.4275 | 538.4366 | 654.2279 |
| 705.8923 | 778.9568 | 811.0705 |
| 864.2536 | 926.5416 | 960.1845 |
| 997.5939 | 1021.7654 | 1078.9209 |
| 1094.2930 | 1112.4947 | 1156.6368 |
| 1195.9138 | 1249.5882 | 1280.6738 |
| 1322.4573 | 1342.1122 | 1359.9739 |
| 1372.6743 | 1376.8650 | 1397.3076 |
| 1419.5827 | 1428.6123 | 1457.1666 |

| | | |
|-----------|-----------|-----------|
| 1485.6671 | 1493.8792 | 1511.2201 |
| 1830.8011 | 2881.9975 | 2886.2551 |
| 2935.8069 | 3013.3117 | 3022.1843 |
| 3041.9867 | 3051.5598 | 3054.1097 |
| 3064.0729 | 3092.9535 | 3098.5604 |

Zero-point correction (Hartree): 0.160577

C6H11O2.ptpmt

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -385.63107196
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -2.892309 | -0.574994 | -0.892781 |
| C | -2.493198 | -0.485064 | 0.414325 |
| C | -1.008767 | -0.160184 | 0.628521 |
| C | -0.600442 | 1.157751 | -0.041246 |
| C | 0.871712 | 1.564031 | 0.133765 |
| C | 1.897924 | 0.619553 | -0.526830 |
| C | 2.211400 | -0.621584 | 0.279135 |
| H | -3.131992 | 0.313678 | 0.853311 |
| H | -2.799918 | -1.396061 | 0.964262 |
| H | -0.812675 | -0.120663 | 1.709254 |
| H | -0.420676 | -0.995043 | 0.231113 |
| H | -0.838329 | 1.089692 | -1.109600 |
| H | -1.227262 | 1.966862 | 0.359229 |
| H | 1.004539 | 2.564958 | -0.291868 |
| H | 1.107353 | 1.660140 | 1.203732 |
| H | 1.592395 | 0.318315 | -1.534018 |
| H | 2.853787 | 1.157716 | -0.620271 |
| O | 2.264256 | -1.747843 | -0.163287 |
| H | 2.425427 | -0.423913 | 1.357388 |

Rotational constants (GHz): 3.0225300 1.0220900 0.8583500
 Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 42.5157 | 59.9008 | 78.7337 |
| 119.2516 | 141.8569 | 230.1725 |
| 288.6440 | 316.3008 | 402.7824 |
| 493.6669 | 511.6302 | 554.8029 |
| 740.4572 | 780.8630 | 814.3063 |
| 901.8387 | 926.6214 | 976.1187 |
| 996.5026 | 1044.7557 | 1079.1638 |
| 1100.5562 | 1121.4602 | 1159.5110 |
| 1194.0486 | 1242.4309 | 1272.7406 |
| 1320.0117 | 1341.1270 | 1354.8998 |
| 1363.6041 | 1376.0553 | 1391.4294 |
| 1421.9518 | 1430.5635 | 1468.5357 |
| 1496.2168 | 1502.6409 | 1512.4865 |
| 1833.8822 | 2860.5541 | 2882.3592 |
| 2940.9820 | 3016.1137 | 3022.0963 |
| 3027.2544 | 3032.0136 | 3073.6781 |
| 3080.8322 | 3096.6931 | 3106.2141 |

Zero-point correction (Hartree): 0.160711

C6H11O2.ptppc

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -385.63299191
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -2.598353 | 1.402575 | -0.153406 |
| C | -2.747139 | 0.042381 | -0.088904 |
| C | -1.467201 | -0.769834 | -0.320966 |
| C | -0.387764 | -0.474479 | 0.727519 |
| C | 0.950372 | -1.194545 | 0.487834 |
| C | 1.755160 | -0.664140 | -0.704550 |
| C | 2.408872 | 0.680820 | -0.470680 |
| H | -3.157477 | -0.160076 | 0.925162 |
| H | -3.566452 | -0.270945 | -0.766059 |
| H | -1.722065 | -1.838915 | -0.316971 |
| H | -1.103598 | -0.539735 | -1.330479 |
| H | -0.221540 | 0.606750 | 0.775899 |
| H | -0.768831 | -0.769980 | 1.714533 |
| H | 1.570522 | -1.094559 | 1.384774 |
| H | 0.768763 | -2.267540 | 0.346088 |
| H | 2.569639 | -1.356163 | -0.970293 |
| H | 1.151708 | -0.586544 | -1.620338 |
| O | 2.407351 | 1.279267 | 0.582855 |
| H | 2.933554 | 1.101748 | -1.359429 |

Rotational constants (GHz): 3.3941700 0.9660600 0.8515900
 Vibrational harmonic frequencies (cm-1):

| | | |
|----------|-----------|-----------|
| 39.1620 | 46.7648 | 109.4665 |
| 139.1917 | 179.4985 | 207.1672 |
| 259.5053 | 320.6620 | 386.8785 |
| 439.6819 | 536.5587 | 657.0410 |
| 711.0676 | 769.4556 | 832.7666 |
| 851.9340 | 926.9511 | 945.7407 |
| 978.0068 | 1051.7461 | 1072.5178 |

| | | |
|-----------|-----------|-----------|
| 1093.5001 | 1113.0646 | 1154.0770 |
| 1191.9804 | 1232.9363 | 1294.9474 |
| 1318.0115 | 1335.3583 | 1360.7546 |
| 1374.0251 | 1385.6805 | 1394.4712 |
| 1416.0890 | 1428.9173 | 1458.9681 |
| 1493.1326 | 1495.2978 | 1517.4413 |
| 1832.7539 | 2884.6894 | 2887.2804 |
| 2932.4001 | 3016.7213 | 3026.9781 |
| 3032.9269 | 3044.2413 | 3050.5306 |
| 3069.7751 | 3094.5454 | 3104.5710 |

Zero-point correction (Hartree): 0.160606

C6H11O2.ptppt

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -385.63130312
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 2.618265 | 1.244962 | -0.484461 |
| C | 2.645090 | 0.130864 | 0.311388 |
| C | 1.274632 | -0.468501 | 0.654393 |
| C | 0.465208 | -0.829747 | -0.596917 |
| C | -0.893454 | -1.493402 | -0.317508 |
| C | -1.892713 | -0.624183 | 0.472520 |
| C | -2.281646 | 0.635131 | -0.269222 |
| H | 3.255577 | -0.605843 | -0.257557 |
| H | 3.249247 | 0.326625 | 1.218643 |
| H | 1.429033 | -1.356732 | 1.282900 |
| H | 0.728791 | 0.260360 | 1.265007 |
| H | 0.329896 | 0.080949 | -1.192938 |
| H | 1.057831 | -1.513568 | -1.220248 |
| H | -1.351741 | -1.776407 | -1.274414 |
| H | -0.739524 | -2.430001 | 0.232585 |
| H | -2.814535 | -1.204411 | 0.627069 |
| H | -1.512965 | -0.340803 | 1.458131 |
| O | -2.229976 | 1.754361 | 0.190137 |
| H | -2.640622 | 0.464279 | -1.312512 |

Rotational constants (GHz): 2.9763000 1.0344500 0.8541300
 Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 25.7616 | 43.2810 | 74.5746 |
| 141.7237 | 170.3726 | 219.4318 |
| 257.6458 | 337.9819 | 428.4625 |
| 504.4148 | 523.0018 | 563.9224 |
| 747.4516 | 781.6449 | 826.1254 |
| 887.0588 | 919.1603 | 974.8911 |
| 1006.2167 | 1046.3962 | 1077.4673 |
| 1100.6076 | 1118.5413 | 1153.9734 |
| 1196.8062 | 1225.8376 | 1289.0513 |
| 1309.6065 | 1335.3266 | 1356.5187 |
| 1364.8212 | 1374.7335 | 1392.1592 |
| 1421.1946 | 1431.2540 | 1479.7427 |
| 1494.8054 | 1501.3669 | 1513.1564 |
| 1836.7939 | 2865.5541 | 2880.3581 |
| 2940.4823 | 3024.1117 | 3026.4124 |
| 3032.7547 | 3038.9621 | 3066.0297 |
| 3077.3956 | 3092.2216 | 3117.4526 |

Zero-point correction (Hartree): 0.160873

C6H11O2.ptptc

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -385.63391943
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 3.338836 | 0.788743 | -0.565927 |
| C | 3.003157 | -0.124111 | 0.398959 |
| C | 1.505447 | -0.226327 | 0.712205 |
| C | 0.678138 | -0.636922 | -0.512468 |
| C | -0.839083 | -0.689161 | -0.279170 |
| C | -1.481813 | 0.677314 | -0.031165 |
| C | -2.984826 | 0.634076 | 0.121470 |
| H | 3.388608 | -1.098030 | 0.023293 |
| H | 3.607041 | 0.059044 | 1.309523 |
| H | 1.362943 | -0.948016 | 1.528328 |
| H | 1.174848 | 0.747622 | 1.093971 |
| H | 0.908056 | 0.054637 | -1.333071 |
| H | 1.014073 | -1.628376 | -0.845960 |
| H | -1.324231 | -1.144693 | -1.149338 |
| H | -1.068258 | -1.350959 | 0.565035 |
| H | -1.257488 | 1.379601 | -0.849541 |
| H | -1.084985 | 1.167175 | 0.870621 |
| O | -3.656783 | -0.372937 | 0.070423 |
| H | -3.463150 | 1.626333 | 0.292181 |

Rotational constants (GHz): 6.5985400 0.6730200 0.6556100
 Vibrational harmonic frequencies (cm-1):

| | | |
|----------|----------|----------|
| 36.2037 | 48.5524 | 114.1544 |
| 137.6833 | 173.8740 | 193.3108 |

| | | |
|-----------|-----------|-----------|
| 241.8799 | 276.2218 | 400.3826 |
| 439.9557 | 544.3995 | 667.4261 |
| 703.6077 | 771.3116 | 826.9275 |
| 874.6024 | 912.8505 | 940.8987 |
| 999.5175 | 1038.5498 | 1079.3728 |
| 1096.1754 | 1122.7779 | 1158.5793 |
| 1187.5837 | 1260.2214 | 1301.5669 |
| 1315.1716 | 1332.9298 | 1349.0888 |
| 1361.2096 | 1377.4256 | 1408.5625 |
| 1417.9489 | 1428.4950 | 1464.1817 |
| 1495.0176 | 1503.3091 | 1513.5148 |
| 1833.1141 | 2884.4096 | 2885.2145 |
| 2935.4737 | 3014.6702 | 3026.3803 |
| 3034.4077 | 3042.8838 | 3051.3165 |
| 3066.4092 | 3084.9711 | 3095.4908 |

Zero-point correction (Hartree): 0.160543

C6H11O2.ptppt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -385.63212144

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -3.316629 | -0.499613 | -0.914476 |
| C | -2.992975 | -0.295917 | 0.401012 |
| C | -1.491039 | -0.230912 | 0.704800 |
| C | -0.788379 | 0.893139 | -0.065722 |
| C | 0.728822 | 0.978370 | 0.160620 |
| C | 1.515499 | -0.237811 | -0.367957 |
| C | 3.008793 | -0.011985 | -0.297490 |
| H | -3.487438 | 0.662555 | 0.675073 |
| H | -3.511347 | -1.044071 | 1.032279 |
| H | -1.354651 | -0.096935 | 1.786744 |
| H | -1.052130 | -1.203160 | 0.451073 |
| H | -0.997209 | 0.764595 | -1.135056 |
| H | -1.236938 | 1.854016 | 0.222093 |
| H | 1.105936 | 1.884245 | -0.332437 |
| H | 0.937208 | 1.103571 | 1.231410 |
| H | 1.254445 | -0.397941 | -1.425379 |
| H | 1.284561 | -1.154389 | 0.181469 |
| O | 3.792915 | -0.730986 | 0.280831 |
| H | 3.362953 | 0.903001 | -0.829680 |

Rotational constants (GHz): 5.8679000 0.6536000 0.6417500

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 41.6648 | 60.0854 | 70.7022 |
| 110.2758 | 143.9366 | 241.2655 |
| 267.7738 | 273.5950 | 414.6069 |
| 469.8860 | 517.1222 | 563.0049 |
| 761.2260 | 769.4804 | 835.2834 |
| 884.4874 | 923.8385 | 987.6046 |
| 1001.2109 | 1062.0951 | 1074.4380 |
| 1096.6509 | 1129.1043 | 1158.6970 |
| 1191.2429 | 1260.2986 | 1282.5343 |
| 1314.6961 | 1326.9793 | 1349.7100 |
| 1361.6216 | 1378.0667 | 1395.1003 |
| 1419.0072 | 1433.8018 | 1477.8712 |
| 1494.2858 | 1507.8648 | 1511.6236 |
| 1837.2935 | 2868.7727 | 2884.7324 |
| 2937.9754 | 3017.5202 | 3024.3916 |
| 3032.8204 | 3036.0653 | 3062.5368 |
| 3073.3573 | 3090.2603 | 3120.8160 |

Zero-point correction (Hartree): 0.160723

C6H11O2.pttmc

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -385.63433814

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -2.808873 | 1.327400 | 0.204322 |
| C | -2.879646 | -0.038646 | 0.136180 |
| C | -1.654605 | -0.735117 | -0.469138 |
| C | -0.358202 | -0.422725 | 0.284894 |
| C | 0.875198 | -1.085900 | -0.342209 |
| C | 2.177768 | -0.786084 | 0.405519 |
| C | 2.705377 | 0.620273 | 0.221775 |
| H | -3.025925 | -0.366167 | 1.189982 |
| H | -3.819266 | -0.344532 | -0.364486 |
| H | -1.841784 | -1.818094 | -0.483908 |
| H | -1.559209 | -0.419626 | -1.516124 |
| H | -0.222186 | 0.662967 | 0.309143 |
| H | -0.457398 | -0.754954 | 1.329420 |
| H | 0.729095 | -2.173013 | -0.375978 |
| H | 0.980956 | -0.747822 | -1.379633 |
| H | 2.078884 | -0.967305 | 1.486579 |
| H | 2.987318 | -1.459330 | 0.082660 |
| O | 2.226266 | 1.450290 | -0.519494 |

| | | | | |
|--|-----------|-----------|-----------|-----------|
| H | 3.615022 | 0.855550 | 0.821591 | |
| Rotational constants (GHz): | 3.7771600 | | 0.8787400 | 0.7639300 |
| Vibrational harmonic frequencies (cm-1): | | | | |
| 45.5698 | | 62.4353 | | 113.7097 |
| 133.6025 | | 152.4118 | | 200.6599 |
| 253.1637 | | 309.3005 | | 384.2159 |
| 495.8467 | | 531.2870 | | 666.7235 |
| 708.4434 | | 766.5578 | | 837.8850 |
| 881.0177 | | 917.9748 | | 948.6448 |
| 996.2606 | | 1048.5049 | | 1075.9054 |
| 1096.6921 | | 1107.4680 | | 1160.6909 |
| 1207.5532 | | 1237.8965 | | 1300.7916 |
| 1311.0113 | | 1339.7640 | | 1359.1030 |
| 1366.4965 | | 1385.2647 | | 1392.4540 |
| 1419.8477 | | 1429.6625 | | 1458.4200 |
| 1493.2416 | | 1496.7921 | | 1518.3818 |
| 1833.4215 | | 2880.3834 | | 2884.1834 |
| 2936.3987 | | 3011.4118 | | 3014.3706 |
| 3027.4576 | | 3038.0816 | | 3045.8259 |
| 3071.4061 | | 3085.3239 | | 3111.2681 |

Zero-point correction (Hartree): 0.160727

C6H11O2.pttmt

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -385.63291938
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | | |
|---|-----------|-----------|-----------|--|
| O | 2.794069 | 1.429502 | 0.270367 | |
| C | 2.918696 | 0.168602 | -0.250007 | |
| C | 1.814238 | -0.816881 | 0.151341 | |
| C | 0.419625 | -0.347936 | -0.275991 | |
| C | -0.706218 | -1.258420 | 0.230383 | |
| C | -2.106141 | -0.813041 | -0.229764 | |
| C | -2.529921 | 0.507658 | 0.375830 | |
| H | 2.929238 | 0.311586 | -1.353358 | |
| H | 3.928976 | -0.228755 | -0.030050 | |
| H | 2.040231 | -1.799187 | -0.285735 | |
| | | | | |
| H | 1.847193 | -0.944160 | 1.241355 | |
| H | 0.272016 | 0.675908 | 0.090010 | |
| H | 0.372720 | -0.289707 | -1.372895 | |
| H | -0.533454 | -2.286299 | -0.111433 | |
| H | -0.680878 | -1.295918 | 1.328609 | |
| H | -2.172507 | -0.731422 | -1.319473 | |
| H | -2.845281 | -1.561086 | 0.094399 | |
| O | -2.997932 | 1.437579 | -0.242101 | |
| H | -2.389022 | 0.572499 | 1.481692 | |

Rotational constants (GHz): 3.6528300 0.8176800 0.7017600
 Vibrational harmonic frequencies (cm-1):

| | | | | |
|-----------|--|-----------|--|-----------|
| 47.1123 | | 51.6542 | | 81.2738 |
| 135.8864 | | 154.4270 | | 180.6753 |
| 284.7590 | | 309.9874 | | 409.7223 |
| 483.6766 | | 529.2088 | | 536.9081 |
| 741.6630 | | 768.9976 | | 825.0351 |
| 912.8166 | | 934.0733 | | 972.5346 |
| 1018.6868 | | 1037.5678 | | 1081.5774 |
| 1094.6208 | | 1110.1985 | | 1169.1412 |
| 1203.5365 | | 1228.2253 | | 1294.0486 |
| 1304.7753 | | 1335.5101 | | 1353.6716 |
| 1362.5882 | | 1368.3498 | | 1391.2049 |
| 1420.6227 | | 1432.2868 | | 1472.1662 |
| 1494.5644 | | 1501.4615 | | 1518.3866 |
| 1838.0934 | | 2863.7346 | | 2886.4254 |
| 2938.0445 | | 3018.8203 | | 3023.2333 |
| 3028.3432 | | 3034.8721 | | 3059.3309 |
| 3069.4898 | | 3087.4244 | | 3106.1935 |

Zero-point correction (Hartree): 0.160628

C6H11O2.pttpc

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -385.63528859
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | | |
|---|-----------|-----------|-----------|--|
| O | -3.208996 | 0.006382 | -1.019506 | |
| C | -2.801445 | 0.525318 | 0.181200 | |
| C | -1.598442 | -0.174827 | 0.824943 | |
| C | -0.352590 | -0.145296 | -0.065931 | |
| C | 0.821997 | -0.943477 | 0.514730 | |
| C | 2.070858 | -0.925900 | -0.371644 | |
| C | 2.812722 | 0.391811 | -0.400882 | |
| H | -2.554043 | 1.587931 | -0.038871 | |
| H | -3.662495 | 0.595919 | 0.874315 | |
| H | -1.389887 | 0.303185 | 1.791561 | |
| H | -1.880670 | -1.213574 | 1.042636 | |
| H | -0.623215 | -0.545766 | -1.051341 | |

| | | | | |
|--|-----------|-----------|-----------|-----------|
| H | -0.039827 | 0.894684 | -0.218128 | |
| H | 1.085500 | -0.542644 | 1.500783 | |
| H | 0.513179 | -1.985012 | 0.668473 | |
| H | 2.802657 | -1.681794 | -0.046474 | |
| H | 1.834287 | -1.196698 | -1.411963 | |
| O | 2.521501 | 1.369538 | 0.253903 | |
| H | 3.695872 | 0.410641 | -1.080659 | |
| Rotational constants (GHz): | 4.3692600 | | 0.7833500 | 0.7532000 |
| Vibrational harmonic frequencies (cm-1): | | | | |
| 45.4086 | | 72.0077 | | 107.4232 |
| 119.8454 | | 164.9954 | | 202.8047 |
| 252.9419 | | 312.0240 | | 383.3914 |
| 504.5078 | | 560.8281 | | 662.2096 |
| 712.9998 | | 762.3382 | | 856.0001 |
| 868.4762 | | 915.3994 | | 953.1060 |
| 1005.1618 | | 1034.2011 | | 1083.9930 |
| 1094.8143 | | 1115.5803 | | 1157.7350 |
| 1197.8030 | | 1253.2785 | | 1287.6915 |
| 1318.2254 | | 1341.0360 | | 1358.9528 |
| 1366.1244 | | 1385.4980 | | 1392.4031 |
| 1419.8285 | | 1429.7281 | | 1457.2354 |
| 1493.7584 | | 1496.8623 | | 1518.5580 |
| 1831.2108 | | 2883.3996 | | 2885.4028 |
| 2938.3389 | | 3014.2429 | | 3030.0210 |
| 3036.9022 | | 3041.5059 | | 3049.4177 |
| 3065.6481 | | 3078.7406 | | 3099.7982 |
| Zero-point correction (Hartree): | 0.160884 | | | |

C6H11O2.pttpt

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -385.63301915
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | | |
|--|-----------|-----------|-----------|-----------|
| O | -3.143188 | -0.857875 | 0.807721 | |
| C | -2.865939 | -0.363705 | -0.439371 | |
| C | -1.741449 | 0.677982 | -0.495071 | |
| C | -0.405764 | 0.133659 | 0.021579 | |
| C | 0.689265 | 1.203756 | 0.113774 | |
| C | 2.036453 | 0.655494 | 0.622107 | |
| C | 2.692629 | -0.275302 | -0.373545 | |
| H | -2.598326 | -1.255797 | -1.048194 | |
| H | -3.796740 | 0.005209 | -0.912828 | |
| H | -1.639928 | 1.033593 | -1.529562 | |
| H | -2.046986 | 1.545015 | 0.105314 | |
| H | -0.570746 | -0.310520 | 1.010752 | |
| H | -0.070188 | -0.686748 | -0.629105 | |
| H | 0.837747 | 1.670456 | -0.870658 | |
| H | 0.359248 | 2.007574 | 0.782686 | |
| H | 2.729855 | 1.495255 | 0.778080 | |
| H | 1.927683 | 0.127533 | 1.574727 | |
| O | 3.099384 | -1.388697 | -0.127183 | |
| H | 2.787641 | 0.149700 | -1.402351 | |
| Rotational constants (GHz): | 4.1306700 | | 0.7496100 | 0.6945600 |
| Vibrational harmonic frequencies (cm-1): | | | | |
| 42.7885 | | 51.0683 | | 82.4459 |
| 120.5064 | | 150.7745 | | 184.3658 |
| 291.4287 | | 309.4139 | | 409.2380 |
| 493.9946 | | 527.2538 | | 556.2904 |
| 742.3976 | | 773.1136 | | 830.9531 |
| 903.1799 | | 942.7956 | | 976.0891 |
| 1011.8293 | | 1036.2305 | | 1079.5345 |
| 1094.6351 | | 1121.3025 | | 1162.3425 |
| 1192.5580 | | 1239.6618 | | 1282.5405 |
| 1309.8168 | | 1334.4934 | | 1353.7393 |
| 1361.3297 | | 1365.7785 | | 1390.4760 |
| 1420.6548 | | 1432.7369 | | 1473.0114 |
| 1495.0141 | | 1500.8041 | | 1518.3450 |
| 1838.0165 | | 2858.2321 | | 2886.3155 |
| 2939.4740 | | 3019.8327 | | 3023.3365 |
| 3027.1521 | | 3032.3972 | | 3064.2838 |
| 3070.0977 | | 3089.3805 | | 3109.7335 |
| Zero-point correction (Hartree): | 0.160664 | | | |

C6H11O2.ptttc

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -385.63528873
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | | |
|---|-----------|-----------|-----------|--|
| O | 3.482667 | -0.729895 | -0.623771 | |
| C | 3.147487 | 0.283927 | 0.234695 | |
| C | 1.722614 | 0.830011 | 0.082933 | |
| C | 0.650856 | -0.247725 | 0.277924 | |
| C | -0.772114 | 0.262862 | 0.026724 | |
| C | -1.835532 | -0.819831 | 0.212241 | |

| | | | |
|--|-----------|-----------|-----------|
| C | -3.251813 | -0.349780 | -0.026074 |
| H | 3.290440 | -0.145524 | 1.251556 |
| H | 3.908019 | 1.087496 | 0.183041 |
| H | 1.580610 | 1.648843 | 0.801240 |
| H | 1.626609 | 1.271893 | -0.917271 |
| H | 0.876087 | -1.083048 | -0.396997 |
| H | 0.722813 | -0.650350 | 1.299255 |
| H | -0.996573 | 1.101581 | 0.696779 |
| H | -0.849779 | 0.667389 | -0.989505 |
| H | -1.658841 | -1.676456 | -0.456920 |
| H | -1.802287 | -1.248971 | 1.226174 |
| O | -3.562049 | 0.780748 | -0.332506 |
| H | -4.031037 | -1.136458 | 0.102212 |
| Rotational constants (GHz): | 7.0988200 | 0.6266500 | 0.6008600 |
| Vibrational harmonic frequencies (cm-1): | | | |
| 39.2629 | 80.3890 | | 107.8449 |
| 113.2017 | 149.1854 | | 188.8706 |
| 211.3698 | 337.5193 | | 359.6922 |
| 479.8672 | 529.5510 | | 673.5900 |
| 707.3178 | 752.7861 | | 836.6287 |
| 885.4518 | 921.6418 | | 953.6032 |
| 1005.1169 | 1058.6186 | | 1067.7517 |
| 1094.6162 | 1112.0047 | | 1166.0707 |
| 1200.8839 | 1260.6694 | | 1282.0501 |
| 1324.4784 | 1333.0241 | | 1338.2372 |
| 1363.3663 | 1372.4807 | | 1404.8911 |
| 1421.4742 | 1427.3972 | | 1463.5800 |
| 1495.6914 | 1500.5375 | | 1519.9783 |
| 1833.1359 | 2882.2248 | | 2884.8320 |
| 2938.2614 | 3010.4106 | | 3015.2061 |
| 3033.7881 | 3035.9749 | | 3050.6247 |
| 3062.1505 | 3077.8114 | | 3095.7561 |
| Zero-point correction (Hartree): | 0.160522 | | |

C6H11O2.ptttt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -385.63318550
Electronic state : 2-A
Cartesian coordinates (Angs):

| | | | |
|--|-----------|-----------|-----------|
| O | 3.455233 | -1.080286 | -0.274130 |
| C | 3.235437 | 0.215336 | 0.112280 |
| C | 1.862625 | 0.788188 | -0.261713 |
| C | 0.703863 | -0.022062 | 0.328822 |
| C | -0.674636 | 0.471775 | -0.125596 |
| C | -1.830722 | -0.356884 | 0.465156 |
| C | -3.183520 | 0.205541 | 0.092733 |
| H | 3.366068 | 0.211251 | 1.217381 |
| H | 4.063655 | 0.858479 | -0.244339 |
| H | 1.813398 | 1.833295 | 0.073443 |
| H | 1.783605 | 0.806273 | -1.356465 |
| H | 0.835474 | -1.072779 | 0.043900 |
| H | 0.757223 | 0.009844 | 1.426881 |
| H | -0.799475 | 1.526148 | 0.158639 |
| H | -0.731245 | 0.440222 | -1.221405 |
| H | -1.758181 | -0.339847 | 1.563531 |
| H | -1.786349 | -1.400981 | 0.140421 |
| O | -4.067257 | -0.415099 | -0.454974 |
| H | -3.326260 | 1.279811 | 0.360750 |
| Rotational constants (GHz): | 7.7179300 | 0.5811400 | 0.5635500 |
| Vibrational harmonic frequencies (cm-1): | | | |
| 45.6072 | 54.9449 | | 81.8510 |
| 124.9576 | 132.9412 | | 161.1253 |
| 250.4229 | 329.4316 | | 380.0659 |
| 481.5274 | 521.8852 | | 546.4659 |
| 742.8974 | 775.3738 | | 844.1224 |
| 900.9813 | 938.9193 | | 1001.1631 |
| 1004.1022 | 1054.7955 | | 1072.1818 |
| 1094.2233 | 1121.1343 | | 1166.7744 |
| 1200.3176 | 1254.2766 | | 1276.7631 |
| 1314.1183 | 1331.0730 | | 1339.8797 |
| 1362.0454 | 1369.7714 | | 1393.9287 |
| 1418.6093 | 1435.7483 | | 1477.4844 |
| 1495.0505 | 1504.5872 | | 1521.2738 |
| 1838.3533 | 2866.5487 | | 2884.7760 |
| 2938.9882 | 3016.6937 | | 3018.3057 |
| 3025.3211 | 3032.9472 | | 3061.6334 |
| 3068.8735 | 3089.2971 | | 3112.2397 |
| Zero-point correction (Hartree): | 0.160558 | | |

C6H11O2.tpmmc

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -385.62905139
Electronic state : 2-A
Cartesian coordinates (Angs):

| | | | |
|---|----------|-----------|----------|
| O | 3.066533 | -0.976556 | 0.314462 |
|---|----------|-----------|----------|

| | | | |
|---|-----------|-----------|-----------|
| C | 1.836299 | -0.631009 | -0.172769 |
| C | 1.488790 | 0.862417 | -0.070701 |
| C | 0.124253 | 1.239541 | -0.689728 |
| C | -1.053024 | 1.339655 | 0.298310 |
| C | -1.421488 | 0.056708 | 1.051830 |
| C | -1.989959 | -1.054626 | 0.198675 |
| H | 1.859982 | -0.936404 | -1.242881 |
| H | 1.054774 | -1.287007 | 0.258087 |
| H | 1.529405 | 1.159789 | 0.985359 |
| H | 2.295680 | 1.410759 | -0.569168 |
| H | 0.218253 | 2.217212 | -1.175821 |
| H | -0.137532 | 0.534004 | -1.486636 |
| H | -0.828518 | 2.117156 | 1.039403 |
| H | -1.937983 | 1.679091 | -0.251757 |
| H | -0.571435 | -0.356397 | 1.614625 |
| H | -2.178280 | 0.266249 | 1.823997 |
| O | -2.188019 | -0.985414 | -0.995456 |
| H | -2.241689 | -1.984809 | 0.759036 |
| Rotational constants (GHz): | 2.9259300 | 1.1013900 | 0.9591500 |
| Vibrational harmonic frequencies (cm ⁻¹): | | | |
| 34.7078 | 73.7249 | | 87.8076 |
| 125.0329 | 170.1791 | | 231.0134 |
| 268.6812 | 306.9297 | | 386.2565 |
| 477.4501 | 564.4216 | | 658.2037 |
| 719.1983 | 754.5450 | | 843.7238 |
| 872.0210 | 892.9007 | | 950.3409 |
| 1015.0075 | 1062.1952 | | 1066.7982 |
| 1086.3604 | 1106.5416 | | 1159.3182 |
| 1214.7752 | 1227.9285 | | 1272.9291 |
| 1310.9943 | 1334.9573 | | 1366.2952 |
| 1371.7352 | 1390.4962 | | 1396.2172 |
| 1401.2264 | 1430.8317 | | 1461.0334 |
| 1494.5739 | 1506.2036 | | 1512.0464 |
| 1829.8249 | 2882.1066 | | 2884.6412 |
| 2940.7516 | 3016.9001 | | 3040.5090 |
| 3041.8666 | 3047.2990 | | 3051.4231 |
| 3085.1161 | 3091.5229 | | 3095.3768 |
| Zero-point correction (Hartree): | 0.160868 | | |

C6H11O2.tpmmt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -385.62998379

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 2.834388 | -0.900907 | 0.503901 |
| C | 1.772519 | -0.477857 | -0.238086 |
| C | 1.345675 | 0.981276 | 0.008917 |
| C | 0.045288 | 1.386100 | -0.722793 |
| C | -1.210740 | 1.445293 | 0.165891 |
| C | -1.588726 | 0.120904 | 0.872905 |
| C | -1.968688 | -0.947909 | -0.121283 |
| H | 1.938533 | -0.668734 | -1.318076 |
| H | 0.944242 | -1.180691 | 0.009735 |
| H | 1.250847 | 1.134961 | 1.090951 |
| H | 2.172062 | 1.623651 | -0.315392 |
| H | 0.170205 | 2.378032 | -1.171184 |
| H | -0.129912 | 0.703589 | -1.565821 |
| H | -1.065408 | 2.205622 | 0.942659 |
| H | -2.063252 | 1.784560 | -0.437344 |
| H | -0.762864 | -0.244938 | 1.489711 |
| H | -2.450333 | 0.306508 | 1.527281 |
| O | -1.260803 | -1.883377 | -0.434324 |
| H | -2.964773 | -0.815137 | -0.602442 |
| Rotational constants (GHz): | 2.5253600 | 1.3429300 | 1.0040000 |
| Vibrational harmonic frequencies (cm ⁻¹): | | | |
| 73.4685 | 81.8180 | | 90.0839 |
| 120.1199 | 169.9764 | | 228.2977 |
| 287.5185 | 341.7541 | | 407.9532 |
| 495.1569 | 513.4893 | | 670.0879 |
| 771.2849 | 796.5783 | | 863.1782 |
| 892.9921 | 939.2772 | | 982.7254 |
| 1012.6778 | 1051.3191 | | 1091.0978 |
| 1098.1759 | 1103.1524 | | 1170.2489 |
| 1205.0814 | 1219.1792 | | 1280.7691 |
| 1301.4608 | 1337.7407 | | 1346.0438 |
| 1374.4779 | 1379.7682 | | 1390.8861 |
| 1398.3425 | 1430.7025 | | 1489.9069 |
| 1499.6992 | 1509.9810 | | 1511.5343 |
| 1821.9321 | 2866.5311 | | 2893.9518 |
| 2921.1363 | 3032.2042 | | 3035.4547 |
| 3047.6595 | 3048.1010 | | 3072.7516 |
| 3083.0813 | 3091.3057 | | 3119.9400 |
| Zero-point correction (Hartree): | 0.161663 | | |

C6H11O2.tpmmpc

```

-----
E(UB+HF-LYP/6-31G(d,p)) (Hartree): -385.63337911
Electronic state : 2-A
Cartesian coordinates (Angs):
O      3.560277      0.604256      -0.342697
C      2.210018      0.574895      -0.125781
C      1.677982      -0.734216      0.476477
C      0.157416      -0.741900      0.693020
C      -0.660948     -0.785572     -0.607142
C      -2.174266     -0.798472     -0.372293
C      -2.752194      0.521374      0.089074
H      1.882275      1.456990      0.459626
H      1.768702      0.751525     -1.131223
H      1.981184     -1.565846     -0.171918
H      2.184278     -0.886950      1.437078
H      -0.106716     -1.613839      1.305952
H      -0.133615      0.143266      1.271598
H      -0.420853      0.080699     -1.234100
H      -0.381752     -1.678447     -1.180361
H      -2.719243     -1.068270     -1.290171
H      -2.466311     -1.565222      0.361427
O      -2.121668      1.549484      0.210939
H      -3.844872      0.499514      0.306032
Rotational constants (GHz):  4.0801200      0.8509700      0.7665400
Vibrational harmonic frequencies (cm-1):
  35.0488      80.2279      88.3769
 133.0973      154.3264      242.8909
 261.7383      290.5493      346.3373
 512.8163      610.8862      660.5889
 708.4336      780.9963      823.2487
 876.6668      910.6438      961.5692
1021.5940     1043.4783     1079.5247
1086.7045     1113.4899     1154.1264
1204.1254     1245.6221     1291.0374
1314.0918     1347.1057     1351.8521
1369.6415     1383.9022     1392.0068
1416.6101     1429.0772     1457.2142
1494.1386     1500.8773     1510.9133
1830.3788     2890.1514     2892.9207
2933.9869     3015.2539     3032.4925
3039.6470     3044.7082     3049.0797
3073.4247     3088.0898     3097.0138
Zero-point correction (Hartree): 0.161004
    
```

C6H11O2.tpmp

```

-----
E(UB+HF-LYP/6-31G(d,p)) (Hartree): -385.62793481
Electronic state : 2-A
Cartesian coordinates (Angs):
O      2.812131      0.794716      -0.057181
C      1.727872      0.135591      0.444439
C      1.114336     -0.900710     -0.517179
C      -0.003700     -1.773461      0.092631
C      -1.458507     -1.319639     -0.128250
C      -1.855734      0.035293      0.503460
C      -1.513969      1.225806     -0.360312
H      1.958139     -0.319892      1.429450
H      1.001224      0.944930      0.676577
H      0.767117     -0.386869     -1.422263
H      1.937123     -1.549516     -0.838469
H      0.076244     -2.784082     -0.324717
H      0.172161     -1.889420      1.171866
H      -1.672503     -1.290152     -1.206047
H      -2.117208     -2.091822      0.284704
H      -2.948952      0.054470      0.621775
H      -1.411509      0.170102      1.494811
O      -0.790834      2.143585     -0.034075
H      -1.993999      1.218557     -1.366367
Rotational constants (GHz):  2.3432500      1.5031800      1.0004800
Vibrational harmonic frequencies (cm-1):
  60.4364      86.5879      99.0535
 113.7331      167.8324      255.5054
 286.2786      328.1078      400.5891
 476.1302      515.9073      680.6466
 752.0245      810.4272      848.6149
 885.9699      956.8800      974.6211
1023.5001     1049.5961     1093.5675
1103.6413     1104.0027     1165.3364
1204.6368     1249.5460     1273.6067
1300.9423     1334.2325     1350.1207
1377.3182     1387.0473     1393.7540
1397.8316     1431.2291     1481.8234
1499.2940     1504.8546     1507.0619
1824.4277     2884.0076     2890.8866
2921.7050     3022.0230     3025.2872
    
```

3030.7839 3045.7314 3071.9514
3079.1460 3089.0785 3107.7764
Zero-point correction (Hartree): 0.161579

C6H11O2.tpmtc

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -385.62938417

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -3.334980 | -1.107964 | -0.318463 |
| C | -2.289958 | -0.495359 | 0.316734 |
| C | -1.712118 | 0.731598 | -0.404547 |
| C | -0.540955 | 1.416705 | 0.330898 |
| C | 0.870732 | 0.939848 | -0.050093 |
| C | 1.191888 | -0.518129 | 0.286451 |
| C | 2.639536 | -0.896000 | 0.055672 |
| H | -2.573121 | -0.251324 | 1.361392 |
| H | -1.526826 | -1.292876 | 0.442718 |
| H | -1.413972 | 0.437989 | -1.418687 |
| H | -2.536918 | 1.443615 | -0.524034 |
| H | -0.584778 | 2.492733 | 0.128061 |
| H | -0.681657 | 1.318927 | 1.417913 |
| H | 1.030578 | 1.096403 | -1.123735 |
| H | 1.608953 | 1.575204 | 0.451409 |
| H | 0.585941 | -1.225435 | -0.299443 |
| H | 0.965446 | -0.751578 | 1.339338 |
| O | 3.495938 | -0.136596 | -0.340080 |
| H | 2.883947 | -1.959169 | 0.282726 |

Rotational constants (GHz): 4.3112400 0.7955000 0.7069100

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 37.8491 | 53.4634 | 82.5951 |
| 118.8907 | 181.4335 | 186.0815 |
| 246.1842 | 288.1273 | 396.6187 |
| 446.9792 | 508.1019 | 679.0382 |
| 684.7251 | 781.1639 | 832.8362 |
| 863.7141 | 913.4398 | 961.9859 |
| 994.8044 | 1053.4842 | 1080.7952 |
| 1087.9059 | 1108.6428 | 1161.5347 |
| 1212.8579 | 1249.8922 | 1286.5026 |
| 1319.7813 | 1328.3800 | 1339.7494 |
| 1372.1691 | 1390.6909 | 1397.1592 |
| 1410.2797 | 1428.2971 | 1465.7325 |
| 1497.3613 | 1503.3647 | 1506.0282 |
| 1834.4098 | 2888.9552 | 2904.4003 |
| 2921.3052 | 3008.4108 | 3015.0262 |
| 3040.7095 | 3045.2616 | 3052.8438 |
| 3076.0724 | 3089.1825 | 3096.5544 |

Zero-point correction (Hartree): 0.160455

C6H11O2.tpmtt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -385.62768671

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -3.151289 | -1.407774 | -0.149600 |
| C | -2.127914 | -0.652075 | 0.352890 |
| C | -1.811212 | 0.620262 | -0.449100 |
| C | -0.728541 | 1.530578 | 0.163012 |
| C | 0.731734 | 1.199279 | -0.194102 |
| C | 1.271984 | -0.134487 | 0.357545 |
| C | 2.772412 | -0.241450 | 0.187738 |
| H | -2.311513 | -0.420924 | 1.422264 |
| H | -1.259890 | -1.343695 | 0.383740 |
| H | -1.542831 | 0.336906 | -1.474285 |
| H | -2.749309 | 1.182749 | -0.523373 |
| H | -0.916992 | 2.557359 | -0.171480 |
| H | -0.839485 | 1.551660 | 1.257343 |
| H | 0.847340 | 1.206224 | -1.285557 |
| H | 1.365979 | 2.012598 | 0.184162 |
| H | 0.820248 | -1.003598 | -0.128404 |
| H | 1.060349 | -0.191910 | 1.436460 |
| O | 3.342203 | -1.145229 | -0.380781 |
| H | 3.348005 | 0.604013 | 0.634288 |

Rotational constants (GHz): 3.4239500 0.8289900 0.7041200

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 49.5597 | 63.5917 | 78.6787 |
| 97.7834 | 110.8939 | 226.6842 |
| 282.3719 | 293.9082 | 413.5396 |
| 472.1019 | 527.2729 | 550.0742 |
| 764.0729 | 778.8503 | 851.3750 |
| 863.3596 | 928.2090 | 988.0142 |
| 1023.4546 | 1055.8950 | 1084.1273 |
| 1095.9692 | 1105.4638 | 1167.8673 |
| 1214.9778 | 1247.2499 | 1281.2762 |
| 1308.9244 | 1327.1485 | 1341.2185 |

| | | |
|-----------|-----------|-----------|
| 1375.7810 | 1393.0066 | 1396.0618 |
| 1402.8514 | 1432.3465 | 1477.1475 |
| 1498.0238 | 1500.0671 | 1508.2207 |
| 1839.2233 | 2871.1498 | 2909.6741 |
| 2927.0219 | 3015.4226 | 3018.5449 |
| 3028.6803 | 3045.6767 | 3067.6240 |
| 3075.8587 | 3090.1089 | 3116.5157 |

Zero-point correction (Hartree): 0.160800

C6H11O2.tppmc

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -385.63285510
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 2.828139 | -0.939122 | 0.112427 |
| C | 1.843832 | -0.141284 | -0.393846 |
| C | 1.114931 | 0.715646 | 0.655066 |
| C | 0.100133 | 1.702528 | 0.057084 |
| C | -1.126642 | 1.096440 | -0.651274 |
| C | -2.053146 | 0.270959 | 0.253787 |
| C | -1.757703 | -1.209784 | 0.326415 |
| H | 2.210761 | 0.473913 | -1.240710 |
| H | 1.119675 | -0.854043 | -0.846816 |
| H | 0.641069 | 0.045998 | 1.382506 |
| H | 1.871744 | 1.283415 | 1.209695 |
| H | -0.252747 | 2.367732 | 0.856609 |
| H | 0.621414 | 2.350965 | -0.660240 |
| H | -1.705693 | 1.921689 | -1.080337 |
| H | -0.813639 | 0.469692 | -1.493644 |
| H | -2.077903 | 0.659189 | 1.282855 |
| H | -3.098321 | 0.336021 | -0.087867 |
| O | -0.934596 | -1.797101 | -0.344000 |
| H | -2.393126 | -1.771814 | 1.047144 |

Rotational constants (GHz): 2.6577900 1.3891200 1.0201700
 Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 59.5942 | 87.7259 | 139.2971 |
| 149.9234 | 159.8058 | 223.7392 |
| 271.0774 | 320.9640 | 406.0462 |
| 495.6669 | 649.9540 | 692.1332 |
| 717.5600 | 805.4602 | 821.6559 |
| 880.9898 | 934.8206 | 989.4122 |
| 1019.1174 | 1036.3142 | 1092.9973 |
| 1103.9902 | 1108.5015 | 1157.5446 |
| 1192.7866 | 1253.9394 | 1258.5382 |
| 1314.9025 | 1334.4159 | 1364.4153 |
| 1375.1573 | 1394.2020 | 1401.5571 |
| 1402.8898 | 1428.3236 | 1455.3244 |
| 1496.6020 | 1503.4896 | 1506.6990 |
| 1824.9619 | 2887.6722 | 2902.6329 |
| 2926.5946 | 3013.6876 | 3024.3590 |
| 3043.1966 | 3046.4435 | 3056.9691 |
| 3064.7776 | 3090.6926 | 3099.3678 |

Zero-point correction (Hartree): 0.161725

C6H11O2.tppmt

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -385.62845227
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 2.856479 | -1.220034 | -0.221748 |
| C | 2.077266 | -0.110763 | -0.403418 |
| C | 1.151525 | 0.230635 | 0.774233 |
| C | 0.317820 | 1.503956 | 0.554262 |
| C | -0.772500 | 1.436145 | -0.532077 |
| C | -1.981449 | 0.542033 | -0.190546 |
| C | -1.736150 | -0.944004 | -0.336204 |
| H | 2.689446 | 0.762519 | -0.706890 |
| H | 1.483055 | -0.348332 | -1.313589 |
| H | 0.516833 | -0.635931 | 0.988710 |
| H | 1.783381 | 0.370332 | 1.659328 |
| H | -0.155821 | 1.783528 | 1.503752 |
| H | 0.998336 | 2.330148 | 0.306241 |
| H | -1.143782 | 2.452237 | -0.705913 |
| H | -0.343130 | 1.113970 | -1.491219 |
| H | -2.360884 | 0.734781 | 0.818283 |
| H | -2.794019 | 0.776234 | -0.895616 |
| O | -2.080630 | -1.786495 | 0.462047 |
| H | -1.219271 | -1.235259 | -1.282974 |

Rotational constants (GHz): 2.5580900 1.1863300 0.9177100
 Vibrational harmonic frequencies (cm-1):

| | | |
|----------|----------|----------|
| 34.8903 | 77.1304 | 85.2257 |
| 97.2098 | 167.3035 | 234.0434 |
| 297.4307 | 320.4748 | 409.9624 |
| 469.6145 | 527.1673 | 632.5670 |
| 732.1844 | 779.6492 | 840.0454 |

| | | |
|-----------|-----------|-----------|
| 873.1308 | 937.1539 | 984.9684 |
| 1014.7042 | 1042.5736 | 1084.4534 |
| 1099.0643 | 1116.4105 | 1144.8443 |
| 1190.7296 | 1242.5960 | 1257.2386 |
| 1307.6841 | 1333.6870 | 1354.5238 |
| 1369.6349 | 1384.4653 | 1398.1297 |
| 1398.8047 | 1428.3326 | 1467.4670 |
| 1499.5993 | 1502.4939 | 1510.4308 |
| 1834.9339 | 2854.9006 | 2884.9259 |
| 2926.3919 | 3016.2781 | 3027.5896 |
| 3030.6319 | 3055.9334 | 3070.3596 |
| 3079.8946 | 3104.2459 | 3104.9152 |

Zero-point correction (Hartree): 0.160928

C6H11O2.tpppc

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -385.63288882

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 3.833675 | -0.062699 | -0.336955 |
| C | 2.592918 | 0.350243 | 0.064334 |
| C | 1.540531 | -0.764959 | 0.162766 |
| C | 0.159834 | -0.280455 | 0.629132 |
| C | -0.557637 | 0.637448 | -0.373433 |
| C | -1.952491 | 1.071218 | 0.088068 |
| C | -3.002631 | -0.017467 | 0.050337 |
| H | 2.647323 | 0.945007 | 0.998552 |
| H | 2.297818 | 1.090446 | -0.712021 |
| H | 1.463533 | -1.261485 | -0.811954 |
| H | 1.918491 | -1.515999 | 0.866505 |
| H | -0.471500 | -1.154846 | 0.815155 |
| H | 0.262058 | 0.242179 | 1.591912 |
| H | 0.038907 | 1.539466 | -0.557035 |
| H | -0.650549 | 0.117854 | -1.334430 |
| H | -1.934469 | 1.479972 | 1.109967 |
| H | -2.340814 | 1.892820 | -0.533607 |
| O | -2.822339 | -1.142925 | -0.361358 |
| H | -4.004633 | 0.293405 | 0.426246 |

Rotational constants (GHz): 5.9223900 0.7272800 0.6841300

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 39.7328 | 83.6792 | 90.6803 |
| 112.8965 | 153.7417 | 227.6029 |
| 254.5014 | 300.2127 | 343.7562 |
| 516.2478 | 657.7471 | 665.7447 |
| 711.5494 | 765.2277 | 847.1383 |
| 877.9718 | 917.9551 | 962.7594 |
| 1026.6868 | 1049.3745 | 1063.3902 |
| 1090.1034 | 1101.2591 | 1159.1192 |
| 1200.6762 | 1246.3321 | 1273.3482 |
| 1319.4519 | 1344.7023 | 1348.1425 |
| 1368.8563 | 1387.0653 | 1392.2706 |
| 1412.8602 | 1428.9893 | 1457.4971 |
| 1492.4960 | 1501.3408 | 1507.0620 |
| 1831.9028 | 2886.1622 | 2887.6835 |
| 2926.9651 | 3014.3694 | 3017.2272 |
| 3038.6066 | 3046.8290 | 3049.9126 |
| 3083.0747 | 3093.2024 | 3104.1078 |

Zero-point correction (Hartree): 0.161021

C6H11O2.tpppt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -385.63285515

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 2.828519 | -0.938287 | 0.111959 |
| C | 1.843757 | -0.140767 | -0.393933 |
| C | 1.114590 | 0.715512 | 0.655303 |
| C | 0.099482 | 1.702336 | 0.057742 |
| C | -1.126929 | 1.096349 | -0.651363 |
| C | -2.053690 | 0.270377 | 0.252957 |
| C | -1.756710 | -1.209988 | 0.326935 |
| H | 2.210301 | 0.474837 | -1.240676 |
| H | 1.119896 | -0.853723 | -0.847066 |
| H | 0.640962 | 0.045453 | 1.382516 |
| H | 1.871223 | 1.283326 | 1.210131 |
| H | -0.253874 | 2.366818 | 0.857657 |
| H | 0.620658 | 2.351505 | -0.658991 |
| H | -1.705940 | 1.921748 | -1.080196 |
| H | -0.813599 | 0.470038 | -1.493930 |
| H | -2.080653 | 0.659427 | 1.281634 |
| H | -3.098368 | 0.333795 | -0.090579 |
| O | -0.933864 | -1.797244 | -0.343862 |
| H | -2.390847 | -1.771895 | 1.048892 |

Rotational constants (GHz): 2.6581400 1.3891400 1.0202600

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 59.5088 | 87.7716 | 139.2929 |
| 149.8483 | 159.8168 | 223.6492 |
| 271.0201 | 320.9430 | 406.0061 |
| 495.6648 | 649.7647 | 692.3050 |
| 717.5289 | 805.4203 | 821.5946 |
| 880.9197 | 934.8417 | 989.3633 |
| 1019.0364 | 1036.2732 | 1093.0068 |
| 1103.9740 | 1108.5041 | 1157.5017 |
| 1192.7466 | 1253.9374 | 1258.5632 |
| 1314.8789 | 1334.4250 | 1364.4399 |
| 1375.2119 | 1394.1987 | 1401.5651 |
| 1402.8661 | 1428.3405 | 1455.3086 |
| 1496.5451 | 1503.4790 | 1506.6809 |
| 1824.9355 | 2887.6639 | 2902.6082 |
| 2926.5431 | 3013.5945 | 3024.3592 |
| 3043.3278 | 3046.4674 | 3056.9718 |
| 3064.7762 | 3090.6843 | 3099.4010 |

Zero-point correction (Hartree): 0.161723

C6H11O2.tpptc

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -385.63195389

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 3.281378 | -1.229441 | 0.176400 |
| C | 2.297471 | -0.491127 | -0.421458 |
| C | 1.702266 | 0.621521 | 0.455335 |
| C | 0.579164 | 1.415577 | -0.232056 |
| C | -0.714830 | 0.635427 | -0.519810 |
| C | -1.463691 | 0.179901 | 0.734446 |
| C | -2.765341 | -0.534078 | 0.448150 |
| H | 2.624594 | -0.103686 | -1.406930 |
| H | 1.517467 | -1.243070 | -0.674758 |
| H | 1.359020 | 0.175139 | 1.395855 |
| H | 2.516021 | 1.306574 | 0.721256 |
| H | 0.338308 | 2.289687 | 0.387145 |
| H | 0.960507 | 1.819226 | -1.179767 |
| H | -1.386580 | 1.263793 | -1.114734 |
| H | -0.511859 | -0.239031 | -1.149463 |
| H | -1.696966 | 1.031057 | 1.393561 |
| H | -0.860130 | -0.496253 | 1.358614 |
| O | -3.199222 | -0.759249 | -0.660466 |
| H | -3.327862 | -0.857238 | 1.354106 |

Rotational constants (GHz): 3.9313700 0.7935700 0.7362500

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 32.5224 | 46.3956 | 87.9242 |
| 162.0926 | 174.2815 | 201.2840 |
| 226.7776 | 306.2570 | 404.0252 |
| 488.1696 | 648.7440 | 666.2066 |
| 689.4404 | 768.8588 | 865.6951 |
| 880.8045 | 895.3899 | 952.2632 |
| 995.6021 | 1053.2630 | 1080.2964 |
| 1090.9968 | 1108.8182 | 1152.2297 |
| 1187.8079 | 1232.4978 | 1290.9556 |
| 1309.4785 | 1327.8634 | 1342.3403 |
| 1366.5159 | 1389.4535 | 1395.7144 |
| 1408.7177 | 1427.6535 | 1463.8464 |
| 1499.7755 | 1504.4331 | 1507.3214 |
| 1832.7402 | 2886.0227 | 2889.0921 |
| 2932.1311 | 3013.5580 | 3027.9581 |
| 3040.1950 | 3047.6236 | 3055.8560 |
| 3068.3633 | 3093.5870 | 3094.8383 |

Zero-point correction (Hartree): 0.160872

C6H11O2.tpptt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -385.62991526

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 3.190728 | -1.385670 | 0.080793 |
| C | 2.280839 | -0.504607 | -0.435753 |
| C | 1.703939 | 0.493249 | 0.580321 |
| C | 0.708646 | 1.493274 | -0.029406 |
| C | -0.600084 | 0.890447 | -0.570225 |
| C | -1.475294 | 0.221605 | 0.508441 |
| C | -2.829955 | -0.171195 | -0.037392 |
| H | 2.682022 | 0.009830 | -1.331949 |
| H | 1.476180 | -1.159091 | -0.837805 |
| H | 1.248334 | -0.069725 | 1.402615 |
| H | 2.544127 | 1.047404 | 1.014975 |
| H | 0.461174 | 2.248270 | 0.727801 |
| H | 1.203740 | 2.036805 | -0.845606 |
| H | -1.177138 | 1.691837 | -1.050199 |
| H | -0.386890 | 0.161072 | -1.362257 |
| H | -1.006065 | -0.671547 | 0.930210 |

| | | | | |
|---|-----------|-----------|-----------|--|
| H | -1.641696 | 0.939024 | 1.326540 | |
| O | -3.280546 | -1.294784 | -0.030154 | |
| H | -3.413789 | 0.673119 | -0.475348 | |
| Rotational constants (GHz): | 3.5378000 | 0.8058800 | 0.7040800 | |
| Vibrational harmonic frequencies (cm ⁻¹): | | | | |
| 35.5357 | 63.0037 | | 70.1134 | |
| 92.0669 | 159.9178 | | 210.3587 | |
| 283.1138 | 310.9888 | | 417.8486 | |
| 483.9338 | 528.9841 | | 653.0653 | |
| 750.2593 | 780.6150 | | 868.9028 | |
| 883.4440 | 924.8542 | | 988.6716 | |
| 1009.3597 | 1063.5468 | | 1082.0545 | |
| 1091.9212 | 1114.1682 | | 1159.8980 | |
| 1190.1787 | 1240.4932 | | 1286.4080 | |
| 1294.7299 | 1329.4534 | | 1341.0259 | |
| 1368.7479 | 1388.7705 | | 1395.4477 | |
| 1401.2758 | 1433.2355 | | 1478.4324 | |
| 1498.7112 | 1504.9655 | | 1510.5040 | |
| 1838.2716 | 2870.0756 | | 2887.5985 | |
| 2929.4620 | 3018.8108 | | 3027.4738 | |
| 3034.8150 | 3053.1494 | | 3062.9284 | |
| 3075.6453 | 3098.4915 | | 3119.4009 | |
| Zero-point correction (Hartree): 0.161078 | | | | |

C6H11O2.tptmc

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -385.63337785

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 3.569932 | 0.596051 | -0.340214 |
| C | 2.217487 | 0.571768 | -0.136098 |
| C | 1.679053 | -0.725355 | 0.486068 |
| C | 0.157685 | -0.726162 | 0.696789 |
| C | -0.656379 | -0.777555 | -0.605814 |
| C | -2.170319 | -0.803387 | -0.375850 |
| C | -2.761913 | 0.510284 | 0.085792 |
| H | 1.884507 | 1.465169 | 0.428849 |
| H | 1.786938 | 0.728713 | -1.149460 |
| H | 1.982896 | -1.568845 | -0.146521 |
| H | 2.180845 | -0.862755 | 1.451346 |
| H | -0.110889 | -1.592664 | 1.315539 |
| H | -0.132999 | 0.164208 | 1.267420 |
| H | -0.421480 | 0.090315 | -1.232567 |
| H | -0.368218 | -1.668561 | -1.177595 |
| H | -2.709935 | -1.076593 | -1.295888 |
| H | -2.458001 | -1.573858 | 0.355721 |
| O | -2.141436 | 1.543867 | 0.212718 |
| H | -3.855321 | 0.477967 | 0.297792 |

| | | | |
|---|-----------|-----------|-----------|
| Rotational constants (GHz): | 4.1120300 | 0.8459000 | 0.7641200 |
| Vibrational harmonic frequencies (cm ⁻¹): | | | |
| 35.6768 | 79.7041 | | 89.2535 |
| 131.4793 | 153.8325 | | 243.1001 |
| 260.3956 | 290.7460 | | 346.1339 |
| 512.9564 | 611.5847 | | 660.5740 |
| 708.3273 | 781.4062 | | 823.2600 |
| 876.6430 | 909.4305 | | 962.2113 |
| 1020.5887 | 1043.4903 | | 1079.4353 |
| 1086.6975 | 1113.2745 | | 1153.6910 |
| 1203.8494 | 1245.5792 | | 1291.1843 |
| 1313.1814 | 1346.8082 | | 1351.1570 |
| 1369.7831 | 1383.8442 | | 1392.0944 |
| 1416.1926 | 1429.0540 | | 1457.1184 |
| 1494.0752 | 1500.5675 | | 1511.0070 |
| 1830.4852 | 2889.9273 | | 2892.6297 |
| 2933.9124 | 3015.0719 | | 3032.2499 |
| 3039.3061 | 3044.6128 | | 3048.6452 |
| 3073.4996 | 3087.9283 | | 3096.9759 |
| Zero-point correction (Hartree): 0.160986 | | | |

C6H11O2.tptmt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -385.62910716

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -3.732886 | -0.731651 | -0.237673 |
| C | -2.382342 | -0.672361 | -0.029553 |
| C | -1.849066 | 0.716703 | 0.353143 |
| C | -0.332349 | 0.758322 | 0.594711 |
| C | 0.507722 | 0.537365 | -0.674061 |
| C | 2.030276 | 0.734643 | -0.482222 |
| C | 2.650193 | -0.303724 | 0.427341 |
| H | -2.056504 | -1.448677 | 0.691836 |
| H | -1.945796 | -1.006814 | -0.996206 |
| H | -2.131403 | 1.428190 | -0.432608 |

| | | | | |
|--|-----------|-----------|-----------|--|
| H | -2.371348 | 1.032789 | 1.263742 | |
| H | -0.073212 | 1.734521 | 1.024473 | |
| H | -0.069278 | 0.014062 | 1.358762 | |
| H | 0.337549 | -0.467861 | -1.079792 | |
| H | 0.173388 | 1.240086 | -1.447664 | |
| H | 2.541890 | 0.675700 | -1.447420 | |
| H | 2.211933 | 1.729186 | -0.050606 | |
| O | 3.390357 | -1.184715 | 0.047051 | |
| H | 2.376413 | -0.225949 | 1.504305 | |
| Rotational constants (GHz): | 4.7713000 | 0.7012600 | 0.6609700 | |
| Vibrational harmonic frequencies (cm-1): | | | | |
| 20.1687 | 42.7799 | | 88.1787 | |
| 108.4521 | 127.9125 | | 237.5634 | |
| 255.9513 | 307.1119 | | 384.8965 | |
| 491.4695 | 540.9582 | | 629.6431 | |
| 749.1709 | 814.7529 | | 834.4164 | |
| 885.8571 | 941.8271 | | 972.8242 | |
| 1028.3541 | 1055.5585 | | 1074.9753 | |
| 1085.3561 | 1111.9416 | | 1156.1607 | |
| 1190.6804 | 1244.6178 | | 1288.3595 | |
| 1301.8906 | 1337.9942 | | 1347.3383 | |
| 1353.3734 | 1373.4166 | | 1389.7205 | |
| 1409.8790 | 1438.8784 | | 1483.3466 | |
| 1498.2435 | 1503.6136 | | 1514.0580 | |
| 1833.0775 | 2889.3116 | | 2890.4460 | |
| 2928.5423 | 3026.6192 | | 3031.0523 | |
| 3038.8157 | 3045.4613 | | 3060.0792 | |
| 3083.4537 | 3093.2032 | | 3114.4460 | |
| Zero-point correction (Hartree): | 0.160967 | | | |

C6H11O2.tptpc

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -385.63337774
Electronic state : 2-A
Cartesian coordinates (Angs):

| | | | | |
|--|-----------|-----------|-----------|--|
| O | 3.570356 | 0.596298 | -0.339241 | |
| C | 2.217625 | 0.571380 | -0.137065 | |
| C | 1.679213 | -0.725192 | 0.486251 | |
| C | 0.157824 | -0.726007 | 0.696735 | |
| C | -0.656109 | -0.776690 | -0.605978 | |
| C | -2.170049 | -0.803520 | -0.376078 | |
| C | -2.762369 | 0.509670 | 0.086010 | |
| H | 1.883241 | 1.465400 | 0.426093 | |
| H | 1.788425 | 0.726615 | -1.151258 | |
| H | 1.983254 | -1.569323 | -0.145396 | |
| H | 2.180860 | -0.861539 | 1.451752 | |
| H | -0.110860 | -1.592817 | 1.315010 | |
| H | -0.132880 | 0.164087 | 1.267794 | |
| H | -0.421678 | 0.091915 | -1.231882 | |
| H | -0.367435 | -1.666997 | -1.178593 | |
| H | -2.709477 | -1.076719 | -1.296227 | |
| H | -2.457289 | -1.574396 | 0.355234 | |
| O | -2.142516 | 1.543619 | 0.212979 | |
| H | -3.855693 | 0.476593 | 0.298323 | |
| Rotational constants (GHz): | 4.1134300 | 0.8456900 | 0.7640100 | |
| Vibrational harmonic frequencies (cm-1): | | | | |
| 35.7284 | 79.6009 | | 89.3253 | |
| 131.3619 | 153.7894 | | 243.1732 | |
| 260.2906 | 290.8163 | | 346.1212 | |
| 512.9316 | 611.2740 | | 660.6443 | |
| 708.2528 | 781.4196 | | 823.2558 | |
| 876.6672 | 909.3353 | | 962.2578 | |
| 1020.5087 | 1043.4798 | | 1079.4138 | |
| 1086.7133 | 1113.2426 | | 1153.6573 | |
| 1203.8594 | 1245.6108 | | 1291.2061 | |
| 1313.0858 | 1346.7890 | | 1351.1670 | |
| 1369.8191 | 1383.8494 | | 1392.1316 | |
| 1416.2001 | 1429.0515 | | 1457.1199 | |
| 1494.0758 | 1500.5586 | | 1510.9921 | |
| 1830.4989 | 2889.9409 | | 2892.6249 | |
| 2933.7823 | 3015.0899 | | 3032.2354 | |
| 3039.3245 | 3044.5878 | | 3048.6520 | |
| 3073.4803 | 3087.9182 | | 3096.9801 | |
| Zero-point correction (Hartree): | 0.160984 | | | |

C6H11O2.tptpt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -385.62910717
Electronic state : 2-A
Cartesian coordinates (Angs):

| | | | | |
|---|-----------|-----------|-----------|--|
| O | -3.733915 | -0.731846 | -0.238227 | |
| C | -2.383532 | -0.672720 | -0.029086 | |
| C | -1.850158 | 0.716580 | 0.352667 | |
| C | -0.333525 | 0.758101 | 0.594817 | |

| | | | |
|---|-----------|-----------|-----------|
| C | 0.506962 | 0.536908 | -0.673624 |
| C | 2.029495 | 0.733768 | -0.481412 |
| C | 2.650012 | -0.305409 | 0.426648 |
| H | -2.058384 | -1.448423 | 0.693269 |
| H | -1.946366 | -1.008148 | -0.995138 |
| H | -2.132072 | 1.427442 | -0.433796 |
| H | -2.372747 | 1.033528 | 1.262789 |
| H | -0.074436 | 1.734328 | 1.024548 |
| H | -0.070833 | 0.013947 | 1.359095 |
| H | 0.336394 | -0.468193 | -1.079547 |
| H | 0.173134 | 1.239789 | -1.447297 |
| H | 2.541393 | 0.676880 | -1.446580 |
| H | 2.210998 | 1.727542 | -0.047914 |
| O | 3.397379 | -1.180430 | 0.046741 |
| H | 2.369689 | -0.233856 | 1.502402 |

Rotational constants (GHz): 4.7802900 0.7003900 0.6603000
 Vibrational harmonic frequencies (cm-1):
 20.6232 42.5423 88.1042
 108.4130 127.7072 237.4287
 256.0227 307.0732 384.5328
 491.0527 541.2610 629.9590
 749.1822 814.5607 834.1583
 885.7023 941.6483 972.9954
 1028.3834 1055.7274 1075.0074
 1085.3860 1112.0191 1156.2145
 1190.6969 1244.6289 1288.3993
 1301.8883 1337.9919 1347.3053
 1353.3955 1373.3781 1389.7093
 1409.8820 1439.0016 1483.0862
 1498.2662 1503.6098 1514.0937
 1833.2651 2889.1742 2890.1103
 2928.5543 3026.6282 3030.8486
 3038.7616 3045.4828 3060.0467
 3083.3758 3093.2190 3114.4290
 Zero-point correction (Hartree): 0.160964

C6H11O2.tpttc

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -385.63337797

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 3.569829 | 0.596417 | -0.340356 |
| C | 2.217433 | 0.571833 | -0.135661 |
| C | 1.679195 | -0.725664 | 0.485659 |
| C | 0.157854 | -0.726706 | 0.696628 |
| C | -0.656371 | -0.777392 | -0.605925 |
| C | -2.170261 | -0.803355 | -0.375704 |
| C | -2.761975 | 0.510374 | 0.085671 |
| H | 1.885250 | 1.464805 | 0.430512 |
| H | 1.785993 | 0.730431 | -1.148344 |
| H | 1.982878 | -1.568726 | -0.147593 |
| H | 2.181154 | -0.863808 | 1.450739 |
| H | -0.110613 | -1.593569 | 1.314906 |
| H | -0.132810 | 0.163351 | 1.267757 |
| H | -0.421620 | 0.090883 | -1.232172 |
| H | -0.368253 | -1.668039 | -1.178265 |
| H | -2.710022 | -1.076968 | -1.295477 |
| H | -2.457750 | -1.573589 | 0.356191 |
| O | -2.141577 | 1.543937 | 0.212917 |
| H | -3.855476 | 0.477857 | 0.297255 |

Rotational constants (GHz): 4.1114400 0.8459100 0.7640900
 Vibrational harmonic frequencies (cm-1):
 35.6158 79.7153 89.1840
 131.4955 153.7338 243.0736
 260.3814 290.7033 346.1873
 512.6338 609.1592 660.4569
 708.2944 781.3402 822.8568
 876.4871 909.4402 962.0249
 1020.6319 1043.4526 1079.3396
 1086.6911 1113.3951 1153.6732
 1204.0028 1245.7784 1291.2637
 1313.1901 1346.7628 1351.2329
 1369.9642 1383.8396 1392.1922
 1416.1860 1429.0587 1457.1038
 1494.0655 1500.5772 1510.9930
 1830.6273 2889.7580 2893.0140
 2933.5026 3015.3182 3032.2960
 3039.4262 3044.5880 3048.7974
 3073.5137 3087.9168 3097.0012
 Zero-point correction (Hartree): 0.160980

C6H11O2.tpttt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -385.63087659

```

Electronic state : 2-A
Cartesian coordinates (Angs):
O      -3.767083    -0.477744    -0.349072
C      -2.401253    -0.533842    -0.299673
C      -1.752313     0.397458     0.735518
C      -0.219171     0.315282     0.773035
C       0.477488     0.878601    -0.475317
C       2.014662     0.854579    -0.371972
C       2.573958    -0.551222    -0.378169
H      -2.048364    -1.578802    -0.186862
H      -2.085160    -0.253968    -1.328744
H      -2.077935     1.425337     0.533495
H      -2.154542     0.130237     1.719688
H       0.142007     0.863132     1.652261
H       0.087328    -0.729039     0.929005
H       0.174147     0.318317    -1.370754
H       0.150614     1.912462    -0.640002
H       2.441080     1.372398    -1.243785
H       2.368654     1.365621     0.529021
O       3.345041    -0.998333     0.440902
H       2.218286    -1.182217    -1.228486
Rotational constants (GHz):   4.9199000    0.7037800    0.6824600
Vibrational harmonic frequencies (cm-1):
   36.8410           55.7073           89.4777
  104.3972          136.5059          241.9929
  270.8449          301.1625          372.3257
  489.9790          557.6441          637.2726
  742.3893          769.5646          843.0395
  879.9847          953.1144          987.7775
 1025.3595         1044.2326         1074.5295
 1088.5769         1115.7326         1156.0403
 1195.0551         1234.6374         1282.1586
 1305.3609         1340.8954         1344.9545
 1358.8503         1373.2791         1389.8762
 1412.7208         1432.1926         1474.1464
 1496.4047         1503.4335         1510.7761
 1838.9158         2859.8649         2887.6536
 2928.7690         3022.0352         3026.4306
 3030.4673         3046.6484         3062.7487
 3081.1326         3092.8943         3108.8983
Zero-point correction (Hartree): 0.160874
    
```

C6H11O2.ttpmc

```

-----
E(UB+HF-LYP/6-31G(d,p)) (Hartree): -385.63163001
Electronic state : 2-A
Cartesian coordinates (Angs):
O       3.250578    -1.017835     0.189989
C       2.541659     0.143848     0.048720
C       1.023402    -0.019472    -0.095497
C       0.299645     1.332632    -0.129304
C      -1.211192     1.270721    -0.411388
C      -2.029488     0.491182     0.628011
C      -2.189399    -0.988275     0.347746
H       2.777712     0.727069     0.967809
H       2.967779     0.762868    -0.766537
H       0.810419    -0.584942    -1.009509
H       0.669839    -0.637325     0.738001
H       0.464103     1.855269     0.825202
H       0.761865     1.965672    -0.899508
H      -1.591213     2.297245    -0.461755
H      -1.384155     0.819441    -1.394714
H      -1.623365     0.602921     1.644298
H      -3.055808     0.884911     0.697044
O      -1.838780    -1.547013    -0.668507
H      -2.699323    -1.558163     1.158089
Rotational constants (GHz):   3.2323200    0.9932700    0.8282700
Vibrational harmonic frequencies (cm-1):
   66.4850           78.0356           95.6650
  124.8572          155.6554          173.8083
  279.7455          294.7561          424.4101
  458.9365          564.6611          652.6220
  707.9773          766.9175          823.7978
  883.5654          933.9154          978.3352
 1021.0470         1038.3363         1058.2483
 1087.8574         1107.7016         1159.3372
 1229.0769         1241.8590         1265.4246
 1317.1339         1329.4997         1370.9549
 1373.3189         1378.0125         1397.8138
 1413.5928         1428.1906         1458.9373
 1492.9236         1498.9649         1510.8394
 1832.5193         2872.7153         2890.0537
 2926.3009         3008.4345         3013.9524
 3041.4357         3044.6565         3056.8033
 3059.8354         3098.3302         3104.8199
    
```

Zero-point correction (Hartree): 0.160823

C6H11O2.ttpmt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -385.63021904

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -3.235192 | -1.071209 | 0.157955 |
| C | -2.524152 | 0.031864 | -0.227419 |
| C | -1.064599 | 0.077611 | 0.241975 |
| C | -0.339026 | 1.342689 | -0.235840 |
| C | 1.096102 | 1.517535 | 0.288917 |
| C | 2.125313 | 0.510989 | -0.263301 |
| C | 2.044944 | -0.874468 | 0.340172 |
| H | -2.578348 | 0.051947 | -1.338180 |

| | | | |
|---|-----------|-----------|-----------|
| H | -3.077494 | 0.947243 | 0.068386 |
| H | -1.056076 | 0.032158 | 1.338847 |
| H | -0.565102 | -0.828737 | -0.116534 |
| H | -0.321650 | 1.363459 | -1.334937 |
| H | -0.922201 | 2.221620 | 0.072299 |
| H | 1.438891 | 2.526184 | 0.032257 |
| H | 1.094460 | 1.470548 | 1.387204 |
| H | 2.065745 | 0.419808 | -1.352895 |
| H | 3.133460 | 0.880896 | -0.020716 |
| O | 2.083239 | -1.908016 | -0.290041 |
| H | 1.972436 | -0.888645 | 1.453932 |

Rotational constants (GHz): 2.8920300 0.9999200 0.7851800

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 44.5916 | 66.0839 | 87.8502 |
| 95.2578 | 123.3383 | 194.8863 |
| 276.3810 | 306.9904 | 315.7128 |
| 438.4283 | 457.2948 | 524.3704 |
| 743.4659 | 757.4930 | 831.6631 |
| 891.8830 | 943.5923 | 1006.7790 |
| 1020.4091 | 1025.8093 | 1086.5134 |
| 1088.1594 | 1108.2671 | 1165.3895 |
| 1228.7728 | 1237.5676 | 1283.6066 |
| 1302.7384 | 1331.9650 | 1354.7744 |
| 1364.9108 | 1392.9210 | 1397.2728 |
| 1415.4840 | 1429.1100 | 1468.3251 |
| 1497.6825 | 1502.8801 | 1513.3990 |
| 1833.5827 | 2868.1550 | 2888.8176 |
| 2916.4196 | 3016.6327 | 3016.9964 |
| 3028.2338 | 3043.7046 | 3054.8762 |
| 3079.4509 | 3103.1666 | 3105.3226 |

Zero-point correction (Hartree): 0.160104

C6H11O2.ttppc

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -385.63304960

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -3.614111 | -0.497464 | 0.584687 |
| C | -2.585048 | -0.363335 | -0.306791 |
| C | -1.340279 | 0.360596 | 0.220927 |
| C | -0.210714 | 0.409782 | -0.815596 |
| C | 1.028904 | 1.208661 | -0.376758 |
| C | 1.802410 | 0.611757 | 0.804838 |
| C | 2.539258 | -0.673400 | 0.500749 |
| H | -2.326175 | -1.402737 | -0.609111 |
| H | -2.955060 | 0.090035 | -1.248862 |
| H | -1.630165 | 1.378570 | 0.513085 |
| H | -1.020343 | -0.149367 | 1.137258 |
| H | 0.097776 | -0.607205 | -1.084531 |
| H | -0.597026 | 0.864415 | -1.738125 |
| H | 1.713389 | 1.288703 | -1.228178 |
| H | 0.727302 | 2.231053 | -0.116544 |
| H | 2.561225 | 1.319928 | 1.172545 |
| H | 1.158397 | 0.425908 | 1.676574 |
| O | 2.587805 | -1.208373 | -0.586030 |
| H | 3.073934 | -1.116973 | 1.372414 |

Rotational constants (GHz): 4.1089800 0.7955400 0.7638200

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 36.3989 | 67.6043 | 93.2094 |
| 126.2167 | 166.6075 | 191.0920 |
| 253.4379 | 316.3263 | 420.6021 |
| 447.7183 | 497.3857 | 654.1251 |
| 716.3131 | 756.6491 | 822.7119 |
| 877.8081 | 929.0828 | 968.9652 |
| 1012.5839 | 1020.9778 | 1080.4227 |
| 1092.1227 | 1114.4707 | 1146.3968 |
| 1214.9866 | 1256.3640 | 1268.8835 |
| 1311.5520 | 1332.1344 | 1363.5836 |
| 1377.3995 | 1390.7251 | 1395.7436 |

| | | |
|-----------|-----------|-----------|
| 1409.2199 | 1429.9872 | 1459.7663 |
| 1492.7793 | 1502.1428 | 1517.1455 |
| 1830.5765 | 2882.7648 | 2885.3154 |
| 2923.1610 | 3019.1692 | 3029.5753 |
| 3039.4919 | 3044.8344 | 3050.8965 |
| 3075.6493 | 3091.6906 | 3097.9945 |

Zero-point correction (Hartree): 0.160617

C6H11O2.ttppt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -385.63117263

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 3.460054 | 0.786005 | 0.435677 |
| C | 2.525928 | 0.201805 | -0.375071 |
| C | 1.241590 | -0.261658 | 0.323084 |
| C | 0.237863 | -0.884149 | -0.655935 |
| C | -1.018174 | -1.474770 | 0.006973 |
| C | -1.905847 | -0.443156 | 0.737749 |
| C | -2.469659 | 0.583887 | -0.216813 |
| H | 2.290582 | 0.965827 | -1.148876 |
| H | 2.994553 | -0.616679 | -0.959321 |
| H | 1.512223 | -0.991403 | 1.097325 |
| H | 0.804211 | 0.601161 | 0.836987 |
| H | -0.057951 | -0.130467 | -1.399312 |
| H | 0.734585 | -1.685064 | -1.220431 |
| H | -1.620675 | -1.982118 | -0.757963 |
| H | -0.723236 | -2.248826 | 0.725681 |
| H | -2.752090 | -0.972395 | 1.198085 |
| H | -1.361780 | 0.078993 | 1.529491 |
| O | -2.257498 | 1.775237 | -0.160127 |
| H | -3.111071 | 0.159277 | -1.025991 |

Rotational constants (GHz): 3.3497200 0.8858000 0.7692300

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 23.4329 | 56.1962 | 69.6527 |
| 106.3573 | 145.4441 | 213.4789 |
| 254.6349 | 357.9061 | 396.7587 |
| 459.5816 | 477.9053 | 503.8809 |
| 748.4162 | 784.1403 | 827.0835 |
| 898.0704 | 949.2103 | 1000.3740 |
| 1011.0999 | 1026.4878 | 1084.5977 |
| 1088.3389 | 1120.2664 | 1154.4745 |
| 1206.6106 | 1251.4656 | 1269.7131 |
| 1302.3386 | 1330.6784 | 1347.8833 |
| 1368.2444 | 1389.2776 | 1391.5405 |
| 1413.3173 | 1432.7970 | 1482.9010 |
| 1498.2973 | 1502.8189 | 1514.3468 |
| 1835.2201 | 2866.3174 | 2885.5589 |
| 2919.7067 | 3020.9854 | 3031.6515 |
| 3039.5337 | 3043.8994 | 3056.3082 |
| 3078.5801 | 3100.6225 | 3121.7188 |

Zero-point correction (Hartree): 0.160520

C6H11O2.ttpptc

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -385.63318669

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 3.872767 | -0.763360 | -0.293191 |
| C | 2.964148 | 0.174308 | 0.115720 |
| C | 1.501238 | -0.124154 | -0.233431 |
| C | 0.536392 | 0.931920 | 0.321255 |
| C | -0.929870 | 0.743268 | -0.095914 |
| C | -1.579626 | -0.529892 | 0.450564 |
| C | -3.049009 | -0.661511 | 0.119786 |
| H | 3.092379 | 0.239550 | 1.219432 |
| H | 3.273220 | 1.179803 | -0.235616 |
| H | 1.409546 | -0.176679 | -1.326077 |
| H | 1.259566 | -1.122059 | 0.150371 |
| H | 0.604697 | 0.948636 | 1.419077 |
| H | 0.864372 | 1.925055 | -0.014749 |
| H | -1.517837 | 1.603920 | 0.240871 |
| H | -1.007688 | 0.742430 | -1.189816 |
| H | -1.488720 | -0.588287 | 1.547133 |
| H | -1.085571 | -1.440938 | 0.081237 |
| O | -3.689161 | 0.147224 | -0.515762 |
| H | -3.532450 | -1.585969 | 0.511878 |

Rotational constants (GHz): 7.1026100 0.6240200 0.6007200

Vibrational harmonic frequencies (cm-1):

| | | |
|----------|----------|----------|
| 38.1020 | 71.5947 | 81.4644 |
| 127.9437 | 177.3941 | 192.7964 |
| 205.0927 | 273.3912 | 427.5463 |
| 463.2519 | 496.9065 | 670.8002 |
| 700.0990 | 754.3041 | 839.1018 |
| 873.1180 | 936.1518 | 970.8912 |

| | | |
|-----------|-----------|-----------|
| 1011.9500 | 1031.5212 | 1080.4863 |
| 1090.4912 | 1111.3840 | 1162.6182 |
| 1220.9631 | 1256.5477 | 1292.0400 |
| 1307.2387 | 1326.3432 | 1344.6486 |
| 1367.1385 | 1388.5346 | 1408.9616 |
| 1409.5477 | 1428.4520 | 1464.5039 |
| 1496.8693 | 1503.2513 | 1512.6422 |
| 1833.2956 | 2881.8256 | 2886.4079 |
| 2923.5917 | 3011.0536 | 3014.5670 |
| 3041.1796 | 3044.8833 | 3045.4048 |
| 3060.5127 | 3091.6481 | 3097.2002 |

Zero-point correction (Hartree): 0.160492

C6H11O2.ttptt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -385.63116778

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 3.785864 | -1.033866 | -0.045347 |
| C | 2.977369 | 0.057816 | 0.116284 |
| C | 1.493552 | -0.165766 | -0.199799 |
| C | 0.644581 | 1.085425 | 0.058868 |
| C | -0.830319 | 0.953133 | -0.351775 |
| C | -1.615850 | -0.100717 | 0.452704 |
| C | -3.095237 | -0.058041 | 0.140510 |
| H | 3.105899 | 0.359352 | 1.179789 |
| H | 3.390990 | 0.920632 | -0.444594 |
| H | 1.405012 | -0.466154 | -1.251892 |
| H | 1.141684 | -1.013198 | 0.399226 |
| H | 0.699355 | 1.353689 | 1.124045 |
| H | 1.079363 | 1.932495 | -0.489334 |
| H | -1.318594 | 1.929250 | -0.230715 |
| H | -0.891437 | 0.709429 | -1.420328 |
| H | -1.501145 | 0.112244 | 1.526992 |
| H | -1.257427 | -1.116889 | 0.268169 |
| O | -3.752164 | -1.003077 | -0.234824 |
| H | -3.567882 | 0.943594 | 0.279256 |

Rotational constants (GHz): 5.7444500 0.6256000 0.5839900

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 54.3080 | 60.5049 | 78.1861 |
| 89.3985 | 128.4527 | 203.6861 |
| 259.9595 | 277.7388 | 420.3532 |
| 471.3704 | 486.1521 | 523.5365 |
| 751.1274 | 765.1116 | 830.1281 |
| 915.3473 | 937.8044 | 1011.2008 |
| 1012.8769 | 1042.9899 | 1080.2559 |
| 1089.5035 | 1121.1088 | 1161.7344 |
| 1224.3436 | 1255.6249 | 1286.3676 |
| 1291.5051 | 1325.6218 | 1340.1128 |
| 1367.8392 | 1389.7270 | 1398.0090 |
| 1411.6838 | 1433.1152 | 1478.7602 |
| 1496.0952 | 1508.3689 | 1511.9967 |
| 1838.5946 | 2869.0671 | 2883.1358 |
| 2922.9903 | 3013.9804 | 3015.5299 |
| 3030.8234 | 3045.2186 | 3051.9975 |
| 3071.7965 | 3096.2993 | 3123.5745 |

Zero-point correction (Hartree): 0.160508

C6H11O2.ttttc

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -385.63438022

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 3.932318 | 0.312619 | -0.169992 |
| C | 2.691123 | 0.366195 | 0.404021 |
| C | 1.577184 | -0.364109 | -0.353993 |
| C | 0.212338 | -0.235254 | 0.331626 |
| C | -0.905001 | -0.970412 | -0.421578 |
| C | -2.273475 | -0.879190 | 0.260025 |
| C | -2.928272 | 0.482997 | 0.200318 |
| H | 2.753173 | 0.035978 | 1.461349 |
| H | 2.454161 | 1.449878 | 0.490249 |
| H | 1.530218 | 0.037971 | -1.373334 |
| H | 1.856708 | -1.421745 | -0.445871 |
| H | 0.278968 | -0.630440 | 1.356310 |
| H | -0.056102 | 0.824018 | 0.420290 |
| H | -0.987694 | -0.560117 | -1.434737 |
| H | -0.635491 | -2.028324 | -0.530106 |
| H | -2.989707 | -1.584255 | -0.189762 |
| H | -2.221179 | -1.174780 | 1.319263 |
| O | -2.471923 | 1.450248 | -0.370121 |
| H | -3.909594 | 0.547528 | 0.724737 |

Rotational constants (GHz): 5.1498400 0.7122400 0.6617200

Vibrational harmonic frequencies (cm-1):

| | | |
|---------|---------|----------|
| 58.0567 | 66.3633 | 111.3026 |
|---------|---------|----------|

| | | |
|-----------|-----------|-----------|
| 121.8024 | 139.3758 | 176.1174 |
| 246.9603 | 320.9048 | 352.0667 |
| 396.8478 | 503.6206 | 658.2328 |
| 716.9560 | 750.5117 | 832.5501 |
| 864.9698 | 947.6894 | 973.9083 |
| 1020.3418 | 1042.5880 | 1066.4697 |
| 1089.8944 | 1107.8477 | 1157.5550 |
| 1225.1747 | 1260.9780 | 1274.5137 |
| 1312.3648 | 1340.8496 | 1349.3076 |
| 1373.0710 | 1386.0037 | 1401.0036 |
| 1416.3094 | 1429.5362 | 1456.6436 |
| 1495.0093 | 1501.8326 | 1518.3050 |
| 1831.1716 | 2885.7543 | 2886.5779 |
| 2919.4294 | 3012.9229 | 3015.9155 |
| 3037.7143 | 3040.1797 | 3048.0440 |
| 3071.6568 | 3085.0593 | 3098.9765 |

Zero-point correction (Hartree): 0.160377

C6H11O2.tttpt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -385.63235935

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 4.010249 | -0.338024 | 0.185329 |
| C | 2.724629 | -0.594840 | -0.206397 |
| C | 1.689297 | 0.465944 | 0.183965 |
| C | 0.267714 | 0.098553 | -0.255421 |
| C | -0.770385 | 1.168663 | 0.108350 |
| C | -2.201154 | 0.810060 | -0.338195 |
| C | -2.764135 | -0.368207 | 0.425076 |
| H | 2.707718 | -0.801415 | -1.296393 |
| H | 2.464274 | -1.580013 | 0.239572 |
| H | 1.729447 | 0.606142 | 1.271321 |
| H | 1.986822 | 1.421843 | -0.265822 |
| H | 0.247355 | -0.064832 | -1.342245 |
| H | -0.019528 | -0.861800 | 0.196181 |
| H | -0.760117 | 1.336902 | 1.194354 |
| H | -0.487275 | 2.124240 | -0.348760 |
| H | -2.862383 | 1.666761 | -0.141832 |
| H | -2.247958 | 0.585734 | -1.408601 |
| O | -3.223406 | -1.369521 | -0.077516 |
| H | -2.728898 | -0.254231 | 1.535453 |

Rotational constants (GHz): 5.1801300 0.6613000 0.6109200

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 43.9221 | 58.9965 | 76.5486 |
| 122.6338 | 132.2056 | 151.7690 |
| 267.1538 | 335.5961 | 342.1999 |
| 378.2506 | 487.4326 | 540.6292 |
| 734.7106 | 776.5044 | 804.4313 |
| 930.1351 | 944.1524 | 1005.9317 |
| 1029.3830 | 1032.8682 | 1064.4106 |
| 1089.3424 | 1109.6964 | 1167.4341 |
| 1214.1826 | 1254.9445 | 1270.8389 |
| 1302.7848 | 1333.4571 | 1346.9857 |
| 1355.2464 | 1372.2782 | 1406.4672 |
| 1415.6507 | 1432.7036 | 1474.6336 |
| 1497.7983 | 1501.3131 | 1517.4089 |
| 1837.5308 | 2863.0138 | 2888.8434 |
| 2919.4362 | 3015.8891 | 3026.0875 |
| 3031.3548 | 3042.1936 | 3046.7983 |
| 3077.0759 | 3089.8162 | 3108.5779 |

Zero-point correction (Hartree): 0.160086

C6H11O2.ttttc

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -385.63428392

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 4.162423 | -0.502264 | 0.012708 |
| C | 3.062078 | 0.310760 | -0.020418 |
| C | 1.707385 | -0.405695 | -0.002970 |
| C | 0.521138 | 0.565356 | 0.001941 |
| C | -0.837500 | -0.145151 | -0.000235 |
| C | -2.019740 | 0.824130 | 0.006189 |
| C | -3.374411 | 0.153414 | 0.002600 |
| H | 3.162143 | 0.975764 | 0.866188 |
| H | 3.143360 | 1.014321 | -0.874287 |
| H | 1.651123 | -1.062274 | -0.880414 |
| H | 1.670292 | -1.057998 | 0.878042 |
| H | 0.589211 | 1.221161 | 0.882596 |
| H | 0.587488 | 1.228660 | -0.873044 |
| H | -0.915863 | -0.798374 | -0.877260 |
| H | -0.913923 | -0.807877 | 0.869775 |
| H | -1.989929 | 1.491969 | 0.881597 |
| H | -1.990601 | 1.502430 | -0.861175 |

```

O      -3.550701    -1.045138    -0.005541
H      -4.240770     0.854547     0.008004
Rotational constants (GHz):    8.6356700    0.5708200    0.5443200
Vibrational harmonic frequencies (cm-1):
 49.8048      69.4928      86.1306
128.0287     139.5968     188.0526
192.5286     290.2165     377.3958
395.3756     503.5617     673.1702
704.8071     742.5815     815.9582
897.6474     929.1274    1005.1208
1022.7300    1040.4469    1067.3371
1086.3596    1106.3580    1166.5142
1237.2156    1248.3634    1288.6865
1314.1528    1328.8039    1336.6378
1363.7189    1387.1030    1407.4126
1418.5695    1427.0949    1464.3197
1498.0261    1502.3803    1519.1074
1833.5345    2883.2133    2885.8123
2919.8602    3006.9216    3011.2469
3035.1353    3037.4628    3043.9338
3055.0012    3087.2775    3097.5678
Zero-point correction (Hartree): 0.160194
    
```

C6H11O2.ttttt

```

-----
E(UB+HF-LYP/6-31G(d,p)) (Hartree): -385.63238348
Electronic state : 2-A
Cartesian coordinates (Angs):
O      -4.270968    -0.365006    -0.110207
C      -3.122685     0.374851    -0.031242
C      -1.817776    -0.429043    -0.001642
C      -0.572111     0.463123     0.046828
C       0.738395    -0.332835     0.092435
C       1.986055     0.569054     0.129992
C       3.262120    -0.228646     0.277776
H      -3.143258     1.054238    -0.911833
H      -3.192901     1.073878     0.827427
H      -1.839603    -1.093045     0.871836
H      -1.789494    -1.076551    -0.886576
H      -0.560823     1.127048    -0.829147
H      -0.623769     1.121727     0.925872
H       0.734552    -0.988974     0.973638
H       0.795240    -0.993315    -0.782326
H       2.066226     1.186774    -0.769899
H       1.915887     1.241931     0.998456
O       4.210430    -0.164653    -0.472248
H       3.278255    -0.915459     1.157312
Rotational constants (GHz):    12.0345400    0.5161300    0.5089600
Vibrational harmonic frequencies (cm-1):
 44.1084      61.2035      84.0306
102.4000     136.6559     149.5356
242.6876     278.0243     350.2105
406.5910     490.9031     535.9067
739.0704     767.8998     826.9454
913.3968     978.1729    1020.7009
1028.7974    1033.5191    1063.0269
1088.2357    1115.0365    1169.9625
1237.0092    1244.0203    1284.4652
1300.9584    1328.1011    1341.7029
1355.6951    1378.3524    1406.0316
1415.3144    1434.9766    1477.5917
1499.8646    1505.4264    1521.5854
1838.2287    2870.8120    2888.0717
2919.7697    3014.5909    3017.0801
3030.5951    3042.9176    3046.4399
3071.9745    3091.3227    3110.5324
Zero-point correction (Hartree): 0.160156
    
```

C6H11O2.1-7Hshift.BB

```

-----
E(UB+HF-LYP/6-31G(d,p)) (Hartree): -385.62500873
Electronic state : 2-A
Cartesian coordinates (Angs):
O      -0.728448    -1.778648    -0.292056
H       0.603472    -1.189582    -0.240014
C       1.540099    -0.491031    -0.016630
C      -1.548458    -1.026592     0.540810
C       1.179928     0.722669     0.817916
C      -1.990623     0.334895    -0.039586
C       0.258328     1.717067     0.065424
C      -0.893821     1.127081    -0.771437
O       2.631596    -0.772139    -0.432375
H      -2.444910    -1.648998     0.717049
H      -1.099928    -0.905668     1.543440
H       0.676227     0.352766     1.718467
    
```

| | | | | |
|--|-----------|-----------|-----------|--|
| H | 2.107350 | 1.215190 | 1.125455 | |
| H | -2.794680 | 0.154992 | -0.763318 | |
| H | -2.427796 | 0.938127 | 0.768254 | |
| H | -0.144772 | 2.419819 | 0.805002 | |
| H | 0.889033 | 2.308264 | -0.608659 | |
| H | -1.374364 | 1.968526 | -1.284777 | |
| H | -0.487538 | 0.488333 | -1.564431 | |
| Rotational constants (GHz): | 2.6173700 | 1.5955100 | 1.1573000 | |
| Vibrational harmonic frequencies (cm-1): | | | | |
| i302.8851 | 52.5160 | | 114.9227 | |
| 209.1122 | 224.5160 | | 263.9075 | |
| 294.4427 | 371.0932 | | 481.6893 | |
| 493.5366 | 550.7299 | | 737.8420 | |
| 773.9321 | 795.0759 | | 866.1066 | |
| 894.4912 | 953.7092 | | 975.9338 | |
| 1007.3626 | 1035.9577 | | 1059.4065 | |
| 1106.7478 | 1127.1413 | | 1178.8644 | |
| 1194.5369 | 1214.4506 | | 1266.6566 | |
| 1286.7844 | 1307.0627 | | 1334.7138 | |
| 1377.3518 | 1390.2104 | | 1392.4751 | |
| 1412.1745 | 1446.9416 | | 1481.4854 | |
| 1488.9668 | 1503.5769 | | 1508.3259 | |
| 1702.5633 | 1867.7906 | | 2944.2009 | |
| 2966.5168 | 3029.8643 | | 3041.2166 | |
| 3046.7846 | 3056.2914 | | 3076.1138 | |
| 3079.7785 | 3091.1720 | | 3116.9304 | |
| Zero-point correction (Hartree): | 0.159914 | | | |

C6H11O2.1-7Hshift.CR

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -385.62696035
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | | |
|--|-----------|-----------|-----------|--|
| O | 0.672999 | -1.497808 | 0.880335 | |
| H | -0.680638 | -1.072246 | 0.501821 | |
| C | -1.572862 | -0.471253 | 0.010134 | |
| C | 1.513511 | -1.220614 | -0.194901 | |
| C | -1.498655 | 1.026535 | 0.260041 | |
| C | 2.021454 | 0.225119 | -0.278301 | |
| C | -0.080942 | 1.535339 | 0.556652 | |
| C | 0.951200 | 1.292048 | -0.578377 | |
| O | -2.419729 | -1.034942 | -0.629459 | |
| H | 2.379120 | -1.897411 | -0.068964 | |
| H | 1.052421 | -1.524075 | -1.153555 | |
| H | -1.954687 | 1.530743 | -0.600090 | |
| H | -2.154806 | 1.217635 | 1.122042 | |
| H | 2.524221 | 0.470367 | 0.666045 | |
| H | 2.788667 | 0.267837 | -1.063490 | |
| H | -0.158792 | 2.609449 | 0.757731 | |
| H | 0.275470 | 1.072489 | 1.482257 | |
| H | 1.471314 | 2.232703 | -0.791573 | |
| H | 0.429311 | 1.031472 | -1.510728 | |
| Rotational constants (GHz): | 2.5386300 | 1.5961700 | 1.1547800 | |
| Vibrational harmonic frequencies (cm-1): | | | | |
| i290.2498 | 55.0319 | | 103.4739 | |
| 148.5694 | 231.0665 | | 290.2290 | |
| 338.6113 | 362.7766 | | 410.6349 | |
| 484.6970 | 535.3686 | | 738.7808 | |
| 756.0189 | 830.0883 | | 850.0976 | |
| 904.6438 | 927.5353 | | 998.4693 | |
| 1031.0839 | 1056.1935 | | 1072.6019 | |
| 1105.5975 | 1134.7061 | | 1177.7358 | |
| 1208.2589 | 1241.3026 | | 1271.3391 | |
| 1297.8367 | 1310.2877 | | 1346.8148 | |
| 1370.0760 | 1382.6038 | | 1398.3396 | |
| 1404.5823 | 1440.7023 | | 1454.5854 | |
| 1485.8414 | 1498.5498 | | 1508.2768 | |
| 1756.9480 | 1863.4337 | | 2940.5442 | |
| 2966.6593 | 3021.0374 | | 3028.7884 | |
| 3029.6917 | 3056.4811 | | 3072.3496 | |
| 3078.0562 | 3086.3441 | | 3107.6785 | |
| Zero-point correction (Hartree): | 0.159862 | | | |

C4H9O2.mmm

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.23868662
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | | |
|---|-----------|-----------|-----------|--|
| O | -1.134273 | 1.334782 | 0.190145 | |
| C | -0.925586 | 0.098630 | -0.247192 | |
| C | 0.151462 | -0.654780 | 0.605180 | |
| C | 1.521939 | 0.022945 | 0.631587 | |
| C | 2.262993 | 0.017473 | -0.710301 | |
| O | -2.066254 | -0.733174 | -0.329195 | |
| H | -0.490586 | 0.214333 | -1.272830 | |

| | | | | |
|--|-----------|-----------|-----------|--|
| H | -0.268554 | -0.735617 | 1.612437 | |
| H | 0.209556 | -1.667371 | 0.192397 | |
| H | 1.403695 | 1.052216 | 0.986874 | |
| H | 2.133931 | -0.496373 | 1.379845 | |
| H | 1.735512 | 0.601753 | -1.472088 | |
| H | 2.383776 | -1.001704 | -1.094829 | |
| H | 3.261515 | 0.453239 | -0.606028 | |
| H | -2.829488 | -0.138956 | -0.289026 | |
| Rotational constants (GHz): | 6.4799700 | 2.0075100 | 1.8624700 | |
| Vibrational harmonic frequencies (cm-1): | | | | |
| 52.6933 | 126.4037 | | 169.0777 | |
| 204.4132 | 271.3698 | | 343.0690 | |
| 396.5712 | 463.6042 | | 572.4554 | |
| 739.0034 | 824.0101 | | 863.4239 | |
| 897.4669 | 966.8966 | | 1030.4799 | |
| 1063.3176 | 1096.3488 | | 1153.8203 | |
| 1179.2016 | 1239.5015 | | 1250.8175 | |
| 1288.1481 | 1311.7259 | | 1368.1528 | |
| 1392.0493 | 1430.0781 | | 1494.1805 | |
| 1496.5790 | 1515.6532 | | 1520.1055 | |
| 2778.0941 | 3040.1499 | | 3043.0988 | |
| 3065.5871 | 3086.3999 | | 3110.8111 | |
| 3114.6245 | 3119.8648 | | 3802.6463 | |
| Zero-point correction (Hartree): | 0.127308 | | | |

C4H9O2.mmp

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.23329933
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | | |
|--|-----------|-----------|-----------|--|
| O | -1.028833 | 1.358944 | 0.252495 | |
| C | -0.934325 | 0.138856 | -0.255486 | |
| C | 0.121098 | -0.698511 | 0.559206 | |
| C | 1.515336 | -0.074071 | 0.637026 | |
| C | 2.232213 | 0.056742 | -0.711434 | |
| O | -2.184380 | -0.528026 | -0.288722 | |
| H | -0.532654 | 0.245699 | -1.291839 | |
| H | -0.308583 | -0.828720 | 1.556904 | |
| H | 0.167185 | -1.689718 | 0.089036 | |
| H | 1.436649 | 0.909764 | 1.110295 | |
| H | 2.120512 | -0.697582 | 1.307372 | |
| H | 1.716964 | 0.755611 | -1.378414 | |
| H | 2.302038 | -0.910153 | -1.223820 | |
| H | 3.251081 | 0.432154 | -0.575633 | |
| H | -2.053415 | -1.402498 | -0.679956 | |
| Rotational constants (GHz): | 6.5042300 | 2.0222100 | 1.8758000 | |
| Vibrational harmonic frequencies (cm-1): | | | | |
| 49.9836 | 132.9959 | | 208.8814 | |
| 220.4638 | 276.6025 | | 333.4896 | |
| 387.4726 | 457.9630 | | 574.7649 | |
| 736.9075 | 824.4743 | | 863.2161 | |
| 893.7102 | 979.3214 | | 1038.1648 | |
| 1066.9598 | 1099.3899 | | 1148.7969 | |
| 1169.1201 | 1225.0481 | | 1260.0331 | |
| 1281.3590 | 1322.7483 | | 1379.9366 | |
| 1405.1516 | 1428.3420 | | 1493.1740 | |
| 1496.2590 | 1515.7753 | | 1521.8893 | |
| 2817.3488 | 3035.4298 | | 3040.3369 | |
| 3043.5173 | 3091.1190 | | 3109.2203 | |
| 3115.3499 | 3118.0982 | | 3810.5457 | |
| Zero-point correction (Hartree): | 0.127517 | | | |

C4H9O2.mmt

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.23869063
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | | |
|--|-----------|-----------|-----------|--|
| O | -1.122820 | 1.330704 | 0.223676 | |
| C | -0.924291 | 0.105042 | -0.245752 | |
| C | 0.149854 | -0.676950 | 0.585329 | |
| C | 1.522594 | -0.005282 | 0.633784 | |
| C | 2.257471 | 0.044052 | -0.710639 | |
| O | -2.071139 | -0.716445 | -0.345725 | |
| H | -0.490783 | 0.241466 | -1.269285 | |
| H | -0.271892 | -0.786390 | 1.589140 | |
| H | 0.205036 | -1.676972 | 0.142496 | |
| H | 1.410017 | 1.008343 | 1.032997 | |
| H | 2.135932 | -0.558477 | 1.356278 | |
| H | 1.731454 | 0.667241 | -1.441895 | |
| H | 2.367731 | -0.957504 | -1.141868 | |
| H | 3.260194 | 0.466103 | -0.591436 | |
| H | -2.829787 | -0.119054 | -0.276359 | |
| Rotational constants (GHz): | 6.4808300 | 2.0109300 | 1.8660300 | |
| Vibrational harmonic frequencies (cm-1): | | | | |
| 51.4508 | 128.7581 | | 166.1389 | |

| | | |
|-----------|-----------|-----------|
| 205.4258 | 272.5725 | 343.3772 |
| 397.2999 | 464.0930 | 572.1606 |
| 738.4393 | 824.1523 | 864.3019 |
| 896.7662 | 966.8738 | 1031.0520 |
| 1063.9502 | 1096.5702 | 1153.8195 |
| 1179.5438 | 1240.5454 | 1250.6705 |
| 1287.3158 | 1311.4200 | 1368.5213 |
| 1391.9035 | 1429.4917 | 1494.5959 |
| 1496.5415 | 1515.8204 | 1520.5382 |
| 2779.9701 | 3040.2125 | 3042.8681 |
| 3065.5917 | 3086.7001 | 3111.1551 |
| 3114.8449 | 3119.9512 | 3803.0031 |

Zero-point correction (Hartree): 0.127323

C4H9O2.mpm

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.23863153

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 0.729006 | 1.344322 | 0.055307 |
| C | 1.013807 | 0.077648 | 0.318804 |
| C | -0.097298 | -0.881557 | -0.272945 |
| C | -1.499623 | -0.690103 | 0.305938 |
| C | -2.251626 | 0.540515 | -0.210525 |
| O | 2.269959 | -0.378905 | -0.145910 |
| H | 0.974906 | -0.075271 | 1.423031 |
| H | -0.083548 | -0.737279 | -1.358173 |
| H | 0.284423 | -1.886250 | -0.069503 |
| H | -2.076625 | -1.592287 | 0.063339 |
| H | -1.441697 | -0.660768 | 1.402246 |
| H | -2.368265 | 0.497909 | -1.299427 |
| H | -1.714307 | 1.460012 | 0.032644 |
| H | -3.252986 | 0.597602 | 0.228317 |
| H | 2.694826 | 0.393976 | -0.545281 |

Rotational constants (GHz): 7.0263000 2.1338900 1.7759200
 Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 63.0531 | 89.2139 | 144.0319 |
| 215.1033 | 274.3903 | 330.9668 |
| 402.2922 | 445.6860 | 575.3808 |
| 731.6422 | 827.4115 | 835.7249 |
| 908.5412 | 965.1461 | 1032.0089 |
| 1070.6917 | 1106.7762 | 1148.8403 |
| 1186.0613 | 1238.5239 | 1259.1031 |
| 1281.8487 | 1317.2516 | 1367.7072 |
| 1387.1198 | 1427.7958 | 1489.2754 |
| 1495.6843 | 1512.8580 | 1526.4719 |
| 2829.0944 | 3027.8207 | 3045.5198 |
| 3056.0892 | 3072.0492 | 3109.7482 |
| 3122.7217 | 3142.6499 | 3803.1186 |

Zero-point correction (Hartree): 0.127271

C4H9O2.mpp

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.23318892

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 0.671062 | 1.367452 | 0.067783 |
| C | 1.027757 | 0.114380 | 0.310432 |
| C | -0.071425 | -0.872570 | -0.249894 |
| C | -1.475882 | -0.693703 | 0.333423 |
| C | -2.263774 | 0.489340 | -0.236983 |
| O | 2.295028 | -0.192120 | -0.243937 |
| H | 1.043036 | -0.036372 | 1.416255 |
| H | -0.067892 | -0.752382 | -1.337937 |
| H | 0.306437 | -1.878514 | -0.030819 |
| H | -2.031308 | -1.621371 | 0.143086 |
| H | -1.408443 | -0.606120 | 1.426102 |
| H | -2.391266 | 0.387313 | -1.320589 |
| H | -1.746452 | 1.432290 | -0.046692 |
| H | -3.261122 | 0.544187 | 0.211196 |
| H | 2.528237 | -1.096380 | 0.006771 |

Rotational constants (GHz): 7.0488700 2.1291700 1.7806000
 Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 62.8281 | 141.2458 | 208.7865 |
| 228.6507 | 272.1210 | 326.0401 |
| 391.7266 | 441.8262 | 582.9094 |
| 735.7904 | 825.9426 | 841.5683 |
| 909.7159 | 980.5205 | 1039.1738 |
| 1074.2814 | 1108.3148 | 1138.0396 |
| 1182.9827 | 1220.2076 | 1253.3398 |
| 1281.0508 | 1327.9440 | 1386.3354 |
| 1394.3431 | 1429.6637 | 1489.9820 |
| 1497.0416 | 1512.6725 | 1526.9787 |
| 2821.5385 | 3027.3163 | 3044.9296 |

3046.1397 3061.5915 3107.7818
3112.1338 3144.5147 3810.3397
Zero-point correction (Hartree): 0.127551

C4H9O2.mtm

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.23955657
Electronic state : 2-A
Cartesian coordinates (Angs):
O 1.379971 1.276245 -0.276429
C 1.154544 0.080816 0.262292
C -0.238845 -0.496085 -0.146247
C -1.413742 0.374563 0.294455
C -2.762427 -0.203184 -0.146576
O 2.129598 -0.908469 0.001679
H 1.103578 0.262037 1.367702
H -0.218814 -0.616962 -1.234652
H -0.293446 -1.498445 0.290982
H -1.401004 0.480743 1.387509

H -1.284861 1.382608 -0.113571
H -2.925818 -1.202565 0.272077
H -2.820468 -0.288084 -1.237335
H -3.589614 0.433961 0.181400
H 2.916715 -0.432161 -0.299652
Rotational constants (GHz): 8.1472800 1.7523700 1.5364200
Vibrational harmonic frequencies (cm-1):
85.8292 117.0050 172.6250
182.2541 248.3622 316.5729
400.9041 448.6268 571.0479
753.0842 844.3004 862.9792
922.1001 962.0391 1027.0978
1052.7861 1116.0392 1162.9059
1178.8111 1235.9488 1259.0685
1294.1564 1319.5200 1334.4545
1400.5196 1429.3266 1497.8880
1509.4020 1513.8633 1525.1903
2764.8242 3034.0790 3040.3415
3063.1965 3083.6319 3107.1551
3116.4281 3119.7861 3802.5806
Zero-point correction (Hartree): 0.127297

C4H9O2.mtp

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.23411336
Electronic state : 2-A
Cartesian coordinates (Angs):
O 1.334264 1.306646 -0.260517
C 1.175868 0.098879 0.266312
C -0.221591 -0.482905 -0.155272
C -1.406980 0.374805 0.285060
C -2.751617 -0.229379 -0.133040
O 2.225610 -0.781136 -0.093666
H 1.143995 0.228120 1.376047
H -0.194925 -0.598095 -1.243732
H -0.290623 -1.489669 0.276986
H -1.384060 0.497981 1.376081
H -1.295406 1.377454 -0.139156
H -2.898846 -1.223342 0.304599
H -2.818804 -0.333510 -1.221498
H -3.583484 0.402859 0.192249
H 2.069084 -1.634275 0.333528
Rotational constants (GHz): 8.1219200 1.7541200 1.5366300
Vibrational harmonic frequencies (cm-1):
82.2304 120.1699 179.4682
235.3047 247.8281 313.1293
379.6333 450.6494 574.1405
750.5416 840.9572 858.7228
918.9298 974.5041 1032.7990
1053.8663 1116.0656 1146.2688
1182.0806 1229.1859 1261.8058
1275.3400 1323.9475 1358.6110
1407.9409 1428.5137 1496.0834
1508.2219 1513.8545 1524.3865
2805.7267 3035.3953 3036.9980
3041.1033 3089.1478 3102.9629
3117.2077 3117.6146 3811.8902
Zero-point correction (Hartree): 0.127448

C4H9O2.pmm

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.23960796
Electronic state : 2-A
Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 0.889597 | 1.344187 | 0.327909 |
| C | 1.100786 | 0.030251 | 0.341238 |
| C | -0.148762 | -0.787731 | 0.813687 |
| C | -1.320285 | -0.725169 | -0.171145 |
| C | -1.940359 | 0.663699 | -0.329076 |
| O | 1.569961 | -0.530063 | -0.870270 |
| H | 1.871428 | -0.132221 | 1.138815 |
| H | 0.189361 | -1.821468 | 0.936439 |
| H | -0.432920 | -0.401956 | 1.798007 |
| H | -0.979198 | -1.098383 | -1.142277 |
| H | -2.083893 | -1.429931 | 0.184177 |
| H | -1.200270 | 1.386429 | -0.692006 |
| H | -2.326419 | 1.040802 | 0.624305 |
| H | -2.769018 | 0.644995 | -1.044698 |
| H | 1.906191 | 0.212445 | -1.392095 |
| Rotational constants (GHz): | 5.1458700 | 2.5878800 | 2.2657900 |
| Vibrational harmonic frequencies (cm ⁻¹): | | | |
| 71.4984 | 149.4627 | | 208.0274 |
| 216.3637 | 278.1062 | | 343.7384 |
| 398.7540 | 513.3040 | | 626.6247 |
| 737.4849 | 809.9316 | | 844.9508 |
| 912.4021 | 967.9614 | | 1018.2879 |
| 1069.4558 | 1092.4271 | | 1124.3371 |
| 1186.4860 | 1241.7618 | | 1282.3617 |
| 1293.0411 | 1306.9048 | | 1366.2075 |
| 1385.1794 | 1432.3537 | | 1483.9462 |
| 1493.5051 | 1511.9458 | | 1512.4074 |
| 2766.2797 | 3032.5700 | | 3036.4660 |
| 3065.3472 | 3086.7524 | | 3105.5580 |
| 3112.6285 | 3120.4059 | | 3807.1389 |
| Zero-point correction (Hartree): | 0.127606 | | |

C4H9O2.pmp

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.23404148

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 0.833745 | 1.396017 | 0.234940 |
| C | 1.118963 | 0.102409 | 0.320489 |
| C | -0.117760 | -0.706278 | 0.868371 |
| C | -1.293655 | -0.759837 | -0.111334 |
| C | -1.961760 | 0.591625 | -0.367568 |
| O | 1.584370 | -0.422667 | -0.912539 |
| H | 1.911432 | -0.000783 | 1.101544 |
| H | 0.239852 | -1.719802 | 1.089653 |
| H | -0.409968 | -0.247352 | 1.818256 |
| H | -0.943475 | -1.184987 | -1.058250 |
| H | -2.029811 | -1.465709 | 0.295807 |
| H | -1.246559 | 1.306054 | -0.789509 |
| H | -2.356521 | 1.023701 | 0.558485 |
| H | -2.792774 | 0.489020 | -1.073058 |
| H | 1.808174 | -1.354448 | -0.781885 |
| Rotational constants (GHz): | 5.1388500 | 2.5835400 | 2.2718900 |
| Vibrational harmonic frequencies (cm ⁻¹): | | | |
| 69.5626 | 149.3464 | | 214.8488 |
| 252.8644 | 274.5909 | | 335.2017 |
| 402.7447 | 519.1701 | | 614.0888 |
| 729.8536 | 806.7834 | | 843.8133 |
| 916.6714 | 977.2000 | | 1021.7148 |
| 1069.8126 | 1093.4559 | | 1132.3129 |
| 1171.1652 | 1227.1377 | | 1244.5655 |
| 1299.2651 | 1341.1355 | | 1374.3128 |
| 1390.7981 | 1432.2255 | | 1489.4516 |
| 1492.0555 | 1511.7011 | | 1513.0489 |
| 2805.1032 | 3031.3951 | | 3038.3388 |
| 3045.7932 | 3080.3981 | | 3103.5161 |
| 3112.9837 | 3114.9782 | | 3808.2032 |
| Zero-point correction (Hartree): | 0.127695 | | |

C4H9O2.ppm

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.23726129

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 1.444437 | -0.576110 | 1.009260 |
| C | 1.145615 | -0.150008 | -0.214339 |
| C | -0.153168 | -0.801735 | -0.789652 |
| C | -1.390776 | -0.671984 | 0.110230 |
| C | -1.926144 | 0.750464 | 0.299088 |
| O | 1.078168 | 1.253620 | -0.383187 |
| H | 1.978877 | -0.545133 | -0.855711 |
| H | -0.325868 | -0.341167 | -1.768247 |
| H | 0.075192 | -1.859978 | -0.949368 |
| H | -2.176934 | -1.294047 | -0.337353 |
| H | -1.164353 | -1.120095 | 1.084971 |

| | | | | |
|---|-----------|-----------|-----------|-----------|
| H | -2.169676 | 1.211664 | -0.664326 | |
| H | -1.192856 | 1.393234 | 0.790683 | |
| H | -2.837483 | 0.740202 | 0.906128 | |
| H | 1.579096 | 1.634813 | 0.352675 | |
| Rotational constants (GHz): | 5.0507800 | | 2.5542200 | 2.2265800 |
| Vibrational harmonic frequencies (cm-1): | | | | |
| 50.7359 | | 138.1850 | | 213.2471 |
| 237.9082 | | 274.4558 | | 342.0258 |
| 386.7504 | | 502.6726 | | 587.9600 |
| 744.7394 | | 810.9537 | | 868.1011 |
| 889.8936 | | 955.9970 | | 1016.2929 |
| 1059.3427 | | 1093.2324 | | 1153.0935 |
| 1178.8646 | | 1235.3516 | | 1281.9127 |
| 1306.6635 | | 1313.7984 | | 1374.1177 |
| 1387.8604 | | 1433.1088 | | 1482.4318 |
| 1498.2535 | | 1512.0320 | | 1518.6639 |
| 2738.0764 | | 3033.7043 | | 3047.7780 |
| 3060.4511 | | 3076.0994 | | 3110.8512 |
| 3116.0311 | | 3142.5176 | | 3799.0802 |
| Zero-point correction (Hartree): 0.127516 | | | | |

C4H9O2.ppp

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.23206898
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | | |
|---|-----------|-----------|-----------|-----------|
| O | -1.482666 | -0.654363 | -0.943286 | |
| C | -1.171947 | -0.086170 | 0.214712 | |
| C | 0.116192 | -0.750145 | 0.823073 | |
| C | 1.356116 | -0.712047 | -0.081687 | |
| C | 1.951323 | 0.678573 | -0.326571 | |
| O | -1.074815 | 1.325836 | 0.109188 | |
| H | -2.001123 | -0.347277 | 0.919746 | |
| H | 0.318989 | -0.256268 | 1.783094 | |
| H | -0.151149 | -1.788060 | 1.043761 | |
| H | 2.115891 | -1.350925 | 0.386971 | |
| H | 1.105231 | -1.184322 | -1.038258 | |
| H | 2.230601 | 1.159550 | 0.619280 | |
| H | 1.240395 | 1.330698 | -0.837901 | |
| H | 2.857280 | 0.607548 | -0.936887 | |
| H | -0.766370 | 1.676009 | 0.955816 | |
| Rotational constants (GHz): | 5.0584800 | | 2.5728300 | 2.2026800 |
| Vibrational harmonic frequencies (cm-1): | | | | |
| 62.8685 | | 145.1750 | | 218.9402 |
| 242.4372 | | 273.5379 | | 336.8805 |
| 383.9386 | | 509.8446 | | 574.6992 |
| 736.2919 | | 809.6884 | | 870.5807 |
| 892.4489 | | 966.8538 | | 1019.2968 |
| 1061.9067 | | 1091.0021 | | 1154.4864 |
| 1166.0518 | | 1232.8856 | | 1250.6060 |
| 1310.6309 | | 1331.7545 | | 1378.7222 |
| 1391.3876 | | 1430.3398 | | 1489.0538 |
| 1499.8888 | | 1514.2536 | | 1526.1936 |
| 2783.4721 | | 3032.3718 | | 3036.7187 |
| 3038.3034 | | 3080.9767 | | 3101.8057 |
| 3106.0580 | | 3146.6740 | | 3815.1179 |
| Zero-point correction (Hartree): 0.127610 | | | | |

C4H9O2.ptm

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.23905452
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | | |
|--|-----------|-----------|-----------|-----------|
| O | -1.580998 | -1.142394 | -0.408658 | |
| C | -1.245480 | -0.104506 | 0.354518 | |
| C | 0.265111 | -0.113021 | 0.747544 | |
| C | 1.191949 | -0.007669 | -0.467443 | |
| C | 2.666813 | 0.065744 | -0.063309 | |
| O | -1.569354 | 1.171884 | -0.162880 | |
| H | -1.807062 | -0.259985 | 1.312844 | |
| H | 0.419324 | 0.733170 | 1.425824 | |
| H | 0.452778 | -1.035218 | 1.306744 | |
| H | 1.025904 | -0.873225 | -1.119874 | |
| H | 0.915788 | 0.881299 | -1.043896 | |
| H | 2.974121 | -0.825112 | 0.496076 | |
| H | 2.862810 | 0.938747 | 0.569591 | |
| H | 3.312647 | 0.143490 | -0.943746 | |
| H | -2.223844 | 1.017625 | -0.859122 | |
| Rotational constants (GHz): | 6.9148400 | | 1.9193600 | 1.7519200 |
| Vibrational harmonic frequencies (cm-1): | | | | |
| 90.9431 | | 112.7080 | | 176.6588 |
| 217.7237 | | 249.0658 | | 312.3962 |
| 373.5698 | | 517.7305 | | 603.5439 |
| 754.5978 | | 812.2273 | | 854.5650 |
| 907.4805 | | 961.1465 | | 1020.8707 |

| | | |
|-----------|-----------|-----------|
| 1052.6104 | 1090.7565 | 1149.7996 |
| 1186.5068 | 1248.5510 | 1281.0715 |
| 1299.4552 | 1320.0268 | 1336.0907 |
| 1393.3874 | 1427.9427 | 1489.0027 |
| 1509.7146 | 1513.2796 | 1523.4960 |
| 2758.8983 | 3037.7658 | 3048.4178 |
| 3062.2842 | 3087.1100 | 3106.0966 |
| 3113.5035 | 3121.3842 | 3804.6141 |

Zero-point correction (Hartree): 0.127411

C4H9O2.ptp

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.23340563
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -1.546914 | -1.184373 | -0.370415 |
| C | -1.271725 | -0.095941 | 0.339322 |
| C | 0.245465 | -0.093138 | 0.745083 |
| C | 1.185140 | -0.033323 | -0.462711 |
| C | 2.655303 | 0.071952 | -0.048480 |
| O | -1.637954 | 1.092068 | -0.344266 |
| H | -1.846604 | -0.177698 | 1.293933 |
| H | 0.405780 | 0.772477 | 1.401840 |
| H | 0.427731 | -0.992583 | 1.341727 |
| H | 1.030859 | -0.928251 | -1.076028 |
| H | 0.905699 | 0.821841 | -1.087116 |
| H | 2.963586 | -0.788083 | 0.556565 |
| H | 2.840235 | 0.976023 | 0.543438 |
| H | 3.308924 | 0.111769 | -0.925497 |
| H | -1.442360 | 1.845648 | 0.229307 |

Rotational constants (GHz): 6.8336800 1.9302600 1.7560400
 Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 92.2495 | 112.6428 | 189.4496 |
| 240.4477 | 254.0958 | 310.1728 |
| 361.2086 | 527.5244 | 586.2118 |
| 753.6455 | 800.6574 | 856.5028 |
| 910.2103 | 972.2928 | 1022.8108 |
| 1053.5645 | 1091.2054 | 1155.0355 |
| 1167.9030 | 1226.3727 | 1256.6338 |
| 1310.1294 | 1327.6099 | 1360.9298 |
| 1398.7423 | 1428.0833 | 1495.2284 |
| 1508.6648 | 1512.7904 | 1523.7694 |
| 2806.2318 | 3031.8390 | 3037.3481 |
| 3058.5395 | 3085.7740 | 3099.6786 |
| 3113.9689 | 3117.5581 | 3809.7866 |

Zero-point correction (Hartree): 0.127503

C4H9O2.tmm

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.23729093
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -2.244720 | -0.422441 | -0.173886 |
| C | -1.059783 | -0.025672 | 0.280253 |
| C | 0.080679 | -0.938414 | -0.289482 |
| C | 1.472444 | -0.688543 | 0.310885 |
| C | 2.196232 | 0.567519 | -0.185097 |
| O | -0.751414 | 1.337088 | 0.057055 |
| H | -1.070012 | -0.213298 | 1.384510 |
| H | -0.239166 | -1.965454 | -0.092808 |
| H | 0.090617 | -0.790844 | -1.374763 |
| H | 1.396581 | -0.669695 | 1.406362 |
| H | 2.082646 | -1.568778 | 0.069517 |
| H | 1.646943 | 1.474344 | 0.072843 |
| H | 2.310686 | 0.545572 | -1.274825 |
| H | 3.198301 | 0.629083 | 0.252177 |
| H | -1.584963 | 1.752553 | -0.207720 |

Rotational constants (GHz): 6.5892200 2.2307100 1.8049500
 Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 45.9198 | 104.0620 | 147.4571 |
| 223.0027 | 283.7046 | 322.8138 |
| 394.1978 | 468.4656 | 563.1531 |
| 734.9554 | 801.1194 | 883.1579 |
| 899.8082 | 969.8460 | 1043.7219 |
| 1076.0628 | 1087.8888 | 1157.7552 |
| 1184.3119 | 1239.0685 | 1281.0382 |
| 1291.6932 | 1311.8204 | 1354.7343 |
| 1384.4938 | 1430.4582 | 1485.5490 |
| 1497.3063 | 1511.9121 | 1526.0845 |
| 2776.8900 | 3026.6173 | 3045.8022 |
| 3055.2729 | 3071.1176 | 3107.5160 |
| 3122.4426 | 3154.9207 | 3799.8730 |

Zero-point correction (Hartree): 0.127272

C4H9O2.tmp

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.23042762
Electronic state : 2-A
Cartesian coordinates (Angs):
O -2.239669 -0.454561 0.016423
C -1.034800 0.038362 0.287993
C 0.036450 -0.922747 -0.355086
C 1.467351 -0.780081 0.185926
C 2.161343 0.571785 -0.024677
O -0.900837 1.371205 -0.170596
H -0.885838 -0.010308 1.393513
H -0.310286 -1.944869 -0.182229
H 0.002583 -0.731188 -1.432493
H 1.480070 -1.035892 1.253497
H 2.062981 -1.555207 -0.312354
H 1.782757 1.349480 0.649926
H 2.050297 0.928493 -1.053825
H 3.232123 0.488144 0.185179
H -0.072705 1.734278 0.167235
Rotational constants (GHz): 6.3645700 2.2650800 1.7981200
Vibrational harmonic frequencies (cm-1):
48.5715 120.5790 183.2884
251.6154 283.2033 302.6034
389.3591 471.5963 570.1498
732.1126 779.3146 889.0593
897.9148 979.7261 1046.6579
1076.6518 1084.5230 1144.2119
1172.6134 1217.6830 1262.3040
1290.0173 1354.1955 1367.7383
1386.2241 1429.3403 1486.3564
1497.0620 1512.1336 1530.3330
2818.1102 3032.4441 3034.1274
3061.1374 3074.9414 3099.5283
3121.7141 3128.1261 3837.3903
Zero-point correction (Hartree): 0.127497

C4H9O2.tmt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.23729102
Electronic state : 2-A
Cartesian coordinates (Angs):
O -2.245628 -0.422899 -0.170887
C -1.059068 -0.025561 0.279211
C 0.080784 -0.937831 -0.290912
C 1.472736 -0.689554 0.309701
C 2.196314 0.568113 -0.182558
O -0.751351 1.336821 0.053460
H -1.068523 -0.212292 1.383856
H -0.239448 -1.964958 -0.095296
H 0.090928 -0.789250 -1.376069
H 1.397123 -0.674020 1.405264
H 2.083041 -1.568944 0.065574
H 1.647430 1.474202 0.078828
H 2.309917 0.549937 -1.272437
H 3.198720 0.628018 0.254175
H -1.587951 1.754930 -0.197132
Rotational constants (GHz): 6.5918500 2.2304900 1.8043700
Vibrational harmonic frequencies (cm-1):
46.9028 109.4797 148.5839
223.2416 284.1569 322.5636
393.8829 468.4821 563.7567
735.3164 801.2624 883.3768
899.8988 970.4240 1043.5479
1076.2366 1087.5139 1157.5998
1184.2129 1238.7306 1281.5704
1291.8753 1311.9249 1354.9656
1384.6268 1430.5375 1485.5140
1497.3310 1511.9506 1526.0234
2774.5040 3026.5738 3045.8406
3055.2155 3071.0564 3107.5616
3122.3452 3154.8233 3799.8737
Zero-point correction (Hartree): 0.127289

C4H9O2.tpm

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.23895620
Electronic state : 2-A
Cartesian coordinates (Angs):
O 2.076185 -0.693156 -0.390325
C 0.946098 -0.003671 -0.293085
C -0.133632 -0.829379 0.489635
C -1.467897 -0.091053 0.640187
C -2.191561 0.191129 -0.678982
O 1.053905 1.279048 0.295763
H 0.554215 0.112500 -1.334346

| | | | | |
|--|-----------|-----------|-----------|-----------|
| H | -0.257060 | -1.778033 | -0.041926 | |
| H | 0.297514 | -1.043990 | 1.472233 | |
| H | -2.109118 | -0.709381 | 1.282026 | |
| H | -1.294185 | 0.845770 | 1.178603 | |
| H | -2.359305 | -0.729180 | -1.250327 | |
| H | -1.623755 | 0.882019 | -1.311619 | |
| H | -3.167743 | 0.651233 | -0.496439 | |
| H | 2.000661 | 1.479771 | 0.311754 | |
| Rotational constants (GHz): | 6.2433700 | | 2.1206500 | 1.9305000 |
| Vibrational harmonic frequencies (cm-1): | | | | |
| 61.9967 | | 103.4968 | | 147.5140 |
| 208.2898 | | 271.7146 | | 332.0296 |
| 415.6914 | | 486.8416 | | 556.1653 |
| 735.3605 | | 799.9532 | | 865.8113 |
| 911.9150 | | 969.4132 | | 1032.6381 |
| 1065.6539 | | 1114.1784 | | 1141.8238 |
| 1190.0756 | | 1248.4128 | | 1284.1043 |
| 1291.4724 | | 1295.1730 | | 1351.8310 |
| 1382.7873 | | 1430.9035 | | 1485.7681 |
| 1496.1800 | | 1513.1818 | | 1519.6658 |
| 2795.0611 | | 3037.0826 | | 3039.3743 |
| 3068.0844 | | 3092.5074 | | 3111.3436 |
| 3114.0237 | | 3125.2099 | | 3805.6423 |
| Zero-point correction (Hartree): | 0.127346 | | | |

C4H9O2.tpp

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.23313948
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | | |
|--|-----------|-----------|-----------|-----------|
| O | 2.091485 | -0.673683 | -0.374867 | |
| C | 0.970965 | 0.034679 | -0.309293 | |
| C | -0.096026 | -0.854941 | 0.437212 | |
| C | -1.444045 | -0.152860 | 0.638507 | |
| C | -2.194430 | 0.182007 | -0.654479 | |
| O | 1.157576 | 1.278971 | 0.344438 | |
| H | 0.592294 | 0.197295 | -1.344051 | |
| H | -0.213621 | -1.776261 | -0.141197 | |
| H | 0.343008 | -1.114553 | 1.404649 | |
| H | -2.066944 | -0.814003 | 1.253842 | |
| H | -1.290944 | 0.753374 | 1.236862 | |
| H | -2.358531 | -0.715331 | -1.260932 | |
| H | -1.650457 | 0.902035 | -1.277411 | |
| H | -3.172991 | 0.620905 | -0.436750 | |
| H | 0.406901 | 1.850922 | 0.136736 | |
| Rotational constants (GHz): | 6.1796400 | | 2.1259900 | 1.9160100 |
| Vibrational harmonic frequencies (cm-1): | | | | |
| 68.9702 | | 127.7982 | | 195.0950 |
| 212.4959 | | 287.6977 | | 318.0564 |
| 415.1858 | | 490.2529 | | 555.3571 |
| 732.5648 | | 797.4104 | | 863.1809 |
| 910.6841 | | 977.3540 | | 1040.0032 |
| 1061.6123 | | 1105.6694 | | 1153.1230 |
| 1168.8469 | | 1222.8825 | | 1262.4755 |
| 1291.2792 | | 1346.7974 | | 1365.1623 |
| 1386.7828 | | 1433.4238 | | 1485.6252 |
| 1506.5516 | | 1515.2703 | | 1518.8542 |
| 2848.9548 | | 3037.9106 | | 3042.6199 |
| 3067.2109 | | 3077.9319 | | 3103.9589 |
| 3118.1770 | | 3128.6079 | | 3820.0837 |
| Zero-point correction (Hartree): | 0.127718 | | | |

C4H9O2.ttm

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.23942518
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | | |
|--|-----------|-----------|-----------|-----------|
| O | -2.111607 | -0.952363 | -0.071167 | |
| C | -1.181068 | -0.073490 | 0.286178 | |
| C | 0.238588 | -0.575662 | -0.146961 | |
| C | 1.357382 | 0.365133 | 0.305796 | |
| C | 2.735355 | -0.118921 | -0.157665 | |
| O | -1.367119 | 1.245848 | -0.191487 | |
| H | -1.169404 | -0.049187 | 1.404686 | |
| H | 0.367404 | -1.579679 | 0.268692 | |
| H | 0.220931 | -0.659870 | -1.238754 | |
| H | 1.158373 | 1.367745 | -0.084873 | |
| H | 1.343845 | 0.446928 | 1.400788 | |
| H | 2.789005 | -0.177209 | -1.250390 | |
| H | 2.965223 | -1.113891 | 0.239443 | |
| H | 3.522827 | 0.563630 | 0.177297 | |
| H | -2.269944 | 1.271294 | -0.539755 | |
| Rotational constants (GHz): | 7.8659300 | | 1.8067600 | 1.5684600 |
| Vibrational harmonic frequencies (cm-1): | | | | |
| 93.4056 | | 96.5562 | | 128.2502 |

| | | |
|-----------|-----------|-----------|
| 192.7990 | 248.3816 | 322.8123 |
| 377.4616 | 488.4447 | 556.6091 |
| 755.9324 | 794.4607 | 873.0351 |
| 924.2031 | 965.8654 | 1040.6718 |
| 1062.2026 | 1111.4650 | 1155.2731 |
| 1191.3667 | 1252.8985 | 1282.0298 |
| 1295.1659 | 1299.1312 | 1331.6141 |
| 1388.0400 | 1426.1692 | 1491.2216 |
| 1508.8451 | 1512.3516 | 1523.1706 |
| 2791.5502 | 3035.5262 | 3039.9547 |
| 3064.3367 | 3092.7964 | 3109.8665 |
| 3115.2753 | 3126.3109 | 3805.1163 |

Zero-point correction (Hartree): 0.127283

C4H9O2.ttp

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.23394807

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -2.087546 | -0.981416 | -0.075936 |
| C | -1.207130 | -0.057728 | 0.292702 |
| C | 0.218887 | -0.589120 | -0.114646 |
| C | 1.339606 | 0.390795 | 0.244240 |
| C | 2.723521 | -0.152287 | -0.127625 |
| O | -1.480123 | 1.205668 | -0.289260 |
| H | -1.209743 | 0.023366 | 1.404291 |
| H | 0.363958 | -1.552038 | 0.384056 |
| H | 0.195219 | -0.766111 | -1.194381 |
| H | 1.169857 | 1.339107 | -0.279422 |
| H | 1.309133 | 0.609065 | 1.320780 |
| H | 2.792931 | -0.354028 | -1.201755 |
| H | 2.939192 | -1.086758 | 0.401311 |
| H | 3.508601 | 0.565927 | 0.128846 |
| H | -0.977103 | 1.877487 | 0.189812 |

Rotational constants (GHz): 7.6675200 1.8211500 1.5678900

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 92.2415 | 110.6872 | 183.9532 |
| 218.3128 | 247.6896 | 324.3689 |
| 360.6459 | 494.4400 | 558.5880 |
| 759.7121 | 790.4259 | 875.6161 |
| 926.9914 | 974.3146 | 1043.4376 |
| 1067.1291 | 1104.8624 | 1157.5479 |
| 1179.5485 | 1227.6490 | 1272.1477 |
| 1294.0783 | 1328.5662 | 1374.8470 |
| 1384.6789 | 1427.3752 | 1491.3958 |
| 1510.1602 | 1511.7319 | 1523.8091 |
| 2840.5409 | 3024.0718 | 3043.8698 |

| | | |
|-----------|-----------|-----------|
| 3069.0163 | 3070.8406 | 3114.5253 |
| 3117.9301 | 3128.0416 | 3818.2920 |

Zero-point correction (Hartree): 0.127678

C4H9O2.1-5Hshift.a.m

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.20967775

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| C | -1.729973 | -0.688263 | 0.505111 |
| C | -1.543293 | 0.615618 | -0.239503 |
| C | -0.115990 | 1.127353 | -0.022113 |
| C | 0.949083 | 0.053873 | -0.397503 |
| O | 0.443792 | -1.234867 | -0.468395 |
| H | -1.675736 | -0.618613 | 1.593855 |
| H | -2.529840 | -1.346159 | 0.162051 |
| H | -2.259029 | 1.372773 | 0.113955 |
| H | -1.739480 | 0.466076 | -1.307236 |
| H | 0.043087 | 1.350258 | 1.038758 |
| H | 0.073635 | 2.049621 | -0.578869 |
| O | 1.982562 | 0.186759 | 0.562238 |
| H | 1.349852 | 0.262316 | -1.407606 |
| H | -0.625407 | -1.254582 | 0.145002 |
| H | 2.593119 | -0.548316 | 0.413391 |

Rotational constants (GHz): 5.9511900 2.6632700 2.1910000

Vibrational harmonic frequencies (cm-1):

| | | |
|------------|-----------|-----------|
| i1578.5068 | 44.3675 | 245.6350 |
| 305.1067 | 382.8313 | 447.6199 |
| 470.4787 | 521.8310 | 602.9916 |
| 632.2109 | 816.3994 | 865.3213 |
| 908.4142 | 926.0184 | 1028.4785 |
| 1046.5776 | 1078.5973 | 1105.2077 |
| 1131.5192 | 1196.7335 | 1228.7057 |
| 1238.7716 | 1273.5197 | 1337.4908 |
| 1358.6219 | 1378.3619 | 1397.6714 |
| 1468.0614 | 1484.7969 | 1505.2402 |
| 1554.3494 | 2934.9161 | 3016.5189 |

| | | |
|-----------|-----------|-----------|
| 3065.2730 | 3081.9345 | 3096.5232 |
| 3117.9761 | 3180.4234 | 3808.7709 |

Zero-point correction (Hartree): 0.123669

C4H9O2.1-5Hshift.a.p

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.20312855

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| C | 1.846838 | -0.620377 | -0.403890 |
| C | 1.520430 | 0.700015 | 0.260151 |
| C | 0.074275 | 1.075079 | -0.074304 |
| C | -0.937628 | -0.022016 | 0.382916 |
| O | -0.410308 | -1.291277 | 0.301558 |
| H | 1.918451 | -0.590623 | -1.493278 |
| H | 2.627461 | -1.229506 | 0.053865 |
| H | 2.197850 | 1.492274 | -0.091411 |
| H | 1.656826 | 0.623595 | 1.345220 |
| H | -0.045485 | 1.158001 | -1.161033 |
| H | -0.212384 | 2.038177 | 0.362715 |
| O | -2.100873 | 0.033089 | -0.436729 |
| H | -1.224290 | 0.162946 | 1.436992 |
| H | 0.732266 | -1.223366 | -0.155179 |
| H | -2.584737 | 0.837801 | -0.205766 |

Rotational constants (GHz): 6.3233300 2.5741700 2.0821600

Vibrational harmonic frequencies (cm-1):

| | | |
|------------|-----------|-----------|
| i1617.4276 | 46.1797 | 158.7904 |
| 245.8037 | 359.1498 | 416.0378 |
| 460.8629 | 509.8461 | 573.7235 |
| 637.6115 | 814.0658 | 874.6621 |
| 920.2063 | 929.2094 | 1022.8786 |
| 1041.7144 | 1078.6800 | 1098.7030 |
| 1126.6190 | 1174.9501 | 1216.7913 |
| 1246.4806 | 1270.0738 | 1329.8697 |
| 1335.7360 | 1368.2800 | 1425.9153 |
| 1469.0123 | 1487.2173 | 1506.6970 |
| 1553.6207 | 2916.0165 | 3016.8029 |
| 3051.4092 | 3076.6825 | 3097.7473 |
| 3102.7153 | 3181.8097 | 3807.4471 |

Zero-point correction (Hartree): 0.122907

C4H9O2.1-5Hshift.a.t

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.20906867

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| C | 1.885826 | 0.660935 | 0.251332 |
| C | 1.522318 | -0.732212 | -0.223461 |
| C | 0.082759 | -1.051531 | 0.194016 |
| C | -0.908517 | -0.011138 | -0.381571 |
| O | -0.468318 | 1.294239 | -0.133853 |
| H | 2.054521 | 0.756402 | 1.326366 |
| H | 2.626647 | 1.207083 | -0.334836 |
| H | 2.211053 | -1.477945 | 0.198565 |
| H | 1.617821 | -0.797019 | -1.314101 |
| H | -0.004494 | -1.019008 | 1.288798 |
| H | -0.233820 | -2.048164 | -0.128573 |
| O | -2.198196 | -0.178310 | 0.166738 |
| H | -1.038351 | -0.181936 | -1.462398 |
| H | 0.764707 | 1.247311 | 0.058932 |
| H | -2.160286 | 0.189519 | 1.062265 |

Rotational constants (GHz): 6.5705000 2.5391500 2.0206200

Vibrational harmonic frequencies (cm-1):

| | | |
|------------|-----------|-----------|
| i1541.6206 | 87.4811 | 243.3201 |
| 265.4919 | 357.3108 | 384.3835 |
| 464.9083 | 501.4973 | 536.9204 |
| 656.5386 | 817.1109 | 878.6802 |
| 915.3250 | 926.1251 | 1020.9679 |
| 1061.1458 | 1073.0290 | 1096.7848 |
| 1125.2701 | 1184.1632 | 1233.0448 |
| 1240.1313 | 1301.5176 | 1336.2755 |
| 1361.3694 | 1374.2814 | 1433.2342 |
| 1468.3372 | 1488.1697 | 1500.3818 |
| 1544.5488 | 2997.9256 | 3023.5985 |
| 3037.3429 | 3074.7489 | 3095.3388 |
| 3110.2055 | 3176.7062 | 3785.5970 |

Zero-point correction (Hartree): 0.123429

C4H9O2.1-5Hshift.b.m

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.21628582

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|----------|----------|----------|
| C | 1.699419 | 0.707120 | 0.301653 |
|---|----------|----------|----------|

| | | | |
|---|-----------|-----------|-----------|
| C | 1.284775 | -0.749666 | 0.283462 |
| C | 0.135246 | -0.974596 | -0.716464 |
| C | -1.007315 | 0.006410 | -0.396781 |
| O | -0.580765 | 1.321642 | -0.411881 |
| H | 2.307231 | 1.036638 | -0.544052 |
| H | 2.056816 | 1.105034 | 1.252590 |
| H | 2.135565 | -1.388500 | 0.005086 |
| H | 0.950337 | -1.057235 | 1.277572 |
| H | 0.471309 | -0.781328 | -1.741339 |
| H | -0.238214 | -2.001713 | -0.668264 |
| H | -1.781029 | -0.059335 | -1.186266 |
| O | -1.553705 | -0.378780 | 0.854082 |
| H | 0.555272 | 1.283072 | 0.063643 |
| H | -2.054274 | 0.384860 | 1.172199 |
| Rotational constants (GHz): 5.0291000 3.0095800 2.5232000 | | | |
| Vibrational harmonic frequencies (cm-1): | | | |
| i1554.0641 | 122.1108 | | 233.5330 |
| 307.6305 | 391.5982 | | 409.9484 |
| 469.8142 | 527.0603 | | 597.4109 |
| 710.8099 | 836.1725 | | 855.1476 |
| 902.4668 | 931.1963 | | 1005.3290 |
| 1045.1543 | 1068.4770 | | 1101.1053 |
| 1147.2724 | 1196.6163 | | 1210.0876 |
| 1241.4923 | 1261.1692 | | 1346.9240 |
| 1359.1030 | 1373.8312 | | 1387.3669 |
| 1465.1687 | 1484.0997 | | 1498.9169 |
| 1546.7936 | 2932.1326 | | 3019.8180 |
| 3066.4308 | 3094.6506 | | 3110.3960 |
| 3123.8770 | 3178.2354 | | 3814.0657 |
| Zero-point correction (Hartree): 0.123872 | | | |

C4H9O2.1-5Hshift.b.p

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.20990013

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| C | -1.725699 | 0.635663 | -0.332523 |
| C | -1.254128 | -0.801099 | -0.245991 |
| C | -0.099586 | -0.927091 | 0.764058 |
| C | 1.010881 | 0.084078 | 0.384943 |
| O | 0.524092 | 1.364843 | 0.359270 |
| H | -2.354673 | 0.976590 | 0.492756 |
| H | -2.086328 | 0.976521 | -1.303711 |
| H | -2.077648 | -1.463023 | 0.058552 |
| H | -0.903183 | -1.137079 | -1.225646 |
| H | -0.444748 | -0.691175 | 1.777607 |
| H | 0.302232 | -1.947423 | 0.783999 |
| H | 1.799845 | 0.066824 | 1.161784 |
| O | 1.575653 | -0.226486 | -0.887215 |
| H | -0.602423 | 1.265621 | -0.113518 |
| H | 1.980160 | -1.103014 | -0.831182 |
| Rotational constants (GHz): 5.0227200 2.9936800 2.5265400 | | | |
| Vibrational harmonic frequencies (cm-1): | | | |
| i1579.0997 | 122.1978 | | 233.1893 |
| 260.5696 | 397.6338 | | 414.4053 |
| 468.4308 | 519.7173 | | 596.4638 |
| 702.6391 | 834.4011 | | 855.6796 |
| 907.4025 | 934.8223 | | 1002.0827 |
| 1051.0867 | 1065.6704 | | 1106.0083 |
| 1148.9255 | 1196.4912 | | 1200.6352 |
| 1239.0424 | 1255.6052 | | 1299.7782 |
| 1353.4641 | 1376.4284 | | 1399.5543 |
| 1464.8864 | 1485.3830 | | 1502.1516 |
| 1562.3182 | 2929.6651 | | 3020.3931 |
| 3049.7510 | 3089.5027 | | 3097.0882 |
| 3111.4410 | 3182.2108 | | 3806.3142 |
| Zero-point correction (Hartree): 0.123576 | | | |

C4H9O2.mmm

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.21504878

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -1.133435 | -1.482025 | -0.627825 |
| C | -0.937911 | -0.802205 | 0.538896 |
| C | -0.224406 | 0.564250 | 0.402268 |
| C | 1.040903 | 0.501735 | -0.451255 |
| C | 2.161711 | -0.350746 | 0.150784 |
| H | -1.872984 | -0.696922 | 1.125919 |
| H | -0.291034 | -1.473018 | 1.145038 |
| O | -1.086897 | 1.513146 | -0.215716 |
| H | 0.038654 | 0.890554 | 1.425175 |
| H | 0.761740 | 0.120835 | -1.438444 |
| H | 1.384633 | 1.532492 | -0.589663 |
| H | 1.886125 | -1.409283 | 0.205517 |

| | | | | |
|---|-----------|-----------|-----------|--|
| H | 2.425477 | -0.017800 | 1.161724 | |
| H | 3.065743 | -0.285603 | -0.462046 | |
| H | -1.877480 | 1.611572 | 0.330951 | |
| Rotational constants (GHz): | 4.1406500 | 2.9377900 | 2.0503000 | |
| Vibrational harmonic frequencies (cm ⁻¹): | | | | |
| 56.4076 | 140.2561 | | 220.4406 | |
| 245.1204 | 288.7145 | | 293.9421 | |
| 383.3143 | 460.3223 | | 598.5192 | |
| 762.0216 | 791.4525 | | 852.3866 | |
| 925.4197 | 1028.5935 | | 1043.5700 | |
| 1070.7308 | 1076.4814 | | 1134.8682 | |
| 1169.5203 | 1203.5465 | | 1260.6092 | |
| 1306.5524 | 1358.9891 | | 1385.9283 | |
| 1399.2732 | 1428.3226 | | 1453.4112 | |
| 1500.6947 | 1515.1439 | | 1522.1646 | |
| 2891.5063 | 2928.2240 | | 2952.6705 | |
| 3041.8196 | 3066.8578 | | 3098.6639 | |
| 3119.4604 | 3122.6322 | | 3810.8382 | |
| Zero-point correction (Hartree): 0.127371 | | | | |

C4H9O2.mmp

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.21606732
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | | |
|---|-----------|-----------|-----------|--|
| O | -1.126213 | -1.477335 | -0.631557 | |
| C | -0.951926 | -0.788665 | 0.538461 | |
| C | -0.227709 | 0.559077 | 0.418251 | |
| C | 1.034972 | 0.488116 | -0.447718 | |
| C | 2.157610 | -0.373298 | 0.140798 | |
| H | -1.928642 | -0.643507 | 1.037278 | |
| H | -0.395664 | -1.468780 | 1.215652 | |
| O | -1.192583 | 1.450933 | -0.134917 | |
| H | 0.047622 | 0.878300 | 1.440673 | |
| H | 0.741601 | 0.113479 | -1.433517 | |
| H | 1.404727 | 1.513610 | -0.589663 | |
| H | 1.870657 | -1.428334 | 0.197051 | |
| H | 2.431378 | -0.045169 | 1.150509 | |
| H | 3.057132 | -0.315226 | -0.479392 | |
| H | -0.756129 | 2.295471 | -0.305549 | |
| Rotational constants (GHz): | 4.1757700 | 2.9339000 | 2.0513600 | |
| Vibrational harmonic frequencies (cm ⁻¹): | | | | |
| 70.2314 | 141.0281 | | 214.7287 | |
| 237.5064 | 268.2351 | | 300.5213 | |
| 360.8946 | 451.2718 | | 519.5293 | |
| 657.8197 | 777.8761 | | 851.6286 | |
| 937.1417 | 1019.3601 | | 1039.9288 | |
| 1070.0320 | 1100.9825 | | 1148.9909 | |
| 1193.7239 | 1249.1199 | | 1289.8123 | |
| 1340.1886 | 1359.9905 | | 1371.4971 | |
| 1417.8613 | 1424.9706 | | 1445.2474 | |
| 1498.5611 | 1514.7279 | | 1520.9004 | |
| 2919.5845 | 2949.0040 | | 2961.8249 | |
| 3024.2860 | 3043.6816 | | 3096.5074 | |
| 3115.8944 | 3121.3859 | | 3817.3843 | |
| Zero-point correction (Hartree): 0.127222 | | | | |

C4H9O2.mmt

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.22065226
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | | |
|---|-----------|-----------|-----------|--|
| O | -1.575759 | -1.100388 | -0.621391 | |
| C | -0.887266 | -0.834620 | 0.533159 | |
| C | -0.117490 | 0.504540 | 0.453238 | |
| C | 1.109666 | 0.422343 | -0.471218 | |
| C | 2.247913 | -0.460985 | 0.051217 | |
| H | -1.683089 | -0.716774 | 1.300080 | |
| H | -0.275225 | -1.692126 | 0.861470 | |
| O | -1.018432 | 1.508674 | 0.022730 | |
| H | 0.207357 | 0.785290 | 1.463751 | |
| H | 0.775631 | 0.068246 | -1.456237 | |
| H | 1.467803 | 1.447860 | -0.612752 | |
| H | 1.952930 | -1.512623 | 0.133056 | |
| H | 2.583534 | -0.132072 | 1.041614 | |
| H | 3.111379 | -0.418079 | -0.619502 | |
| H | -1.503731 | 1.116320 | -0.720573 | |
| Rotational constants (GHz): | 4.7877100 | 2.6186900 | 2.0122100 | |
| Vibrational harmonic frequencies (cm ⁻¹): | | | | |
| 81.4849 | 140.1994 | | 233.9080 | |
| 249.4301 | 277.7032 | | 385.8961 | |
| 446.3865 | 464.1532 | | 658.8267 | |
| 766.3756 | 802.8832 | | 850.4267 | |
| 930.1997 | 1037.3003 | | 1053.4749 | |
| 1075.9383 | 1087.8107 | | 1129.1650 | |

| | | |
|-----------|-----------|-----------|
| 1155.0581 | 1239.5905 | 1280.2390 |
| 1319.2784 | 1352.5155 | 1382.1025 |
| 1400.3844 | 1429.0509 | 1437.0139 |
| 1501.3762 | 1515.8386 | 1520.1637 |
| 2897.1617 | 2990.5173 | 3032.9795 |
| 3042.8486 | 3051.5354 | 3086.4976 |
| 3112.0552 | 3119.6672 | 3751.0544 |

Zero-point correction (Hartree): 0.128235

C4H9O2.mpm

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.21494462

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -1.200962 | -1.301812 | -0.484661 |
| C | -1.411141 | -0.339900 | 0.434026 |
| C | -0.219072 | 0.727291 | 0.443465 |
| C | 1.146776 | 0.108250 | 0.738667 |
| C | 1.721212 | -0.748471 | -0.391740 |
| H | -2.312977 | 0.262790 | 0.203914 |
| H | -1.481546 | -0.711482 | 1.474164 |
| O | -0.130066 | 1.442242 | -0.761182 |
| H | -0.503381 | 1.387914 | 1.280569 |
| H | 1.830223 | 0.939180 | 0.955445 |
| H | 1.062625 | -0.476708 | 1.662464 |
| H | 1.832640 | -0.160087 | -1.305514 |
| H | 1.060957 | -1.593466 | -0.610858 |
| H | 2.703925 | -1.141843 | -0.112025 |
| H | -0.970891 | 1.887243 | -0.927923 |

Rotational constants (GHz): 4.1529400 3.1266400 2.4020100

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 81.3537 | 140.6400 | 221.7858 |
| 242.6201 | 279.5978 | 316.3808 |
| 367.7587 | 468.3364 | 642.5117 |
| 727.7674 | 804.1171 | 806.8903 |
| 865.6013 | 976.0874 | 1036.6311 |
| 1078.2653 | 1107.5321 | 1147.1652 |
| 1217.0397 | 1248.7046 | 1298.4305 |
| 1303.5656 | 1379.3025 | 1386.6824 |
| 1414.2232 | 1437.3787 | 1487.3721 |
| 1505.6850 | 1521.0244 | 1541.5406 |
| 2901.8873 | 2950.7959 | 2970.9242 |
| 3042.0621 | 3051.2363 | 3080.4938 |
| 3120.3780 | 3143.6673 | 3819.2870 |

Zero-point correction (Hartree): 0.127880

C4H9O2.mpp

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.21477593

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -1.327258 | -1.249795 | -0.458082 |
| C | -1.354360 | -0.250896 | 0.471305 |
| C | -0.184605 | 0.747995 | 0.447217 |
| C | 1.188250 | 0.102406 | 0.702136 |
| C | 1.657992 | -0.875896 | -0.379272 |
| H | -2.275064 | 0.321886 | 0.227445 |
| H | -1.511266 | -0.638563 | 1.496444 |
| O | -0.249556 | 1.421724 | -0.802510 |
| H | -0.382614 | 1.454108 | 1.274639 |
| H | 1.922067 | 0.915902 | 0.804141 |
| H | 1.161379 | -0.392777 | 1.682011 |
| H | 1.650477 | -0.399592 | -1.363314 |
| H | 1.005185 | -1.751111 | -0.440325 |
| H | 2.675588 | -1.221067 | -0.169690 |
| H | 0.525087 | 1.994125 | -0.874933 |

Rotational constants (GHz): 4.1191900 3.1159000 2.3845900

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 96.0101 | 139.0992 | 215.4555 |
| 231.1828 | 267.8470 | 299.9099 |
| 354.7796 | 473.9333 | 727.5403 |
| 747.0373 | 783.8576 | 824.4158 |
| 922.0837 | 1001.6648 | 1064.1895 |
| 1078.8318 | 1096.9257 | 1124.4589 |
| 1184.4408 | 1217.0830 | 1293.0190 |
| 1330.0365 | 1360.3768 | 1386.2058 |
| 1397.7574 | 1431.5901 | 1441.0976 |
| 1495.8530 | 1508.2580 | 1517.6340 |
| 2898.4310 | 2944.8268 | 2954.5727 |
| 3014.8729 | 3053.7959 | 3056.9630 |
| 3123.6087 | 3135.5276 | 3817.4162 |

Zero-point correction (Hartree): 0.127606

C4H9O2.mpt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.22148955
Electronic state : 2-A
Cartesian coordinates (Angs):
O -1.318199 -1.172608 -0.438173
C -1.231790 -0.346887 0.646662
C -0.177978 0.780031 0.434326
C 1.258384 0.258418 0.628937
C 1.685522 -0.801894 -0.388084
H -2.219755 0.159026 0.690057
H -1.099843 -0.887145 1.599841
O -0.379774 1.352930 -0.840382
H -0.368329 1.567390 1.174623
H 1.928750 1.123653 0.560773
H 1.353036 -0.132173 1.651093
H 1.666173 -0.395884 -1.403774
H 1.026139 -1.678572 -0.366497
H 2.703561 -1.148738 -0.185255
H -0.610776 0.611864 -1.423463
Rotational constants (GHz): 4.3087000 3.0594800 2.4889600
Vibrational harmonic frequencies (cm-1):
111.3629 131.3788 224.3633
247.0899 303.9299 365.2893
490.4309 495.7020 706.5056
766.4599 781.1961 863.0554
923.3971 991.3089 1058.1954
1077.8233 1085.0960 1135.9596
1143.0316 1229.2128 1286.7010
1335.2726 1341.7559 1387.1330
1416.0064 1433.0915 1439.0721
1488.9215 1508.8651 1519.2562
2897.7542 2991.3175 3033.0848
3037.1248 3055.8182 3076.5071
3107.0692 3126.7271 3743.1335
Zero-point correction (Hartree): 0.128387

C4H9O2.mtm

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.21573767
Electronic state : 2-A
Cartesian coordinates (Angs):
O -2.003826 -0.701679 -0.637458
C -1.528078 -0.134265 0.510869
C -0.058528 0.336129 0.466693
C 0.885214 -0.755957 -0.033025
C 2.352828 -0.321397 -0.053531
H -2.194128 0.677019 0.869324
H -1.621831 -0.935120 1.277123
O 0.079299 1.453574 -0.406384
H 0.223493 0.617618 1.497841
H 0.760749 -1.637252 0.609708
H 0.555580 -1.048495 -1.035121
H 2.706197 -0.060716 0.951220
H 2.484786 0.554620 -0.693041
H 2.992578 -1.124386 -0.432953
H -0.419818 2.194492 -0.039404
Rotational constants (GHz): 5.9038700 2.2780900 1.9249100
Vibrational harmonic frequencies (cm-1):
91.7398 120.4868 206.8140
223.3215 271.7620 309.0400
356.9939 458.3164 607.1005
736.6134 781.8728 845.4167
940.9624 994.8907 1057.2250
1069.7600 1086.0074 1117.0634
1191.5145 1215.4640 1259.6519
1327.4196 1345.4592 1382.7304
1395.6556 1424.2726 1452.6011
1496.1614 1509.9193 1523.6427
2887.3526 2926.4648 2953.8105
3043.6618 3045.7626 3097.7370
3114.6926 3142.4367 3817.4647
Zero-point correction (Hartree): 0.127188

C4H9O2.mtp

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.21642276
Electronic state : 2-A
Cartesian coordinates (Angs):
O -1.991985 -0.700341 -0.647659
C -1.536553 -0.104756 0.497353
C -0.070029 0.343830 0.481537
C 0.866417 -0.770020 -0.001823
C 2.337385 -0.348260 -0.073215
H -2.190048 0.750899 0.753255
H -1.701724 -0.836462 1.315708
O -0.033614 1.494052 -0.359681

| | | | | |
|--|-----------|-----------|-----------|--|
| H | 0.200252 | 0.621710 | 1.517228 | |
| H | 0.764760 | -1.626480 | 0.678295 | |
| H | 0.515319 | -1.100195 | -0.984805 | |
| H | 2.706966 | -0.001082 | 0.899366 | |
| H | 2.489901 | 0.456166 | -0.802179 | |
| H | 2.970436 | -1.183315 | -0.387630 | |
| H | 0.865604 | 1.844313 | -0.353627 | |
| Rotational constants (GHz): | 5.8475000 | 2.2942100 | 1.9270400 | |
| Vibrational harmonic frequencies (cm-1): | | | | |
| 98.0252 | 119.4456 | | 199.2313 | |
| 230.4459 | 276.9063 | | 313.3235 | |
| 355.0200 | 462.6475 | | 519.5596 | |
| 680.6686 | 775.8284 | | 841.0650 | |
| 941.2241 | 992.4288 | | 1044.1420 | |
| 1065.4034 | 1093.5330 | | 1158.6432 | |
| 1200.2272 | 1243.1699 | | 1295.4870 | |
| 1337.8603 | 1360.5961 | | 1377.9962 | |
| 1410.1224 | 1422.6045 | | 1440.8855 | |
| 1496.7506 | 1513.8865 | | 1524.6866 | |
| 2912.8214 | 2949.7738 | | 2958.6332 | |
| 3035.2757 | 3038.7507 | | 3089.9814 | |
| 3110.8408 | 3118.6019 | | 3831.7678 | |
| Zero-point correction (Hartree): | 0.127209 | | | |

C4H9O2.mtt

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.22213685
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | | |
|--|-----------|-----------|-----------|--|
| O | -2.024751 | -0.372018 | -0.726676 | |
| C | -1.463646 | -0.417026 | 0.521044 | |
| C | -0.045128 | 0.199006 | 0.542895 | |
| C | 0.974590 | -0.735631 | -0.128221 | |
| C | 2.390660 | -0.157348 | -0.136408 | |
| H | -2.122762 | 0.233581 | 1.136016 | |
| H | -1.516026 | -1.424038 | 0.971742 | |
| O | -0.096762 | 1.471050 | -0.077666 | |
| H | 0.250959 | 0.372841 | 1.585825 | |
| H | 0.962005 | -1.705445 | 0.387736 | |
| H | 0.635842 | -0.926220 | -1.156355 | |
| H | 2.768449 | -0.022615 | 0.883785 | |
| H | 2.399049 | 0.819940 | -0.625919 | |
| H | 3.085402 | -0.817607 | -0.664856 | |
| H | -0.629671 | 1.343307 | -0.879093 | |
| Rotational constants (GHz): | 6.3470000 | 2.2240000 | 1.9563400 | |
| Vibrational harmonic frequencies (cm-1): | | | | |
| 109.3023 | 120.5485 | | 224.9836 | |
| 227.0263 | 298.5749 | | 364.9805 | |
| 452.1923 | 483.3636 | | 677.0242 | |
| 771.3336 | 811.6473 | | 854.9661 | |
| 941.1843 | 995.6174 | | 1067.0765 | |
| 1075.3501 | 1101.0172 | | 1118.7895 | |
| 1150.9272 | 1234.8541 | | 1287.5614 | |
| 1316.9097 | 1362.5781 | | 1384.2632 | |
| 1402.1597 | 1420.1983 | | 1437.4321 | |
| 1495.4875 | 1508.8037 | | 1522.7471 | |
| 2893.1956 | 2980.1194 | | 3022.0472 | |
| 3045.6266 | 3046.6580 | | 3065.7615 | |
| 3112.5489 | 3138.2643 | | 3745.8664 | |
| Zero-point correction (Hartree): | 0.128190 | | | |

C4H9O2.pmm

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.21703604
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | | |
|--|-----------|-----------|-----------|--|
| O | 0.229383 | 1.943049 | -0.104587 | |
| C | -0.774525 | 1.116858 | 0.265608 | |
| C | -0.531260 | -0.348829 | -0.314544 | |
| C | 0.692895 | -1.024421 | 0.296224 | |
| C | 2.029321 | -0.399371 | -0.108415 | |
| H | -0.917361 | 1.014112 | 1.355653 | |
| H | -1.727647 | 1.432984 | -0.202485 | |
| O | -1.654971 | -1.142239 | 0.006086 | |
| H | -0.405197 | -0.238084 | -1.401141 | |
| H | 0.579246 | -1.022761 | 1.387538 | |
| H | 0.656029 | -2.074875 | -0.016417 | |
| H | 2.086152 | 0.652233 | 0.189072 | |
| H | 2.179872 | -0.448432 | -1.192373 | |
| H | 2.858733 | -0.931947 | 0.367479 | |
| H | -2.403709 | -0.855137 | -0.532550 | |
| Rotational constants (GHz): | 3.8211300 | 3.3419700 | 1.9342200 | |
| Vibrational harmonic frequencies (cm-1): | | | | |
| 80.9801 | 149.5968 | | 209.9445 | |

| | | |
|-----------|-----------|-----------|
| 237.8376 | 303.3765 | 333.9922 |
| 371.7674 | 425.0124 | 503.3313 |
| 583.5793 | 785.7671 | 873.1786 |
| 896.0777 | 1037.0489 | 1063.0355 |
| 1094.8073 | 1104.6492 | 1124.5085 |
| 1192.3591 | 1262.1125 | 1284.4948 |
| 1305.9734 | 1337.4300 | 1357.1848 |
| 1428.7879 | 1442.9491 | 1497.1353 |
| 1507.8159 | 1520.6306 | 1526.9552 |
| 2910.7408 | 2983.7089 | 3023.9943 |
| 3044.7352 | 3047.1286 | 3082.9975 |
| 3116.2273 | 3122.9832 | 3816.9617 |

Zero-point correction (Hartree): 0.127559

C4H9O2.pmp

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.21759031

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 0.079975 | 2.021555 | -0.132947 |
| C | -0.775883 | 1.041274 | 0.271926 |
| C | -0.514979 | -0.353878 | -0.320724 |
| C | 0.733231 | -1.024089 | 0.266007 |
| C | 2.051018 | -0.320328 | -0.072635 |
| H | -0.875729 | 0.992035 | 1.373512 |
| H | -1.778871 | 1.365065 | -0.083835 |
| O | -1.695388 | -1.095909 | -0.021901 |
| H | -0.389047 | -0.230841 | -1.409188 |
| H | 0.603184 | -1.096072 | 1.353956 |
| H | 0.769612 | -2.058025 | -0.108756 |
| H | 2.069213 | 0.706812 | 0.305143 |
| H | 2.208246 | -0.270205 | -1.155250 |
| H | 2.898932 | -0.855465 | 0.366170 |
| H | -1.542563 | -2.016336 | -0.270422 |

Rotational constants (GHz): 3.7142100 3.3599900 1.9069700

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 95.7977 | 136.6155 | 207.6079 |
| 233.7351 | 266.8381 | 319.1098 |
| 401.7106 | 415.5223 | 531.9981 |
| 743.7263 | 793.3370 | 879.4403 |
| 970.3175 | 1043.4730 | 1045.6953 |
| 1075.2025 | 1114.0131 | 1122.6169 |
| 1182.1944 | 1230.9174 | 1280.2277 |
| 1332.2949 | 1337.3622 | 1363.3302 |
| 1401.0147 | 1424.1843 | 1441.2041 |
| 1496.0524 | 1510.5850 | 1515.6962 |
| 2888.5798 | 2948.1550 | 2989.2623 |
| 3011.6506 | 3047.7339 | 3060.7034 |
| 3118.0857 | 3120.4364 | 3822.2128 |

Zero-point correction (Hartree): 0.127392

C4H9O2.pmt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.21784251

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 0.390654 | 1.927146 | -0.085799 |
| C | -0.677139 | 1.159588 | 0.246785 |
| C | -0.569181 | -0.300754 | -0.337716 |
| C | 0.601470 | -1.085768 | 0.261618 |
| C | 1.987120 | -0.532290 | -0.077532 |
| H | -0.873962 | 1.095422 | 1.335897 |
| H | -1.576610 | 1.571367 | -0.248171 |
| O | -1.804460 | -0.961754 | -0.136915 |
| H | -0.446892 | -0.204093 | -1.421292 |
| H | 0.471963 | -1.122843 | 1.354373 |
| H | 0.508609 | -2.117629 | -0.099034 |
| H | 2.104861 | 0.499011 | 0.271541 |
| H | 2.161333 | -0.537887 | -1.158390 |
| H | 2.768154 | -1.138395 | 0.392275 |
| H | -1.860627 | -1.212752 | 0.795577 |

Rotational constants (GHz): 3.8506300 3.3021500 1.9318000

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 73.4349 | 152.4432 | 197.3185 |
| 225.4061 | 244.4319 | 319.0391 |
| 378.0390 | 411.7577 | 465.4624 |
| 586.4316 | 799.4527 | 862.0203 |
| 921.8154 | 1018.6778 | 1055.7606 |
| 1084.4802 | 1092.6704 | 1142.3986 |
| 1183.0399 | 1260.8994 | 1279.0562 |
| 1314.9357 | 1338.0613 | 1383.6473 |
| 1420.5061 | 1434.9953 | 1481.1444 |
| 1495.1088 | 1510.1682 | 1515.6894 |
| 2908.8897 | 2960.5694 | 3009.0905 |
| 3045.5397 | 3067.0648 | 3091.5894 |

3116.9933 3120.7743 3797.5288
Zero-point correction (Hartree): 0.127045

C4H9O2.ppm

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.21655594

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -1.995897 | -0.978125 | 0.088718 |
| C | -1.296729 | 0.072496 | -0.423638 |
| C | -0.121060 | 0.568111 | 0.458152 |
| C | 0.930355 | -0.510716 | 0.719420 |
| C | 1.735152 | -0.933768 | -0.515097 |
| H | -0.867636 | -0.299902 | -1.378502 |
| H | -1.953792 | 0.916431 | -0.717193 |
| O | 0.511261 | 1.672826 | -0.180200 |
| H | -0.547939 | 0.875292 | 1.426313 |
| H | 1.615838 | -0.129718 | 1.485192 |
| H | 0.410969 | -1.372802 | 1.152392 |
| H | 2.224168 | -0.071725 | -0.975657 |
| H | 1.105827 | -1.411818 | -1.274170 |
| H | 2.507152 | -1.657476 | -0.236170 |
| H | -0.103805 | 2.417366 | -0.183375 |

Rotational constants (GHz): 4.3532000 2.7848100 2.0483100

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 70.5110 | 144.3401 | 225.3523 |
| 247.5030 | 260.4983 | 289.0409 |
| 382.6771 | 468.5679 | 569.2644 |
| 706.1139 | 784.5226 | 854.1809 |
| 949.0959 | 993.7427 | 1052.9816 |
| 1058.6611 | 1123.3051 | 1145.6467 |
| 1151.2434 | 1189.1436 | 1245.9378 |
| 1315.0251 | 1365.2715 | 1387.8159 |
| 1391.2035 | 1423.2352 | 1445.6261 |
| 1491.0023 | 1516.1649 | 1521.7255 |
| 2896.6415 | 2927.9438 | 2992.4890 |
| 3049.7481 | 3056.4629 | 3095.9689 |
| 3113.7072 | 3140.6858 | 3819.0273 |

Zero-point correction (Hartree): 0.127263

C4H9O2.ppp

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.21744077

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -1.973824 | -0.956841 | 0.102611 |
| C | -1.297105 | 0.117534 | -0.395581 |
| C | -0.108733 | 0.595632 | 0.451127 |
| C | 0.925746 | -0.505059 | 0.724166 |
| C | 1.656787 | -1.019149 | -0.520813 |
| H | -0.947746 | -0.163237 | -1.412083 |
| H | -1.992351 | 0.956322 | -0.593934 |
| O | 0.429156 | 1.701196 | -0.274155 |
| H | -0.513649 | 0.933308 | 1.419568 |
| H | 1.659108 | -0.112761 | 1.443028 |
| H | 0.407345 | -1.326270 | 1.232644 |
| H | 2.105284 | -0.192028 | -1.078648 |
| H | 0.981871 | -1.551790 | -1.198889 |
| H | 2.452921 | -1.716175 | -0.242221 |
| H | 1.144387 | 2.084036 | 0.249502 |

Rotational constants (GHz): 4.2297000 2.8683400 2.0728600

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 70.7845 | 140.4606 | 221.0173 |
| 238.8457 | 278.2384 | 279.1838 |
| 371.3586 | 450.6422 | 510.0153 |
| 620.3913 | 784.6001 | 814.5868 |
| 972.4718 | 994.2596 | 1036.4868 |
| 1082.8429 | 1118.7369 | 1141.5329 |
| 1155.5157 | 1256.4667 | 1298.4513 |
| 1320.1792 | 1353.0373 | 1394.0763 |
| 1397.6352 | 1432.7610 | 1440.1807 |
| 1494.8249 | 1514.2751 | 1523.2148 |
| 2905.6931 | 2943.4292 | 2984.1484 |
| 3027.1301 | 3052.2839 | 3082.3344 |
| 3117.6744 | 3130.8639 | 3822.9143 |

Zero-point correction (Hartree): 0.127061

C4H9O2.ppt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.21648194

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -1.944193 | -1.001786 | 0.073048 |
| C | -1.298670 | 0.093613 | -0.420493 |
| C | -0.125387 | 0.600710 | 0.455695 |

| | | | |
|---|-----------|-----------|-----------|
| C | 0.920890 | -0.490442 | 0.732498 |
| C | 1.688313 | -0.987321 | -0.499338 |
| H | -0.993869 | -0.033619 | -1.478753 |
| H | -2.062778 | 0.899292 | -0.440839 |
| O | 0.427313 | 1.775132 | -0.124320 |
| H | -0.547616 | 0.920370 | 1.414352 |
| H | 1.631148 | -0.094524 | 1.467522 |
| H | 0.399792 | -1.330135 | 1.207963 |
| H | 2.243497 | -0.177976 | -0.989232 |
| H | 1.028126 | -1.445982 | -1.242972 |
| H | 2.426120 | -1.741559 | -0.210676 |
| H | 0.899748 | 1.517998 | -0.927356 |
| Rotational constants (GHz): | 4.1704100 | 2.8679700 | 2.0572700 |
| Vibrational harmonic frequencies (cm ⁻¹): | | | |
| 65.3412 | 135.2815 | | 206.0697 |
| 249.4260 | 266.9632 | | 295.1930 |
| 387.3301 | 424.6719 | | 564.7027 |
| 709.4102 | 774.2465 | | 799.9215 |
| 942.1329 | 998.3357 | | 1049.3186 |
| 1051.4428 | 1110.1786 | | 1131.9282 |
| 1152.1765 | 1200.9063 | | 1284.8908 |
| 1313.8465 | 1355.8923 | | 1384.1877 |
| 1396.0979 | 1417.9768 | | 1431.4412 |
| 1489.1726 | 1514.8884 | | 1522.9328 |
| 2900.3258 | 2934.2290 | | 3037.6274 |
| 3048.3137 | 3079.9606 | | 3086.5723 |
| 3107.0239 | 3123.2152 | | 3807.8406 |
| Zero-point correction (Hartree): | 0.127011 | | |

C4H9O2.ptm

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.21823959
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 2.112976 | -1.036920 | -0.191750 |
| C | 1.557601 | 0.161363 | 0.147826 |
| C | 0.082909 | 0.353020 | -0.275917 |
| C | -0.836938 | -0.675335 | 0.371979 |
| C | -2.272503 | -0.621680 | -0.156364 |
| H | 1.596887 | 0.199351 | 1.258919 |
| H | 2.183869 | 1.015541 | -0.180515 |
| O | -0.351101 | 1.651591 | 0.122583 |
| H | 0.028388 | 0.245394 | -1.371858 |
| H | -0.396848 | -1.664963 | 0.206148 |
| H | -0.830200 | -0.497522 | 1.455836 |
| H | -2.308515 | -0.846537 | -1.228702 |
| H | -2.701106 | 0.372977 | -0.006039 |
| H | -2.908362 | -1.349954 | 0.356592 |
| H | 0.054471 | 2.304143 | -0.462185 |
| Rotational constants (GHz): | 5.2719000 | 2.3589200 | 1.7598300 |
| Vibrational harmonic frequencies (cm ⁻¹): | | | |
| 96.5229 | 128.1774 | | 204.3914 |
| 242.3466 | 261.1963 | | 279.6062 |
| 415.5884 | 461.5183 | | 521.0307 |
| 671.6166 | 784.3381 | | 874.6661 |
| 995.0869 | 1001.7156 | | 1048.7688 |
| 1066.4439 | 1107.4136 | | 1139.1707 |
| 1160.9430 | 1219.8456 | | 1261.9813 |
| 1324.4157 | 1342.7114 | | 1364.2373 |
| 1386.8334 | 1420.7577 | | 1451.5969 |
| 1494.1148 | 1509.8459 | | 1523.3607 |
| 2886.1273 | 2928.2209 | | 2987.8159 |
| 3038.1199 | 3046.1334 | | 3091.4631 |
| 3112.9986 | 3133.9444 | | 3822.2959 |
| Zero-point correction (Hartree): | 0.127139 | | |

C4H9O2.ptp

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.21853855
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 2.125520 | -1.010414 | -0.165573 |
| C | 1.555591 | 0.191698 | 0.135936 |
| C | 0.091926 | 0.354986 | -0.292944 |
| C | -0.809681 | -0.709483 | 0.337553 |
| C | -2.269617 | -0.626386 | -0.118141 |
| H | 1.637120 | 0.331540 | 1.235875 |
| H | 2.173412 | 1.016638 | -0.270198 |
| O | -0.254804 | 1.681638 | 0.100502 |
| H | 0.049310 | 0.254156 | -1.391236 |
| H | -0.391141 | -1.690729 | 0.085356 |
| H | -0.753751 | -0.605942 | 1.429371 |
| H | -2.356164 | -0.731469 | -1.206045 |
| H | -2.727278 | 0.328631 | 0.166957 |

| | | | | |
|--|-----------|-----------|-----------|--|
| H | -2.872221 | -1.416643 | 0.339382 | |
| H | -1.134330 | 1.879133 | -0.243319 | |
| Rotational constants (GHz): | 5.3057800 | 2.3659100 | 1.7574700 | |
| Vibrational harmonic frequencies (cm-1): | | | | |
| 96.3613 | 116.1112 | | 213.8150 | |
| 236.1111 | 252.2591 | | 276.2063 | |
| 399.4916 | 429.7544 | | 503.4782 | |
| 543.0860 | 777.7264 | | 850.7058 | |
| 997.0040 | 1001.9241 | | 1031.0367 | |
| 1075.6096 | 1108.3731 | | 1142.1423 | |
| 1191.9075 | 1253.9481 | | 1302.4498 | |
| 1325.2029 | 1336.2415 | | 1379.3928 | |
| 1419.1163 | 1423.2714 | | 1438.0647 | |
| 1493.9935 | 1514.6554 | | 1523.1550 | |
| 2897.2046 | 2939.5947 | | 2976.8042 | |
| 3035.0980 | 3038.9136 | | 3082.6918 | |
| 3104.7176 | 3119.0026 | | 3836.1172 | |
| Zero-point correction (Hartree): | 0.126855 | | | |

C4H9O2.ptt

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.21848964
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | | |
|--|-----------|-----------|-----------|--|
| O | 2.121825 | -1.018024 | -0.149520 | |
| C | 1.557617 | 0.187779 | 0.149197 | |
| C | 0.089776 | 0.352563 | -0.299921 | |
| C | -0.817168 | -0.693997 | 0.353790 | |
| C | -2.267205 | -0.628464 | -0.131814 | |
| H | 1.678927 | 0.448617 | 1.221654 | |
| H | 2.168649 | 0.941049 | -0.392414 | |
| O | -0.339980 | 1.687436 | -0.049788 | |
| H | 0.054789 | 0.233877 | -1.389280 | |
| H | -0.386438 | -1.683280 | 0.155669 | |
| H | -0.777951 | -0.556393 | 1.446252 | |
| H | -2.331630 | -0.846472 | -1.203513 | |
| H | -2.686778 | 0.368979 | 0.027562 | |
| H | -2.894505 | -1.353712 | 0.395474 | |
| H | -0.457942 | 1.784753 | 0.905554 | |
| Rotational constants (GHz): | 5.2717000 | 2.3581300 | 1.7610700 | |
| Vibrational harmonic frequencies (cm-1): | | | | |
| 107.9635 | 120.9201 | | 198.6723 | |
| 229.7992 | 259.7978 | | 310.7439 | |
| 416.1010 | 456.2530 | | 495.4383 | |
| 686.1199 | 785.0977 | | 840.1609 | |
| 992.3360 | 1006.3971 | | 1049.2533 | |
| 1068.7758 | 1106.2553 | | 1119.0173 | |
| 1173.3097 | 1208.8464 | | 1271.4605 | |
| 1332.5827 | 1351.2124 | | 1375.8662 | |
| 1396.0161 | 1416.3302 | | 1425.5829 | |
| 1496.4636 | 1508.8035 | | 1521.1175 | |
| 2894.9259 | 2921.7752 | | 3001.5474 | |
| 3049.5954 | 3064.9977 | | 3076.4851 | |
| 3117.4187 | 3130.2235 | | 3792.6812 | |
| Zero-point correction (Hartree): | 0.127068 | | | |

C4H9O2.tmm

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.22117214
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | | |
|--|-----------|-----------|-----------|--|
| O | 2.186556 | -0.804718 | -0.092348 | |
| C | 0.853139 | -0.871682 | 0.212208 | |
| C | 0.072762 | 0.359514 | -0.310307 | |
| C | -1.331050 | 0.488005 | 0.279986 | |
| C | -2.298025 | -0.625078 | -0.139431 | |
| H | 0.408253 | -1.838996 | -0.075736 | |
| H | 0.826358 | -0.833611 | 1.324107 | |
| O | 0.800386 | 1.523653 | 0.023451 | |
| H | -0.007726 | 0.251653 | -1.407531 | |
| H | -1.246453 | 0.534813 | 1.373437 | |
| H | -1.723357 | 1.460235 | -0.038621 | |
| H | -1.987783 | -1.607630 | 0.232016 | |
| H | -2.377100 | -0.693010 | -1.230335 | |
| H | -3.301170 | -0.432633 | 0.252411 | |
| H | 1.732469 | 1.303145 | -0.133314 | |
| Rotational constants (GHz): | 5.7765700 | 2.3069500 | 1.7678500 | |
| Vibrational harmonic frequencies (cm-1): | | | | |
| 94.5448 | 124.8367 | | 205.0401 | |
| 244.5247 | 286.8887 | | 409.7890 | |
| 462.8788 | 490.6476 | | 549.5803 | |
| 770.6427 | 803.4569 | | 893.0789 | |
| 935.3174 | 1047.3134 | | 1061.4690 | |
| 1078.5602 | 1111.6926 | | 1121.1084 | |
| 1183.6070 | 1250.9027 | | 1281.5728 | |

| | | |
|-----------|-----------|-----------|
| 1307.8215 | 1351.0240 | 1380.3135 |
| 1394.3970 | 1430.6814 | 1449.2940 |
| 1504.0524 | 1516.1322 | 1522.3194 |
| 2880.9353 | 2952.8843 | 2994.9160 |
| 3042.9882 | 3046.1244 | 3084.7544 |
| 3112.8615 | 3121.3284 | 3747.6190 |

Zero-point correction (Hartree): 0.128142

C4H9O2.tmp

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.21517582

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 2.146259 | -0.960363 | -0.235212 |
| C | 0.945970 | -0.722919 | 0.377602 |
| C | 0.103417 | 0.382747 | -0.266932 |
| C | -1.339003 | 0.426051 | 0.259294 |
| C | -2.214628 | -0.756282 | -0.171149 |
| H | 0.406823 | -1.691198 | 0.325442 |
| H | 1.076451 | -0.520214 | 1.457832 |
| O | 0.796978 | 1.590562 | 0.034574 |
| H | 0.096612 | 0.197852 | -1.354115 |
| H | -1.311783 | 0.508147 | 1.353588 |
| H | -1.795662 | 1.358061 | -0.101492 |
| H | -1.860005 | -1.706181 | 0.243301 |
| H | -2.236448 | -0.859438 | -1.261902 |
| H | -3.245595 | -0.621647 | 0.169720 |
| H | 0.349174 | 2.315444 | -0.420157 |

Rotational constants (GHz): 5.0852800 2.3792100 1.7610700

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 95.3836 | 110.8142 | 213.8680 |
| 244.1544 | 260.5846 | 288.0656 |
| 397.2869 | 470.9335 | 488.1428 |
| 708.4732 | 775.0146 | 888.8039 |
| 953.8280 | 1024.4256 | 1048.5700 |
| 1087.6272 | 1117.9814 | 1133.8505 |
| 1173.9439 | 1261.3586 | 1272.0228 |
| 1337.5354 | 1348.2625 | 1370.3498 |
| 1391.4142 | 1428.3219 | 1442.1418 |
| 1500.4485 | 1515.7278 | 1520.1169 |
| 2920.9115 | 2957.7355 | 2988.6240 |
| 3026.5327 | 3045.5478 | 3066.5043 |
| 3111.7905 | 3120.0209 | 3817.9544 |

Zero-point correction (Hartree): 0.127407

C4H9O2.tmt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.21488120

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 2.143886 | -0.965517 | -0.205894 |
| C | 0.930352 | -0.741168 | 0.375330 |
| C | 0.106951 | 0.387137 | -0.285617 |
| C | -1.336429 | 0.447973 | 0.233890 |
| C | -2.215919 | -0.746313 | -0.152854 |
| H | 0.382695 | -1.698493 | 0.243180 |
| H | 0.997911 | -0.580201 | 1.471459 |
| O | 0.766986 | 1.635993 | -0.119453 |
| H | 0.109315 | 0.205207 | -1.366396 |
| H | -1.318435 | 0.557766 | 1.328899 |
| H | -1.772097 | 1.372810 | -0.160351 |
| H | -1.869271 | -1.682863 | 0.297449 |
| H | -2.236089 | -0.887014 | -1.239176 |
| H | -3.246680 | -0.592194 | 0.180349 |
| H | 0.755954 | 1.855401 | 0.822870 |

Rotational constants (GHz): 5.0166800 2.3859500 1.7603300

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 94.9927 | 111.8986 | 217.6424 |
| 233.0153 | 267.9605 | 290.7138 |
| 409.6731 | 468.8150 | 475.3581 |
| 769.0996 | 836.2777 | 850.5829 |
| 939.7775 | 1009.5586 | 1046.1814 |
| 1055.3452 | 1113.5630 | 1123.2886 |
| 1174.8688 | 1214.2859 | 1267.0506 |
| 1322.8888 | 1341.3547 | 1381.4421 |
| 1406.4163 | 1428.4594 | 1433.9266 |
| 1501.7009 | 1515.4192 | 1520.2682 |
| 2894.3428 | 2927.7166 | 3013.6886 |
| 3045.8700 | 3074.0451 | 3083.9453 |
| 3114.2260 | 3120.5908 | 3789.6700 |

Zero-point correction (Hartree): 0.127317

C4H9O2.tpm

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.22157961

Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -2.285477 | -0.351333 | -0.246368 |
| C | -1.037424 | -0.813362 | 0.062416 |
| C | -0.113712 | 0.326966 | 0.566991 |
| C | 1.355069 | -0.085848 | 0.687442 |
| C | 2.033057 | -0.436048 | -0.641359 |
| H | -1.053775 | -1.687440 | 0.737255 |
| H | -0.629655 | -1.166081 | -0.909428 |
| O | -0.220216 | 1.423547 | -0.316279 |
| H | -0.479696 | 0.602775 | 1.571628 |
| H | 1.887948 | 0.749820 | 1.155942 |
| H | 1.422525 | -0.927033 | 1.389939 |
| H | 1.924365 | 0.385372 | -1.353665 |
| H | 1.610787 | -1.338767 | -1.098051 |
| H | 3.100740 | -0.622985 | -0.491047 |
| H | -1.159631 | 1.476379 | -0.554333 |

Rotational constants (GHz): 5.9974200 2.2845300 2.0226700
 Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 102.1859 | 123.1806 | 210.1382 |
| 239.8037 | 301.4150 | 355.3468 |
| 495.8096 | 517.0849 | 586.9072 |
| 770.8547 | 803.8322 | 888.3940 |
| 938.5642 | 993.6019 | 1059.9430 |
| 1089.3000 | 1102.5170 | 1127.2026 |
| 1170.4700 | 1250.3900 | 1278.8176 |
| 1304.5921 | 1383.4690 | 1391.9317 |
| 1399.6015 | 1419.2928 | 1445.3941 |
| 1492.8111 | 1514.0611 | 1522.4410 |
| 2895.8338 | 2962.3910 | 2985.3937 |
| 3042.6630 | 3047.9549 | 3080.0377 |
| 3111.1526 | 3143.2319 | 3747.7165 |

Zero-point correction (Hartree): 0.128251

C4H9O2.tpp

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.21495514
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -2.395294 | -0.408480 | -0.068920 |
| C | -1.062178 | -0.711303 | -0.106536 |
| C | -0.139843 | 0.363899 | 0.480934 |
| C | 1.293528 | -0.138899 | 0.728575 |
| C | 2.039719 | -0.569262 | -0.539262 |
| H | -0.884215 | -1.698716 | 0.362475 |
| H | -0.812848 | -0.859138 | -1.177426 |
| O | -0.173492 | 1.450390 | -0.440719 |
| H | -0.578892 | 0.666343 | 1.445423 |
| H | 1.852385 | 0.668280 | 1.222015 |
| H | 1.259510 | -0.963111 | 1.453705 |
| H | 2.016009 | 0.230299 | -1.284670 |
| H | 1.596281 | -1.462293 | -0.992906 |
| H | 3.085520 | -0.802280 | -0.317110 |
| H | 0.229178 | 2.218722 | -0.016662 |

Rotational constants (GHz): 5.7895500 2.2520500 1.9436400
 Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 112.6588 | 114.5722 | 206.9375 |
| 233.4934 | 267.3411 | 312.8262 |
| 367.7213 | 437.0394 | 519.3045 |
| 622.4184 | 788.2128 | 870.1047 |
| 944.0381 | 993.9889 | 1044.6550 |
| 1092.6429 | 1097.5423 | 1120.1448 |
| 1175.5537 | 1277.3605 | 1285.7134 |
| 1314.9226 | 1364.7561 | 1374.9248 |
| 1395.2204 | 1432.3240 | 1439.8618 |
| 1498.4309 | 1515.3541 | 1525.2005 |
| 2918.6847 | 2950.4846 | 2992.9290 |
| 3027.0736 | 3051.8862 | 3059.9825 |
| 3115.9726 | 3136.2032 | 3822.6651 |

Zero-point correction (Hartree): 0.127170

C4H9O2.tpt

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.21347880
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -2.408711 | -0.394222 | -0.093462 |
| C | -1.077824 | -0.704121 | -0.156752 |
| C | -0.147622 | 0.344470 | 0.488280 |
| C | 1.281509 | -0.173343 | 0.733818 |
| C | 2.076560 | -0.525694 | -0.531025 |
| H | -0.991814 | -1.655177 | 0.412897 |
| H | -0.761824 | -0.953983 | -1.188654 |
| O | -0.160727 | 1.553312 | -0.262539 |

| | | | | |
|--|-----------|-----------|-----------|--|
| H | -0.598468 | 0.608562 | 1.451211 | |
| H | 1.817579 | 0.605244 | 1.287916 | |
| H | 1.230570 | -1.048913 | 1.394606 | |
| H | 2.158682 | 0.336063 | -1.203308 | |
| H | 1.626265 | -1.351031 | -1.092489 | |
| H | 3.096816 | -0.825033 | -0.273725 | |
| H | 0.181958 | 1.363668 | -1.146370 | |
| Rotational constants (GHz): | 5.7639000 | 2.2190800 | 1.9131700 | |
| Vibrational harmonic frequencies (cm-1): | | | | |
| 85.7966 | 109.5669 | | 209.3303 | |
| 243.5412 | 290.3098 | | 306.1877 | |
| 373.1014 | 436.3965 | | 590.4028 | |
| 750.4411 | 779.8235 | | 837.1066 | |
| 930.9128 | 997.6951 | | 1052.9032 | |
| 1059.1782 | 1099.8075 | | 1133.0697 | |
| 1153.2289 | 1216.5056 | | 1293.3738 | |
| 1307.9543 | 1347.2915 | | 1385.2177 | |
| 1401.0747 | 1432.4457 | | 1435.3029 | |
| 1492.3733 | 1516.6464 | | 1524.6310 | |
| 2891.6419 | 2941.8093 | | 3037.8949 | |
| 3045.4688 | 3078.9386 | | 3084.1496 | |
| 3111.7939 | 3122.5565 | | 3804.6419 | |
| Zero-point correction (Hartree): | 0.127374 | | | |

C4H9O2.ttm

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.22266423
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | | |
|--|-----------|-----------|-----------|--|
| O | -2.470437 | 0.014797 | 0.169715 | |
| C | -1.351337 | -0.727537 | -0.088683 | |
| C | -0.051451 | 0.026799 | 0.281436 | |
| C | 1.194450 | -0.666839 | -0.261303 | |
| C | 2.493987 | 0.019307 | 0.170426 | |
| H | -1.404510 | -1.743210 | 0.341904 | |
| H | -1.355252 | -0.853583 | -1.194016 | |
| O | -0.119408 | 1.335104 | -0.248119 | |
| H | 0.003626 | 0.057163 | 1.385071 | |
| H | 1.189427 | -1.712057 | 0.075843 | |
| H | 1.126021 | -0.681261 | -1.356899 | |
| H | 2.602680 | 0.009071 | 1.260861 | |
| H | 2.503011 | 1.061516 | -0.158393 | |
| H | 3.365637 | -0.485650 | -0.257359 | |
| H | -1.025767 | 1.638425 | -0.081037 | |
| Rotational constants (GHz): | 8.1342000 | 1.9908600 | 1.7151800 | |
| Vibrational harmonic frequencies (cm-1): | | | | |
| 96.9641 | 136.0156 | | 193.3570 | |
| 235.1707 | 303.6979 | | 391.2086 | |
| 464.3964 | 481.7463 | | 548.8630 | |
| 782.3344 | 809.8520 | | 908.2776 | |
| 958.1833 | 996.0425 | | 1071.9716 | |
| 1076.6033 | 1116.9643 | | 1127.1122 | |
| 1176.9209 | 1252.2845 | | 1283.6636 | |
| 1317.5414 | 1346.2146 | | 1390.1109 | |
| 1392.3076 | 1424.4711 | | 1452.4221 | |
| 1488.6929 | 1510.1966 | | 1523.1332 | |
| 2884.1126 | 2953.5422 | | 2982.8406 | |
| 3030.5732 | 3048.9449 | | 3071.6528 | |
| 3115.1008 | 3140.4795 | | 3753.7266 | |
| Zero-point correction (Hartree): | 0.128119 | | | |

C4H9O2.ttp

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.21614661
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | | |
|--|-----------|-----------|-----------|--|
| O | 2.533609 | -0.073852 | -0.329719 | |
| C | 1.394211 | -0.568391 | 0.244394 | |
| C | 0.088076 | 0.069392 | -0.234677 | |
| C | -1.139816 | -0.736883 | 0.212236 | |
| C | -2.468792 | -0.099158 | -0.201823 | |
| H | 1.387257 | -1.663396 | 0.067205 | |
| H | 1.474923 | -0.470164 | 1.345544 | |
| O | 0.086045 | 1.388934 | 0.305238 | |
| H | 0.122769 | 0.104679 | -1.336169 | |
| H | -1.069954 | -1.748332 | -0.210204 | |
| H | -1.108487 | -0.844391 | 1.304500 | |
| H | -2.536170 | 0.013983 | -1.290572 | |
| H | -2.588369 | 0.890598 | 0.251810 | |
| H | -3.318591 | -0.708206 | 0.120349 | |
| H | -0.562686 | 1.914811 | -0.177401 | |
| Rotational constants (GHz): | 7.6532800 | 1.9578700 | 1.6914800 | |
| Vibrational harmonic frequencies (cm-1): | | | | |
| 90.6439 | 117.7445 | | 137.7102 | |

| | | |
|-----------|-----------|-----------|
| 187.7436 | 239.3574 | 278.2629 |
| 308.4940 | 399.2631 | 487.6430 |
| 541.4432 | 781.6906 | 894.9805 |
| 956.4556 | 1006.7541 | 1032.0682 |
| 1089.0157 | 1107.4245 | 1139.8682 |
| 1174.7167 | 1270.9019 | 1287.4620 |
| 1324.3293 | 1357.1121 | 1390.8549 |
| 1402.6931 | 1420.4188 | 1442.8890 |
| 1491.1040 | 1513.2611 | 1526.0794 |
| 2918.0448 | 2944.1621 | 2991.2287 |
| 3029.3086 | 3039.9420 | 3069.3230 |
| 3108.5641 | 3120.4829 | 3839.4506 |

Zero-point correction (Hartree): 0.126345

C4H9O2.ttt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.21587699

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 2.528957 | -0.083355 | -0.328038 |
| C | 1.394538 | -0.575591 | 0.252073 |
| C | 0.082362 | 0.069549 | -0.236763 |
| C | -1.148035 | -0.707038 | 0.252218 |
| C | -2.469119 | -0.102280 | -0.230662 |
| H | 1.387760 | -1.651495 | -0.028384 |
| H | 1.450437 | -0.565438 | 1.360449 |
| O | 0.034509 | 1.442235 | 0.137765 |
| H | 0.108485 | 0.078635 | -1.332724 |
| H | -1.066480 | -1.750050 | -0.081716 |
| H | -1.132535 | -0.738623 | 1.352621 |
| H | -2.542125 | -0.141971 | -1.322974 |
| H | -2.543419 | 0.947027 | 0.066388 |
| H | -3.326128 | -0.642230 | 0.183307 |
| H | -0.002207 | 1.485272 | 1.104015 |

Rotational constants (GHz): 7.5356100 1.9578000 1.6930200

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 98.7400 | 119.2647 | 192.5412 |
| 219.4588 | 299.9980 | 312.5169 |
| 386.4673 | 453.7988 | 517.8246 |
| 773.8026 | 793.4936 | 870.2764 |
| 969.1414 | 998.4100 | 1046.7189 |
| 1070.1444 | 1107.5559 | 1128.2057 |
| 1158.4349 | 1218.3029 | 1268.4701 |
| 1311.5635 | 1360.9372 | 1388.9588 |
| 1398.1856 | 1421.7754 | 1433.7636 |
| 1496.1421 | 1508.7467 | 1522.7062 |
| 2889.2036 | 2924.1233 | 3007.6561 |
| 3051.1521 | 3054.6750 | 3077.2191 |
| 3118.3264 | 3137.2255 | 3786.4418 |

Zero-point correction (Hartree): 0.127332

C4H9O2.l-5Hshift.a.m

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.19837493

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| C | 1.572903 | -0.606714 | -0.384219 |
| C | 1.144216 | 0.426171 | 0.638646 |
| C | -0.341175 | 0.769947 | 0.458882 |
| C | -1.156632 | -0.541897 | 0.521857 |
| O | -0.731491 | -1.483949 | -0.416632 |
| H | 1.714595 | -0.221451 | -1.393739 |
| H | 2.358994 | -1.297596 | -0.076370 |
| H | 1.727256 | 1.350829 | 0.528697 |
| H | 1.301030 | 0.057394 | 1.658161 |
| O | -0.457566 | 1.426675 | -0.794274 |
| H | -0.681705 | 1.424930 | 1.278825 |
| H | -2.213495 | -0.308511 | 0.303183 |
| H | -1.117632 | -0.922160 | 1.558894 |
| H | 0.487467 | -1.302145 | -0.503818 |
| H | -1.379933 | 1.391859 | -1.077583 |

Rotational constants (GHz): 3.9174100 3.7483500 2.6305700

Vibrational harmonic frequencies (cm-1):

| | | |
|------------|-----------|-----------|
| i1547.0177 | 98.0247 | 168.2898 |
| 217.1250 | 365.2133 | 378.7708 |
| 408.4126 | 532.7770 | 582.2443 |
| 761.8073 | 813.3334 | 851.5564 |
| 905.7859 | 985.8141 | 1016.2609 |
| 1047.6855 | 1100.4562 | 1106.6863 |
| 1148.1946 | 1192.9838 | 1200.1209 |
| 1236.3233 | 1267.3350 | 1348.2848 |
| 1355.8308 | 1396.5807 | 1413.9482 |
| 1461.1978 | 1483.7895 | 1511.4105 |
| 1552.1122 | 2948.1255 | 2982.5283 |
| 2985.2830 | 3034.0491 | 3092.1220 |

3109.4252 3195.2790 3823.1230
Zero-point correction (Hartree): 0.123199

C4H9O2.1-5Hshift.a.p

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.19680382

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| C | 1.565627 | -0.639374 | -0.371971 |
| C | 1.135874 | 0.384802 | 0.656484 |
| C | -0.344520 | 0.764569 | 0.451683 |
| C | -1.191519 | -0.522361 | 0.478863 |
| O | -0.738856 | -1.494138 | -0.419319 |
| H | 1.702066 | -0.251916 | -1.381711 |
| H | 2.354298 | -1.329366 | -0.069707 |
| H | 1.751842 | 1.295845 | 0.592014 |
| H | 1.264276 | -0.008301 | 1.671905 |
| O | -0.556514 | 1.394667 | -0.804286 |
| H | -0.683484 | 1.412269 | 1.277077 |
| H | -2.217546 | -0.252417 | 0.188200 |
| H | -1.213511 | -0.890517 | 1.520121 |
| H | 0.474343 | -1.330060 | -0.489996 |
| H | -0.062096 | 2.224419 | -0.809419 |

Rotational constants (GHz): 3.8622600 3.7845700 2.6004500

Vibrational harmonic frequencies (cm-1):

| | | |
|------------|-----------|-----------|
| i1566.7199 | 138.9016 | 190.1241 |
| 278.1793 | 362.2591 | 375.6316 |
| 403.4478 | 530.7005 | 583.9544 |
| 753.6060 | 819.8496 | 841.3623 |
| 907.1314 | 973.0304 | 1013.5580 |
| 1053.7891 | 1085.7742 | 1115.8250 |
| 1141.7348 | 1184.1691 | 1205.9021 |
| 1237.1840 | 1266.3320 | 1332.8479 |
| 1372.5889 | 1384.4811 | 1428.0509 |
| 1463.6774 | 1486.5280 | 1504.0015 |
| 1556.6548 | 2957.6163 | 2987.1702 |
| 3002.4425 | 3032.6258 | 3076.1790 |
| 3109.0156 | 3193.2363 | 3816.0335 |

Zero-point correction (Hartree): 0.123398

C4H9O2.1-5Hshift.a.t

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.20327693

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| C | -1.606042 | 0.568650 | -0.363361 |
| C | -1.164559 | -0.541518 | 0.567481 |
| C | 0.360713 | -0.790536 | 0.442689 |
| C | 1.075374 | 0.562073 | 0.644386 |
| O | 0.710528 | 1.426462 | -0.402022 |
| H | -1.780559 | 0.270528 | -1.398389 |
| H | -2.374538 | 1.246323 | 0.010265 |
| H | -1.675443 | -1.482323 | 0.325032 |
| H | -1.399712 | -0.292175 | 1.608546 |
| O | 0.697812 | -1.318396 | -0.825975 |
| H | 0.685370 | -1.518450 | 1.195201 |
| H | 2.160615 | 0.404142 | 0.568082 |
| H | 0.852905 | 0.980243 | 1.639463 |
| H | -0.512799 | 1.283342 | -0.460883 |
| H | 0.784526 | -0.548160 | -1.410502 |

Rotational constants (GHz): 4.0157300 3.7008300 2.6969900

Vibrational harmonic frequencies (cm-1):

| | | |
|------------|-----------|-----------|
| i1574.8687 | 145.0869 | 203.1456 |
| 366.6114 | 383.4557 | 445.0998 |
| 519.8787 | 544.1952 | 587.8509 |
| 761.0761 | 814.5297 | 827.4925 |
| 905.6490 | 981.0594 | 1015.8791 |
| 1049.7524 | 1080.4662 | 1118.5508 |
| 1139.3961 | 1192.1541 | 1228.1494 |
| 1240.1956 | 1283.0195 | 1315.1330 |
| 1356.9462 | 1375.9901 | 1435.9368 |
| 1461.6360 | 1485.3975 | 1498.4655 |
| 1549.0350 | 2987.5360 | 3036.7392 |
| 3046.6473 | 3074.1601 | 3088.9542 |
| 3104.1989 | 3185.9040 | 3745.8345 |

Zero-point correction (Hartree): 0.124345

C4H9O2.1-5Hshift.b.m

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.19935731

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| C | 1.619073 | -0.996060 | -0.065069 |
| C | 0.152830 | -1.245877 | 0.213780 |
| C | -0.702977 | -0.094068 | -0.332025 |

| | | | |
|---|-----------|-----------|-----------|
| C | -0.158508 | 1.233987 | 0.246889 |
| O | 1.183423 | 1.427177 | -0.095009 |
| H | 1.949683 | -1.215788 | -1.081997 |
| H | 2.324160 | -1.351724 | 0.687022 |
| H | -0.189371 | -2.184649 | -0.242468 |
| H | -0.036577 | -1.322566 | 1.290504 |
| H | -0.600036 | -0.054907 | -1.428670 |
| O | -2.046967 | -0.325052 | 0.054144 |
| H | -0.731402 | 2.070140 | -0.186785 |
| H | -0.334252 | 1.235344 | 1.336529 |
| H | 1.672696 | 0.308406 | -0.022156 |
| H | -2.609057 | 0.310849 | -0.406509 |
| Rotational constants (GHz): 4.6655900 3.1840400 2.0504900 | | | |
| Vibrational harmonic frequencies (cm-1): | | | |
| i1588.2527 | 156.9169 | 206.9635 | |
| 281.7927 | 352.7101 | 412.1147 | |
| 437.9581 | 472.3087 | 507.4428 | |
| 632.4366 | 829.8097 | 854.2178 | |
| 964.9160 | 985.1302 | 1067.0612 | |
| 1079.2558 | 1091.8620 | 1126.7976 | |
| 1149.9191 | 1187.2068 | 1197.2752 | |
| 1241.7424 | 1274.4004 | 1325.5839 | |
| 1338.8324 | 1377.2353 | 1434.2653 | |
| 1471.2025 | 1492.5818 | 1510.7242 | |
| 1561.7732 | 2967.0095 | 2989.5890 | |
| 3013.4469 | 3032.9110 | 3088.6219 | |
| 3101.7429 | 3182.8925 | 3821.7981 | |
| Zero-point correction (Hartree): 0.123523 | | | |

C4H9O2.1-5Hshift.b.p

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.19872153

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| C | 1.599694 | -1.031951 | -0.049974 |
| C | 0.126793 | -1.244768 | 0.223901 |
| C | -0.706594 | -0.070332 | -0.332664 |
| C | -0.134858 | 1.242880 | 0.232542 |
| O | 1.213631 | 1.396371 | -0.109996 |
| H | 1.930674 | -1.265160 | -1.063717 |
| H | 2.292451 | -1.398765 | 0.708249 |
| H | -0.226526 | -2.184729 | -0.227285 |
| H | -0.068549 | -1.309638 | 1.300169 |
| H | -0.603869 | -0.039887 | -1.429418 |
| O | -2.068338 | -0.134689 | 0.056243 |
| H | -0.690287 | 2.081669 | -0.211385 |
| H | -0.308886 | 1.261178 | 1.322059 |
| H | 1.681459 | 0.269269 | -0.016190 |
| H | -2.479016 | -0.882369 | -0.395290 |
| Rotational constants (GHz): 4.6717300 3.1825400 2.0506400 | | | |
| Vibrational harmonic frequencies (cm-1): | | | |
| i1580.7538 | 155.9589 | 204.5109 | |
| 233.3456 | 353.5572 | 410.7069 | |
| 437.3185 | 471.4555 | 509.7467 | |
| 634.3522 | 829.8063 | 853.2485 | |
| 966.2177 | 983.7386 | 1050.8810 | |
| 1080.9956 | 1104.2351 | 1127.0511 | |
| 1147.6242 | 1185.4775 | 1209.2112 | |
| 1228.4846 | 1262.1903 | 1311.6543 | |
| 1360.9193 | 1386.0803 | 1427.8495 | |
| 1469.2994 | 1492.2175 | 1510.7792 | |
| 1561.8487 | 2974.7718 | 2994.9985 | |
| 3006.7611 | 3040.6038 | 3086.1380 | |
| 3101.2558 | 3182.6440 | 3827.8997 | |
| Zero-point correction (Hartree): 0.123422 | | | |

C4H9O2.1-5Hshift.b.t

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.19992271

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| C | 1.614106 | -1.010503 | -0.050146 |
| C | 0.144555 | -1.248922 | 0.211393 |
| C | -0.706451 | -0.088350 | -0.349505 |
| C | -0.159187 | 1.245413 | 0.215638 |
| O | 1.195452 | 1.417178 | -0.074662 |
| H | 1.952672 | -1.233932 | -1.063375 |
| H | 2.310031 | -1.365294 | 0.710733 |
| H | -0.203708 | -2.185533 | -0.244330 |
| H | -0.044292 | -1.324535 | 1.291243 |
| H | -0.609502 | -0.062494 | -1.440775 |
| O | -2.088009 | -0.240045 | -0.091453 |
| H | -0.716683 | 2.067849 | -0.255382 |
| H | -0.368300 | 1.276514 | 1.303625 |
| H | 1.671330 | 0.296153 | -0.005027 |

| | | | | |
|---|-----------|-----------|-----------|-----------|
| H | -2.209216 | -0.271625 | 0.867923 | |
| Rotational constants (GHz): | 4.6424800 | | 3.1606900 | 2.0447000 |
| Vibrational harmonic frequencies (cm-1): | | | | |
| i1584.9478 | | 155.8089 | | 201.1334 |
| 307.8724 | | 382.5054 | | 409.0423 |
| 432.2055 | | 469.1175 | | 502.3575 |
| 630.5486 | | 828.2139 | | 840.5110 |
| 964.1335 | | 990.0476 | | 1071.3902 |
| 1082.5326 | | 1090.8471 | | 1120.9170 |
| 1148.5593 | | 1182.2133 | | 1202.3840 |
| 1238.5144 | | 1268.9214 | | 1319.2117 |
| 1366.5162 | | 1382.9899 | | 1423.9190 |
| 1469.0074 | | 1489.8318 | | 1508.6636 |
| 1561.9578 | | 2919.8367 | | 3021.5878 |
| 3033.7937 | | 3060.3329 | | 3083.1772 |
| 3102.9385 | | 3184.7282 | | 3792.1132 |
| Zero-point correction (Hartree): 0.123569 | | | | |

C4H9O2.mmm

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.21972585
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | | |
|---|-----------|-----------|-----------|-----------|
| O | -1.904728 | 0.593514 | -0.333812 | |
| C | -1.353501 | -0.665348 | -0.327400 | |
| C | -0.264206 | -0.837204 | 0.738861 | |
| C | 0.951442 | 0.076904 | 0.475815 | |
| C | 1.876479 | -0.429522 | -0.627685 | |
| H | 2.682194 | 0.291294 | -0.791808 | |
| O | 0.536647 | 1.387516 | 0.101488 | |
| H | 1.529834 | 0.127327 | 1.414181 | |
| H | -2.199847 | -1.342483 | -0.084921 | |
| H | -1.020036 | -0.968349 | -1.335139 | |
| H | -0.707574 | -0.579413 | 1.708764 | |
| H | 0.058012 | -1.883821 | 0.798394 | |
| H | 2.321799 | -1.390754 | -0.351545 | |
| H | 1.337793 | -0.547654 | -1.572737 | |
| H | -0.318806 | 1.576622 | 0.515854 | |
| Rotational constants (GHz): | 5.5039600 | | 2.6608400 | 2.2400400 |
| Vibrational harmonic frequencies (cm-1): | | | | |
| 80.9743 | | 163.5466 | | 234.8332 |
| 241.2926 | | 305.1810 | | 358.7212 |
| 416.2330 | | 446.4729 | | 599.6916 |
| 779.0010 | | 873.2231 | | 892.5304 |
| 960.2383 | | 966.0241 | | 1038.2386 |
| 1080.6907 | | 1113.5977 | | 1139.6913 |
| 1162.8285 | | 1224.3597 | | 1298.3066 |
| 1335.2368 | | 1360.1299 | | 1384.2440 |
| 1407.2537 | | 1412.1992 | | 1449.7455 |
| 1485.9038 | | 1500.5392 | | 1515.5632 |
| 2905.9089 | | 2967.8397 | | 2980.0350 |
| 3045.4153 | | 3054.3953 | | 3090.5356 |
| 3128.5796 | | 3135.1076 | | 3763.6374 |
| Zero-point correction (Hartree): 0.128256 | | | | |

C4H9O2.mmp

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.21436969
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | | |
|--|-----------|-----------|-----------|-----------|
| O | -1.971426 | 0.613508 | -0.449699 | |
| C | -1.411322 | -0.615312 | -0.228190 | |
| C | -0.330819 | -0.632836 | 0.869243 | |
| C | 0.985858 | 0.041920 | 0.463129 | |
| C | 1.722100 | -0.660950 | -0.681301 | |
| H | 2.677163 | -0.161145 | -0.883699 | |
| O | 0.663823 | 1.387491 | 0.126134 | |
| H | 1.641365 | 0.024086 | 1.351620 | |
| H | -2.260537 | -1.234910 | 0.132255 | |
| H | -1.063677 | -1.102756 | -1.157495 | |
| H | -0.733624 | -0.114573 | 1.745508 | |
| H | -0.121634 | -1.670565 | 1.157338 | |
| H | 1.945869 | -1.703238 | -0.430260 | |
| H | 1.133990 | -0.641453 | -1.603346 | |
| H | 1.447008 | 1.799632 | -0.260693 | |
| Rotational constants (GHz): | 5.2736600 | | 2.5514500 | 2.2074800 |
| Vibrational harmonic frequencies (cm-1): | | | | |
| 39.8806 | | 115.3951 | | 242.9714 |
| 265.2100 | | 287.8256 | | 347.7360 |
| 396.8322 | | 431.5861 | | 587.2725 |
| 774.7520 | | 870.3011 | | 886.7968 |
| 954.6258 | | 971.0043 | | 1045.8956 |
| 1077.4763 | | 1092.3633 | | 1132.0762 |
| 1168.5419 | | 1231.7484 | | 1254.7822 |
| 1354.1060 | | 1378.3241 | | 1389.2711 |

| | | |
|-----------|-----------|-----------|
| 1415.4707 | 1423.5739 | 1432.9559 |
| 1472.3019 | 1508.1678 | 1515.5248 |
| 2895.5715 | 2958.6335 | 2960.0472 |
| 3040.4420 | 3052.8581 | 3104.4225 |
| 3108.3484 | 3131.3195 | 3817.5062 |

Zero-point correction (Hartree): 0.127882

C4H9O2.mmt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.22079580
Electronic state : 2-A
Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -1.698016 | 0.680458 | -0.658087 |
| C | -1.503207 | -0.534039 | -0.044068 |
| C | -0.340951 | -0.591247 | 0.960161 |
| C | 0.996005 | -0.030574 | 0.436067 |
| C | 1.509072 | -0.733597 | -0.827929 |
| H | 2.484475 | -0.323538 | -1.102492 |
| O | 0.923993 | 1.378222 | 0.251432 |
| H | 1.739845 | -0.178257 | 1.229390 |
| H | -2.446214 | -0.916041 | 0.387553 |
| H | -1.298279 | -1.216245 | -0.899792 |
| H | -0.621949 | -0.015918 | 1.849769 |
| H | -0.217745 | -1.634873 | 1.277456 |
| H | 1.619521 | -1.813587 | -0.673833 |
| H | 0.836738 | -0.574561 | -1.678212 |
| H | 0.130275 | 1.540328 | -0.281986 |

Rotational constants (GHz): 4.8438400 2.6602900 2.3924100
Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 85.9337 | 176.1001 | 237.0164 |
| 269.8572 | 366.1143 | 379.1915 |
| 443.2586 | 487.5697 | 599.3948 |
| 749.7382 | 791.5619 | 878.1339 |
| 945.5334 | 961.0002 | 1031.9560 |
| 1070.9829 | 1083.0871 | 1151.6666 |
| 1180.7849 | 1205.3150 | 1276.1035 |
| 1340.9285 | 1378.5883 | 1385.9657 |
| 1395.5302 | 1421.5661 | 1453.8794 |
| 1483.4265 | 1505.3832 | 1519.8590 |
| 2880.7501 | 2964.5424 | 3037.3917 |
| 3041.9514 | 3051.0409 | 3092.5234 |
| 3109.7035 | 3132.6650 | 3751.1682 |

Zero-point correction (Hartree): 0.128300

C4H9O2.mpm

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.21702369
Electronic state : 2-A
Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 2.174630 | 0.629482 | -0.127472 |
| C | 1.637817 | -0.580116 | 0.220307 |
| C | 0.232721 | -0.876865 | -0.321564 |
| C | -0.880302 | -0.033189 | 0.325657 |
| C | -0.810936 | 1.443693 | -0.043159 |
| H | -1.619615 | 1.989348 | 0.450942 |
| O | -2.164260 | -0.489925 | -0.099757 |
| H | -0.791841 | -0.130335 | 1.422922 |
| H | 2.353317 | -1.318199 | -0.205156 |
| H | 1.698472 | -0.745555 | 1.314351 |
| H | 0.218428 | -0.724671 | -1.406749 |
| H | 0.018808 | -1.939836 | -0.137047 |
| H | 0.146387 | 1.882761 | 0.250012 |
| H | -0.924910 | 1.562847 | -1.125134 |
| H | -2.257809 | -1.413950 | 0.166243 |

Rotational constants (GHz): 6.4891900 2.2015500 1.7698000
Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 72.3725 | 141.7699 | 224.9709 |
| 252.6717 | 312.8982 | 328.1963 |
| 393.4463 | 455.6525 | 525.7479 |
| 690.5923 | 848.7892 | 886.9794 |
| 936.8914 | 973.8857 | 1035.9364 |
| 1075.4765 | 1096.7564 | 1143.7802 |
| 1175.9804 | 1225.8510 | 1287.2915 |
| 1328.5464 | 1349.4389 | 1381.9025 |
| 1403.1825 | 1411.9699 | 1451.4681 |
| 1483.8732 | 1493.0246 | 1514.9402 |
| 2886.3344 | 2933.9863 | 2952.7692 |
| 3021.7047 | 3056.6013 | 3093.3715 |
| 3132.5874 | 3139.2638 | 3811.7641 |

Zero-point correction (Hartree): 0.127424

C4H9O2.mpp

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.21762412
Electronic state : 2-A

```

Cartesian coordinates (Angs):
O      2.172392      0.658058      -0.089904
C      1.647332      -0.571123      0.209685
C      0.247598      -0.869925      -0.335915
C      -0.865371     -0.046233      0.320268
C      -0.848235     1.429101      -0.080047
H      -1.649301     1.978088      0.430547
O      -2.087910     -0.673207     -0.071838
H      -0.745273     -0.119350     1.416779
H      2.374883     -1.291382     -0.224953
H      1.713054     -0.762335     1.299720
H      0.233369     -0.704877     -1.419517
H      0.021555     -1.929032     -0.163538
H      0.103321     1.904685     0.174138
H      -0.998845     1.525276     -1.160146
H      -2.816557     -0.130803     0.256952
Rotational constants (GHz):      6.4323900      2.2119300      1.7713700
Vibrational harmonic frequencies (cm-1):
66.6140      143.9507      235.0130
267.9399      300.6094      322.3666
389.0974      447.7978      511.6751
611.0027      833.9517      888.8938
927.6082      981.7305      1028.2665
1090.4110     1100.5294     1130.7166
1175.5956     1241.0078     1286.2933
1339.8182     1365.7967     1377.4580
1390.5430     1427.0998     1438.6266
1486.9930     1503.8366     1513.6590
2890.4737     2928.5801     2947.8256
3036.7537     3052.6731     3100.1768
3108.4220     3131.8067     3813.4997
Zero-point correction (Hartree): 0.127202

```

C4H9O2.mpt

```

-----
E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.21776953
Electronic state : 2-A
Cartesian coordinates (Angs):
O      2.172511      0.638096      -0.144901
C      1.644347      -0.570684      0.220602
C      0.238644      -0.885317      -0.307281
C      -0.879812     -0.045360      0.334556
C      -0.820454     1.436566      -0.037058
H      -1.632711     1.979157      0.454991
O      -2.157157     -0.603862      0.024253
H      -0.801010     -0.144346      1.425503
H      2.363391     -1.310773     -0.195266
H      1.712195     -0.719738      1.316513
H      0.230782     -0.742942     -1.396531
H      0.015543     -1.940735     -0.110619
H      0.133518     1.890453      0.247028
H      -0.926979     1.563596     -1.122131
H      -2.313911     -0.459778     -0.919221
Rotational constants (GHz):      6.4383400      2.1909500      1.7671000
Vibrational harmonic frequencies (cm-1):
71.0853      141.4294      229.8113
268.7180      302.7274      326.5640
401.2542      454.2308      518.9250
671.8723      834.7005      887.2234
930.7748      974.1332      1027.8447
1088.6084     1110.4897     1115.2613
1173.6200     1219.8763     1295.1628
1341.4784     1356.0239     1374.9794
1399.1646     1421.6964     1434.1457
1484.0385     1502.0469     1509.8065
2886.4852     2935.4753     3032.5497
3035.9116     3045.1235     3088.9688
3109.4315     3134.7660     3796.6901
Zero-point correction (Hartree): 0.127425

```

C4H9O2.mtm

```

-----
E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.21989739
Electronic state : 2-A
Cartesian coordinates (Angs):
O      2.032768      0.471785      -0.569105
C      1.626095      -0.465968     -0.343370
C      0.197059     -1.004163      0.129790
C      -0.790401     0.094971     -0.307079
C      -2.240086     -0.340529     -0.137397
H      -2.916469     0.436979     -0.502513
O      -0.608259     1.285218      0.460544
H      -0.605014     0.313575     -1.369259
H      2.363108     -1.276230      0.478500
H      1.623253      0.107144      1.297887

```


| | | | | |
|--|-----------|-----------|-----------|--|
| H | 0.218106 | -1.795537 | -0.629737 | |
| H | -0.135012 | -1.466377 | 1.067943 | |
| H | -2.438519 | -1.265104 | -0.689417 | |
| H | -2.459937 | -0.514857 | 0.921147 | |
| H | 0.198411 | 1.698508 | 0.121831 | |
| Rotational constants (GHz): | 6.5998300 | 2.3009000 | 1.9477300 | |
| Vibrational harmonic frequencies (cm-1): | | | | |
| 83.6324 | 125.5083 | | 207.3916 | |
| 242.0535 | 316.4745 | | 398.9292 | |
| 466.9771 | 496.1996 | | 586.4499 | |
| 747.0636 | 845.0415 | | 905.3081 | |
| 949.4398 | 958.1572 | | 1050.7953 | |
| 1057.3472 | 1120.6576 | | 1137.3278 | |
| 1175.6741 | 1229.1296 | | 1247.8760 | |
| 1303.3130 | 1356.4344 | | 1397.9425 | |
| 1411.9043 | 1414.7708 | | 1444.3557 | |
| 1492.1655 | 1499.4320 | | 1514.9853 | |
| 2873.7438 | 2984.9919 | | 3006.9904 | |
| 3040.6005 | 3050.9179 | | 3087.3016 | |
| 3122.8039 | 3134.8921 | | 3795.2408 | |
| Zero-point correction (Hartree): | 0.128216 | | | |

C4H9O2.mtp

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.22072038
Electronic state : 2-A
Cartesian coordinates (Angs):

| | | | | |
|--|-----------|-----------|-----------|--|
| O | 2.202750 | -0.100428 | -0.818513 | |
| C | 1.667995 | 0.015178 | 0.434315 | |
| C | 0.290913 | -0.642909 | 0.608853 | |
| C | -0.771371 | 0.017437 | -0.266756 | |
| C | -2.118711 | -0.702119 | -0.213375 | |
| H | -2.858951 | -0.190999 | -0.839943 | |
| O | -0.887857 | 1.364413 | 0.209675 | |
| H | -0.395398 | 0.018586 | -1.301726 | |
| H | 2.388533 | -0.301889 | 1.211317 | |
| H | 1.544184 | 1.110415 | 0.583388 | |
| H | 0.366125 | -1.707619 | 0.360354 | |
| H | -0.013408 | -0.568493 | 1.660716 | |
| H | -2.032356 | -1.732032 | -0.575974 | |
| H | -2.500633 | -0.723363 | 0.812519 | |
| H | -1.430195 | 1.857993 | -0.418169 | |
| Rotational constants (GHz): | 6.3204500 | 2.0848300 | 1.8906900 | |
| Vibrational harmonic frequencies (cm-1): | | | | |
| 86.3633 | 135.3368 | | 221.9341 | |
| 248.2165 | 286.7181 | | 330.0626 | |
| 419.7995 | 470.9214 | | 533.9738 | |
| 707.5505 | 845.4778 | | 883.4353 | |
| 938.9750 | 979.3458 | | 1065.9114 | |
| 1089.7079 | 1096.6447 | | 1115.1401 | |
| 1169.5577 | 1220.8550 | | 1285.1828 | |
| 1313.0877 | 1357.0261 | | 1380.7713 | |
| 1401.2365 | 1422.8264 | | 1439.1452 | |
| 1480.5731 | 1506.1100 | | 1512.5717 | |
| 2893.0990 | 2956.0034 | | 3004.7616 | |
| 3038.9478 | 3048.5455 | | 3097.5629 | |
| 3107.2950 | 3124.0126 | | 3825.9375 | |
| Zero-point correction (Hartree): | 0.127670 | | | |

C4H9O2.mtt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.22019337
Electronic state : 2-A
Cartesian coordinates (Angs):

| | | | | |
|--|-----------|-----------|-----------|--|
| O | 2.222728 | -0.181297 | -0.788901 | |
| C | 1.666145 | 0.068854 | 0.434383 | |
| C | 0.293939 | -0.586572 | 0.652897 | |
| C | -0.771476 | 0.003553 | -0.278969 | |
| C | -2.110909 | -0.725787 | -0.192007 | |
| H | -2.841552 | -0.258468 | -0.858089 | |
| O | -0.926691 | 1.407031 | -0.037912 | |
| H | -0.388585 | -0.055310 | -1.303981 | |
| H | 2.376328 | -0.146639 | 1.254323 | |
| H | 1.521915 | 1.171997 | 0.452135 | |
| H | 0.383504 | -1.667420 | 0.490308 | |
| H | -0.011595 | -0.445572 | 1.700348 | |
| H | -2.008971 | -1.779265 | -0.472488 | |
| H | -2.509236 | -0.692507 | 0.830846 | |
| H | -1.356293 | 1.507024 | 0.823281 | |
| Rotational constants (GHz): | 6.2796100 | 2.0714500 | 1.8760400 | |
| Vibrational harmonic frequencies (cm-1): | | | | |
| 94.6663 | 132.5395 | | 223.1152 | |
| 251.2397 | 327.0850 | | 342.6370 | |
| 429.3571 | 464.4995 | | 537.0600 | |

| | | |
|-----------|-----------|-----------|
| 712.9771 | 842.4355 | 886.3505 |
| 933.2379 | 978.5799 | 1061.4726 |
| 1078.3403 | 1095.4006 | 1137.0719 |
| 1154.1419 | 1218.9617 | 1282.9022 |
| 1336.3020 | 1345.1784 | 1385.4260 |
| 1406.4097 | 1417.9727 | 1436.2493 |
| 1485.5803 | 1506.2346 | 1510.6011 |
| 2888.0088 | 2957.0172 | 3021.2553 |
| 3032.9461 | 3073.3399 | 3083.2930 |
| 3107.0173 | 3132.4551 | 3789.6446 |

Zero-point correction (Hartree): 0.127803

C4H9O2.pmm

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.21757515

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 1.965381 | 0.706486 | -0.353912 |
| C | 1.424592 | -0.543643 | -0.202142 |
| C | 0.318770 | -0.662051 | 0.853698 |
| C | -1.031266 | -0.075450 | 0.397551 |
| C | -0.978390 | 1.411875 | 0.067821 |
| H | -1.968744 | 1.755769 | -0.243482 |
| O | -1.501711 | -0.735608 | -0.782272 |
| H | -1.752222 | -0.222953 | 1.218863 |
| H | 1.091573 | -0.951273 | -1.174042 |
| H | 2.289178 | -1.180587 | 0.086084 |
| H | 0.173507 | -1.724452 | 1.098433 |
| H | 0.648142 | -0.164269 | 1.773364 |
| H | -0.659306 | 1.990596 | 0.939180 |
| H | -0.275895 | 1.609358 | -0.747393 |
| H | -1.657825 | -1.663608 | -0.563100 |

Rotational constants (GHz): 5.1070500 2.5620100 2.1766900

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 82.3350 | 121.8352 | 221.5620 |
| 236.5036 | 322.1369 | 343.6338 |
| 420.3112 | 425.9620 | 520.5046 |
| 704.8677 | 793.9042 | 866.8124 |
| 922.9606 | 979.5329 | 1041.4016 |
| 1073.3334 | 1087.5231 | 1126.6513 |
| 1165.9942 | 1231.5238 | 1286.0113 |
| 1339.7831 | 1363.2573 | 1381.8717 |
| 1401.3113 | 1414.7734 | 1451.2600 |
| 1480.0819 | 1492.1345 | 1515.4288 |
| 2892.8440 | 2966.3106 | 2975.6539 |
| 3022.7614 | 3056.4454 | 3085.8035 |
| 3130.9685 | 3138.0810 | 3810.0854 |

Zero-point correction (Hartree): 0.127336

C4H9O2.pmp

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.21870188

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 1.897735 | 0.793637 | -0.436618 |
| C | 1.487741 | -0.471557 | -0.122786 |
| C | 0.353207 | -0.584390 | 0.909209 |
| C | -1.024980 | -0.153271 | 0.391711 |
| C | -1.145861 | 1.340445 | 0.082029 |
| H | -2.154338 | 1.572923 | -0.283101 |
| O | -1.272161 | -0.952513 | -0.770812 |
| H | -1.762582 | -0.406168 | 1.171982 |
| H | 1.116905 | -0.890801 | -1.084297 |
| H | 2.347923 | -1.112040 | 0.150036 |
| H | 0.288648 | -1.635648 | 1.216000 |
| H | 0.610845 | -0.002211 | 1.801189 |
| H | -0.977474 | 1.938447 | 0.983793 |
| H | -0.415185 | 1.648709 | -0.667822 |
| H | -2.079972 | -0.629566 | -1.189328 |

Rotational constants (GHz): 4.9717900 2.5802500 2.2172900

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 74.3685 | 157.4975 | 232.0970 |
| 259.7976 | 283.8770 | 337.0803 |
| 414.4334 | 432.8486 | 592.9134 |
| 720.0518 | 784.9823 | 873.1252 |
| 936.7660 | 989.4080 | 1051.5342 |
| 1083.7211 | 1101.5673 | 1109.8800 |
| 1173.8787 | 1239.0093 | 1257.0922 |
| 1312.7661 | 1381.8653 | 1390.3798 |
| 1395.9667 | 1425.3483 | 1434.4658 |
| 1480.3192 | 1504.8875 | 1514.0109 |
| 2891.4038 | 2948.5284 | 2970.8381 |
| 3037.7421 | 3051.6140 | 3097.8112 |
| 3106.2128 | 3156.2336 | 3825.4209 |

Zero-point correction (Hartree): 0.127650

C4H9O2.pmt

```

-----
E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.21739443
Electronic state : 2-A
Cartesian coordinates (Angs):
  O      1.849813      0.788675      -0.418142
  C      1.471581      -0.502495      -0.155315
  C      0.348335      -0.649233      0.884675
  C     -1.022501      -0.146512      0.389019
  C     -1.066116      1.357221      0.121381
  H     -2.063420      1.646606      -0.223523
  O     -1.458863      -0.891721      -0.750544
  H     -1.754818      -0.384548      1.170862
  H      1.244966      -1.075665      -1.073072
  H      2.389608      -0.968686      0.263433
  H      0.253212      -1.712186      1.135660
  H      0.632502      -0.110324      1.795999
  H     -0.827242      1.929882      1.022698
  H     -0.335278      1.643908      -0.645880
  H     -1.054929      -0.498512      -1.535256
Rotational constants (GHz):      4.9772200      2.5950400      2.2235300
Vibrational harmonic frequencies (cm-1):
  63.0039      132.3104      226.2643
 254.4679      289.6434      334.0108
 409.0232      424.7864      586.9976
 770.2392      830.2442      882.0061
 902.5253      956.2004      1020.7057
1058.7336      1075.9987      1121.4601
1155.2673      1208.5032      1300.6620
1320.3778      1348.2559      1386.1060
1417.1953      1423.9649      1433.1398
1474.2519      1498.4656      1507.8899
2894.6543      2964.0533      3030.8124
3044.2215      3056.1413      3101.0812
3106.6690      3131.0016      3812.0334
Zero-point correction (Hartree): 0.127471
    
```

C4H9O2.ppm

```

-----
E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.21740955
Electronic state : 2-A
Cartesian coordinates (Angs):
  O     -2.211326      -0.047060      -0.804605
  C     -1.664905      0.124922      0.439328
  C     -0.316346      -0.572358      0.654362
  C      0.793641      -0.055325      -0.277724
  C      1.238210      1.368901      0.035915
  H      2.046201      1.662049      -0.639536
  O      1.961603      -0.866274      -0.161993
  H      0.404531      -0.090831      -1.309278
  H     -1.635595      1.198096      0.708647
  H     -2.419698      -0.300301      1.136648
  H      0.003010      -0.461729      1.698491
  H     -0.460016      -1.644934      0.467961
  H      0.417072      2.081991      -0.082467
  H      1.613174      1.431844      1.062938
  H      1.725501      -1.766347      -0.421897
Rotational constants (GHz):      6.1039000      2.0486100      1.8394100
Vibrational harmonic frequencies (cm-1):
  69.5223      122.2880      225.5325
 247.0090      318.9739      357.8804
 394.5572      458.6395      510.6733
 635.8683      821.5549      880.5837
 941.7964      959.4526      1038.7508
1088.3173      1119.7385      1125.4687
1170.8074      1231.6568      1287.5536
1326.9312      1367.5719      1375.6484
1395.0620      1409.4322      1452.5979
1486.6017      1498.3930      1516.9698
2890.9291      2947.2071      2978.8602
3033.3958      3054.2769      3082.6196
3127.7261      3137.7035      3812.5457
Zero-point correction (Hartree): 0.127352
    
```

C4H9O2.ppp

```

-----
E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.21724875
Electronic state : 2-A
Cartesian coordinates (Angs):
  O     -2.189044      0.040730      -0.826687
  C     -1.679520      0.038470      0.445706
  C     -0.314843      -0.636534      0.613391
  C      0.783898      -0.048491      -0.275021
  C      1.204643      1.367564      0.126222
    
```

| | | | | |
|---|-----------|-----------|-----------|--|
| H | 2.008225 | 1.729913 | -0.525881 | |
| O | 1.885996 | -0.952256 | -0.171665 | |
| H | 0.400598 | -0.030828 | -1.307351 | |
| H | -1.640427 | 1.108367 | 0.744904 | |
| H | -2.427899 | -0.387772 | 1.142367 | |
| H | -0.006902 | -0.581793 | 1.665727 | |
| H | -0.411879 | -1.698823 | 0.363865 | |
| H | 0.378213 | 2.081337 | 0.040901 | |
| H | 1.574138 | 1.378917 | 1.157096 | |
| H | 2.585255 | -0.633166 | -0.756600 | |

Rotational constants (GHz): 6.025000 2.0718500 1.8578100
 Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 58.6519 | 133.5903 | 228.3847 |
| 258.7955 | 305.2429 | 364.3554 |
| 388.3981 | 395.0293 | 466.4545 |
| 556.6179 | 813.6174 | 877.6557 |
| 938.4210 | 966.1868 | 1038.9756 |
| 1087.2624 | 1102.2471 | 1133.7991 |
| 1186.8678 | 1222.5011 | 1298.4272 |
| 1344.6154 | 1356.4946 | 1385.3734 |
| 1403.3413 | 1427.7363 | 1438.6669 |
| 1492.8295 | 1511.3213 | 1514.7574 |
| 2896.2915 | 2936.8024 | 3000.1513 |
| 3038.2865 | 3047.5609 | 3098.6595 |
| 3103.5531 | 3121.3556 | 3815.9136 |

Zero-point correction (Hartree): 0.127020

C4H9O2.ppt

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.21705837

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -2.187688 | 0.074690 | -0.807864 |
| C | -1.679908 | 0.000210 | 0.462343 |
| C | -0.305530 | -0.669804 | 0.584388 |
| C | 0.788594 | -0.038610 | -0.291303 |
| C | 1.178991 | 1.377260 | 0.139104 |
| H | 1.984994 | 1.750071 | -0.498671 |
| O | 1.935642 | -0.887253 | -0.345558 |
| H | 0.415076 | -0.010217 | -1.320380 |
| H | -1.646127 | 1.052283 | 0.819707 |
| H | -2.422366 | -0.471203 | 1.135766 |
| H | 0.003108 | -0.653393 | 1.640602 |
| H | -0.398845 | -1.722214 | 0.294003 |
| H | 0.339612 | 2.077061 | 0.067001 |
| H | 1.533849 | 1.386209 | 1.178377 |
| H | 2.314187 | -0.922429 | 0.543775 |

Rotational constants (GHz): 6.0020000 2.0622000 1.8565500

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 59.5648 | 130.8047 | 225.5125 |
| 256.3095 | 300.3516 | 366.0226 |
| 402.4210 | 428.1684 | 462.2466 |
| 553.2057 | 808.7364 | 878.4558 |
| 939.1525 | 959.5088 | 1042.8180 |
| 1074.6299 | 1091.7326 | 1146.1327 |
| 1186.8093 | 1219.6030 | 1305.1303 |
| 1351.1117 | 1357.2951 | 1370.0997 |
| 1409.4612 | 1419.0361 | 1437.2838 |
| 1491.3103 | 1506.2976 | 1514.3324 |
| 2896.8320 | 2936.4601 | 3018.3257 |
| 3032.1166 | 3078.7269 | 3092.2042 |
| 3105.8708 | 3132.4981 | 3793.9369 |

Zero-point correction (Hartree): 0.127077

C4H9O2.ptm

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.22286134

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -2.087015 | 0.647181 | -0.021727 |
| C | -1.645598 | -0.646499 | 0.127593 |
| C | -0.200753 | -0.915869 | -0.314552 |
| C | 0.822867 | 0.039322 | 0.321886 |
| C | 2.259354 | -0.367134 | 0.012085 |
| H | 2.950820 | 0.365896 | 0.436555 |
| O | 0.653630 | 1.366667 | -0.156314 |
| H | 0.681310 | 0.007844 | 1.419718 |
| H | -1.737711 | -0.819033 | 1.225120 |
| H | -2.366734 | -1.356028 | -0.318013 |
| H | 0.041527 | -1.956173 | -0.061435 |
| H | -0.133821 | -0.822778 | -1.405638 |
| H | 2.491965 | -1.351262 | 0.431358 |
| H | 2.420750 | -0.397365 | -1.070436 |

```

H      -0.296241      1.559196      -0.114979
Rotational constants (GHz):  6.7473000      2.3066500      1.8472400
Vibrational harmonic frequencies (cm-1):
  88.4359           185.4837           233.7541
 252.3471           321.5087           400.8505
 473.8608           499.2612           546.4681
 724.9765           830.9550           909.4808
 943.6715           969.0501          1053.5854
1071.9825           1084.6191          1155.3070
1188.8070           1250.6008          1287.1339
1327.7069           1364.7411          1376.4614
1399.6583           1420.2337          1465.0590
1482.5104           1499.4256          1516.2097
2865.8393           2925.9957          2962.5252
3040.9731           3051.7471          3088.5145
3125.2567           3134.7287          3744.4472
Zero-point correction (Hartree): 0.128179
    
```

C4H9O2.ptp

```

-----
E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.21622181
Electronic state : 2-A
Cartesian coordinates (Angs):
O      -2.179170      0.566126      -0.289680
C      -1.626102     -0.542883      0.288293
C      -0.222999     -0.912113     -0.222051
C       0.863518      0.003801      0.342511
C       2.261890     -0.376940     -0.150674
H       3.017250      0.300200      0.264633
O       0.520981      1.329888     -0.051364
H       0.840787     -0.079392      1.443985
H      -1.648524     -0.502558      1.394991
H      -2.326781     -1.359821      0.009518
H       0.006162     -1.947270      0.059900
H      -0.220696     -0.849290     -1.316221
H       2.528000     -1.396030      0.150143
H       2.309535     -0.309536     -1.242024
H       1.101931      1.944398      0.414956
Rotational constants (GHz):  6.8957300      2.2353700      1.8382800
Vibrational harmonic frequencies (cm-1):
  72.0646           114.6950           230.7013
 251.9303           282.1224           335.8045
 399.3200           463.7115           515.8802
 779.7627           884.5068           898.2533
 946.0179           979.7110          1058.8583
1084.3037           1120.2618          1123.4715
1176.8464           1197.6322          1300.8485
1329.2847           1359.9172          1393.7790
1410.4801           1418.8849          1434.5126
1472.2201           1506.1388          1511.2186
2890.8375           2938.9187          2956.8343
3039.4305           3048.7498          3101.5097
3107.9894           3127.0004          3820.4786
Zero-point correction (Hartree): 0.127771
    
```

C4H9O2.tmm

```

-----
E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.21773280
Electronic state : 2-A
Cartesian coordinates (Angs):
O      -2.646945     -0.008762     -0.119462
C      -1.324783     -0.205353     -0.394232
C      -0.391587     -0.077255      0.822320
C       1.086468      0.117556      0.443007
C       1.708085     -1.071479     -0.284539
H       2.764883     -0.875239     -0.483931
O       1.240974      1.246373     -0.424761
H       1.652694      0.285101      1.373526
H      -1.158662     -1.138006     -0.963366
H      -1.054021      0.608913     -1.104293
H      -0.735045      0.786626      1.406318
H      -0.498164     -0.955608      1.470568
H       1.629605     -1.979780      0.320678
H       1.214736     -1.248870     -1.244583
H       0.962642      2.035155      0.059527
Rotational constants (GHz):  6.3550400      1.9907500      1.8013200
Vibrational harmonic frequencies (cm-1):
  97.2229           125.9987           212.6024
 238.8888           339.1944           353.6108
 389.1318           439.6556           610.8041
 721.8209           827.1211           923.9821
 944.1032           974.1728          1044.0490
1077.6153           1105.5104          1119.9174
1163.0408           1217.3342          1287.8666
    
```

| | | |
|-----------|-----------|-----------|
| 1314.1162 | 1349.4815 | 1381.0742 |
| 1405.0867 | 1413.1013 | 1448.7872 |
| 1494.9274 | 1502.5391 | 1519.1216 |
| 2874.2752 | 2964.4341 | 2984.2650 |
| 3040.7412 | 3059.2080 | 3085.6062 |
| 3134.2244 | 3137.8554 | 3809.5119 |

Zero-point correction (Hartree): 0.127878

C4H9O2.tmp

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.21742346

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -2.663509 | -0.046113 | -0.111418 |
| C | -1.333413 | -0.104214 | -0.415252 |
| C | -0.400594 | -0.096887 | 0.807864 |
| C | 1.079727 | 0.088314 | 0.457932 |
| C | 1.693293 | -1.080990 | -0.319262 |
| H | 2.759442 | -0.902182 | -0.503954 |
| O | 1.160087 | 1.306118 | -0.288654 |
| H | 1.632915 | 0.197112 | 1.405586 |
| H | -1.117202 | -0.931822 | -1.116150 |
| H | -1.132370 | 0.818040 | -1.002913 |
| H | -0.717468 | 0.725091 | 1.458020 |
| H | -0.526783 | -1.027527 | 1.373192 |
| H | 1.611090 | -2.015934 | 0.244927 |
| H | 1.205217 | -1.216583 | -1.288817 |
| H | 2.078459 | 1.436430 | -0.557009 |

Rotational constants (GHz): 6.4017600 1.9875900 1.7939200

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 86.4210 | 107.9321 | 206.2858 |
| 252.0880 | 298.1877 | 340.5532 |
| 385.3875 | 439.1440 | 600.2201 |
| 697.6574 | 824.1051 | 896.5478 |
| 950.2561 | 979.8104 | 1046.5712 |
| 1082.6884 | 1095.1037 | 1126.4430 |
| 1171.1921 | 1240.1756 | 1249.0297 |
| 1338.5329 | 1364.0012 | 1389.9480 |
| 1399.1820 | 1416.5650 | 1428.9150 |
| 1491.0603 | 1509.2948 | 1514.2739 |
| 2896.7479 | 2955.8760 | 2976.6464 |
| 3041.1795 | 3061.0766 | 3105.7196 |
| 3110.1951 | 3130.9652 | 3822.1220 |

Zero-point correction (Hartree): 0.127641

C4H9O2.tmt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.21530021

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -2.671962 | -0.073559 | -0.107659 |
| C | -1.341694 | -0.052073 | -0.418559 |
| C | -0.406978 | -0.152904 | 0.797223 |
| C | 1.079152 | 0.074328 | 0.462568 |
| C | 1.721332 | -1.055783 | -0.345045 |
| H | 2.781896 | -0.844470 | -0.511995 |
| O | 1.257031 | 1.342602 | -0.180566 |
| H | 1.617777 | 0.160453 | 1.414577 |
| H | -1.095978 | -0.780561 | -1.214162 |
| H | -1.181044 | 0.950091 | -0.875954 |
| H | -0.728719 | 0.604713 | 1.519098 |
| H | -0.532861 | -1.132055 | 1.275606 |
| H | 1.641609 | -2.012366 | 0.180752 |
| H | 1.241166 | -1.177886 | -1.323941 |
| H | 1.264730 | 1.198325 | -1.135304 |

Rotational constants (GHz): 6.3748000 1.9567900 1.7701300

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 93.0709 | 95.0654 | 164.4975 |
| 210.7094 | 251.5933 | 332.4287 |
| 372.5702 | 434.3590 | 599.7894 |
| 724.0814 | 810.9747 | 923.7156 |
| 936.7757 | 976.1859 | 1045.3231 |
| 1062.8768 | 1104.1252 | 1121.0015 |
| 1163.5421 | 1226.5943 | 1290.0669 |
| 1319.5978 | 1354.1506 | 1384.4754 |
| 1414.5912 | 1416.4294 | 1429.6193 |
| 1492.6920 | 1506.4824 | 1513.7945 |
| 2877.8191 | 2949.1897 | 3038.8353 |
| 3045.4416 | 3056.4000 | 3106.7198 |
| 3109.9718 | 3129.1624 | 3819.5669 |

Zero-point correction (Hartree): 0.127359

C4H9O2.tpm

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.21608405

Electronic state : 2-A
Cartesian coordinates (Angs):
O 2.791221 -0.195646 -0.119979
C 1.566332 0.328977 0.195906
C 0.366094 -0.523144 -0.239061
C -0.984705 -0.061694 0.328965
C -1.413719 1.319454 -0.156309
H -2.412583 1.549677 0.223652
O -2.025210 -0.954231 -0.065455
H -0.908835 -0.038209 1.431762
H 1.582424 0.427808 1.305041
H 1.494510 1.374124 -0.159508
H 0.305690 -0.539257 -1.333810
H 0.563019 -1.553557 0.085908
H -0.727153 2.098842 0.188160
H -1.450813 1.343066 -1.250329
H -1.778357 -1.845040 0.215587
Rotational constants (GHz): 7.4480700 1.7741300 1.5220800
Vibrational harmonic frequencies (cm-1):
95.1309 111.9640 187.1027
240.0989 318.1255 333.7562
405.4078 450.3387 498.6745
539.7903 830.4148 885.2127
962.1111 1017.6677 1018.4291
1082.0600 1087.9728 1141.1148
1201.7967 1254.8472 1286.3845
1298.5293 1372.3726 1376.1908
1403.4793 1408.5885 1450.4553
1498.3926 1499.0936 1517.5527
2875.1498 2945.5235 2951.0461
3036.8165 3054.1635 3090.2220
3127.7802 3137.2965 3812.3699
Zero-point correction (Hartree): 0.127130

C4H9O2.tpp

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.21593241
Electronic state : 2-A
Cartesian coordinates (Angs):
O 2.787272 -0.159969 -0.173767
C 1.569743 0.270178 0.281210
C 0.368896 -0.537382 -0.224610
C -0.978637 -0.062338 0.323140
C -1.394184 1.319348 -0.189785
H -2.379802 1.596919 0.202535
O -1.925279 -1.055655 -0.069589
H -0.912723 -0.023448 1.425743
H 1.579212 0.348273 1.387331
H 1.508481 1.328497 -0.054371
H 0.348967 -0.513946 -1.320116
H 0.503325 -1.583532 0.070614
H -0.693617 2.101803 0.121899
H -1.451309 1.316544 -1.283126
H -2.793380 -0.784952 0.256607
Rotational constants (GHz): 7.3559100 1.7860800 1.5360400
Vibrational harmonic frequencies (cm-1):
80.7971 103.9820 190.7003
256.9958 303.3129 334.1056
403.6977 456.2845 492.3342
538.8905 832.4200 871.7506
967.1072 1012.2475 1024.4798
1084.5242 1088.5859 1135.6070
1196.2098 1246.3691 1287.7755
1310.8023 1374.8660 1384.8800
1393.2756 1423.3268 1437.5667
1499.4443 1509.4150 1515.5527
2890.9126 2923.9227 2950.3819
3038.3283 3061.3529 3102.9743
3109.5226 3124.2140 3812.3173
Zero-point correction (Hartree): 0.127056

C4H9O2.tpt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.21625482
Electronic state : 2-A
Cartesian coordinates (Angs):
O 2.784034 -0.168278 -0.187861
C 1.573765 0.272846 0.275149
C 0.365324 -0.545630 -0.201157
C -0.988648 -0.056082 0.334520
C -1.389539 1.327206 -0.186081
H -2.380770 1.593176 0.190690
O -2.009205 -1.015946 0.062206
H -0.940820 -0.019877 1.430850
H 1.588202 0.380128 1.378044

| | | | | |
|--|-----------|-----------|-----------|--|
| H | 1.509043 | 1.319341 | -0.095036 | |
| H | 0.354082 | -0.547036 | -1.299780 | |
| H | 0.501328 | -1.583845 | 0.120701 | |
| H | -0.686687 | 2.107161 | 0.127057 | |
| H | -1.426811 | 1.333250 | -1.283099 | |
| H | -2.081608 | -1.098556 | -0.898783 | |
| Rotational constants (GHz): | 7.3083500 | 1.7708400 | 1.5285000 | |
| Vibrational harmonic frequencies (cm-1): | | | | |
| 91.5235 | 107.7135 | | 186.1154 | |
| 254.7114 | 304.2261 | | 337.0772 | |
| 405.1229 | 459.8619 | | 492.3854 | |
| 609.6717 | 837.5495 | | 873.7017 | |
| 963.1430 | 1013.2958 | | 1017.5297 | |
| 1083.8399 | 1087.5344 | | 1136.4633 | |
| 1190.1274 | 1230.9004 | | 1291.8021 | |
| 1330.2961 | 1368.8780 | | 1379.3949 | |
| 1392.1048 | 1418.5164 | | 1432.9080 | |
| 1498.1762 | 1505.7790 | | 1514.5996 | |
| 2892.0930 | 2932.8870 | | 3033.8175 | |
| 3034.8600 | 3047.5480 | | 3098.1683 | |
| 3104.2918 | 3132.6966 | | 3796.1990 | |
| Zero-point correction (Hartree): | 0.127321 | | | |

C4H9O2.ttp

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.21955241

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | | |
|--|-----------|-----------|-----------|--|
| O | -2.758645 | -0.244361 | -0.202233 | |
| C | -1.567173 | 0.217517 | 0.274542 | |
| C | -0.338088 | -0.609353 | -0.131895 | |
| C | 0.969102 | 0.031373 | 0.329810 | |
| C | 2.197101 | -0.792058 | -0.060483 | |
| H | 3.118948 | -0.302220 | 0.274951 | |
| O | 1.005673 | 1.331212 | -0.267684 | |
| H | 0.942475 | 0.130099 | 1.429654 | |
| H | -1.457742 | 1.236327 | -0.157216 | |
| H | -1.604143 | 0.389581 | 1.369052 | |
| H | -0.420887 | -1.615542 | 0.295056 | |
| H | -0.328792 | -0.713099 | -1.222852 | |
| H | 2.166925 | -1.787737 | 0.394440 | |
| H | 2.247865 | -0.905849 | -1.147865 | |
| H | 1.793487 | 1.788768 | 0.052270 | |
| Rotational constants (GHz): | 7.7397100 | 1.8196600 | 1.5775500 | |
| Vibrational harmonic frequencies (cm-1): | | | | |
| 102.9366 | 118.9270 | | 180.0343 | |
| 251.2799 | 298.7378 | | 339.5813 | |
| 401.0036 | 475.6202 | | 499.6822 | |
| 696.1549 | 859.6158 | | 897.7240 | |
| 948.0749 | 1010.1376 | | 1043.5457 | |
| 1089.7537 | 1100.9983 | | 1124.6735 | |
| 1167.2030 | 1225.4749 | | 1292.9709 | |
| 1308.4185 | 1357.7629 | | 1382.2760 | |
| 1395.2622 | 1422.7141 | | 1433.8025 | |
| 1489.5490 | 1506.7164 | | 1511.7877 | |
| 2895.0431 | 2930.4129 | | 2959.9526 | |
| 3039.4991 | 3056.0733 | | 3104.6518 | |
| 3107.7332 | 3128.4368 | | 3822.1631 | |
| Zero-point correction (Hartree): | 0.127524 | | | |

C4H9O2.ttt

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.21988096

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | | |
|--|-----------|-----------|-----------|--|
| O | -2.745145 | -0.219792 | -0.251857 | |
| C | -1.568915 | 0.172288 | 0.314137 | |
| C | -0.332193 | -0.625131 | -0.127290 | |
| C | 0.971984 | 0.034998 | 0.337906 | |
| C | 2.212918 | -0.760262 | -0.067897 | |
| H | 3.118681 | -0.247397 | 0.267109 | |
| O | 1.047278 | 1.388130 | -0.123903 | |
| H | 0.952836 | 0.128816 | 1.431502 | |
| H | -1.424239 | 1.226305 | -0.013884 | |
| H | -1.640892 | 0.240074 | 1.417571 | |
| H | -0.395916 | -1.647807 | 0.264006 | |
| H | -0.341370 | -0.702749 | -1.223058 | |
| H | 2.200269 | -1.765247 | 0.366418 | |
| H | 2.263352 | -0.871020 | -1.158601 | |
| H | 1.147453 | 1.360962 | -1.086128 | |
| Rotational constants (GHz): | 7.6049400 | 1.8150000 | 1.5793000 | |
| Vibrational harmonic frequencies (cm-1): | | | | |
| 101.6563 | 128.2277 | | 183.6567 | |
| 252.0959 | 328.0893 | | 348.4719 | |
| 398.8267 | 480.3565 | | 503.5251 | |

| | | |
|-----------|-----------|-----------|
| 716.1277 | 855.6795 | 914.4410 |
| 938.5730 | 1001.1283 | 1044.6447 |
| 1084.6698 | 1102.8118 | 1127.9890 |
| 1161.3886 | 1201.2135 | 1296.2342 |
| 1329.3210 | 1349.8640 | 1383.9803 |
| 1395.5774 | 1418.4508 | 1428.1517 |
| 1493.7863 | 1506.4396 | 1510.1862 |
| 2879.1926 | 2937.7208 | 3033.7874 |
| 3037.2323 | 3050.1006 | 3085.5953 |
| 3109.4698 | 3133.7324 | 3789.9783 |

Zero-point correction (Hartree): 0.127674

C4H9O2.1-5Hshift.a.m

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.19610687

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| C | -0.438671 | 1.387297 | 0.001122 |
| C | -0.869539 | -0.022227 | 0.355268 |
| C | 0.132609 | -1.033509 | -0.238524 |
| C | 1.555946 | -0.668822 | 0.203454 |
| O | 1.893083 | 0.637777 | -0.194983 |
| H | -0.735226 | 1.684453 | -1.006088 |
| H | -0.621875 | 2.159445 | 0.748918 |
| O | -2.187600 | -0.215651 | -0.158649 |
| H | -0.866616 | -0.134886 | 1.452168 |
| H | 0.060364 | -0.989596 | -1.331467 |
| H | -0.116173 | -2.055121 | 0.077796 |
| H | 2.279323 | -1.343569 | -0.277164 |
| H | 1.655245 | -0.803149 | 1.295085 |
| H | 0.860172 | 1.260349 | -0.077709 |
| H | -2.441148 | -1.131375 | 0.019599 |

Rotational constants (GHz): 6.5119700 2.5018000 1.9613600

Vibrational harmonic frequencies (cm-1):

| | | |
|------------|----------|----------|
| i1617.0510 | 110.9514 | 255.8332 |
| 274.1670 | 344.2083 | 409.5568 |
| 425.5653 | 480.5896 | 530.0204 |
| 643.9970 | 834.1546 | 888.4438 |

| | | |
|-----------|-----------|-----------|
| 943.1147 | 971.0133 | 1025.3359 |
| 1060.0600 | 1071.6230 | 1127.5602 |
| 1137.0697 | 1169.5126 | 1217.9333 |
| 1234.0885 | 1279.0476 | 1326.9217 |
| 1377.9853 | 1392.8124 | 1422.8342 |
| 1468.4844 | 1496.9218 | 1511.4135 |
| 1547.3344 | 2962.8280 | 2981.5532 |
| 3028.9984 | 3042.0236 | 3096.4981 |
| 3105.7805 | 3193.1595 | 3803.3475 |

Zero-point correction (Hartree): 0.123460

C4H9O2.1-5Hshift.a.p

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.19715685

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| C | -0.464370 | 1.370856 | -0.020313 |
| C | -0.860216 | -0.049093 | 0.351201 |
| C | 0.152371 | -1.040165 | -0.236406 |
| C | 1.567006 | -0.644786 | 0.207094 |
| O | 1.883796 | 0.670598 | -0.183269 |
| H | -0.739991 | 1.639866 | -1.042152 |
| H | -0.693361 | 2.155205 | 0.704433 |
| O | -2.145691 | -0.400464 | -0.165878 |
| H | -0.851064 | -0.152165 | 1.448767 |
| H | 0.079462 | -1.002127 | -1.329390 |
| H | -0.087587 | -2.059710 | 0.083045 |
| H | 2.303227 | -1.303020 | -0.277315 |
| H | 1.669719 | -0.782202 | 1.297852 |
| H | 0.830229 | 1.278745 | -0.069544 |
| H | -2.784222 | 0.243461 | 0.168028 |

Rotational constants (GHz): 6.5070900 2.5102500 1.9656500

Vibrational harmonic frequencies (cm-1):

| | | |
|------------|-----------|-----------|
| i1620.8952 | 116.5800 | 256.2110 |
| 313.7988 | 335.3220 | 419.5763 |
| 427.2904 | 481.3733 | 532.7877 |
| 642.6957 | 834.2503 | 887.4596 |
| 939.8576 | 970.9820 | 1020.8457 |
| 1069.7052 | 1073.2299 | 1118.2916 |
| 1144.5222 | 1171.1462 | 1211.5149 |
| 1235.3300 | 1287.3620 | 1337.4985 |
| 1379.1227 | 1389.5301 | 1414.1980 |
| 1466.0855 | 1499.2121 | 1510.8005 |
| 1539.2053 | 2964.2191 | 2984.7687 |
| 3028.8261 | 3062.7410 | 3091.3601 |
| 3113.1949 | 3177.7880 | 3809.5626 |

Zero-point correction (Hartree): 0.123609

C4H9O2.1-5Hshift.a.t

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.19679334

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| C | -0.453188 | 1.378433 | -0.007116 |
| C | -0.863398 | -0.040156 | 0.355075 |
| C | 0.143041 | -1.039536 | -0.241341 |
| C | 1.563386 | -0.658622 | 0.199397 |
| O | 1.886033 | 0.658147 | -0.185217 |
| H | -0.695501 | 1.662694 | -1.034972 |
| H | -0.705957 | 2.159851 | 0.710820 |
| O | -2.211255 | -0.326208 | -0.022964 |
| H | -0.856832 | -0.149499 | 1.445722 |
| H | 0.083823 | -0.999652 | -1.338128 |
| H | -0.105987 | -2.058597 | 0.072769 |
| H | 2.297887 | -1.316734 | -0.287030 |
| H | 1.663899 | -0.802147 | 1.289371 |
| H | 0.845018 | 1.277062 | -0.041745 |
| H | -2.263624 | -0.269201 | -0.987451 |

Rotational constants (GHz): 6.4977000 2.4830700 1.9558600

Vibrational harmonic frequencies (cm-1):

| | | |
|------------|-----------|-----------|
| i1638.3081 | 118.3990 | 252.2061 |
| 277.5083 | 343.8268 | 416.8706 |
| 427.4450 | 477.0073 | 528.8707 |
| 638.0928 | 826.5599 | 885.6287 |
| 937.9188 | 968.4532 | 1025.0320 |
| 1063.0679 | 1087.4531 | 1101.2174 |
| 1139.4794 | 1173.6795 | 1214.2438 |
| 1229.0940 | 1298.7982 | 1346.6388 |
| 1372.0412 | 1391.7122 | 1426.9846 |
| 1466.5246 | 1495.0616 | 1511.1267 |
| 1537.7058 | 2967.8617 | 3025.9786 |
| 3039.1337 | 3067.6351 | 3087.7744 |
| 3103.8636 | 3176.6047 | 3792.7003 |

Zero-point correction (Hartree): 0.123568

C4H9O2.1-5Hshift.b.m

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.19878537

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| C | -0.579241 | 1.420916 | 0.214315 |
| C | -0.996585 | -0.017253 | 0.418079 |
| C | 0.232652 | -0.869504 | 0.794245 |
| C | 1.330970 | -0.668008 | -0.264603 |
| O | 1.690416 | 0.684912 | -0.365550 |
| H | -0.428649 | 1.987476 | 1.133941 |
| H | -1.160720 | 1.955220 | -0.537181 |
| H | -1.730225 | -0.072602 | 1.244222 |
| O | -1.592366 | -0.457109 | -0.799123 |
| H | 0.605657 | -0.549819 | 1.774449 |
| H | -0.041685 | -1.929882 | 0.875251 |
| H | 2.233415 | -1.219566 | 0.039898 |
| H | 0.989148 | -1.076940 | -1.228372 |
| H | 0.633827 | 1.279910 | -0.252872 |
| H | -1.811948 | -1.393123 | -0.704168 |

Rotational constants (GHz): 5.0539300 2.9471800 2.4480000

Vibrational harmonic frequencies (cm-1):

| | | |
|------------|-----------|-----------|
| i1597.6759 | 126.4051 | 245.3888 |
| 305.7388 | 377.9843 | 402.1164 |
| 446.9255 | 500.0072 | 598.6398 |
| 684.4373 | 821.9426 | 881.9729 |
| 910.4755 | 969.9464 | 998.3257 |
| 1061.5482 | 1073.3477 | 1103.3897 |
| 1163.2383 | 1193.0535 | 1200.9881 |
| 1243.8642 | 1251.4550 | 1318.4361 |
| 1366.4950 | 1391.6080 | 1407.8007 |
| 1457.4910 | 1489.2191 | 1505.3171 |
| 1557.7344 | 2936.0139 | 2990.2438 |
| 3028.5127 | 3041.6525 | 3090.9861 |
| 3111.5634 | 3199.7501 | 3815.9396 |

Zero-point correction (Hartree): 0.123636

C4H9O2.1-5Hshift.b.p

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.19857570

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| C | -0.606727 | 1.402908 | 0.236145 |
| C | -0.989824 | -0.053992 | 0.423312 |
| C | 0.254863 | -0.878561 | 0.784177 |
| C | 1.347650 | -0.640758 | -0.274153 |

| | | | |
|--|-----------|-----------|-----------|
| O | 1.672045 | 0.723704 | -0.371509 |
| H | -0.468545 | 1.963935 | 1.162415 |
| H | -1.191567 | 1.956358 | -0.502445 |
| H | -1.714150 | -0.136720 | 1.255905 |
| O | -1.533748 | -0.629647 | -0.759172 |
| H | 0.620640 | -0.559045 | 1.766390 |
| H | -0.007433 | -1.940021 | 0.840838 |
| H | 2.264465 | -1.166547 | 0.033226 |
| H | 1.019435 | -1.055980 | -1.238453 |
| H | 0.608957 | 1.290093 | -0.239389 |
| H | -2.273953 | -0.082118 | -1.049924 |
| Rotational constants (GHz): | 5.0362600 | 2.9613800 | 2.4474100 |
| Vibrational harmonic frequencies (cm-1): | | | |
| i1608.4597 | 120.5885 | | 245.8027 |
| 292.3258 | 376.2051 | | 391.8811 |
| 438.4829 | 503.0352 | | 594.1947 |
| 684.4644 | 819.4823 | | 880.2420 |
| 902.8713 | 975.9290 | | 1001.6945 |
| 1048.7069 | 1062.1468 | | 1117.6755 |
| 1157.9486 | 1186.4772 | | 1191.0990 |
| 1245.5402 | 1254.7637 | | 1344.2276 |
| 1365.2882 | 1383.5202 | | 1399.1759 |
| 1458.8296 | 1483.8748 | | 1509.0618 |
| 1553.9586 | 2930.8378 | | 2998.8490 |
| 3037.6346 | 3065.6910 | | 3090.3896 |
| 3116.2739 | 3173.3986 | | 3822.3716 |
| Zero-point correction (Hartree): | 0.123534 | | |

C4H9O2.1-5Hshift.b.t

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.19863450
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | |
|--|-----------|-----------|-----------|
| C | -0.654381 | 1.390757 | 0.262223 |
| C | -1.004757 | -0.076369 | 0.406840 |
| C | 0.255677 | -0.864190 | 0.816065 |
| C | 1.367056 | -0.622545 | -0.223506 |
| O | 1.625788 | 0.746059 | -0.402878 |
| H | -0.485975 | 1.925776 | 1.198678 |
| H | -1.277451 | 1.946031 | -0.440611 |
| H | -1.768703 | -0.202823 | 1.187715 |
| O | -1.601671 | -0.603926 | -0.773183 |
| H | 0.597033 | -0.517185 | 1.798529 |
| H | 0.025932 | -1.932103 | 0.888141 |
| H | 2.298485 | -1.089690 | 0.129272 |
| H | 1.096085 | -1.118380 | -1.173141 |
| H | 0.553618 | 1.301857 | -0.232743 |
| H | -1.013531 | -0.416455 | -1.517094 |
| Rotational constants (GHz): | 4.9786400 | 2.9386600 | 2.4694900 |
| Vibrational harmonic frequencies (cm-1): | | | |
| i1600.0036 | 98.2187 | | 243.1145 |
| 294.9201 | 379.8956 | | 406.1284 |
| 439.6627 | 506.9684 | | 582.6307 |
| 685.0976 | 808.2004 | | 876.3024 |
| 898.5752 | 971.2993 | | 993.8612 |
| 1060.1555 | 1071.0907 | | 1110.8108 |
| 1154.2093 | 1183.9728 | | 1200.1338 |
| 1233.3791 | 1283.7371 | | 1300.6332 |
| 1361.7151 | 1380.9522 | | 1410.9746 |
| 1455.7429 | 1485.3081 | | 1523.1941 |
| 1555.5164 | 2951.7635 | | 3022.2622 |
| 3024.3014 | 3060.4213 | | 3100.8466 |
| 3113.8740 | 3186.1726 | | 3808.7240 |
| Zero-point correction (Hartree): | 0.123533 | | |

C4H9O2.pmmm

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.21218810
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 1.623083 | -1.245334 | 0.130029 |
| C | 1.828922 | 0.095776 | -0.050878 |
| C | 0.621474 | 0.915905 | -0.524412 |
| C | -0.516887 | 0.978989 | 0.507360 |
| C | -1.345509 | -0.308334 | 0.587634 |
| O | -1.994429 | -0.619070 | -0.640274 |
| H | -2.622904 | 0.090780 | -0.826975 |
| H | 2.297831 | 0.544581 | 0.848491 |
| H | 2.630268 | 0.141453 | -0.822094 |
| H | 0.974143 | 1.930266 | -0.751350 |
| H | 0.234367 | 0.485280 | -1.454225 |
| H | -0.113605 | 1.209539 | 1.503913 |
| H | -1.188786 | 1.811979 | 0.254749 |
| H | -0.696877 | -1.163558 | 0.798620 |
| H | -2.071672 | -0.229099 | 1.412601 |

```

Rotational constants (GHz):      5.5473100      2.2054600      1.8996000
Vibrational harmonic frequencies (cm-1):
  57.5334      122.9611      170.1696
 265.2923      312.0003      353.3295
 439.3233      493.0483      643.4004
 808.2941      826.4471      890.5150
 976.4674      1017.8343      1034.6524
1092.9184      1110.4516      1132.7836
1198.8167      1209.9802      1311.8588
1351.8573      1364.1985      1382.2368
1385.9502      1404.7092      1433.3986
1487.2652      1494.1464      1517.5412
2879.5466      2923.5127      2990.1351
3015.7755      3042.0991      3052.7329
3101.4919      3104.1433      3807.4639
Zero-point correction (Hartree): 0.128047
  
```

C4H9O2.pmpm

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.21726536

Electronic state : 2-A

Cartesian coordinates (Angs):

```

O      1.235368      -1.292839      0.209698
C      1.651263      0.016473      0.150262
C      0.692859      0.987754      -0.544961
C     -0.624477      1.224430      0.213798
C     -1.395141      -0.066174      0.537840
O     -1.547281      -0.918667      -0.584187
H     -0.697975      -1.376938      -0.677131
H      1.946705      0.356338      1.162473
H      2.616260      -0.027902      -0.401470
H      1.208725      1.944446      -0.693997
H      0.466249      0.588436      -1.539743
H     -0.431120      1.763279      1.152242
H     -1.256288      1.876581      -0.400700
H     -0.901550      -0.597441      1.368007
H     -2.402734      0.190350      0.884601
  
```

```

Rotational constants (GHz):      4.7693100      2.9112200      2.1631200
Vibrational harmonic frequencies (cm-1):
 110.2331      160.5783      173.0152
 254.4978      329.4430      454.8969
 511.6676      571.8572      671.1302
 787.5024      820.8994      896.0757
 998.4257      1012.6078      1027.1721
1085.0826      1113.4004      1154.2393
1213.2400      1232.8235      1301.3599
1354.1310      1365.0264      1388.0210
1390.5541      1424.5728      1439.5678
1488.0009      1497.4970      1515.2746
2888.2877      2938.3243      2981.1008
3028.0463      3050.7055      3072.3280
3083.8832      3099.8014      3760.1736
Zero-point correction (Hartree): 0.129048
  
```

C4H9O2.pmmt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.21288711

Electronic state : 2-A

Cartesian coordinates (Angs):

```

O      1.461902      -1.295440      0.161552
C      1.785959      0.027344      0.013009
C      0.670116      0.915478      -0.561462
C     -0.514597      1.084913      0.402044
C     -1.321601      -0.193225      0.604238
O     -1.925252      -0.535682      -0.637913
H     -2.173541      -1.466959      -0.606714
H      2.210993      0.457636      0.941293
H      2.629769      0.009963      -0.712408
H      1.101263      1.897362      -0.793895
H      0.311565      0.476635      -1.497683
H     -0.159932      1.437012      1.380478
H     -1.188854      1.857585      0.013081
H     -0.658395      -0.998678      0.957455
H     -2.085321      -0.028641      1.382315
  
```

```

Rotational constants (GHz):      5.3242200      2.3819500      1.9871400
Vibrational harmonic frequencies (cm-1):
  62.6598      124.7061      162.9311
 200.8417      266.0687      340.4407
 430.9208      501.5500      774.7725
 800.7584      852.8913      907.5306
 952.4919      1036.5088      1059.4658
1065.7439      1100.7048      1147.0153
1160.6082      1234.4353      1282.9754
1316.8747      1333.0642      1368.4531
1390.6793      1410.5452      1461.2620
  
```

| | | |
|-----------|-----------|-----------|
| 1482.3963 | 1487.2182 | 1522.8265 |
| 2879.1792 | 2936.2092 | 2971.8659 |
| 3003.6079 | 3035.1716 | 3048.9777 |
| 3080.6022 | 3113.5569 | 3841.3187 |

Zero-point correction (Hartree): 0.127919

C4H9O2.pmpm

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.21763101
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -1.366379 | -1.255247 | 0.231135 |
| C | -1.664652 | 0.003693 | -0.227093 |
| C | -0.749418 | 1.146719 | 0.247021 |
| C | 0.698692 | 1.158470 | -0.273623 |
| C | 1.633950 | 0.071916 | 0.276026 |
| O | 1.391489 | -1.219464 | -0.243385 |
| H | 0.507658 | -1.486130 | 0.060235 |
| H | -1.587852 | -0.098428 | -1.333601 |
| H | -2.727896 | 0.237029 | -0.038981 |
| H | -1.244306 | 2.078270 | -0.057623 |
| H | -0.752761 | 1.146360 | 1.345344 |
| H | 0.703203 | 1.094274 | -1.370012 |
| H | 1.131697 | 2.134590 | -0.016591 |
| H | 2.663117 | 0.322860 | -0.004788 |
| H | 1.594825 | 0.084081 | 1.380028 |

Rotational constants (GHz): 4.7303200 2.8869400 1.9651300
 Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 65.5537 | 129.8626 | 210.3689 |
| 280.4017 | 326.9658 | 451.9610 |
| 469.6576 | 550.0616 | 761.1446 |
| 778.8740 | 874.4936 | 916.4872 |
| 937.7883 | 1037.2880 | 1055.3836 |
| 1097.0508 | 1116.1393 | 1157.9487 |
| 1205.4423 | 1233.2256 | 1289.1716 |
| 1320.6082 | 1384.5135 | 1387.8410 |
| 1402.3015 | 1419.5743 | 1459.2658 |
| 1484.7637 | 1488.7094 | 1519.4324 |
| 2875.9852 | 2961.3061 | 2970.6847 |
| 3025.7521 | 3033.4562 | 3067.4467 |
| 3075.3743 | 3077.9154 | 3700.8451 |

Zero-point correction (Hartree): 0.128947

C4H9O2.pmpp

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.21005475
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 1.355662 | -1.207545 | -0.386680 |
| C | 1.550549 | -0.053216 | 0.326959 |
| C | 0.767954 | 1.174701 | -0.166651 |
| C | -0.726917 | 1.188517 | 0.188054 |
| C | -1.551788 | 0.018398 | -0.357395 |
| O | -1.231572 | -1.232973 | 0.239452 |
| H | -1.409280 | -1.162856 | 1.186878 |
| H | 1.415432 | -0.212417 | 1.414024 |
| H | 2.637033 | 0.146378 | 0.204512 |
| H | 1.233945 | 2.074731 | 0.255973 |
| H | 0.892034 | 1.232288 | -1.255221 |
| H | -0.847343 | 1.223777 | 1.282161 |
| H | -1.167208 | 2.121139 | -0.189259 |
| H | -2.624030 | 0.243329 | -0.239431 |
| H | -1.362090 | -0.112624 | -1.427608 |

Rotational constants (GHz): 4.5939800 3.0650000 2.0764800
 Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 66.7322 | 124.8071 | 151.2314 |
| 291.2299 | 307.9760 | 351.2996 |
| 457.1135 | 493.5504 | 769.1946 |
| 810.9972 | 869.6911 | 932.1389 |
| 948.4972 | 1036.8835 | 1062.6101 |
| 1099.5835 | 1113.9950 | 1138.7840 |
| 1200.3775 | 1273.4599 | 1287.9631 |
| 1370.9154 | 1382.9150 | 1387.2354 |
| 1395.3867 | 1406.5798 | 1427.7816 |
| 1483.0645 | 1492.3865 | 1518.3186 |
| 2896.0062 | 2945.4406 | 2988.5235 |
| 3008.1921 | 3033.4331 | 3058.5175 |
| 3081.5051 | 3097.9267 | 3806.7178 |

Zero-point correction (Hartree): 0.128874

C4H9O2.pmtm

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.21249504
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | |
|--|-----------|-----------|-----------|
| O | 1.641109 | -1.311626 | -0.102468 |
| C | 1.870728 | -0.028590 | 0.319706 |
| C | 0.953010 | 1.037183 | -0.299877 |
| C | -0.507414 | 0.927792 | 0.162564 |
| C | -1.222605 | -0.345355 | -0.299848 |
| O | -2.588798 | -0.371467 | 0.093191 |
| H | -2.616738 | -0.408755 | 1.057960 |
| H | 1.888812 | 0.043288 | 1.425132 |
| H | 2.919082 | 0.168766 | 0.004831 |
| H | 1.345357 | 2.025847 | -0.030432 |
| H | 1.011969 | 0.953140 | -1.392021 |
| H | -0.543861 | 0.981915 | 1.261931 |
| H | -1.075353 | 1.789722 | -0.206794 |
| H | -1.225787 | -0.395110 | -1.394017 |
| H | -0.684271 | -1.240251 | 0.052362 |
| Rotational constants (GHz): | 6.4762100 | 1.9259300 | 1.6045300 |
| Vibrational harmonic frequencies (cm-1): | | | |
| 89.8810 | 102.9987 | | 127.5941 |
| 264.7599 | 309.7173 | | 316.1381 |
| 411.1018 | 492.7502 | | 763.5171 |
| 801.6917 | 837.9321 | | 906.3611 |
| 995.0513 | 1032.6147 | | 1061.9654 |
| 1082.3129 | 1099.9749 | | 1130.3014 |
| 1162.1313 | 1245.8988 | | 1308.4438 |
| 1329.5027 | 1356.8867 | | 1371.6884 |
| 1396.1010 | 1406.2497 | | 1434.8154 |
| 1485.9360 | 1497.6953 | | 1518.7886 |
| 2887.6154 | 2937.6733 | | 2982.1128 |
| 3006.4244 | 3040.9924 | | 3074.6127 |
| 3086.2170 | 3094.3724 | | 3814.6864 |
| Zero-point correction (Hartree): | 0.128182 | | |

C4H9O2.pmtp

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.21240182
Electronic state : 2-A
Cartesian coordinates (Angs):

| | | | |
|--|-----------|-----------|-----------|
| O | -1.692662 | -1.295534 | 0.103721 |
| C | -1.883259 | -0.002190 | -0.303448 |
| C | -0.932869 | 1.038558 | 0.303729 |
| C | 0.517860 | 0.904857 | -0.184390 |
| C | 1.231756 | -0.366337 | 0.286699 |
| O | 2.554785 | -0.461334 | -0.225001 |
| H | 3.056199 | 0.291091 | 0.115179 |
| H | -1.906683 | 0.061626 | -1.409781 |
| H | -2.928815 | 0.225569 | 0.001163 |
| H | -1.309865 | 2.037122 | 0.048359 |
| H | -0.975987 | 0.950476 | 1.396757 |
| H | 0.550820 | 0.936238 | -1.281534 |
| H | 1.089162 | 1.776763 | 0.165741 |
| H | 1.219488 | -0.414745 | 1.388159 |
| H | 0.707766 | -1.258526 | -0.069349 |
| Rotational constants (GHz): | 6.5123600 | 1.9085400 | 1.5889400 |
| Vibrational harmonic frequencies (cm-1): | | | |
| 87.0879 | 108.2216 | | 130.0156 |
| 262.4420 | 300.7494 | | 329.0549 |
| 414.9564 | 480.1699 | | 659.8178 |
| 790.5764 | 821.5448 | | 920.2735 |
| 990.5914 | 1011.9368 | | 1067.2762 |
| 1083.4914 | 1101.0094 | | 1139.3403 |
| 1208.1971 | 1227.6171 | | 1321.6712 |
| 1342.2064 | 1360.4782 | | 1369.7196 |
| 1390.8526 | 1397.7865 | | 1437.2788 |
| 1485.9744 | 1499.7689 | | 1522.0658 |
| 2885.8085 | 2932.5722 | | 2986.1228 |
| 3017.3405 | 3038.6916 | | 3061.6652 |
| 3083.0234 | 3097.8821 | | 3810.5442 |
| Zero-point correction (Hartree): | 0.127978 | | |

C4H9O2.pmtt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.21257976
Electronic state : 2-A
Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -1.624533 | -1.320642 | 0.099889 |
| C | -1.863992 | -0.037444 | -0.317808 |
| C | -0.957419 | 1.033501 | 0.307441 |
| C | 0.502077 | 0.939242 | -0.157608 |
| C | 1.211376 | -0.337490 | 0.279747 |
| O | 2.541813 | -0.279659 | -0.219860 |
| H | 2.988465 | -1.099358 | 0.024639 |
| H | -1.878242 | 0.035497 | -1.422945 |
| H | -2.916218 | 0.149204 | -0.008792 |
| H | -1.357413 | 2.020594 | 0.043750 |

| | | | | |
|--|-----------|-----------|-----------|--|
| H | -1.017399 | 0.942775 | 1.399249 | |
| H | 0.552662 | 1.005832 | -1.252475 | |
| H | 1.067362 | 1.794726 | 0.230608 | |
| H | 1.195824 | -0.413226 | 1.379673 | |
| H | 0.674474 | -1.220495 | -0.104567 | |
| Rotational constants (GHz): | 6.4905600 | 1.9544900 | 1.6182700 | |
| Vibrational harmonic frequencies (cm-1): | | | | |
| 95.6021 | 110.9950 | | 126.1132 | |
| 270.0968 | 282.3676 | | 315.5716 | |
| 411.8793 | 494.8579 | | 759.2962 | |
| 807.1329 | 837.1896 | | 919.5422 | |
| 984.4928 | 1046.1513 | | 1053.5819 | |
| 1087.0679 | 1099.5153 | | 1162.5467 | |
| 1193.8209 | 1236.3169 | | 1278.9183 | |
| 1319.3650 | 1342.2233 | | 1365.6171 | |
| 1373.7059 | 1400.4534 | | 1471.1556 | |
| 1486.7659 | 1505.6726 | | 1530.5565 | |
| 2886.2007 | 2940.5052 | | 2969.5141 | |
| 2996.8395 | 3039.4396 | | 3041.1387 | |
| 3082.2368 | 3089.8203 | | 3829.6597 | |
| Zero-point correction (Hartree): | 0.128133 | | | |

C4H9O2.ppm

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.21568744
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | | |
|--|-----------|-----------|-----------|--|
| O | -1.806849 | -0.781568 | 0.675162 | |
| C | -1.457713 | -0.191232 | -0.503287 | |
| C | -0.639894 | 1.109539 | -0.365914 | |
| C | 0.592836 | 0.981771 | 0.539544 | |
| C | 1.729470 | 0.124969 | -0.024310 | |
| O | 1.365213 | -1.231597 | -0.280037 | |
| H | 1.032497 | -1.605028 | 0.547827 | |
| H | -0.803562 | -0.952392 | -0.986226 | |
| H | -2.324199 | -0.061360 | -1.178631 | |
| H | -0.345626 | 1.438265 | -1.371758 | |
| H | -1.302056 | 1.886778 | 0.035061 | |
| H | 0.998274 | 1.981341 | 0.743339 | |
| H | 0.275561 | 0.574529 | 1.508377 | |
| H | 2.059679 | 0.521238 | -0.991421 | |
| H | 2.594324 | 0.171670 | 0.656234 | |
| Rotational constants (GHz): | 5.0561600 | 2.5373800 | 2.0342800 | |
| Vibrational harmonic frequencies (cm-1): | | | | |
| 46.2423 | 124.2356 | | 223.7912 | |
| 258.3969 | 321.9562 | | 383.8866 | |
| 468.1189 | 525.1644 | | 739.2582 | |
| 802.5922 | 872.7070 | | 926.4655 | |
| 944.6302 | 1014.8195 | | 1067.9221 | |
| 1098.2623 | 1120.4842 | | 1141.2931 | |
| 1186.7248 | 1240.4682 | | 1291.6473 | |
| 1307.1339 | 1379.0506 | | 1382.1023 | |
| 1390.8621 | 1413.9101 | | 1432.8812 | |
| 1491.3923 | 1495.7067 | | 1522.3250 | |
| 2866.5425 | 2954.8106 | | 2996.0238 | |
| 3034.1159 | 3039.2100 | | 3070.0415 | |
| 3076.9935 | 3088.2271 | | 3801.7620 | |
| Zero-point correction (Hartree): | 0.128813 | | | |

C4H9O2.pmp

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.21377247
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | | |
|--|-----------|-----------|-----------|--|
| O | 2.069775 | -0.561161 | -0.713359 | |
| C | 1.453050 | -0.337029 | 0.483130 | |
| C | 0.609308 | 0.950014 | 0.541922 | |
| C | -0.533478 | 0.978528 | -0.484756 | |
| C | -1.778746 | 0.200222 | -0.073942 | |
| O | -1.441594 | -1.176949 | 0.092527 | |
| H | -2.228171 | -1.649092 | 0.391680 | |
| H | 0.773134 | -1.207183 | 0.610028 | |
| H | 2.170007 | -0.398288 | 1.324853 | |
| H | 0.215569 | 1.067496 | 1.560950 | |
| H | 1.280516 | 1.799362 | 0.366705 | |
| H | -0.843975 | 2.014978 | -0.665463 | |
| H | -0.157111 | 0.589261 | -1.437998 | |
| H | -2.181230 | 0.618298 | 0.863994 | |
| H | -2.554982 | 0.319642 | -0.846219 | |
| Rotational constants (GHz): | 5.5424400 | 2.2637800 | 1.9283300 | |
| Vibrational harmonic frequencies (cm-1): | | | | |
| 70.1321 | 118.5700 | | 193.0356 | |
| 259.2677 | 290.9539 | | 323.8651 | |
| 459.4441 | 507.3159 | | 727.1748 | |
| 814.9150 | 868.2965 | | 913.7216 | |

| | | |
|-----------|-----------|-----------|
| 953.4331 | 1020.6613 | 1079.9509 |
| 1101.1304 | 1113.9506 | 1163.0520 |
| 1184.4181 | 1247.5833 | 1294.5723 |
| 1301.8584 | 1329.7581 | 1375.2569 |
| 1382.9264 | 1410.2467 | 1463.9755 |
| 1492.5253 | 1495.0013 | 1536.1673 |
| 2896.0099 | 2943.2214 | 2975.1017 |
| 3008.7528 | 3032.5878 | 3050.0133 |
| 3078.8573 | 3094.6291 | 3830.1778 |

Zero-point correction (Hartree): 0.128494

C4H9O2.ppm

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.21377247

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 2.069753 | -0.561291 | -0.713300 |
| C | 1.453025 | -0.337019 | 0.483169 |
| C | 0.609354 | 0.950100 | 0.541842 |
| C | -0.533428 | 0.978502 | -0.484807 |
| C | -1.778694 | 0.200234 | -0.073870 |
| O | -1.441728 | -1.176962 | 0.092371 |
| H | -2.228052 | -1.648917 | 0.392466 |
| H | 0.773062 | -1.207094 | 0.610163 |
| H | 2.170000 | -0.398228 | 1.324887 |
| H | 0.215686 | 1.067710 | 1.560881 |
| H | 1.280633 | 1.799375 | 0.366533 |
| H | -0.843992 | 2.014911 | -0.665684 |
| H | -0.157055 | 0.589147 | -1.438008 |
| H | -2.180937 | 0.618320 | 0.864167 |
| H | -2.555090 | 0.319904 | -0.845972 |

Rotational constants (GHz): 5.5422900 2.2637900 1.9283000

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 70.1120 | 118.5253 | 193.0136 |
| 259.1886 | 290.9337 | 323.8551 |
| 459.4428 | 507.3055 | 727.1205 |
| 814.9100 | 868.2859 | 913.7279 |
| 953.4356 | 1020.6652 | 1079.9797 |
| 1101.1197 | 1113.9396 | 1163.0892 |
| 1184.3414 | 1247.6508 | 1294.5411 |
| 1301.8561 | 1329.7492 | 1375.2595 |
| 1382.9294 | 1410.2543 | 1463.9851 |
| 1492.5311 | 1495.0112 | 1536.1902 |
| 2896.1661 | 2943.2149 | 2975.0516 |
| 3008.6140 | 3032.5860 | 3049.9735 |
| 3078.8459 | 3094.6151 | 3830.2712 |

Zero-point correction (Hartree): 0.128494

C4H9O2.ppm

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.21144947

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -2.378944 | -0.598770 | -0.325980 |
| C | -1.596107 | 0.522084 | -0.397512 |
| C | -0.535341 | 0.643639 | 0.708747 |
| C | 0.425412 | -0.552347 | 0.781934 |
| C | 1.455347 | -0.620903 | -0.350703 |
| O | 2.396868 | 0.446330 | -0.325968 |
| H | 1.931852 | 1.264669 | -0.538588 |
| H | -1.111962 | 0.448152 | -1.396786 |
| H | -2.219193 | 1.433892 | -0.472280 |
| H | 0.017570 | 1.583505 | 0.568329 |
| H | -1.060184 | 0.748618 | 1.665347 |
| H | 0.970672 | -0.522389 | 1.731954 |
| H | -0.170189 | -1.473378 | 0.778619 |
| H | 2.047847 | -1.534997 | -0.244431 |
| H | 0.954329 | -0.683388 | -1.331366 |

Rotational constants (GHz): 7.3484600 1.7275700 1.6903000

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 50.7618 | 103.7698 | 197.2544 |
| 221.2061 | 278.7284 | 352.8626 |
| 457.4815 | 532.8409 | 637.7708 |
| 773.6621 | 826.2988 | 914.6758 |
| 950.0299 | 1025.6453 | 1072.0439 |
| 1081.8194 | 1107.1714 | 1128.6253 |
| 1192.5855 | 1225.1455 | 1308.5915 |
| 1325.4223 | 1372.2797 | 1378.5562 |
| 1395.6982 | 1407.3911 | 1428.4324 |
| 1486.8375 | 1502.0707 | 1520.6076 |
| 2884.2222 | 2946.3394 | 2980.8342 |
| 3028.5081 | 3050.8662 | 3081.3574 |
| 3094.6590 | 3098.1641 | 3828.1768 |

Zero-point correction (Hartree): 0.128146

C4H9O2.pppp

```

-----
E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.21364602
Electronic state : 2-A
Cartesian coordinates (Angs):
O      2.240811      0.646339      -0.405426
C      1.533075      -0.524976      -0.395771
C      0.526236      -0.676951      0.755138
C      -0.437821      0.508559      0.893374
C      -1.405137      0.667670      -0.284022
O      -2.122783      -0.524384      -0.590947
H      -2.661817      -0.748940      0.179006
H      0.993756      -0.522879      -1.369221
H      2.206022      -1.400557      -0.467970
H      -0.040178      -1.601291      0.593767
H      1.087005      -0.800955      1.689264
H      -1.016532      0.392740      1.820485
H      0.138718      1.435141      0.998680
H      -2.090920      1.506203      -0.086456
H      -0.858403      0.919077      -1.198888
Rotational constants (GHz):      6.4690400      1.8779600      1.8712600
Vibrational harmonic frequencies (cm-1):
13.9591      110.4864      210.2681
238.5244      327.3501      343.2123
464.7908      568.8027      664.7327
775.5192      834.9465      925.5378
957.5074      1017.6157      1072.1999
1080.5083      1113.4624      1140.4464
1161.2001      1248.6174      1294.5295
1324.4340      1376.0763      1381.3845
1387.3241      1414.9251      1428.4018
1489.7948      1494.2915      1527.6288
2885.1197      2948.3965      3000.6233
3028.0975      3052.7249      3080.9295

3093.5775      3098.7191      3808.5179
Zero-point correction (Hartree): 0.128455

```

C4H9O2.pppt

```

-----
E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.21300589
Electronic state : 2-A
Cartesian coordinates (Angs):
O      -1.988185      -0.600992      0.723254
C      -1.446613      -0.382975      -0.513822
C      -0.576905      0.875769      -0.648523
C      0.475793      1.031746      0.459379
C      1.354481      -0.200234      0.659124
O      1.868785      -0.601517      -0.610027
H      2.423796      -1.379681      -0.477232
H      -0.802999      -1.274597      -0.688106
H      -2.212602      -0.439896      -1.310433
H      -0.084927      0.837643      -1.626260
H      -1.228485      1.758087      -0.651198
H      1.109427      1.893952      0.221481
H      -0.018157      1.245015      1.413593
H      2.168265      0.040688      1.360509
H      0.760350      -1.006968      1.114881
Rotational constants (GHz):      5.6064200      2.1648500      2.0851200
Vibrational harmonic frequencies (cm-1):
36.5435      124.2646      195.4435
249.0346      299.6847      328.2279
452.5181      586.6675      684.9448
784.4791      841.3943      923.2339
966.6677      1044.8120      1069.6815
1081.8596      1110.7130      1147.4382
1203.4095      1236.1187      1282.0751
1282.5250      1332.0956      1384.2046
1390.2577      1410.7529      1460.4492
1486.3856      1498.9044      1548.3472
2877.8034      2948.5511      2992.7172
3020.8826      3049.7111      3060.4265
3093.8397      3107.7421      3830.1080
Zero-point correction (Hartree): 0.128545

```

C4H9O2.pptm

```

-----
E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.21172871
Electronic state : 2-A
Cartesian coordinates (Angs):
O      2.160109      -1.012156      -0.409008
C      1.812912      -0.040248      0.489902
C      0.849938      1.031763      -0.046100
C      -0.467813      0.461140      -0.589069
C      -1.435646      -0.017322      0.497006

```

| | | | | |
|--|-----------|-----------|-----------|--|
| O | -2.626651 | -0.578151 | -0.035723 | |
| H | -3.059286 | 0.103291 | -0.566595 | |
| H | 1.351624 | -0.596918 | 1.334977 | |
| H | 2.718018 | 0.411970 | 0.939810 | |
| H | 0.658164 | 1.761900 | 0.752573 | |
| H | 1.368408 | 1.575627 | -0.844276 | |
| H | -0.972401 | 1.231616 | -1.188638 | |
| H | -0.246932 | -0.372765 | -1.264401 | |
| H | -0.983826 | -0.817066 | 1.094032 | |
| H | -1.657781 | 0.812802 | 1.189934 | |
| Rotational constants (GHz): | 7.3581300 | 1.6362500 | 1.5201700 | |
| Vibrational harmonic frequencies (cm-1): | | | | |
| 63.9163 | 90.1485 | | 168.8100 | |
| 238.8410 | 291.8275 | | 328.6104 | |
| 442.7564 | 516.1086 | | 609.2880 | |
| 772.5503 | 860.2215 | | 873.5330 | |
| 1002.7158 | 1024.6932 | | 1082.2931 | |
| 1097.2885 | 1105.4361 | | 1131.0984 | |
| 1178.4384 | 1266.0847 | | 1321.1623 | |
| 1332.8477 | 1356.4327 | | 1370.0867 | |
| 1393.9196 | 1407.3801 | | 1439.1642 | |
| 1494.2940 | 1505.2709 | | 1528.6567 | |
| 2892.2792 | 2941.6388 | | 2970.2976 | |
| 3026.1060 | 3034.8207 | | 3078.1220 | |
| 3082.5108 | 3099.4557 | | 3812.0658 | |
| Zero-point correction (Hartree): | 0.128104 | | | |

C4H9O2.pptp

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.21214890
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | | |
|--|-----------|-----------|-----------|--|
| O | 2.104755 | -1.070388 | -0.342336 | |
| C | 1.814251 | -0.020469 | 0.485801 | |
| C | 0.864385 | 1.036043 | -0.103565 | |
| C | -0.465604 | 0.461327 | -0.611027 | |
| C | -1.430565 | 0.032085 | 0.497387 | |
| O | -2.670064 | -0.440507 | -0.011263 | |
| H | -2.485380 | -1.216113 | -0.556922 | |
| H | 1.357789 | -0.499166 | 1.380539 | |
| H | 2.742504 | 0.437107 | 0.878948 | |
| H | 0.689209 | 1.810980 | 0.655311 | |
| H | 1.385833 | 1.528608 | -0.932632 | |
| H | -0.977836 | 1.201552 | -1.235588 | |
| H | -0.242977 | -0.400203 | -1.254854 | |
| H | -0.961304 | -0.721174 | 1.152212 | |
| H | -1.680160 | 0.891651 | 1.130197 | |
| Rotational constants (GHz): | 7.2704000 | 1.6525100 | 1.5279300 | |
| Vibrational harmonic frequencies (cm-1): | | | | |
| 58.0902 | 88.2417 | | 171.2180 | |
| 238.9408 | 289.7281 | | 326.6781 | |
| 440.7209 | 522.1907 | | 630.3603 | |
| 775.1459 | 860.1675 | | 870.8964 | |
| 1012.5589 | 1021.7601 | | 1076.6757 | |
| 1087.4988 | 1103.2768 | | 1145.9944 | |
| 1170.4500 | 1278.3943 | | 1298.8460 | |
| 1336.2309 | 1356.1882 | | 1369.2043 | |
| 1391.1857 | 1409.4524 | | 1435.9898 | |
| 1494.0380 | 1503.3929 | | 1528.2611 | |
| 2885.4528 | 2944.0227 | | 2978.8295 | |
| 3035.5380 | 3039.2131 | | 3071.8526 | |
| 3082.7279 | 3095.9644 | | 3811.9146 | |
| Zero-point correction (Hartree): | 0.128118 | | | |

C4H9O2.pptt

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.21100500
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | | |
|---|-----------|-----------|-----------|--|
| O | 2.154705 | -1.024349 | -0.397935 | |
| C | 1.810009 | -0.047910 | 0.497089 | |
| C | 0.855275 | 1.029333 | -0.043302 | |
| C | -0.464729 | 0.474116 | -0.593778 | |
| C | -1.430681 | -0.012694 | 0.481599 | |
| O | -2.611746 | -0.459382 | -0.170912 | |
| H | -3.220028 | -0.792519 | 0.500070 | |
| H | 1.340274 | -0.601381 | 1.339974 | |
| H | 2.715744 | 0.398858 | 0.951469 | |
| H | 0.668289 | 1.762276 | 0.753971 | |
| H | 1.380355 | 1.568439 | -0.840430 | |
| H | -0.977409 | 1.245711 | -1.178828 | |
| H | -0.248259 | -0.353249 | -1.278387 | |
| H | -0.973861 | -0.826260 | 1.069640 | |
| H | -1.648020 | 0.810908 | 1.183641 | |

```

Rotational constants (GHz):    7.4304200    1.6400500    1.5277700
Vibrational harmonic frequencies (cm-1):
    63.0595          85.2154          171.0866
    240.0791        274.6036        305.1522
    440.5428        516.9839        603.3314
    783.3873        864.2882        870.9765
    1008.9772       1028.0282       1076.1183
    1096.6249       1109.9536       1142.6553
    1221.3051       1247.7019       1296.9317
    1322.4790       1335.3457       1364.7562
    1372.7592       1403.3084       1472.0537
    1494.9369       1511.0420       1541.2348
    2888.3136       2939.7759       2963.1641
    2989.2910       3032.5307       3060.2968
    3083.1079       3107.0258       3828.2820
Zero-point correction (Hartree): 0.127934
    
```

C4H9O2.ptmm

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.21400653

Electronic state : 2-A

Cartesian coordinates (Angs):

```

O    -2.622307    0.588626    -0.072399
C    -1.916374    -0.564985    0.149765
C    -0.461964    -0.550471    -0.332331
C    0.360553    0.582164    0.288218
C    1.806337    0.620534    -0.209554
O    2.518609    -0.586843    0.043301
H    2.594493    -0.686027    1.001356
H    -1.955945    -0.707891    1.253225
H    -2.476082    -1.434811    -0.246040
H    0.004461    -1.517021    -0.109347
H    -0.459667    -0.449183    -1.425636
H    -0.122878    1.542370    0.070962
H    0.361222    0.481436    1.385162
H    1.824321    0.745622    -1.298064
H    2.328336    1.487775    0.224576
    
```

```

Rotational constants (GHz):    10.1891200    1.5014500    1.3924300
Vibrational harmonic frequencies (cm-1):
    55.3070          114.6382          168.0290
    236.5917        279.2151        325.9634
    470.1489        531.7821        571.4052
    777.4818        852.0579        913.1232
    948.5754        1009.5159        1076.8854
    1094.8885       1101.9827       1116.2400
    1210.1192       1244.9258       1317.8173
    1328.3867       1362.8128       1369.2371
    1390.8467       1417.4545       1425.3737
    1493.0602       1507.9953       1520.8882
    2878.5373       2939.5467       2995.0793
    3005.8185       3043.3509       3073.3172
    3084.3819       3095.7856       3810.1996
Zero-point correction (Hartree): 0.127933
    
```

C4H9O2.ptmp

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.21327552

Electronic state : 2-A

Cartesian coordinates (Angs):

```

O    2.609248    -0.593380    -0.173015
C    1.929304    0.541028    0.181958
C    0.458492    0.585088    -0.251901
C    -0.362607    -0.573574    0.323058
C    -1.798683    -0.630640    -0.201591
O    -2.571442    0.514110    0.144816
H    -2.254022    1.257342    -0.382458
H    2.003843    0.583909    1.291261
H    2.488983    1.436102    -0.152921
H    0.034877    1.548928    0.061270
H    0.424955    0.560770    -1.350123
H    0.143934    -1.515980    0.080490
H    -0.391790    -0.495122    1.417911
H    -1.792058    -0.789181    -1.292684
    
```

```

Rotational constants (GHz):    10.2471200    1.4952800    1.3843800
Vibrational harmonic frequencies (cm-1):
    62.8093          109.5945          161.4692
    232.8688        275.3285        307.1481
    465.7302        523.4521        566.6015
    773.7591        847.7422        918.5386
    949.5178        1009.4701       1083.0614
    1088.3257       1099.8450       1144.9586
    1214.7586       1235.6393       1322.0902
    1326.9041       1363.7585       1373.1801
    
```

| | | |
|-----------|-----------|-----------|
| 1395.0734 | 1416.5648 | 1425.5505 |
| 1490.7781 | 1506.0873 | 1518.6324 |
| 2887.2420 | 2939.8093 | 2986.5036 |
| 3023.1176 | 3037.1115 | 3061.8657 |
| 3088.8681 | 3093.6380 | 3828.7303 |

Zero-point correction (Hartree): 0.127933

C4H9O2.ptmt

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.21372528
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 2.617099 | 0.591455 | 0.107260 |
| C | 1.920182 | -0.559354 | -0.154987 |
| C | 0.460346 | -0.565260 | 0.311489 |
| C | -0.358442 | 0.575211 | -0.300634 |
| C | -1.795368 | 0.623739 | 0.200594 |
| O | -2.438231 | -0.591346 | -0.173829 |
| H | -3.334937 | -0.580578 | 0.182066 |
| H | 1.968315 | -0.665460 | -1.262260 |
| H | 2.479767 | -1.439266 | 0.217590 |
| H | 0.004759 | -1.529562 | 0.060927 |
| H | 0.447289 | -0.484688 | 1.406842 |
| H | 0.130550 | 1.530368 | -0.076952 |
| H | -0.376336 | 0.472984 | -1.394021 |
| H | -1.801411 | 0.754333 | 1.295789 |
| H | -2.309245 | 1.494974 | -0.236196 |

Rotational constants (GHz): 10.2868300 1.5168400 1.4029900
 Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 57.8530 | 114.8415 | 165.4811 |
| 234.2434 | 268.3520 | 300.0708 |
| 464.1285 | 535.9578 | 591.2282 |
| 776.3887 | 862.7500 | 919.3335 |
| 956.7809 | 1030.1837 | 1066.6790 |
| 1095.5038 | 1102.0840 | 1163.6371 |
| 1199.0430 | 1259.8455 | 1280.5277 |
| 1327.5681 | 1332.5654 | 1364.3335 |
| 1368.3774 | 1419.8138 | 1461.3381 |
| 1491.5726 | 1505.6863 | 1536.3680 |
| 2879.0021 | 2940.8279 | 2974.0252 |
| 3003.9276 | 3035.2248 | 3045.1150 |
| 3084.6452 | 3102.9581 | 3832.1205 |

Zero-point correction (Hartree): 0.127920

C4H9O2.ptpm

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.21255646
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -2.381890 | -0.597130 | -0.685828 |
| C | -1.989163 | 0.166495 | 0.380515 |
| C | -0.492296 | 0.118041 | 0.711877 |
| C | 0.389253 | 0.581911 | -0.452467 |
| C | 1.891588 | 0.488776 | -0.170371 |
| O | 2.350999 | -0.842891 | 0.025828 |
| H | 2.011365 | -1.155790 | 0.873067 |
| H | -2.296116 | 1.205075 | 0.125963 |
| H | -2.615374 | -0.079293 | 1.261019 |
| H | -0.310128 | 0.734176 | 1.604095 |
| H | -0.241480 | -0.916712 | 0.979626 |
| H | 0.151588 | -0.021204 | -1.335635 |
| H | 0.148720 | 1.625749 | -0.700946 |
| H | 2.449256 | 0.867239 | -1.033198 |
| H | 2.153014 | 1.129585 | 0.688687 |

Rotational constants (GHz): 8.2691200 1.5369300 1.5069900
 Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 59.6766 | 113.4593 | 148.5957 |
| 234.8011 | 271.5473 | 309.1653 |
| 415.5904 | 439.3814 | 560.7171 |
| 781.3074 | 836.5716 | 895.2158 |
| 958.5271 | 1006.0067 | 1081.7166 |
| 1094.6169 | 1108.1672 | 1155.0423 |
| 1185.1575 | 1265.4957 | 1317.0147 |
| 1334.4684 | 1360.1593 | 1380.0420 |
| 1394.5951 | 1415.7334 | 1427.1793 |
| 1488.4514 | 1502.6393 | 1517.9874 |
| 2887.1935 | 2933.5861 | 2979.1920 |
| 3022.4996 | 3026.3428 | 3066.1579 |
| 3089.6490 | 3099.0163 | 3829.6091 |

Zero-point correction (Hartree): 0.127560

C4H9O2.ptpp

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.21424572
 Electronic state : 2-A

Cartesian coordinates (Angs):
O 2.299125 0.844193 -0.448213
C 1.981891 -0.264634 0.291762
C 0.495929 -0.421969 0.634276
C -0.398438 -0.478590 -0.607509
C -1.892183 -0.401379 -0.282183
O -2.248808 0.779420 0.427550
H -2.036189 1.534748 -0.136606
H 2.330620 -1.122058 -0.327159
H 2.623580 -0.316210 1.192920
H 0.366754 -1.327897 1.241953
H 0.184358 0.422234 1.259110
H -0.126483 0.353217 -1.271797
H -0.207858 -1.400693 -1.174943
H -2.479671 -0.501178 -1.208796
H -2.180833 -1.231636 0.372549
Rotational constants (GHz): 7.8021000 1.6047700 1.5477400
Vibrational harmonic frequencies (cm-1):
59.7817 127.0183 176.4628
228.6728 297.4997 341.3653
448.9054 521.2083 574.4589
785.6598 845.8422 900.1528
964.4011 1009.8158 1074.5084
1089.1279 1102.5948 1146.6374
1182.5914 1274.5843 1303.5541
1333.5886 1363.0271 1369.7161
1388.9752 1419.4011 1428.3975
1496.3908 1510.6962 1522.3235
2877.0344 2939.3624 2992.4715
3024.5250 3038.5611 3058.8047
3083.4079 3099.2233 3808.4001
Zero-point correction (Hartree): 0.128054

C4H9O2.ptpt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.21288461
Electronic state : 2-A
Cartesian coordinates (Angs):
O -2.355955 -0.718870 -0.575429
C -1.985240 0.215445 0.354593
C -0.489183 0.261515 0.688423
C 0.386657 0.512506 -0.543116
C 1.880489 0.451726 -0.246343
O 2.188846 -0.854895 0.226497
H 3.129183 -0.884950 0.440016
H -2.310263 1.185361 -0.086561
H -2.608765 0.119998 1.265085
H -0.325216 1.044007 1.442694
H -0.197343 -0.688448 1.147954
H 0.144080 -0.234407 -1.306887
H 0.161545 1.498094 -0.973762
H 2.445333 0.686349 -1.162847
H 2.141984 1.216961 0.504426
Rotational constants (GHz): 8.1695300 1.5808100 1.5422100
Vibrational harmonic frequencies (cm-1):
61.9791 125.1165 162.6723
223.5989 271.3317 304.4968
439.5172 538.0200 576.4604
784.7122 850.6194 908.6732
971.4650 1010.6704 1083.9846
1093.9444 1118.1891 1144.1104
1215.9112 1248.7200 1295.1018
1314.4966 1336.2506 1366.0052
1369.0628 1419.4111 1462.1161
1493.1475 1506.5143 1537.8839
2871.6575 2937.1005 2968.6379
3001.4921 3032.2431 3035.0350
3092.6981 3107.9324 3832.6931
Zero-point correction (Hartree): 0.127836

C4H9O2.pttm

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.21351618
Electronic state : 2-A
Cartesian coordinates (Angs):
O 2.421597 -0.959754 -0.291146
C 2.112899 0.255638 0.258388
C 0.743558 0.825695 -0.132902
C -0.412940 -0.102359 0.252294
C -1.772066 0.385199 -0.251892
O -2.845052 -0.451930 0.156226
H -2.691324 -1.328139 -0.220542
H 2.164854 0.095968 1.358414
H 2.932205 0.974717 0.061338
H 0.623779 1.808981 0.341728

| | | | | |
|--|-----------|-----------|-----------|--|
| H | 0.741236 | 0.998381 | -1.217228 | |
| H | -0.206435 | -1.100263 | -0.157707 | |
| H | -0.464627 | -0.212392 | 1.343314 | |
| H | -1.996137 | 1.374136 | 0.163681 | |
| H | -1.744615 | 0.497045 | -1.348964 | |
| Rotational constants (GHz): | 9.9878600 | 1.3893300 | 1.2909700 | |
| Vibrational harmonic frequencies (cm-1): | | | | |
| 90.5883 | 96.1289 | | 155.3290 | |
| 188.0333 | 307.9683 | | 328.9100 | |
| 438.1142 | 483.2056 | | 535.3955 | |
| 767.1938 | 855.4395 | | 919.7085 | |
| 989.3368 | 1027.9693 | | 1081.4744 | |
| 1092.0584 | 1095.6487 | | 1154.6437 | |
| 1192.9105 | 1287.4982 | | 1299.4050 | |
| 1329.2461 | 1361.6445 | | 1367.1328 | |
| 1389.1690 | 1413.7131 | | 1436.1352 | |
| 1495.6204 | 1510.4919 | | 1531.3332 | |
| 2885.0778 | 2936.9214 | | 2979.6158 | |
| 3028.2439 | 3035.3523 | | 3061.5224 | |
| 3074.7012 | 3091.8616 | | 3812.3211 | |
| Zero-point correction (Hartree): | 0.127867 | | | |

C4H9O2.pttp

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.21295830
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | | |
|--|------------|-----------|-----------|--|
| O | 2.441256 | -0.937871 | -0.317856 | |
| C | 2.110833 | 0.249948 | 0.277449 | |
| C | 0.740894 | 0.822691 | -0.107504 | |
| C | -0.412343 | -0.132231 | 0.218251 | |
| C | -1.774112 | 0.390974 | -0.241843 | |
| O | -2.832737 | -0.523602 | 0.005882 | |
| H | -2.884387 | -0.661903 | 0.960471 | |
| H | 2.153699 | 0.048506 | 1.370950 | |
| H | 2.924656 | 0.984615 | 0.117607 | |
| H | 0.606120 | 1.784188 | 0.406835 | |
| H | 0.749991 | 1.041385 | -1.183230 | |
| H | -0.223176 | -1.102338 | -0.253727 | |
| H | -0.443918 | -0.309267 | 1.304728 | |
| H | -1.975996 | 1.372328 | 0.220539 | |
| H | -1.766781 | 0.545973 | -1.326497 | |
| Rotational constants (GHz): | 10.0350200 | 1.3831500 | 1.2891700 | |
| Vibrational harmonic frequencies (cm-1): | | | | |
| 91.4607 | 95.4358 | | 152.0751 | |
| 188.7615 | 310.4092 | | 314.7787 | |
| 433.0369 | 455.8070 | | 526.8412 | |
| 766.0153 | 854.8597 | | 917.0975 | |
| 982.7268 | 1031.4929 | | 1087.0383 | |
| 1095.0612 | 1104.6704 | | 1126.7219 | |
| 1208.7291 | 1273.1557 | | 1312.0663 | |
| 1328.5294 | 1360.8604 | | 1369.0771 | |
| 1391.0057 | 1413.8724 | | 1437.1614 | |
| 1494.9281 | 1510.8497 | | 1531.4012 | |
| 2885.0895 | 2935.1106 | | 2975.4795 | |
| 3006.4225 | 3030.9692 | | 3070.5869 | |
| 3080.3584 | 3101.6508 | | 3813.8406 | |
| Zero-point correction (Hartree): | 0.127726 | | | |

C4H9O2.pttt

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.21245828
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | | |
|--|------------|-----------|-----------|--|
| O | 2.443329 | -0.933858 | -0.323644 | |
| C | 2.109336 | 0.251568 | 0.274617 | |
| C | 0.739330 | 0.822287 | -0.112919 | |
| C | -0.411352 | -0.126068 | 0.235907 | |
| C | -1.765479 | 0.376399 | -0.247302 | |
| O | -2.750064 | -0.568623 | 0.151751 | |
| H | -3.607975 | -0.262278 | -0.166537 | |
| H | 2.146681 | 0.044898 | 1.367270 | |
| H | 2.922454 | 0.988341 | 0.121414 | |
| H | 0.609618 | 1.791287 | 0.388516 | |
| H | 0.746801 | 1.025780 | -1.191884 | |
| H | -0.216554 | -1.108492 | -0.207698 | |
| H | -0.463967 | -0.273023 | 1.322617 | |
| H | -1.969143 | 1.371838 | 0.183229 | |
| H | -1.745044 | 0.496373 | -1.343600 | |
| Rotational constants (GHz): | 10.0875500 | 1.3959600 | 1.2993200 | |
| Vibrational harmonic frequencies (cm-1): | | | | |
| 91.4084 | 93.9813 | | 150.6768 | |
| 188.8268 | 271.2856 | | 315.1798 | |
| 432.4431 | 469.8074 | | 528.6628 | |
| 771.3812 | 864.9038 | | 920.6148 | |

| | | |
|-----------|-----------|-----------|
| 983.7575 | 1034.6731 | 1079.8251 |
| 1095.8174 | 1104.0019 | 1176.0555 |
| 1220.2533 | 1253.8386 | 1303.7960 |
| 1319.7471 | 1323.9251 | 1362.0524 |
| 1372.4745 | 1410.2382 | 1472.7934 |
| 1496.3190 | 1517.5825 | 1543.5838 |
| 2886.1996 | 2935.5738 | 2965.5698 |
| 2992.1792 | 3028.8004 | 3044.5312 |
| 3067.7677 | 3103.3120 | 3828.5097 |

Zero-point correction (Hartree): 0.127628

C4H9O2.tpm

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.21390857

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -2.611053 | -0.456720 | -0.206445 |
| C | -1.342577 | -0.321070 | 0.271457 |
| C | -0.611605 | 0.955792 | -0.180146 |
| C | 0.835741 | 1.068627 | 0.322201 |
| C | 1.819755 | 0.079849 | -0.309958 |
| O | 1.530494 | -1.289337 | -0.024365 |
| H | 1.658840 | -1.425976 | 0.923640 |
| H | -1.309773 | -0.440126 | 1.374445 |
| H | -0.788297 | -1.208245 | -0.106489 |
| H | -0.635111 | 0.997362 | -1.276114 |
| H | -1.187173 | 1.818196 | 0.177382 |
| H | 1.207310 | 2.081713 | 0.120113 |
| H | 0.863683 | 0.954872 | 1.417059 |
| H | 1.780298 | 0.160873 | -1.401779 |
| H | 2.846805 | 0.330605 | -0.003099 |

Rotational constants (GHz): 6.1582100 1.9907500 1.6283300

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 98.5470 | 114.2118 | 153.9021 |
| 271.3063 | 310.0127 | 356.9210 |
| 420.4257 | 518.0653 | 705.9009 |
| 807.2130 | 875.6105 | 907.6581 |
| 963.1776 | 1031.7636 | 1063.3955 |
| 1094.2098 | 1103.5314 | 1126.0874 |
| 1193.3553 | 1269.3292 | 1279.6825 |
| 1340.8215 | 1368.5065 | 1384.4327 |
| 1390.6358 | 1395.9013 | 1425.9190 |
| 1489.6125 | 1499.1953 | 1520.3052 |
| 2887.1675 | 2916.3869 | 3001.0402 |
| 3011.9800 | 3042.5446 | 3063.3369 |
| 3086.1918 | 3091.8276 | 3811.5690 |

Zero-point correction (Hartree): 0.128470

C4H9O2.tpmt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.21369021

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -2.617170 | -0.466905 | -0.213279 |
| C | -1.360018 | -0.310025 | 0.290388 |
| C | -0.609258 | 0.933420 | -0.216040 |
| C | 0.826395 | 1.070622 | 0.314862 |
| C | 1.833237 | 0.092635 | -0.282075 |
| O | 1.495243 | -1.232156 | 0.128582 |
| H | 2.093696 | -1.849466 | -0.309894 |
| H | -1.360096 | -0.364034 | 1.397908 |
| H | -0.802940 | -1.224356 | -0.007907 |
| H | -0.608002 | 0.914636 | -1.313261 |
| H | -1.187982 | 1.817599 | 0.078070 |
| H | 1.190970 | 2.083627 | 0.104199 |
| H | 0.838442 | 0.958742 | 1.407294 |
| H | 1.822697 | 0.178912 | -1.380922 |
| H | 2.846486 | 0.356922 | 0.059279 |

Rotational constants (GHz): 6.2945500 1.9813800 1.6275000

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 87.8864 | 102.1365 | 155.1371 |
| 267.2489 | 284.7027 | 328.0093 |
| 413.4434 | 512.0951 | 674.9022 |
| 811.9889 | 870.1454 | 905.7841 |
| 970.4992 | 1042.2216 | 1066.5195 |
| 1097.1607 | 1103.0198 | 1173.9915 |
| 1195.7099 | 1251.2472 | 1292.1759 |
| 1307.7040 | 1343.9544 | 1364.4302 |
| 1385.9642 | 1396.7613 | 1461.9948 |
| 1488.3038 | 1500.1799 | 1536.3707 |
| 2898.1146 | 2927.6255 | 2980.7987 |
| 3011.1699 | 3039.5804 | 3041.2300 |
| 3078.9221 | 3085.6491 | 3829.3557 |

Zero-point correction (Hartree): 0.128225

C4H9O2.tppm

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.21081010
Electronic state : 2-A
Cartesian coordinates (Angs):
O -2.698968 -0.604057 -0.035199
C -1.571978 0.015125 0.431132
C -0.571299 0.442317 -0.653931
C 0.726009 1.051352 -0.099892
C 1.664909 0.049534 0.583948
O 2.191287 -0.924845 -0.306714
H 1.473057 -1.510345 -0.576618
H -1.823729 0.856676 1.106714
H -1.114125 -0.740797 1.107756
H -0.351396 -0.423832 -1.290876
H -1.071099 1.170664 -1.302497
H 1.278752 1.523485 -0.919841
H 0.483462 1.849709 0.615798
H 2.533736 0.583203 0.982327
H 1.166937 -0.427511 1.444997
Rotational constants (GHz): 7.2069100 1.6419800 1.5280100
Vibrational harmonic frequencies (cm-1):
62.7385 88.5043 166.6261
239.9918 290.5435 327.3935
434.4641 506.9500 651.3189
774.3090 856.3976 907.9976
960.2960 1037.8582 1072.2843
1090.9060 1097.2112 1130.5026
1194.1005 1231.3737 1303.8228
1332.9914 1361.3735 1385.2661
1390.5352 1396.2892 1428.5760
1484.9487 1511.1770 1520.2442
2880.7080 2933.7804 2977.7271
3029.3807 3046.2800 3085.7847
3089.4935 3094.3250 3828.0056

Zero-point correction (Hartree): 0.128039

C4H9O2.tppp

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.21211738
Electronic state : 2-A
Cartesian coordinates (Angs):
O -2.695078 -0.540045 -0.071417
C -1.504383 -0.088712 0.427697
C -0.562310 0.527399 -0.617791
C 0.740345 1.080625 -0.023170
C 1.662847 0.014348 0.579905
O 1.959180 -1.046749 -0.319504
H 2.426012 -0.670908 -1.077488
H -1.659948 0.586823 1.293126
H -1.038704 -0.998022 0.867516
H -0.333515 -0.234182 -1.369528
H -1.103200 1.333850 -1.126254
H 1.287934 1.620030 -0.808820
H 0.519672 1.826949 0.753245
H 2.582359 0.492720 0.952701
H 1.187586 -0.464872 1.443022
Rotational constants (GHz): 6.9067000 1.7255800 1.5843400
Vibrational harmonic frequencies (cm-1):
46.0144 95.0263 183.3627
230.3193 313.4786 329.5999
430.3823 537.5734 666.0892
774.1781 863.4690 929.3055
960.8185 1039.4556 1060.4447
1091.8047 1103.5920 1150.2269
1170.3046 1251.9856 1314.8970
1324.4073 1367.5549 1381.1019
1391.3138 1405.7074 1431.0415
1492.9294 1499.7302 1526.0253
2890.3528 2926.6369 2995.7368
3021.9666 3050.8682 3062.2182
3085.4736 3113.8302 3810.9905

Zero-point correction (Hartree): 0.128307

C4H9O2.tppt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.21135799
Electronic state : 2-A
Cartesian coordinates (Angs):
O -2.695271 -0.566687 -0.062466
C -1.516765 -0.080313 0.433498
C -0.570877 0.514664 -0.620583
C 0.731118 1.078829 -0.033328

| | | | | |
|--|-----------|-----------|-----------|-----------|
| C | 1.659042 | 0.028103 | 0.572099 | |
| O | 1.981643 | -0.915215 | -0.442191 | |
| H | 2.554373 | -1.590658 | -0.059213 | |
| H | -1.689364 | 0.619374 | 1.276176 | |
| H | -1.044277 | -0.970060 | 0.905991 | |
| H | -0.340399 | -0.255177 | -1.362353 | |
| H | -1.109264 | 1.315621 | -1.140622 | |
| H | 1.279884 | 1.602110 | -0.824776 | |
| H | 0.508006 | 1.825675 | 0.740970 | |
| H | 2.562778 | 0.524729 | 0.959923 | |
| H | 1.172183 | -0.464094 | 1.431042 | |
| Rotational constants (GHz): | | | | 7.0532700 |
| Vibrational harmonic frequencies (cm-1): | | | | 1.7107000 |
| | 44.5197 | 91.2917 | 180.3828 | 1.5816500 |
| | 231.6903 | 279.7413 | 325.1251 | |
| | 427.3512 | 521.7305 | 671.6530 | |
| | 781.1393 | 865.1352 | 933.1504 | |
| | 966.8779 | 1044.0139 | 1075.0799 | |
| | 1086.4130 | 1104.6967 | 1149.5535 | |
| | 1202.0298 | 1251.6033 | 1272.7753 | |
| | 1318.9580 | 1337.2919 | 1365.6917 | |
| | 1392.1511 | 1398.5685 | 1464.5046 | |
| | 1487.7368 | 1502.9681 | 1540.5582 | |
| | 2884.9378 | 2925.9715 | 2972.3530 | |
| | 3001.6046 | 3037.3203 | 3059.8955 | |
| | 3085.5932 | 3122.0465 | 3832.4859 | |
| Zero-point correction (Hartree): | | | | 0.128116 |

C4H9O2.tptm

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.21122557
Electronic state : 2-A
Cartesian coordinates (Angs):

| | | | | |
|--|-----------|-----------|-----------|------------|
| O | 2.959139 | -0.358857 | 0.119864 | |
| C | 1.654624 | -0.379243 | -0.290687 | |
| C | 0.790955 | 0.777441 | 0.235507 | |
| C | -0.663681 | 0.740560 | -0.256669 | |
| C | -1.502044 | -0.394929 | 0.339209 | |
| O | -2.830768 | -0.415974 | -0.161009 | |
| H | -3.250561 | 0.418768 | 0.084712 | |
| H | 1.591334 | -0.465771 | -1.394275 | |
| H | 1.270095 | -1.357889 | 0.071327 | |
| H | 0.828948 | 0.770972 | 1.332014 | |
| H | 1.261167 | 1.713867 | -0.085543 | |
| H | -1.146209 | 1.695445 | -0.005941 | |
| H | -0.695134 | 0.659550 | -1.351103 | |
| H | -1.079930 | -1.370217 | 0.073469 | |
| H | -1.485801 | -0.329052 | 1.440337 | |
| Rotational constants (GHz): | | | | 11.0957900 |
| Vibrational harmonic frequencies (cm-1): | | | | 1.3462100 |
| | 85.6302 | 90.2523 | 117.8925 | 1.2742800 |
| | 251.6307 | 292.5786 | 321.8726 | |
| | 367.1393 | 534.7830 | 594.6531 | |
| | 767.8824 | 831.1414 | 920.7422 | |
| | 993.8905 | 1055.0604 | 1065.4205 | |
| | 1087.7914 | 1092.0804 | 1161.0578 | |
| | 1185.1388 | 1270.0332 | 1313.3063 | |
| | 1336.5642 | 1349.0797 | 1374.5421 | |
| | 1387.4566 | 1401.4364 | 1438.5728 | |
| | 1499.1688 | 1504.7840 | 1528.9406 | |
| | 2893.9102 | 2927.4002 | 2978.9314 | |
| | 3024.6314 | 3046.8314 | 3065.3266 | |
| | 3088.6416 | 3093.3251 | 3812.2092 | |
| Zero-point correction (Hartree): | | | | 0.127923 |

C4H9O2.tptp

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.21094215
Electronic state : 2-A
Cartesian coordinates (Angs):

| | | | | |
|---|-----------|-----------|-----------|--|
| O | -2.959767 | -0.364077 | -0.107213 | |
| C | -1.650739 | -0.386021 | 0.287782 | |
| C | -0.794547 | 0.776943 | -0.237151 | |
| C | 0.663977 | 0.748671 | 0.244175 | |
| C | 1.502952 | -0.391220 | -0.341570 | |
| O | 2.870726 | -0.312454 | 0.033419 | |
| H | 2.918440 | -0.391934 | 0.995008 | |
| H | -1.572737 | -0.485185 | 1.389716 | |
| H | -1.269545 | -1.359336 | -0.092167 | |
| H | -0.837404 | 0.776249 | -1.333270 | |
| H | -1.267058 | 1.709751 | 0.091106 | |
| H | 1.155263 | 1.692332 | -0.017873 | |
| H | 0.686945 | 0.684528 | 1.343249 | |
| H | 1.076015 | -1.370780 | -0.069008 | |
| H | 1.492554 | -0.333613 | -1.435825 | |

Rotational constants (GHz): 11.2139600 1.3390000 1.2722000
 Vibrational harmonic frequencies (cm⁻¹):
 87.6423 90.3576 117.7778
 249.7619 294.8156 317.6077
 361.3242 538.1984 609.4410
 770.6562 833.6061 920.1235
 988.3065 1052.4381 1082.2888
 1085.1772 1104.2503 1119.7602
 1208.8312 1274.0952 1299.3827
 1337.5102 1350.7724 1374.1514
 1383.8170 1404.2628 1435.5925
 1499.5543 1504.9711 1528.3451
 2891.4681 2923.1418 2981.0744
 3008.2942 3049.0495 3075.8087
 3090.8824 3094.4288 3813.0292
 Zero-point correction (Hartree): 0.127924

C4H9O2.tppt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.21064523

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 2.955534 | -0.380583 | 0.112161 |
| C | 1.652675 | -0.375119 | -0.304178 |
| C | 0.794275 | 0.768356 | 0.257988 |
| C | -0.660426 | 0.756593 | -0.232189 |
| C | -1.500798 | -0.387183 | 0.327414 |
| O | -2.818517 | -0.240629 | -0.184060 |
| H | -3.360557 | -0.958452 | 0.165524 |
| H | 1.591562 | -0.424532 | -1.410221 |
| H | 1.259201 | -1.362300 | 0.024456 |
| H | 0.835761 | 0.730301 | 1.353691 |
| H | 1.267280 | 1.711968 | -0.036930 |
| H | -1.149987 | 1.696244 | 0.046740 |
| H | -0.692797 | 0.707151 | -1.328485 |
| H | -1.071600 | -1.360745 | 0.036515 |
| H | -1.489355 | -0.345817 | 1.429688 |

Rotational constants (GHz): 11.2820400 1.3487400 1.2796500

Vibrational harmonic frequencies (cm⁻¹):
 82.3920 89.8128 119.2437
 254.3168 280.6387 299.5546
 358.6248 538.6048 602.2427
 778.9822 835.9120 924.3946
 987.0253 1061.4635 1073.6095
 1082.3692 1104.9354 1159.9541
 1233.3781 1246.9877 1290.2055
 1316.7818 1337.2916 1364.6614
 1373.7296 1387.9031 1471.3625
 1501.7033 1509.1894 1542.3273
 2889.1851 2926.3305 2967.9804
 2992.9187 3044.2019 3047.9297
 3090.9704 3094.3568 3829.0761
 Zero-point correction (Hartree): 0.127788

C4H9O2.ttpm

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.21265985

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -2.927397 | -0.546937 | 0.099549 |
| C | -1.899994 | 0.308437 | -0.190892 |
| C | -0.505811 | -0.161049 | 0.239949 |
| C | 0.603218 | 0.817776 | -0.161428 |
| C | 1.999565 | 0.382440 | 0.294154 |
| O | 2.430611 | -0.835022 | -0.300411 |
| H | 1.920661 | -1.555834 | 0.089156 |
| H | -1.936870 | 0.450169 | -1.293645 |
| H | -2.130624 | 1.319294 | 0.202845 |
| H | -0.510484 | -0.301792 | 1.329285 |
| H | -0.327012 | -1.145056 | -0.210279 |
| H | 0.615606 | 0.936773 | -1.252809 |
| H | 0.395440 | 1.809951 | 0.264162 |
| H | 2.735443 | 1.135035 | -0.007096 |
| H | 2.030261 | 0.321517 | 1.394579 |

Rotational constants (GHz): 10.1725100 1.3803500 1.2845300

Vibrational harmonic frequencies (cm⁻¹):
 88.8125 95.0286 141.9887
 195.6590 305.1116 327.5553
 420.7155 480.7295 503.0463
 760.8385 876.7041 892.0647
 996.9054 1027.7708 1068.0680
 1089.6007 1095.0275 1159.4797
 1215.8542 1263.1930 1303.4757
 1323.8964 1362.7991 1388.0423
 1398.0193 1411.7138 1425.0215

| | | |
|-----------|-----------|-----------|
| 1489.5278 | 1511.4061 | 1517.2229 |
| 2887.7192 | 2923.6918 | 2986.0800 |
| 3022.4860 | 3034.8620 | 3063.7066 |
| 3087.3973 | 3092.7243 | 3831.3368 |

Zero-point correction (Hartree): 0.127726

C4H9O2.tttp

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.21286137

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 2.929728 | -0.526686 | -0.138071 |
| C | 1.883456 | 0.254310 | 0.272000 |
| C | 0.511111 | -0.128460 | -0.291177 |
| C | -0.604602 | 0.819047 | 0.161333 |
| C | -1.996274 | 0.377630 | -0.301674 |
| O | -2.357018 | -0.917052 | 0.164216 |
| H | -2.424677 | -0.875524 | 1.127171 |
| H | 1.869476 | 0.320920 | 1.379265 |
| H | 2.158654 | 1.286425 | -0.042153 |
| H | 0.574679 | -0.143173 | -1.386221 |
| H | 0.267679 | -1.149147 | 0.022558 |
| H | -0.605058 | 0.897625 | 1.259902 |
| H | -0.419058 | 1.835785 | -0.213383 |
| H | -2.743206 | 1.130488 | -0.004186 |
| H | -2.022311 | 0.311340 | -1.395010 |

Rotational constants (GHz): 9.9582600 1.3902300 1.3001400

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 83.3873 | 93.1120 | 154.8633 |
| 193.6557 | 310.9116 | 329.8394 |
| 427.5667 | 498.8724 | 516.9665 |
| 762.9400 | 881.1101 | 899.1619 |
| 982.0986 | 1023.4321 | 1077.3285 |
| 1092.2434 | 1101.2027 | 1120.8569 |
| 1221.1628 | 1272.5641 | 1288.5846 |
| 1324.6973 | 1367.1769 | 1384.9792 |
| 1391.5317 | 1411.8399 | 1425.7267 |
| 1494.1048 | 1513.2328 | 1520.7405 |
| 2876.7286 | 2919.6840 | 2992.9499 |
| 3005.8298 | 3044.9073 | 3053.5650 |
| 3086.5976 | 3105.8298 | 3810.5079 |

Zero-point correction (Hartree): 0.127720

C4H9O2.ttpt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.21252521

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -2.928518 | -0.542952 | 0.123324 |
| C | -1.891734 | 0.278891 | -0.227572 |
| C | -0.510301 | -0.141101 | 0.284140 |
| C | 0.600388 | 0.813591 | -0.168110 |
| C | 1.988883 | 0.384808 | 0.292871 |
| O | 2.286209 | -0.869685 | -0.309190 |
| H | 3.132388 | -1.179087 | 0.035809 |
| H | -1.901423 | 0.299186 | -1.340324 |
| H | -2.133871 | 1.326470 | 0.046836 |
| H | -0.544049 | -0.181926 | 1.380817 |
| H | -0.292072 | -1.154595 | -0.065358 |
| H | 0.611131 | 0.883279 | -1.264127 |
| H | 0.409666 | 1.826885 | 0.210979 |
| H | 2.726159 | 1.150079 | 0.001112 |
| H | 2.007129 | 0.313669 | 1.393205 |

Rotational constants (GHz): 10.1402700 1.3994700 1.3060700

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 79.3899 | 95.5838 | 150.4439 |
| 191.3015 | 261.4155 | 317.9959 |
| 400.7200 | 475.8632 | 499.1336 |
| 760.8579 | 886.8701 | 908.3058 |
| 989.6034 | 1026.6047 | 1073.4819 |
| 1087.7761 | 1119.1046 | 1149.0238 |
| 1236.2308 | 1257.6968 | 1280.6751 |
| 1309.8968 | 1336.6082 | 1365.0583 |
| 1386.9145 | 1413.4059 | 1461.3905 |
| 1490.4466 | 1512.1528 | 1536.7595 |
| 2881.4280 | 2916.0312 | 2974.1769 |
| 3002.5709 | 3030.2131 | 3044.4944 |
| 3068.7929 | 3115.6718 | 3832.7150 |

Zero-point correction (Hartree): 0.127411

C4H9O2.tttp

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.21257065

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|--|------------|-----------|-----------|
| O | 3.163621 | 0.211927 | 0.007983 |
| C | 1.966231 | -0.449264 | -0.006323 |
| C | 0.717272 | 0.439165 | 0.022441 |
| C | -0.584585 | -0.368534 | -0.028738 |
| C | -1.836368 | 0.511007 | 0.018830 |
| O | -3.040902 | -0.233522 | -0.093414 |
| H | -3.104202 | -0.810008 | 0.679013 |
| H | 1.979274 | -1.074090 | -0.926527 |
| H | 1.950932 | -1.202189 | 0.808524 |
| H | 0.749504 | 1.050598 | 0.933381 |
| H | 0.768225 | 1.135364 | -0.823749 |
| H | -0.623693 | -0.974936 | -0.942926 |
| H | -0.613428 | -1.075522 | 0.814678 |
| H | -1.826484 | 1.126109 | 0.934056 |
| H | -1.837186 | 1.203189 | -0.830262 |
| Rotational constants (GHz): | 17.7662800 | 1.1535500 | 1.1158600 |
| Vibrational harmonic frequencies (cm-1): | | | |
| 81.2197 | 110.5311 | | 136.8328 |
| 156.7022 | 309.8370 | | 335.6692 |
| 349.7270 | 377.7033 | | 534.7306 |
| 754.2766 | 829.7860 | | 981.9427 |
| 989.8152 | 1045.5714 | | 1071.6475 |
| 1085.4378 | 1091.0134 | | 1137.8873 |
| 1241.4247 | 1263.7432 | | 1303.0161 |
| 1328.1659 | 1350.0424 | | 1375.0396 |
| 1400.8047 | 1410.9602 | | 1434.9883 |
| 1500.7030 | 1510.2516 | | 1530.5648 |
| 2888.6927 | 2918.9034 | | 2983.9900 |
| 3008.4687 | 3041.6259 | | 3060.4058 |
| 3083.3405 | 3094.5092 | | 3814.6318 |
| Zero-point correction (Hartree): | 0.127406 | | |

C4H9O2.tttt

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.21221502
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | |
|--|------------|-----------|-----------|
| O | 3.163344 | 0.215654 | -0.005552 |
| C | 1.964710 | -0.443868 | 0.007559 |
| C | 0.715800 | 0.443923 | 0.003461 |
| C | -0.581880 | -0.370513 | -0.001986 |
| C | -1.831411 | 0.501027 | 0.001919 |
| O | -2.962913 | -0.359861 | -0.003222 |
| H | -3.757928 | 0.187119 | -0.001451 |
| H | 1.968726 | -1.125591 | -0.870531 |
| H | 1.958957 | -1.147460 | 0.866210 |
| H | 0.753485 | 1.096417 | 0.885114 |
| H | 0.761696 | 1.100489 | -0.874496 |
| H | -0.619764 | -1.021909 | -0.884842 |
| H | -0.621354 | -1.031447 | 0.873623 |
| H | -1.825703 | 1.151583 | 0.892456 |
| H | -1.824871 | 1.161035 | -0.881600 |
| Rotational constants (GHz): | 17.9095300 | 1.1641400 | 1.1233400 |
| Vibrational harmonic frequencies (cm-1): | | | |
| 70.1663 | 100.5744 | | 128.9284 |
| 138.9184 | 206.4724 | | 276.5248 |
| 349.7477 | 353.3230 | | 532.2117 |
| 757.3936 | 839.2448 | | 987.8447 |
| 990.7553 | 1050.5100 | | 1056.2348 |
| 1084.9750 | 1099.4273 | | 1200.4176 |
| 1228.5625 | 1264.5244 | | 1291.4603 |
| 1312.8773 | 1325.8511 | | 1351.7917 |
| 1386.0446 | 1419.2049 | | 1472.4219 |
| 1503.2165 | 1516.1499 | | 1543.9624 |
| 2894.3473 | 2914.4456 | | 2971.0203 |
| 2997.8590 | 3034.1947 | | 3043.1780 |
| 3069.1062 | 3091.9001 | | 3828.3616 |
| Zero-point correction (Hartree): | 0.126858 | | |

C4H9O2.1-5Hshift.a.m

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.20464684
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| C | -1.099480 | -0.091659 | 0.387109 |
| C | -0.349970 | 1.130269 | -0.110929 |
| C | 1.146043 | 1.011737 | 0.212333 |
| C | 1.690512 | -0.315435 | -0.350983 |
| O | 0.999442 | -1.413488 | 0.172049 |
| H | -1.249851 | -0.107889 | 1.477033 |
| O | -2.270640 | -0.300693 | -0.335505 |
| H | -0.774760 | 2.046456 | 0.320687 |
| H | -0.495495 | 1.188411 | -1.196801 |
| H | 1.299741 | 1.024478 | 1.298486 |

| | | | | |
|--|-----------|-----------|-----------|--|
| H | 1.700251 | 1.857906 | -0.209380 | |
| H | 2.747811 | -0.426798 | -0.059936 | |
| H | 1.656194 | -0.285196 | -1.455833 | |
| H | -0.257634 | -0.989590 | 0.219281 | |
| H | -2.779298 | -1.003807 | 0.088941 | |
| Rotational constants (GHz): | 5.7175300 | 2.4802800 | 1.9113500 | |
| Vibrational harmonic frequencies (cm-1): | | | | |
| i1122.6262 | 122.4311 | | 225.0165 | |
| 307.5653 | 364.3590 | | 393.1244 | |
| 446.5601 | 487.1989 | | 588.3313 | |
| 823.2161 | 850.2754 | | 912.8007 | |
| 933.8661 | 996.4201 | | 1062.4381 | |
| 1080.0631 | 1133.8907 | | 1163.2783 | |
| 1190.9564 | 1206.6934 | | 1265.2930 | |
| 1285.8070 | 1339.0159 | | 1364.2692 | |
| 1378.7900 | 1388.1490 | | 1431.3961 | |
| 1488.2211 | 1495.1506 | | 1508.6064 | |
| 1637.7737 | 2945.7537 | | 3000.4475 | |
| 3018.2810 | 3032.5804 | | 3048.5855 | |
| 3080.5548 | 3098.1322 | | 3822.4444 | |
| Zero-point correction (Hartree): | 0.125112 | | | |

C4H9O2.1-5Hshift.a.t

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.20447403
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | | |
|--|-----------|-----------|-----------|--|
| C | 1.103354 | -0.102540 | -0.405377 | |
| C | 0.361895 | 1.120403 | 0.124338 | |
| C | -1.132017 | 1.022053 | -0.207851 | |
| C | -1.696034 | -0.303187 | 0.343958 | |
| O | -1.008729 | -1.407154 | -0.168458 | |
| H | 1.248893 | -0.094793 | -1.489766 | |
| O | 2.325832 | -0.400528 | 0.182727 | |
| H | 0.801622 | 2.041111 | -0.281927 | |
| H | 0.486082 | 1.165071 | 1.217345 | |
| H | -1.275477 | 1.044542 | -1.294890 | |
| H | -1.680929 | 1.870359 | 0.216126 | |
| H | -2.750975 | -0.400362 | 0.040407 | |
| H | -1.676794 | -0.271361 | 1.450295 | |
| H | 0.252067 | -0.994037 | -0.244583 | |
| H | 2.235496 | -0.319451 | 1.142438 | |
| Rotational constants (GHz): | 5.7097400 | 2.4596300 | 1.9017400 | |
| Vibrational harmonic frequencies (cm-1): | | | | |
| i1107.6994 | 127.4151 | | 204.2710 | |
| 306.6981 | 370.9551 | | 408.1728 | |
| 450.7655 | 488.3313 | | 588.2975 | |
| 817.6237 | 848.6494 | | 907.4158 | |
| 935.5692 | 996.9829 | | 1061.7228 | |
| 1083.6399 | 1112.5398 | | 1164.1494 | |
| 1187.4525 | 1210.2447 | | 1261.3492 | |
| 1299.9599 | 1352.4069 | | 1354.2274 | |
| 1383.1689 | 1387.2355 | | 1429.1746 | |
| 1484.2788 | 1494.2139 | | 1511.4677 | |
| 1636.7387 | 2932.4162 | | 3001.3485 | |
| 3007.5635 | 3047.9292 | | 3060.7355 | |
| 3098.8819 | 3106.2789 | | 3800.2787 | |
| Zero-point correction (Hartree): | 0.125118 | | | |

C4H9O2.1-5Hshift.s.p

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.20375305
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | | |
|--|-----------|-----------|-----------|--|
| C | 1.133295 | -0.180390 | 0.527867 | |
| C | 0.369175 | 1.127679 | 0.447284 | |
| C | -0.830306 | 0.979708 | -0.504614 | |
| C | -1.722381 | -0.176614 | -0.012656 | |
| O | -1.011251 | -1.376243 | 0.099037 | |
| O | 1.960001 | -0.337283 | -0.583440 | |
| H | 1.647932 | -0.360533 | 1.483376 | |
| H | 1.043648 | 1.925790 | 0.112083 | |
| H | 0.014554 | 1.392138 | 1.450979 | |
| H | -0.466763 | 0.755118 | -1.513195 | |
| H | -1.413462 | 1.906434 | -0.552923 | |
| H | -2.529990 | -0.342432 | -0.745064 | |
| H | -2.199822 | 0.113765 | 0.942095 | |
| H | 0.199979 | -0.997596 | 0.468986 | |
| H | 2.415228 | -1.186773 | -0.518403 | |
| Rotational constants (GHz): | 5.3071700 | 2.7243000 | 2.1576300 | |
| Vibrational harmonic frequencies (cm-1): | | | | |
| i1174.3812 | 122.3455 | | 165.1913 | |
| 283.1742 | 350.3813 | | 405.9351 | |
| 495.7822 | 513.5941 | | 671.8067 | |
| 839.4634 | 861.7475 | | 900.4591 | |

| | | |
|-----------|-----------|-----------|
| 943.5095 | 1013.4123 | 1056.9673 |
| 1086.1557 | 1091.1526 | 1167.4839 |
| 1188.9522 | 1211.8150 | 1248.4517 |
| 1261.4310 | 1300.3862 | 1351.2811 |
| 1370.5589 | 1386.4858 | 1429.2365 |
| 1479.9109 | 1493.0427 | 1508.4319 |
| 1621.2543 | 2938.8389 | 2994.3444 |
| 3016.9361 | 3041.9861 | 3058.9485 |
| 3086.2891 | 3109.8144 | 3823.3294 |

Zero-point correction (Hartree): 0.125049

C4H9O2.1-5Hshift.s.t

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -308.20417479

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| C | 1.160673 | -0.114780 | 0.549259 |
| C | 0.364112 | 1.177428 | 0.389210 |
| C | -0.861676 | 0.966054 | -0.513787 |
| C | -1.689768 | -0.216784 | 0.026559 |
| O | -0.919037 | -1.379403 | 0.137102 |
| O | 1.968358 | -0.483607 | -0.520594 |
| H | 1.760881 | -0.171261 | 1.461102 |
| H | 1.020587 | 1.963203 | -0.007216 |
| H | 0.028556 | 1.501629 | 1.382303 |
| H | -0.546678 | 0.745686 | -1.542663 |

| | | | |
|---|-----------|-----------|-----------|
| H | -1.477910 | 1.871164 | -0.556480 |
| H | -2.509889 | -0.437113 | -0.675908 |
| H | -2.152365 | 0.071648 | 0.988385 |
| H | 0.233198 | -0.946948 | 0.617118 |
| H | 1.409002 | -0.565435 | -1.306140 |

Rotational constants (GHz): 5.1689300 2.8119900 2.1935400

Vibrational harmonic frequencies (cm-1):

| | | |
|------------|-----------|-----------|
| i1222.2685 | 97.7136 | 151.5301 |
| 291.4240 | 361.0330 | 417.3593 |
| 498.2344 | 517.0307 | 654.3976 |
| 826.9500 | 857.3007 | 890.0224 |
| 937.2512 | 1014.6887 | 1050.2102 |
| 1076.7110 | 1108.9504 | 1149.6282 |
| 1197.1508 | 1204.9181 | 1257.1460 |
| 1280.6012 | 1340.0555 | 1351.8180 |
| 1377.3823 | 1385.3362 | 1434.8016 |
| 1478.1526 | 1497.6959 | 1505.5500 |
| 1605.8614 | 2948.3672 | 3002.7095 |
| 3033.5485 | 3037.6801 | 3079.9197 |
| 3092.8099 | 3115.6079 | 3797.2884 |

Zero-point correction (Hartree): 0.125128

C5H11O2.pmmmm

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.52877391

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 1.823705 | -1.320939 | -0.025862 |
| C | 2.176962 | -0.003573 | -0.159950 |
| C | 1.037641 | 0.941054 | -0.571834 |
| C | -0.009761 | 1.151182 | 0.534017 |
| C | -0.736745 | -0.118728 | 1.004711 |
| C | -1.566412 | -0.810361 | -0.081078 |
| O | -2.486778 | 0.064639 | -0.728122 |
| H | -3.114718 | 0.372583 | -0.061466 |
| H | 2.717952 | 0.369844 | 0.731484 |
| H | 2.939033 | -0.020090 | -0.970827 |
| H | 1.475100 | 1.911898 | -0.838380 |
| H | 0.565764 | 0.546145 | -1.477983 |
| H | 0.474087 | 1.623643 | 1.399566 |
| H | -0.756444 | 1.863545 | 0.165426 |
| H | -0.019033 | -0.850626 | 1.400483 |
| H | -1.393562 | 0.147231 | 1.846403 |
| H | -0.910755 | -1.189575 | -0.869540 |
| H | -2.082951 | -1.681650 | 0.351507 |

Rotational constants (GHz): 4.2599400 1.5064100 1.3575600

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 43.8563 | 85.7908 | 131.0500 |
| 188.7552 | 235.4144 | 322.9025 |
| 330.6325 | 378.4566 | 461.5074 |
| 543.5064 | 740.8956 | 761.7367 |
| 829.8033 | 877.6839 | 907.5530 |
| 962.9661 | 999.1911 | 1043.4845 |
| 1065.6005 | 1091.5703 | 1113.1482 |
| 1135.5246 | 1163.9599 | 1182.0094 |
| 1261.7779 | 1325.9046 | 1331.9374 |
| 1365.0673 | 1377.5628 | 1392.9366 |

| | | |
|-----------|-----------|-----------|
| 1404.2026 | 1410.2229 | 1426.6065 |
| 1483.2687 | 1489.3632 | 1494.9520 |
| 1531.2408 | 2880.1584 | 2940.0518 |
| 2995.6765 | 3012.2669 | 3033.5413 |
| 3044.3347 | 3048.8240 | 3084.8362 |
| 3098.2473 | 3114.0544 | 3808.8305 |

Zero-point correction (Hartree): 0.157086

C5H11O2.pmmmp

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.52737667

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 1.824361 | -1.329710 | -0.070709 |
| C | 2.179691 | -0.009540 | -0.159592 |
| C | 1.044857 | 0.948739 | -0.551648 |
| C | -0.000441 | 1.136847 | 0.562016 |
| C | -0.740202 | -0.134955 | 1.009225 |
| C | -1.588387 | -0.802326 | -0.078661 |
| O | -2.600073 | 0.053233 | -0.605134 |
| H | -2.173124 | 0.699540 | -1.180233 |
| H | 2.709469 | 0.335286 | 0.749691 |
| H | 2.952821 | -0.000529 | -0.959742 |
| H | 1.484330 | 1.923550 | -0.799800 |
| H | 0.580969 | 0.567571 | -1.469510 |
| H | 0.493724 | 1.582647 | 1.435352 |
| H | -0.739211 | 1.879303 | 0.232032 |
| H | -0.021930 | -0.878229 | 1.382304 |
| H | -1.393938 | 0.124689 | 1.850957 |
| H | -0.941282 | -1.197340 | -0.874812 |
| H | -2.119237 | -1.657271 | 0.352473 |

Rotational constants (GHz): 4.2785200 1.4852000 1.3360500

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 52.2815 | 84.3394 | 127.4315 |
| 179.3255 | 230.1194 | 274.1342 |
| 331.1561 | 383.0145 | 460.3016 |
| 528.9398 | 742.7688 | 757.9048 |
| 823.0427 | 874.0205 | 915.6978 |
| 955.0202 | 1005.7324 | 1048.2656 |
| 1078.0133 | 1089.4089 | 1110.9609 |
| 1138.2826 | 1155.9521 | 1207.1738 |
| 1248.0572 | 1320.1207 | 1337.9062 |
| 1365.2478 | 1381.0717 | 1393.4539 |
| 1399.5095 | 1406.5691 | 1428.2369 |
| 1482.0490 | 1486.0783 | 1507.2994 |
| 1528.3357 | 2883.3229 | 2942.6887 |
| 3020.8492 | 3024.2958 | 3028.8614 |
| 3040.8506 | 3062.8684 | 3075.7456 |
| 3084.4008 | 3095.4421 | 3831.2686 |

Zero-point correction (Hartree): 0.157029

C5H11O2.pmmmt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.52818239

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 1.794336 | -1.337027 | -0.011842 |
| C | 2.157969 | -0.026326 | -0.179325 |
| C | 1.024141 | 0.922189 | -0.597737 |
| C | -0.001862 | 1.179296 | 0.517851 |
| C | -0.744045 | -0.062300 | 1.038283 |
| C | -1.555164 | -0.804176 | -0.019128 |
| O | -2.457059 | 0.120127 | -0.624387 |
| H | -2.943219 | -0.345293 | -1.315583 |
| H | 2.713729 | 0.360954 | 0.696945 |
| H | 2.910291 | -0.069286 | -0.998595 |
| H | 1.470997 | 1.878623 | -0.899019 |
| H | 0.531717 | 0.508996 | -1.485006 |
| H | 0.505887 | 1.663016 | 1.363545 |
| H | -0.741965 | 1.895702 | 0.146245 |
| H | -0.036834 | -0.778547 | 1.477772 |
| H | -1.419115 | 0.250172 | 1.844770 |
| H | -0.876581 | -1.248036 | -0.761908 |
| H | -2.099360 | -1.633199 | 0.461006 |

Rotational constants (GHz): 4.2040800 1.5341900 1.3796400

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 45.7097 | 85.3678 | 127.8535 |
| 183.3872 | 233.4257 | 272.7428 |
| 325.2417 | 378.4304 | 457.5917 |
| 536.1455 | 743.5761 | 759.7134 |
| 831.8785 | 874.8883 | 916.4315 |
| 970.3110 | 991.1754 | 1063.4676 |
| 1080.4151 | 1088.0577 | 1110.0748 |
| 1140.7207 | 1170.9066 | 1207.5552 |
| 1258.1333 | 1288.3655 | 1326.9446 |

| | | |
|-----------|-----------|-----------|
| 1337.5948 | 1365.4814 | 1389.1953 |
| 1402.8757 | 1409.0012 | 1461.1692 |
| 1482.2178 | 1487.7338 | 1497.2203 |
| 1546.9267 | 2877.5752 | 2940.0795 |
| 2988.3348 | 3024.6402 | 3031.4124 |
| 3035.3992 | 3042.8831 | 3073.3670 |
| 3091.5942 | 3098.4259 | 3831.6438 |

Zero-point correction (Hartree): 0.156928

C5H11O2.pmmpp

 Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -0.845614 | -1.522880 | -0.399948 |
| C | -1.800905 | -0.569267 | -0.137891 |
| C | -1.325762 | 0.629508 | 0.693662 |
| C | -0.370755 | 1.569939 | -0.058065 |
| C | 0.858742 | 0.908266 | -0.703221 |
| C | 1.825477 | 0.166560 | 0.254445 |
| O | 1.664392 | -1.240205 | 0.284917 |
| H | 0.713224 | -1.427040 | 0.354394 |
| H | -2.299829 | -0.258219 | -1.074426 |
| H | -2.587628 | -1.117484 | 0.429457 |
| H | -2.207150 | 1.194018 | 1.022929 |
| H | -0.851252 | 0.237693 | 1.598804 |
| H | -0.935344 | 2.096126 | -0.840400 |
| H | -0.037568 | 2.348809 | 0.641734 |
| H | 0.541116 | 0.179962 | -1.461250 |
| H | 1.402618 | 1.682871 | -1.257972 |
| H | 2.859431 | 0.348466 | -0.058198 |
| H | 1.731380 | 0.589443 | 1.271594 |

Rotational constants (GHz): 3.2356537 2.2250154 1.5457812

C5H11O2.pmmpp

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.53388295
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -1.223659 | -1.295097 | -0.672218 |
| C | -1.914313 | -0.259561 | -0.088141 |
| C | -1.081246 | 0.659203 | 0.821743 |
| C | -0.057287 | 1.507515 | 0.043721 |
| C | 0.956047 | 0.725183 | -0.807581 |
| C | 1.939391 | -0.166564 | -0.040027 |
| O | 1.329033 | -1.189575 | 0.731966 |
| H | 0.584834 | -1.542603 | 0.216965 |
| H | -2.496607 | 0.307698 | -0.837596 |
| H | -2.671676 | -0.780506 | 0.539534 |
| H | -1.775385 | 1.324882 | 1.350405 |
| H | -0.568907 | 0.043637 | 1.564726 |
| H | -0.599430 | 2.201372 | -0.613627 |
| H | 0.485698 | 2.133534 | 0.764591 |
| H | 0.419838 | 0.105415 | -1.543155 |
| H | 1.543604 | 1.440438 | -1.399018 |
| H | 2.656521 | -0.594068 | -0.761348 |
| H | 2.522961 | 0.442922 | 0.662254 |

Rotational constants (GHz): 3.3784500 2.0715500 1.6478400

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 120.2663 | 136.6207 | 152.8696 |
| 203.6391 | 275.5984 | 332.7058 |
| 365.0254 | 463.0938 | 525.2352 |
| 586.7230 | 764.8561 | 811.2212 |
| 841.0353 | 843.9677 | 926.0264 |
| 957.2112 | 1002.1140 | 1043.0841 |
| 1075.9935 | 1096.5263 | 1121.4890 |
| 1136.5153 | 1193.7599 | 1203.8108 |
| 1289.5384 | 1305.6226 | 1336.7103 |
| 1370.5225 | 1390.7121 | 1396.2916 |
| 1408.0205 | 1415.4710 | 1458.1482 |
| 1489.9748 | 1495.1046 | 1501.5607 |
| 1531.4809 | 2879.1575 | 2962.3182 |
| 2972.9576 | 2998.8121 | 3021.0648 |
| 3048.4787 | 3049.7520 | 3057.5106 |
| 3064.9869 | 3132.7193 | 3717.5489 |

Zero-point correction (Hartree): 0.158273

C5H11O2.pmmpt

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.52566158
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 1.935136 | -0.844171 | 0.998156 |
| C | 2.173338 | -0.243197 | -0.209424 |
| C | 0.951473 | 0.268796 | -0.987720 |
| C | 0.069453 | 1.270271 | -0.219381 |
| C | -0.888284 | 0.660795 | 0.823563 |

| | | | |
|--|-----------|-----------|-----------|
| C | -2.144005 | 0.012969 | 0.248808 |
| O | -1.788092 | -1.145990 | -0.502843 |
| H | -2.595298 | -1.523563 | -0.872990 |
| H | 2.823130 | 0.621256 | 0.062873 |
| H | 2.820418 | -0.876836 | -0.846926 |
| H | 1.338846 | 0.745055 | -1.898921 |
| H | 0.345934 | -0.584525 | -1.305577 |
| H | 0.718675 | 2.001395 | 0.282617 |
| H | -0.522247 | 1.846839 | -0.943635 |
| H | -0.352347 | -0.071110 | 1.434437 |
| H | -1.227321 | 1.457576 | 1.498946 |
| H | -2.820551 | -0.254816 | 1.076570 |
| H | -2.677451 | 0.742212 | -0.384971 |
| Rotational constants (GHz): | 3.9482300 | 1.4835900 | 1.4074200 |
| Vibrational harmonic frequencies (cm-1): | | | |
| 43.8688 | 77.9893 | | 122.3128 |
| 182.7105 | 257.5545 | | 283.2609 |
| 327.0011 | 338.4113 | | 466.0215 |
| 498.8701 | 688.9781 | | 781.6503 |
| 831.6982 | 856.1166 | | 911.3003 |
| 964.4828 | 1003.0419 | | 1056.7850 |
| 1074.2171 | 1102.6074 | | 1116.3907 |
| 1165.4556 | 1190.5470 | | 1241.5112 |
| 1259.9274 | 1283.9525 | | 1319.9223 |
| 1340.7510 | 1373.8559 | | 1381.5747 |
| 1406.8110 | 1412.2397 | | 1464.0186 |
| 1496.9529 | 1497.8708 | | 1503.8810 |
| 1535.2258 | 2857.4940 | | 2938.0997 |
| 2966.3247 | 2998.6698 | | 3015.3488 |
| 3033.4239 | 3043.6176 | | 3053.8976 |
| 3119.8478 | 3122.0016 | | 3827.4632 |
| Zero-point correction (Hartree): | 0.156820 | | |

C5H11O2.pmmtm

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.52798224

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|--|-----------|-----------|-----------|
| O | -1.253580 | -1.611731 | -0.167473 |
| C | -2.104534 | -0.542567 | -0.060338 |
| C | -1.501830 | 0.709183 | 0.594575 |
| C | -0.446272 | 1.401911 | -0.287227 |
| C | 0.766717 | 0.540596 | -0.673890 |
| C | 1.640397 | 0.097569 | 0.502112 |
| O | 2.805600 | -0.598372 | 0.074566 |
| H | 2.513696 | -1.427956 | -0.325397 |
| H | -2.590299 | -0.306121 | -1.026991 |
| H | -2.925574 | -0.925840 | 0.585471 |
| H | -2.315213 | 1.416279 | 0.802613 |
| H | -1.075659 | 0.420962 | 1.561943 |
| H | -0.934361 | 1.752692 | -1.206466 |
| H | -0.099033 | 2.305454 | 0.231716 |
| H | 0.426469 | -0.356664 | -1.212403 |
| H | 1.399103 | 1.099929 | -1.374041 |
| H | 2.003155 | 0.974663 | 1.051172 |
| H | 1.054682 | -0.512727 | 1.204249 |
| Rotational constants (GHz): | 3.9969600 | 1.5045800 | 1.2339400 |
| Vibrational harmonic frequencies (cm-1): | | | |
| 58.0733 | 86.3659 | | 117.7067 |
| 175.5956 | 231.5636 | | 302.3572 |
| 336.5359 | 351.0208 | | 455.6231 |
| 510.0449 | 752.3073 | | 767.9379 |
| 838.4676 | 864.2321 | | 915.0196 |
| 961.4943 | 1042.3856 | | 1046.5069 |
| 1083.1343 | 1092.2532 | | 1106.5147 |
| 1132.4201 | 1170.6219 | | 1193.1454 |
| 1291.9697 | 1310.6036 | | 1338.3575 |
| 1350.6808 | 1378.4636 | | 1385.1022 |
| 1404.8536 | 1410.1721 | | 1437.0617 |
| 1490.9089 | 1496.5670 | | 1502.7443 |
| 1525.2668 | 2883.7915 | | 2942.9914 |
| 3008.1073 | 3019.3759 | | 3025.9715 |
| 3044.0591 | 3062.4419 | | 3066.2842 |
| 3085.9406 | 3095.9362 | | 3812.7188 |
| Zero-point correction (Hartree): | 0.157106 | | |

Rotational constants (GHz): 3.9969600 1.5045800 1.2339400

Vibrational harmonic frequencies (cm-1):

C5H11O2.pmmtp

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.52691779

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -1.344377 | -1.596448 | -0.200865 |
| C | -2.142128 | -0.490756 | -0.069632 |
| C | -1.481929 | 0.719192 | 0.606375 |
| C | -0.409628 | 1.393629 | -0.268350 |

| | | | |
|---|-----------|-----------|-----------|
| C | 0.781503 | 0.507362 | -0.668161 |
| C | 1.627502 | 0.012436 | 0.507804 |
| O | 2.776612 | -0.711410 | 0.087954 |
| H | 3.314264 | -0.118506 | -0.453029 |
| H | -2.618059 | -0.214020 | -1.030935 |
| H | -2.981600 | -0.847835 | 0.567524 |
| H | -2.263405 | 1.453628 | 0.840867 |
| H | -1.057388 | 0.391116 | 1.561947 |
| H | -0.889410 | 1.770212 | -1.181829 |
| H | -0.037821 | 2.280240 | 0.262774 |
| H | 0.441495 | -0.366072 | -1.238815 |
| H | 1.427237 | 1.087366 | -1.344410 |
| H | 1.905179 | 0.863745 | 1.154243 |
| H | 1.049711 | -0.688183 | 1.116736 |

Rotational constants (GHz): 4.0483600 1.4753300 1.2210700

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 62.9006 | 98.0530 | 113.1356 |
| 171.2872 | 233.4831 | 310.6197 |
| 330.9002 | 354.8241 | 457.6461 |
| 510.7718 | 750.4434 | 759.0883 |
| 836.6363 | 863.5521 | 912.3625 |
| 968.4120 | 1033.8655 | 1067.9785 |
| 1072.2027 | 1091.4464 | 1107.1232 |
| 1154.1904 | 1171.2783 | 1195.5510 |
| 1284.8171 | 1327.4684 | 1339.3307 |
| 1347.5950 | 1378.2034 | 1390.1141 |
| 1400.5015 | 1406.5938 | 1440.8105 |
| 1490.1779 | 1496.4939 | 1502.6171 |
| 1528.4088 | 2883.6435 | 2938.6744 |
| 2964.8777 | 3010.9025 | 3025.7758 |
| 3042.7634 | 3055.5792 | 3070.8824 |
| 3093.6345 | 3113.1196 | 3809.7945 |

Zero-point correction (Hartree): 0.157126

C5H11O2.pmmtt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.52652433

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -1.317376 | -1.608229 | -0.196363 |
| C | -2.126697 | -0.509388 | -0.075780 |
| C | -1.489151 | 0.705647 | 0.612394 |
| C | -0.421002 | 1.402913 | -0.250011 |
| C | 0.776246 | 0.536148 | -0.668363 |
| C | 1.609703 | 0.005550 | 0.492810 |
| O | 2.787185 | -0.576202 | -0.057763 |
| H | 3.249601 | -1.042122 | 0.649272 |
| H | -2.590372 | -0.236046 | -1.043900 |
| H | -2.972577 | -0.876089 | 0.547481 |
| H | -2.283260 | 1.426268 | 0.847694 |
| H | -1.066439 | 0.376259 | 1.568624 |
| H | -0.903708 | 1.790976 | -1.157076 |
| H | -0.057372 | 2.283359 | 0.296502 |
| H | 0.443520 | -0.318543 | -1.271045 |
| H | 1.438053 | 1.130108 | -1.310581 |
| H | 1.860433 | 0.832578 | 1.180781 |
| H | 1.029064 | -0.736526 | 1.058957 |

Rotational constants (GHz): 4.0618500 1.4849800 1.2278500

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 68.3012 | 101.2891 | 112.7252 |
| 165.3218 | 233.5877 | 257.9236 |
| 318.8991 | 348.6301 | 455.6596 |
| 513.4552 | 751.4704 | 765.4801 |
| 839.0758 | 867.9962 | 910.9030 |
| 972.4945 | 1028.3092 | 1069.5908 |
| 1077.6654 | 1094.5559 | 1108.0095 |
| 1164.1378 | 1172.4532 | 1230.8017 |
| 1261.1401 | 1306.1778 | 1325.6010 |
| 1339.8008 | 1358.0513 | 1382.9772 |
| 1392.0438 | 1402.1936 | 1470.0926 |
| 1489.9972 | 1497.5142 | 1505.3793 |
| 1542.4485 | 2882.1139 | 2939.8230 |
| 2959.4400 | 3025.0153 | 3029.1528 |
| 3035.8766 | 3043.0880 | 3061.8351 |
| 3084.6017 | 3091.5118 | 3830.1367 |

Zero-point correction (Hartree): 0.156931

C5H11O2.pmpmm

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.53144743

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -1.104951 | -1.287184 | 0.745221 |
| C | -1.712546 | -0.631388 | -0.291896 |
| C | -1.500984 | 0.916202 | -0.110944 |

| | | | |
|--|-----------|-----------|-----------|
| C | -0.069251 | 1.408530 | -0.353782 |
| C | 0.989201 | 0.889753 | 0.648018 |
| C | 1.977160 | -0.110436 | 0.033275 |
| O | 1.346947 | -1.195698 | -0.624629 |
| H | 0.670416 | -1.546747 | -0.020074 |
| H | -1.310170 | -0.923092 | -1.273784 |
| H | -2.803107 | -0.794686 | -0.251422 |
| H | -2.186915 | 1.386260 | -0.825839 |
| H | -1.841246 | 1.182433 | 0.895712 |
| H | 0.229172 | 1.141224 | -1.374311 |
| H | -0.105313 | 2.504611 | -0.318892 |
| H | 1.565853 | 1.725838 | 1.063593 |
| H | 0.488089 | 0.417594 | 1.504768 |
| H | 2.584868 | 0.393673 | -0.728697 |
| H | 2.670905 | -0.460023 | 0.816183 |
| Rotational constants (GHz): | 3.4052900 | 2.1306700 | 1.5766400 |
| Vibrational harmonic frequencies (cm-1): | | | |
| 98.7628 | 126.7574 | | 173.8146 |
| 193.2104 | 279.5912 | | 310.4988 |
| 335.8291 | 470.2264 | | 504.0805 |
| 637.9833 | 740.7313 | | 779.3170 |
| 799.8603 | 865.5572 | | 925.9326 |
| 954.4763 | 1006.1866 | | 1030.0685 |
| 1078.4524 | 1113.3093 | | 1129.3304 |
| 1175.0430 | 1204.1224 | | 1246.1280 |
| 1272.6750 | 1302.5991 | | 1321.5811 |
| 1361.3372 | 1367.5806 | | 1401.5903 |
| 1409.3870 | 1462.9648 | | 1485.4317 |
| 1494.1286 | 1501.7891 | | 1526.1690 |
| 1529.9542 | 2959.6985 | | 2980.0273 |
| 3024.1223 | 3030.1372 | | 3037.2425 |
| 3052.9379 | 3056.1038 | | 3073.2851 |
| 3082.3240 | 3105.7088 | | 3691.2469 |
| Zero-point correction (Hartree): | 0.158809 | | |

C5H11O2.pmpmt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.53057801

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|--|-----------|-----------|-----------|
| O | -1.580067 | -1.226350 | -0.507685 |
| C | -2.042765 | -0.036690 | 0.001715 |
| C | -0.997253 | 0.885083 | 0.630300 |
| C | 0.088297 | 1.371378 | -0.369933 |
| C | 1.528079 | 0.946473 | -0.027730 |
| C | 1.848310 | -0.535574 | -0.263834 |
| O | 1.109990 | -1.428595 | 0.553875 |
| H | 0.228707 | -1.525954 | 0.157127 |
| H | -2.612505 | 0.467916 | -0.805998 |
| H | -2.836940 | -0.310287 | 0.729502 |
| H | -1.528658 | 1.741503 | 1.063129 |
| H | -0.527011 | 0.351888 | 1.462242 |
| H | -0.151989 | 1.013965 | -1.381495 |
| H | 0.054479 | 2.464926 | -0.428164 |
| H | 2.225132 | 1.536881 | -0.638541 |
| H | 1.744112 | 1.193832 | 1.019824 |
| H | 1.710025 | -0.770428 | -1.332804 |
| H | 2.907262 | -0.708706 | -0.037451 |
| Rotational constants (GHz): | 3.4480400 | 1.9886100 | 1.4498500 |
| Vibrational harmonic frequencies (cm-1): | | | |
| 45.9734 | 107.1792 | | 170.0050 |
| 175.4719 | 274.0398 | | 304.9755 |
| 332.7619 | 436.5747 | | 487.9193 |
| 551.9616 | 656.9726 | | 745.4091 |
| 834.3062 | 882.6882 | | 888.8412 |
| 953.3935 | 1019.0111 | | 1058.5874 |
| 1072.4135 | 1099.3157 | | 1112.1361 |
| 1164.3415 | 1200.9119 | | 1252.0639 |
| 1286.8210 | 1309.9386 | | 1345.9888 |
| 1358.9603 | 1392.7352 | | 1397.1219 |
| 1406.7268 | 1425.0546 | | 1448.1501 |
| 1490.4712 | 1499.1866 | | 1500.8315 |
| 1516.5939 | 2898.3417 | | 2917.2100 |
| 2978.5661 | 3022.4914 | | 3025.2932 |
| 3048.6355 | 3066.8007 | | 3071.9061 |
| 3078.5136 | 3107.9887 | | 3710.5305 |
| Zero-point correction (Hartree): | 0.157495 | | |

C5H11O2.pmtmm

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.52924869

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|----------|
| O | -1.965269 | -1.348541 | 0.350399 |
|---|-----------|-----------|----------|

| | | | | |
|--|-----------|-----------|-----------|-----------|
| C | -2.192887 | -0.269882 | -0.462042 | |
| C | -1.529040 | 1.041288 | -0.006023 | |
| C | -0.001307 | 1.029885 | -0.164817 | |
| C | 0.725477 | 0.036101 | 0.748300 | |
| C | 2.229327 | -0.041650 | 0.471008 | |
| O | 2.532710 | -0.441226 | -0.861726 | |
| H | 2.194892 | -1.338884 | -0.979821 | |
| H | -1.966057 | -0.488477 | -1.523739 | |
| H | -3.296937 | -0.138628 | -0.418266 | |
| H | -1.951406 | 1.860453 | -0.602119 | |
| H | -1.806350 | 1.223066 | 1.039642 | |
| H | 0.260505 | 0.806270 | -1.206561 | |
| H | 0.380521 | 2.040796 | 0.032556 | |
| H | 0.571936 | 0.307895 | 1.801607 | |
| H | 0.288281 | -0.967603 | 0.636290 | |
| H | 2.686510 | 0.947792 | 0.588315 | |
| H | 2.709164 | -0.708995 | 1.204149 | |
| Rotational constants (GHz): | 4.5602900 | | 1.2751700 | 1.1712000 |
| Vibrational harmonic frequencies (cm-1): | | | | |
| 50.2363 | | 89.9929 | | 123.9763 |
| 163.9684 | | 240.3892 | | 305.5881 |
| 334.7571 | | 342.8366 | | 443.3273 |
| 533.6795 | | 756.9030 | | 793.8290 |
| 848.6978 | | 868.7876 | | 906.1686 |
| 945.6103 | | 1016.1422 | | 1045.6598 |
| 1065.8357 | | 1096.3689 | | 1100.5476 |
| 1133.9442 | | 1152.3148 | | 1207.9488 |
| 1281.8464 | | 1310.5936 | | 1328.1489 |
| 1347.9055 | | 1371.7012 | | 1391.3370 |
| 1409.1184 | | 1416.0586 | | 1425.0411 |
| 1485.6199 | | 1487.1325 | | 1508.6927 |
| 1521.3678 | | 2881.5850 | | 2942.7764 |
| 2994.2039 | | 3007.7307 | | 3030.1314 |
| 3039.7391 | | 3051.5046 | | 3073.3876 |
| 3081.1856 | | 3089.2085 | | 3809.3749 |
| Zero-point correction (Hartree): | 0.156858 | | | |

C5H11O2.pmtmp

```

-----
E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.52781915
Electronic state : 2-A
Cartesian coordinates (Angs):
O      2.060909      -1.353826      -0.120262
C      2.233025      -0.142312      0.494482
C      1.510431      1.039329      -0.172131
C      -0.015572      0.995434      0.003845
C      -0.699909      -0.204211      -0.663254
C      -2.222691      -0.208560      -0.493563
O      -2.642942      -0.323279      0.861541
H      -2.438410      0.507451      1.307562
H      2.014365      -0.192767      1.579030
H      3.330485      0.028657      0.430551
H      1.900106      1.969896      0.260748
H      1.768678      1.043694      -1.238134
H      -0.243404      0.992109      1.079979
H      -0.439903      1.926004      -0.399299
H      -0.468333      -0.208557      -1.736906
H      -0.297942      -1.140376      -0.256037
H      -2.654360      0.689786      -0.966526
H      -2.646722      -1.077136      -1.007474
Rotational constants (GHz):      4.7757200      1.2299800      1.1359500
Vibrational harmonic frequencies (cm-1):
50.1964      93.9972      118.0896
148.6055      242.3453      291.4972
311.2001      344.5083      449.8787
526.1579      752.2633      795.3035
831.5021      875.6058      901.2823
961.9183      1010.1358      1061.5429
1073.3061      1091.6229      1103.5526
1150.2632      1173.3125      1199.6391
1278.9272      1319.4171      1334.8271
1350.2193      1375.8202      1393.8132
1403.5286      1414.9439      1423.9516
1481.1199      1487.2974      1507.2526
1517.0614      2884.5532      2942.5968
2978.3251      3008.1707      3032.4841
3035.4865      3046.4798      3078.4961
3087.1737      3093.8149      3831.7834
Zero-point correction (Hartree): 0.156887

```

C5H11O2.pmtmt

```

-----
E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.52817375
Electronic state : 2-A
Cartesian coordinates (Angs):

```

| | | | |
|---|-----------|-----------|-----------|
| O | 2.032532 | -1.352065 | -0.239054 |
| C | 2.208802 | -0.205938 | 0.489826 |
| C | 1.517589 | 1.045236 | -0.076054 |
| C | -0.010205 | 1.018279 | 0.081598 |
| C | -0.707685 | -0.096286 | -0.707791 |
| C | -2.217260 | -0.123690 | -0.495949 |
| O | -2.470841 | -0.385645 | 0.881054 |
| H | -3.425683 | -0.377382 | 1.018714 |
| H | 1.966940 | -0.354558 | 1.560132 |
| H | 3.310238 | -0.048963 | 0.462555 |
| H | 1.920283 | 1.924038 | 0.444377 |
| H | 1.793699 | 1.140269 | -1.133752 |
| H | -0.269179 | 0.914816 | 1.142125 |
| H | -0.412389 | 1.989712 | -0.238155 |
| H | -0.508420 | 0.020513 | -1.781020 |
| H | -0.299640 | -1.074461 | -0.423308 |
| H | -2.652768 | 0.843173 | -0.801410 |
| H | -2.664054 | -0.901074 | -1.136045 |
| Rotational constants (GHz): | 4.6934900 | 1.2609500 | 1.1638300 |
| Vibrational harmonic frequencies (cm ⁻¹): | | | |
| 53.5937 | 94.1215 | | 122.5848 |
| 161.2306 | 231.8975 | | 283.4703 |
| 307.1532 | 346.7263 | | 447.2055 |
| 522.0186 | 750.8056 | | 795.0706 |
| 830.2979 | 880.8532 | | 917.4905 |
| 965.0506 | 1011.9814 | | 1057.5505 |
| 1084.1434 | 1096.4750 | | 1106.5402 |
| 1149.1064 | 1162.5093 | | 1237.5687 |
| 1255.7638 | 1298.9768 | | 1324.9399 |
| 1340.5531 | 1352.1449 | | 1374.0313 |
| 1404.1782 | 1418.5518 | | 1459.9907 |
| 1483.5445 | 1486.6368 | | 1509.9005 |
| 1536.4218 | 2880.2675 | | 2944.6429 |
| 2968.6468 | 3002.4757 | | 3023.9452 |
| 3037.8496 | 3039.3906 | | 3066.6805 |
| 3079.1349 | 3092.4606 | | 3832.3730 |
| Zero-point correction (Hartree): | 0.156804 | | |

C5H11O2.pmtpm

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.52804745

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 2.284793 | -1.217794 | -0.169176 |
| C | 2.397329 | 0.062187 | 0.303561 |
| C | 1.391031 | 1.068160 | -0.279167 |
| C | -0.047819 | 0.835418 | 0.207846 |
| C | -0.675392 | -0.480254 | -0.269340 |
| C | -2.092679 | -0.708502 | 0.264591 |
| O | -3.029641 | 0.268114 | -0.178089 |
| H | -2.830273 | 1.097394 | 0.273010 |
| H | 2.409545 | 0.097435 | 1.410645 |
| H | 3.422078 | 0.365683 | -0.006040 |
| H | 1.714245 | 2.078150 | 0.004550 |
| H | 1.434471 | 1.007967 | -1.373231 |
| H | -0.063966 | 0.873416 | 1.308109 |
| H | -0.665347 | 1.674324 | -0.139818 |
| H | -0.702813 | -0.495509 | -1.365907 |
| H | -0.047993 | -1.328412 | 0.037243 |
| H | -2.472863 | -1.667706 | -0.101148 |
| H | -2.073115 | -0.767350 | 1.365763 |
| Rotational constants (GHz): | 5.8791700 | 1.1547200 | 1.0226100 |
| Vibrational harmonic frequencies (cm ⁻¹): | | | |
| 52.5453 | 91.8383 | | 120.9762 |
| 138.9017 | 243.6032 | | 290.6767 |
| 307.7722 | 347.4131 | | 457.2503 |
| 516.0764 | 756.2537 | | 781.7214 |
| 830.7196 | 875.5531 | | 923.6263 |
| 953.9220 | 1004.9276 | | 1056.3986 |
| 1066.6777 | 1091.4038 | | 1100.1310 |
| 1148.1004 | 1157.3330 | | 1231.1379 |
| 1251.3639 | 1324.2580 | | 1327.3307 |
| 1348.0286 | 1375.8720 | | 1394.1825 |
| 1405.2059 | 1412.5950 | | 1426.0328 |
| 1481.2681 | 1486.6056 | | 1506.1835 |
| 1517.2074 | 2883.0027 | | 2939.9696 |
| 2981.5750 | 3004.9412 | | 3027.5238 |
| 3037.5858 | 3050.6882 | | 3080.1375 |
| 3089.3104 | 3094.3479 | | 3831.7469 |
| Zero-point correction (Hartree): | 0.156788 | | |

C5H11O2.pmtpp

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.52909453

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 2.281955 | -1.208345 | -0.225458 |
| C | 2.408118 | 0.064062 | 0.264742 |
| C | 1.374242 | 1.074191 | -0.259593 |
| C | -0.043400 | 0.821861 | 0.273823 |
| C | -0.669859 | -0.499826 | -0.185989 |
| C | -2.109078 | -0.680865 | 0.303617 |
| O | -2.984920 | 0.354659 | -0.132388 |
| H | -3.029716 | 0.310598 | -1.096607 |
| H | 2.463835 | 0.079021 | 1.370924 |
| H | 3.419363 | 0.376788 | -0.078849 |
| H | 1.700707 | 2.080584 | 0.033143 |
| H | 1.381592 | 1.037172 | -1.356042 |
| H | -0.025287 | 0.849097 | 1.373359 |
| H | -0.698690 | 1.643548 | -0.035827 |
| H | -0.652297 | -0.553687 | -1.284841 |
| H | -0.070272 | -1.353077 | 0.159408 |
| H | -2.484132 | -1.670863 | -0.000107 |
| H | -2.141520 | -0.646236 | 1.398600 |

Rotational constants (GHz): 5.8906500 1.1576000 1.0292000

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 49.7746 | 89.8785 | 119.6757 |
| 154.5378 | 242.9307 | 291.0554 |
| 331.4896 | 348.1663 | 458.9309 |
| 526.0221 | 757.6685 | 781.7964 |
| 828.1136 | 878.6575 | 921.8462 |
| 947.2863 | 1005.8163 | 1046.0359 |
| 1073.1376 | 1096.8425 | 1101.4526 |
| 1116.3408 | 1151.8972 | 1239.2590 |
| 1252.5290 | 1322.0721 | 1326.3598 |
| 1348.8000 | 1372.8154 | 1390.3035 |
| 1404.6345 | 1413.5924 | 1426.2518 |
| 1483.9657 | 1487.0713 | 1509.1037 |
| 1520.5664 | 2880.7623 | 2939.7089 |
| 2995.8038 | 3013.9680 | 3021.7378 |
| 3036.5382 | 3050.8003 | 3081.6245 |
| 3082.8816 | 3090.2198 | 3809.4646 |

Zero-point correction (Hartree): 0.156784

C5H11O2.pmtpt

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.52833378

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 2.286274 | -1.212497 | -0.199141 |
| C | 2.405373 | 0.063010 | 0.284360 |
| C | 1.380966 | 1.071594 | -0.262346 |
| C | -0.045586 | 0.827415 | 0.251311 |
| C | -0.672959 | -0.485431 | -0.233395 |
| C | -2.094071 | -0.692713 | 0.276887 |
| O | -2.908565 | 0.362866 | -0.225854 |
| H | -3.800361 | 0.247925 | 0.123894 |
| H | 2.444852 | 0.086852 | 1.391192 |
| H | 3.420995 | 0.373135 | -0.048730 |
| H | 1.706831 | 2.078490 | 0.029584 |
| H | 1.403575 | 1.028729 | -1.358164 |
| H | -0.039544 | 0.843649 | 1.351697 |
| H | -0.687963 | 1.657184 | -0.061961 |
| H | -0.688879 | -0.503629 | -1.330310 |
| H | -0.062681 | -1.342490 | 0.080466 |
| H | -2.465950 | -1.673937 | -0.058775 |
| H | -2.094882 | -0.702110 | 1.380175 |

Rotational constants (GHz): 5.9209800 1.1661900 1.0338400

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 52.7144 | 92.0825 | 120.9320 |
| 149.5461 | 233.4532 | 282.6735 |
| 294.1180 | 348.2670 | 455.0006 |
| 513.3459 | 756.6481 | 783.7663 |
| 834.2352 | 878.7077 | 927.4948 |
| 960.7385 | 999.6639 | 1056.8438 |
| 1068.6491 | 1095.6126 | 1102.9716 |
| 1144.3548 | 1170.5446 | 1221.9666 |
| 1267.6465 | 1288.4069 | 1324.1232 |
| 1336.4362 | 1350.2017 | 1374.2287 |
| 1406.6148 | 1416.6697 | 1460.9389 |
| 1482.0991 | 1486.6106 | 1507.5247 |
| 1536.5997 | 2879.3893 | 2938.4409 |
| 2970.7320 | 3003.2906 | 3013.8688 |
| 3034.3762 | 3039.8198 | 3074.2088 |
| 3084.9504 | 3097.3053 | 3831.1537 |

Zero-point correction (Hartree): 0.156624

C5H11O2.pmttm

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.52807815

Electronic state : 2-A
Cartesian coordinates (Angs):
O 1.875934 -1.525810 -0.064205
C 2.357501 -0.302204 0.317198
C 1.692119 0.906245 -0.359877
C 0.253353 1.155317 0.119640
C -0.734583 0.032750 -0.221043
C -2.158154 0.336130 0.252283
O -3.066498 -0.727455 0.004705
H -3.080109 -0.885344 -0.948212
H 2.377160 -0.190668 1.419091
H 3.427845 -0.337791 0.015099
H 2.302058 1.795337 -0.153874
H 1.708467 0.745238 -1.444689
H 0.261835 1.314949 1.207791
H -0.101504 2.097471 -0.319641
H -0.740901 -0.129004 -1.309139
H -0.412514 -0.916260 0.225126
H -2.168585 0.484877 1.337996
H -2.510647 1.277893 -0.202766
Rotational constants (GHz): 4.9537600 1.1677400 0.9995300
Vibrational harmonic frequencies (cm-1):
69.0849 79.5505 110.5777
147.1838 191.9861 303.8891
318.7436 370.6938 441.9153
478.3260 750.5044 785.9112
830.2999 863.8105 940.1805
976.7227 1036.9858 1065.6765
1074.0740 1086.2766 1103.4813
1138.0500 1162.5425 1236.1705
1277.4548 1317.1361 1326.1161
1341.1914 1374.1234 1385.3833
1402.2663 1411.8378 1432.5599
1484.1407 1492.5498 1505.9541
1528.6194 2883.1141 2940.1190
2971.1513 3013.1034 3020.7671
3035.8855 3051.0738 3068.6974
3084.7251 3088.8892 3813.7979
Zero-point correction (Hartree): 0.156768

C5H11O2.pmttp

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.52842428
Electronic state : 2-A
Cartesian coordinates (Angs):
O -1.846582 1.529584 -0.070776
C -2.351785 0.316874 0.315075
C -1.698195 -0.906908 -0.348070
C -0.260540 -1.158356 0.133965
C 0.741099 -0.069304 -0.268611
C 2.145067 -0.318946 0.286380
O 3.092084 0.648171 -0.144764
H 2.783863 1.512959 0.156164
H -2.383613 0.210216 1.417136
H -3.417190 0.365253 -0.002152
H -2.316231 -1.786227 -0.125455
H -1.715122 -0.763388 -1.435099
H -0.265492 -1.269058 1.228523
H 0.078001 -2.124124 -0.264346
H 0.801295 0.003169 -1.361405
H 0.384907 0.910924 0.082106
H 2.106148 -0.379136 1.387522
H 2.525541 -1.282779 -0.071108
Rotational constants (GHz): 4.9498900 1.1719700 1.0027400
Vibrational harmonic frequencies (cm-1):
69.9849 84.1920 112.9787
143.6405 192.1835 305.7046
324.5149 365.3350 443.4540
475.8876 751.1067 798.1813
828.6220 866.4550 935.3657
981.8336 1038.9613 1051.9766
1067.8189 1086.4966 1104.4486
1140.6507 1163.3999 1220.9722
1294.1682 1302.1395 1330.1623
1336.5820 1371.7785 1385.9970
1407.0678 1413.8661 1436.3671
1484.8037 1493.1497 1506.0773
1530.0341 2882.8743 2940.2474
2974.1172 3008.5451 3015.7935
3038.2658 3054.7442 3069.5528
3085.9133 3090.4513 3811.6079
Zero-point correction (Hartree): 0.156780

C5H11O2.pmttt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.52708807
Electronic state : 2-A
Cartesian coordinates (Angs):
O 1.884170 -1.525871 -0.057876
C 2.361634 -0.299440 0.318285
C 1.689520 0.906561 -0.357519
C 0.251673 1.151168 0.126904
C -0.739458 0.044521 -0.251312
C -2.144971 0.314646 0.272093
O -2.984646 -0.752321 -0.149533
H -3.873311 -0.587075 0.188331
H 2.385956 -0.184039 1.419893
H 3.430444 -0.331191 0.010135
H 2.298355 1.796419 -0.151482
H 1.702831 0.746957 -1.442444
H 0.261718 1.281221 1.219380
H -0.096620 2.107328 -0.286612
H -0.786122 -0.062083 -1.341932
H -0.402880 -0.925491 0.135406
H -2.121436 0.395162 1.372224
H -2.505512 1.283586 -0.114335
Rotational constants (GHz): 4.9714400 1.1747700 1.0050200
Vibrational harmonic frequencies (cm-1):
65.6931 81.7159 111.2575
138.9253 192.9618 270.6347
308.1375 371.5019 437.1299
476.4673 754.4630 792.0740
832.8306 868.9544 942.2440
983.8092 1031.0784 1064.0891
1073.6002 1088.9806 1104.1936
1157.4556 1195.1922 1228.7898
1262.0644 1307.5514 1319.5248
1326.8410 1341.3697 1374.4872
1401.1449 1409.7168 1471.0033
1484.4575 1495.9094 1510.1452
1541.9575 2881.9090 2937.5465
2962.2319 2987.9805 3012.8328
3034.8040 3043.5629 3051.6304
3085.6639 3091.0394 3828.2861
Zero-point correction (Hartree): 0.156592

C5H11O2.ppmmm

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.52738332
Electronic state : 2-A
Cartesian coordinates (Angs):
O 2.359372 -0.708155 -0.605246
C 1.634526 -0.443677 0.521515
C 1.004606 0.964589 0.543391
C -0.023203 1.182188 -0.583014
C -1.495764 0.956491 -0.190154
C -1.816661 -0.380065 0.484606
O -1.324800 -1.520130 -0.215680
H -1.632861 -1.471287 -1.130239
H 0.825354 -1.207797 0.488270
H 2.212996 -0.655179 1.440992
H 0.556568 1.141647 1.530532
H 1.823816 1.686148 0.446623
H 0.061133 2.204106 -0.969711
H 0.251228 0.525926 -1.417337
H -1.822701 1.753048 0.492858
H -2.119374 1.061305 -1.089999
H -1.350027 -0.431793 1.474307
H -2.903727 -0.456997 0.643043
Rotational constants (GHz): 3.6167800 1.7324500 1.3890500
Vibrational harmonic frequencies (cm-1):
85.1836 94.5744 145.6822
167.7661 224.1688 287.2162
318.3290 389.6940 474.9185
541.3145 749.6999 770.8822
831.5772 860.9921 922.2937
987.6571 1000.3455 1056.6036
1078.9255 1110.7386 1116.6608
1143.5885 1172.3502 1222.6621
1279.2779 1301.2149 1324.4898
1356.3902 1374.9997 1385.0884
1403.2097 1406.6372 1433.8685
1493.8964 1497.9139 1513.1663
1528.5845 2876.4449 2949.5219
2998.8507 3018.1524 3036.5799
3046.6249 3054.2353 3080.2655
3086.3641 3088.6904 3813.2189
Zero-point correction (Hartree): 0.157425

C5H11O2.ppmmp


```

-----
E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.53020791
Electronic state : 2-A
Cartesian coordinates (Angs):
O      1.306656      -1.421912      -0.384245
C      1.684932      -0.453293      0.504835
C      1.399473      1.004982      0.083766
C      0.071363      1.260191      -0.646994
C     -1.232859      1.125202      0.158873
C     -1.606859     -0.299397      0.603079
O     -1.562614     -1.248590     -0.442575
H     -0.629078     -1.380602     -0.681415
H      1.084303     -0.701059      1.410403
H      2.735193     -0.581775      0.822504
H      1.477726      1.635023      0.979603
H      2.218213      1.313253     -0.578574
H      0.114440      2.281604     -1.043236
H      0.013229      0.604075     -1.522372
H     -1.198903      1.772631      1.046917
H     -2.045722      1.503482     -0.472843
H     -0.980384     -0.612556      1.456888
H     -2.637651     -0.296175      0.975333
Rotational constants (GHz):      3.2354300      2.1627900      1.5367700
Vibrational harmonic frequencies (cm-1):
  73.1684      147.1731      160.6765
 217.9515      264.6822      283.7670
 383.3399      496.1713      548.5271
 582.5763      721.9290      778.9688
 809.9964      861.4944      938.3873
 954.0508      1011.1707     1059.0315
1077.0669      1114.3956     1127.1491
1149.4912      1193.5399     1223.6197
1247.6877      1300.8989     1328.2018
1377.5844      1387.3356     1397.7865
1409.1418      1418.3791     1447.6247
1487.1748      1497.8325     1507.0488
1523.9582      2858.7696     2958.3798
2969.3476      3024.2113     3034.8028
3051.6482      3069.5567     3074.8495
3080.1322      3094.5808     3684.8795
Zero-point correction (Hartree): 0.158128

```

C5H11O2.ppmmt

```

-----
E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.52614599
Electronic state : 2-A
Cartesian coordinates (Angs):
O      2.378147      -0.733013      -0.583514
C      1.618099     -0.460009      0.518497
C      1.021606      0.961787      0.533064
C     -0.013976      1.192673     -0.583346
C     -1.483559      0.973862     -0.175177
C     -1.804183     -0.365436      0.481553
O     -1.372718     -1.419535     -0.378546
H     -1.674777     -2.257726     -0.006945
H      0.791359     -1.201856      0.447129
H      2.158439     -0.696463      1.455460
H      0.587301      1.157912      1.523158
H      1.857147      1.662404      0.422503
H      0.072055      2.218322     -0.960102
H      0.239929      0.539066     -1.424973
H     -1.790267      1.759365      0.529153
H     -2.116383      1.084717     -1.063929
H     -1.308301     -0.436139      1.463705
H     -2.887861     -0.426486      0.663777
Rotational constants (GHz):      3.6384700      1.7245700      1.3828000
Vibrational harmonic frequencies (cm-1):
  87.0917      96.8856      137.6337
 164.7032      233.9098      291.4747
 324.1523      394.8100      469.3441
 527.8288      748.5534      777.9450
 827.0780      858.9716      929.5381
 985.0050      1006.8327     1055.2765
1094.3840      1103.8386     1116.9958
1159.3445      1175.5966     1243.3353
1258.6376      1292.2984     1312.7481
1332.6620      1367.4481     1385.2505
1397.3954      1405.7818     1459.6689
1489.6131      1497.3975     1513.9631
1537.6860      2878.3840     2943.9174
2977.7145      3014.2270     3033.0108
3034.5824      3052.7736     3077.2866
3083.8029      3097.9269     3826.7647
Zero-point correction (Hartree): 0.157379

```

C5H11O2.ppmppm

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.53114873

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -1.486382 | -1.224921 | 0.624983 |
| C | -1.619058 | -0.498426 | -0.527170 |
| C | -1.384738 | 1.013337 | -0.171814 |
| C | -0.050082 | 1.360868 | 0.502154 |
| C | 1.236824 | 1.032765 | -0.292193 |
| C | 1.944458 | -0.270794 | 0.105173 |
| O | 1.231774 | -1.455552 | -0.200793 |
| H | 0.447737 | -1.503103 | 0.372991 |
| H | -0.840798 | -0.787372 | -1.251616 |
| H | -2.623960 | -0.587755 | -0.968854 |
| H | -1.485318 | 1.548752 | -1.124057 |
| H | -2.212293 | 1.329650 | 0.471331 |
| H | -0.081971 | 2.440211 | 0.694507 |
| H | -0.006157 | 0.885825 | 1.490051 |
| H | 1.024939 | 1.010604 | -1.369542 |
| H | 1.959848 | 1.844841 | -0.141004 |
| H | 2.891465 | -0.339423 | -0.442263 |
| H | 2.198941 | -0.224947 | 1.178037 |

Rotational constants (GHz): 3.3092200 2.1396100 1.4916100

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 100.3141 | 141.5485 | 185.3145 |
| 214.7426 | 239.3947 | 312.2681 |
| 340.8117 | 458.7481 | 474.8179 |
| 693.9105 | 727.6665 | 772.9520 |
| 833.0618 | 858.3132 | 909.1751 |
| 964.6424 | 980.2012 | 1025.9886 |
| 1080.9537 | 1103.2486 | 1121.4343 |
| 1174.7164 | 1225.3371 | 1260.3250 |
| 1272.5379 | 1299.6320 | 1310.9626 |
| 1372.8849 | 1380.6341 | 1397.0991 |
| 1421.4596 | 1443.5030 | 1484.1230 |
| 1491.8385 | 1502.6627 | 1516.8352 |
| 1531.7757 | 2968.1478 | 2974.2412 |
| 3025.4952 | 3028.9076 | 3039.6357 |
| 3049.3093 | 3071.5843 | 3075.4180 |
| 3079.7041 | 3105.7538 | 3688.5054 |

Zero-point correction (Hartree): 0.158862

C5H11O2.ppmpp

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.52867410

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 2.149009 | -0.637297 | -0.919462 |
| C | 1.607002 | -0.607978 | 0.328376 |
| C | 1.063540 | 0.764271 | 0.773056 |
| C | 0.067335 | 1.404664 | -0.210279 |
| C | -1.413441 | 0.997400 | -0.090839 |
| C | -1.790575 | -0.431643 | -0.491767 |
| O | -1.350000 | -1.439854 | 0.421101 |
| H | -1.727325 | -1.238606 | 1.287675 |
| H | 0.750481 | -1.321115 | 0.282823 |
| H | 2.291886 | -1.038598 | 1.085149 |
| H | 0.617910 | 0.658200 | 1.771600 |
| H | 1.922952 | 1.435844 | 0.890503 |
| H | 0.112406 | 2.493046 | -0.083437 |
| H | 0.422679 | 1.204005 | -1.228854 |
| H | -1.770632 | 1.181848 | 0.934754 |
| H | -2.000666 | 1.670382 | -0.730552 |
| H | -2.881674 | -0.497837 | -0.621486 |
| H | -1.333245 | -0.690245 | -1.452572 |

Rotational constants (GHz): 3.3946000 1.7975500 1.4477200

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 59.0926 | 76.8344 | 167.0761 |
| 198.8117 | 252.3054 | 297.6618 |
| 338.4599 | 375.8563 | 481.8318 |
| 502.4015 | 740.2790 | 773.5771 |
| 861.3914 | 875.7571 | 898.7103 |
| 974.7904 | 990.2613 | 1063.4515 |
| 1081.8066 | 1103.6266 | 1126.5807 |
| 1134.8427 | 1170.1124 | 1255.5587 |
| 1271.9537 | 1307.9711 | 1320.2865 |
| 1379.0344 | 1380.9679 | 1393.5146 |
| 1403.1635 | 1409.4851 | 1430.2424 |
| 1486.5410 | 1497.2089 | 1500.9566 |
| 1520.2890 | 2845.7246 | 2935.3961 |
| 2998.4271 | 3008.4911 | 3030.6263 |
| 3038.5511 | 3054.9623 | 3074.3464 |
| 3080.4549 | 3096.0286 | 3811.5655 |

Zero-point correction (Hartree): 0.157370

C5H11O2.ppmpt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.52858701

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -2.050880 | -0.745461 | 0.929248 |
| C | -1.589139 | -0.612815 | -0.343725 |
| C | -1.115073 | 0.800465 | -0.732998 |
| C | -0.096748 | 1.420827 | 0.238460 |
| C | 1.381496 | 1.017726 | 0.075307 |
| C | 1.772922 | -0.404714 | 0.468567 |
| O | 1.383863 | -1.314819 | -0.567146 |
| H | 1.642295 | -2.205078 | -0.295787 |
| H | -0.702236 | -1.288725 | -0.392860 |
| H | -2.299728 | -1.024070 | -1.087269 |
| H | -0.708522 | 0.760834 | -1.751813 |
| H | -2.000348 | 1.447566 | -0.774673 |
| H | -0.145294 | 2.511310 | 0.130951 |
| H | -0.426415 | 1.202028 | 1.262063 |
| H | 1.711662 | 1.184397 | -0.958535 |
| H | 1.980575 | 1.691704 | 0.701492 |
| H | 2.863074 | -0.452740 | 0.609938 |
| H | 1.300329 | -0.673923 | 1.426003 |

Rotational constants (GHz): 3.3506400 1.8395000 1.4665500

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 51.7423 | 73.0021 | 163.2628 |
| 205.1158 | 256.9557 | 312.9801 |
| 350.7901 | 374.1662 | 461.4157 |
| 507.5093 | 741.0699 | 772.7498 |
| 864.5963 | 873.7088 | 912.1259 |
| 967.9248 | 996.8206 | 1075.4545 |
| 1090.7432 | 1101.5173 | 1129.0815 |
| 1150.8808 | 1201.1818 | 1240.6046 |
| 1274.9431 | 1282.5307 | 1322.8871 |
| 1327.3440 | 1381.6629 | 1389.2912 |
| 1403.4469 | 1412.3641 | 1461.1492 |
| 1482.2352 | 1496.1263 | 1501.9326 |
| 1531.3919 | 2835.5521 | 2936.6138 |
| 2991.6169 | 3021.9465 | 3033.5368 |
| 3038.1991 | 3043.0681 | 3072.3201 |
| 3076.9425 | 3084.2663 | 3820.8907 |

Zero-point correction (Hartree): 0.157416

C5H11O2.ppmtm

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.52468806

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 2.419078 | -0.964674 | -0.719053 |
| C | 1.873182 | -0.647562 | 0.494351 |
| C | 1.351118 | 0.794263 | 0.619543 |
| C | 0.329607 | 1.202256 | -0.459047 |
| C | -1.149955 | 0.913560 | -0.147747 |
| C | -1.543374 | -0.562149 | -0.041170 |
| O | -2.950870 | -0.743823 | 0.040074 |
| H | -3.261190 | -0.279902 | 0.828644 |
| H | 1.047150 | -1.380922 | 0.620421 |
| H | 2.573599 | -0.899086 | 1.314584 |
| H | 0.935723 | 0.934566 | 1.627146 |
| H | 2.224443 | 1.454326 | 0.554890 |
| H | 0.422077 | 2.280061 | -0.634425 |
| H | 0.617164 | 0.719569 | -1.401877 |
| H | -1.429299 | 1.424508 | 0.786807 |
| H | -1.770992 | 1.353987 | -0.937184 |
| H | -1.225743 | -1.101823 | -0.940350 |
| H | -1.042075 | -1.039510 | 0.817594 |

Rotational constants (GHz): 4.3958800 1.2473900 1.0969800

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 43.7828 | 94.2585 | 130.3238 |
| 159.4444 | 240.1114 | 276.7943 |
| 316.0796 | 361.1976 | 465.8632 |
| 509.8970 | 655.3297 | 784.9792 |
| 797.5445 | 875.3477 | 892.8501 |
| 975.9613 | 1028.3608 | 1055.4384 |
| 1080.5761 | 1103.1905 | 1117.4083 |
| 1151.4832 | 1153.7544 | 1255.9581 |
| 1281.1432 | 1323.0475 | 1331.5379 |
| 1358.1339 | 1366.5615 | 1381.6932 |
| 1402.3168 | 1408.7272 | 1432.2032 |
| 1491.9863 | 1502.9701 | 1509.7230 |
| 1530.3075 | 2896.9626 | 2939.4698 |
| 2974.7937 | 3006.2044 | 3031.8798 |

3043.9877 3070.2659 3077.2264
3083.7176 3089.0796 3812.4167
Zero-point correction (Hartree): 0.156903

C5H11O2.ppmtp

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.52495563
Electronic state : 2-A
Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 2.436838 | -0.927705 | -0.748399 |
| C | 1.876830 | -0.659164 | 0.470798 |
| C | 1.338513 | 0.772065 | 0.641911 |
| C | 0.325084 | 1.207105 | -0.434151 |
| C | -1.155039 | 0.918904 | -0.126773 |
| C | -1.542172 | -0.559239 | -0.033876 |
| O | -2.933095 | -0.744909 | 0.191352 |
| H | -3.404626 | -0.360015 | -0.558954 |
| H | 1.059197 | -1.406455 | 0.562650 |
| H | 2.572751 | -0.932026 | 1.287874 |
| H | 0.909542 | 0.871554 | 1.648354 |
| H | 2.205934 | 1.442205 | 0.611754 |
| H | 0.424249 | 2.287176 | -0.590427 |
| H | 0.614677 | 0.739511 | -1.384188 |
| H | -1.449271 | 1.413139 | 0.808019 |
| H | -1.764340 | 1.376419 | -0.920344 |
| H | -1.205053 | -1.093449 | -0.938398 |
| H | -1.052300 | -1.035168 | 0.822590 |

Rotational constants (GHz): 4.4193500 1.2444400 1.0981900

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 42.6378 | 96.8030 | 128.0279 |
| 156.4054 | 238.2443 | 275.2196 |
| 315.5310 | 362.2597 | 466.7192 |
| 510.7065 | 655.2989 | 781.2549 |
| 798.9987 | 874.6975 | 895.5398 |
| 972.8557 | 1034.1004 | 1053.3629 |
| 1085.9244 | 1103.1055 | 1108.7100 |
| 1136.4710 | 1177.6522 | 1236.7630 |
| 1286.4093 | 1322.8316 | 1336.5848 |
| 1358.2626 | 1365.9821 | 1382.5406 |
| 1396.9653 | 1413.5402 | 1433.5570 |
| 1491.5866 | 1501.5626 | 1509.3821 |
| 1530.9674 | 2901.5528 | 2941.0342 |
| 2978.6546 | 3013.7902 | 3034.7150 |
| 3042.9342 | 3061.9433 | 3077.9831 |
| 3083.2387 | 3088.3572 | 3811.6248 |

Zero-point correction (Hartree): 0.156905

C5H11O2.ppmtt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.52427969
Electronic state : 2-A
Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 2.351815 | -1.022343 | -0.727769 |
| C | 1.866496 | -0.648636 | 0.495458 |
| C | 1.380188 | 0.807154 | 0.594317 |
| C | 0.334661 | 1.211096 | -0.462087 |
| C | -1.137666 | 0.929368 | -0.117691 |
| C | -1.532919 | -0.541266 | -0.029885 |
| O | -2.946728 | -0.593838 | 0.115335 |
| H | -3.210928 | -1.520638 | 0.166790 |
| H | 1.032502 | -1.358592 | 0.685881 |
| H | 2.597522 | -0.888113 | 1.292485 |
| H | 0.998645 | 0.983835 | 1.609398 |
| H | 2.264994 | 1.445866 | 0.484223 |
| H | 0.426242 | 2.288538 | -0.640411 |
| H | 0.602185 | 0.726556 | -1.409982 |
| H | -1.403606 | 1.419108 | 0.827957 |
| H | -1.773790 | 1.382179 | -0.887762 |
| H | -1.200728 | -1.070201 | -0.938944 |
| H | -1.038289 | -1.025381 | 0.829170 |

Rotational constants (GHz): 4.3714200 1.2671000 1.1066800

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 36.4399 | 93.7395 | 125.3820 |
| 164.5904 | 246.2576 | 277.2007 |
| 285.7437 | 354.0946 | 466.7955 |
| 513.7238 | 634.2004 | 792.6681 |
| 798.8173 | 872.1616 | 896.4597 |
| 977.1395 | 1019.3928 | 1060.8559 |
| 1085.7699 | 1104.7435 | 1124.2805 |
| 1144.2314 | 1201.4696 | 1244.9318 |
| 1276.9205 | 1301.5506 | 1325.1633 |
| 1337.2255 | 1365.0128 | 1374.8718 |
| 1386.0993 | 1408.7618 | 1466.0141 |
| 1492.7786 | 1505.4452 | 1511.0853 |

| | | |
|-----------|-----------|-----------|
| 1541.8794 | 2897.4160 | 2937.1985 |
| 2964.6839 | 2993.1297 | 3032.9680 |
| 3040.5907 | 3043.5117 | 3075.9779 |
| 3082.2816 | 3088.4250 | 3827.1550 |

Zero-point correction (Hartree): 0.156732

C5H11O2.pppmm

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.52802329

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 2.351166 | -0.255786 | -0.884438 |
| C | 1.605870 | -0.759924 | 0.142974 |
| C | 0.903728 | 0.275401 | 1.034350 |
| C | 0.138213 | 1.359521 | 0.259294 |
| C | -0.978702 | 0.880513 | -0.686393 |
| C | -2.054445 | -0.003531 | -0.046878 |
| O | -1.626151 | -1.349352 | 0.186260 |
| H | -1.620325 | -1.802064 | -0.666713 |
| H | 0.819721 | -1.369121 | -0.356222 |
| H | 2.177534 | -1.495194 | 0.741251 |
| H | 0.234288 | -0.271025 | 1.707816 |
| H | 1.659109 | 0.764307 | 1.662708 |
| H | -0.297486 | 2.055784 | 0.988287 |
| H | 0.858213 | 1.938034 | -0.329748 |
| H | -1.470869 | 1.768076 | -1.106319 |
| H | -0.549381 | 0.346671 | -1.545364 |
| H | -2.335648 | 0.390859 | 0.936414 |
| H | -2.963258 | 0.002898 | -0.666773 |

Rotational constants (GHz): 3.7646200 1.6413800 1.4375900

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 59.6381 | 84.8449 | 149.9687 |
| 194.4390 | 224.9716 | 312.5241 |
| 336.7872 | 376.0443 | 477.0260 |
| 558.0776 | 694.4254 | 768.7009 |
| 823.9840 | 875.1291 | 911.3306 |
| 965.2673 | 999.9823 | 1040.8151 |
| 1085.4980 | 1092.4175 | 1120.8724 |
| 1145.2083 | 1147.5117 | 1245.0745 |
| 1256.4949 | 1293.8740 | 1331.1233 |
| 1379.1686 | 1381.3462 | 1395.1419 |
| 1403.0072 | 1414.8066 | 1423.2850 |
| 1489.7336 | 1497.8349 | 1502.1977 |
| 1517.9387 | 2882.1838 | 2945.0448 |
| 3007.2519 | 3030.2409 | 3031.6139 |
| 3047.3251 | 3064.2127 | 3081.7989 |
| 3085.4725 | 3100.3735 | 3820.6048 |

Zero-point correction (Hartree): 0.157359

C5H11O2.pppmp

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.52681112

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 2.313253 | -0.171271 | -0.931259 |
| C | 1.591940 | -0.771933 | 0.058812 |
| C | 0.922813 | 0.186414 | 1.058498 |
| C | 0.114992 | 1.321516 | 0.404426 |
| C | -0.939800 | 0.917930 | -0.641620 |
| C | -2.061542 | -0.009959 | -0.171602 |
| O | -1.630915 | -1.360770 | 0.040548 |
| H | -1.413759 | -1.466081 | 0.973168 |
| H | 0.790269 | -1.330597 | -0.475782 |
| H | 2.178891 | -1.556606 | 0.574462 |
| H | 0.297550 | -0.412487 | 1.734330 |
| H | 1.700717 | 0.630677 | 1.692149 |
| H | -0.368798 | 1.904175 | 1.200182 |
| H | 0.823834 | 1.998364 | -0.084478 |
| H | -1.409620 | 1.837297 | -1.017163 |
| H | -0.452797 | 0.454212 | -1.507424 |
| H | -2.541668 | 0.392599 | 0.733016 |
| H | -2.833736 | -0.059035 | -0.947853 |

Rotational constants (GHz): 3.7410700 1.6474400 1.4616700

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 73.5033 | 83.5830 | 153.6006 |
| 162.5408 | 213.4261 | 257.9496 |
| 325.8126 | 367.0054 | 482.0266 |
| 559.8295 | 705.7102 | 775.4041 |
| 824.4136 | 872.1144 | 901.9136 |
| 961.7509 | 996.2751 | 1053.6344 |
| 1075.5580 | 1097.9547 | 1123.4583 |
| 1141.4815 | 1160.8307 | 1246.7543 |
| 1257.9411 | 1298.7104 | 1325.7366 |
| 1377.1289 | 1385.1470 | 1394.1823 |
| 1407.9263 | 1412.8208 | 1425.6064 |

| | | |
|-----------|-----------|-----------|
| 1492.2591 | 1499.2606 | 1504.8006 |
| 1517.8281 | 2873.5391 | 2941.8392 |
| 3009.0129 | 3026.4193 | 3032.9126 |
| 3039.5320 | 3066.4100 | 3076.8079 |
| 3086.0912 | 3095.1059 | 3856.5683 |

Zero-point correction (Hartree): 0.157239

C5H11O2.pppmt

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.52854226
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 2.380471 | -0.147881 | -0.880869 |
| C | 1.616625 | -0.774287 | 0.062675 |
| C | 0.893887 | 0.150605 | 1.055297 |
| C | 0.124861 | 1.304302 | 0.391885 |
| C | -0.951258 | 0.918338 | -0.639398 |
| C | -2.074578 | 0.019683 | -0.132834 |
| O | -1.567862 | -1.305958 | 0.035485 |
| H | -2.279014 | -1.864261 | 0.372683 |
| H | 0.847260 | -1.325307 | -0.522862 |
| H | 2.182818 | -1.569839 | 0.584759 |
| H | 0.221587 | -0.471797 | 1.654912 |
| H | 1.638181 | 0.575299 | 1.741329 |
| H | -0.342049 | 1.907438 | 1.182315 |
| H | 0.848552 | 1.956743 | -0.108971 |
| H | -1.409520 | 1.842101 | -1.015201 |
| H | -0.492616 | 0.432486 | -1.508851 |
| H | -2.472018 | 0.412865 | 0.817639 |
| H | -2.901278 | 0.023143 | -0.860437 |

Rotational constants (GHz): 3.8706700 1.6292400 1.4437600
 Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 61.9357 | 79.3048 | 148.3364 |
| 201.0945 | 245.5441 | 254.9354 |
| 335.9192 | 369.1700 | 475.1293 |
| 556.6211 | 704.5058 | 779.2119 |
| 826.8092 | 879.5398 | 922.8426 |
| 961.1893 | 1003.5911 | 1053.5024 |
| 1089.6673 | 1101.9254 | 1124.4843 |
| 1142.9822 | 1190.1183 | 1234.4910 |
| 1266.1914 | 1273.3050 | 1316.8363 |
| 1334.5268 | 1382.0972 | 1386.1440 |
| 1406.6373 | 1416.2186 | 1461.1418 |
| 1489.6867 | 1495.3481 | 1503.3575 |
| 1536.2018 | 2888.2591 | 2941.7988 |
| 2977.6649 | 3008.8393 | 3030.4410 |
| 3044.5598 | 3048.1240 | 3081.0058 |
| 3089.7004 | 3104.0988 | 3830.0676 |

Zero-point correction (Hartree): 0.157319

C5H11O2.ppppm

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.52647527
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 2.944098 | -0.450396 | -0.265401 |
| C | 2.110282 | 0.136117 | 0.647862 |
| C | 0.942840 | 0.934404 | 0.044653 |
| C | 0.054307 | 0.098873 | -0.891445 |
| C | -0.856539 | -0.932361 | -0.201132 |
| C | -1.983293 | -0.332820 | 0.648832 |
| O | -2.910026 | 0.435208 | -0.108924 |
| H | -2.453977 | 1.225306 | -0.423686 |
| H | 1.726543 | -0.714746 | 1.253201 |
| H | 2.688011 | 0.737877 | 1.375555 |
| H | 0.362472 | 1.374036 | 0.866696 |
| H | 1.369608 | 1.775423 | -0.515065 |
| H | -0.565980 | 0.769268 | -1.500918 |
| H | 0.711521 | -0.419072 | -1.598671 |
| H | -1.315509 | -1.565332 | -0.969546 |
| H | -0.261110 | -1.602089 | 0.434752 |
| H | -2.569570 | -1.141879 | 1.096470 |
| H | -1.570162 | 0.257447 | 1.483188 |

Rotational constants (GHz): 6.3830000 1.0988400 1.0795500
 Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 31.7638 | 65.1322 | 123.2009 |
| 201.8392 | 220.9591 | 293.4175 |
| 325.3576 | 402.3833 | 483.8114 |
| 534.1458 | 632.8440 | 742.3316 |
| 799.9174 | 865.9513 | 910.6083 |
| 973.4717 | 990.0615 | 1050.0576 |
| 1081.1485 | 1088.9630 | 1111.7909 |
| 1152.4279 | 1166.7915 | 1216.1138 |
| 1264.9143 | 1322.4614 | 1333.2265 |

| | | |
|-----------|-----------|-----------|
| 1368.0855 | 1375.2602 | 1394.3546 |
| 1397.0984 | 1408.8432 | 1431.4983 |
| 1491.9237 | 1495.4579 | 1511.6552 |
| 1523.8271 | 2888.9150 | 2944.7560 |
| 2985.1421 | 3031.6654 | 3037.5915 |
| 3043.2532 | 3078.6234 | 3082.4220 |
| 3089.5684 | 3092.8518 | 3829.1241 |

Zero-point correction (Hartree): 0.156936

C5H11O2.ppppp

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.52745445

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 2.955476 | -0.477755 | -0.279235 |
| C | 2.147236 | 0.175385 | 0.612569 |
| C | 0.963739 | 0.931288 | -0.011511 |
| C | 0.043638 | 0.041492 | -0.861140 |
| C | -0.853862 | -0.922068 | -0.066403 |
| C | -2.002274 | -0.237867 | 0.683308 |
| O | -2.852688 | 0.520385 | -0.169354 |
| H | -3.249871 | -0.089905 | -0.804663 |
| H | 1.781269 | -0.631737 | 1.285865 |
| H | 2.744701 | 0.824637 | 1.281345 |
| H | 0.406530 | 1.432726 | 0.790423 |
| H | 1.374396 | 1.729736 | -0.641208 |
| H | -0.603652 | 0.676980 | -1.474607 |
| H | 0.675146 | -0.532170 | -1.548819 |
| H | -1.284156 | -1.659885 | -0.759108 |
| H | -0.266863 | -1.508187 | 0.654705 |
| H | -2.574382 | -0.991730 | 1.247675 |
| H | -1.616286 | 0.479121 | 1.416162 |

Rotational constants (GHz): 6.5066200 1.0899400 1.0719800

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 35.2736 | 67.4624 | 119.8839 |
| 193.5829 | 209.9295 | 309.5652 |
| 333.9257 | 390.1102 | 485.9575 |
| 536.1596 | 619.1349 | 743.0276 |
| 803.3298 | 864.8465 | 917.3202 |
| 972.0868 | 986.9399 | 1044.1554 |
| 1077.1178 | 1099.9940 | 1104.9145 |
| 1132.8668 | 1185.2644 | 1196.5154 |
| 1273.7496 | 1315.2997 | 1341.0049 |
| 1369.0815 | 1374.4744 | 1380.8622 |
| 1406.4545 | 1409.8193 | 1428.1821 |
| 1491.5987 | 1491.9513 | 1499.5597 |
| 1522.5579 | 2879.8281 | 2942.5645 |
| 2990.7528 | 3017.4454 | 3040.7833 |
| 3045.9505 | 3060.6889 | 3079.7510 |
| 3086.1866 | 3102.2139 | 3808.9680 |

Zero-point correction (Hartree): 0.156713

C5H11O2.ppppt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.52645709

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 2.859211 | 0.523152 | 0.035850 |
| C | 2.000382 | -0.297853 | -0.644976 |
| C | 0.903870 | -0.953224 | 0.207665 |
| C | 0.048189 | 0.039397 | 1.008053 |
| C | -0.829676 | 0.992508 | 0.178421 |
| C | -1.866466 | 0.301831 | -0.702616 |
| O | -2.695647 | -0.500982 | 0.129995 |
| H | -3.349479 | -0.940055 | -0.427283 |
| H | 1.549192 | 0.365213 | -1.416642 |
| H | 2.560911 | -1.045339 | -1.239817 |
| H | 0.279532 | -1.576933 | -0.445042 |
| H | 1.392793 | -1.642808 | 0.906900 |
| H | -0.602463 | -0.525429 | 1.682927 |
| H | 0.718884 | 0.638025 | 1.634432 |
| H | -1.359996 | 1.662150 | 0.866048 |
| H | -0.212661 | 1.637647 | -0.460907 |
| H | -2.455707 | 1.065765 | -1.235099 |
| H | -1.367314 | -0.311554 | -1.471566 |

Rotational constants (GHz): 5.7918400 1.1826500 1.1590400

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 8.7727 | 58.0716 | 121.2332 |
| 190.3967 | 227.8015 | 273.8987 |
| 310.0891 | 393.2003 | 480.8390 |
| 551.3722 | 601.3747 | 732.5790 |
| 798.9920 | 865.9083 | 915.7307 |
| 974.3259 | 1003.1086 | 1044.2879 |
| 1078.8930 | 1100.1318 | 1118.0087 |
| 1148.0971 | 1175.1996 | 1233.2267 |

| | | |
|-----------|-----------|-----------|
| 1260.2773 | 1293.3531 | 1316.9847 |
| 1340.2627 | 1371.5123 | 1378.4007 |
| 1403.9643 | 1410.6429 | 1462.2348 |
| 1488.9940 | 1493.9390 | 1499.6926 |
| 1539.2305 | 2878.2526 | 2937.1036 |
| 2970.9199 | 2998.6396 | 3038.8296 |
| 3041.3866 | 3060.0687 | 3077.5009 |
| 3083.0634 | 3108.8631 | 3832.0052 |

Zero-point correction (Hartree): 0.156491

C5H11O2.ppptm

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.52686741
 Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 2.848661 | -0.527346 | -0.650570 |
| C | 2.041044 | -0.646546 | 0.448395 |
| C | 1.194968 | 0.595286 | 0.771375 |
| C | 0.294873 | 1.042654 | -0.392028 |
| C | -0.904307 | 0.126507 | -0.691695 |
| C | -1.997811 | 0.147591 | 0.380220 |
| O | -3.070568 | -0.738280 | 0.088689 |
| H | -3.456332 | -0.462899 | -0.753128 |
| H | 1.384910 | -1.513329 | 0.212139 |
| H | 2.621720 | -0.988489 | 1.326648 |
| H | 0.611309 | 0.393466 | 1.678522 |
| H | 1.884171 | 1.409825 | 1.025195 |
| H | -0.072661 | 2.057245 | -0.190244 |
| H | 0.923246 | 1.115396 | -1.286614 |
| H | -1.351636 | 0.438186 | -1.646510 |
| H | -0.581630 | -0.912211 | -0.836963 |
| H | -1.603505 | -0.186272 | 1.345631 |
| H | -2.356943 | 1.181135 | 0.522773 |

| | | | |
|--|-----------|-----------|-----------|
| Rotational constants (GHz): | 5.6994100 | 1.0489600 | 1.0267000 |
| Vibrational harmonic frequencies (cm-1): | | | |
| 32.6072 | 83.6923 | 101.2077 | |
| 184.5621 | 231.4693 | 288.3608 | |
| 324.7566 | 372.3610 | 469.7361 | |
| 529.9656 | 629.2826 | 748.6272 | |
| 822.0497 | 848.3007 | 920.0451 | |
| 965.0734 | 1044.2842 | 1055.6622 | |
| 1077.7928 | 1086.0903 | 1106.6615 | |
| 1138.6144 | 1190.3058 | 1210.2123 | |
| 1293.7996 | 1318.8059 | 1334.3354 | |
| 1354.1118 | 1370.9326 | 1386.4395 | |
| 1398.4002 | 1413.4151 | 1436.8468 | |
| 1497.6108 | 1499.5000 | 1506.7982 | |
| 1530.3079 | 2888.4833 | 2944.9931 | |
| 2976.5426 | 3021.2765 | 3036.8306 | |
| 3045.9328 | 3067.3760 | 3079.5194 | |
| 3091.1650 | 3093.4027 | 3812.1835 | |

Zero-point correction (Hartree): 0.156876

C5H11O2.ppptp

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.52626200
 Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 2.852018 | -0.554344 | -0.624772 |
| C | 2.043605 | -0.625485 | 0.477995 |
| C | 1.196167 | 0.628095 | 0.746565 |
| C | 0.295234 | 1.025459 | -0.434541 |
| C | -0.908881 | 0.105010 | -0.700423 |
| C | -1.997464 | 0.155483 | 0.375811 |
| O | -3.148028 | -0.604841 | 0.028816 |
| H | -2.873732 | -1.526167 | -0.065977 |
| H | 1.389451 | -1.503222 | 0.279219 |
| H | 2.624802 | -0.928272 | 1.370270 |
| H | 0.612950 | 0.465597 | 1.661792 |
| H | 1.885475 | 1.452846 | 0.964642 |
| H | -0.070736 | 2.047977 | -0.275823 |
| H | 0.923267 | 1.059948 | -1.331770 |
| H | -1.373066 | 0.384066 | -1.653454 |
| H | -0.573299 | -0.936167 | -0.822617 |
| H | -1.598067 | -0.160424 | 1.353281 |
| H | -2.350936 | 1.185916 | 0.495639 |

| | | | |
|--|-----------|-----------|-----------|
| Rotational constants (GHz): | 5.7818300 | 1.0406100 | 1.0186000 |
| Vibrational harmonic frequencies (cm-1): | | | |
| 31.4917 | 83.0603 | 101.1005 | |
| 183.7723 | 227.1366 | 282.6332 | |
| 320.8196 | 369.0980 | 468.0927 | |
| 528.6748 | 616.8782 | 748.0837 | |
| 822.1664 | 844.9541 | 916.4839 | |
| 968.7069 | 1035.9284 | 1051.2355 | |

| | | |
|-----------|-----------|-----------|
| 1082.4317 | 1084.9814 | 1111.4511 |
| 1136.5396 | 1172.2629 | 1226.3112 |
| 1301.5214 | 1311.8296 | 1330.3789 |
| 1355.0538 | 1370.3040 | 1382.8305 |
| 1404.2394 | 1410.5550 | 1435.2139 |
| 1497.6950 | 1499.2097 | 1506.4645 |
| 1529.7305 | 2886.4737 | 2944.0771 |
| 2985.7853 | 3012.0649 | 3039.5791 |
| 3047.0350 | 3071.8988 | 3080.7511 |
| 3089.0002 | 3091.6859 | 3813.8941 |

Zero-point correction (Hartree): 0.156764

C5H11O2.ppptt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.52601341

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 2.875062 | -0.513256 | -0.626136 |
| C | 2.046796 | -0.645510 | 0.455774 |
| C | 1.189403 | 0.590455 | 0.771815 |
| C | 0.294472 | 1.029082 | -0.399212 |
| C | -0.905130 | 0.115130 | -0.699330 |
| C | -2.005528 | 0.160539 | 0.355941 |
| O | -3.048811 | -0.707918 | -0.070080 |
| H | -3.751300 | -0.681608 | 0.591025 |
| H | 1.397539 | -1.511160 | 0.197313 |
| H | 2.611126 | -0.993594 | 1.342324 |
| H | 0.600046 | 0.383900 | 1.674391 |
| H | 1.871488 | 1.409321 | 1.031099 |
| H | -0.069502 | 2.047469 | -0.210514 |
| H | 0.927598 | 1.090951 | -1.291368 |
| H | -1.351970 | 0.405229 | -1.657256 |
| H | -0.586069 | -0.927882 | -0.820432 |
| H | -1.613168 | -0.149000 | 1.338451 |
| H | -2.365870 | 1.197593 | 0.464770 |

Rotational constants (GHz): 5.8166900 1.0445400 1.0229900

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 33.8443 | 76.1590 | 100.0429 |
| 184.7848 | 230.4072 | 280.7093 |
| 295.8067 | 365.9827 | 468.6405 |
| 527.5759 | 636.5537 | 755.7492 |
| 828.7286 | 849.7799 | 921.9419 |
| 966.9253 | 1046.5124 | 1055.5109 |
| 1070.3124 | 1090.2759 | 1112.2794 |
| 1164.5571 | 1185.5070 | 1236.9720 |
| 1264.5014 | 1305.3720 | 1326.0834 |
| 1332.2956 | 1362.0653 | 1372.3362 |
| 1392.1365 | 1409.5628 | 1469.5331 |
| 1496.6027 | 1502.2374 | 1510.9932 |
| 1542.6126 | 2888.5962 | 2943.8617 |
| 2968.9434 | 2995.1521 | 3036.0129 |
| 3045.0163 | 3047.0559 | 3079.5585 |
| 3089.2209 | 3090.8910 | 3828.0715 |

Zero-point correction (Hartree): 0.156702

C5H11O2.pptmm

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.52848248

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 2.693456 | -0.866614 | -0.600830 |
| C | 2.375442 | -0.015165 | 0.422890 |
| C | 1.313975 | 1.044912 | 0.087721 |
| C | -0.003099 | 0.464427 | -0.442484 |
| C | -0.824782 | -0.310849 | 0.596222 |
| C | -2.196720 | -0.742189 | 0.068920 |
| O | -3.009527 | 0.351822 | -0.342328 |
| H | -3.189187 | 0.892159 | 0.438283 |
| H | 2.008076 | -0.688435 | 1.229221 |
| H | 3.288088 | 0.438977 | 0.855008 |
| H | 1.136142 | 1.652203 | 0.986330 |
| H | 1.742306 | 1.720558 | -0.662871 |
| H | -0.626371 | 1.274431 | -0.835467 |
| H | 0.224491 | -0.194188 | -1.289699 |
| H | -0.289778 | -1.211064 | 0.928046 |
| H | -0.968255 | 0.308201 | 1.496083 |
| H | -2.073966 | -1.365109 | -0.824007 |
| H | -2.711873 | -1.356212 | 0.824723 |

Rotational constants (GHz): 6.4228200 1.0409400 0.9912300

Vibrational harmonic frequencies (cm-1):

| | | |
|----------|----------|----------|
| 41.3118 | 63.4896 | 133.3517 |
| 184.3373 | 235.9483 | 253.7757 |
| 330.9045 | 373.2315 | 497.4901 |
| 535.0598 | 625.0218 | 755.6988 |
| 825.7835 | 860.4327 | 924.5140 |

| | | |
|-----------|-----------|-----------|
| 945.3494 | 1013.4843 | 1052.6086 |
| 1080.2976 | 1093.8976 | 1105.8348 |
| 1137.3043 | 1160.2945 | 1251.4091 |
| 1275.7249 | 1313.6469 | 1336.2524 |
| 1348.9637 | 1373.9446 | 1387.7531 |
| 1401.8645 | 1415.8757 | 1427.0588 |
| 1492.9433 | 1497.0256 | 1511.0942 |
| 1521.6305 | 2884.0480 | 2942.0075 |
| 2990.9887 | 3004.6049 | 3030.2540 |
| 3051.1211 | 3052.7237 | 3076.6542 |
| 3086.9692 | 3102.0238 | 3809.3579 |

Zero-point correction (Hartree): 0.156773

C5H11O2.pptmp

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.52810701

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 2.644221 | -0.870580 | -0.693530 |
| C | 2.376970 | -0.079008 | 0.390935 |
| C | 1.345414 | 1.033858 | 0.148071 |
| C | -0.005066 | 0.521962 | -0.372229 |
| C | -0.844902 | -0.231426 | 0.668619 |
| C | -2.184209 | -0.734491 | 0.119963 |
| O | -3.052857 | 0.313236 | -0.296278 |
| H | -2.703182 | 0.681235 | -1.116822 |
| H | 2.006630 | -0.790363 | 1.162054 |
| H | 3.313546 | 0.317662 | 0.827970 |
| H | 1.210491 | 1.596593 | 1.081670 |
| H | 1.776001 | 1.733978 | -0.578250 |
| H | -0.583379 | 1.380423 | -0.736417 |
| H | 0.184556 | -0.126773 | -1.237594 |
| H | -0.291665 | -1.100561 | 1.050357 |
| H | -1.042064 | 0.423755 | 1.527199 |
| H | -2.005195 | -1.450392 | -0.698965 |
| H | -2.725895 | -1.272172 | 0.905108 |

Rotational constants (GHz): 6.2653000 1.0388500 0.9956300

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 43.9869 | 65.4811 | 121.1127 |
| 182.6875 | 231.9234 | 254.0458 |
| 306.2056 | 367.7803 | 493.5263 |
| 526.6515 | 629.8012 | 752.3237 |
| 821.0981 | 866.7095 | 923.2441 |
| 940.1003 | 1025.9419 | 1043.1677 |
| 1086.2387 | 1101.7865 | 1107.8510 |
| 1138.5502 | 1177.9708 | 1236.3013 |
| 1280.9842 | 1315.9913 | 1340.2690 |
| 1350.0517 | 1371.4180 | 1397.3389 |
| 1398.9647 | 1413.8990 | 1426.2227 |
| 1488.2179 | 1495.3400 | 1508.1900 |
| 1516.6819 | 2887.7035 | 2944.5469 |
| 2988.1155 | 3024.5698 | 3033.5463 |
| 3036.1460 | 3062.1755 | 3078.2229 |
| 3084.0511 | 3090.8349 | 3831.2912 |

Zero-point correction (Hartree): 0.156759

C5H11O2.pptmt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.52805058

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 2.680302 | -0.868709 | -0.628742 |
| C | 2.375008 | -0.035293 | 0.413712 |
| C | 1.323529 | 1.042509 | 0.105287 |
| C | -0.003358 | 0.488421 | -0.429130 |
| C | -0.823894 | -0.296838 | 0.603810 |
| C | -2.183858 | -0.737791 | 0.073324 |
| O | -2.948497 | 0.428595 | -0.215114 |
| H | -3.775228 | 0.152928 | -0.628899 |
| H | 2.002077 | -0.722069 | 1.206048 |
| H | 3.293434 | 0.399594 | 0.853352 |
| H | 1.156216 | 1.633370 | 1.016438 |
| H | 1.755931 | 1.728477 | -0.633597 |
| H | -0.618198 | 1.315202 | -0.798193 |
| H | 0.212364 | -0.156249 | -1.290562 |
| H | -0.284099 | -1.195372 | 0.930239 |
| H | -0.988002 | 0.319404 | 1.497932 |
| H | -2.044523 | -1.355330 | -0.829461 |
| H | -2.688976 | -1.365095 | 0.825534 |

Rotational constants (GHz): 6.4470200 1.0491800 0.9969900

Vibrational harmonic frequencies (cm-1):

| | | |
|----------|----------|----------|
| 42.2838 | 62.3911 | 129.8856 |
| 181.8147 | 234.1245 | 240.2313 |
| 285.3753 | 372.5206 | 489.3391 |
| 527.9509 | 629.6946 | 755.9385 |

| | | |
|-----------|-----------|-----------|
| 830.7061 | 860.2612 | 935.5920 |
| 958.6459 | 1012.7978 | 1053.2022 |
| 1087.1821 | 1100.1738 | 1108.6406 |
| 1156.9740 | 1172.3196 | 1248.7179 |
| 1275.0956 | 1293.1264 | 1320.5830 |
| 1344.0625 | 1351.2565 | 1374.5417 |
| 1400.1707 | 1418.2675 | 1461.0289 |
| 1490.5458 | 1496.0817 | 1509.6277 |
| 1537.1433 | 2883.8122 | 2941.7056 |
| 2974.8724 | 3002.8718 | 3031.4196 |
| 3034.5509 | 3049.5739 | 3070.4537 |
| 3077.5295 | 3107.4852 | 3833.3547 |

Zero-point correction (Hartree): 0.156638

C5H11O2.pptpm

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.52805647

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -2.302177 | 1.337815 | -0.083125 |
| C | -2.235702 | 0.092401 | 0.481441 |
| C | -1.480261 | -0.955843 | -0.351082 |
| C | -0.029867 | -0.560070 | -0.663305 |
| C | 0.928814 | -0.672408 | 0.530653 |
| C | 2.366791 | -0.261076 | 0.198015 |
| O | 2.501744 | 1.120003 | -0.109594 |
| H | 2.029775 | 1.290230 | -0.934172 |
| H | -1.721969 | 0.260128 | 1.453619 |
| H | -3.243826 | -0.260424 | 0.772100 |
| H | -1.513145 | -1.917587 | 0.178897 |
| H | -2.033270 | -1.096504 | -1.287626 |
| H | 0.345820 | -1.189113 | -1.481227 |
| H | -0.044200 | 0.471855 | -1.037674 |
| H | 0.582781 | -0.045921 | 1.362511 |
| H | 0.938282 | -1.709550 | 0.894501 |
| H | 3.010834 | -0.431702 | 1.066818 |
| H | 2.753736 | -0.891973 | -0.620328 |

Rotational constants (GHz): 4.6673100 1.2101800 1.0687200

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 44.0499 | 66.5032 | 141.1278 |
| 166.0708 | 242.7107 | 265.7363 |
| 316.4743 | 364.1162 | 479.5371 |
| 532.4684 | 642.5509 | 766.0534 |
| 828.6210 | 843.9863 | 925.9852 |
| 939.3149 | 1039.0213 | 1047.7111 |
| 1085.8156 | 1094.8628 | 1106.4541 |
| 1142.2768 | 1185.3225 | 1220.1440 |
| 1292.5340 | 1310.6310 | 1343.4417 |
| 1350.0337 | 1371.5406 | 1392.1794 |
| 1398.7884 | 1415.9764 | 1427.0889 |
| 1488.4784 | 1496.8151 | 1507.6030 |
| 1519.1640 | 2891.5760 | 2945.8418 |
| 2977.1263 | 3023.9072 | 3031.0626 |
| 3035.2734 | 3062.5414 | 3079.3670 |
| 3083.0279 | 3091.1554 | 3827.8727 |

Zero-point correction (Hartree): 0.156852

C5H11O2.pptpm

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.52824712

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -2.223241 | 1.365184 | -0.077116 |
| C | -2.247548 | 0.099119 | 0.442215 |
| C | -1.484908 | -0.960323 | -0.370223 |
| C | -0.019391 | -0.600967 | -0.650116 |
| C | 0.887766 | -0.610530 | 0.587112 |
| C | 2.343104 | -0.255173 | 0.267317 |
| O | 2.489310 | 1.012709 | -0.359836 |
| H | 2.143921 | 1.683134 | 0.244355 |
| H | -1.789904 | 0.214511 | 1.450033 |
| H | -3.285149 | -0.219949 | 0.659585 |
| H | -1.555815 | -1.919091 | 0.162405 |
| H | -2.013367 | -1.094735 | -1.321985 |
| H | 0.384024 | -1.307924 | -1.386607 |
| H | 0.023084 | 0.387884 | -1.116919 |
| H | 0.514101 | 0.098561 | 1.341131 |
| H | 0.868742 | -1.599958 | 1.066063 |
| H | 2.951634 | -0.318985 | 1.183972 |
| H | 2.756046 | -0.979349 | -0.444245 |

Rotational constants (GHz): 4.6595300 1.2271800 1.0899800

Vibrational harmonic frequencies (cm-1):

| | | |
|----------|----------|----------|
| 44.1026 | 55.5831 | 148.6052 |
| 178.0569 | 233.1944 | 261.5055 |

| | | |
|-----------|-----------|-----------|
| 325.2623 | 361.8287 | 490.5759 |
| 543.9191 | 632.3724 | 769.5296 |
| 832.9126 | 841.4918 | 920.3458 |
| 941.8564 | 1029.4729 | 1052.5837 |
| 1079.9240 | 1097.7901 | 1109.3791 |
| 1137.2210 | 1159.5830 | 1241.8343 |
| 1291.4936 | 1301.2708 | 1334.4221 |
| 1351.5393 | 1374.0284 | 1389.6280 |
| 1399.7828 | 1417.3162 | 1428.2298 |
| 1492.7132 | 1496.9594 | 1509.5186 |
| 1522.4696 | 2884.0448 | 2943.0753 |
| 2986.9491 | 3010.8582 | 3029.8642 |
| 3041.7078 | 3049.1599 | 3075.4430 |
| 3082.6429 | 3109.6330 | 3808.9509 |

Zero-point correction (Hartree): 0.156785

C5H11O2.pptpt

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.52735220
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -2.344228 | 1.326478 | -0.111497 |
| C | -2.228411 | 0.099615 | 0.484809 |
| C | -1.473247 | -0.954745 | -0.339493 |
| C | -0.024956 | -0.562915 | -0.664992 |
| C | 0.937168 | -0.677539 | 0.525441 |
| C | 2.364926 | -0.261659 | 0.188206 |
| O | 2.357771 | 1.121665 | -0.144636 |
| H | 3.245620 | 1.369995 | -0.428873 |
| H | -1.692406 | 0.306425 | 1.437163 |
| H | -3.219749 | -0.267722 | 0.814716 |
| H | -1.505229 | -1.911133 | 0.201496 |
| H | -2.032338 | -1.106252 | -1.270839 |
| H | 0.344764 | -1.201252 | -1.478306 |
| H | -0.013175 | 0.464303 | -1.043323 |
| H | 0.595232 | -0.052656 | 1.360601 |
| H | 0.957701 | -1.712746 | 0.892788 |
| H | 3.020918 | -0.458788 | 1.051773 |
| H | 2.737443 | -0.871865 | -0.651965 |

Rotational constants (GHz): 4.6971600 1.2191300 1.0744300
 Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 43.1881 | 64.9612 | 145.4565 |
| 165.2155 | 230.2539 | 255.4610 |
| 294.1277 | 365.0754 | 477.6111 |
| 525.2814 | 615.2641 | 763.6068 |
| 837.4044 | 844.2384 | 934.6860 |
| 948.8334 | 1038.3260 | 1064.1375 |
| 1064.9035 | 1098.8222 | 1112.1109 |
| 1159.5988 | 1169.2050 | 1253.0336 |
| 1265.3720 | 1307.2276 | 1322.0620 |
| 1343.6748 | 1353.9676 | 1371.9672 |
| 1398.2308 | 1417.1578 | 1460.9961 |
| 1489.9967 | 1495.9857 | 1511.9517 |
| 1537.0687 | 2891.6892 | 2938.8947 |
| 2970.0931 | 2998.3240 | 3026.4665 |
| 3032.8954 | 3038.8733 | 3070.4774 |
| 3076.4664 | 3107.8608 | 3832.9601 |

Zero-point correction (Hartree): 0.156582

C5H11O2.ppttm

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.52811461
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -2.544965 | -1.095507 | 0.616077 |
| C | -2.294714 | -0.361121 | -0.511827 |
| C | -1.564876 | 0.970987 | -0.277086 |
| C | -0.235626 | 0.826652 | 0.477567 |
| C | 0.881782 | 0.147116 | -0.325929 |
| C | 2.201906 | 0.072132 | 0.444940 |
| O | 3.255204 | -0.510660 | -0.311063 |
| H | 3.011964 | -1.427392 | -0.493873 |
| H | -1.674664 | -1.036241 | -1.142493 |
| H | -3.219306 | -0.223618 | -1.104820 |
| H | -1.406474 | 1.457550 | -1.249088 |
| H | -2.237048 | 1.624069 | 0.292738 |
| H | 0.103903 | 1.824003 | 0.785202 |
| H | -0.424996 | 0.263822 | 1.399907 |
| H | 0.582087 | -0.874605 | -0.602441 |
| H | 1.058795 | 0.685979 | -1.265668 |
| H | 2.544298 | 1.082172 | 0.696536 |
| H | 2.048704 | -0.460996 | 1.397888 |

Rotational constants (GHz): 5.7376000 1.0004600 0.9451100
 Vibrational harmonic frequencies (cm-1):

| | | |
|---------|---------|----------|
| 46.2720 | 69.3933 | 123.2941 |
|---------|---------|----------|

| | | |
|-----------|-----------|-----------|
| 151.5550 | 216.0804 | 257.9514 |
| 314.3083 | 396.5282 | 444.0694 |
| 519.6649 | 633.2560 | 752.7596 |
| 822.7367 | 876.5579 | 899.9259 |
| 1010.6432 | 1028.1815 | 1040.8453 |
| 1084.2118 | 1097.7266 | 1114.0526 |
| 1136.7216 | 1161.8880 | 1255.9529 |
| 1284.7610 | 1312.7285 | 1333.8875 |
| 1337.1369 | 1372.7518 | 1384.1025 |
| 1402.1823 | 1412.2958 | 1431.9698 |
| 1494.0931 | 1499.4329 | 1507.2048 |
| 1529.3101 | 2887.2696 | 2944.6921 |
| 2984.6624 | 3013.6432 | 3034.3773 |
| 3039.8246 | 3059.3248 | 3076.3600 |
| 3081.7202 | 3092.0515 | 3813.9126 |

Zero-point correction (Hartree): 0.156702

C5H11O2.ppttp

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.52804494

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -2.600023 | -1.093496 | 0.552927 |
| C | -2.295881 | -0.328844 | -0.541042 |
| C | -1.551530 | 0.980085 | -0.233016 |
| C | -0.233348 | 0.775946 | 0.527312 |
| C | 0.895194 | 0.165752 | -0.315268 |
| C | 2.198183 | -0.000672 | 0.469929 |
| O | 3.230120 | -0.616213 | -0.289419 |
| H | 3.433171 | -0.034439 | -1.033293 |
| H | -1.666610 | -0.994261 | -1.172545 |
| H | -3.197155 | -0.153613 | -1.159586 |
| H | -1.375289 | 1.513673 | -1.177099 |
| H | -2.222342 | 1.611887 | 0.361694 |
| H | 0.099958 | 1.742593 | 0.926401 |
| H | -0.435659 | 0.135095 | 1.394534 |
| H | 0.608637 | -0.819227 | -0.703976 |
| H | 1.083976 | 0.804977 | -1.191543 |
| H | 2.521906 | 0.975312 | 0.869248 |
| H | 2.032929 | -0.657924 | 1.330618 |

Rotational constants (GHz): 5.7897700 0.9914800 0.9412700

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 53.8067 | 74.3236 | 120.5044 |
| 150.5784 | 215.3336 | 261.9135 |
| 316.8993 | 398.5404 | 443.9459 |
| 515.4966 | 638.8890 | 754.0066 |
| 825.1704 | 879.5503 | 898.1583 |
| 1003.5213 | 1035.7391 | 1050.7550 |
| 1082.8257 | 1094.8881 | 1102.3259 |
| 1145.0510 | 1161.4919 | 1264.5114 |
| 1276.2388 | 1325.1434 | 1328.2838 |
| 1337.5257 | 1372.7877 | 1385.9851 |
| 1399.1482 | 1411.8298 | 1433.8805 |
| 1494.1850 | 1501.0553 | 1509.6765 |
| 1530.8533 | 2890.1000 | 2944.0506 |
| 2979.2163 | 3007.6994 | 3032.7979 |
| 3037.9743 | 3064.0175 | 3077.7039 |
| 3081.3202 | 3093.4369 | 3813.0895 |

Zero-point correction (Hartree): 0.156775

C5H11O2.ppttt

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.52766548

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -2.583442 | -1.088670 | 0.591543 |
| C | -2.291623 | -0.351481 | -0.524435 |
| C | -1.556069 | 0.971433 | -0.257237 |
| C | -0.233862 | 0.800136 | 0.504156 |
| C | 0.889653 | 0.164995 | -0.325191 |
| C | 2.192652 | 0.030265 | 0.452927 |
| O | 3.156785 | -0.565879 | -0.406665 |
| H | 3.979626 | -0.665008 | 0.087596 |
| H | -1.658660 | -1.028529 | -1.139747 |
| H | -3.196773 | -0.200988 | -1.143779 |
| H | -1.385866 | 1.476980 | -1.217516 |
| H | -2.229915 | 1.616026 | 0.320137 |
| H | 0.096699 | 1.782993 | 0.864131 |
| H | -0.430701 | 0.191754 | 1.395802 |
| H | 0.603385 | -0.835230 | -0.673187 |
| H | 1.083586 | 0.765361 | -1.223393 |
| H | 2.523702 | 1.024882 | 0.796588 |
| H | 2.023662 | -0.583934 | 1.353017 |

Rotational constants (GHz): 5.7833300 1.0011400 0.9505000

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 51.3552 | 71.7938 | 117.4488 |
| 152.1835 | 215.5207 | 262.6538 |
| 275.9473 | 401.6501 | 438.6700 |
| 516.3119 | 643.3041 | 757.4164 |
| 832.0291 | 879.9067 | 904.3613 |
| 1011.0157 | 1028.2973 | 1048.9931 |
| 1082.2662 | 1099.0924 | 1114.5654 |
| 1145.5252 | 1210.3648 | 1240.2180 |
| 1277.1000 | 1298.9712 | 1323.3546 |
| 1333.5865 | 1339.2308 | 1373.5254 |
| 1394.9435 | 1410.4099 | 1470.0393 |
| 1494.2133 | 1502.7567 | 1514.4922 |
| 1543.0522 | 2889.9753 | 2944.1215 |
| 2968.7163 | 2996.3779 | 3031.3705 |
| 3036.9278 | 3041.7511 | 3068.2584 |
| 3079.4613 | 3091.2097 | 3829.0050 |

Zero-point correction (Hartree): 0.156633

C5H11O2.ptmmm

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.52902981

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 3.102332 | 0.363868 | -0.325505 |
| C | 2.303656 | -0.665989 | 0.096134 |
| C | 0.919316 | -0.256522 | 0.615518 |
| C | 0.098068 | 0.491069 | -0.441503 |
| C | -1.226201 | 1.070835 | 0.075024 |
| C | -2.250589 | 0.017387 | 0.510310 |
| O | -2.539477 | -0.936272 | -0.506874 |
| H | -2.917409 | -0.458388 | -1.256905 |
| H | 2.196585 | -1.322362 | -0.796419 |
| H | 2.850675 | -1.298347 | 0.822400 |
| H | 0.397091 | -1.161300 | 0.950980 |
| H | 1.058065 | 0.377296 | 1.501864 |
| H | 0.717103 | 1.301456 | -0.842611 |
| H | -0.118082 | -0.188610 | -1.275381 |
| H | -1.039936 | 1.745883 | 0.922100 |
| H | -1.676204 | 1.692663 | -0.712815 |
| H | -1.867956 | -0.566986 | 1.353628 |
| H | -3.168269 | 0.517244 | 0.859285 |

Rotational constants (GHz): 6.2756200 1.0543500 1.0044500

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 45.6488 | 58.4859 | 129.5953 |
| 185.4207 | 233.3866 | 255.7145 |
| 335.1915 | 379.2062 | 497.8564 |
| 536.1061 | 560.0068 | 740.5152 |
| 832.1098 | 860.3774 | 905.0477 |
| 977.1402 | 1005.1878 | 1030.1597 |
| 1087.7016 | 1097.4311 | 1106.8368 |
| 1130.4963 | 1191.6329 | 1224.4159 |
| 1287.9508 | 1325.2171 | 1338.0344 |
| 1364.7231 | 1366.4570 | 1381.5348 |
| 1401.5597 | 1417.4301 | 1427.7703 |
| 1490.8565 | 1497.3741 | 1507.4041 |
| 1524.6248 | 2881.8580 | 2938.8965 |
| 2992.5878 | 3015.9424 | 3033.0608 |
| 3042.9184 | 3056.1615 | 3072.2532 |
| 3092.4269 | 3096.7052 | 3809.7628 |

Zero-point correction (Hartree): 0.156668

C5H11O2.ptmmp

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.52752640

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 3.106322 | 0.369610 | -0.325229 |
| C | 2.318915 | -0.661680 | 0.113255 |
| C | 0.927756 | -0.256508 | 0.618485 |
| C | 0.104059 | 0.469069 | -0.453550 |
| C | -1.221818 | 1.065716 | 0.044048 |
| C | -2.261814 | 0.038172 | 0.504703 |
| O | -2.696268 | -0.827579 | -0.538152 |
| H | -1.952242 | -1.388772 | -0.788715 |
| H | 2.229276 | -1.343842 | -0.761472 |
| H | 2.872017 | -1.265757 | 0.858854 |
| H | 0.414998 | -1.158426 | 0.978785 |
| H | 1.055903 | 0.396852 | 1.491481 |
| H | 0.725672 | 1.270615 | -0.867634 |
| H | -0.093775 | -0.214808 | -1.292817 |
| H | -1.021763 | 1.754461 | 0.876730 |
| H | -1.668485 | 1.662199 | -0.760310 |
| H | -1.882642 | -0.537137 | 1.364868 |
| H | -3.161982 | 0.559752 | 0.845630 |

Rotational constants (GHz): 6.4381300 1.0321000 0.9872800

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 47.9070 | 61.2299 | 126.0636 |
| 172.4518 | 240.0792 | 251.1965 |
| 281.7864 | 389.1725 | 482.8401 |
| 506.0184 | 544.6919 | 742.0514 |
| 824.0966 | 856.7056 | 897.8259 |
| 971.1466 | 1002.4317 | 1046.9641 |
| 1084.0459 | 1089.1996 | 1103.8147 |
| 1153.4200 | 1177.4726 | 1231.2794 |
| 1278.0633 | 1325.9851 | 1331.7527 |
| 1362.3125 | 1369.8890 | 1390.9438 |
| 1396.7244 | 1411.5747 | 1429.0951 |
| 1487.0542 | 1496.6045 | 1519.0421 |
| 1521.0077 | 2883.4335 | 2938.6602 |
| 2988.4377 | 3014.0128 | 3029.3838 |
| 3034.4826 | 3068.9655 | 3080.9821 |
| 3089.1633 | 3093.0170 | 3827.8802 |

Zero-point correction (Hartree): 0.156402

C5H11O2.ptmmt

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.52807745
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 3.109766 | 0.366137 | -0.265894 |
| C | 2.294424 | -0.677785 | 0.082912 |
| C | 0.900200 | -0.284618 | 0.588228 |
| C | 0.102480 | 0.504833 | -0.456133 |
| C | -1.223813 | 1.086593 | 0.054587 |
| C | -2.243516 | 0.043445 | 0.503083 |
| O | -2.502922 | -0.827399 | -0.593717 |
| H | -3.142246 | -1.490764 | -0.307312 |
| H | 2.205197 | -1.287131 | -0.844287 |
| H | 2.819993 | -1.349963 | 0.789294 |
| H | 0.369239 | -1.201003 | 0.876160 |
| H | 1.022374 | 0.311818 | 1.502644 |
| H | 0.734828 | 1.323729 | -0.818086 |
| H | -0.105528 | -0.141554 | -1.317118 |
| H | -1.037827 | 1.765046 | 0.898272 |
| H | -1.678771 | 1.688823 | -0.741031 |
| H | -1.857644 | -0.517311 | 1.369980 |
| H | -3.163013 | 0.553600 | 0.832307 |

Rotational constants (GHz): 6.3345400 1.0623700 1.0091700
 Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 44.9843 | 58.7084 | 130.1815 |
| 185.1408 | 234.0430 | 253.2257 |
| 277.7054 | 382.2340 | 490.7506 |
| 531.8589 | 556.7610 | 744.5090 |
| 829.9391 | 866.5322 | 910.5360 |
| 976.8688 | 1008.9036 | 1050.3691 |
| 1081.2770 | 1099.8882 | 1117.1319 |
| 1142.5355 | 1213.6835 | 1236.1679 |
| 1263.7378 | 1304.2102 | 1329.9103 |
| 1341.1545 | 1365.6823 | 1369.0338 |
| 1400.5149 | 1416.3065 | 1461.3058 |
| 1487.1517 | 1496.3445 | 1510.9615 |
| 1540.1666 | 2881.6219 | 2936.2753 |
| 2978.5085 | 3003.6924 | 3031.1618 |
| 3037.2230 | 3050.3716 | 3069.8041 |
| 3081.2812 | 3098.7242 | 3831.8069 |

Zero-point correction (Hartree): 0.156535

C5H11O2.ptmpm

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.52627487
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -3.037965 | 0.332864 | -0.401738 |
| C | -2.286694 | -0.589982 | 0.274360 |
| C | -0.779481 | -0.550131 | -0.022469 |
| C | -0.159387 | 0.816146 | 0.307000 |
| C | 1.242839 | 1.082299 | -0.263984 |
| C | 2.372349 | 0.185279 | 0.255227 |
| O | 2.376253 | -1.127516 | -0.296890 |
| H | 1.632998 | -1.614660 | 0.076143 |
| H | -2.468341 | -0.366000 | 1.349336 |
| H | -2.710756 | -1.603717 | 0.139263 |
| H | -0.310856 | -1.359012 | 0.556456 |
| H | -0.627794 | -0.789018 | -1.082288 |
| H | -0.842652 | 1.580696 | -0.081615 |
| H | -0.138953 | 0.949070 | 1.398917 |
| H | 1.222692 | 1.000769 | -1.358353 |
| H | 1.510421 | 2.122623 | -0.033719 |
| H | 3.335532 | 0.618904 | -0.033800 |
| H | 2.353650 | 0.155894 | 1.357882 |

Rotational constants (GHz): 5.8744300 1.1250900 1.0068200
 Vibrational harmonic frequencies (cm⁻¹):
 48.6598 71.9241 128.3801
 153.9874 229.8453 254.4034
 288.5749 365.7853 472.6018
 518.4494 605.2730 771.4289
 799.8548 889.2237 932.3327
 941.1823 986.6232 1047.0553
 1088.1235 1092.0336 1105.7337
 1147.8165 1185.5353 1253.5995
 1262.1493 1324.9284 1327.5834
 1367.4969 1369.9297 1391.9462
 1399.0677 1415.7580 1430.6210
 1482.6800 1491.3268 1508.8543
 1518.1112 2882.5735 2944.0219
 2979.5846 3015.1665 3016.6053
 3029.6988 3070.0592 3074.2202
 3084.8426 3087.8290 3849.3105
 Zero-point correction (Hartree): 0.156516

C5H11O2.ptmpp

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.52887349

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -3.087537 | 0.363134 | -0.176743 |
| C | -2.245095 | -0.637730 | 0.231779 |
| C | -0.787845 | -0.502610 | -0.225649 |
| C | -0.146260 | 0.809265 | 0.245213 |
| C | 1.266487 | 1.080061 | -0.295672 |
| C | 2.376982 | 0.193932 | 0.277242 |
| O | 2.247693 | -1.191736 | -0.031899 |
| H | 2.282252 | -1.280696 | -0.993389 |
| H | -2.300381 | -0.609425 | 1.343563 |
| H | -2.671319 | -1.626777 | -0.026298 |
| H | -0.212772 | -1.362300 | 0.132258 |
| H | -0.770384 | -0.546760 | -1.323582 |
| H | -0.807402 | 1.631517 | -0.052532 |
| H | -0.115198 | 0.824274 | 1.344856 |
| H | 1.267144 | 0.995931 | -1.393366 |
| H | 1.538438 | 2.121879 | -0.077444 |
| H | 3.355867 | 0.576308 | -0.054375 |
| H | 2.366906 | 0.247352 | 1.371975 |

Rotational constants (GHz): 5.8972800 1.1396800 1.0113600

Vibrational harmonic frequencies (cm⁻¹):
 53.4905 92.9581 123.6015
 155.1646 235.8426 292.7996
 339.1834 347.7751 487.4654
 527.3005 584.7721 782.2352
 800.2985 895.5140 920.3705
 938.6206 999.0046 1032.5283
 1086.1335 1102.5059 1105.6852
 1114.4272 1207.5340 1231.0070
 1284.5779 1319.4214 1333.9191
 1360.1524 1367.8607 1387.3324
 1400.2571 1414.5389 1429.9898
 1489.1621 1499.4310 1514.1570
 1521.8581 2877.3326 2939.1343
 2988.7215 3009.5400 3015.7537
 3035.6230 3054.2705 3075.2579
 3082.4684 3108.6901 3812.1413
 Zero-point correction (Hartree): 0.156687

C5H11O2.ptmpt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.52792644

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -3.095367 | 0.365207 | -0.153058 |
| C | -2.251410 | -0.648697 | 0.220217 |
| C | -0.797152 | -0.504757 | -0.243647 |
| C | -0.150624 | 0.794280 | 0.253559 |
| C | 1.256947 | 1.080266 | -0.294193 |
| C | 2.376289 | 0.210448 | 0.269786 |
| O | 2.207567 | -1.132924 | -0.176824 |
| H | 2.917655 | -1.666071 | 0.201216 |
| H | -2.298860 | -0.646181 | 1.333134 |
| H | -2.681208 | -1.630348 | -0.059180 |
| H | -0.222041 | -1.374738 | 0.087874 |
| H | -0.781529 | -0.525876 | -1.341191 |
| H | -0.813452 | 1.623603 | -0.020108 |
| H | -0.112115 | 0.786031 | 1.353521 |
| H | 1.261365 | 0.986608 | -1.387896 |
| H | 1.518688 | 2.122729 | -0.070229 |
| H | 3.346893 | 0.611644 | -0.064092 |

| | | | | |
|---|-----------|-----------|-----------|-----------|
| H | 2.362708 | 0.265092 | 1.371678 | |
| Rotational constants (GHz): | 5.9996700 | | 1.1379400 | 1.0107500 |
| Vibrational harmonic frequencies (cm ⁻¹): | | | | |
| | 46.0106 | 89.5452 | | 123.2199 |
| | 154.7119 | 234.0577 | | 269.5467 |
| | 308.9941 | 347.7405 | | 474.5494 |
| | 524.3984 | 596.3362 | | 780.2052 |
| | 804.3880 | 900.1113 | | 927.8217 |
| | 933.0128 | 1006.2508 | | 1042.0275 |
| | 1085.7685 | 1098.3531 | | 1106.4667 |
| | 1164.7419 | 1212.3291 | | 1224.7415 |
| | 1271.0513 | 1302.7268 | | 1330.7594 |
| | 1334.8845 | 1360.2247 | | 1369.3477 |
| | 1399.9299 | 1417.2789 | | 1464.9479 |
| | 1485.9281 | 1496.5724 | | 1513.2813 |
| | 1536.4774 | 2872.2722 | | 2939.0457 |
| | 2970.0896 | 2999.8043 | | 3010.4953 |
| | 3036.8115 | 3048.2952 | | 3074.2517 |
| | 3077.5956 | 3111.9429 | | 3827.2563 |
| Zero-point correction (Hartree): 0.156525 | | | | |

C5H11O2.ptmtm

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.52778646

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | | |
|---|-----------|-----------|-----------|-----------|
| O | -3.221731 | 0.549827 | -0.225877 | |
| C | -2.535782 | -0.583304 | 0.122382 | |
| C | -1.048043 | -0.591699 | -0.254148 | |
| C | -0.277926 | 0.572381 | 0.383768 | |
| C | 1.163773 | 0.745801 | -0.116751 | |
| C | 2.106148 | -0.405314 | 0.245448 | |
| O | 3.455906 | -0.143220 | -0.117969 | |
| H | 3.484108 | -0.032876 | -1.077234 | |
| H | -2.652476 | -0.656691 | 1.226777 | |
| H | -3.065803 | -1.478739 | -0.256754 | |
| H | -0.623696 | -1.560573 | 0.038248 | |
| H | -0.970748 | -0.532596 | -1.348082 | |
| H | -0.839318 | 1.492111 | 0.184331 | |
| H | -0.270951 | 0.448141 | 1.476589 | |
| H | 1.156186 | 0.873367 | -1.209994 | |
| H | 1.588644 | 1.666760 | 0.299767 | |
| H | 2.116543 | -0.548537 | 1.332268 | |
| H | 1.755096 | -1.350408 | -0.199340 | |
| Rotational constants (GHz): | 9.3093900 | | 0.8787000 | 0.8426200 |
| Vibrational harmonic frequencies (cm ⁻¹): | | | | |
| | 51.7398 | 91.5714 | | 99.7701 |
| | 152.2651 | 243.5937 | | 251.1246 |
| | 304.2972 | 334.3440 | | 463.7002 |
| | 537.4575 | 587.5832 | | 754.7456 |
| | 798.3840 | 876.7303 | | 923.2572 |
| | 961.1509 | 1035.4723 | | 1070.8693 |
| | 1084.1007 | 1086.3958 | | 1099.6437 |
| | 1131.2394 | 1212.5639 | | 1230.5897 |
| | 1305.1313 | 1314.9104 | | 1335.1961 |
| | 1355.2263 | 1366.5847 | | 1370.5049 |
| | 1401.0993 | 1416.6608 | | 1435.6220 |
| | 1494.2291 | 1503.1837 | | 1513.1027 |
| | 1530.2750 | 2883.3112 | | 2939.9671 |
| | 2988.0835 | 3011.1594 | | 3020.8820 |
| | 3035.9665 | 3067.7483 | | 3071.4193 |
| | 3086.5844 | 3090.0959 | | 3813.2061 |
| Zero-point correction (Hartree): 0.156585 | | | | |

C5H11O2.ptmtp

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.52801160

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | | |
|---|-----------|-----------|-----------|--|
| O | -3.222947 | 0.548688 | -0.218776 | |
| C | -2.533793 | -0.580348 | 0.136674 | |
| C | -1.048728 | -0.592913 | -0.249567 | |
| C | -0.275855 | 0.582725 | 0.362702 | |
| C | 1.163539 | 0.738103 | -0.149642 | |
| C | 2.101767 | -0.404864 | 0.247512 | |
| O | 3.423510 | -0.227864 | -0.244036 | |
| H | 3.763334 | 0.599103 | 0.122077 | |
| H | -2.643657 | -0.641963 | 1.242575 | |
| H | -3.065873 | -1.479989 | -0.229329 | |
| H | -0.621239 | -1.555917 | 0.057468 | |
| H | -0.977087 | -0.552881 | -1.344468 | |
| H | -0.836140 | 1.499142 | 0.146103 | |
| H | -0.266426 | 0.480559 | 1.458041 | |
| H | 1.168405 | 0.830778 | -1.243042 | |
| H | 1.579059 | 1.677758 | 0.242941 | |

| | | | | |
|--|-----------|-----------|-----------|-----------|
| H | 2.093973 | -0.526756 | 1.344653 | |
| H | 1.759569 | -1.352645 | -0.180605 | |
| Rotational constants (GHz): | 9.2645700 | | 0.8822900 | 0.8441400 |
| Vibrational harmonic frequencies (cm-1): | | | | |
| | 51.7197 | 92.9903 | | 99.0911 |
| | 152.3893 | 244.1959 | | 255.6430 |
| | 301.3513 | 344.3261 | | 464.9560 |
| | 536.1540 | 587.1982 | | 753.1031 |
| | 797.7512 | 877.1947 | | 927.7969 |
| | 960.7407 | 1037.2912 | | 1059.1101 |
| | 1085.3329 | 1088.4024 | | 1098.2806 |
| | 1151.2320 | 1208.8030 | | 1219.4759 |
| | 1304.4151 | 1320.7580 | | 1337.4259 |
| | 1353.7094 | 1366.2811 | | 1371.6700 |
| | 1398.8871 | 1418.7475 | | 1437.8535 |
| | 1494.2343 | 1502.4308 | | 1512.9118 |
| | 1530.4227 | 2882.2622 | | 2940.2568 |
| | 2970.9373 | 3014.9012 | | 3019.6359 |
| | 3036.5618 | 3067.4145 | | 3071.4975 |
| | 3091.0158 | 3094.0955 | | 3810.3266 |
| Zero-point correction (Hartree): | 0.156608 | | | |

C5H11O2.ptmtt

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.52717022
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | | |
|--|-----------|-----------|-----------|-----------|
| O | -3.225774 | 0.542761 | -0.212765 | |
| C | -2.532706 | -0.589202 | 0.125202 | |
| C | -1.047081 | -0.589876 | -0.259128 | |
| C | -0.276662 | 0.574126 | 0.378395 | |
| C | 1.161386 | 0.750837 | -0.127864 | |
| C | 2.098268 | -0.398252 | 0.229192 | |
| O | 3.400511 | -0.050527 | -0.226146 | |
| H | 3.995816 | -0.782554 | -0.023836 | |
| H | -2.642796 | -0.667290 | 1.230108 | |
| H | -3.061129 | -1.485368 | -0.254633 | |
| H | -0.618324 | -1.558667 | 0.028114 | |
| H | -0.974288 | -0.527183 | -1.352975 | |
| H | -0.839427 | 1.493288 | 0.180500 | |
| H | -0.269013 | 0.449162 | 1.471378 | |
| H | 1.164943 | 0.878101 | -1.217792 | |
| H | 1.588006 | 1.668889 | 0.293185 | |
| H | 2.085039 | -0.557464 | 1.321440 | |
| H | 1.754048 | -1.334583 | -0.238977 | |
| Rotational constants (GHz): | 9.3741800 | | 0.8840900 | 0.8460600 |
| Vibrational harmonic frequencies (cm-1): | | | | |
| | 52.5944 | 85.9796 | | 97.9850 |
| | 152.4915 | 243.5562 | | 258.9735 |
| | 279.2815 | 321.6212 | | 464.6246 |
| | 539.2001 | 587.9616 | | 757.7858 |
| | 806.6428 | 877.1766 | | 930.6837 |
| | 956.4305 | 1044.8807 | | 1063.5921 |
| | 1074.4417 | 1092.2321 | | 1102.7383 |
| | 1183.4858 | 1203.8886 | | 1241.8759 |
| | 1269.9122 | 1312.6702 | | 1327.7074 |
| | 1334.0192 | 1362.3349 | | 1369.9556 |
| | 1375.2599 | 1416.5904 | | 1470.4324 |
| | 1494.1664 | 1507.6980 | | 1514.1547 |
| | 1542.7776 | 2881.4581 | | 2938.9903 |
| | 2965.0813 | 2996.3856 | | 3016.4888 |
| | 3034.9679 | 3045.4517 | | 3070.1219 |
| | 3088.4173 | 3091.5230 | | 3828.2673 |
| Zero-point correction (Hartree): | 0.156453 | | | |

C5H11O2.ptpmm

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.52826730
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | | |
|---|-----------|-----------|-----------|--|
| O | 2.664359 | -0.336365 | 0.937308 | |
| C | 2.330487 | -0.213740 | -0.385858 | |
| C | 0.826940 | -0.159906 | -0.683966 | |
| C | 0.125764 | 0.995434 | 0.042345 | |
| C | -1.395602 | 1.075915 | -0.164037 | |
| C | -2.218378 | -0.033618 | 0.499830 | |
| O | -2.010020 | -1.334272 | -0.045634 | |
| H | -2.274417 | -1.306623 | -0.974548 | |
| H | 2.817386 | 0.737593 | -0.700657 | |
| H | 2.845611 | -0.986904 | -0.988516 | |
| H | 0.694499 | -0.062435 | -1.771319 | |
| H | 0.368860 | -1.110369 | -0.395206 | |
| H | 0.343918 | 0.913061 | 1.114327 | |
| H | 0.572168 | 1.944718 | -0.286744 | |
| H | -1.756099 | 2.031812 | 0.239985 | |

| | | | | |
|---|-----------|-----------|-----------|--|
| H | -1.629556 | 1.101076 | -1.239903 | |
| H | -1.945911 | -0.116353 | 1.557895 | |
| H | -3.286430 | 0.235007 | 0.461406 | |
| Rotational constants (GHz): | 4.7064300 | 1.2235700 | 1.1264900 | |
| Vibrational harmonic frequencies (cm ⁻¹): | | | | |
| 54.4828 | 83.2243 | | 146.2975 | |
| 152.4181 | 235.3149 | | 295.8426 | |
| 332.4731 | 338.3041 | | 471.7736 | |
| 538.3072 | 602.7789 | | 782.6189 | |
| 805.9932 | 886.7370 | | 919.1462 | |
| 953.2807 | 976.9094 | | 1055.6215 | |
| 1080.8343 | 1093.5154 | | 1106.8012 | |
| 1146.5168 | 1176.2017 | | 1263.1857 | |
| 1273.7949 | 1316.2013 | | 1336.7927 | |
| 1363.4312 | 1370.7219 | | 1388.4734 | |
| 1398.7406 | 1417.2006 | | 1430.3522 | |
| 1490.8522 | 1501.1791 | | 1516.6114 | |
| 1521.7031 | 2870.0090 | | 2939.7561 | |
| 2988.0166 | 3006.7231 | | 3020.4295 | |
| 3026.6309 | 3052.8992 | | 3073.5054 | |
| 3087.7920 | 3113.8333 | | 3810.9963 | |
| Zero-point correction (Hartree): | 0.156773 | | | |

C5H11O2.ptpmp

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.53057813
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | | |
|---|-----------|-----------|-----------|--|
| O | -1.571673 | -1.229983 | -0.508064 | |
| C | -2.039067 | -0.040772 | -0.002199 | |
| C | -0.999928 | 0.885774 | 0.630226 | |
| C | 0.087167 | 1.378643 | -0.365221 | |
| C | 1.526126 | 0.946144 | -0.029324 | |
| C | 1.841742 | -0.536409 | -0.268243 | |
| O | 1.111723 | -1.427697 | 0.558706 | |
| H | 0.228397 | -1.529221 | 0.167644 | |
| H | -2.610233 | 0.461861 | -0.809899 | |
| H | -2.832713 | -0.318694 | 0.724892 | |
| H | -1.538264 | 1.739485 | 1.059864 | |
| H | -0.530311 | 0.356077 | 1.464779 | |
| H | -0.155585 | 1.034762 | -1.380894 | |
| H | 0.057734 | 2.472960 | -0.410273 | |
| H | 2.222807 | 1.535532 | -0.641600 | |
| H | 1.747061 | 1.190684 | 1.017885 | |
| H | 1.691387 | -0.772188 | -1.335352 | |
| H | 2.903085 | -0.710100 | -0.053621 | |
| Rotational constants (GHz): | 3.4359100 | 1.9953600 | 1.4518800 | |
| Vibrational harmonic frequencies (cm ⁻¹): | | | | |
| 47.9052 | 106.9143 | | 171.6239 | |
| 175.4020 | 275.8943 | | 305.6448 | |
| 332.7978 | 438.5205 | | 488.7138 | |
| 553.3320 | 657.3754 | | 745.4664 | |
| 833.8713 | 882.6060 | | 889.1289 | |
| 953.4753 | 1019.1307 | | 1058.8821 | |
| 1071.7074 | 1099.7484 | | 1112.4044 | |
| 1164.3286 | 1201.7351 | | 1251.1420 | |
| 1287.4704 | 1309.1513 | | 1346.4830 | |
| 1359.7017 | 1393.1545 | | 1396.4792 | |
| 1406.4307 | 1425.1247 | | 1448.7642 | |
| 1490.0915 | 1499.2987 | | 1501.1673 | |
| 1516.6733 | 2896.1000 | | 2918.7688 | |
| 2978.9828 | 3022.4091 | | 3025.0404 | |
| 3048.3999 | 3066.4901 | | 3071.5487 | |
| 3078.3529 | 3107.9658 | | 3710.6455 | |
| Zero-point correction (Hartree): | 0.157518 | | | |

C5H11O2.ptpmt

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.52782273
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | | |
|---|-----------|-----------|-----------|--|
| O | 2.639061 | -0.435140 | 0.931093 | |
| C | 2.338252 | -0.176817 | -0.381225 | |
| C | 0.843083 | -0.094515 | -0.709938 | |
| C | 0.124489 | 0.993984 | 0.097139 | |
| C | -1.395255 | 1.082482 | -0.121855 | |
| C | -2.218351 | -0.052174 | 0.481747 | |
| O | -1.987898 | -1.252093 | -0.253655 | |
| H | -2.461415 | -1.969045 | 0.185874 | |
| H | 2.830286 | 0.802292 | -0.583204 | |
| H | 2.872334 | -0.882926 | -1.046520 | |
| H | 0.733146 | 0.095637 | -1.786585 | |
| H | 0.378787 | -1.065960 | -0.519108 | |
| H | 0.331459 | 0.830419 | 1.162459 | |

| | | | | |
|--|-----------|-----------|-----------|-----------|
| H | 0.567549 | 1.969164 | -0.151321 | |
| H | -1.760196 | 2.016052 | 0.325891 | |
| H | -1.623929 | 1.142338 | -1.194132 | |
| H | -1.944984 | -0.178865 | 1.542388 | |
| H | -3.285644 | 0.221002 | 0.449549 | |
| Rotational constants (GHz): | 4.7218700 | | 1.2279500 | 1.1315500 |
| Vibrational harmonic frequencies (cm-1): | | | | |
| 46.4579 | | 79.1707 | | 142.2079 |
| 152.7122 | | 236.0179 | | 269.3255 |
| 316.3799 | | 341.8492 | | 454.6327 |
| 533.9909 | | 593.0718 | | 778.9149 |
| 809.9517 | | 885.5343 | | 926.1352 |
| 956.8608 | | 981.2306 | | 1058.0465 |
| 1087.5420 | | 1099.7730 | | 1112.7672 |
| 1171.7670 | | 1182.9264 | | 1246.3750 |
| 1280.4312 | | 1297.0173 | | 1322.4764 |
| 1340.2208 | | 1363.2861 | | 1371.0723 |
| 1398.0071 | | 1419.3558 | | 1465.3184 |
| 1487.1808 | | 1498.7268 | | 1514.0849 |
| 1536.3276 | | 2868.5012 | | 2938.6661 |
| 2974.3875 | | 3002.7379 | | 3017.2479 |
| 3037.2385 | | 3037.5774 | | 3065.0434 |
| 3078.7462 | | 3120.1846 | | 3826.8107 |
| Zero-point correction (Hartree): | 0.156565 | | | |

C5H11O2.ptppm

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.52812395
Electronic state : 2-A
Cartesian coordinates (Angs):

| | | | | |
|--|-----------|-----------|-----------|-----------|
| O | 2.349223 | 1.202203 | -0.223560 | |
| C | 2.381469 | -0.105762 | 0.186341 | |
| C | 1.014785 | -0.700599 | 0.544330 | |
| C | 0.057235 | -0.709486 | -0.654905 | |
| C | -1.408687 | -1.020643 | -0.315824 | |
| C | -2.109245 | 0.061027 | 0.516927 | |
| O | -2.143967 | 1.328051 | -0.127562 | |
| H | -1.249069 | 1.690678 | -0.124907 | |
| H | 2.847336 | -0.666479 | -0.653848 | |
| H | 3.115818 | -0.214679 | 1.008525 | |
| H | 1.152887 | -1.717782 | 0.934647 | |
| H | 0.601286 | -0.106074 | 1.368471 | |
| H | 0.111888 | 0.267401 | -1.152097 | |
| H | 0.418073 | -1.437574 | -1.393251 | |
| H | -1.968608 | -1.143508 | -1.250479 | |
| H | -1.476546 | -1.976224 | 0.223221 | |
| H | -3.155611 | -0.222779 | 0.670746 | |
| H | -1.652849 | 0.137765 | 1.516726 | |
| Rotational constants (GHz): | 4.3570300 | | 1.3084500 | 1.1249200 |
| Vibrational harmonic frequencies (cm-1): | | | | |
| 9.3814 | | 62.8884 | | 143.5317 |
| 195.0401 | | 235.2226 | | 282.2234 |
| 332.8515 | | 374.3741 | | 465.3063 |
| 494.6409 | | 562.8909 | | 745.6485 |
| 815.7445 | | 857.4610 | | 915.0224 |
| 945.8830 | | 1027.9558 | | 1039.1719 |
| 1085.1678 | | 1099.8481 | | 1109.3633 |
| 1132.7812 | | 1193.3472 | | 1219.7133 |
| 1295.6397 | | 1319.5573 | | 1336.0339 |
| 1358.6056 | | 1378.9365 | | 1392.9220 |
| 1399.4512 | | 1411.9506 | | 1429.9494 |
| 1490.5202 | | 1497.2134 | | 1520.1432 |
| 1523.9912 | | 2889.5812 | | 2937.5586 |
| 2993.4405 | | 3027.1375 | | 3033.7236 |
| 3038.5988 | | 3064.5871 | | 3079.0734 |
| 3085.4274 | | 3090.6186 | | 3822.0607 |
| Zero-point correction (Hartree): | 0.156652 | | | |

C5H11O2.ptppp

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.52802140
Electronic state : 2-A
Cartesian coordinates (Angs):

| | | | | |
|---|-----------|-----------|-----------|--|
| O | 2.578813 | 1.087932 | -0.300381 | |
| C | 2.423416 | -0.151225 | 0.261510 | |
| C | 0.978535 | -0.560945 | 0.574898 | |
| C | 0.077752 | -0.539616 | -0.665253 | |
| C | -1.371020 | -0.981082 | -0.408196 | |
| C | -2.173166 | -0.044453 | 0.501756 | |
| O | -2.195155 | 1.301660 | 0.043275 | |
| H | -2.603382 | 1.307861 | -0.832515 | |
| H | 2.867883 | -0.852138 | -0.480623 | |
| H | 3.083562 | -0.253179 | 1.145245 | |
| H | 0.992603 | -1.563887 | 1.024770 | |

| | | | | |
|--|-----------|-----------|-----------|-----------|
| H | 0.590137 | 0.122723 | 1.338978 | |
| H | 0.080022 | 0.474534 | -1.077131 | |
| H | 0.512585 | -1.193357 | -1.433957 | |
| H | -1.894172 | -1.062757 | -1.372379 | |
| H | -1.389986 | -1.989325 | 0.029744 | |
| H | -3.193848 | -0.441346 | 0.625306 | |
| H | -1.727770 | -0.001944 | 1.501133 | |
| Rotational constants (GHz): | 4.7533600 | | 1.2051700 | 1.0828900 |
| Vibrational harmonic frequencies (cm-1): | | | | |
| 42.5638 | | 60.0974 | | 134.4180 |
| 184.9346 | | 231.9395 | | 263.4215 |
| 323.3966 | | 370.3488 | | 491.9915 |
| 509.4265 | | 559.7059 | | 746.8421 |
| 828.1112 | | 856.7075 | | 913.1192 |
| 949.2593 | | 1015.0637 | | 1045.8225 |
| 1087.3356 | | 1095.8587 | | 1109.5468 |
| 1151.7318 | | 1168.5384 | | 1235.3202 |
| 1303.7484 | | 1312.2070 | | 1344.7399 |
| 1365.5872 | | 1367.9952 | | 1381.4281 |
| 1403.5290 | | 1418.4532 | | 1431.7663 |
| 1492.3701 | | 1496.8113 | | 1508.5590 |
| 1526.5166 | | 2878.8079 | | 2935.6424 |
| 2988.4898 | | 3012.6410 | | 3028.7804 |
| 3032.1362 | | 3048.3489 | | 3079.5870 |
| 3094.2018 | | 3106.1400 | | 3810.2826 |
| Zero-point correction (Hartree): | 0.156611 | | | |

C5H11O2.ptppt

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.52728202
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | | |
|--|-----------|-----------|-----------|-----------|
| O | 2.530995 | 1.173125 | -0.209239 | |
| C | 2.445148 | -0.131951 | 0.197773 | |
| C | 1.034183 | -0.627761 | 0.536496 | |
| C | 0.078289 | -0.550891 | -0.660028 | |
| C | -1.361107 | -0.995732 | -0.355789 | |
| C | -2.148677 | -0.028729 | 0.524145 | |
| O | -2.267937 | 1.204245 | -0.176408 | |
| H | -2.673024 | 1.851303 | 0.413331 | |
| H | 2.872063 | -0.724549 | -0.641958 | |
| H | 3.157796 | -0.309657 | 1.027702 | |
| H | 1.106289 | -1.661302 | 0.904077 | |
| H | 0.656630 | -0.024230 | 1.371119 | |
| H | 0.063500 | 0.476742 | -1.036595 | |
| H | 0.476350 | -1.178335 | -1.469399 | |
| H | -1.910693 | -1.106859 | -1.298246 | |
| H | -1.360809 | -1.982519 | 0.127367 | |
| H | -3.139551 | -0.460435 | 0.740589 | |
| H | -1.640033 | 0.111275 | 1.491595 | |
| Rotational constants (GHz): | 4.7413300 | | 1.2035500 | 1.0706300 |
| Vibrational harmonic frequencies (cm-1): | | | | |
| 33.8099 | | 59.0894 | | 134.2098 |
| 174.0812 | | 235.4537 | | 250.1102 |
| 275.7436 | | 376.6669 | | 446.6168 |
| 479.4058 | | 550.0085 | | 755.3317 |
| 818.1159 | | 865.9736 | | 917.5344 |
| 952.9259 | | 1028.1204 | | 1053.8169 |
| 1073.9384 | | 1096.1997 | | 1115.2331 |
| 1165.7972 | | 1180.7335 | | 1251.2364 |
| 1266.6134 | | 1315.0249 | | 1320.6042 |
| 1347.5122 | | 1362.2801 | | 1375.5361 |
| 1400.3315 | | 1415.1092 | | 1461.9842 |
| 1489.7128 | | 1494.0200 | | 1511.7194 |
| 1537.9404 | | 2882.6214 | | 2930.5615 |
| 2977.8707 | | 3003.4107 | | 3026.1692 |
| 3029.2496 | | 3037.4706 | | 3074.4553 |
| 3080.4207 | | 3108.8344 | | 3834.0472 |
| Zero-point correction (Hartree): | 0.156222 | | | |

C5H11O2.ptptm

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.52780165
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | | |
|---|-----------|-----------|-----------|--|
| O | -2.893020 | -0.811693 | -0.620455 | |
| C | -2.588987 | 0.062001 | 0.390219 | |
| C | -1.096896 | 0.194712 | 0.718003 | |
| C | -0.273139 | 0.667791 | -0.486885 | |
| C | 1.237466 | 0.778568 | -0.228250 | |
| C | 1.942088 | -0.564138 | -0.011928 | |
| O | 3.335665 | -0.417939 | 0.228539 | |
| H | 3.724340 | -0.000372 | -0.551113 | |
| H | -3.001690 | 1.040777 | 0.058177 | |
| H | -3.191194 | -0.181908 | 1.287496 | |

| | | | | |
|--|-----------|-----------|-----------|--|
| H | -0.980949 | 0.893774 | 1.557645 | |
| H | -0.740576 | -0.780159 | 1.071760 | |
| H | -0.460827 | -0.015941 | -1.324439 | |
| H | -0.648884 | 1.649459 | -0.806212 | |
| H | 1.706577 | 1.276691 | -1.089257 | |
| H | 1.431416 | 1.418807 | 0.641892 | |
| H | 1.548215 | -1.070587 | 0.874726 | |
| H | 1.749221 | -1.227096 | -0.872292 | |
| Rotational constants (GHz): | 7.0907600 | 0.9243200 | 0.9035900 | |
| Vibrational harmonic frequencies (cm-1): | | | | |
| 47.5597 | 81.6649 | | 119.3692 | |
| 142.1355 | 237.0713 | | 271.5070 | |
| 300.0710 | 340.4705 | | 451.3994 | |
| 464.8487 | 578.1195 | | 759.8171 | |
| 789.4942 | 882.6504 | | 899.1045 | |
| 982.8082 | 1014.9838 | | 1059.6188 | |
| 1085.2041 | 1096.3906 | | 1114.5836 | |
| 1151.2767 | 1172.7482 | | 1249.4207 | |
| 1308.6526 | 1316.4823 | | 1343.0590 | |
| 1354.5482 | 1362.1017 | | 1376.5941 | |
| 1398.5433 | 1419.9650 | | 1439.7661 | |
| 1495.0163 | 1501.6248 | | 1514.0166 | |
| 1529.7126 | 2883.0538 | | 2936.4210 | |
| 2979.8682 | 3015.1325 | | 3030.1295 | |
| 3036.2608 | 3060.6438 | | 3070.8090 | |
| 3089.2970 | 3099.8179 | | 3811.9817 | |
| Zero-point correction (Hartree): | 0.156432 | | | |

C5H11O2.ptptp

```
-----
E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.52746829
Electronic state : 2-A
Cartesian coordinates (Angs):
O      -2.900115      -0.870682      -0.524366
C      -2.590343      0.104582      0.386522
C      -1.096926      0.263848      0.696320
C      -0.274660      0.614222      -0.551203
C      1.237832      0.747783      -0.313739
C      1.948270      -0.566776      0.022383
O      3.360037      -0.415990      0.110477
H      3.544561      0.191619      0.838363
H      -2.996858      1.044309      -0.049698
H      -3.192902      -0.037239      1.305223
H      -0.977893      1.042563      1.462618
H      -0.741782      -0.672312      1.143311
H      -0.464676      -0.147957      -1.317235
H      -0.650198      1.560210      -0.964523
H      1.714381      1.159488      -1.211209
H      1.420930      1.472488      0.494647
H      1.541677      -1.006931      0.946651

H      1.778344      -1.294810      -0.778739
Rotational constants (GHz): 7.1134100 0.9215400 0.8992700
Vibrational harmonic frequencies (cm-1):
49.4675      83.4503      119.3844
142.5086      236.5790      270.1919
303.4073      327.9021      450.0046
457.1670      575.0448      762.7253
790.5660      881.8918      897.7334
976.7046      1024.9520      1064.5615
1082.0899      1095.7901      1106.9892
1146.7494      1174.1235      1261.3808
1298.4876      1323.5288      1332.9238
1358.5708      1363.3969      1374.4290
1401.8776      1417.7981      1437.8789
1495.5210      1503.3208      1513.6926
1529.9535      2882.9087      2936.0763
2995.0595      3008.4335      3028.0758
3033.5015      3068.7256      3071.9217
3088.6699      3090.6311      3813.7956
Zero-point correction (Hartree): 0.156397
```

C5H11O2.ptptt

```
-----
E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.52711262
Electronic state : 2-A
Cartesian coordinates (Angs):
O      -2.890356      -0.847881      -0.584823
C      -2.589305      0.070322      0.386698
C      -1.098359      0.217665      0.712275
C      -0.273511      0.658653      -0.504278
C      1.236629      0.779583      -0.252991
C      1.940791      -0.551440      -0.009565
O      3.330125      -0.281177      0.139197
H      3.782863      -1.117591      0.302399
```

| | | | |
|--|-----------|-----------|-----------|
| H | -3.000890 | 1.033460 | 0.010526 |
| H | -3.194760 | -0.133865 | 1.291815 |
| H | -0.985781 | 0.941425 | 1.531292 |
| H | -0.739564 | -0.745343 | 1.095219 |
| H | -0.462435 | -0.045199 | -1.324774 |
| H | -0.649283 | 1.632185 | -0.847564 |
| H | 1.714916 | 1.251124 | -1.119561 |
| H | 1.429688 | 1.437846 | 0.603838 |
| H | 1.537294 | -1.043150 | 0.889883 |
| H | 1.752329 | -1.227118 | -0.860898 |
| Rotational constants (GHz): | 7.1624200 | 0.9268400 | 0.9035800 |
| Vibrational harmonic frequencies (cm-1): | | | |
| 48.0377 | 76.2160 | | 119.5527 |
| 141.6623 | 237.4751 | | 275.2967 |
| 280.2503 | 312.6217 | | 443.8225 |
| 451.1461 | 577.0605 | | 765.8353 |
| 796.5404 | 885.2861 | | 897.5127 |
| 983.6438 | 1015.7474 | | 1070.7576 |
| 1078.0712 | 1096.6913 | | 1130.8012 |
| 1144.3846 | 1212.0163 | | 1248.0653 |
| 1278.3246 | 1315.1998 | | 1324.0814 |
| 1339.7875 | 1361.3051 | | 1369.7796 |
| 1377.7545 | 1417.8114 | | 1472.1739 |
| 1495.1041 | 1508.2316 | | 1515.1362 |
| 1543.0449 | 2883.3306 | | 2934.5743 |
| 2973.1617 | 3003.2716 | | 3027.1808 |
| 3035.4755 | 3042.6945 | | 3066.4749 |
| 3086.0215 | 3090.4054 | | 3828.1970 |
| Zero-point correction (Hartree): | 0.156230 | | |

C5H11O2.pttmm

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.52940871
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | |
|--|-----------|-----------|-----------|
| O | -2.668225 | 1.212223 | -0.157967 |
| C | -2.593983 | -0.104733 | 0.211970 |
| C | -1.335451 | -0.847261 | -0.253102 |
| C | -0.045953 | -0.227133 | 0.293642 |
| C | 1.228046 | -0.873518 | -0.260632 |
| C | 2.513857 | -0.216391 | 0.248742 |
| O | 2.591532 | 1.172707 | -0.048142 |
| H | 2.577118 | 1.268526 | -1.009532 |
| H | -2.649391 | -0.095200 | 1.323286 |
| H | -3.521832 | -0.629851 | -0.089538 |
| H | -1.417327 | -1.900972 | 0.048062 |
| H | -1.318914 | -0.837707 | -1.351067 |
| H | -0.037719 | 0.842836 | 0.061873 |
| H | -0.040585 | -0.303526 | 1.390963 |
| H | 1.257758 | -1.942115 | -0.004583 |
| H | 1.215116 | -0.827915 | -1.360668 |
| H | 2.560799 | -0.282078 | 1.341779 |
| H | 3.389433 | -0.757219 | -0.145426 |
| Rotational constants (GHz): | 5.5391800 | 1.0456200 | 0.9267300 |
| Vibrational harmonic frequencies (cm-1): | | | |
| 62.4271 | 72.0794 | | 140.0912 |
| 162.4371 | 191.1470 | | 305.2856 |
| 312.0489 | 336.4390 | | 456.6564 |
| 519.3681 | 522.5822 | | 755.6989 |
| 823.4238 | 883.8318 | | 920.4215 |
| 938.9332 | 1009.4903 | | 1065.7018 |
| 1091.7951 | 1094.3013 | | 1106.4102 |
| 1120.5427 | 1200.2267 | | 1239.5041 |
| 1299.9757 | 1310.2807 | | 1331.4183 |
| 1361.6316 | 1366.1995 | | 1385.3044 |
| 1396.9887 | 1420.7420 | | 1427.9729 |
| 1494.5606 | 1496.2616 | | 1521.7853 |
| 1522.1867 | 2885.5118 | | 2934.2658 |
| 2987.7594 | 3007.4218 | | 3020.6707 |
| 3028.5828 | 3046.8889 | | 3066.4882 |
| 3082.1075 | 3103.7373 | | 3810.3505 |
| Zero-point correction (Hartree): | 0.156373 | | |

C5H11O2.pttmp

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.52917571
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -2.666235 | 1.209282 | -0.163418 |
| C | -2.602512 | -0.108148 | 0.205844 |
| C | -1.339474 | -0.855986 | -0.239921 |
| C | -0.051246 | -0.203506 | 0.272011 |
| C | 1.225853 | -0.875318 | -0.246808 |
| C | 2.513521 | -0.216976 | 0.258232 |
| O | 2.687558 | 1.114961 | -0.208503 |

| | | | | |
|--|-----------|-----------|-----------|--|
| H | 2.003379 | 1.663908 | 0.194101 | |
| H | -2.666396 | -0.091121 | 1.317184 | |
| H | -3.527170 | -0.634960 | -0.100742 | |
| H | -1.407952 | -1.896692 | 0.104936 | |
| H | -1.326177 | -0.889824 | -1.336883 | |
| H | -0.069459 | 0.851102 | -0.030391 | |
| H | -0.049975 | -0.215897 | 1.372579 | |
| H | 1.235255 | -1.932498 | 0.053636 | |
| H | 1.232805 | -0.855690 | -1.344035 | |
| H | 2.546855 | -0.259918 | 1.360139 | |
| H | 3.381399 | -0.772745 | -0.111309 | |
| Rotational constants (GHz): | 5.6335700 | 1.0346300 | 0.9182000 | |
| Vibrational harmonic frequencies (cm-1): | | | | |
| 62.8431 | 73.5022 | | 128.8266 | |
| 163.1167 | 186.5461 | | 300.5358 | |
| 308.7985 | 336.4067 | | 495.6398 | |
| 512.7296 | 552.0473 | | 753.8188 | |
| 826.7869 | 873.4312 | | 920.9572 | |
| 945.6545 | 1015.7719 | | 1057.3331 | |
| 1091.4262 | 1094.5348 | | 1101.0834 | |
| 1156.1768 | 1201.7299 | | 1224.6006 | |
| 1297.3384 | 1310.4966 | | 1338.0246 | |
| 1355.6903 | 1366.4000 | | 1390.2944 | |
| 1395.0194 | 1421.0050 | | 1427.2304 | |
| 1489.5352 | 1495.3329 | | 1518.4226 | |
| 1519.0084 | 2879.8911 | | 2939.8632 | |
| 2978.3538 | 3010.1980 | | 3026.0045 | |
| 3033.8408 | 3059.2076 | | 3072.8091 | |
| 3086.2821 | 3091.9455 | | 3828.9050 | |
| Zero-point correction (Hartree): | 0.156545 | | | |

C5H11O2.pttmt

```

-----
E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.52860681
Electronic state : 2-A
Cartesian coordinates (Angs):
O      -2.689562      1.211167      -0.147499
C      -2.602217      -0.108199      0.210399
C      -1.336501      -0.836894      -0.256768
C      -0.050589      -0.201485      0.280835
C      1.222815      -0.872774      -0.246144
C      2.505389      -0.224244      0.262366
O      2.549434      1.113605      -0.221004
H      3.325354      1.546282      0.155086
H      -2.656945      -0.105611      1.322099
H      -3.524560      -0.641537      -0.093742
H      -1.406759      -1.889772      0.051120
H      -1.322884      -0.833506      -1.354567
H      -0.037915      0.859387      0.013058
H      -0.054960      -0.246636      1.380443
H      1.237898      -1.933864      0.038223
H      1.232442      -0.839651      -1.343282
H      2.520606      -0.249501      1.365215
H      3.375368      -0.802198      -0.089758
Rotational constants (GHz): 5.6714200 1.0413700 0.9254600
Vibrational harmonic frequencies (cm-1):
59.7168      74.0481      135.1001
161.0051      188.2576      265.5546
311.0045      327.5251      462.3467
502.6284      522.0317      753.6866
826.0359      893.7547      916.9172
952.1076      1019.2557      1071.6818
1075.6279      1095.5612      1114.4095
1159.7770      1197.9796      1255.3764
1268.7461      1307.8813      1320.7099
1338.8456      1361.4533      1365.5982
1394.8358      1421.9788      1462.3204
1490.6250      1495.7114      1521.1158
1537.2024      2881.7785      2933.4169
2969.9659      2998.4646      3013.2292
3025.5382      3033.3627      3067.8380
3072.5276      3110.9758      3833.2786
Zero-point correction (Hartree): 0.156211

```

C5H11O2.pttpm

```

-----
E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.52916744
Electronic state : 2-A
Cartesian coordinates (Angs):
O      -2.856616      -0.835917      0.671820
C      -2.569396      -0.061031      -0.420944
C      -1.314984      0.812301      -0.296553
C      -0.048028      -0.002311      -0.015835
C      1.198818      0.862111      0.203740
C      2.461906      0.052728      0.511825

```


| | | | | |
|---|-----------|-----------|-----------|--|
| O | 2.863169 | -0.796190 | -0.558340 | |
| H | 2.239455 | -1.530951 | -0.604874 | |
| H | -2.454151 | -0.784795 | -1.258719 | |
| H | -3.460434 | 0.530340 | -0.709211 | |
| H | -1.199488 | 1.396111 | -1.219727 | |
| H | -1.477104 | 1.536270 | 0.512717 | |
| H | -0.230130 | -0.630177 | 0.866234 | |
| H | 0.128226 | -0.685584 | -0.859357 | |
| H | 1.386193 | 1.475930 | -0.686810 | |
| H | 1.022072 | 1.556576 | 1.037030 | |
| H | 3.303642 | 0.732591 | 0.679836 | |
| H | 2.319404 | -0.522248 | 1.441644 | |
| Rotational constants (GHz): | 6.2603100 | 0.9593800 | 0.9184400 | |
| Vibrational harmonic frequencies (cm ⁻¹): | | | | |
| 54.0898 | 85.6041 | | 113.1529 | |
| 155.1699 | 197.2279 | | 297.6289 | |
| 311.5029 | 324.6124 | | 494.6347 | |
| 503.5805 | 539.8224 | | 753.9365 | |
| 831.3020 | 880.5427 | | 898.0953 | |
| 965.6396 | 1003.3259 | | 1055.4167 | |
| 1089.9421 | 1096.0014 | | 1105.2975 | |
| 1161.1427 | 1181.4178 | | 1245.2356 | |
| 1284.6717 | 1319.0992 | | 1335.5533 | |
| 1358.6152 | 1364.7630 | | 1391.5210 | |
| 1398.1605 | 1419.5146 | | 1424.8436 | |
| 1489.0108 | 1495.2646 | | 1517.8271 | |
| 1519.1062 | 2881.5081 | | 2938.9368 | |
| 2987.2915 | 3014.5265 | | 3026.1460 | |
| 3034.7317 | 3055.1276 | | 3070.7124 | |
| 3084.9301 | 3091.1301 | | 3831.3439 | |
| Zero-point correction (Hartree): | 0.156461 | | | |

C5H11O2.pttpp

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.52957032

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | | |
|---|-----------|-----------|-----------|--|
| O | 2.906545 | -0.760661 | -0.685071 | |
| C | 2.556497 | -0.085451 | 0.454452 | |
| C | 1.297880 | 0.783521 | 0.341437 | |
| C | 0.050383 | -0.027920 | -0.021048 | |
| C | -1.191413 | 0.834122 | -0.271148 | |
| C | -2.454503 | 0.010971 | -0.537821 | |
| O | -2.797034 | -0.855192 | 0.539326 | |
| H | -3.007792 | -0.301677 | 1.302698 | |
| H | 2.408521 | -0.878696 | 1.220879 | |
| H | 3.425411 | 0.486798 | 0.834744 | |
| H | 1.150557 | 1.313426 | 1.292828 | |
| H | 1.480159 | 1.554029 | -0.419490 | |
| H | 0.270825 | -0.622013 | -0.916905 | |
| H | -0.174276 | -0.745576 | 0.777870 | |
| H | -1.371087 | 1.491298 | 0.594204 | |
| H | -1.021699 | 1.502487 | -1.126808 | |
| H | -3.291942 | 0.681411 | -0.788702 | |
| H | -2.297819 | -0.646119 | -1.400591 | |
| Rotational constants (GHz): | 6.3201900 | 0.9541400 | 0.9251700 | |
| Vibrational harmonic frequencies (cm ⁻¹): | | | | |
| 57.6472 | 84.8250 | | 117.1002 | |
| 165.9079 | 193.4727 | | 303.5408 | |
| 318.8597 | 334.8688 | | 488.1039 | |
| 513.8383 | 532.7118 | | 753.7650 | |
| 832.2826 | 884.4171 | | 900.2594 | |
| 963.7069 | 998.4116 | | 1068.8218 | |
| 1085.8146 | 1093.0514 | | 1098.7891 | |
| 1141.2501 | 1183.3659 | | 1256.7878 | |
| 1278.3143 | 1321.8801 | | 1331.0025 | |
| 1358.5797 | 1365.4854 | | 1387.4444 | |
| 1396.4213 | 1419.3244 | | 1425.1919 | |
| 1494.0802 | 1496.2062 | | 1520.7197 | |
| 1521.6183 | 2884.3674 | | 2936.4468 | |
| 2990.8890 | 3005.6667 | | 3027.1004 | |
| 3042.5474 | 3047.8972 | | 3062.9395 | |
| 3084.0863 | 3092.1855 | | 3809.8476 | |
| Zero-point correction (Hartree): | 0.156446 | | | |

C5H11O2.pttpt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.52920615

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | | |
|---|-----------|-----------|-----------|--|
| O | -2.896987 | -0.778013 | 0.692853 | |
| C | -2.561261 | -0.089615 | -0.443181 | |
| C | -1.304845 | 0.783017 | -0.336621 | |
| C | -0.050800 | -0.025354 | 0.010541 | |
| C | 1.189821 | 0.846282 | 0.235595 | |

| | | | |
|--|-----------|-----------|-----------|
| C | 2.449802 | 0.039411 | 0.528029 |
| O | 2.747138 | -0.753345 | -0.617618 |
| H | 3.498713 | -1.319824 | -0.405499 |
| H | -2.417409 | -0.875395 | -1.218281 |
| H | -3.436357 | 0.482201 | -0.809912 |
| H | -1.167344 | 1.316344 | -1.287232 |
| H | -1.483023 | 1.549695 | 0.429303 |
| H | -0.257375 | -0.614787 | 0.913110 |
| H | 0.162438 | -0.742851 | -0.790837 |
| H | 1.377489 | 1.467085 | -0.650346 |
| H | 1.018745 | 1.534597 | 1.074137 |
| H | 3.281164 | 0.724205 | 0.761092 |
| H | 2.285458 | -0.592852 | 1.416394 |
| Rotational constants (GHz): | 6.3869300 | 0.9584300 | 0.9285900 |
| Vibrational harmonic frequencies (cm-1): | | | |
| 57.4318 | 83.3890 | | 117.1772 |
| 161.2302 | 193.5918 | | 264.3010 |
| 314.4912 | 323.5321 | | 489.5807 |
| 499.7875 | 532.9239 | | 752.8289 |
| 832.2118 | 894.9495 | | 905.5517 |
| 974.8824 | 998.2112 | | 1068.4524 |
| 1085.4615 | 1095.0365 | | 1125.0379 |
| 1143.9271 | 1205.0183 | | 1247.9755 |
| 1279.3668 | 1296.6139 | | 1326.8356 |
| 1339.0548 | 1358.2153 | | 1365.2073 |
| 1394.2961 | 1420.5479 | | 1460.6665 |
| 1489.7628 | 1496.2126 | | 1520.6437 |
| 1536.2682 | 2882.5348 | | 2935.4442 |
| 2974.0724 | 3002.6240 | | 3027.8405 |
| 3032.5748 | 3044.4089 | | 3062.3560 |
| 3069.6211 | 3096.0754 | | 3832.3752 |
| Zero-point correction (Hartree): | 0.156306 | | |

C5H11O2.ptttm

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.52905966
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | |
|--|-----------|-----------|-----------|
| O | 3.042231 | -0.957057 | -0.352491 |
| C | 2.748397 | 0.247285 | 0.230278 |
| C | 1.372354 | 0.828305 | -0.118011 |
| C | 0.219360 | -0.104491 | 0.267949 |
| C | -1.156000 | 0.412436 | -0.169406 |
| C | -2.300625 | -0.522068 | 0.228040 |
| O | -3.569418 | -0.072199 | -0.228610 |
| H | -3.744558 | 0.781396 | 0.188237 |
| H | 2.821675 | 0.058310 | 1.324726 |
| H | 3.565322 | 0.969547 | 0.035508 |
| H | 1.265346 | 1.800954 | 0.381557 |
| H | 1.344516 | 1.026253 | -1.197297 |
| H | 0.407673 | -1.087627 | -0.180740 |
| H | 0.225874 | -0.256795 | 1.357351 |
| H | -1.334542 | 1.404598 | 0.273045 |
| H | -1.181058 | 0.548577 | -1.257798 |
| H | -2.154798 | -1.506659 | -0.229669 |
| H | -2.298872 | -0.673304 | 1.320788 |
| Rotational constants (GHz): | 9.1281500 | 0.8268500 | 0.7917400 |
| Vibrational harmonic frequencies (cm-1): | | | |
| 65.7631 | 81.2696 | | 119.9662 |
| 155.3962 | 163.3890 | | 263.4490 |
| 318.8373 | 354.2538 | | 437.3844 |
| 484.3987 | 555.6787 | | 751.5431 |
| 797.4841 | 892.3975 | | 927.9613 |
| 991.3721 | 1033.2517 | | 1053.3198 |
| 1084.9570 | 1095.8689 | | 1096.2665 |
| 1149.2509 | 1191.5982 | | 1265.6982 |
| 1277.8841 | 1327.7717 | | 1332.5886 |
| 1343.2564 | 1364.5084 | | 1374.7517 |
| 1399.9974 | 1419.4043 | | 1434.5928 |
| 1494.6303 | 1503.7115 | | 1516.4155 |
| 1532.0123 | 2881.8617 | | 2937.7232 |
| 2977.8241 | 3008.1063 | | 3017.0652 |
| 3031.6936 | 3063.2242 | | 3067.6845 |
| 3081.9864 | 3093.2504 | | 3813.6829 |
| Zero-point correction (Hartree): | 0.156342 | | |

C5H11O2.ptttp

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.52921449
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | |
|---|----------|-----------|-----------|
| O | 3.033249 | -0.956922 | -0.384555 |
| C | 2.749729 | 0.235700 | 0.226895 |
| C | 1.374376 | 0.830846 | -0.099395 |
| C | 0.219545 | -0.102983 | 0.278538 |

| | | | |
|---|-----------|-----------|-----------|
| C | -1.156231 | 0.427171 | -0.141175 |
| C | -2.301002 | -0.516037 | 0.234834 |
| O | -3.581135 | 0.001343 | -0.103788 |
| H | -3.611062 | 0.101676 | -1.064032 |
| H | 2.829579 | 0.022804 | 1.316434 |
| H | 3.569230 | 0.957701 | 0.042229 |
| H | 1.275917 | 1.794486 | 0.418566 |
| H | 1.339976 | 1.048741 | -1.174827 |
| H | 0.402791 | -1.080944 | -0.183882 |
| H | 0.229857 | -0.269522 | 1.365615 |
| H | -1.347059 | 1.404970 | 0.319098 |
| H | -1.167775 | 0.587683 | -1.229878 |
| H | -2.134865 | -1.506390 | -0.221016 |
| H | -2.322003 | -0.664743 | 1.320244 |

Rotational constants (GHz): 9.1238000 0.8261400 0.7926600

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 63.0860 | 80.2574 | 120.5455 |
| 153.8027 | 163.7386 | 262.6888 |
| 317.6688 | 353.9816 | 437.4812 |
| 483.7655 | 555.6070 | 751.1534 |
| 797.3039 | 893.4779 | 925.6570 |
| 995.4725 | 1026.5270 | 1052.9571 |
| 1084.6416 | 1094.6889 | 1113.4423 |
| 1129.2379 | 1199.7616 | 1255.3678 |
| 1288.9819 | 1321.6968 | 1332.8341 |
| 1345.9803 | 1363.7868 | 1374.3461 |
| 1398.8697 | 1419.4928 | 1434.8932 |
| 1494.4919 | 1503.8693 | 1516.3021 |
| 1531.8502 | 2882.4757 | 2937.7124 |
| 2982.5796 | 3010.5281 | 3020.7949 |
| 3033.3177 | 3057.6278 | 3067.3149 |
| 3080.6820 | 3091.3353 | 3813.9794 |

Zero-point correction (Hartree): 0.156323

C5H11O2.ptttt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.52858389

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 3.038218 | -0.957001 | -0.376426 |
| C | 2.748936 | 0.235851 | 0.232040 |
| C | 1.373318 | 0.827494 | -0.098797 |
| C | 0.218663 | -0.109785 | 0.270966 |
| C | -1.153625 | 0.427100 | -0.149117 |
| C | -2.295763 | -0.513392 | 0.214686 |
| O | -3.512134 | 0.087145 | -0.214089 |
| H | -4.236194 | -0.512347 | 0.003869 |
| H | 2.824487 | 0.022397 | 1.321973 |
| H | 3.567198 | 0.960230 | 0.051218 |
| H | 1.270401 | 1.789332 | 0.421770 |
| H | 1.342068 | 1.048943 | -1.173443 |
| H | 0.403182 | -1.083483 | -0.199832 |
| H | 0.229412 | -0.285237 | 1.356883 |
| H | -1.343600 | 1.399608 | 0.322740 |
| H | -1.177004 | 0.596251 | -1.232964 |
| H | -2.138656 | -1.491186 | -0.270538 |
| H | -2.299131 | -0.689269 | 1.303780 |

Rotational constants (GHz): 9.2172400 0.8311900 0.7961000

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 62.6553 | 80.6298 | 121.4177 |
| 148.3649 | 163.4195 | 264.9824 |
| 274.8224 | 357.9054 | 434.6181 |
| 489.8430 | 555.2781 | 754.3252 |
| 806.0516 | 896.0590 | 932.2546 |
| 998.0391 | 1019.8669 | 1057.6992 |
| 1079.0604 | 1095.1342 | 1111.5905 |
| 1181.4610 | 1209.2080 | 1243.7934 |
| 1281.0005 | 1301.3804 | 1324.4129 |
| 1333.1468 | 1351.2717 | 1364.8325 |
| 1381.3066 | 1419.5263 | 1470.7855 |
| 1494.9105 | 1507.9313 | 1521.1361 |
| 1543.7586 | 2880.2517 | 2937.5466 |
| 2967.8007 | 2994.9056 | 3016.0313 |
| 3032.0706 | 3041.7592 | 3061.7722 |
| 3075.4934 | 3092.3169 | 3828.8277 |

Zero-point correction (Hartree): 0.156197

C5H11O2.tpmmm

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.52672677

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -2.718262 | -0.745685 | -0.372969 |
| C | -1.640508 | -0.302345 | 0.333280 |

| | | | | |
|--|-----------|-----------|-----------|--|
| C | -1.002402 | 1.001585 | -0.181653 | |
| C | 0.341242 | 1.333497 | 0.499547 | |
| C | 1.596441 | 0.864348 | -0.260402 | |
| C | 1.636202 | -0.623203 | -0.619373 | |
| O | 1.386201 | -1.487328 | 0.487240 | |
| H | 2.038764 | -1.294953 | 1.173435 | |
| H | -1.874253 | -0.229257 | 1.415516 | |
| H | -0.900695 | -1.133098 | 0.297618 | |
| H | -0.885518 | 0.925202 | -1.269732 | |
| H | -1.719823 | 1.812219 | -0.008940 | |
| H | 0.426035 | 2.416787 | 0.640683 | |
| H | 0.349409 | 0.901432 | 1.508949 | |
| H | 1.695212 | 1.433548 | -1.194893 | |
| H | 2.484930 | 1.112855 | 0.338464 | |
| H | 0.856246 | -0.861847 | -1.349542 | |
| H | 2.600331 | -0.862083 | -1.094120 | |
| Rotational constants (GHz): | 3.6237700 | 1.6042300 | 1.2716300 | |
| Vibrational harmonic frequencies (cm-1): | | | | |
| 76.4214 | 95.1471 | | 134.5346 | |
| 184.2109 | 230.4567 | | 287.3223 | |
| 314.6513 | 359.1415 | | 461.6488 | |
| 550.5575 | 673.9100 | | 756.5807 | |
| 814.9989 | 891.8555 | | 905.3593 | |
| 992.0537 | 1002.5364 | | 1056.4475 | |
| 1092.3658 | 1098.5731 | | 1112.8011 | |
| 1129.6924 | 1202.3998 | | 1224.8832 | |
| 1273.8207 | 1314.1791 | | 1340.4252 | |
| 1365.5482 | 1374.4855 | | 1374.9800 | |
| 1395.2371 | 1404.1973 | | 1435.7256 | |
| 1493.0630 | 1505.9125 | | 1507.3578 | |
| 1530.4790 | 2883.6343 | | 2916.4716 | |
| 3002.6303 | 3018.6170 | | 3035.5065 | |
| 3045.7428 | 3056.5427 | | 3079.4667 | |
| 3087.9975 | 3096.9850 | | 3810.8955 | |
| Zero-point correction (Hartree): | 0.157190 | | | |

C5H11O2.tpmmp

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.52332728

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | | |
|--|-----------|-----------|-----------|--|
| O | -2.870566 | -0.740741 | -0.294971 | |
| C | -1.622076 | -0.467565 | 0.191772 | |
| C | -1.110409 | 0.956037 | -0.080528 | |
| C | 0.265816 | 1.280653 | 0.535244 | |
| C | 1.498643 | 0.934870 | -0.321790 | |
| C | 1.710110 | -0.550684 | -0.629849 | |
| O | 1.866533 | -1.358294 | 0.530418 | |
| H | 1.066656 | -1.280654 | 1.065019 | |
| H | -1.583265 | -0.708537 | 1.275376 | |
| H | -0.965836 | -1.236489 | -0.269809 | |
| H | -1.098381 | 1.125164 | -1.164226 | |
| H | -1.861876 | 1.641201 | 0.328619 | |
| H | 0.306932 | 2.354627 | 0.747648 | |
| H | 0.353454 | 0.797549 | 1.520377 | |
| H | 1.433424 | 1.474690 | -1.276479 | |
| H | 2.393134 | 1.307570 | 0.191927 | |
| H | 0.897930 | -0.927473 | -1.273399 | |
| H | 2.637585 | -0.675245 | -1.197724 | |
| Rotational constants (GHz): | 3.8153800 | 1.4451500 | 1.1844900 | |
| Vibrational harmonic frequencies (cm-1): | | | | |
| 45.2202 | 76.3827 | | 104.8647 | |
| 191.7195 | 216.5117 | | 266.3821 | |
| 294.7784 | 373.1942 | | 437.3082 | |
| 484.4713 | 532.1842 | | 763.1965 | |
| 798.9243 | 848.7818 | | 895.4759 | |
| 990.0514 | 1023.4845 | | 1044.4728 | |
| 1075.8688 | 1089.9628 | | 1112.3123 | |
| 1162.0720 | 1189.3761 | | 1227.0016 | |
| 1297.3261 | 1299.4197 | | 1336.9836 | |
| 1376.7416 | 1377.8129 | | 1390.1115 | |
| 1395.6964 | 1399.9369 | | 1433.0713 | |
| 1488.8024 | 1501.1407 | | 1508.9383 | |
| 1528.4172 | 2893.6096 | | 2911.4502 | |
| 2983.5746 | 3012.0367 | | 3032.1710 | |
| 3047.4459 | 3077.6043 | | 3079.9019 | |
| 3091.6095 | 3094.5384 | | 3825.4809 | |
| Zero-point correction (Hartree): | 0.156346 | | | |

C5H11O2.tpmmt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.52653030

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | | |
|---|----------|-----------|----------|--|
| O | 2.660509 | -0.782451 | 0.393164 | |
|---|----------|-----------|----------|--|

| | | | | |
|--|-----------|-----------|-----------|-----------|
| C | 1.631804 | -0.277733 | -0.343048 | |
| C | 1.000119 | 1.022308 | 0.188974 | |
| C | -0.344856 | 1.359543 | -0.486379 | |
| C | -1.598287 | 0.856267 | 0.255978 | |
| C | -1.613333 | -0.629146 | 0.601811 | |
| O | -1.403143 | -1.383781 | -0.593109 | |
| H | -1.489520 | -2.320886 | -0.377247 | |
| H | 1.912163 | -0.176061 | -1.411587 | |
| H | 0.862470 | -1.083192 | -0.368963 | |
| H | 0.885581 | 0.931148 | 1.276264 | |
| H | 1.717789 | 1.834734 | 0.025032 | |
| H | -0.441285 | 2.445933 | -0.593139 | |
| H | -0.350005 | 0.956297 | -1.506590 | |
| H | -1.712244 | 1.408914 | 1.198171 | |
| H | -2.482641 | 1.083060 | -0.351632 | |
| H | -0.832932 | -0.853565 | 1.345752 | |
| H | -2.580994 | -0.883963 | 1.059482 | |
| Rotational constants (GHz): | 3.5860500 | | 1.6400100 | 1.2914600 |
| Vibrational harmonic frequencies (cm-1): | | | | |
| 72.5298 | | 99.8247 | | 145.1984 |
| 183.8658 | | 243.4481 | | 291.2963 |
| 336.0081 | | 367.3454 | | 456.5951 |
| 541.7088 | | 681.7532 | | 763.4423 |
| 814.8281 | | 898.0461 | | 907.3960 |
| 992.1838 | | 1009.4034 | | 1061.9872 |
| 1091.7306 | | 1099.0219 | | 1116.9615 |
| 1163.7708 | | 1190.3963 | | 1247.7466 |
| 1264.2674 | | 1285.7714 | | 1327.9316 |
| 1341.9130 | | 1369.1854 | | 1374.6829 |
| 1389.5135 | | 1401.1287 | | 1462.8383 |
| 1489.6011 | | 1506.8336 | | 1508.8162 |
| 1541.2228 | | 2866.4718 | | 2918.4278 |
| 2991.7401 | | 3021.4064 | | 3038.3237 |
| 3043.0268 | | 3046.3657 | | 3077.3674 |
| 3086.6510 | | 3087.9183 | | 3826.1173 |
| Zero-point correction (Hartree): | 0.157294 | | | |

C5H11O2.tpmpp

```

-----
E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.52497769
Electronic state : 2-A
Cartesian coordinates (Angs):
O      -2.794649      -0.764836      -0.330354
C      -1.564287      -0.455859      0.167535
C      -1.172279      1.025618      0.043478
C       0.277866      1.339708      0.450634
C       1.359972      0.833943     -0.537306
C       2.166472     -0.380495     -0.070373
O       1.378643     -1.554017      0.133621
H       0.978130     -1.499400      1.009826
H      -1.441268     -0.818004      1.210338
H      -0.852682     -1.081394     -0.418180
H      -1.346163     1.339133     -0.992716
H      -1.861450      1.608604      0.666576
H       0.366670      2.426669      0.551940
H       0.470576      0.942064      1.459223
H       0.897867      0.593317     -1.503141
H       2.080107      1.637618     -0.738147
H       2.901270     -0.645592     -0.837961
H       2.728526     -0.129678      0.842297
Rotational constants (GHz): 3.8132200 1.5306800 1.1906700
Vibrational harmonic frequencies (cm-1):
58.2699      107.2414      141.4356
156.6132      230.7977      282.8383
336.3054      357.8544      465.3644
504.3705      727.0694      750.7905
831.7723      885.7231      942.6971
991.9272      1018.9217     1054.5617
1080.2600     1096.0881     1109.2476
1138.9835     1194.2166     1232.9778
1264.6653     1302.1194     1333.5275
1365.8682     1366.4402     1391.3325
1395.3457     1398.1220     1424.8649
1492.5168     1503.7131     1507.7346
1515.4966     2868.8408     2902.5823
3003.4659     3008.3325     3034.4933
3045.4227     3070.8308     3082.4553
3090.5169     3092.6309     3834.2877
Zero-point correction (Hartree): 0.157175

```

C5H11O2.tpmpp

```

-----
E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.52756408
Electronic state : 2-A
Cartesian coordinates (Angs):

```

| | | | | |
|---|-----------|-----------|-----------|--|
| O | -2.769597 | -0.715704 | -0.127561 | |
| C | -1.597205 | -0.257190 | 0.386699 | |
| C | -1.008503 | 0.964904 | -0.340186 | |
| C | 0.325867 | 1.482983 | 0.229761 | |
| C | 1.622650 | 0.801253 | -0.251474 | |
| C | 1.949276 | -0.588759 | 0.300759 | |
| O | 1.100072 | -1.638228 | -0.164777 | |
| H | 1.164494 | -1.668493 | -1.128734 | |
| H | -1.662691 | -0.084342 | 1.480947 | |
| H | -0.885136 | -1.109287 | 0.284021 | |
| H | -0.906390 | 0.723191 | -1.405585 | |
| H | -1.752629 | 1.768379 | -0.279450 | |
| H | 0.410170 | 2.544805 | -0.030535 | |
| H | 0.291765 | 1.453981 | 1.328977 | |
| H | 1.630858 | 0.759611 | -1.351598 | |
| H | 2.466249 | 1.449418 | 0.022991 | |
| H | 2.999312 | -0.828296 | 0.072747 | |
| H | 1.847696 | -0.596657 | 1.391568 | |
| Rotational constants (GHz): | 3.6396800 | 1.6246700 | 1.2184500 | |
| Vibrational harmonic frequencies (cm ⁻¹): | | | | |
| 64.4362 | 104.5381 | | 110.9510 | |
| 204.4589 | 249.0524 | | 310.5193 | |
| 329.7870 | 362.6330 | | 471.5817 | |
| 488.3519 | 722.8942 | | 768.4982 | |
| 846.9939 | 865.6507 | | 949.6645 | |
| 974.3574 | 1005.7856 | | 1061.6156 | |
| 1097.6703 | 1104.1821 | | 1118.4987 | |
| 1129.3359 | 1187.4018 | | 1254.3002 | |
| 1281.6567 | 1307.6740 | | 1339.4062 | |
| 1367.0978 | 1383.0014 | | 1391.6674 | |
| 1398.4358 | 1401.5998 | | 1429.6258 | |
| 1487.1582 | 1497.4772 | | 1502.2292 | |
| 1519.0531 | 2850.0999 | | 2915.9226 | |
| 2999.5726 | 3012.0919 | | 3018.9551 | |
| 3039.2574 | 3053.8135 | | 3068.5166 | |
| 3082.8978 | 3089.4305 | | 3811.0610 | |
| Zero-point correction (Hartree): | 0.157264 | | | |

C5H11O2.tpmp

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.52680899

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | | |
|---|-----------|-----------|-----------|--|
| O | -2.772368 | -0.730874 | -0.103442 | |
| C | -1.577632 | -0.284256 | 0.369105 | |
| C | -1.024737 | 0.964266 | -0.339891 | |
| C | 0.305321 | 1.493764 | 0.228132 | |
| C | 1.609346 | 0.817572 | -0.241783 | |
| C | 1.934209 | -0.566364 | 0.313445 | |
| O | 1.127177 | -1.550067 | -0.337777 | |
| H | 1.357615 | -2.417121 | 0.019476 | |
| H | -1.591862 | -0.151816 | 1.471338 | |
| H | -0.867612 | -1.124991 | 0.192668 | |
| H | -0.927720 | 0.744947 | -1.409512 | |
| H | -1.782615 | 1.752177 | -0.249607 | |
| H | 0.383641 | 2.553685 | -0.042386 | |
| H | 0.266834 | 1.476244 | 1.327858 | |
| H | 1.627522 | 0.755952 | -1.337479 | |
| H | 2.444134 | 1.470782 | 0.043935 | |
| H | 2.998881 | -0.780960 | 0.135578 | |
| H | 1.773662 | -0.581271 | 1.403825 | |
| Rotational constants (GHz): | 3.6551700 | 1.6287900 | 1.2211000 | |
| Vibrational harmonic frequencies (cm ⁻¹): | | | | |
| 57.9890 | 98.0943 | | 111.1048 | |
| 194.0869 | 252.5393 | | 309.8334 | |
| 322.0004 | 350.2760 | | 455.0880 | |
| 483.4483 | 721.9591 | | 770.0856 | |
| 852.6939 | 864.6851 | | 956.2440 | |
| 968.3078 | 1008.7415 | | 1079.5421 | |
| 1093.1298 | 1106.4954 | | 1119.6901 | |
| 1155.3951 | 1207.3474 | | 1241.0439 | |
| 1272.6801 | 1296.1427 | | 1321.9786 | |
| 1341.9415 | 1367.7213 | | 1394.4029 | |
| 1397.0850 | 1401.8493 | | 1460.1804 | |
| 1482.4931 | 1497.9435 | | 1500.9319 | |
| 1532.8276 | 2855.7623 | | 2910.7912 | |
| 2983.2295 | 3013.2843 | | 3016.8260 | |
| 3038.1596 | 3042.9288 | | 3067.6342 | |
| 3079.3407 | 3091.7778 | | 3824.6626 | |
| Zero-point correction (Hartree): | 0.157131 | | | |

C5H11O2.tpm

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.52379456

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -2.987747 | -1.026708 | -0.225334 |
| C | -1.850236 | -0.502613 | 0.324114 |
| C | -1.329837 | 0.774164 | -0.353543 |
| C | -0.081523 | 1.398917 | 0.301408 |
| C | 1.285306 | 0.867448 | -0.168144 |
| C | 1.615642 | -0.578867 | 0.211612 |
| O | 2.968340 | -0.916396 | -0.064232 |
| H | 3.102584 | -0.839517 | -1.017832 |
| H | -1.986939 | -0.354343 | 1.414990 |
| H | -1.106089 | -1.326062 | 0.270165 |
| H | -1.144591 | 0.561703 | -1.413900 |
| H | -2.151614 | 1.499432 | -0.326325 |
| H | -0.095629 | 2.476495 | 0.102892 |
| H | -0.153061 | 1.302730 | 1.395021 |
| H | 1.356437 | 0.975953 | -1.260836 |
| H | 2.075965 | 1.497239 | 0.257160 |
| H | 1.491223 | -0.720479 | 1.291468 |
| H | 0.930856 | -1.282620 | -0.288951 |

Rotational constants (GHz): 4.5278700 1.1389700 0.9665500

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 51.1705 | 88.6238 | 93.8690 |
| 134.0871 | 226.0010 | 281.9880 |
| 308.7723 | 329.0629 | 453.8703 |
| 490.0559 | 530.1756 | 772.5844 |
| 804.2020 | 843.4277 | 941.1896 |
| 967.0686 | 1046.8261 | 1070.7301 |
| 1074.7198 | 1089.5445 | 1101.4204 |
| 1143.6742 | 1202.7003 | 1252.3020 |
| 1286.6751 | 1322.4432 | 1333.3680 |
| 1357.9483 | 1373.0580 | 1386.4094 |
| 1396.5201 | 1406.9046 | 1433.4161 |
| 1496.5383 | 1502.7151 | 1507.2233 |
| 1528.1981 | 2898.1256 | 2921.6894 |
| 2983.9321 | 3012.8033 | 3021.5572 |
| 3044.4213 | 3068.6161 | 3076.1159 |
| 3085.1259 | 3089.3658 | 3812.7951 |

Zero-point correction (Hartree): 0.156383

C5H11O2.tpmtp

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.52374317

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -2.984470 | -1.022732 | -0.215239 |
| C | -1.865109 | -0.474009 | 0.347894 |
| C | -1.307309 | 0.759152 | -0.378979 |
| C | -0.074318 | 1.401274 | 0.289869 |
| C | 1.297642 | 0.870719 | -0.163370 |
| C | 1.598867 | -0.588497 | 0.188934 |
| O | 2.904246 | -0.985447 | -0.206063 |
| H | 3.536001 | -0.424794 | 0.262946 |
| H | -2.050326 | -0.259520 | 1.420704 |
| H | -1.125893 | -1.302482 | 0.379944 |
| H | -1.086154 | 0.487609 | -1.418528 |
| H | -2.121069 | 1.492472 | -0.420821 |
| H | -0.091569 | 2.477708 | 0.086133 |
| H | -0.160372 | 1.309750 | 1.383085 |
| H | 1.405932 | 0.995009 | -1.248058 |
| H | 2.076280 | 1.496532 | 0.297418 |
| H | 1.437037 | -0.755117 | 1.268183 |
| H | 0.923293 | -1.263561 | -0.346680 |

Rotational constants (GHz): 4.4949700 1.1492300 0.9718700

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 46.7468 | 91.3302 | 96.0937 |
| 134.0934 | 224.9199 | 285.8130 |
| 302.3366 | 338.3609 | 442.4063 |
| 477.5396 | 515.2434 | 768.3059 |
| 807.7817 | 841.0664 | 943.1642 |
| 970.7533 | 1034.3884 | 1074.9365 |
| 1085.0626 | 1087.1588 | 1104.6530 |
| 1139.8979 | 1211.5278 | 1237.9819 |
| 1290.3802 | 1323.5036 | 1333.7645 |
| 1357.0771 | 1371.3093 | 1389.7484 |
| 1399.7282 | 1404.6423 | 1436.3685 |
| 1495.8668 | 1502.8261 | 1506.9024 |
| 1529.9308 | 2904.2949 | 2920.9500 |
| 2969.6909 | 3012.5564 | 3018.4583 |
| 3046.4610 | 3067.0485 | 3077.3377 |
| 3089.3371 | 3092.5106 | 3812.2123 |

Zero-point correction (Hartree): 0.156315

C5H11O2.tpmtt

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.52324737

Electronic state : 2-A
Cartesian coordinates (Angs):
O -2.980329 -1.033657 -0.222268
C -1.846290 -0.501573 0.327360
C -1.326554 0.773400 -0.353444
C -0.080756 1.399543 0.305568
C 1.285764 0.875829 -0.168276
C 1.603825 -0.573441 0.185773
O 2.957897 -0.811344 -0.176415
H 3.164193 -1.735125 0.011931
H -1.987756 -0.348860 1.417151
H -1.098845 -1.322363 0.279657
H -1.135807 0.557401 -1.411934
H -2.149689 1.497356 -0.331618
H -0.097916 2.477840 0.111511
H -0.154473 1.299058 1.398869
H 1.373911 0.995821 -1.255285
H 2.076132 1.493032 0.275485
H 1.442764 -0.736638 1.265489
H 0.931007 -1.260064 -0.353676
Rotational constants (GHz): 4.5686500 1.1463200 0.9710400
Vibrational harmonic frequencies (cm-1):
45.8945 90.6026 93.7004
132.1354 230.9846 276.1052
293.2316 316.5653 447.8210
484.6872 521.6355 776.4978
811.2943 843.8716 944.4316
966.6552 1044.3984 1061.1176
1086.4802 1095.2738 1099.3511
1179.9501 1210.8756 1248.4359
1275.2518 1298.3533 1325.7823
1336.5627 1372.3495 1375.1471
1391.7027 1396.4745 1466.8672
1498.2618 1503.2324 1510.4394
1541.4626 2898.1581 2920.1633
2963.7579 2993.1786 3017.2925
3043.9017 3045.5556 3076.8582
3087.4008 3091.2537 3826.9315
Zero-point correction (Hartree): 0.156187

C5H11O2.tppmm

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.52629241
Electronic state : 2-A
Cartesian coordinates (Angs):
O -2.793277 -0.742257 0.035655
C -1.658467 -0.099850 0.444238
C -0.904277 0.644921 -0.666414
C 0.275575 1.488474 -0.155303
C 1.390413 0.749034 0.609320
C 2.062198 -0.399286 -0.151385
O 1.252562 -1.572285 -0.249060
H 1.276692 -2.017697 0.607203
H -1.848859 0.543811 1.326888
H -1.005954 -0.919078 0.816867
H -0.570904 -0.092101 -1.402505
H -1.615412 1.309099 -1.172569
H 0.728414 1.999370 -1.015384
H -0.110676 2.286258 0.494051
H 2.164702 1.482088 0.873230
H 1.014352 0.359441 1.566285
H 2.270806 -0.096292 -1.183963
H 3.029904 -0.638321 0.314397
Rotational constants (GHz): 3.7858100 1.5630600 1.2477800
Vibrational harmonic frequencies (cm-1):
67.2972 102.4969 128.5546
182.5423 218.3024 304.4028
327.7559 352.1170 453.6049
520.8433 686.3678 788.2497
805.6874 880.3428 940.5979
981.2342 990.6452 1061.6766
1077.8247 1097.4440 1110.4900
1143.9103 1163.3668 1241.5955
1270.8602 1312.9075 1328.7168
1365.9703 1391.5012 1394.8815
1401.1746 1406.8939 1424.0710
1493.2454 1497.1209 1504.8973
1518.2927 2891.7940 2927.9747
3005.6765 3021.6497 3026.2204
3052.4036 3055.8431 3065.5123
3083.8640 3115.3261 3823.3655
Zero-point correction (Hartree): 0.157211

C5H11O2.tppmp

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.52640224
Electronic state : 2-A
Cartesian coordinates (Angs):
O 2.743699 -0.742225 -0.071546
C 1.619533 -0.075919 -0.466372
C 0.905806 0.689429 0.660116
C -0.321397 1.495774 0.199675
C -1.402273 0.740058 -0.596524
C -2.043666 -0.469570 0.089770
O -1.193888 -1.619341 0.129392
H -0.676725 -1.592067 0.942512
H 1.806990 0.567482 -1.348675
H 0.940200 -0.878866 -0.831789
H 0.640749 -0.025508 1.448946
H 1.628025 1.376332 1.117458
H -0.784231 1.951862 1.085084
H 0.024647 2.334750 -0.418546
H -2.204154 1.452113 -0.834602
H -1.003845 0.402485 -1.561512
H -2.390108 -0.200717 1.099240
H -2.928054 -0.773975 -0.480874
Rotational constants (GHz): 3.7153000 1.6109500 1.2693600
Vibrational harmonic frequencies (cm-1):
79.2399 114.7646 157.9645
205.3391 223.9574 315.6463
315.9280 346.0001 457.6009
525.6031 722.5073 792.0612
805.9687 879.1489 935.6950
988.5630 996.8363 1063.1167
1083.3805 1103.6817 1112.2030
1136.9364 1179.4230 1250.8441
1262.3286 1312.6010 1332.3401
1358.4511 1391.0815 1394.1853
1402.7216 1409.8124 1426.5859
1491.8263 1498.7824 1514.8269
1516.9603 2875.5236 2937.6147
3007.4029 3025.5275 3034.5673
3042.5935 3060.5331 3078.4885
3082.1872 3086.1396 3850.2821
Zero-point correction (Hartree): 0.157617

C5H11O2.tppmt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.52738334
Electronic state : 2-A
Cartesian coordinates (Angs):
O 2.780275 -0.736442 -0.053740
C 1.650613 -0.079803 -0.451895
C 0.897018 0.637229 0.679137
C -0.294632 1.480681 0.195983
C -1.394891 0.751658 -0.599187
C -2.062354 -0.423243 0.109415
O -1.162574 -1.530744 0.102412
H -1.552255 -2.250119 0.613978
H 1.846904 0.589808 -1.313750
H 0.995582 -0.886089 -0.848733
H 0.572668 -0.118899 1.399544
H 1.605120 1.295963 1.196946
H -0.754700 1.958577 1.071351
H 0.080540 2.303355 -0.428199
H -2.175905 1.481196 -0.848484
H -1.006287 0.384650 -1.557548
H -2.332081 -0.137050 1.139268
H -2.995711 -0.683035 -0.414465
Rotational constants (GHz): 3.8423100 1.5851200 1.2646200
Vibrational harmonic frequencies (cm-1):
73.3059 105.9788 134.2560
192.8093 214.9315 251.7648
320.5455 354.2992 453.3436
519.3750 705.6314 796.3984
808.5673 887.2715 957.2808
977.4982 997.4783 1078.9613
1085.7884 1101.3333 1111.8565
1162.6046 1188.4872 1236.3951
1268.7074 1292.8311 1326.2192
1331.2268 1365.5618 1394.4513
1401.8072 1409.7078 1461.2825
1491.4832 1496.4787 1504.5447
1536.0202 2890.2693 2928.3141
2979.5551 3009.5007 3022.8729
3042.8075 3051.9850 3058.1856
3083.2575 3114.4013 3832.4068
Zero-point correction (Hartree): 0.157216

C5H11O2.tpppm

```

-----
E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.52573694
Electronic state : 2-A
Cartesian coordinates (Angs):
O      -3.107305      -0.780531      -0.020972
C      -2.069140       0.036831       0.332342
C      -0.980648       0.199217      -0.739324
C       0.175259       1.118616      -0.310603
C       1.064432       0.594800       0.831917
C       1.852635      -0.677481       0.498381
O       2.756514      -0.504443      -0.586844
H       2.242161      -0.462650      -1.402167
H      -2.434201       1.018580       0.694741
H      -1.647514      -0.445327       1.241847
H      -0.619900      -0.798694      -1.016236
H      -1.456710       0.613012      -1.636245
H       0.812147       1.321516      -1.181176
H      -0.234752       2.094809      -0.019894
H       1.783396       1.377966       1.099839
H       0.464779       0.405269       1.733139
H       2.471614      -0.954392       1.358072
H       1.170082      -1.522194       0.314327
Rotational constants (GHz):    5.3672800    1.0911100    1.0639700
Vibrational harmonic frequencies (cm-1):
    37.3840           87.5234           95.2831
   180.2651          231.2253          289.8074
   309.7534          376.4029          462.2441
   531.4121          654.9054          740.7717
   808.2790          887.9312          918.1573
   956.3140          1019.7975         1055.0071
  1083.5437          1099.8750         1104.9394
  1126.3562          1196.6194         1212.8116
  1266.7074          1321.4570         1334.6789
  1366.5616          1381.7723         1388.3738
  1396.4138          1402.5578         1429.1365
  1491.6037          1500.1753         1510.4312
  1522.9331          2886.5781         2932.2063
  2995.5013          3030.2022         3033.2538
  3048.2723          3067.1395         3080.7330
  3089.8135          3092.9843         3831.2978
Zero-point correction (Hartree): 0.156891
    
```

C5H11O2.tpppp

```

-----
E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.52660425
Electronic state : 2-A
Cartesian coordinates (Angs):
O      -3.167290      -0.729942      -0.096582
C      -2.117040       0.039665       0.322815
C      -1.000577       0.233583      -0.714608
C       0.171973       1.088276      -0.207522
C       1.041546       0.438322       0.883127
C       1.884785      -0.742382       0.388111
O       2.740728      -0.399434      -0.695552

H       3.370281       0.260303      -0.375923
H      -2.463646       1.008280       0.735606
H      -1.727601      -0.507919       1.209814
H      -0.658173      -0.752038      -1.049024
H      -1.444196       0.717561      -1.592748
H       0.822192       1.330144      -1.054902
H      -0.217502       2.044249       0.167782
H       1.718066       1.199701       1.297781
H       0.429442       0.098441       1.730278
H       2.456270      -1.164617       1.229868
H       1.243249      -1.543882       0.007001
Rotational constants (GHz):    5.7076200    1.0596400    1.0408300
Vibrational harmonic frequencies (cm-1):
    32.5911           89.5229           96.1817
   183.5277          236.0843          293.2527
   331.2392          374.4185          466.3476
   530.3877          664.0067          745.0269
   815.8579          889.4347          920.8468
   962.5929          1012.5702         1050.0721
  1084.1259          1094.2286         1103.0694
  1132.2619          1181.4069         1211.7942
  1269.3488          1323.1474         1340.0350
  1361.9916          1378.5996         1384.9798
  1396.9775          1408.4339         1429.5302
  1493.9939          1498.1087         1502.6927
  1525.9434          2882.3064         2930.0338
  2994.4602          3017.5495         3036.6838
  3051.0552          3054.0788         3090.6249
  3093.1743          3100.3729         3809.3026
Zero-point correction (Hartree): 0.156907
    
```

C5H11O2.tpppt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.52612814

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -3.104844 | -0.785081 | -0.033736 |
| C | -2.067109 | 0.029375 | 0.329302 |
| C | -0.983192 | 0.213515 | -0.743560 |
| C | 0.175748 | 1.122807 | -0.305506 |
| C | 1.056241 | 0.582196 | 0.835739 |
| C | 1.832944 | -0.684073 | 0.485405 |
| O | 2.672417 | -0.392190 | -0.626148 |
| H | 3.127504 | -1.202930 | -0.883744 |
| H | -2.429169 | 1.002985 | 0.715828 |
| H | -1.638702 | -0.475508 | 1.223780 |
| H | -0.619601 | -0.774805 | -1.046561 |
| H | -1.463004 | 0.647372 | -1.628991 |
| H | 0.820233 | 1.310664 | -1.169859 |
| H | -0.229161 | 2.098167 | -0.003223 |
| H | 1.781149 | 1.355724 | 1.116038 |
| H | 0.459073 | 0.380422 | 1.735167 |
| H | 2.424595 | -0.999191 | 1.360010 |
| H | 1.138710 | -1.507650 | 0.252346 |

Rotational constants (GHz): 5.4093000 1.1021700 1.0740100

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 23.6522 | 90.1796 | 97.9001 |
| 182.1682 | 239.5953 | 273.2335 |
| 296.0773 | 375.2624 | 459.0502 |
| 532.3376 | 671.8993 | 747.5133 |
| 817.6710 | 897.3286 | 921.7623 |
| 970.8526 | 1019.3902 | 1058.2222 |
| 1083.5483 | 1094.1110 | 1105.0899 |
| 1164.8079 | 1173.8127 | 1230.5025 |
| 1263.0206 | 1291.4365 | 1329.7946 |
| 1339.2366 | 1359.8038 | 1387.3706 |
| 1394.4825 | 1405.5434 | 1463.1462 |
| 1490.8785 | 1498.6498 | 1505.6618 |
| 1541.6706 | 2880.3592 | 2931.4693 |
| 2979.8162 | 3004.9487 | 3032.6006 |
| 3041.5928 | 3053.0470 | 3079.6991 |
| 3096.0306 | 3103.1001 | 3833.3383 |

Zero-point correction (Hartree): 0.156812

C5H11O2.tppptm

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.52586992

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 3.035522 | -1.028838 | 0.089219 |
| C | 1.996901 | -0.307577 | -0.432124 |
| C | 1.240494 | 0.559989 | 0.585437 |
| C | 0.083676 | 1.366930 | -0.028589 |
| C | -1.091930 | 0.538738 | -0.576688 |
| C | -1.875751 | -0.228980 | 0.491709 |
| O | -2.940623 | -0.993976 | -0.056055 |
| H | -3.551040 | -0.381546 | -0.486874 |
| H | 2.317703 | 0.282464 | -1.314055 |
| H | 1.321689 | -1.082792 | -0.857297 |
| H | 0.891657 | -0.084717 | 1.399907 |
| H | 1.962736 | 1.253950 | 1.031715 |
| H | -0.295405 | 2.065902 | 0.728469 |
| H | 0.479884 | 1.993577 | -0.838704 |
| H | -1.785213 | 1.218495 | -1.092800 |
| H | -0.751938 | -0.176383 | -1.336369 |
| H | -1.231508 | -0.953472 | 0.999775 |
| H | -2.238091 | 0.472441 | 1.262445 |

Rotational constants (GHz): 4.8597200 1.0756100 0.9686500

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 47.4374 | 87.6337 | 95.8777 |
| 176.8407 | 214.2727 | 293.4913 |
| 312.6862 | 345.8751 | 459.1379 |
| 510.9562 | 665.9522 | 749.2898 |
| 824.5703 | 880.6457 | 916.8497 |
| 984.2401 | 1028.8705 | 1077.0946 |
| 1082.3414 | 1090.9940 | 1107.6163 |
| 1131.4320 | 1179.1977 | 1225.5800 |
| 1288.2382 | 1320.7621 | 1330.2789 |
| 1354.4892 | 1371.0447 | 1389.4677 |
| 1392.6123 | 1404.2317 | 1435.5768 |
| 1497.8436 | 1505.4732 | 1508.3819 |
| 1530.1566 | 2888.2273 | 2930.2998 |
| 2978.1500 | 3018.5201 | 3031.0838 |
| 3050.5108 | 3059.1293 | 3071.6015 |

| | | |
|-----------|-----------|-----------|
| 2970.9581 | 3002.0473 | 3029.7308 |
| 3040.9912 | 3050.7619 | 3067.0677 |
| 3087.3321 | 3094.4883 | 3828.9471 |

Zero-point correction (Hartree): 0.156721

C5H11O2.tptmm

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.52788307

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -3.513176 | -0.186779 | -0.246904 |
| C | -2.237316 | -0.355081 | 0.216809 |
| C | -1.269183 | 0.790475 | -0.114936 |
| C | 0.156179 | 0.568012 | 0.409716 |
| C | 0.912001 | -0.587499 | -0.261210 |
| C | 2.380794 | -0.669479 | 0.166740 |
| O | 3.114131 | 0.516696 | -0.115780 |
| H | 3.138306 | 0.625436 | -1.075585 |
| H | -2.230004 | -0.595142 | 1.299176 |
| H | -1.899582 | -1.296655 | -0.270480 |
| H | -1.261937 | 0.935306 | -1.202425 |
| H | -1.679828 | 1.709711 | 0.319673 |
| H | 0.740299 | 1.483292 | 0.268281 |
| H | 0.125655 | 0.395495 | 1.495424 |
| H | 0.437784 | -1.553220 | -0.038102 |
| H | 0.864339 | -0.472065 | -1.355188 |
| H | 2.447027 | -0.800252 | 1.252785 |
| H | 2.855457 | -1.549804 | -0.294799 |

Rotational constants (GHz): 8.8735300 0.8955100 0.8558300

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 45.6338 | 93.2506 | 98.8382 |
| 157.2983 | 243.7190 | 254.2201 |
| 322.7565 | 328.8603 | 455.4632 |
| 552.8342 | 650.0119 | 754.1883 |
| 823.5199 | 884.6862 | 915.6964 |
| 959.7374 | 1031.8039 | 1053.7121 |
| 1082.2498 | 1092.6347 | 1102.7588 |
| 1117.7253 | 1192.8618 | 1250.1610 |
| 1266.8548 | 1319.2033 | 1337.9193 |
| 1346.0356 | 1366.8654 | 1390.1767 |
| 1391.3531 | 1413.5297 | 1427.4679 |
| 1492.9640 | 1502.3717 | 1512.1072 |
| 1520.8635 | 2882.9390 | 2928.0413 |
| 2993.5661 | 3008.6398 | 3023.9832 |
| 3044.7188 | 3049.3737 | 3083.9280 |
| 3088.7965 | 3095.5908 | 3810.0439 |

Zero-point correction (Hartree): 0.156651

C5H11O2.tptmp

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.52707551

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -3.521172 | -0.218427 | -0.172973 |
| C | -2.228801 | -0.348303 | 0.255306 |
| C | -1.285873 | 0.782212 | -0.184260 |
| C | 0.157391 | 0.613561 | 0.313657 |
| C | 0.915383 | -0.566643 | -0.310718 |
| C | 2.365130 | -0.686833 | 0.171192 |
| O | 3.174057 | 0.426055 | -0.190168 |
| H | 2.920829 | 1.173407 | 0.364890 |
| H | -2.183289 | -0.516313 | 1.350221 |
| H | -1.899158 | -1.317456 | -0.180033 |
| H | -1.308006 | 0.849996 | -1.278511 |
| H | -1.697312 | 1.724580 | 0.196595 |
| H | 0.703903 | 1.539184 | 0.092516 |
| H | 0.156518 | 0.510098 | 1.409457 |
| H | 0.406290 | -1.513303 | -0.082706 |
| H | 0.917521 | -0.462218 | -1.403286 |
| H | 2.384214 | -0.855017 | 1.260822 |
| H | 2.836038 | -1.557945 | -0.295901 |

Rotational constants (GHz): 8.9829800 0.8903000 0.8489300

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 45.9930 | 93.9579 | 98.8288 |
| 144.6322 | 241.4352 | 259.0291 |
| 299.4863 | 323.3952 | 451.5899 |
| 546.8636 | 649.7118 | 750.8324 |
| 819.9009 | 891.8682 | 911.7997 |
| 964.0346 | 1028.9421 | 1061.0157 |
| 1081.8264 | 1092.5499 | 1096.0785 |
| 1144.4008 | 1204.5723 | 1233.2992 |
| 1274.8287 | 1318.3457 | 1343.4324 |
| 1347.9428 | 1370.4989 | 1390.4963 |
| 1397.0606 | 1412.2901 | 1426.6471 |
| 1488.1827 | 1501.6222 | 1509.0879 |

| | | |
|-----------|-----------|-----------|
| 1517.6794 | 2887.5372 | 2928.8104 |
| 2984.6961 | 3010.7733 | 3026.3605 |
| 3045.6638 | 3058.3105 | 3078.6218 |
| 3091.7455 | 3093.4398 | 3833.1224 |

Zero-point correction (Hartree): 0.156677

C5H11O2.tptmt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.52729161

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -3.514721 | -0.199178 | -0.223605 |
| C | -2.232463 | -0.355386 | 0.226575 |
| C | -1.274754 | 0.791737 | -0.131001 |
| C | 0.156115 | 0.587643 | 0.386766 |
| C | 0.909770 | -0.575206 | -0.275014 |
| C | 2.366230 | -0.673219 | 0.166712 |
| O | 3.034304 | 0.515938 | -0.240240 |
| H | 3.941490 | 0.480500 | 0.086121 |
| H | -2.208671 | -0.583814 | 1.311241 |
| H | -1.895937 | -1.298977 | -0.257628 |
| H | -1.275380 | 0.919727 | -1.220305 |
| H | -1.688857 | 1.714583 | 0.292559 |
| H | 0.730970 | 1.504261 | 0.222489 |
| H | 0.133358 | 0.431599 | 1.475603 |
| H | 0.425873 | -1.535306 | -0.051707 |
| H | 0.888078 | -0.455303 | -1.366075 |
| H | 2.413038 | -0.801026 | 1.261383 |
| H | 2.829992 | -1.563738 | -0.287145 |

Rotational constants (GHz): 8.9525500 0.9018300 0.8605000

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 47.8152 | 95.2328 | 98.4439 |
| 152.7193 | 235.0461 | 250.6170 |
| 286.7035 | 323.7511 | 449.4482 |
| 544.8456 | 662.2358 | 753.1737 |
| 829.2250 | 888.7590 | 928.8147 |
| 967.9663 | 1039.0010 | 1055.8860 |
| 1078.1095 | 1085.6705 | 1108.4261 |
| 1165.9167 | 1184.8899 | 1244.7629 |
| 1273.5979 | 1291.3686 | 1326.6113 |
| 1343.3937 | 1348.8818 | 1366.2032 |
| 1391.8504 | 1416.1386 | 1461.7821 |
| 1489.5615 | 1502.2623 | 1510.6974 |
| 1536.4346 | 2883.1433 | 2927.8426 |
| 2972.4588 | 3002.4543 | 3017.5265 |
| 3034.0755 | 3046.7395 | 3072.3118 |
| 3090.8331 | 3103.6888 | 3833.4507 |

Zero-point correction (Hartree): 0.156557

C5H11O2.tptpm

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.52721499

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 3.418083 | -0.445702 | 0.189531 |
| C | 2.069864 | -0.543899 | -0.017700 |
| C | 1.357875 | 0.792073 | -0.279968 |
| C | -0.153838 | 0.652695 | -0.514013 |
| C | -0.952056 | 0.202199 | 0.717676 |
| C | -2.464215 | 0.147130 | 0.477979 |
| O | -2.843513 | -0.815887 | -0.498460 |
| H | -2.586399 | -0.479338 | -1.365373 |
| H | 1.838090 | -1.292200 | -0.802100 |
| H | 1.686941 | -1.009593 | 0.916848 |
| H | 1.554707 | 1.463831 | 0.564433 |
| H | 1.824525 | 1.250223 | -1.160174 |
| H | -0.544703 | 1.620119 | -0.858255 |
| H | -0.323699 | -0.057887 | -1.335829 |
| H | -0.624730 | -0.793216 | 1.043015 |
| H | -0.757145 | 0.890450 | 1.552094 |
| H | -2.973009 | -0.151206 | 1.400380 |
| H | -2.836914 | 1.150337 | 0.212554 |

Rotational constants (GHz): 6.8751100 0.9332200 0.9127300

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 50.1881 | 88.1552 | 114.2380 |
| 140.7562 | 252.5267 | 260.9111 |
| 309.5367 | 316.1194 | 440.2800 |
| 557.2243 | 642.5448 | 765.3598 |
| 823.3859 | 858.3294 | 920.4134 |
| 973.2806 | 1022.7690 | 1064.8303 |
| 1080.6937 | 1094.4889 | 1105.4179 |
| 1151.9914 | 1184.9740 | 1237.6870 |
| 1290.2305 | 1310.5466 | 1344.2997 |
| 1348.7013 | 1370.4116 | 1389.0528 |
| 1397.0264 | 1414.5905 | 1424.6578 |

| | | |
|-----------|-----------|-----------|
| 1488.7139 | 1502.3471 | 1511.0716 |
| 1517.9838 | 2891.1806 | 2929.7128 |
| 2985.2002 | 3014.5407 | 3029.4669 |
| 3041.7239 | 3053.7181 | 3079.2646 |
| 3091.2558 | 3092.7535 | 3833.0126 |

Zero-point correction (Hartree): 0.156755

C5H11O2.tptpp

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.52766253
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 3.395110 | -0.471919 | 0.216155 |
| C | 2.046247 | -0.549964 | 0.002511 |
| C | 1.360218 | 0.789208 | -0.308099 |
| C | -0.152500 | 0.670609 | -0.544000 |
| C | -0.970236 | 0.310314 | 0.703791 |
| C | -2.469921 | 0.183936 | 0.419483 |
| O | -2.773995 | -0.811380 | -0.551526 |
| H | -2.533023 | -1.669238 | -0.178105 |
| H | 1.802113 | -1.319272 | -0.757418 |
| H | 1.652542 | -0.974362 | 0.952739 |
| H | 1.572683 | 1.487505 | 0.510895 |
| H | 1.837238 | 1.204150 | -1.204033 |
| H | -0.522832 | 1.625476 | -0.938992 |
| H | -0.355313 | -0.072991 | -1.324661 |
| H | -0.616189 | -0.637347 | 1.137171 |
| H | -0.823496 | 1.071782 | 1.482588 |
| H | -3.015572 | 0.002928 | 1.358980 |
| H | -2.849917 | 1.123143 | 0.001689 |

Rotational constants (GHz): 6.6147400 0.9511500 0.9210500
 Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 47.4637 | 87.3712 | 115.3125 |
| 155.1558 | 241.0290 | 268.7680 |
| 312.6081 | 333.9597 | 443.0446 |
| 560.7002 | 652.6659 | 765.6891 |
| 827.4131 | 859.7244 | 925.2396 |
| 967.0624 | 1027.7512 | 1062.7037 |
| 1073.3496 | 1092.2411 | 1099.9765 |
| 1146.1786 | 1172.4991 | 1243.5325 |
| 1294.0450 | 1306.0718 | 1341.4217 |
| 1346.4549 | 1368.7443 | 1389.2155 |
| 1392.7978 | 1415.7238 | 1425.9068 |
| 1493.8767 | 1503.1403 | 1512.9487 |
| 1519.6453 | 2885.3993 | 2929.0053 |
| 2994.3276 | 3011.8645 | 3038.0924 |
| 3045.5867 | 3048.8890 | 3077.8724 |
| 3085.5787 | 3091.8667 | 3811.8603 |

Zero-point correction (Hartree): 0.156765

C5H11O2.tptpt

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.52745262
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 3.391647 | -0.471770 | 0.234529 |
| C | 2.045040 | -0.553069 | 0.008078 |
| C | 1.361137 | 0.781261 | -0.326308 |
| C | -0.150832 | 0.658334 | -0.565551 |
| C | -0.966682 | 0.328797 | 0.692629 |
| C | -2.460746 | 0.196322 | 0.419137 |
| O | -2.653001 | -0.910091 | -0.456273 |
| H | -3.590304 | -0.960712 | -0.679214 |
| H | 1.810798 | -1.331834 | -0.745034 |
| H | 1.639358 | -0.970359 | 0.956259 |
| H | 1.570506 | 1.492339 | 0.482695 |
| H | 1.842287 | 1.182310 | -1.226482 |
| H | -0.519107 | 1.604018 | -0.984764 |
| H | -0.349164 | -0.107502 | -1.324883 |
| H | -0.624100 | -0.612896 | 1.139959 |
| H | -0.819640 | 1.110763 | 1.449667 |
| H | -2.999368 | 0.048937 | 1.368969 |
| H | -2.837939 | 1.129953 | -0.031137 |

Rotational constants (GHz): 6.6101800 0.9618700 0.9289200
 Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 47.4740 | 87.3805 | 115.9405 |
| 152.5278 | 234.2665 | 266.1661 |
| 294.2008 | 317.0759 | 437.3549 |
| 551.9658 | 639.8132 | 761.8253 |
| 827.9064 | 866.8711 | 930.5622 |
| 982.9578 | 1022.5649 | 1065.4355 |
| 1082.6426 | 1090.3912 | 1118.1185 |
| 1145.4053 | 1199.3137 | 1250.5865 |
| 1267.0611 | 1302.5517 | 1323.0359 |
| 1346.7148 | 1349.4955 | 1368.8534 |

| | | |
|-----------|-----------|-----------|
| 1388.3149 | 1417.0026 | 1460.8126 |
| 1490.4001 | 1502.6542 | 1512.1731 |
| 1536.7807 | 2887.4437 | 2931.3710 |
| 2972.8468 | 3002.9666 | 3031.7836 |
| 3039.1813 | 3044.3683 | 3068.6036 |
| 3084.1914 | 3093.5812 | 3832.7992 |

Zero-point correction (Hartree): 0.156610

C5H11O2.tpttm

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.52707780

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -3.440928 | -0.694274 | -0.104564 |
| C | -2.161600 | -0.459797 | 0.318725 |
| C | -1.480317 | 0.756902 | -0.325918 |
| C | -0.050368 | 1.006776 | 0.176897 |
| C | 0.965087 | -0.072614 | -0.224163 |
| C | 2.389088 | 0.254179 | 0.232911 |
| O | 3.343539 | -0.711021 | -0.185910 |
| H | 3.120758 | -1.549570 | 0.238562 |
| H | -2.104593 | -0.421553 | 1.425323 |
| H | -1.618361 | -1.393387 | 0.052314 |
| H | -1.486902 | 0.624896 | -1.414514 |
| H | -2.100429 | 1.635670 | -0.112684 |
| H | 0.290112 | 1.974987 | -0.212128 |
| H | -0.061628 | 1.111676 | 1.271626 |
| H | 0.675929 | -1.044503 | 0.202729 |
| H | 0.969950 | -0.200865 | -1.313946 |
| H | 2.713928 | 1.201597 | -0.211483 |
| H | 2.409014 | 0.390738 | 1.327281 |

Rotational constants (GHz): 7.4356800 0.8671700 0.8121200

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 61.2236 | 82.4995 | 88.4325 |
| 140.0402 | 200.7787 | 261.5952 |
| 307.7660 | 325.4741 | 447.6972 |
| 513.5360 | 656.9120 | 749.7129 |
| 822.7221 | 872.5278 | 945.0409 |
| 1002.3563 | 1030.0535 | 1067.8554 |
| 1077.5369 | 1089.2024 | 1095.8502 |
| 1149.2691 | 1178.9286 | 1253.9902 |
| 1288.4979 | 1308.0602 | 1327.9793 |
| 1341.7583 | 1369.4592 | 1386.3222 |
| 1389.9615 | 1410.3918 | 1431.1048 |
| 1496.8931 | 1502.7838 | 1508.2262 |
| 1529.1690 | 2887.7088 | 2927.8462 |
| 2979.5542 | 3010.7269 | 3019.5518 |
| 3045.9346 | 3058.3828 | 3070.6971 |
| 3088.9079 | 3093.7152 | 3814.5744 |

Zero-point correction (Hartree): 0.156531

C5H11O2.tpttp

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.52729545

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -3.437848 | -0.700987 | -0.095024 |
| C | -2.163819 | -0.447677 | 0.333055 |
| C | -1.479076 | 0.747283 | -0.347509 |
| C | -0.050921 | 1.011382 | 0.153021 |
| C | 0.962508 | -0.084646 | -0.205690 |
| C | 2.388284 | 0.257495 | 0.234185 |
| O | 3.316213 | -0.785426 | -0.029244 |
| H | 3.355344 | -0.909559 | -0.986401 |
| H | -2.119757 | -0.369093 | 1.438009 |
| H | -1.614072 | -1.388468 | 0.109131 |
| H | -1.481388 | 0.579632 | -1.431417 |
| H | -2.099286 | 1.633117 | -0.166150 |
| H | 0.293021 | 1.966945 | -0.263698 |
| H | -0.066317 | 1.148987 | 1.243852 |
| H | 0.689038 | -1.041545 | 0.255482 |
| H | 0.951479 | -0.247890 | -1.294062 |
| H | 2.705662 | 1.205504 | -0.231730 |
| H | 2.417496 | 0.410647 | 1.318757 |

Rotational constants (GHz): 7.3675500 0.8690500 0.8142500

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 67.5958 | 81.5219 | 89.0492 |
| 141.6462 | 202.4433 | 263.4263 |
| 322.9198 | 326.8741 | 448.5854 |
| 513.7291 | 651.2027 | 750.2521 |
| 822.3312 | 870.5154 | 944.7453 |
| 1006.1616 | 1021.1737 | 1071.0226 |
| 1083.7439 | 1088.1074 | 1106.6794 |
| 1126.0635 | 1192.3690 | 1260.0908 |
| 1275.8868 | 1317.5449 | 1325.1187 |

| | | |
|-----------|-----------|-----------|
| 1343.3041 | 1370.0728 | 1386.2219 |
| 1389.4677 | 1409.4163 | 1430.8246 |
| 1497.0152 | 1502.3897 | 1508.6557 |
| 1529.3369 | 2888.7787 | 2929.2605 |
| 2980.4823 | 3010.5099 | 3022.7768 |
| 3043.7358 | 3056.5999 | 3071.7860 |
| 3088.5353 | 3092.2744 | 3814.4897 |

Zero-point correction (Hartree): 0.156594

C5H11O2.tpttt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.52676952

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -3.436498 | -0.698630 | -0.090262 |
| C | -2.156153 | -0.456568 | 0.325002 |
| C | -1.479406 | 0.753347 | -0.335869 |
| C | -0.050187 | 1.013898 | 0.162591 |
| C | 0.959575 | -0.076866 | -0.217114 |
| C | 2.380705 | 0.254499 | 0.222125 |
| O | 3.220011 | -0.827306 | -0.160348 |
| H | 4.121758 | -0.620947 | 0.114407 |
| H | -2.096516 | -0.405093 | 1.431153 |
| H | -1.610457 | -1.392396 | 0.071752 |
| H | -1.485422 | 0.606067 | -1.422646 |
| H | -2.102601 | 1.633026 | -0.135337 |
| H | 0.289437 | 1.975360 | -0.244156 |
| H | -0.062971 | 1.138515 | 1.255298 |
| H | 0.686410 | -1.039178 | 0.233198 |
| H | 0.958633 | -0.229421 | -1.303902 |
| H | 2.702845 | 1.198477 | -0.248857 |
| H | 2.403585 | 0.413225 | 1.313566 |

Rotational constants (GHz): 7.3565900 0.8785600 0.8204400

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 66.7984 | 81.7806 | 89.9358 |
| 135.0655 | 203.7735 | 262.8342 |
| 278.8223 | 327.9811 | 443.2538 |
| 516.6491 | 653.2164 | 754.2949 |
| 831.2663 | 873.9743 | 949.9717 |
| 1010.5242 | 1018.6331 | 1070.5737 |
| 1085.4988 | 1086.8898 | 1104.6230 |
| 1168.1926 | 1216.0168 | 1239.8071 |
| 1273.7764 | 1301.4676 | 1321.9149 |
| 1329.4744 | 1342.9380 | 1370.5499 |
| 1389.6186 | 1405.5559 | 1468.4733 |
| 1498.5246 | 1503.7426 | 1514.4873 |
| 1542.5705 | 2888.4105 | 2925.5873 |
| 2966.9146 | 2993.7638 | 3017.5592 |
| 3040.0150 | 3044.7862 | 3057.2574 |
| 3086.3900 | 3092.5938 | 3828.9958 |

Zero-point correction (Hartree): 0.156455

C5H11O2.ttpmm

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.52772987

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 3.203152 | -0.726742 | -0.127294 |
| C | 2.271194 | 0.188909 | 0.281451 |
| C | 0.856281 | -0.014829 | -0.270216 |
| C | -0.104069 | 1.104827 | 0.155681 |
| C | -1.541846 | 0.966653 | -0.373347 |
| C | -2.390901 | -0.125334 | 0.285725 |
| O | -1.916049 | -1.452752 | 0.083771 |
| H | -1.925964 | -1.627895 | -0.866413 |
| H | 2.274104 | 0.269739 | 1.387448 |
| H | 2.677522 | 1.171970 | -0.048669 |
| H | 0.918794 | -0.060967 | -1.365413 |
| H | 0.473919 | -0.981773 | 0.068589 |
| H | -0.135413 | 1.164892 | 1.253471 |
| H | 0.299938 | 2.068387 | -0.185893 |
| H | -2.069790 | 1.918467 | -0.224376 |
| H | -1.522368 | 0.803357 | -1.461600 |
| H | -2.397849 | 0.016419 | 1.372582 |
| H | -3.433681 | -0.028006 | -0.057306 |

Rotational constants (GHz): 5.1027700 1.1288700 0.9795800

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 69.0194 | 90.5749 | 112.0334 |
| 141.5466 | 205.0138 | 300.4267 |
| 338.6138 | 364.4735 | 431.1602 |
| 503.6899 | 508.1143 | 764.9682 |
| 818.8660 | 896.8949 | 910.1520 |
| 974.9239 | 1013.4422 | 1044.3601 |
| 1078.5634 | 1092.3814 | 1106.6481 |
| 1130.4881 | 1211.8859 | 1264.6201 |

| | | |
|-----------|-----------|-----------|
| 1273.6578 | 1310.7710 | 1331.4942 |
| 1367.8676 | 1381.6126 | 1388.8249 |
| 1400.6570 | 1408.1494 | 1431.3180 |
| 1491.1780 | 1499.6633 | 1520.3540 |
| 1521.8906 | 2873.2759 | 2923.5438 |
| 2988.2470 | 3011.1525 | 3012.5699 |
| 3040.9842 | 3050.8774 | 3055.5874 |
| 3082.2719 | 3120.2932 | 3812.2384 |

Zero-point correction (Hartree): 0.156445

C5H11O2.ttpmp

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.52565244
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 3.175504 | -0.799710 | -0.020519 |
| C | 2.314628 | 0.257928 | 0.079028 |
| C | 0.830272 | -0.076718 | -0.122752 |
| C | -0.079438 | 1.136720 | 0.122459 |
| C | -1.542005 | 0.986063 | -0.329828 |
| C | -2.350247 | -0.129245 | 0.345715 |
| O | -2.083543 | -1.430921 | -0.163156 |
| H | -1.203876 | -1.698546 | 0.126421 |
| H | 2.479309 | 0.660868 | 1.103724 |
| H | 2.638517 | 1.087636 | -0.580868 |
| H | 0.693629 | -0.456188 | -1.142799 |
| H | 0.591579 | -0.900440 | 0.562158 |
| H | -0.056524 | 1.392049 | 1.191905 |
| H | 0.348058 | 2.003943 | -0.400223 |
| H | -2.054989 | 1.938522 | -0.139909 |
| H | -1.583950 | 0.818582 | -1.413622 |
| H | -2.211075 | -0.087711 | 1.439248 |
| H | -3.415622 | 0.037845 | 0.155634 |

Rotational constants (GHz): 5.0742800 1.1238100 0.9640900
 Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 68.7632 | 87.4544 | 116.5296 |
| 125.6912 | 208.0112 | 277.4012 |
| 302.6499 | 382.9491 | 435.2466 |
| 492.0380 | 559.9148 | 763.3491 |
| 810.0991 | 898.2354 | 907.7493 |
| 979.2057 | 1024.4433 | 1036.5641 |
| 1079.1175 | 1096.4316 | 1104.9469 |
| 1141.3719 | 1217.7716 | 1244.6567 |
| 1272.1376 | 1314.1861 | 1324.4429 |
| 1370.5711 | 1376.7428 | 1393.1340 |
| 1399.3276 | 1408.2412 | 1431.8528 |
| 1484.1880 | 1496.5849 | 1511.3436 |
| 1518.0561 | 2879.2101 | 2930.5189 |
| 2980.8539 | 3013.0962 | 3030.3365 |
| 3034.9020 | 3047.8222 | 3077.7716 |
| 3087.0048 | 3089.0193 | 3847.4596 |

Zero-point correction (Hartree): 0.156463

C5H11O2.ttpmt

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.52678705
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -3.208014 | 0.737803 | -0.123131 |
| C | -2.276252 | -0.178633 | 0.284995 |
| C | -0.864325 | 0.015993 | -0.278309 |
| C | 0.093846 | -1.099127 | 0.163123 |
| C | 1.533869 | -0.974135 | -0.364184 |
| C | 2.386930 | 0.110611 | 0.287066 |
| O | 1.896853 | 1.393493 | -0.091249 |
| H | 2.427371 | 2.063695 | 0.356797 |
| H | -2.271703 | -0.261788 | 1.390956 |
| H | -2.690045 | -1.158410 | -0.046698 |
| H | -0.927828 | 0.047493 | -1.372997 |
| H | -0.478630 | 0.988316 | 0.039432 |
| H | 0.121422 | -1.148391 | 1.262057 |
| H | -0.310899 | -2.066232 | -0.167912 |
| H | 2.052500 | -1.928221 | -0.203007 |
| H | 1.523702 | -0.803736 | -1.448300 |
| H | 2.365522 | -0.015098 | 1.382952 |
| H | 3.433465 | -0.016248 | -0.034385 |

Rotational constants (GHz): 5.1793400 1.1271200 0.9789600
 Vibrational harmonic frequencies (cm-1):

| | | |
|----------|-----------|-----------|
| 59.9252 | 87.7815 | 110.8578 |
| 140.8887 | 202.6764 | 267.2418 |
| 320.7976 | 361.5853 | 432.2638 |
| 490.2465 | 552.4088 | 762.0451 |
| 824.9236 | 899.4251 | 911.2282 |
| 983.5561 | 1019.3709 | 1043.5945 |

| | | |
|-----------|-----------|-----------|
| 1079.3183 | 1093.9735 | 1110.8601 |
| 1176.3512 | 1205.0769 | 1249.8651 |
| 1278.2348 | 1289.9356 | 1323.3430 |
| 1337.3250 | 1371.1762 | 1373.7034 |
| 1399.7508 | 1410.3289 | 1465.8381 |
| 1487.4085 | 1499.3016 | 1516.9001 |
| 1536.3076 | 2869.7073 | 2920.9792 |
| 2970.0663 | 2999.2120 | 3007.7470 |
| 3033.2886 | 3045.7222 | 3058.6430 |
| 3079.9213 | 3126.5263 | 3828.2180 |

Zero-point correction (Hartree): 0.156318

C5H11O2.ttpm

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.52687716
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -3.309723 | -0.615435 | 0.358649 |
| C | -2.320046 | -0.005750 | -0.362997 |
| C | -0.972254 | 0.143076 | 0.353006 |
| C | 0.103655 | 0.770856 | -0.543408 |
| C | 1.447663 | 1.036931 | 0.153783 |
| C | 2.199999 | -0.220311 | 0.604907 |
| O | 2.560770 | -1.073696 | -0.476152 |
| H | 1.763013 | -1.519068 | -0.786207 |
| H | -2.205358 | -0.625290 | -1.280496 |
| H | -2.683360 | 0.965004 | -0.757502 |
| H | -1.121070 | 0.761900 | 1.247138 |
| H | -0.667064 | -0.847963 | 0.709888 |
| H | 0.276443 | 0.130848 | -1.420991 |
| H | -0.274667 | 1.720160 | -0.945319 |
| H | 2.098505 | 1.593152 | -0.531209 |
| H | 1.285918 | 1.678674 | 1.031043 |
| H | 3.143446 | 0.074077 | 1.076129 |
| H | 1.621714 | -0.767257 | 1.365806 |

Rotational constants (GHz): 5.7196900 1.0019200 0.9455000

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 45.0736 | 74.6631 | 111.6162 |
| 144.0119 | 215.7989 | 258.9460 |
| 280.3148 | 400.2820 | 431.7866 |
| 488.4913 | 517.7522 | 736.9399 |
| 817.7179 | 854.9752 | 941.5113 |
| 979.2906 | 1010.4968 | 1046.7888 |
| 1083.6922 | 1095.5869 | 1104.2936 |
| 1141.3738 | 1195.3318 | 1255.2169 |
| 1271.3553 | 1311.9332 | 1328.9666 |
| 1364.0502 | 1384.8041 | 1392.7549 |
| 1400.3182 | 1404.8372 | 1428.6705 |
| 1489.4126 | 1502.4037 | 1518.4885 |
| 1520.0710 | 2880.7861 | 2923.7751 |
| 3001.0882 | 3017.5862 | 3029.7145 |
| 3043.6955 | 3053.7320 | 3080.6589 |
| 3088.7514 | 3092.8858 | 3830.2601 |

Zero-point correction (Hartree): 0.156266

C5H11O2.ttpm

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.52816646
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 3.324796 | -0.590566 | -0.351224 |
| C | 2.311718 | -0.038593 | 0.384344 |
| C | 0.986435 | 0.165620 | -0.358956 |
| C | -0.106130 | 0.747950 | 0.546702 |
| C | -1.437064 | 1.028493 | -0.167850 |
| C | -2.184232 | -0.230273 | -0.621350 |
| O | -2.445312 | -1.136980 | 0.444735 |
| H | -3.029313 | -0.691126 | 1.072317 |
| H | 2.166475 | -0.732530 | 1.242254 |
| H | 2.660246 | 0.896487 | 0.868707 |
| H | 1.166160 | 0.834611 | -1.210815 |
| H | 0.678735 | -0.800417 | -0.774211 |
| H | -0.298010 | 0.057364 | 1.377508 |
| H | 0.258243 | 1.682665 | 0.994063 |
| H | -2.092814 | 1.599156 | 0.505958 |
| H | -1.269573 | 1.671524 | -1.043078 |
| H | -3.114460 | 0.059330 | -1.135310 |
| H | -1.585922 | -0.795870 | -1.342828 |

Rotational constants (GHz): 5.7132911 1.0074822 0.9529149

C5H11O2.ttppt

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.52760010
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | | |
|---|-----------|-----------|-----------|--|
| O | -3.306037 | -0.628255 | 0.343845 | |
| C | -2.314436 | -0.008545 | -0.366873 | |
| C | -0.970842 | 0.138465 | 0.356884 | |
| C | 0.102559 | 0.780675 | -0.530807 | |
| C | 1.444018 | 1.036332 | 0.174150 | |
| C | 2.182728 | -0.228094 | 0.603366 | |
| O | 2.433701 | -1.010647 | -0.559643 | |
| H | 2.860391 | -1.831357 | -0.285509 | |
| H | -2.188600 | -0.628808 | -1.282635 | |
| H | -2.676796 | 0.961744 | -0.763411 | |
| H | -1.128258 | 0.743642 | 1.259576 | |
| H | -0.658538 | -0.856415 | 0.693766 | |
| H | 0.285175 | 0.144399 | -1.404897 | |
| H | -0.274998 | 1.738315 | -0.914753 | |
| H | 2.100533 | 1.599719 | -0.499794 | |
| H | 1.289698 | 1.661906 | 1.063553 | |
| H | 3.123064 | 0.054909 | 1.103148 | |
| H | 1.582860 | -0.789829 | 1.337022 | |
| Rotational constants (GHz): | 5.7191700 | 1.0153300 | 0.9593200 | |
| Vibrational harmonic frequencies (cm ⁻¹): | | | | |
| 41.7032 | 70.8808 | | 113.5028 | |
| 149.2549 | 221.9351 | | 255.3918 | |
| 282.6093 | 399.5261 | | 439.0178 | |
| 520.8975 | 527.1282 | | 740.8408 | |
| 825.2668 | 865.7852 | | 949.2480 | |
| 993.5500 | 1010.2992 | | 1051.3002 | |
| 1085.5769 | 1088.0456 | | 1118.6285 | |
| 1147.8373 | 1223.9999 | | 1244.5801 | |
| 1270.5651 | 1290.9490 | | 1320.7589 | |
| 1339.8836 | 1368.0042 | | 1381.4047 | |
| 1400.4738 | 1407.2089 | | 1463.2035 | |
| 1489.3487 | 1499.4876 | | 1511.6159 | |
| 1538.9895 | 2879.3920 | | 2922.9006 | |
| 2982.1239 | 3008.0458 | | 3028.0559 | |
| 3039.6564 | 3039.7811 | | 3073.7882 | |
| 3084.2197 | 3097.3556 | | 3832.7982 | |
| Zero-point correction (Hartree): | 0.156366 | | | |

C5H11O2.ttptm

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.52704030

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | | |
|---|-----------|-----------|-----------|--|
| O | 3.458820 | -0.782055 | -0.111661 | |
| C | 2.532522 | 0.185685 | 0.166267 | |
| C | 1.088194 | -0.146928 | -0.226936 | |
| C | 0.103233 | 0.960705 | 0.171468 | |
| C | -1.339016 | 0.734317 | -0.308582 | |
| C | -2.039044 | -0.465734 | 0.336025 | |
| O | -3.371075 | -0.635549 | -0.128779 | |
| H | -3.865424 | 0.162499 | 0.099378 | |
| H | 2.605599 | 0.346564 | 1.265247 | |
| H | 2.859314 | 1.157914 | -0.255861 | |
| H | 1.052110 | -0.305584 | -1.312461 | |
| H | 0.820865 | -1.102050 | 0.238670 | |
| H | 0.109186 | 1.079218 | 1.265105 | |
| H | 0.459258 | 1.917049 | -0.234912 | |
| H | -1.929604 | 1.635942 | -0.089976 | |
| H | -1.359398 | 0.607078 | -1.398166 | |
| H | -1.523665 | -1.397241 | 0.082044 | |
| H | -2.005533 | -0.368813 | 1.434999 | |
| Rotational constants (GHz): | 7.9892500 | 0.8516700 | 0.8025300 | |
| Vibrational harmonic frequencies (cm ⁻¹): | | | | |
| 71.8119 | 78.1251 | | 89.6214 | |
| 128.7206 | 209.9589 | | 262.9762 | |
| 299.7355 | 341.5674 | | 436.7642 | |
| 502.4259 | 528.7402 | | 745.1909 | |
| 791.1262 | 885.2148 | | 941.1312 | |
| 1006.1704 | 1011.5225 | | 1067.9576 | |
| 1078.3287 | 1090.6825 | | 1094.0925 | |
| 1160.4426 | 1196.0076 | | 1253.5520 | |
| 1290.2728 | 1313.5407 | | 1330.7820 | |
| 1356.2543 | 1367.1925 | | 1383.9585 | |
| 1397.6697 | 1411.0098 | | 1438.4993 | |
| 1496.1570 | 1502.7356 | | 1512.5394 | |
| 1530.0631 | 2880.4876 | | 2922.0257 | |
| 2972.7808 | 3011.7125 | | 3020.2864 | |
| 3045.2562 | 3049.2980 | | 3071.1218 | |
| 3093.6414 | 3101.2742 | | 3811.0092 | |
| Zero-point correction (Hartree): | 0.156240 | | | |

C5H11O2.ttptp

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.52693808

Electronic state : 2-A

```

Cartesian coordinates (Angs):
O      3.459469      -0.787510      -0.115381
C      2.534438       0.180430       0.166179
C      1.089540      -0.149725      -0.226934
C      0.106367       0.961318       0.166924
C     -1.339348       0.737987      -0.304716
C     -2.047215      -0.450151       0.353536
O     -3.419524      -0.534498      -0.009554
H     -3.461727      -0.698462      -0.960556
H      2.608423       0.339489       1.265261
H      2.862021       1.153136      -0.254307
H      1.055290      -0.310966      -1.312418
H      0.819532      -1.103235       0.240411
H      0.114601       1.087212       1.259521
H      0.462971       1.914488      -0.246424
H     -1.935735       1.634381      -0.097964
H     -1.348593       0.602366     -1.396695
H     -1.521562      -1.391641       0.129675
H     -2.037470      -0.329857       1.443044
Rotational constants (GHz):      8.0735600      0.8460500      0.8003400
Vibrational harmonic frequencies (cm-1):
  70.9236      78.1117      87.2996
 128.3198     208.6882     258.5564
 302.7265     331.6864     434.6857
 498.6025     527.0270     746.1819
 791.2605     883.8006     940.9432
1001.4036    1011.6594    1065.1601
1086.3928    1089.0460    1112.9978
1119.7396    1215.4917    1252.6741
1294.1584    1307.8544    1326.4298
1357.8645    1366.5506    1383.8961
1398.4867    1410.9521    1435.4462
1496.7029    1503.0997    1512.9017
1529.7034    2881.7295    2921.8878
2996.1133    3013.1965    3016.6947
3042.8497    3051.6305    3070.5513
3088.2282    3094.7609    3814.2698
Zero-point correction (Hartree): 0.156190

```

C5H11O2.ttptt

```

-----
E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.52650185
Electronic state : 2-A
Cartesian coordinates (Angs):
O      3.454446      -0.792390      -0.122125
C      2.533248       0.178084       0.164117
C      1.086126      -0.145910      -0.225611
C      0.105289       0.958851       0.190714
C     -1.337962       0.751738      -0.290862
C     -2.033678      -0.463708      -0.313408
O     -3.380785      -0.456317      -0.143673
H     -3.818666      -1.245572       0.197660
H      2.610379       0.329122       1.264365
H      2.862145       1.152440      -0.251049
H      1.044158      -0.291943      -1.312820
H      0.819247      -1.106216       0.229938
H      0.114033       1.061206       1.285932
H      0.464789       1.919753      -0.201697
H     -1.938212       1.634288      -0.040134
H     -1.361437       0.659606     -1.383970
H     -1.520163      -1.390622       0.012886
H     -1.983706      -0.406729       1.414674
Rotational constants (GHz):      8.1573100      0.8519900      0.8039900
Vibrational harmonic frequencies (cm-1):
  71.9800      79.0088      88.2032
 127.3443     209.2548     268.4796
 281.2950     317.6797     438.5845
 513.1907     532.0842     748.5186
 802.8341     885.7007     942.5907
1004.4644    1011.3588    1069.8866
1081.5397    1087.5392    1108.9413
1172.2238    1229.5694    1245.7018
1271.0694    1299.5648    1323.8333
1327.8637    1367.5664    1371.9252
1381.5136    1408.1443    1471.5518
1496.8810    1508.1618    1513.5344
1543.3821    2879.1028    2923.4378
2966.3541    3002.8195    3014.4344
3040.9203    3043.9758    3054.7155
3089.7558    3093.7227    3829.3099
Zero-point correction (Hartree): 0.156149

```

C5H11O2.tttpm

```

-----
E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.52820457

```

```
Electronic state : 2-A
Cartesian coordinates (Angs):
O      -3.680936   -0.035170   -0.142709
C      -2.427202   -0.487367    0.168103
C      -1.275261    0.460230   -0.184247
C       0.094950   -0.083061    0.236746
C       1.257209    0.845499   -0.137121
C       2.630075    0.322902    0.295663
O       3.000556   -0.891445   -0.347428
H       2.456789   -1.600187    0.017074
H      -2.450042   -0.680357    1.263857
H      -2.275036   -1.497528   -0.264175
H      -1.290376    0.637588   -1.266944
H      -1.464256    1.429088    0.294216
H       0.101634   -0.256164    1.323804
H       0.251864   -1.064180   -0.234652
H       1.268505    0.999001   -1.223529
H       1.100967    1.831444    0.322061
H       3.402666    1.048640    0.021637
H       2.661701    0.216355    1.392883
Rotational constants (GHz):      8.9935000      0.8291700      0.7916300
Vibrational harmonic frequencies (cm-1):
  63.5853          77.2018          117.9741
 140.6922          165.3885          265.8619
 304.1655          349.4962          369.0741
 448.7445          540.8823          745.8097
 807.9750          873.2240          922.8525
1008.5846          1018.4354          1051.9961
1077.6876          1089.6653          1095.4164
1158.1573          1210.3974          1248.7279
1282.9602          1310.4486          1338.5554
1348.1557          1373.0577          1395.2571
1401.4681          1417.3541          1425.1031
1489.5404          1501.1758          1516.9477
1518.1971          2882.7743          2921.1854
2982.7931          3003.5619          3030.0054
3036.9737          3044.7617          3077.8594
3090.7138          3093.0362          3832.7478
Zero-point correction (Hartree): 0.155978
```

C5H11O2.tttpp

```
-----
E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.52913601
Electronic state : 2-A
Cartesian coordinates (Angs):
O      -3.666499   -0.085048   -0.207427
C      -2.426059   -0.441283    0.247804
C      -1.267228    0.449124   -0.214287
C       0.093827   -0.043218    0.289027
C       1.263451    0.848583   -0.142974
C       2.628577    0.307361    0.290033
O       2.905124   -0.991280   -0.223829
H       2.952901   -0.920670   -1.186302
H      -2.449026   -0.544245    1.352112
H      -2.273512   -1.487362   -0.099597
H      -1.278631    0.489643   -1.310754
H      -1.454760    1.471890    0.137585
H       0.080295   -0.105711    1.386987
H       0.282313   -1.063023   -0.068874
H       1.254964    0.963813   -1.237642
H       1.140406    1.860307    0.267704
H       3.419391    1.021601    0.010868
H       2.661249    0.200985    1.380335
Rotational constants (GHz):      8.6721500      0.8377800      0.8015700
Vibrational harmonic frequencies (cm-1):
  58.3105          80.9710          118.5912
 135.6386          175.2341          267.9616
 321.3080          328.5662          356.1877
 447.7240          548.1380          746.0385
 809.2201          884.9039          917.9427
1001.9451          1014.2921          1051.2407
1086.5980          1090.1283          1101.6964
1122.1068          1220.3006          1257.7683
1272.5722          1315.8950          1333.3765
1347.3820          1372.4220          1390.9184
1401.1734          1417.2845          1426.4136
1494.4049          1501.7220          1519.9655
1520.8638          2883.7927          2920.0110
2993.2995          3010.3821          3021.0219
3039.2363          3050.1425          3068.2959
3083.1132          3090.5055          3810.1325
Zero-point correction (Hartree): 0.155888
```

C5H11O2.tttpt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.52860158
Electronic state : 2-A
Cartesian coordinates (Angs):
O -3.671744 -0.074459 -0.190564
C -2.427367 -0.454967 0.233726
C -1.270586 0.451162 -0.200584
C 0.093149 -0.061868 0.273487
C 1.257113 0.845382 -0.142383
C 2.620467 0.317504 0.288577
O 2.840646 -0.929423 -0.362607
H 3.682683 -1.286385 -0.055415
H -2.435926 -0.612269 1.331809
H -2.284149 -1.482724 -0.168436
H -1.288112 0.534990 -1.294296
H -1.454388 1.459452 0.193196
H 0.087940 -0.159869 1.369384
H 0.274612 -1.067734 -0.123667
H 1.262310 0.963487 -1.233523
H 1.123609 1.848526 0.283959
H 3.400051 1.048386 0.019960
H 2.643503 0.201918 1.385452
Rotational constants (GHz): 8.8756400 0.8404900 0.8041200
Vibrational harmonic frequencies (cm-1):
60.0953 79.6576 119.1141
137.4395 171.6305 253.2288
292.0424 352.3961 359.2848
445.9977 539.8362 745.4958
809.7833 895.3016 929.4781
1012.9206 1017.1453 1050.1424
1079.6987 1087.9271 1122.4857
1151.6273 1237.6185 1239.9277
1280.7674 1287.2796 1324.1005
1342.0198 1350.2961 1373.2090
1398.9628 1419.7261 1462.0877
1490.7555 1502.3329 1519.5870
1536.7569 2882.7371 2919.5395
2971.6576 3002.1021 3014.4752
3035.5052 3040.1493 3067.1455
3077.5339 3094.4534 3832.1649
Zero-point correction (Hartree): 0.155862

C5H11O2.ttttt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.52835589
Electronic state : 2-A
Cartesian coordinates (Angs):
O 3.795112 -0.315234 0.007526
C 2.628668 0.400516 -0.000958
C 1.340489 -0.429486 -0.022204
C 0.075730 0.436394 0.014483
C -1.221326 -0.380706 -0.030850
C -2.479857 0.488007 0.023090
O -3.679834 -0.264994 -0.086519
H -3.721147 -0.863244 0.670772
H 2.665459 1.039873 0.909097
H 2.653317 1.139511 -0.828144
H 1.343252 -1.051783 -0.926007
H 1.356953 -1.118228 0.831452
H 0.084619 1.057760 0.922108
H 0.089058 1.138785 -0.831480
H -1.255719 -0.986398 -0.944896
H -1.236542 -1.087878 0.812039
H -2.473028 1.102033 0.939712
H -2.490678 1.183042 -0.824071
Rotational constants (GHz): 14.5112200 0.7230600 0.7047900
Vibrational harmonic frequencies (cm-1):
64.8803 91.2924 102.4568
139.2564 159.3846 258.6708
297.6131 324.5203 355.9189
462.8402 521.1245 743.8798
784.0726 884.7926 992.9810
1008.3219 1016.8399 1062.1649
1080.0269 1086.4896 1094.1029
1141.2300 1232.9667 1251.5148
1286.7526 1321.0802 1330.9265
1335.5006 1365.9117 1390.0558
1404.6509 1415.8733 1435.7344
1500.3174 1503.4687 1517.1313
1532.1919 2884.0828 2919.1990
2977.5507 3010.3804 3016.0525
3041.6727 3044.1827 3069.5239
3085.7947 3092.5699 3813.7273
Zero-point correction (Hartree): 0.155944

C5H11O2.ttttt

```

-----
E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.52777210
Electronic state : 2-A
Cartesian coordinates (Angs):
O      3.794781      -0.310455      0.012433
C      2.627374      0.403150     -0.017505
C      1.339941     -0.428016     -0.006509
C      0.074853      0.438153      0.003620
C     -1.218177     -0.385045     -0.004380
C     -2.473823      0.478003      0.007145
O     -3.600715     -0.389072     -0.001916
H     -4.398632      0.153581      0.005420
H      2.667675      1.068294      0.873808
H      2.647278      1.117202     -0.866298
H      1.340428     -1.080773     -0.888547
H      1.358311     -1.086874      0.870156
H      0.087716      1.090873      0.888898
H      0.085927      1.109643     -0.867361
H     -1.249137     -1.030084     -0.891237
H     -1.247119     -1.050895      0.866980
H     -2.472096      1.123395      0.901889
H     -2.473885      1.144381     -0.872065
Rotational constants (GHz): 14.5732900      0.7282600      0.7087600
Vibrational harmonic frequencies (cm-1):
  65.6871      88.4594      103.6900
 141.2769     154.0930     262.9956
 277.3361     303.7554     393.7783
 460.6749     523.4596     746.1678
 792.5376     894.7996     987.2141
1018.9808     1019.6155    1060.1913
1067.9157     1088.7611    1100.5996
1199.4398     1223.1864    1248.7038
1278.0528     1297.8149    1326.0381
1336.2641     1337.0634    1369.4713
1397.9390     1415.2649    1472.3366
1500.9858     1507.1558    1521.3574
1544.2370     2883.0566    2920.0929
2966.5050     2992.7225    3010.1609
3039.5139     3042.4524    3047.9305
3085.5059     3095.2632    3828.0147
Zero-point correction (Hartree): 0.155914
    
```

C5H9O2.1-5Hshift.m.mm

```

-----
E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.52531263
Electronic state : 2-A
Cartesian coordinates (Angs):
C     -0.691079      0.639478     -0.847486
C      0.285120      1.463173     -0.016179
C      1.217002      0.579849      0.836977
C      1.828130     -0.522142     -0.046314
O      0.831853     -1.279002     -0.698795
C     -1.899588      0.020540     -0.163292
H     -0.943276      1.085525     -1.814770
H     -0.270642      2.147565      0.641762
H      0.888525      2.086844     -0.686673
H      0.643041      0.119388      1.645004
H      2.017520      1.179931      1.284857
H      2.396812     -1.225179      0.580426
H      2.529243     -0.080655     -0.774035
H      0.033700     -0.385314     -1.109619
O     -1.561032     -0.834277     -0.915241
H     -2.534221      0.815255      0.255995
H     -2.507525     -0.505230     -0.918002
H     -0.857258     -1.417286      0.581246
Rotational constants (GHz): 3.5648000      2.1005300      1.7952300
Vibrational harmonic frequencies (cm-1):
i1466.0032      112.3279      176.0770
 186.2670      281.3492      329.8497
 416.6431      492.0719      528.1737
 609.1485      691.5556      789.3167
 854.4580      855.2648      899.6778
 928.1572      989.2541     1031.4555
1050.6717      1058.0553     1116.7473
1143.0665      1185.8910     1212.8141
1231.2576      1264.1871     1289.8850
1348.8501      1355.0545     1382.0817
1388.2008      1400.7982     1463.3637
1483.1576      1498.4912     1503.7930
1514.0476      1535.5543     2975.8756
2979.9239      3013.8232     3028.3574
3029.6608      3062.4569     3066.4065
3096.5359      3126.7413     3696.2100
Zero-point correction (Hartree): 0.154170
    
```


C5H9O2.1-5Hshift.m.mp

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.51696491

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| C | 0.594972 | -0.112561 | 0.990031 |
| C | -0.150583 | 1.173652 | 0.642678 |
| C | -1.119065 | 0.953667 | -0.538544 |
| C | -2.022151 | -0.252322 | -0.227806 |
| O | -1.266892 | -1.410026 | 0.001758 |
| C | 1.916416 | -0.382173 | 0.289442 |
| H | 0.677870 | -0.304467 | 2.064948 |
| H | 0.555368 | 1.983389 | 0.399678 |
| H | -0.720961 | 1.515654 | 1.513670 |
| H | -0.549137 | 0.733879 | -1.446323 |
| H | -1.727417 | 1.847894 | -0.717774 |
| H | -2.668161 | -0.454303 | -1.096661 |
| H | -2.681601 | -0.011065 | 0.626013 |
| H | -0.247674 | -0.987456 | 0.584909 |
| O | 1.922301 | -0.115901 | -1.106006 |
| H | 2.708466 | 0.198023 | 0.798680 |
| H | 2.187040 | -1.437604 | 0.398145 |
| H | 1.905405 | 0.841889 | -1.226116 |

Rotational constants (GHz): 3.8515000 1.7583300 1.6355400

Vibrational harmonic frequencies (cm-1):

| | | |
|------------|-----------|-----------|
| i1486.9240 | 86.7955 | 117.0991 |
| 163.0944 | 243.8843 | 312.0632 |
| 328.5772 | 434.6566 | 481.9952 |
| 546.9620 | 611.4768 | 789.0475 |
| 824.1616 | 858.6299 | 904.8186 |
| 917.0464 | 983.8433 | 1034.0948 |
| 1047.6893 | 1069.9603 | 1110.2146 |
| 1129.4998 | 1166.0991 | 1195.0075 |
| 1223.0370 | 1230.6760 | 1268.5175 |
| 1343.3023 | 1347.0607 | 1375.7828 |
| 1386.4749 | 1392.8929 | 1418.3985 |
| 1487.3586 | 1496.2600 | 1498.5337 |
| 1512.5778 | 1565.3875 | 2941.7371 |
| 2947.1109 | 2997.1983 | 3008.7454 |
| 3056.9217 | 3069.6932 | 3085.4548 |
| 3092.3849 | 3115.2113 | 3824.8214 |

Zero-point correction (Hartree): 0.152733

C5H9O2.1-5Hshift.m.mt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.51763580

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| C | -0.600233 | 0.052776 | -0.994672 |
| C | 0.169016 | 1.265066 | -0.476794 |
| C | 1.140139 | 0.869788 | 0.654186 |
| C | 2.008895 | -0.311466 | 0.188208 |
| O | 1.224516 | -1.411597 | -0.186114 |
| C | -1.922825 | -0.275906 | -0.342012 |
| H | -0.688222 | 0.006510 | -2.084413 |
| H | -0.529378 | 2.027527 | -0.106071 |
| H | 0.738103 | 1.715243 | -1.298764 |
| H | 0.565007 | 0.565105 | 1.532573 |
| H | 1.777770 | 1.717274 | 0.932849 |
| H | 2.648197 | -0.640515 | 1.022873 |
| H | 2.676480 | 0.016401 | -0.629963 |
| H | 0.220883 | -0.889455 | -0.709580 |
| O | -1.799055 | -0.194965 | 1.070863 |
| H | -2.680032 | 0.444135 | -0.708117 |
| H | -2.254100 | -1.276013 | -0.663903 |
| H | -2.648350 | -0.435271 | 1.461014 |

Rotational constants (GHz): 3.8561300 1.7897800 1.6631000

Vibrational harmonic frequencies (cm-1):

| | | |
|------------|-----------|-----------|
| i1494.1124 | 81.9237 | 119.4660 |
| 156.0324 | 228.9378 | 269.7168 |
| 322.1832 | 434.7817 | 485.1823 |
| 538.4878 | 615.5276 | 794.9085 |
| 829.2253 | 857.4345 | 911.8423 |
| 923.9094 | 989.3538 | 1038.9120 |
| 1051.8920 | 1083.1553 | 1123.2831 |
| 1145.5539 | 1167.0839 | 1196.1760 |
| 1215.4171 | 1245.7129 | 1248.6713 |
| 1284.2412 | 1348.1567 | 1362.3775 |
| 1382.9889 | 1388.9292 | 1453.8362 |
| 1483.9618 | 1496.2802 | 1510.6018 |
| 1520.7372 | 1564.6835 | 2927.4917 |
| 2944.1001 | 2999.0990 | 3005.0306 |
| 3026.0320 | 3057.5054 | 3072.0297 |
| 3099.6394 | 3126.4830 | 3831.7910 |

Zero-point correction (Hartree): 0.152548

C5H9O2.1-5Hshift.m.pm

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.51855814

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| C | 0.574406 | -0.204438 | 0.689869 |
| C | -0.126787 | 1.132799 | 0.476881 |
| C | -1.285966 | 1.000634 | -0.529666 |
| C | -2.209852 | -0.144690 | -0.080073 |
| O | -1.506815 | -1.353437 | 0.033213 |
| C | 1.611575 | -0.629605 | -0.335829 |
| H | 0.925279 | -0.370144 | 1.712303 |
| H | 0.584169 | 1.897512 | 0.126513 |
| H | -0.519656 | 1.499250 | 1.432179 |
| H | -0.898403 | 0.769899 | -1.528869 |
| H | -1.848988 | 1.938145 | -0.603316 |
| H | -2.995019 | -0.300143 | -0.836261 |
| H | -2.710444 | 0.132970 | 0.864718 |
| H | -0.407207 | -1.011740 | 0.520211 |
| O | 2.847018 | 0.067784 | -0.166175 |
| H | 1.853971 | -1.688162 | -0.206974 |
| H | 1.219895 | -0.506234 | -1.356113 |
| H | 2.694519 | 0.995668 | -0.387792 |

Rotational constants (GHz): 4.9053000 1.4880100 1.2886000

Vibrational harmonic frequencies (cm-1):

| | | |
|------------|-----------|-----------|
| i1485.2959 | 68.8857 | 115.3732 |
| 143.0707 | 253.4776 | 306.1765 |
| 325.0275 | 406.4349 | 483.3784 |
| 522.5849 | 648.0729 | 806.2954 |
| 814.8984 | 870.1842 | 890.7170 |
| 946.5123 | 984.7145 | 1014.8537 |
| 1057.6865 | 1062.5576 | 1101.5932 |
| 1127.6043 | 1167.6483 | 1190.0195 |
| 1214.3056 | 1243.7797 | 1268.9415 |
| 1336.7053 | 1354.3071 | 1370.9138 |
| 1384.7973 | 1396.1823 | 1422.4852 |
| 1486.7257 | 1495.4314 | 1506.5417 |
| 1515.9991 | 1546.9206 | 2955.5918 |
| 2998.1643 | 3013.4457 | 3015.4596 |
| 3052.3560 | 3070.7053 | 3098.2623 |
| 3101.5152 | 3112.9809 | 3814.8659 |

Zero-point correction (Hartree): 0.152831

C5H9O2.1-5Hshift.m.pp

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.51992113

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| C | 0.566771 | -0.239476 | 0.704749 |
| C | -0.095582 | 1.115167 | 0.496148 |
| C | -1.249560 | 1.015770 | -0.519804 |
| C | -2.203004 | -0.112988 | -0.090067 |
| O | -1.529682 | -1.339566 | 0.020189 |
| C | 1.603206 | -0.658229 | -0.323400 |
| H | 0.891759 | -0.428012 | 1.734350 |
| H | 0.654677 | 1.837555 | 0.147393 |
| H | -0.487254 | 1.489016 | 1.449291 |
| H | -0.858061 | 0.788914 | -1.518171 |
| H | -1.792284 | 1.965445 | -0.589054 |
| H | -2.982983 | -0.245875 | -0.856100 |
| H | -2.708005 | 0.166251 | 0.851904 |
| H | -0.427686 | -1.030101 | 0.516777 |
| O | 2.742586 | 0.206402 | -0.317586 |
| H | 1.897504 | -1.705357 | -0.162560 |
| H | 1.189052 | -0.588722 | -1.333078 |
| H | 3.189061 | 0.094741 | 0.532657 |

Rotational constants (GHz): 4.8580700 1.5139300 1.3150600

Vibrational harmonic frequencies (cm-1):

| | | |
|------------|-----------|-----------|
| i1506.7578 | 75.4159 | 123.0529 |
| 146.0181 | 257.1890 | 313.1319 |
| 328.7670 | 425.7257 | 486.0893 |
| 532.5796 | 647.9113 | 809.9727 |
| 815.3783 | 872.2702 | 896.9027 |
| 942.4729 | 992.3086 | 1010.6371 |
| 1047.2111 | 1065.7667 | 1107.1929 |
| 1119.5091 | 1165.2263 | 1186.0868 |
| 1213.1399 | 1248.1329 | 1270.2282 |
| 1341.7828 | 1365.2723 | 1374.0227 |
| 1383.9800 | 1387.4871 | 1419.1790 |
| 1486.3686 | 1495.8583 | 1505.6171 |
| 1519.4647 | 1541.4722 | 2955.2713 |
| 3011.7234 | 3016.9894 | 3031.4030 |
| 3053.3397 | 3069.9932 | 3081.1188 |

3099.7414 3111.3331 3804.5778
 Zero-point correction (Hartree): 0.152989

C5H9O2.1-5Hshift.m.pt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.51838877

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| C | 0.562109 | -0.217048 | 0.725052 |
| C | -0.109121 | 1.127532 | 0.489385 |
| C | -1.251572 | 1.008219 | -0.537231 |
| C | -2.196916 | -0.127691 | -0.107740 |
| O | -1.510149 | -1.345389 | 0.022393 |
| C | 1.595771 | -0.652972 | -0.290488 |
| H | 0.896213 | -0.385037 | 1.752397 |
| H | 0.639805 | 1.852403 | 0.142456 |
| H | -0.513810 | 1.508418 | 1.434123 |
| H | -0.849000 | 0.777443 | -1.530369 |
| H | -1.804293 | 1.951159 | -0.619266 |
| H | -2.966116 | -0.277783 | -0.881219 |
| H | -2.715861 | 0.154265 | 0.825654 |
| H | -0.431774 | -1.018842 | 0.541506 |
| O | 2.723648 | 0.217332 | -0.162874 |
| H | 1.878670 | -1.699629 | -0.102119 |
| H | 1.170818 | -0.604961 | -1.304241 |
| H | 3.385726 | -0.061223 | -0.808940 |

Rotational constants (GHz): 4.8667400 1.5252400 1.3210000

Vibrational harmonic frequencies (cm-1):

| | | |
|------------|-----------|-----------|
| i1529.1407 | 69.5969 | 120.0980 |
| 148.3373 | 232.0393 | 262.6640 |
| 317.7636 | 416.4396 | 485.1952 |
| 530.0055 | 648.2099 | 812.0948 |
| 814.1402 | 869.6423 | 902.4896 |
| 946.5036 | 991.1184 | 1019.7138 |
| 1061.1192 | 1069.1896 | 1095.9441 |
| 1147.6223 | 1171.8352 | 1203.5226 |
| 1221.3511 | 1247.4178 | 1263.3913 |
| 1278.5451 | 1344.4028 | 1365.5821 |
| 1380.4643 | 1385.2348 | 1461.0101 |
| 1485.1903 | 1496.2547 | 1506.1195 |
| 1535.8680 | 1539.2278 | 2956.8101 |
| 2994.6333 | 3013.5624 | 3026.7601 |
| 3031.6790 | 3053.0530 | 3077.1710 |
| 3098.7284 | 3111.0152 | 3813.5689 |

Zero-point correction (Hartree): 0.152688

C5H9O2.1-5Hshift.m.tm

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.51773630

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| C | 0.589086 | 0.388905 | 0.625025 |
| C | -0.577952 | 1.334185 | 0.364104 |
| C | -1.621432 | 0.685070 | -0.567381 |
| C | -2.010605 | -0.689745 | -0.000845 |
| O | -0.890297 | -1.521540 | 0.136512 |
| C | 1.703712 | 0.375114 | -0.403446 |
| H | 0.969959 | 0.421614 | 1.652647 |
| H | -0.221672 | 2.277220 | -0.076416 |
| H | -1.060048 | 1.594110 | 1.313343 |
| H | -1.201249 | 0.549370 | -1.570665 |
| H | -2.507061 | 1.323587 | -0.664156 |
| H | -2.698120 | -1.193169 | -0.698477 |
| H | -2.550059 | -0.557484 | 0.954653 |
| H | 0.013330 | -0.754841 | 0.523456 |
| O | 2.669182 | -0.639660 | -0.185498 |
| H | 1.296415 | 0.189095 | -1.402386 |
| H | 2.173995 | 1.376878 | -0.433257 |
| H | 3.056586 | -0.497951 | 0.688405 |

Rotational constants (GHz): 4.2539800 1.6094200 1.3179500

Vibrational harmonic frequencies (cm-1):

| | | |
|------------|-----------|-----------|
| i1512.7606 | 83.1536 | 113.8181 |
| 124.5190 | 258.3114 | 301.1494 |
| 328.5956 | 399.0995 | 488.3698 |
| 525.3216 | 621.1140 | 793.4437 |
| 835.7470 | 854.9182 | 904.6496 |
| 961.7157 | 987.4199 | 1046.0039 |
| 1069.4075 | 1080.4429 | 1108.0771 |
| 1116.8879 | 1173.6551 | 1191.2434 |
| 1212.3573 | 1248.9124 | 1264.4700 |
| 1335.0661 | 1349.9219 | 1367.6218 |
| 1388.5685 | 1391.7602 | 1426.4809 |
| 1489.5280 | 1495.1857 | 1505.4816 |
| 1507.6451 | 1550.7354 | 2930.3765 |

| | | |
|-----------|-----------|-----------|
| 2950.4034 | 3010.7910 | 3012.9138 |
| 3051.5480 | 3063.8700 | 3077.3496 |
| 3092.1624 | 3100.8858 | 3808.9835 |

Zero-point correction (Hartree): 0.152637

C5H9O2.1-5Hshift.m.tp

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.52099547

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| C | 0.572499 | 0.583091 | 0.675451 |
| C | -0.663950 | 1.388085 | 0.305302 |
| C | -1.588598 | 0.577525 | -0.627975 |
| C | -1.858062 | -0.805549 | -0.009526 |
| O | -0.663284 | -1.499057 | 0.251544 |
| C | 1.672485 | 0.468995 | -0.365850 |
| H | 0.960213 | 0.749563 | 1.684615 |
| H | -0.381299 | 2.331216 | -0.186341 |
| H | -1.213877 | 1.660706 | 1.213259 |
| H | -1.113143 | 0.441760 | -1.605967 |
| H | -2.533848 | 1.106367 | -0.795310 |
| H | -2.433039 | -1.418745 | -0.720432 |
| H | -2.470362 | -0.693492 | 0.902091 |
| H | 0.086286 | -0.588089 | 0.712453 |
| O | 2.511047 | -0.654200 | -0.144766 |
| H | 1.236347 | 0.451309 | -1.376587 |
| H | 2.326154 | 1.350111 | -0.316733 |
| H | 1.948226 | -1.437524 | -0.229683 |

Rotational constants (GHz): 3.9694700 1.7965800 1.4155900

Vibrational harmonic frequencies (cm-1):

| | | |
|------------|-----------|-----------|
| i1398.6832 | 46.3412 | 135.0394 |
| 151.3171 | 275.7542 | 321.3042 |
| 399.3293 | 452.0620 | 495.8357 |
| 526.5139 | 628.9689 | 820.8712 |
| 839.8713 | 857.6289 | 898.4420 |
| 971.0082 | 989.9600 | 1037.5411 |
| 1049.9761 | 1080.1777 | 1095.1352 |
| 1144.0012 | 1174.8936 | 1196.2246 |
| 1231.9503 | 1253.4381 | 1274.6439 |
| 1332.0028 | 1349.9662 | 1370.7266 |
| 1387.3219 | 1408.1793 | 1426.0486 |
| 1486.7502 | 1493.0976 | 1504.5806 |
| 1513.4016 | 1543.0309 | 2964.4521 |
| 2995.9569 | 3010.9776 | 3017.5681 |
| 3049.9315 | 3054.9812 | 3073.0003 |
| 3099.7026 | 3106.1064 | 3788.7582 |

Zero-point correction (Hartree): 0.153377

C5H9O2.1-5Hshift.m.tt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.51754369

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| C | 0.585809 | 0.397617 | 0.628063 |
| C | -0.584994 | 1.334178 | 0.359706 |
| C | -1.625566 | 0.680176 | -0.571451 |
| C | -2.004501 | -0.698323 | -0.006730 |
| O | -0.878260 | -1.521572 | 0.130781 |
| C | 1.686841 | 0.362122 | -0.404730 |
| H | 0.990481 | 0.441498 | 1.643107 |
| H | -0.234007 | 2.279888 | -0.079265 |
| H | -1.069239 | 1.591002 | 1.308729 |
| H | -1.206620 | 0.549409 | -1.576060 |
| H | -2.515933 | 1.312685 | -0.665504 |
| H | -2.687858 | -1.206667 | -0.705101 |
| H | -2.546145 | -0.571024 | 0.948213 |
| H | 0.015172 | -0.746916 | 0.547996 |
| O | 2.654428 | -0.590438 | 0.010387 |
| H | 1.268545 | 0.112631 | -1.392218 |
| H | 2.131463 | 1.372493 | -0.488085 |
| H | 3.299254 | -0.693545 | -0.700302 |

Rotational constants (GHz): 4.2953400 1.6170400 1.3238500

Vibrational harmonic frequencies (cm-1):

| | | |
|------------|-----------|-----------|
| i1497.5764 | 87.6517 | 116.1062 |
| 126.8079 | 239.4959 | 270.9407 |
| 319.6891 | 393.8421 | 489.5847 |
| 527.0203 | 625.0546 | 815.9409 |
| 835.8951 | 856.1219 | 908.4966 |
| 959.2411 | 991.5651 | 1052.9202 |
| 1074.6548 | 1081.6894 | 1115.9361 |
| 1130.9428 | 1181.8746 | 1201.3744 |
| 1221.9650 | 1250.3871 | 1266.2942 |
| 1281.0553 | 1343.3962 | 1354.1369 |
| 1370.7723 | 1389.3509 | 1462.1737 |
| 1490.1207 | 1495.3012 | 1506.4818 |

| | | |
|-----------|-----------|-----------|
| 1521.9790 | 1547.4583 | 2929.4887 |
| 2950.3586 | 3004.2016 | 3009.1521 |
| 3012.7960 | 3050.6488 | 3072.6288 |
| 3097.1219 | 3108.9092 | 3829.1982 |

Zero-point correction (Hartree): 0.152565

C5H9O2.1-5Hshift.p.mm

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.51988200

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| C | 0.568548 | -0.171937 | -0.473318 |
| C | -0.075202 | 1.083615 | 0.091521 |
| C | -1.591212 | 1.077596 | -0.169090 |
| C | -2.189098 | -0.229632 | 0.381809 |
| O | -1.579527 | -1.354993 | -0.193060 |
| H | 0.659165 | -0.153226 | -1.566518 |
| C | 1.814118 | -0.691142 | 0.216416 |
| H | 0.380220 | 1.982507 | -0.344768 |
| H | 0.110078 | 1.134557 | 1.172263 |
| H | -1.787754 | 1.130436 | -1.246912 |
| H | -2.075390 | 1.942123 | 0.299400 |
| H | -3.259183 | -0.279269 | 0.126353 |
| H | -2.110779 | -0.234547 | 1.483740 |
| H | -0.382457 | -1.022783 | -0.316790 |
| O | 2.882172 | 0.259972 | 0.167943 |
| H | 1.617920 | -0.851199 | 1.281322 |
| H | 2.120703 | -1.655792 | -0.213197 |
| H | 3.143391 | 0.356359 | -0.757985 |

Rotational constants (GHz): 5.2194400 1.3974900 1.1889000

Vibrational harmonic frequencies (cm-1):

| | | |
|------------|-----------|-----------|
| i1517.3418 | 72.4570 | 114.9808 |
| 152.1473 | 292.5186 | 302.2965 |
| 322.1414 | 397.5099 | 472.4664 |
| 510.8900 | 586.3688 | 808.5437 |
| 830.9752 | 880.4714 | 899.3009 |
| 970.3266 | 979.4397 | 1014.3268 |
| 1061.0163 | 1070.1758 | 1096.3358 |
| 1128.1920 | 1174.9948 | 1202.9011 |
| 1227.4990 | 1246.2161 | 1267.6078 |
| 1330.3837 | 1362.0709 | 1374.0176 |
| 1386.2181 | 1394.2151 | 1418.6542 |
| 1484.8216 | 1494.2097 | 1507.9664 |
| 1516.8869 | 1546.5411 | 2954.7203 |
| 3010.4196 | 3014.6007 | 3027.6611 |
| 3046.4164 | 3058.5767 | 3073.4872 |
| 3095.2033 | 3099.9002 | 3804.3797 |

Zero-point correction (Hartree): 0.152827

C5H9O2.1-5Hshift.p.mp

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.51931547

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| C | 0.570890 | -0.169696 | -0.474849 |
| C | -0.082487 | 1.087583 | 0.080128 |
| C | -1.599331 | 1.070546 | -0.179905 |
| C | -2.188892 | -0.233628 | 0.385682 |
| O | -1.571861 | -1.360997 | -0.175646 |
| H | 0.678191 | -0.150599 | -1.563948 |
| C | 1.816651 | -0.685491 | 0.218675 |
| H | 0.359243 | 1.988402 | -0.369216 |
| H | 0.092621 | 1.149927 | 1.164123 |
| H | -1.791821 | 1.109348 | -1.258635 |
| H | -2.087940 | 1.938545 | 0.277362 |
| H | -3.258694 | -0.291393 | 0.131006 |
| H | -2.111488 | -0.224484 | 1.487962 |
| H | -0.378502 | -1.020855 | -0.309845 |
| O | 2.935364 | 0.181123 | 0.011821 |
| H | 1.621393 | -0.831447 | 1.292260 |
| H | 2.113872 | -1.651900 | -0.197528 |
| H | 2.754107 | 1.007561 | 0.478674 |

Rotational constants (GHz): 5.2363200 1.3902300 1.1804300

Vibrational harmonic frequencies (cm-1):

| | | |
|------------|-----------|-----------|
| i1509.0390 | 74.7752 | 105.9516 |
| 150.6326 | 287.5059 | 303.1678 |
| 334.2719 | 383.1988 | 471.8107 |
| 508.4708 | 582.7439 | 809.4185 |
| 827.3475 | 880.3494 | 900.4478 |
| 972.0115 | 979.4631 | 1020.6140 |
| 1051.1064 | 1074.5606 | 1110.2764 |
| 1130.2376 | 1179.1590 | 1200.2933 |
| 1223.1270 | 1250.4674 | 1262.8684 |
| 1324.7911 | 1361.9505 | 1375.1357 |
| 1387.3185 | 1395.7162 | 1420.6376 |

| | | |
|-----------|-----------|-----------|
| 1488.4443 | 1494.8615 | 1508.6967 |
| 1515.5975 | 1548.7681 | 2951.6057 |
| 3001.8450 | 3007.3376 | 3010.9910 |
| 3041.5811 | 3054.7743 | 3095.5067 |
| 3098.4519 | 3110.9679 | 3813.3154 |

Zero-point correction (Hartree): 0.152825

C5H9O2.1-5Hshift.p.mt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.51835802

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| C | 0.565915 | -0.153810 | -0.487344 |
| C | -0.085908 | 1.089337 | 0.091120 |
| C | -1.602784 | 1.071316 | -0.162292 |
| C | -2.185813 | -0.242245 | 0.390355 |
| O | -1.565341 | -1.362662 | -0.183124 |
| H | 0.663761 | -0.125991 | -1.577024 |
| C | 1.807815 | -0.676987 | 0.194164 |
| H | 0.363079 | 1.991016 | -0.346287 |
| H | 0.103096 | 1.136437 | 1.171580 |
| H | -1.804309 | 1.124009 | -1.239095 |
| H | -2.093364 | 1.930131 | 0.309895 |
| H | -3.255616 | -0.303340 | 0.136509 |
| H | -2.105471 | -0.245142 | 1.492209 |
| H | -0.384211 | -1.013964 | -0.329851 |
| O | 2.838486 | 0.300741 | 0.026865 |
| H | 1.597988 | -0.849803 | 1.261945 |
| H | 2.100098 | -1.641496 | -0.247935 |
| H | 3.634435 | -0.032152 | 0.462098 |

Rotational constants (GHz): 5.2470700 1.4057000 1.1923100

Vibrational harmonic frequencies (cm-1):

| | | |
|------------|-----------|-----------|
| i1546.1058 | 71.5354 | 109.0443 |
| 151.5258 | 237.9667 | 299.6675 |
| 305.1276 | 374.2569 | 472.0376 |
| 508.5233 | 585.8459 | 803.0448 |
| 833.6944 | 883.2494 | 900.6554 |
| 966.0618 | 996.4554 | 1019.3750 |
| 1068.7418 | 1072.4301 | 1095.0207 |
| 1160.8986 | 1174.1572 | 1214.9181 |
| 1219.8305 | 1241.1772 | 1260.9213 |
| 1279.1306 | 1331.4453 | 1363.5929 |
| 1384.2850 | 1393.1540 | 1461.8546 |
| 1483.6707 | 1494.5232 | 1509.5192 |
| 1534.1970 | 1545.0241 | 2953.9582 |
| 2983.2421 | 3010.8769 | 3018.7322 |
| 3027.0826 | 3047.2793 | 3066.7471 |
| 3095.4511 | 3102.0492 | 3810.0770 |

Zero-point correction (Hartree): 0.152460

C5H9O2.1-5Hshift.p.pm

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.51829007

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| C | 0.570524 | 0.221533 | -0.785985 |
| C | -0.177236 | 1.221547 | 0.080718 |
| C | -1.686643 | 0.926556 | 0.070723 |
| C | -1.912268 | -0.542633 | 0.472401 |
| O | -1.225121 | -1.415845 | -0.382494 |
| H | 0.425290 | 0.393170 | -1.858290 |
| C | 2.023621 | -0.079216 | -0.464598 |
| H | 0.009875 | 2.250096 | -0.261814 |
| H | 0.184528 | 1.155308 | 1.115205 |
| H | -2.090663 | 1.085526 | -0.936281 |
| H | -2.222721 | 1.594600 | 0.754667 |
| H | -2.983063 | -0.784541 | 0.387465 |
| H | -1.622702 | -0.683886 | 1.529007 |
| H | -0.145259 | -0.832144 | -0.595548 |
| O | 2.266102 | -0.444409 | 0.885641 |
| H | 2.366944 | -0.922541 | -1.072327 |
| H | 2.642936 | 0.789926 | -0.756486 |
| H | 2.198996 | 0.349806 | 1.429672 |

Rotational constants (GHz): 4.1526000 1.5942200 1.4129000

Vibrational harmonic frequencies (cm-1):

| | | |
|------------|-----------|-----------|
| i1531.7762 | 68.8331 | 100.2945 |
| 190.4414 | 258.8202 | 290.3092 |
| 309.5306 | 420.2681 | 471.6690 |
| 509.0124 | 603.1773 | 784.8920 |
| 823.2379 | 878.7493 | 903.5166 |
| 919.5298 | 981.9305 | 1012.3559 |
| 1069.4796 | 1077.5921 | 1121.1807 |
| 1140.4152 | 1180.7766 | 1200.4061 |
| 1234.7416 | 1241.8055 | 1267.9062 |
| 1321.7554 | 1361.6096 | 1370.4301 |

| | | |
|-----------|-----------|-----------|
| 1388.4378 | 1403.1332 | 1417.2884 |
| 1481.3829 | 1493.7489 | 1499.3984 |
| 1508.7415 | 1568.5979 | 2938.0748 |
| 2955.6909 | 3008.2585 | 3013.0118 |
| 3045.7699 | 3056.8149 | 3083.8148 |
| 3091.7622 | 3096.4860 | 3831.2195 |

Zero-point correction (Hartree): 0.152629

C5H9O2.1-5Hshift.p.pp

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.52364611

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| C | -0.626732 | 0.726881 | 0.713431 |
| C | 0.312175 | 1.335476 | -0.321451 |
| C | 1.724206 | 0.731431 | -0.192141 |
| C | 1.625202 | -0.802869 | -0.272947 |
| O | 0.752016 | -1.320465 | 0.707072 |
| H | -0.685978 | 1.270748 | 1.661629 |
| C | -1.959405 | 0.195626 | 0.215666 |
| H | 0.363240 | 2.425498 | -0.202037 |
| H | -0.074882 | 1.123901 | -1.324017 |
| H | 2.165139 | 1.010220 | 0.772702 |
| H | 2.388948 | 1.102346 | -0.980344 |
| H | 2.619218 | -1.240272 | -0.091819 |
| H | 1.303226 | -1.093754 | -1.285563 |
| H | -0.000879 | -0.335916 | 0.996377 |
| O | -1.787147 | -0.774759 | -0.805005 |
| H | -2.540489 | -0.203342 | 1.062262 |
| H | -2.554158 | 1.007197 | -0.227523 |
| H | -1.155014 | -1.424099 | -0.453555 |

Rotational constants (GHz): 3.7585400 2.0104600 1.6275000

Vibrational harmonic frequencies (cm-1):

| | | |
|------------|-----------|-----------|
| i1385.0272 | 79.8208 | 135.3106 |
| 174.7041 | 276.1398 | 312.5807 |
| 445.4299 | 454.7273 | 552.9892 |
| 577.6463 | 645.7104 | 803.8728 |
| 826.9946 | 880.3410 | 910.3421 |
| 932.5843 | 988.8804 | 1030.0337 |
| 1040.1610 | 1072.2128 | 1102.4534 |
| 1143.0906 | 1183.8033 | 1207.5683 |
| 1227.1886 | 1247.6654 | 1277.3663 |
| 1321.5511 | 1358.2967 | 1377.9377 |
| 1382.4873 | 1398.2564 | 1450.2736 |
| 1481.7099 | 1495.3630 | 1512.0539 |
| 1513.5450 | 1549.7721 | 2980.4421 |
| 2990.2020 | 3019.4716 | 3033.1371 |
| 3037.7602 | 3049.9361 | 3086.3578 |
| 3096.4502 | 3105.6907 | 3721.4658 |

Zero-point correction (Hartree): 0.153758

C5H9O2.1-5Hshift.p.pt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.51905489

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| C | 0.574789 | 0.293743 | -0.785488 |
| C | -0.183041 | 1.234537 | 0.138191 |
| C | -1.685744 | 0.906964 | 0.134363 |
| C | -1.874986 | -0.588353 | 0.449090 |
| O | -1.197203 | -1.392475 | -0.479068 |
| H | 0.449244 | 0.523199 | -1.848553 |
| C | 2.014371 | -0.014927 | -0.450826 |
| H | -0.026841 | 2.279226 | -0.169669 |
| H | 0.213347 | 1.131299 | 1.153549 |
| H | -2.115564 | 1.116335 | -0.852943 |
| H | -2.222437 | 1.519965 | 0.867757 |
| H | -2.943266 | -0.845656 | 0.375591 |
| H | -1.552527 | -0.791306 | 1.485186 |
| H | -0.129501 | -0.776668 | -0.666970 |
| O | 2.098707 | -0.436901 | 0.903954 |
| H | 2.395507 | -0.785640 | -1.138784 |
| H | 2.623039 | 0.894463 | -0.619546 |
| H | 3.024633 | -0.621986 | 1.103315 |

Rotational constants (GHz): 4.1158700 1.6457100 1.4557300

Vibrational harmonic frequencies (cm-1):

| | | |
|------------|-----------|-----------|
| i1531.4080 | 68.8011 | 108.4058 |
| 185.2916 | 239.5139 | 278.3911 |
| 309.9719 | 429.5977 | 472.2450 |
| 505.8581 | 590.8672 | 788.1333 |
| 829.9151 | 884.8259 | 913.3069 |
| 919.4831 | 992.9386 | 1017.8635 |
| 1072.6593 | 1096.1982 | 1122.7842 |
| 1136.3841 | 1180.3194 | 1208.0508 |
| 1234.3723 | 1240.2869 | 1263.9524 |

| | | |
|-----------|-----------|-----------|
| 1278.0966 | 1329.0790 | 1363.1803 |
| 1386.3726 | 1400.5860 | 1451.7435 |
| 1486.1616 | 1494.2267 | 1506.5479 |
| 1520.7218 | 1564.0029 | 2927.0510 |
| 2962.5573 | 3002.9092 | 3010.1776 |
| 3011.5741 | 3046.2002 | 3084.0583 |
| 3093.3465 | 3105.6508 | 3831.4531 |

Zero-point correction (Hartree): 0.152514

C5H9O2.1-5Hshift.p.tm

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.52080518

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| C | 0.581884 | 0.415811 | -0.412041 |
| C | -0.534766 | 1.322471 | 0.080532 |
| C | -1.911898 | 0.703701 | -0.222186 |
| C | -1.962635 | -0.719788 | 0.360181 |
| O | -0.938375 | -1.524568 | -0.161528 |
| H | 0.757845 | 0.468918 | -1.491312 |
| C | 1.872580 | 0.393287 | 0.379685 |
| H | -0.460425 | 2.314977 | -0.385428 |
| H | -0.439715 | 1.473750 | 1.164422 |
| H | -2.065209 | 0.648600 | -1.306484 |
| H | -2.718700 | 1.314651 | 0.198339 |
| H | -2.917276 | -1.193791 | 0.083171 |
| H | -1.926881 | -0.667962 | 1.463257 |
| H | 0.023607 | -0.727788 | -0.295107 |
| O | 2.817774 | -0.537949 | -0.121649 |
| H | 2.362278 | 1.375735 | 0.317088 |
| H | 1.652637 | 0.218679 | 1.446027 |
| H | 2.425654 | -1.418531 | -0.045588 |

Rotational constants (GHz): 4.5231200 1.5013200 1.2174000

Vibrational harmonic frequencies (cm-1):

| | | |
|------------|-----------|-----------|
| i1446.0133 | 76.4764 | 117.1731 |
| 142.5619 | 265.3115 | 321.4690 |
| 345.7817 | 394.5912 | 483.7989 |
| 495.8637 | 579.5645 | 781.4277 |
| 849.8002 | 873.9241 | 904.1194 |
| 950.3190 | 1003.1036 | 1038.4741 |
| 1073.6752 | 1085.8395 | 1093.0594 |
| 1146.6125 | 1177.0521 | 1214.7662 |
| 1224.9523 | 1234.6664 | 1274.1562 |
| 1301.8122 | 1357.1492 | 1376.7904 |
| 1385.7682 | 1393.1613 | 1421.8168 |
| 1486.9068 | 1495.4133 | 1505.9639 |
| 1511.2840 | 1557.7630 | 2953.1327 |
| 2979.9170 | 3010.4901 | 3017.6060 |
| 3034.9695 | 3047.7809 | 3060.0017 |
| 3096.3951 | 3099.9510 | 3804.6029 |

Zero-point correction (Hartree): 0.152745

C5H9O2.1-5Hshift.p.tp

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.51870415

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| C | 0.579891 | 0.357468 | -0.384990 |
| C | -0.514665 | 1.307352 | 0.075902 |
| C | -1.904507 | 0.726723 | -0.240154 |
| C | -2.001629 | -0.689515 | 0.353093 |
| O | -0.993477 | -1.524513 | -0.148992 |
| H | 0.732324 | 0.374856 | -1.471582 |
| C | 1.880390 | 0.368417 | 0.390785 |
| H | -0.401847 | 2.292209 | -0.399349 |
| H | -0.430486 | 1.469254 | 1.159171 |
| H | -2.045092 | 0.666579 | -1.326078 |
| H | -2.698104 | 1.365554 | 0.164054 |
| H | -2.964762 | -1.140733 | 0.068020 |
| H | -1.979625 | -0.628496 | 1.456259 |
| H | 0.005495 | -0.782752 | -0.230500 |
| O | 2.809366 | -0.616789 | -0.028290 |
| H | 2.321193 | 1.383250 | 0.340482 |
| H | 1.686529 | 0.167057 | 1.450122 |
| H | 3.010387 | -0.459032 | -0.960158 |

Rotational constants (GHz): 4.5826600 1.4735100 1.2058800

Vibrational harmonic frequencies (cm-1):

| | | |
|------------|-----------|-----------|
| i1513.0833 | 80.9410 | 112.1124 |
| 148.1902 | 254.2146 | 308.5533 |
| 321.6041 | 393.5019 | 477.2575 |
| 492.9951 | 570.8941 | 789.0540 |
| 851.9360 | 875.1924 | 904.6485 |
| 949.5360 | 999.8200 | 1049.4286 |
| 1080.2557 | 1084.3075 | 1105.4957 |

| | | |
|-----------|-----------|-----------|
| 1118.8481 | 1181.7427 | 1207.0278 |
| 1237.5591 | 1247.6484 | 1274.6657 |
| 1313.2699 | 1354.5192 | 1371.9843 |
| 1387.3810 | 1396.5274 | 1423.0079 |
| 1487.4128 | 1495.4976 | 1505.1429 |
| 1510.4027 | 1557.4193 | 2924.8802 |
| 2951.2703 | 3011.5055 | 3014.6494 |
| 3045.4514 | 3053.1081 | 3064.9836 |
| 3083.0789 | 3096.8045 | 3811.6836 |

Zero-point correction (Hartree): 0.152586

C5H9O2.1-5Hshift.p.tt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.51839694

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| C | 0.579238 | 0.355971 | -0.391325 |
| C | -0.511569 | 1.305108 | 0.077014 |
| C | -1.902580 | 0.728310 | -0.238819 |
| C | -2.003823 | -0.686426 | 0.357488 |
| O | -0.998453 | -1.525908 | -0.140809 |
| H | 0.757858 | 0.380387 | -1.470790 |
| C | 1.866634 | 0.351293 | 0.393195 |
| H | -0.396707 | 2.290665 | -0.396236 |
| H | -0.427352 | 1.464224 | 1.160932 |
| H | -2.041811 | 0.665965 | -1.324709 |
| H | -2.695249 | 1.369600 | 0.163349 |
| H | -2.969041 | -1.134486 | 0.073702 |
| H | -1.982707 | -0.621392 | 1.460880 |
| H | 0.001293 | -0.780073 | -0.252298 |
| O | 2.758471 | -0.575969 | -0.205768 |
| H | 2.291361 | 1.374110 | 0.392140 |
| H | 1.657597 | 0.097413 | 1.445661 |
| H | 3.557219 | -0.616936 | 0.334665 |

Rotational constants (GHz): 4.6209000 1.4805600 1.2128800

Vibrational harmonic frequencies (cm-1):

| | | |
|------------|-----------|-----------|
| i1493.2970 | 85.4224 | 114.1449 |
| 147.5517 | 252.3067 | 270.0020 |
| 321.7812 | 394.1231 | 479.9972 |
| 492.8994 | 575.7944 | 794.9475 |
| 852.8740 | 882.7008 | 905.2482 |
| 948.5410 | 1010.0370 | 1052.1881 |
| 1080.1872 | 1083.1120 | 1109.2957 |
| 1149.9934 | 1186.6414 | 1211.2223 |
| 1239.3987 | 1249.5073 | 1265.8194 |
| 1282.1040 | 1319.5503 | 1360.5573 |
| 1383.3006 | 1387.4013 | 1461.4705 |
| 1487.8928 | 1495.9183 | 1510.4332 |
| 1522.0497 | 1556.5036 | 2923.9936 |
| 2946.0286 | 2986.0596 | 3008.3045 |
| 3013.9207 | 3045.2926 | 3056.7053 |
| 3096.4028 | 3102.7623 | 3827.7723 |

Zero-point correction (Hartree): 0.152478

C5H9O2.1-6Hshift.ad.m

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.52038943

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 0.917001 | -1.508418 | -0.580750 |
| H | -0.375852 | -1.109691 | -0.533171 |
| C | -1.373660 | -0.420757 | -0.432362 |
| C | 1.577505 | -0.736542 | 0.378642 |
| C | -0.903277 | 1.008421 | -0.672822 |
| C | 1.577462 | 0.773504 | 0.089544 |
| C | 0.221012 | 1.475779 | 0.274005 |
| O | -2.000693 | -0.656543 | 0.790737 |
| H | -2.035871 | -0.797351 | -1.218179 |
| H | 1.193463 | -0.924825 | 1.400735 |
| H | 2.617472 | -1.103054 | 0.376674 |
| H | -0.553825 | 1.079259 | -1.709776 |
| H | -1.766869 | 1.681158 | -0.578320 |
| H | 2.308065 | 1.252487 | 0.754752 |
| H | 1.933924 | 0.922928 | -0.937586 |
| H | 0.359723 | 2.553913 | 0.132239 |
| H | -0.100156 | 1.368147 | 1.322864 |
| H | -1.504780 | -0.205712 | 1.487823 |

Rotational constants (GHz): 3.2719700 2.1388500 1.6085800

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|----------|-----------|
| i806.6009 | 88.3556 | 129.0993 |
| 233.4435 | 295.6683 | 333.0534 |
| 372.1099 | 403.9108 | 473.7782 |
| 533.1370 | 694.7147 | 780.1585 |
| 845.0080 | 865.4988 | 900.6575 |
| 954.3577 | 997.2181 | 1056.4707 |

| | | |
|-----------|-----------|-----------|
| 1070.1649 | 1101.6822 | 1129.4453 |
| 1154.8541 | 1185.4092 | 1234.4509 |
| 1249.9368 | 1288.6704 | 1289.5963 |
| 1352.7618 | 1374.2732 | 1386.3543 |
| 1394.6238 | 1405.7079 | 1433.1201 |
| 1474.8360 | 1478.0540 | 1488.7162 |
| 1508.1445 | 1509.3172 | 2924.0528 |
| 2993.6873 | 2997.3766 | 3029.3904 |
| 3034.1880 | 3071.4804 | 3078.9285 |
| 3084.1012 | 3099.0649 | 3802.1685 |

Zero-point correction (Hartree): 0.153961

C5H9O2.1-6Hshift.ad.t

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.52177279

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -0.898144 | -1.505239 | 0.607807 |
| H | 0.362115 | -1.070358 | 0.585982 |
| C | 1.362557 | -0.382778 | 0.444668 |
| C | -1.558706 | -0.749725 | -0.370234 |
| C | 0.906045 | 1.047898 | 0.648031 |
| C | -1.572551 | 0.763302 | -0.100153 |
| C | -0.225213 | 1.478488 | -0.305960 |
| O | 1.877877 | -0.556284 | -0.842434 |
| H | 2.041802 | -0.742053 | 1.233134 |
| H | -1.159433 | -0.947780 | -1.381763 |
| H | -2.594798 | -1.127418 | -0.366405 |

| | | | |
|---|-----------|-----------|-----------|
| H | 0.578619 | 1.151301 | 1.689903 |
| H | 1.769850 | 1.713381 | 0.514556 |
| H | -2.310680 | 1.222251 | -0.771433 |
| H | -1.931697 | 0.923734 | 0.925008 |
| H | -0.381432 | 2.557041 | -0.183197 |
| H | 0.110998 | 1.330551 | -1.339370 |
| H | 2.204003 | -1.461578 | -0.927516 |

Rotational constants (GHz): 3.2480900 2.1981800 1.6392900

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| i928.0708 | 88.6860 | 125.1851 |
| 220.4805 | 325.3199 | 338.4155 |
| 369.8468 | 391.7618 | 471.7370 |
| 535.7012 | 696.5855 | 783.1046 |
| 842.7220 | 871.0573 | 909.2999 |
| 957.8768 | 1001.7318 | 1054.4395 |
| 1067.7934 | 1093.3401 | 1138.2732 |
| 1163.0297 | 1190.7833 | 1230.5380 |
| 1244.4266 | 1265.7861 | 1295.5368 |
| 1311.8973 | 1374.2070 | 1388.5608 |
| 1397.7583 | 1408.8563 | 1437.4131 |
| 1471.6730 | 1479.3790 | 1488.6313 |
| 1503.3141 | 1522.2757 | 2953.2728 |
| 2997.8106 | 3009.1375 | 3029.9133 |
| 3031.8579 | 3045.6542 | 3070.9011 |
| 3076.6539 | 3091.0793 | 3823.1853 |

Zero-point correction (Hartree): 0.153974

C5H9O2.1-6Hshift.au.m

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.52106655

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 0.596368 | -1.652284 | -0.250924 |
| H | -0.513634 | -0.995435 | 0.138488 |
| C | -1.320052 | -0.118795 | 0.395299 |
| C | 1.676724 | -0.914648 | 0.246369 |
| C | -0.761503 | 1.148200 | -0.235076 |
| C | 1.766673 | 0.520644 | -0.291596 |
| C | 0.673693 | 1.478181 | 0.217207 |
| H | -1.351379 | -0.077145 | 1.489704 |
| O | -2.586129 | -0.499232 | -0.044947 |
| H | 1.698992 | -0.903015 | 1.352314 |
| H | 2.572990 | -1.474461 | -0.069825 |
| H | -0.779728 | 1.037387 | -1.329577 |
| H | -1.432152 | 1.983721 | 0.007955 |
| H | 2.745021 | 0.931576 | -0.009084 |
| H | 1.743152 | 0.479971 | -1.388456 |
| H | 0.913648 | 2.492680 | -0.122076 |
| H | 0.705670 | 1.513564 | 1.315858 |
| H | -2.597701 | -0.458216 | -1.011553 |

Rotational constants (GHz): 3.6513300 1.8949000 1.3579700

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|----------|----------|
| i820.2946 | 100.4548 | 158.9286 |
| 221.8025 | 270.2062 | 333.7108 |
| 344.1738 | 410.3660 | 460.8563 |
| 505.1479 | 670.6203 | 794.2893 |

| | | |
|-----------|-----------|-----------|
| 835.3898 | 854.3692 | 921.6770 |
| 953.9629 | 997.8338 | 1041.6478 |
| 1092.6047 | 1104.4012 | 1121.2146 |
| 1164.5175 | 1190.8292 | 1235.1876 |
| 1262.4997 | 1285.5088 | 1315.4675 |
| 1351.3849 | 1376.5227 | 1384.8200 |
| 1393.4365 | 1405.9409 | 1424.0150 |
| 1472.4816 | 1483.0775 | 1494.5490 |
| 1503.9443 | 1525.3296 | 2942.6564 |
| 2994.5427 | 3011.9100 | 3022.7900 |
| 3031.9763 | 3054.7951 | 3071.8626 |
| 3077.5041 | 3087.3337 | 3799.3717 |

Zero-point correction (Hartree): 0.153908

C5H9O2.1-6Hshift.au.t

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.52066700

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 0.607924 | -1.666254 | -0.253766 |
| H | -0.510028 | -0.986779 | 0.069290 |
| C | -1.311052 | -0.118351 | 0.360730 |
| C | 1.676053 | -0.915375 | 0.248738 |
| C | -0.764258 | 1.168170 | -0.222293 |
| C | 1.759647 | 0.519081 | -0.293893 |
| C | 0.674845 | 1.479653 | 0.227481 |
| H | -1.315585 | -0.122510 | 1.463426 |
| O | -2.557470 | -0.411895 | -0.191760 |
| H | 1.690029 | -0.897743 | 1.355464 |
| H | 2.579562 | -1.468910 | -0.058091 |
| H | -0.808848 | 1.091459 | -1.315601 |
| H | -1.430893 | 1.993481 | 0.062270 |
| H | 2.741808 | 0.928279 | -0.022238 |
| H | 1.723588 | 0.475473 | -1.390020 |
| H | 0.921573 | 2.494723 | -0.105204 |
| H | 0.716038 | 1.506292 | 1.326461 |
| H | -2.922286 | -1.187645 | 0.253876 |

Rotational constants (GHz): 3.6350700 1.9074000 1.3562100

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| i803.6895 | 94.0981 | 170.7947 |
| 232.8949 | 270.0258 | 334.3671 |
| 349.9672 | 377.9920 | 454.9858 |
| 504.9299 | 677.2998 | 792.1283 |
| 837.0576 | 855.7429 | 922.5672 |
| 950.6296 | 1004.0131 | 1037.6958 |
| 1087.9333 | 1100.2671 | 1144.4525 |
| 1162.2110 | 1189.0904 | 1236.6086 |
| 1258.1280 | 1285.5279 | 1299.9635 |
| 1351.8613 | 1358.1033 | 1384.2840 |
| 1394.5583 | 1406.6324 | 1419.7652 |

| | | |
|-----------|-----------|-----------|
| 1472.9841 | 1483.0130 | 1497.9927 |
| 1504.4649 | 1547.9881 | 2934.5539 |
| 2989.3603 | 2992.9274 | 3018.7990 |
| 3032.6767 | 3032.7594 | 3071.7761 |
| 3076.9791 | 3083.8170 | 3820.0103 |

Zero-point correction (Hartree): 0.153792

C5H9O2.1-6Hshift.bd.m

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.51695340

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -0.629982 | -1.546432 | -0.590894 |
| H | 0.541263 | -0.892233 | -0.533009 |
| C | 1.377207 | -0.001271 | -0.400433 |
| C | -1.369903 | -0.996700 | 0.460349 |
| C | 0.647826 | 1.172201 | 0.247478 |
| C | -1.845355 | 0.446337 | 0.206822 |
| C | -0.752585 | 1.376990 | -0.362998 |
| H | 1.664012 | 0.203351 | -1.437660 |
| O | 2.509268 | -0.461969 | 0.264322 |
| H | -2.242253 | -1.655295 | 0.601008 |
| H | -0.811474 | -1.048043 | 1.413655 |
| H | 0.565895 | 1.000967 | 1.331535 |
| H | 1.259779 | 2.075788 | 0.127059 |
| H | -2.691730 | 0.435846 | -0.489431 |
| H | -2.222598 | 0.851356 | 1.155993 |
| H | -1.066079 | 2.417312 | -0.225297 |
| H | -0.681075 | 1.222688 | -1.446353 |
| H | 2.306833 | -0.529870 | 1.207771 |

Rotational constants (GHz): 3.6240100 1.9394800 1.4491300

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|----------|----------|
| i929.7093 | 92.4544 | 151.2479 |
| 239.0137 | 266.7495 | 335.3886 |

| | | |
|-----------|-----------|-----------|
| 359.4712 | 398.2810 | 456.0291 |
| 571.1527 | 630.8487 | 758.6132 |
| 805.3800 | 864.9437 | 913.8364 |
| 973.2909 | 1002.0396 | 1047.1341 |
| 1074.6774 | 1094.6523 | 1118.7276 |
| 1152.1277 | 1186.4561 | 1235.6849 |
| 1260.0801 | 1281.9358 | 1312.6177 |
| 1352.4706 | 1374.7978 | 1382.4419 |
| 1390.4599 | 1415.2373 | 1432.5280 |
| 1474.2600 | 1492.2357 | 1493.3949 |
| 1502.7433 | 1510.7288 | 2938.2539 |
| 3004.4113 | 3012.1554 | 3031.0532 |
| 3046.7173 | 3058.7357 | 3080.5590 |
| 3089.9884 | 3094.2223 | 3801.2999 |

Zero-point correction (Hartree): 0.153916

C5H9O2.1-6Hshift.bd.t

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.51753980

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 0.606510 | -1.548453 | 0.598993 |
| H | -0.544737 | -0.869412 | 0.536319 |
| C | -1.371319 | 0.026115 | 0.389026 |
| C | 1.341564 | -1.015196 | -0.466960 |
| | | | |
| C | -0.631051 | 1.199534 | -0.230515 |
| C | 1.845507 | 0.419331 | -0.218979 |
| C | 0.777901 | 1.365842 | 0.371894 |
| H | -1.681561 | 0.222014 | 1.428211 |
| O | -2.420589 | -0.388679 | -0.428737 |
| H | 2.199373 | -1.690323 | -0.618051 |
| H | 0.762621 | -1.057915 | -1.406207 |
| H | -0.576556 | 1.040851 | -1.314447 |
| H | -1.223344 | 2.111816 | -0.081483 |
| H | 2.704474 | 0.394205 | 0.461721 |
| H | 2.210801 | 0.820558 | -1.174276 |
| H | 1.113072 | 2.400436 | 0.241389 |
| H | 0.715508 | 1.201970 | 1.454769 |
| H | -2.942638 | -1.050896 | 0.043212 |

Rotational constants (GHz): 3.5963200 1.9735400 1.4673900

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| i941.8228 | 82.3067 | 148.0986 |
| 238.7026 | 272.8319 | 345.2978 |
| 363.8141 | 395.3749 | 450.0444 |
| 570.5892 | 641.7586 | 760.5490 |
| 809.4209 | 870.2016 | 913.3535 |
| 981.2899 | 1003.3452 | 1041.8939 |
| 1071.2629 | 1107.3870 | 1116.5684 |
| 1157.6438 | 1192.1820 | 1236.5969 |
| 1262.1840 | 1275.6556 | 1302.1408 |
| 1340.3951 | 1352.5432 | 1382.6946 |
| 1384.5224 | 1413.4287 | 1441.6891 |
| 1475.1840 | 1492.8061 | 1502.1440 |
| 1509.8444 | 1511.3425 | 2962.0778 |
| 2998.7120 | 3006.4267 | 3031.5227 |
| 3035.6886 | 3045.9336 | 3077.8462 |
| 3081.7907 | 3091.9857 | 3818.4283 |

Zero-point correction (Hartree): 0.153930

C5H9O2.1-6Hshift.bu.m

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.51599823

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -0.726157 | -1.570831 | -0.301720 |
| H | 0.448102 | -1.116029 | 0.160831 |
| C | 1.355367 | -0.357968 | 0.490998 |
| C | -1.672039 | -0.747744 | 0.319656 |
| C | 0.707396 | 1.017748 | 0.657972 |
| C | -1.713829 | 0.692765 | -0.229519 |
| C | -0.324865 | 1.331750 | -0.444853 |
| O | 2.352243 | -0.430124 | -0.480000 |
| H | 1.771126 | -0.769915 | 1.415525 |
| H | -2.649911 | -1.229485 | 0.158339 |
| H | -1.529759 | -0.732453 | 1.414715 |
| H | 0.232989 | 1.078500 | 1.644708 |
| H | 1.511679 | 1.765322 | 0.653292 |
| H | -2.254064 | 0.707205 | -1.183141 |
| H | -2.296656 | 1.305520 | 0.471677 |
| H | -0.444975 | 2.416387 | -0.540586 |
| H | 0.072862 | 0.993708 | -1.411839 |
| H | 2.017736 | -0.030424 | -1.295283 |

Rotational constants (GHz): 3.6726100 1.9811300 1.5212000

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 1963.9303 | 95.4021 | 140.9677 |
| 212.2887 | 247.6683 | 291.9250 |
| 369.2317 | 417.4612 | 470.6878 |
| 561.2594 | 684.6046 | 777.1532 |
| 809.6954 | 857.7922 | 898.5903 |
| 953.2947 | 1001.7121 | 1039.2721 |
| 1065.7627 | 1105.7157 | 1127.6914 |
| 1151.6020 | 1194.6340 | 1219.1632 |
| 1270.0853 | 1274.7422 | 1298.9933 |
| 1351.7935 | 1364.8828 | 1383.7948 |
| 1386.8619 | 1412.3654 | 1426.3486 |
| 1472.0473 | 1488.8471 | 1492.1682 |
| 1499.3736 | 1510.3726 | 2955.2773 |
| 3006.2599 | 3025.8246 | 3032.8285 |
| 3035.6498 | 3077.9360 | 3081.4716 |
| 3086.4800 | 3101.5776 | 3796.9739 |

Zero-point correction (Hartree): 0.153837

C5H9O2.1-6Hshift.bu.p

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.51599822

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -0.726144 | -1.570867 | -0.301707 |
| H | 0.448137 | -1.116119 | 0.160858 |
| C | 1.355365 | -0.358008 | 0.490963 |
| C | -1.671940 | -0.747704 | 0.319699 |
| C | 0.707319 | 1.017649 | 0.658110 |
| C | -1.713820 | 0.692707 | -0.229689 |
| C | -0.324852 | 1.331827 | -0.444755 |
| O | 2.352173 | -0.430028 | -0.480115 |
| H | 1.771232 | -0.769986 | 1.415431 |
| H | -2.649839 | -1.229475 | 0.158638 |
| H | -1.529440 | -0.732200 | 1.414726 |
| H | 0.232804 | 1.078183 | 1.644805 |
| H | 1.511563 | 1.765263 | 0.653650 |
| H | -2.253850 | 0.706946 | -1.183430 |
| H | -2.296876 | 1.305473 | 0.471307 |
| H | -0.444991 | 2.416480 | -0.540268 |
| H | 0.073000 | 0.994026 | -1.411775 |
| H | 2.017586 | -0.030266 | -1.295336 |

Rotational constants (GHz): 3.6725300 1.9812000 1.5212700

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 1963.7906 | 95.3854 | 140.9939 |
| 212.2924 | 247.7191 | 291.9130 |
| 369.2417 | 417.4509 | 470.6864 |
| 561.2258 | 684.6288 | 777.1561 |
| 809.7081 | 857.7873 | 898.5801 |
| 953.2991 | 1001.7069 | 1039.2706 |
| 1065.7459 | 1105.7249 | 1127.6946 |
| 1151.6104 | 1194.6306 | 1219.1628 |
| 1270.0860 | 1274.7456 | 1298.9817 |
| 1351.7905 | 1364.8888 | 1383.7920 |
| 1386.8581 | 1412.3625 | 1426.3560 |
| 1472.0251 | 1488.8414 | 1492.1849 |
| 1499.3672 | 1510.3769 | 2955.2842 |
| 3006.2697 | 3025.8156 | 3032.8244 |
| 3035.6611 | 3077.9429 | 3081.4835 |
| 3086.4875 | 3101.5591 | 3796.9769 |

Zero-point correction (Hartree): 0.153837

C5H9O2.1-6Hshift.bu.t

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.51634085

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -0.747362 | -1.585642 | -0.278271 |
| H | 0.428539 | -1.099575 | 0.121194 |
| C | 1.337830 | -0.353099 | 0.477447 |
| C | -1.680223 | -0.731601 | 0.321692 |
| C | 0.706230 | 1.017028 | 0.665445 |
| C | -1.703656 | 0.695297 | -0.260753 |
| C | -0.310746 | 1.336216 | -0.450288 |
| O | 2.293768 | -0.295742 | -0.538571 |
| H | 1.722178 | -0.807137 | 1.404347 |
| H | -2.664176 | -1.204069 | 0.169056 |
| H | -1.539092 | -0.692676 | 1.416895 |
| H | 0.232911 | 1.067933 | 1.653108 |
| H | 1.514868 | 1.758842 | 0.663052 |
| H | -2.215394 | 0.683924 | -1.230062 |
| H | -2.313022 | 1.317108 | 0.409716 |
| H | -0.432715 | 2.421495 | -0.537825 |
| H | 0.122456 | 0.997286 | -1.397154 |
| H | 2.675590 | -1.175098 | -0.658847 |

Rotational constants (GHz): 3.6728600 1.9953300 1.5271700

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| i998.5745 | 84.5086 | 165.7359 |
| 212.6988 | 247.9453 | 301.8451 |
| 361.6172 | 394.7240 | 473.1919 |
| 563.8171 | 689.0497 | 778.9822 |
| 810.7820 | 872.7819 | 898.3417 |
| 960.6730 | 1001.8330 | 1045.0213 |
| 1061.1412 | 1093.9686 | 1137.6794 |
| 1156.9094 | 1198.1259 | 1215.2625 |
| 1263.6656 | 1269.2109 | 1300.9814 |
| 1340.3477 | 1360.8087 | 1382.7650 |
| 1388.5323 | 1394.9420 | 1415.9252 |
| 1471.3626 | 1487.2401 | 1495.8556 |
| 1513.1222 | 1519.3988 | 2949.0750 |
| 3003.4089 | 3003.7960 | 3029.3487 |
| 3042.5435 | 3058.4191 | 3078.0216 |
| 3085.9301 | 3104.0936 | 3819.6222 |

Zero-point correction (Hartree): 0.153788

C5H9O2.1-6Hshift.cd.m

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.51566670

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| C | 0.676433 | 1.062119 | 0.459169 |
| C | -0.712774 | 1.537139 | -0.013592 |
| C | -1.710391 | 0.423490 | -0.415405 |
| C | -1.589131 | -0.881863 | 0.391713 |
| O | -0.555824 | -1.714495 | -0.059095 |
| H | 0.493135 | -0.939478 | -0.366394 |
| C | 1.290019 | -0.008537 | -0.427761 |
| H | 0.597356 | 0.651441 | 1.476664 |
| H | 1.358435 | 1.920266 | 0.523753 |
| H | -1.146157 | 2.140589 | 0.792743 |
| H | -0.590493 | 2.218019 | -0.864973 |
| H | -2.728235 | 0.820005 | -0.319379 |
| H | -1.580742 | 0.151407 | -1.469311 |
| H | -1.512031 | -0.657771 | 1.472185 |
| H | -2.514675 | -1.466089 | 0.258655 |
| O | 2.557402 | -0.445403 | -0.051158 |
| H | 1.335136 | 0.262569 | -1.488005 |
| H | 2.550713 | -0.615861 | 0.901345 |

Rotational constants (GHz): 3.5581800 1.9597300 1.4064400

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| i961.3897 | 88.3797 | 162.1666 |
| 194.0356 | 250.9434 | 296.7361 |
| 362.5100 | 408.4121 | 449.3247 |
| 554.0596 | 648.2152 | 769.1485 |
| 816.8210 | 877.8230 | 922.6377 |
| 967.4103 | 994.3239 | 1034.2932 |
| 1101.0847 | 1110.7233 | 1115.2525 |
| 1157.7055 | 1193.2855 | 1227.0381 |
| 1241.4871 | 1289.7162 | 1303.3274 |
| 1343.2262 | 1362.0178 | 1384.9182 |
| 1393.2506 | 1397.6649 | 1429.6929 |
| 1492.2490 | 1494.9605 | 1505.0866 |
| 1513.6804 | 1529.0804 | 2939.7073 |
| 2993.6230 | 3014.0994 | 3037.8620 |
| 3050.2327 | 3058.2873 | 3074.0017 |
| 3090.5197 | 3096.3740 | 3797.4818 |

Zero-point correction (Hartree): 0.153856

C5H9O2.1-6Hshift.cd.p

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.51566674

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| C | 0.676420 | 1.061969 | 0.459329 |
| C | -0.712688 | 1.537118 | -0.013561 |
| C | -1.710391 | 0.423525 | -0.415451 |
| C | -1.589212 | -0.881908 | 0.391597 |
| O | -0.555741 | -1.714444 | -0.058929 |
| H | 0.493100 | -0.938958 | -0.367208 |
| C | 1.290092 | -0.008356 | -0.427906 |
| H | 0.597039 | 0.650846 | 1.476627 |
| H | 1.358407 | 1.920089 | 0.524448 |
| H | -1.146111 | 2.140602 | 0.792726 |
| H | -0.590255 | 2.217992 | -0.864926 |
| H | -2.728195 | 0.820100 | -0.319254 |
| H | -1.580906 | 0.151555 | -1.469407 |
| H | -1.512501 | -0.657845 | 1.472104 |
| H | -2.514685 | -1.466183 | 0.258187 |
| O | 2.557292 | -0.445657 | -0.051183 |
| H | 1.335494 | 0.263230 | -1.488025 |
| H | 2.550883 | -0.614701 | 0.901571 |

```

Rotational constants (GHz):      3.5582300      1.9597400      1.4064800
Vibrational harmonic frequencies (cm-1):
i958.5617                        88.3369                        162.0438
194.2140                         250.9198                       296.7764
362.4801                         408.1698                       449.3749
554.0987                         648.8322                       769.2874
816.9118                         878.0067                       922.9461
967.3803                         994.3308                      1034.2819
1101.0535                       1110.8116                      1115.4435
1157.8123                       1193.2896                      1227.0221
1241.4616                       1289.7114                      1303.3364
1343.5526                       1362.0124                      1384.9043
1393.2625                       1397.6581                      1429.6955
1492.2740                       1494.9712                      1505.1179
1513.6979                       1529.3223                      2939.6852
2993.5165                       3014.0775                      3037.8630
3050.2341                       3058.2804                      3073.9978
3090.4241                       3096.3512                      3797.5415
Zero-point correction (Hartree): 0.153860

```

C5H9O2.1-6Hshift.cd.t

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.51546006

Electronic state : 2-A

Cartesian coordinates (Angs):

```

C      -0.674190      1.078569      -0.445879
C       0.712277      1.537634      0.048995
C       1.721063      0.417833      0.408584
C       1.584660     -0.879510     -0.408993
O       0.570102     -1.722322      0.064826
H      -0.501323     -0.958740      0.296997
C      -1.287506     -0.021293      0.392746
H      -0.607651      0.704892     -1.474949
H      -1.356993      1.937655     -0.476027
H       1.141661      2.174940     -0.732952
H       0.588212      2.185020      0.926207
H       2.736276      0.816812      0.295122
H       1.616667      0.130470      1.461490
H       1.477164     -0.651691     -1.485152
H       2.514618     -1.462800     -0.304897
O      -2.534121     -0.381233     -0.116460
H      -1.307135      0.200177      1.472405
H      -2.927170     -1.047693      0.462117

```

```

Rotational constants (GHz):      3.5608700      1.9616100      1.4009800
Vibrational harmonic frequencies (cm-1):
i975.1917                        84.6785                        174.8626
200.7700                        255.8645                       292.3232
364.4021                        377.6719                       443.8803
554.4639                        641.7378                       764.8813
814.8725                        880.9127                       918.3279
968.6466                        999.6264                      1031.9953
1093.5411                       1109.7861                      1129.0899
1158.6519                       1200.2210                      1227.5534
1240.1401                       1280.6648                      1304.6349
1339.3876                       1356.8364                      1378.7481
1387.7243                       1396.9425                      1423.9241
1489.5254                       1493.4374                      1504.0119
1514.4000                       1540.6390                      2950.3522
2994.5687                       2996.1368                      3034.6568
3039.9832                       3049.7480                      3066.1756
3080.4860                       3093.9224                      3820.4315
Zero-point correction (Hartree): 0.153699

```

C5H9O2.1-6Hshift.cu.m

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.51537889

Electronic state : 2-A

Cartesian coordinates (Angs):

```

C       0.843692      0.733722      0.930859
C      -0.076056      1.541952     -0.013544
C      -1.204745      0.738397     -0.703108
C      -1.817833     -0.387994      0.151807
O      -1.056639     -1.563160      0.147815
H       0.242190     -1.221519      0.213614
C       1.290612     -0.604663      0.367168
H       0.313216      0.523951      1.866873
H       1.719047      1.342181      1.194729
H      -0.514781      2.357669      0.572478
H       0.527342      2.037503     -0.786091
H      -1.992010      1.438150     -1.007021
H      -0.842374      0.263091     -1.623676
H      -2.023984     -0.018291      1.173589
H      -2.791263     -0.668306     -0.283218
H       1.854754     -1.212762      1.080799
O       2.019194     -0.565071     -0.819665

```

```

H          1.593400      0.055705      -1.426368
Rotational constants (GHz):  3.3095800      2.1167100      1.6604200
Vibrational harmonic frequencies (cm-1):
  1938.1205      88.5162      140.5343
  187.8099      264.3641      299.4263
  380.1193      390.5578      457.9767
  600.0574      656.0959      756.1825
  792.4628      864.8829      932.7043
  951.8109      987.0755      1040.5323
  1077.0892      1099.4445      1108.6892
  1152.0747      1195.6415      1230.6262
  1243.5139      1269.5560      1303.9007
  1347.0173      1358.5370      1381.6571
  1391.1273      1395.8482      1431.3078
  1485.6567      1495.0935      1500.5849
  1516.0010      1518.4982      2942.7911
  2994.8378      3027.3905      3035.8779
  3043.3288      3066.9100      3083.4834
  3090.9223      3102.9052      3809.6558
Zero-point correction (Hartree): 0.153756
    
```

C5H9O2.1-6Hshift.cu.p

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.51537913

Electronic state : 2-A

Cartesian coordinates (Angs):

```

C          0.843752      0.733268      0.931081
C          -0.075926      1.541891      -0.013074
C          -1.204094      0.738419      -0.703469
C          -1.818201      -0.387485      0.151377
O          -1.057477      -1.562931      0.148131
H          0.242137      -1.221545      0.212794
C          1.290506      -0.605009      0.366967
H          0.313212      0.523245      1.867002
H          1.719171      1.341527      1.195174
H          -0.515154      2.357054      0.573349
H          0.527505      2.038152      -0.785142
H          -1.990891      1.438240      -1.008432
H          -0.840947      0.262632      -1.623485
H          -2.024744      -0.017419      1.172947
H          -2.791503      -0.667492      -0.284156
H          1.854395      -1.213395      1.080552
O          2.019527      -0.565035      -0.819601
H          1.594196      0.056223      -1.426131
Rotational constants (GHz):  3.3099200      2.1162400      1.6603100
Vibrational harmonic frequencies (cm-1):
  1935.7018      88.6388      140.5687
  187.7268      264.3257      299.4475
  380.1121      390.6297      457.9027
  600.0743      656.3155      756.1927
  792.5285      864.9281      932.6942
  951.8888      987.0538      1040.5531
  1077.0753      1099.4499      1108.6805
  1152.0882      1195.6404      1230.6903
  1243.4656      1269.6524      1303.9193
  1347.5898      1358.5428      1381.6637
  1391.0869      1395.8277      1431.3207
  1485.6770      1495.0404      1500.6135
  1516.0704      1518.6570      2942.7960
  2994.7327      3027.3939      3035.9070
  3043.3075      3066.9115      3083.4963
  3090.9180      3102.9064      3809.6757
Zero-point correction (Hartree): 0.153759
    
```

C5H9O2.1-6Hshift.cu.t

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -347.51668842

Electronic state : 2-A

Cartesian coordinates (Angs):

```

C          0.844041      0.766877      0.921064
C          -0.081445      1.548052      -0.039240
C          -1.177441      0.713454      -0.737206
C          -1.822625      -0.381780      0.134064
O          -1.055645      -1.554186      0.211145
H          0.222617      -1.198003      0.252640
C          1.277450      -0.578128      0.383897
H          0.328257      0.576184      1.869743
H          1.723994      1.379142      1.158817
H          -0.545743      2.360382      0.533333
H          0.528772      2.025766      -0.812759
H          -1.958405      1.395250      -1.094588
H          -0.762598      0.213246      -1.619311
H          -2.069887      0.023004      1.133022
H          -2.775524      -0.685219      -0.330002
H          1.839794      -1.181863      1.112651
    
```


| | | | | |
|--|-----------|-----------|-----------|-----------|
| O | 1.930755 | -0.445919 | -0.841927 | |
| H | 2.227967 | -1.317902 | -1.132767 | |
| Rotational constants (GHz): | 3.3114000 | 2.1463400 | 1.6881100 | |
| Vibrational harmonic frequencies (cm-1): | | | | |
| i1043.9593 | 97.5621 | | | 139.3807 |
| 176.9909 | 268.7310 | | | 318.3777 |
| 376.4592 | 392.5096 | | | 455.8803 |
| 598.5018 | 655.8962 | | | 756.4919 |
| 796.8789 | 871.7814 | | | 936.5206 |
| 958.1614 | 992.1906 | | | 1042.6550 |
| 1073.2840 | 1089.2318 | | | 1114.3095 |
| 1164.7318 | 1197.4586 | | | 1231.7536 |
| 1240.8766 | 1264.9269 | | | 1304.2978 |
| 1322.6918 | 1360.1302 | | | 1384.6824 |
| 1390.4242 | 1398.3064 | | | 1431.2726 |
| 1485.2130 | 1489.2368 | | | 1503.2429 |
| 1509.5529 | 1520.9161 | | | 2944.1901 |
| 2993.7569 | 3011.9107 | | | 3036.0231 |
| 3045.0704 | 3052.8099 | | | 3075.2787 |
| 3090.2638 | 3103.4837 | | | 3822.1323 |
| Zero-point correction (Hartree): | 0.153745 | | | |

C8H17O.pttttt

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -390.27005718
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | |
|--|-----------|-----------|-----------|
| O | 4.251515 | -1.042136 | -0.487384 |
| C | 4.042386 | 0.115828 | 0.214495 |
| C | 2.704140 | 0.815005 | -0.053334 |
| C | 1.495001 | -0.067007 | 0.275174 |
| C | 0.150968 | 0.569767 | -0.097595 |
| C | -1.056643 | -0.313673 | 0.240387 |
| C | -2.402446 | 0.311741 | -0.147001 |
| C | -3.610348 | -0.570237 | 0.193885 |
| C | -4.950126 | 0.058637 | -0.201714 |
| H | 4.113493 | -0.183746 | 1.284128 |
| H | 4.903745 | 0.798989 | 0.078013 |
| H | 2.672178 | 1.746005 | 0.529377 |
| H | 2.675253 | 1.108012 | -1.111067 |
| H | 1.611844 | -1.022825 | -0.250794 |
| H | 1.500621 | -0.304821 | 1.349209 |
| H | 0.048478 | 1.536813 | 0.415815 |
| H | 0.145040 | 0.796753 | -1.173223 |
| H | -0.947871 | -1.283578 | -0.265556 |
| H | -1.055312 | -0.533397 | 1.317719 |
| H | -2.510646 | 1.283724 | 0.355920 |
| H | -2.405461 | 0.528178 | -1.225078 |
| H | -3.500277 | -1.542170 | -0.306282 |
| H | -3.609766 | -0.783389 | 1.271624 |
| H | -4.994006 | 0.252047 | -1.279727 |
| H | -5.106072 | 1.015173 | 0.310463 |
| H | -5.790952 | -0.595037 | 0.052743 |
| Rotational constants (GHz): | 6.8348500 | 0.3776000 | 0.3686500 |
| Vibrational harmonic frequencies (cm-1): | | | |
| 35.8297 | 53.5041 | | 74.0950 |
| 95.2553 | 120.3292 | | 148.7486 |
| 160.4876 | 194.0601 | | 246.7860 |
| 257.0962 | 312.4443 | | 409.1798 |
| 467.0526 | 484.9336 | | 544.4819 |
| 735.0080 | 743.4990 | | 773.5606 |
| 834.4217 | 897.5762 | | 901.8727 |
| 929.2565 | 981.1106 | | 1015.4673 |
| 1028.6966 | 1039.0133 | | 1064.7555 |
| 1071.1993 | 1094.6598 | | 1102.2229 |
| 1138.8694 | 1192.9288 | | 1223.4854 |
| 1253.3435 | 1271.0519 | | 1302.5429 |
| 1313.5505 | 1329.9302 | | 1338.9315 |
| 1341.3687 | 1348.9326 | | 1364.2221 |
| 1372.7265 | 1398.9900 | | 1415.5888 |
| 1419.1554 | 1426.8302 | | 1493.8877 |
| 1498.1360 | 1499.3765 | | 1503.9371 |
| 1512.5682 | 1513.1027 | | 1522.0403 |
| 1527.9226 | 2881.5996 | | 2935.3556 |
| 3009.2762 | 3010.6524 | | 3014.2195 |
| 3019.8680 | 3027.0159 | | 3030.4172 |
| 3033.3544 | 3038.0474 | | 3040.4760 |
| 3054.4801 | 3063.0761 | | 3071.0110 |
| 3084.2432 | 3105.5028 | | 3111.4178 |
| Zero-point correction (Hartree): | 0.236633 | | |

C8H17O.1-4Hshift.ttt

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -390.23881934
 Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -3.120667 | 1.359683 | -0.353821 |
| C | -3.900943 | 0.218287 | -0.034774 |
| C | -2.906846 | -0.953873 | -0.073846 |
| C | -1.625311 | -0.289568 | 0.448127 |
| C | -0.290647 | -0.701223 | -0.125069 |
| C | 0.894829 | 0.140010 | 0.368713 |
| C | 2.242953 | -0.318507 | -0.200663 |
| C | 3.430780 | 0.520975 | 0.286507 |
| C | 4.774058 | 0.054000 | -0.283331 |
| H | -4.358789 | 0.305833 | 0.965078 |
| H | -4.710845 | 0.127501 | -0.770935 |
| H | -2.750477 | -1.274197 | -1.110199 |
| H | -3.219674 | -1.830474 | 0.506143 |
| H | -2.002717 | 0.872382 | 0.035785 |
| H | -1.615861 | -0.163202 | 1.537170 |
| H | -0.116212 | -1.760163 | 0.134616 |
| H | -0.340866 | -0.671063 | -1.222003 |
| H | 0.723897 | 1.192180 | 0.103395 |
| H | 0.931561 | 0.104663 | 1.466587 |
| H | 2.410851 | -1.372218 | 0.065470 |
| H | 2.203509 | -0.286801 | -1.298905 |
| H | 3.264193 | 1.572831 | 0.017631 |
| H | 3.468299 | 0.491355 | 1.384024 |
| H | 4.779678 | 0.105684 | -1.378118 |
| H | 4.984811 | -0.984094 | -0.001596 |
| H | 5.600738 | 0.671715 | 0.082440 |

Rotational constants (GHz): 5.4301000 0.4352800 0.4185300

Vibrational harmonic frequencies (cm-1):

| | | |
|------------|-----------|-----------|
| 11753.2091 | 43.9822 | 53.9093 |
| 82.6600 | 111.6170 | 134.0004 |
| 169.6383 | 185.7659 | 251.4469 |
| 275.3826 | 287.5374 | 398.3846 |
| 473.4834 | 558.0119 | 611.6688 |
| 732.4003 | 744.5569 | 786.6019 |
| 849.4556 | 884.8512 | 905.6579 |
| 936.3018 | 953.5235 | 999.2184 |
| 1009.8968 | 1032.1140 | 1049.0695 |
| 1066.5289 | 1076.2444 | 1108.7731 |
| 1135.3510 | 1178.6244 | 1203.5219 |
| 1221.2291 | 1227.3793 | 1253.6642 |
| 1256.5716 | 1295.5535 | 1303.8919 |
| 1331.7135 | 1337.9659 | 1341.4134 |
| 1373.4082 | 1383.7296 | 1412.1153 |
| 1416.5899 | 1427.5011 | 1479.4217 |
| 1498.6372 | 1498.9590 | 1502.7668 |
| 1513.9282 | 1514.9509 | 1525.5344 |
| 1530.8238 | 1748.5587 | 2973.1323 |
| 2974.1317 | 3012.1282 | 3020.2120 |
| 3028.4026 | 3038.2832 | 3039.3183 |
| 3042.7763 | 3044.8416 | 3052.8303 |
| 3058.4484 | 3073.1183 | 3077.8861 |
| 3098.2114 | 3107.0626 | 3113.0417 |

Zero-point correction (Hartree): 0.233376

C8H17O.1-5Hshift.ttd

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -390.25497015

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 1.575239 | 1.581247 | -0.287291 |
| C | 2.817106 | 1.085080 | 0.133900 |
| C | 2.681964 | -0.306582 | 0.776623 |
| C | 2.017324 | -1.264465 | -0.231714 |
| C | 0.706210 | -0.686622 | -0.752830 |
| C | -0.526227 | -0.851118 | 0.118576 |
| C | -1.728481 | -0.020941 | -0.350930 |
| C | -2.984097 | -0.229546 | 0.504621 |
| C | -4.179164 | 0.605089 | 0.033333 |
| H | 3.546904 | 1.038380 | -0.694984 |
| H | 3.211272 | 1.795117 | 0.878363 |
| H | 2.067393 | -0.223398 | 1.680654 |
| H | 3.666543 | -0.680147 | 1.081530 |
| H | 1.843772 | -2.241944 | 0.242173 |
| H | 2.706393 | -1.435197 | -1.067494 |
| H | 0.982749 | 0.557920 | -0.730378 |
| H | 0.510878 | -0.903908 | -1.808613 |
| H | -0.803170 | -1.918521 | 0.135429 |
| H | -0.283057 | -0.586407 | 1.155881 |
| H | -1.450488 | 1.041204 | -0.341691 |
| H | -1.956103 | -0.270100 | -1.397367 |
| H | -3.255190 | -1.294397 | 0.498132 |
| H | -2.753975 | 0.018279 | 1.549809 |
| H | -4.455218 | 0.355105 | -0.997547 |
| H | -3.949481 | 1.676224 | 0.061965 |

| | | | | |
|---|-----------|-----------|-----------|-----------|
| H | -5.058936 | 0.436439 | 0.662999 | |
| Rotational constants (GHz): | 3.2455700 | | 0.6240200 | 0.5691600 |
| Vibrational harmonic frequencies (cm ⁻¹): | | | | |
| i1442.9869 | | 45.8952 | | 62.9070 |
| 91.6292 | | 120.9558 | | 149.6840 |
| 175.1251 | | 243.2457 | | 259.9774 |
| 332.4838 | | 362.2223 | | 433.8296 |
| 491.4634 | | 514.8321 | | 622.6394 |
| 737.1939 | | 772.4856 | | 834.0352 |
| 845.0552 | | 858.7913 | | 901.8094 |
| 909.7505 | | 959.2659 | | 985.4237 |
| 994.9983 | | 1032.5490 | | 1058.2044 |
| 1069.3524 | | 1091.4653 | | 1096.1109 |
| 1144.4609 | | 1164.6337 | | 1182.5734 |
| 1217.2907 | | 1227.5416 | | 1251.0766 |
| 1263.2277 | | 1282.0895 | | 1315.9404 |
| 1336.9886 | | 1344.3471 | | 1350.6281 |
| 1369.0388 | | 1385.6212 | | 1398.0866 |
| 1415.3708 | | 1428.0447 | | 1483.4094 |
| 1488.8346 | | 1493.7369 | | 1500.6523 |
| 1507.4497 | | 1510.8792 | | 1512.4847 |
| 1524.5246 | | 1558.8253 | | 2950.2528 |
| 2985.7142 | | 3007.9044 | | 3015.1465 |
| 3017.3806 | | 3024.7128 | | 3039.5254 |
| 3047.2178 | | 3049.9606 | | 3055.0642 |
| 3067.7527 | | 3074.8943 | | 3086.3761 |
| 3099.1373 | | 3107.6924 | | 3112.6867 |
| Zero-point correction (Hartree): | 0.233404 | | | |

C8H17O.1-5Hshift.tt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -390.25547405

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -1.805604 | 1.608855 | -0.122888 |
| C | -2.936634 | 0.981463 | 0.416400 |
| C | -3.145101 | -0.420639 | -0.185231 |
| C | -1.883400 | -1.264925 | 0.064402 |
| C | -0.644602 | -0.553461 | -0.460985 |
| C | 0.675251 | -0.811268 | 0.239961 |
| C | 1.839922 | 0.033672 | -0.293449 |
| C | 3.170860 | -0.247961 | 0.414769 |
| C | 4.327960 | 0.603797 | -0.116640 |
| H | -2.882531 | 0.902692 | 1.517761 |
| H | -3.804870 | 1.615110 | 0.174768 |
| H | -3.321216 | -0.321114 | -1.263302 |
| H | -4.030789 | -0.894043 | 0.254338 |
| H | -1.991058 | -2.251813 | -0.408979 |
| H | -1.776357 | -1.443106 | 1.142855 |
| H | -0.985310 | 0.662637 | -0.285236 |
| H | -0.565052 | -0.592901 | -1.553990 |
| H | 0.554392 | -0.635969 | 1.318028 |
| H | 0.926153 | -1.881050 | 0.138857 |
| H | 1.956281 | -0.147306 | -1.371457 |
| H | 1.588525 | 1.097759 | -0.188823 |
| H | 3.050958 | -0.070829 | 1.492314 |
| H | 3.420100 | -1.312825 | 0.308760 |
| H | 4.120838 | 1.672923 | 0.005998 |
| H | 4.496955 | 0.421521 | -1.184141 |
| H | 5.262272 | 0.383406 | 0.409988 |

| | | | |
|---|-----------|-----------|-----------|
| Rotational constants (GHz): | 3.6558000 | 0.5670600 | 0.5159000 |
| Vibrational harmonic frequencies (cm ⁻¹): | | | |
| i1439.5444 | | 44.1639 | 67.3286 |
| 88.1145 | | 116.3438 | 144.7503 |
| 191.7337 | | 252.2829 | 288.8189 |
| 300.4120 | | 330.2685 | 452.3247 |
| 477.9052 | | 482.2860 | 583.3221 |
| 734.5484 | | 762.6301 | 809.2044 |
| 852.0119 | | 888.1347 | 901.7640 |
| 911.2978 | | 947.0659 | 979.0912 |
| 1018.9229 | | 1036.5164 | 1063.9268 |
| 1069.3606 | | 1084.3559 | 1104.9750 |
| 1138.2966 | | 1172.4715 | 1192.9831 |
| 1219.3820 | | 1239.0966 | 1249.5232 |
| 1274.2278 | | 1274.3643 | 1316.9766 |
| 1329.3521 | | 1338.7764 | 1357.2703 |
| 1374.3649 | | 1386.8911 | 1400.4494 |
| 1416.6823 | | 1428.5936 | 1482.6484 |
| 1488.3009 | | 1494.8588 | 1500.9610 |
| 1510.7536 | | 1511.1532 | 1513.9908 |
| 1524.8429 | | 1560.6045 | 2948.3109 |
| 2979.5585 | | 3007.0253 | 3013.4584 |
| 3018.4297 | | 3025.5700 | 3039.1498 |
| 3040.3204 | | 3046.2269 | 3047.9456 |
| 3056.4003 | | 3071.0101 | 3078.3811 |

3096.1406 3108.0673 3113.0619
 Zero-point correction (Hartree): 0.233218

C8H17O.1-6Hshift.t

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -390.25626601

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -0.837071 | 1.615118 | -0.283732 |
| C | -2.138964 | 1.417732 | 0.205106 |
| C | -2.823159 | 0.143496 | -0.310989 |
| C | -2.250476 | -1.176698 | 0.235569 |
| C | -0.807392 | -1.498881 | -0.199702 |
| C | 0.235630 | -0.553167 | 0.370082 |
| C | 1.639367 | -0.649001 | -0.200294 |
| C | 2.620410 | 0.373767 | 0.389165 |
| C | 4.025994 | 0.270492 | -0.210423 |
| H | -2.172867 | 1.440610 | 1.309677 |
| H | -2.704417 | 2.297329 | -0.141430 |
| H | -2.771559 | 0.144646 | -1.407637 |
| H | -3.886478 | 0.198683 | -0.042164 |
| H | -2.901724 | -1.997013 | -0.090075 |
| H | -2.302825 | -1.165674 | 1.334096 |
| H | -0.747271 | -1.486116 | -1.296560 |
| H | -0.561342 | -2.527366 | 0.106723 |

| | | | |
|---|-----------|-----------|-----------|
| H | -0.172474 | 0.592622 | 0.070964 |
| H | 0.224288 | -0.533328 | 1.468010 |
| H | 2.023836 | -1.668136 | -0.024386 |
| H | 1.594747 | -0.531490 | -1.291906 |
| H | 2.221628 | 1.383085 | 0.228317 |
| H | 2.673759 | 0.235809 | 1.477603 |
| H | 4.007681 | 0.440289 | -1.292992 |
| H | 4.460437 | -0.721330 | -0.039229 |
| H | 4.702689 | 1.009994 | 0.229763 |

Rotational constants (GHz): 2.9124700 0.7313600 0.6183900

Vibrational harmonic frequencies (cm-1):

| | | |
|------------|-----------|-----------|
| i1300.3012 | 55.2087 | 70.7759 |
| 86.7796 | 131.9310 | 191.6624 |
| 213.6814 | 247.0212 | 264.0541 |
| 337.8907 | 353.3434 | 395.0403 |
| 453.7850 | 506.2986 | 601.7570 |
| 742.3999 | 779.8370 | 792.0976 |
| 832.6972 | 864.7600 | 898.5797 |
| 912.9594 | 951.5676 | 986.4515 |
| 1010.0666 | 1046.3921 | 1060.5790 |
| 1084.2596 | 1088.4602 | 1107.9224 |
| 1128.6941 | 1165.3233 | 1211.3352 |
| 1225.0930 | 1247.8090 | 1264.0118 |
| 1283.3641 | 1294.5107 | 1305.3805 |
| 1335.5907 | 1350.9770 | 1380.8612 |
| 1394.5561 | 1396.4566 | 1405.3548 |
| 1409.0956 | 1424.6529 | 1451.9688 |
| 1480.2219 | 1481.3084 | 1484.4523 |
| 1493.8614 | 1502.0859 | 1506.2896 |
| 1512.8990 | 1522.2535 | 2952.9281 |
| 2981.3170 | 3002.9079 | 3010.2094 |
| 3019.7152 | 3030.1825 | 3032.3920 |
| 3037.9266 | 3041.4270 | 3047.3672 |
| 3061.6028 | 3068.3845 | 3073.2342 |
| 3077.4125 | 3107.1247 | 3113.8520 |

Zero-point correction (Hartree): 0.233249

C8H17O.1-7Hshift.BB.tt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -390.25168875

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -0.069405 | -1.662290 | -0.287204 |
| H | 0.499771 | -0.533915 | -0.346987 |
| C | 1.001483 | 0.626764 | -0.218953 |
| C | -1.121116 | -1.531260 | 0.631886 |
| C | 0.009528 | 1.431048 | 0.601000 |
| C | -2.346404 | -0.765701 | 0.089454 |
| C | -1.357485 | 1.674154 | -0.071735 |
| C | -2.015404 | 0.467844 | -0.768120 |
| C | 2.369085 | 0.401644 | 0.402300 |
| C | 3.261927 | -0.541540 | -0.411267 |
| H | 1.061011 | 0.955247 | -1.264965 |
| H | -1.417148 | -2.561051 | 0.889709 |
| H | -0.768451 | -1.088342 | 1.577662 |
| H | -0.127271 | 0.941780 | 1.574099 |
| H | 0.459421 | 2.408811 | 0.838083 |
| H | -2.932318 | -1.449545 | -0.537255 |
| H | -2.992217 | -0.488297 | 0.934384 |

| | | | | |
|--|-----------|-----------|-----------|--|
| H | -2.045230 | 2.083324 | 0.680188 | |
| H | -1.237093 | 2.461631 | -0.827777 | |
| H | -2.948057 | 0.820652 | -1.225651 | |
| H | -1.382207 | 0.135446 | -1.598444 | |
| H | 2.867414 | 1.377743 | 0.519269 | |
| H | 2.242999 | 0.007004 | 1.419389 | |
| H | 3.429641 | -0.153829 | -1.422463 | |
| H | 2.795334 | -1.527071 | -0.502465 | |
| H | 4.239957 | -0.668985 | 0.063463 | |
| Rotational constants (GHz): | 2.2379700 | 1.0310000 | 0.7983100 | |
| Vibrational harmonic frequencies (cm-1): | | | | |
| i1418.2280 | 65.6473 | | 81.3263 | |
| 122.0127 | 163.9061 | | 232.1813 | |
| 255.8858 | 261.7845 | | 286.2175 | |
| 311.3602 | 375.1260 | | 402.5324 | |
| 495.0044 | 561.5289 | | 573.4337 | |
| 737.9550 | 764.7297 | | 793.5458 | |
| 808.4771 | 857.0247 | | 889.6068 | |
| 909.2770 | 952.8106 | | 976.4183 | |
| 1011.8932 | 1033.1782 | | 1057.0961 | |
| 1082.3763 | 1097.8152 | | 1125.0962 | |
| 1137.3904 | 1161.5707 | | 1196.5649 | |
| 1215.6338 | 1235.0906 | | 1265.3141 | |
| 1280.6087 | 1300.6257 | | 1308.6288 | |
| 1320.3709 | 1365.6425 | | 1384.0873 | |
| 1394.6767 | 1399.0674 | | 1402.7181 | |
| 1415.5439 | 1425.8294 | | 1452.5679 | |
| 1468.3849 | 1486.2834 | | 1493.0776 | |
| 1495.0759 | 1505.2424 | | 1512.3988 | |
| 1513.3223 | 1523.3713 | | 2977.2231 | |
| 2989.9958 | 2996.8067 | | 3005.1494 | |
| 3025.8894 | 3027.2621 | | 3041.2869 | |
| 3044.7218 | 3046.4003 | | 3047.3322 | |
| 3060.6249 | 3068.2791 | | 3070.8982 | |
| 3092.1286 | 3113.4568 | | 3128.1039 | |
| Zero-point correction (Hartree): | 0.233922 | | | |

C8H17O.1-7Hshift.CR.t

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -390.25103746

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | | |
|--|-----------|-----------|-----------|--|
| O | 0.064138 | 1.678486 | -0.353017 | |
| C | -1.099755 | 1.676607 | 0.426806 | |
| C | -2.283137 | 0.888809 | -0.158950 | |
| C | -2.382800 | -0.607714 | 0.193863 | |
| C | -1.345717 | -1.588126 | -0.392635 | |
| C | 0.047381 | -1.596120 | 0.271233 | |
| C | 1.064169 | -0.634746 | -0.316643 | |
| C | 2.372305 | -0.483012 | 0.441006 | |
| C | 3.315655 | 0.558160 | -0.171096 | |
| H | -0.904567 | 1.363847 | 1.468683 | |
| H | -1.379023 | 2.742127 | 0.483738 | |
| H | -2.265137 | 1.025387 | -1.247760 | |
| H | -3.208471 | 1.362138 | 0.197297 | |
| H | -3.372994 | -0.947372 | -0.136547 | |
| H | -2.386056 | -0.714666 | 1.288637 | |
| H | -1.238919 | -1.415903 | -1.472446 | |
| H | -1.770388 | -2.594568 | -0.292472 | |
| H | 0.472288 | -2.609524 | 0.186499 | |
| H | -0.057591 | -1.415490 | 1.350159 | |
| H | 0.557553 | 0.510329 | -0.348954 | |
| H | 1.219881 | -0.807824 | -1.389935 | |
| H | 2.155476 | -0.219088 | 1.484791 | |
| H | 2.873298 | -1.464147 | 0.478664 | |
| H | 2.837427 | 1.541881 | -0.189626 | |
| H | 3.581203 | 0.294404 | -1.201072 | |
| H | 4.244313 | 0.637435 | 0.402982 | |
| Rotational constants (GHz): | 2.1978500 | 1.0066100 | 0.7466400 | |
| Vibrational harmonic frequencies (cm-1): | | | | |
| i1283.1179 | 48.7332 | | 80.0992 | |
| 104.5146 | 123.5711 | | 176.4416 | |
| 241.4598 | 281.3961 | | 293.5323 | |
| 309.9503 | 377.2197 | | 410.3424 | |
| 462.1382 | 468.1024 | | 567.8220 | |
| 736.2266 | 756.2316 | | 800.2195 | |
| 825.0739 | 862.5470 | | 899.8303 | |
| 915.0398 | 961.3010 | | 981.9411 | |
| 996.7545 | 1046.2584 | | 1054.9211 | |
| 1088.4062 | 1101.5341 | | 1115.0255 | |
| 1137.0962 | 1160.1007 | | 1198.2856 | |
| 1210.3027 | 1251.3393 | | 1260.9039 | |
| 1287.9544 | 1297.0252 | | 1311.1766 | |
| 1317.4678 | 1370.3709 | | 1385.1141 | |
| 1390.9603 | 1394.2146 | | 1402.3584 | |

| | | |
|-----------|-----------|-----------|
| 1410.0502 | 1425.0102 | 1434.1631 |
| 1469.1755 | 1482.3910 | 1484.2430 |
| 1491.8617 | 1501.2096 | 1503.1743 |
| 1512.6769 | 1524.4878 | 2953.8859 |
| 2986.4444 | 2992.9556 | 2994.1430 |
| 3014.4473 | 3027.2289 | 3028.3980 |
| 3039.4904 | 3044.2415 | 3046.1947 |
| 3058.1330 | 3062.6559 | 3068.2505 |
| 3076.6334 | 3113.0671 | 3130.6679 |

Zero-point correction (Hartree): 0.233140

C8H17O.1-8Hshift

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -390.24752864

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 0.341083 | -1.551136 | -0.785636 |
| C | 1.460871 | -1.670127 | 0.053877 |
| C | 2.372996 | -0.437277 | 0.115438 |
| C | 1.658744 | 0.832249 | 0.610938 |
| C | 0.826351 | 1.568131 | -0.473872 |
| C | -0.561380 | 2.052326 | -0.002314 |
| C | -1.699154 | 1.039125 | -0.224741 |
| C | -1.527756 | -0.330836 | 0.410644 |
| C | -2.680192 | -1.297076 | 0.210630 |
| H | 1.157715 | -1.956494 | 1.076657 |
| H | 2.027836 | -2.529954 | -0.340449 |
| H | 2.809111 | -0.256803 | -0.875536 |
| H | 3.208784 | -0.680891 | 0.785677 |
| H | 2.401376 | 1.526558 | 1.021694 |
| H | 1.017941 | 0.562998 | 1.460908 |
| H | 0.693872 | 0.910498 | -1.339087 |
| H | 1.403808 | 2.428599 | -0.831559 |
| H | -0.832373 | 2.969630 | -0.539259 |
| H | -0.514863 | 2.331072 | 1.059663 |
| H | -1.852930 | 0.904170 | -1.304749 |
| H | -2.638552 | 1.474604 | 0.154579 |
| H | -0.562206 | -0.897269 | -0.180668 |
| H | -1.197266 | -0.283418 | 1.455162 |
| H | -2.922486 | -1.409523 | -0.851469 |
| H | -3.584810 | -0.935519 | 0.719924 |
| H | -2.446508 | -2.288257 | 0.609998 |

Rotational constants (GHz): 1.8086300 1.2681100 0.8330600

Vibrational harmonic frequencies (cm-1):

| | | |
|------------|-----------|-----------|
| i1435.3212 | 92.1861 | 137.4458 |
| 140.2732 | 163.0028 | 180.7037 |
| 222.2125 | 240.9452 | 305.0137 |
| 320.8981 | 343.1404 | 373.1326 |
| 481.6160 | 510.4195 | 582.1616 |
| 730.2204 | 798.2589 | 816.9848 |
| 842.0275 | 880.4228 | 894.4293 |
| 906.6336 | 957.9256 | 973.7420 |
| 1013.4234 | 1042.5213 | 1072.6886 |
| 1082.8648 | 1096.5492 | 1110.6307 |
| 1134.4875 | 1149.0280 | 1198.8375 |
| 1205.5870 | 1227.9649 | 1265.8649 |
| 1268.8575 | 1295.0216 | 1322.3727 |
| 1341.6833 | 1352.5989 | 1383.7175 |
| 1389.1174 | 1401.5416 | 1405.4208 |
| 1412.6004 | 1420.2173 | 1426.4430 |
| 1464.1578 | 1481.1963 | 1493.0423 |
| 1498.6858 | 1504.0843 | 1506.9157 |
| 1513.0198 | 1521.3536 | 2959.1175 |
| 2986.8809 | 2998.4161 | 3021.9625 |
| 3023.8499 | 3027.5868 | 3034.2876 |
| 3039.2716 | 3045.2954 | 3064.7139 |
| 3068.4911 | 3071.1700 | 3077.6605 |
| 3093.6411 | 3100.2208 | 3126.3778 |

Zero-point correction (Hartree): 0.233820

C8H17O.1-8Hshift.TBCd.t

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -390.24886371

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| C | -2.185037 | -0.834346 | -0.223461 |
| C | -0.955209 | -1.751677 | -0.275571 |
| O | -0.081406 | -1.653340 | 0.821151 |
| H | 0.803467 | -0.774347 | 0.599654 |
| C | 1.752895 | 0.018452 | 0.339390 |
| C | 1.226590 | 1.140925 | -0.536273 |
| C | 0.191554 | 2.063652 | 0.129989 |
| C | -1.087525 | 1.370193 | 0.634750 |
| C | -1.917228 | 0.660441 | -0.469803 |
| H | -2.896931 | -1.195366 | -0.979211 |

| | | | |
|-----------------------------|-----------|-----------|-----------|
| H | -2.670136 | -0.970346 | 0.751919 |
| H | -0.414206 | -1.608926 | -1.227851 |
| H | -1.292254 | -2.802105 | -0.288056 |
| C | 2.827552 | -0.858265 | -0.273540 |
| H | 2.009376 | 0.357220 | 1.351177 |
| H | 0.819738 | 0.714668 | -1.463807 |
| H | 2.083969 | 1.754844 | -0.857746 |
| H | -0.081615 | 2.850452 | -0.586004 |
| H | 0.670971 | 2.576100 | 0.975170 |
| H | -1.707992 | 2.129390 | 1.125563 |
| H | -0.825760 | 0.647808 | 1.413024 |
| H | -1.421017 | 0.769658 | -1.443997 |
| H | -2.882939 | 1.167458 | -0.581333 |
| H | 3.746141 | -0.282035 | -0.454329 |
| H | 2.506297 | -1.267960 | -1.237873 |
| H | 3.082586 | -1.696045 | 0.381615 |
| Rotational constants (GHz): | 1.8133500 | 1.2874200 | 0.8628100 |

Vibrational harmonic frequencies (cm-1):

| | | |
|------------|-----------|-----------|
| i1419.8651 | 66.7574 | 92.0231 |
| 139.8710 | 200.1769 | 202.2787 |
| 221.9272 | 270.2527 | 309.5533 |
| 331.3042 | 352.3745 | 390.4234 |
| 477.0593 | 499.5512 | 567.5686 |
| 739.3668 | 765.5526 | 814.2996 |
| 837.7402 | 858.8630 | 887.2469 |
| 900.6863 | 937.8393 | 977.3642 |
| 1022.6510 | 1047.1420 | 1064.4315 |
| 1079.9803 | 1092.5542 | 1115.2574 |
| 1131.6255 | 1145.8188 | 1185.4940 |
| 1214.2813 | 1221.3268 | 1253.7464 |
| 1280.0378 | 1299.1093 | 1319.9459 |
| 1333.3149 | 1362.9235 | 1385.7649 |
| 1397.1579 | 1403.0416 | 1404.1991 |
| 1408.1054 | 1419.1033 | 1433.8639 |
| 1463.3678 | 1482.3031 | 1487.9737 |
| 1499.1822 | 1502.6092 | 1503.7856 |
| 1512.8395 | 1519.0112 | 2959.8755 |
| 2990.4922 | 2991.6367 | 3020.8550 |
| 3022.6446 | 3023.9851 | 3029.1594 |
| 3039.3580 | 3047.5060 | 3058.6721 |
| 3064.8264 | 3067.8049 | 3075.2818 |
| 3087.9522 | 3107.9666 | 3125.3269 |

Zero-point correction (Hartree): 0.233616

C8H17O.4me.pttttt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -429.58379691

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|-----------------------------|-----------|-----------|-----------|
| O | -3.938145 | -0.927382 | -1.119311 |
| C | -3.881884 | -0.351653 | 0.122107 |
| C | -2.509803 | -0.409586 | 0.808645 |
| C | -1.370211 | 0.248234 | 0.006243 |
| C | -0.001293 | -0.190013 | 0.565316 |
| C | 1.216502 | 0.248579 | -0.259875 |
| C | 2.541318 | -0.301918 | 0.284500 |
| C | 3.767376 | 0.130376 | -0.529835 |
| C | 5.085313 | -0.423243 | 0.021323 |
| H | -4.194597 | 0.701926 | -0.047717 |
| H | -4.682330 | -0.756804 | 0.771536 |
| H | -2.594160 | 0.053184 | 1.802487 |
| H | -2.272232 | -1.467522 | 0.978373 |
| H | -1.452111 | -0.130603 | -1.022493 |
| C | -1.515744 | 1.778341 | -0.029645 |
| H | 0.103803 | 0.184000 | 1.595166 |
| H | 0.006880 | -1.286318 | 0.640965 |
| H | 1.086226 | -0.082860 | -1.300156 |
| H | 1.275490 | 1.344141 | -0.294364 |
| H | 2.668220 | 0.021538 | 1.327876 |
| H | 2.494855 | -1.400121 | 0.312968 |
| H | 3.641375 | -0.193169 | -1.572069 |
| H | 3.814529 | 1.227651 | -0.557524 |
| H | 5.082282 | -1.519283 | 0.029286 |
| H | 5.256475 | -0.087332 | 1.050577 |
| H | 5.940227 | -0.097957 | -0.580612 |
| H | -2.490420 | 2.087981 | -0.421529 |
| H | -0.757581 | 2.241619 | -0.667200 |
| H | -1.411212 | 2.204288 | 0.976249 |
| Rotational constants (GHz): | 3.5416600 | 0.3658900 | 0.3573800 |

Vibrational harmonic frequencies (cm-1):

| | | |
|----------|----------|----------|
| 36.9421 | 54.7123 | 62.8373 |
| 81.4263 | 115.6800 | 140.5770 |
| 146.1997 | 206.4102 | 226.0263 |
| 254.3350 | 255.9043 | 272.3260 |

| | | |
|-----------|-----------|-----------|
| 374.5842 | 402.0517 | 435.7411 |
| 482.7155 | 527.7276 | 599.1438 |
| 737.9543 | 761.3453 | 820.8329 |
| 848.8424 | 868.8048 | 900.9910 |
| 931.1818 | 956.5879 | 966.2240 |
| 1013.9770 | 1041.4795 | 1049.0179 |
| 1064.5864 | 1072.7960 | 1091.8680 |
| 1113.7120 | 1142.4897 | 1185.2769 |
| 1187.7069 | 1224.9590 | 1252.8521 |
| 1275.0906 | 1306.7479 | 1312.5745 |
| 1336.0026 | 1339.1371 | 1342.6450 |
| 1360.9909 | 1367.9718 | 1391.8320 |
| 1400.5012 | 1407.0938 | 1416.2217 |
| 1427.8688 | 1429.0463 | 1486.9940 |
| 1498.2346 | 1499.4541 | 1505.2135 |
| 1509.4472 | 1514.5461 | 1516.7070 |
| 1520.9171 | 1526.7872 | 2890.6416 |
| 2937.7932 | 3004.8354 | 3011.7713 |
| 3019.9606 | 3021.4734 | 3027.2807 |
| 3030.0605 | 3037.5684 | 3038.5022 |
| 3038.8510 | 3043.2690 | 3059.0580 |
| 3069.7087 | 3077.2011 | 3101.8177 |
| 3106.7408 | 3111.6389 | 3123.1791 |

Zero-point correction (Hartree): 0.265070

C8H17O.1-4Hshift.4me.tttt

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -429.55724810

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -2.792278 | -1.215773 | -1.064312 |
| C | -3.649802 | -0.694278 | -0.064946 |
| C | -2.708863 | -0.103570 | 1.000243 |
| C | -1.506146 | 0.374695 | 0.153312 |
| C | -0.134035 | 0.042061 | 0.719962 |
| C | 1.059768 | 0.282113 | -0.215859 |
| C | 2.390507 | -0.191346 | 0.382968 |
| C | 3.595395 | 0.053190 | -0.534333 |
| C | 4.919453 | -0.429166 | 0.066515 |
| H | -4.323167 | 0.080448 | -0.468866 |
| H | -4.276478 | -1.508700 | 0.324461 |
| H | -2.381156 | -0.890812 | 1.687642 |
| H | -3.163624 | 0.695912 | 1.598492 |
| H | -1.774673 | -0.448126 | -0.777575 |
| C | -1.672607 | 1.766110 | -0.433324 |
| H | 0.005676 | 0.631796 | 1.642989 |
| H | -0.136738 | -1.008991 | 1.036719 |
| H | 0.882484 | -0.238987 | -1.167027 |
| H | 1.137718 | 1.349169 | -0.460171 |
| H | 2.558612 | 0.315757 | 1.344270 |
| H | 2.323865 | -1.263882 | 0.614900 |
| H | 3.424716 | -0.449678 | -1.495897 |
| H | 3.665120 | 1.125757 | -0.761723 |
| H | 4.892499 | -1.505441 | 0.271820 |
| H | 5.135298 | 0.080999 | 1.012387 |
| H | 5.758837 | -0.241370 | -0.610943 |
| H | -2.675184 | 1.907580 | -0.848016 |
| H | -0.949134 | 1.971706 | -1.227063 |
| H | -1.528469 | 2.524203 | 0.350868 |

Rotational constants (GHz): 3.0786300 0.4156500 0.4041000

Vibrational harmonic frequencies (cm-1):

| | | |
|------------|-----------|-----------|
| 11615.5926 | 39.6156 | 55.2167 |
| 88.1579 | 99.3984 | 129.8373 |
| 146.8384 | 182.2407 | 201.6252 |
| 235.7263 | 249.0294 | 277.1255 |
| 305.2983 | 390.0902 | 399.1431 |
| 487.4325 | 583.5357 | 621.3645 |
| 736.3541 | 757.2051 | 797.4318 |
| 845.1487 | 891.8532 | 908.0875 |
| 941.2086 | 958.0225 | 959.5268 |
| 1013.2235 | 1015.8243 | 1030.5046 |
| 1049.2465 | 1063.8102 | 1071.4539 |
| 1108.8740 | 1140.3796 | 1153.6761 |
| 1191.4466 | 1199.8149 | 1226.6218 |
| 1238.4841 | 1273.0471 | 1282.3017 |
| 1312.1839 | 1333.2986 | 1337.8541 |
| 1340.5405 | 1352.1091 | 1374.1994 |
| 1399.8871 | 1415.4384 | 1419.6101 |
| 1429.8794 | 1476.8895 | 1492.6055 |
| 1499.2604 | 1502.2982 | 1503.8341 |
| 1508.8475 | 1513.9436 | 1516.0524 |
| 1526.1782 | 1533.0540 | 1743.2060 |
| 2971.3468 | 2973.5196 | 3012.2092 |
| 3016.4119 | 3023.0404 | 3030.3937 |
| 3036.1240 | 3038.9279 | 3039.4868 |

| | | |
|-----------|-----------|-----------|
| 3047.6767 | 3050.3205 | 3061.2124 |
| 3079.0821 | 3096.9005 | 3097.8790 |
| 3106.9346 | 3112.9252 | 3130.0696 |

Zero-point correction (Hartree): 0.261536

C8H17O.5me.pttttt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -429.58372519

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 4.002742 | -1.601706 | -0.253933 |
| C | 4.012214 | -0.275482 | 0.088669 |
| C | 2.757839 | 0.516844 | -0.303155 |
| C | 1.483822 | -0.055223 | 0.329800 |
| C | 0.161448 | 0.544496 | -0.188696 |
| C | -1.033765 | -0.245874 | 0.383835 |
| C | -2.401001 | 0.090070 | -0.227463 |
| C | -3.533255 | -0.798831 | 0.304831 |
| C | -4.899285 | -0.468764 | -0.305030 |
| H | 4.138653 | -0.270876 | 1.194610 |
| H | 4.939319 | 0.204087 | -0.282083 |
| H | 2.912069 | 1.564639 | -0.016718 |
| H | 2.670119 | 0.500040 | -1.397757 |
| H | 1.481385 | -1.136698 | 0.146423 |
| H | 1.532022 | 0.072065 | 1.422314 |
| C | 0.055861 | 2.047703 | 0.115226 |
| H | 0.148923 | 0.417696 | -1.282866 |
| H | -0.842009 | -1.317973 | 0.237505 |
| H | -1.074762 | -0.093179 | 1.472802 |
| H | -2.656341 | 1.140307 | -0.034989 |
| H | -2.344468 | -0.013817 | -1.320882 |
| H | -3.288917 | -1.851699 | 0.108335 |
| H | -3.586673 | -0.700206 | 1.397749 |
| H | -4.886530 | -0.589916 | -1.394323 |
| H | -5.188933 | 0.566907 | -0.092704 |
| H | -5.684082 | -1.120864 | 0.092343 |
| H | -0.871273 | 2.476339 | -0.276368 |
| H | 0.882819 | 2.611054 | -0.328021 |
| H | 0.073468 | 2.226111 | 1.197992 |

Rotational constants (GHz): 3.0333100 0.3893300 0.3574900

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 38.6051 | 52.5021 | 66.2256 |
| 84.7681 | 99.9222 | 136.8813 |
| 152.1849 | 191.2009 | 239.7915 |
| 249.1930 | 261.8711 | 294.7505 |
| 314.4070 | 409.8672 | 455.3713 |
| 483.1036 | 520.6482 | 563.1952 |
| 737.1687 | 776.1486 | 788.9481 |
| 856.0251 | 906.6215 | 909.1205 |
| 918.7369 | 927.2063 | 976.6515 |
| 1007.8538 | 1025.6135 | 1051.8645 |
| 1068.5909 | 1080.4844 | 1096.0033 |
| 1106.3122 | 1142.1720 | 1178.3024 |
| 1202.5036 | 1233.4714 | 1251.2548 |
| 1272.4270 | 1301.5260 | 1321.0534 |
| 1328.6346 | 1338.0010 | 1347.1287 |
| 1365.1971 | 1370.7247 | 1387.6164 |
| 1391.1878 | 1411.4929 | 1415.9269 |
| 1425.4972 | 1428.0727 | 1489.5287 |
| 1497.1634 | 1501.2719 | 1509.4623 |
| 1512.5868 | 1513.3152 | 1513.5257 |
| 1521.5413 | 1526.2686 | 2881.2290 |
| 2936.8171 | 2995.4388 | 3005.0598 |
| 3012.2607 | 3016.9637 | 3026.7342 |
| 3035.9845 | 3038.0362 | 3038.9379 |
| 3040.4852 | 3049.8100 | 3064.9048 |
| 3072.7906 | 3084.6747 | 3105.8032 |
| 3108.0059 | 3111.4129 | 3122.6678 |

Zero-point correction (Hartree): 0.264934

C8H17O.1-5Hshift.5me.ttt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -429.57278984

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -1.690888 | -1.480577 | 0.844668 |
| C | -2.744921 | -1.369260 | -0.069663 |
| C | -3.082552 | 0.103623 | -0.362771 |
| C | -1.827173 | 0.812647 | -0.902897 |
| C | -0.626058 | 0.622044 | 0.031645 |
| C | 0.712638 | 0.469275 | -0.688860 |
| C | 1.899714 | 0.046054 | 0.187994 |
| C | 3.184540 | -0.184624 | -0.618630 |
| C | 4.376231 | -0.595585 | 0.251812 |
| H | -2.530914 | -1.893596 | -1.019493 |

| | | | |
|---|-----------|-----------|-----------|
| H | -3.620700 | -1.860589 | 0.384850 |
| H | -3.420586 | 0.581000 | 0.564433 |
| H | -3.906537 | 0.167047 | -1.083284 |
| H | -2.032274 | 1.884088 | -1.043113 |
| H | -1.590423 | 0.404385 | -1.893748 |
| H | -0.909046 | -0.497213 | 0.515319 |
| C | -0.620089 | 1.567599 | 1.226580 |
| H | 0.590794 | -0.261817 | -1.499245 |
| H | 0.950661 | 1.426864 | -1.183288 |
| H | 2.092780 | 0.807809 | 0.954176 |
| H | 1.638050 | -0.874475 | 0.727748 |
| H | 3.001162 | -0.957164 | -1.377806 |
| H | 3.433933 | 0.730935 | -1.172700 |
| H | 4.169024 | -1.525586 | 0.793248 |
| H | 4.607046 | 0.174730 | 0.996567 |
| H | 5.276276 | -0.755120 | -0.350973 |
| H | 0.092175 | 1.255281 | 1.995049 |
| H | -1.606658 | 1.624495 | 1.695272 |
| H | -0.341632 | 2.582905 | 0.908380 |
| Rotational constants (GHz): | 2.3474100 | 0.5426300 | 0.5097600 |
| Vibrational harmonic frequencies (cm ⁻¹): | | | |
| i1228.1900 | 42.6736 | | 64.5693 |
| 95.8164 | 109.1206 | | 137.6521 |
| 147.1347 | 199.5651 | | 247.5060 |
| 277.1564 | 281.0835 | | 298.5307 |
| 309.0830 | 403.5513 | | 459.1528 |
| 492.5175 | 508.3251 | | 607.0011 |
| 739.1271 | 783.6816 | | 802.5534 |
| 855.3998 | 894.5212 | | 907.3928 |
| 919.0936 | 929.9590 | | 950.0398 |
| 1009.7984 | 1016.9099 | | 1026.1616 |
| 1062.6544 | 1070.9060 | | 1086.1261 |
| 1105.3661 | 1150.7654 | | 1162.2834 |
| 1187.3256 | 1199.6442 | | 1215.9485 |
| 1244.5119 | 1257.2553 | | 1290.4292 |
| 1296.7627 | 1329.9275 | | 1340.3632 |
| 1353.4501 | 1367.4972 | | 1378.7498 |
| 1385.7460 | 1413.8160 | | 1418.9770 |
| 1428.7860 | 1478.5652 | | 1487.7583 |
| 1492.5643 | 1497.8560 | | 1501.8784 |
| 1505.0026 | 1511.4149 | | 1512.4664 |
| 1513.6937 | 1524.7702 | | 1560.2210 |
| 2943.8548 | 2978.0382 | | 3000.5734 |
| 3013.6742 | 3020.3910 | | 3021.0767 |
| 3030.3300 | 3039.9609 | | 3044.0201 |
| 3049.4738 | 3050.4841 | | 3064.1504 |
| 3077.8906 | 3095.9719 | | 3102.2068 |
| 3108.1190 | 3112.8918 | | 3132.2133 |
| Zero-point correction (Hartree): | 0.261383 | | |

C8H17O.6me.pttttt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -429.58357816

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|-----------------------------|-----------|-----------|-----------|
| O | -4.457217 | 0.816570 | -0.158008 |
| C | -4.126892 | -0.442659 | 0.269282 |
| C | -2.759207 | -0.957427 | -0.194999 |
| C | -1.599920 | -0.065688 | 0.263940 |
| C | -0.240160 | -0.517575 | -0.284831 |
| C | 0.976353 | 0.284835 | 0.222922 |
| C | 2.283589 | -0.396264 | -0.233240 |
| C | 3.573952 | 0.175016 | 0.370895 |
| C | 4.821878 | -0.613052 | -0.042408 |
| H | -4.158535 | -0.381943 | 1.380280 |
| H | -4.943381 | -1.150035 | 0.023955 |
| H | -2.626668 | -1.983610 | 0.174665 |
| H | -2.769329 | -1.020099 | -1.291124 |
| H | -1.821156 | 0.961479 | -0.045730 |
| H | -1.563756 | -0.056973 | 1.363605 |
| H | -0.091310 | -1.575444 | -0.025648 |
| H | -0.261898 | -0.477104 | -1.384082 |
| C | 0.912782 | 1.757731 | -0.212234 |
| H | 0.955456 | 0.255308 | 1.324177 |
| H | 2.226700 | -1.464476 | 0.020428 |
| H | 2.346630 | -0.351160 | -1.331026 |
| H | 3.698691 | 1.223117 | 0.073154 |
| H | 3.489290 | 0.177282 | 1.466529 |
| H | 4.950577 | -0.608445 | -1.130949 |
| H | 4.754405 | -1.659702 | 0.276091 |
| H | 5.728861 | -0.188479 | 0.400526 |
| H | 1.754367 | 2.333741 | 0.183430 |
| H | -0.002908 | 2.244220 | 0.136102 |
| H | 0.937455 | 1.840266 | -1.306277 |
| Rotational constants (GHz): | 3.9896600 | 0.3693400 | 0.3489900 |

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 32.4630 | 57.5306 | 70.5908 |
| 90.6216 | 106.6920 | 126.8077 |
| 146.3637 | 192.3517 | 233.7815 |
| 254.6174 | 263.2118 | 306.6844 |
| 327.4366 | 385.1148 | 446.2598 |
| 482.2771 | 517.2331 | 546.5522 |
| 746.3631 | 755.4263 | 820.7858 |
| 851.1214 | 880.4754 | 902.6555 |
| 916.1740 | 958.2038 | 969.2058 |
| 1005.4705 | 1039.2061 | 1049.1616 |
| 1056.5826 | 1085.2058 | 1094.7089 |
| 1104.6218 | 1148.9172 | 1179.6293 |
| 1200.3105 | 1221.7926 | 1256.4308 |
| 1284.1553 | 1308.6218 | 1312.1682 |
| 1336.3213 | 1340.0019 | 1346.6996 |
| 1364.2422 | 1368.3310 | 1387.3713 |
| 1394.5881 | 1408.7430 | 1417.7439 |
| 1426.5470 | 1430.5357 | 1489.5879 |
| 1494.4040 | 1500.8090 | 1507.5996 |
| 1512.4794 | 1513.9768 | 1517.8109 |
| 1521.6653 | 1525.8754 | 2881.1634 |
| 2935.6642 | 2992.2828 | 3004.0270 |
| 3010.1018 | 3016.2744 | 3028.2955 |
| 3030.1906 | 3038.3633 | 3039.0359 |
| 3040.6460 | 3048.3928 | 3067.4170 |
| 3072.3167 | 3094.4702 | 3107.1244 |
| 3110.4822 | 3111.8567 | 3125.6526 |

Zero-point correction (Hartree): 0.264935

C8H17O.1-6Hshift.6me.tt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -429.57259889

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -0.811557 | 1.715856 | 0.168710 |
| C | -2.165378 | 1.436411 | 0.401294 |
| C | -2.780361 | 0.417198 | -0.569353 |
| C | -2.301559 | -1.033861 | -0.384245 |
| C | -0.821418 | -1.291726 | -0.732720 |
| C | 0.207130 | -0.598721 | 0.166385 |
| C | 1.582027 | -0.472231 | -0.494614 |
| C | 2.612907 | 0.380300 | 0.259618 |
| C | 3.916962 | 0.554842 | -0.525986 |
| H | -2.350678 | 1.120058 | 1.444423 |
| H | -2.676524 | 2.405274 | 0.276503 |
| H | -2.575021 | 0.750346 | -1.595139 |
| H | -3.870357 | 0.442051 | -0.438180 |
| H | -2.913853 | -1.682578 | -1.022759 |
| H | -2.508563 | -1.352407 | 0.646408 |
| H | -0.650634 | -0.977967 | -1.770703 |
| H | -0.633860 | -2.376584 | -0.707092 |
| H | -0.186390 | 0.565035 | 0.230436 |
| C | 0.234764 | -1.120405 | 1.598462 |
| H | 1.989238 | -1.486608 | -0.647054 |
| H | 1.443084 | -0.051001 | -1.499109 |
| H | 2.175081 | 1.363880 | 0.471973 |
| H | 2.838323 | -0.074798 | 1.231628 |
| H | 3.737433 | 1.048603 | -1.487727 |
| H | 4.388642 | -0.412567 | -0.734700 |
| H | 4.638335 | 1.162585 | 0.029815 |
| H | -0.767041 | -1.178677 | 2.033457 |
| H | 0.841963 | -0.489056 | 2.252307 |
| H | 0.662830 | -2.133280 | 1.622781 |

Rotational constants (GHz): 2.0337900 0.6862300 0.6153100

Vibrational harmonic frequencies (cm-1):

| | | |
|------------|-----------|-----------|
| i1009.9059 | 52.6943 | 70.7938 |
| 88.8010 | 101.3307 | 148.5599 |
| 193.7671 | 218.6150 | 246.0250 |
| 259.4612 | 314.0926 | 329.2202 |
| 349.4943 | 391.4589 | 410.9578 |
| 470.1628 | 523.4561 | 625.5958 |
| 746.2997 | 779.3322 | 799.6640 |
| 845.8877 | 874.3729 | 889.1575 |
| 911.0272 | 951.0756 | 954.5740 |
| 977.5265 | 1021.7684 | 1040.9943 |
| 1060.6643 | 1083.4809 | 1094.3041 |
| 1103.3489 | 1146.7273 | 1170.5101 |
| 1184.5460 | 1203.1312 | 1233.7306 |
| 1258.5295 | 1273.7807 | 1283.0025 |
| 1309.3727 | 1325.2856 | 1347.4053 |
| 1377.7873 | 1382.9947 | 1395.5844 |
| 1405.4343 | 1406.1420 | 1420.7258 |
| 1422.6622 | 1429.3148 | 1475.3369 |
| 1477.9399 | 1482.8857 | 1490.8355 |

| | | |
|-----------|-----------|-----------|
| 1498.6806 | 1503.8068 | 1508.0998 |
| 1512.7109 | 1516.3685 | 1523.2998 |
| 2948.8853 | 2980.2324 | 3000.0452 |
| 3001.6250 | 3020.2403 | 3028.8923 |
| 3033.1500 | 3037.9055 | 3040.3501 |
| 3047.6734 | 3056.7125 | 3068.0353 |
| 3077.1305 | 3078.4684 | 3102.1823 |
| 3107.8389 | 3113.6033 | 3133.1645 |

Zero-point correction (Hartree): 0.261467

C8H17O.7me.pttttt

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -429.58358842
 Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 4.515295 | -1.198201 | -0.228293 |
| C | 4.308079 | 0.103054 | 0.147335 |
| C | 2.964932 | 0.706121 | -0.280912 |
| C | 1.761838 | -0.062056 | 0.276303 |
| C | 0.412053 | 0.465961 | -0.225997 |
| C | -0.783798 | -0.307516 | 0.346743 |
| C | -2.165930 | 0.106992 | -0.199805 |
| C | -3.245802 | -0.880837 | 0.290176 |
| C | -4.628215 | -0.703251 | -0.348782 |
| H | 4.391007 | 0.095211 | 1.257291 |
| H | 5.165612 | 0.727242 | -0.172681 |
| H | 2.933636 | 1.756420 | 0.040532 |
| H | 2.925735 | 0.714633 | -1.378169 |
| H | 1.872470 | -1.120069 | 0.007897 |
| H | 1.782747 | -0.020386 | 1.375401 |
| H | 0.329792 | 1.531287 | 0.025612 |
| H | 0.388340 | 0.409249 | -1.323883 |
| H | -0.634747 | -1.376794 | 0.141622 |
| H | -0.788548 | -0.209026 | 1.442716 |
| C | -2.514809 | 1.559491 | 0.161949 |
| H | -2.124319 | 0.031562 | -1.298256 |
| H | -2.896216 | -1.902753 | 0.092224 |
| H | -3.334110 | -0.798474 | 1.383154 |
| H | -4.569862 | -0.770417 | -1.441535 |
| H | -5.077642 | 0.263049 | -0.099710 |
| H | -5.318891 | -1.481140 | -0.006754 |
| H | -3.486896 | 1.855192 | -0.243483 |
| H | -1.775564 | 2.264914 | -0.228890 |
| H | -2.554982 | 1.688150 | 1.251210 |

Rotational constants (GHz): 3.8635800 0.3524100 0.3336100

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 32.4233 | 44.5702 | 70.0492 |
| 87.5301 | 111.0366 | 122.9428 |
| 154.8703 | 203.2693 | 215.6416 |
| 242.6838 | 262.8485 | 313.9731 |
| 339.6237 | 408.0214 | 443.3609 |
| 474.6403 | 498.6221 | 545.3952 |
| 740.6097 | 774.2388 | 781.2566 |
| 830.1672 | 883.5049 | 906.8736 |
| 928.3394 | 970.0525 | 987.6198 |
| 1004.8836 | 1029.1133 | 1050.0769 |
| 1054.2245 | 1071.0993 | 1094.5134 |
| 1105.3099 | 1153.1035 | 1179.4501 |
| 1197.7484 | 1214.6545 | 1255.3578 |
| 1290.1683 | 1299.9083 | 1315.4719 |
| 1331.7511 | 1337.4811 | 1349.4543 |
| 1363.8073 | 1372.5901 | 1388.0502 |
| 1392.3658 | 1406.0811 | 1418.2148 |
| 1425.5765 | 1427.1360 | 1490.2854 |
| 1494.4443 | 1501.1471 | 1505.9453 |
| 1510.0999 | 1512.8968 | 1520.0962 |
| 1523.3819 | 1527.9900 | 2881.6030 |
| 2935.1348 | 2993.8558 | 3007.6800 |
| 3013.3102 | 3019.3021 | 3023.6087 |
| 3030.6891 | 3038.7997 | 3041.4618 |
| 3042.3099 | 3054.8072 | 3059.3120 |
| 3067.6372 | 3085.5683 | 3107.8228 |
| 3108.2343 | 3116.5664 | 3124.5828 |

Zero-point correction (Hartree): 0.264815

C8H17O.1-7Hshift.7me.t

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -429.56799353
 Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|----------|-----------|-----------|
| O | 0.194258 | 1.622189 | 0.661412 |
| C | 1.333600 | 1.768179 | -0.137394 |
| C | 2.495047 | 0.821419 | 0.197179 |
| C | 2.469134 | -0.582816 | -0.435425 |
| C | 1.406865 | -1.597983 | 0.041049 |

| | | | |
|---|-----------|-----------|-----------|
| C | 0.007649 | -1.482910 | -0.602691 |
| C | -0.998259 | -0.538557 | 0.061317 |
| C | -2.112685 | -0.093860 | -0.890367 |
| C | -3.031927 | 1.008550 | -0.351091 |
| H | 1.094833 | 1.722946 | -1.215700 |
| H | 1.659246 | 2.806258 | 0.049401 |
| H | 2.555132 | 0.743581 | 1.290355 |
| H | 3.424875 | 1.306181 | -0.131558 |
| H | 3.453310 | -1.030837 | -0.246969 |
| H | 2.398221 | -0.482032 | -1.528477 |
| H | 1.328846 | -1.564953 | 1.135162 |
| H | 1.792906 | -2.596974 | -0.195690 |
| H | -0.453913 | -2.483331 | -0.615164 |
| H | 0.129428 | -1.203270 | -1.657608 |
| H | -0.397821 | 0.494740 | 0.336084 |
| C | -1.488924 | -1.027694 | 1.420197 |
| H | -1.652298 | 0.250599 | -1.825410 |
| H | -2.711553 | -0.979336 | -1.160789 |
| H | -2.441187 | 1.875062 | -0.038802 |
| H | -3.618642 | 0.670407 | 0.508609 |
| H | -3.738392 | 1.333150 | -1.121867 |
| H | -2.059031 | -0.258451 | 1.947248 |
| H | -0.658938 | -1.323423 | 2.068076 |
| H | -2.142081 | -1.903791 | 1.295156 |
| Rotational constants (GHz): | 1.7012500 | 0.8864600 | 0.7061400 |
| Vibrational harmonic frequencies (cm ⁻¹): | | | |
| i929.0056 | 51.7834 | | 76.9171 |
| 84.3477 | 122.4953 | | 183.8549 |
| 199.7223 | 217.9477 | | 254.8601 |
| 282.5230 | 311.5357 | | 322.2419 |
| 373.9189 | 380.1159 | | 449.2042 |
| 457.8645 | 482.8448 | | 621.1774 |
| 742.7866 | 768.5208 | | 796.8735 |
| 838.0849 | 849.4168 | | 888.8041 |
| 923.9882 | 956.1667 | | 978.4967 |
| 993.1977 | 1011.7946 | | 1028.8886 |
| 1061.5102 | 1084.4067 | | 1105.5149 |
| 1114.4123 | 1151.3134 | | 1159.1508 |
| 1184.9963 | 1204.2639 | | 1240.9782 |
| 1257.9324 | 1262.9055 | | 1296.3879 |
| 1303.6501 | 1324.3386 | | 1366.0077 |
| 1376.4691 | 1387.4416 | | 1393.5429 |
| 1398.2444 | 1401.7299 | | 1414.4937 |
| 1421.1838 | 1424.0198 | | 1462.0976 |
| 1481.0118 | 1482.5195 | | 1491.9983 |
| 1495.0368 | 1502.5716 | | 1502.9433 |
| 1507.7209 | 1520.1727 | | 1526.2368 |
| 2950.9162 | 2984.9697 | | 2988.1106 |
| 2994.0345 | 3014.5501 | | 3020.4540 |
| 3026.0942 | 3035.8186 | | 3046.9055 |
| 3050.3337 | 3054.0873 | | 3060.2365 |
| 3072.2769 | 3077.6160 | | 3103.7685 |
| 3117.1751 | 3129.9549 | | 3135.5900 |
| Zero-point correction (Hartree): | 0.261580 | | |

C8H17O.1-7Hshift.BB.7me.tt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -429.56809086

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -0.256625 | 1.614397 | 0.663757 |
| H | 0.370566 | 0.504440 | 0.408317 |
| C | 0.933275 | -0.522793 | -0.032414 |
| C | -1.268613 | 1.718295 | -0.300811 |
| C | -0.084306 | -1.151970 | -0.985144 |
| C | -2.493067 | 0.814025 | -0.037419 |
| C | -1.439657 | -1.581571 | -0.385146 |
| C | -2.158004 | -0.574056 | 0.533865 |
| C | 2.157325 | 0.029560 | -0.769324 |
| C | 3.056694 | 0.957920 | 0.056131 |
| C | 1.263662 | -1.363771 | 1.194608 |
| H | -1.582258 | 2.775131 | -0.289896 |
| H | -0.866334 | 1.550230 | -1.313151 |
| H | -0.255369 | -0.457741 | -1.816895 |
| H | 0.382810 | -2.037626 | -1.446760 |
| H | -3.143964 | 1.314840 | 0.690019 |
| H | -3.076379 | 0.724654 | -0.964482 |
| H | -2.103354 | -1.847304 | -1.218820 |
| H | -1.301676 | -2.508308 | 0.186602 |
| H | -3.095762 | -1.040974 | 0.860121 |
| H | -1.568546 | -0.417972 | 1.443566 |
| H | 2.747332 | -0.822213 | -1.145658 |
| H | 1.811867 | 0.570212 | -1.659673 |
| H | 3.519299 | 0.439749 | 0.901903 |
| H | 2.475971 | 1.798589 | 0.447441 |

| | | | | |
|--|-----------|-----------|-----------|--|
| H | 3.865824 | 1.359343 | -0.562487 | |
| H | 0.365273 | -1.683888 | 1.728222 | |
| H | 1.894425 | -0.819788 | 1.902463 | |
| H | 1.809423 | -2.270376 | 0.893044 | |
| Rotational constants (GHz): | 1.7420500 | 0.9328900 | 0.7417300 | |
| Vibrational harmonic frequencies (cm-1): | | | | |
| i1217.1658 | 73.0361 | | 85.6018 | |
| 110.7985 | 160.7910 | | 192.0849 | |
| 198.3949 | 232.3918 | | 260.5529 | |
| 270.9559 | 281.0385 | | 320.6419 | |
| 369.7395 | 375.2623 | | 430.5672 | |
| 520.8315 | 559.6467 | | 583.2177 | |
| 733.9145 | 767.9011 | | 787.1085 | |
| 800.5405 | 855.6769 | | 871.0572 | |
| 924.3321 | 942.7880 | | 978.8632 | |
| 997.8470 | 1011.5292 | | 1023.4707 | |
| 1057.6756 | 1083.1671 | | 1091.7717 | |
| 1122.4213 | 1150.2737 | | 1158.9126 | |
| 1199.1600 | 1202.7935 | | 1222.0860 | |
| 1254.7402 | 1256.1292 | | 1301.7048 | |
| 1306.4524 | 1323.3432 | | 1368.1522 | |
| 1370.8203 | 1385.1735 | | 1394.0815 | |
| 1398.4768 | 1413.8760 | | 1416.5221 | |
| 1424.4103 | 1429.8973 | | 1469.2486 | |
| 1483.3761 | 1491.1720 | | 1496.3724 | |
| 1497.4217 | 1505.1488 | | 1507.6192 | |
| 1510.9805 | 1520.9540 | | 1525.4911 | |
| 2974.9753 | 2987.7177 | | 2994.5347 | |
| 3001.0839 | 3017.0429 | | 3027.5903 | |
| 3028.8097 | 3044.6454 | | 3049.0894 | |
| 3050.7878 | 3055.4457 | | 3068.9333 | |
| 3071.4043 | 3093.7623 | | 3104.9830 | |
| 3117.2952 | 3130.9776 | | 3139.0759 | |
| Zero-point correction (Hartree): | 0.262032 | | | |

C8H17O.8me.pttttt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -429.58521612

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | | |
|--|-----------|-----------|-----------|--|
| O | -4.566471 | 1.187118 | -0.292432 | |
| C | -4.422932 | -0.083071 | 0.200781 | |
| C | -3.120329 | -0.795054 | -0.183676 | |
| C | -1.870106 | -0.042812 | 0.284611 | |
| C | -0.557618 | -0.678922 | -0.187917 | |
| C | 0.691099 | 0.076923 | 0.286107 | |
| C | 2.000867 | -0.555725 | -0.203372 | |
| C | 3.290409 | 0.104505 | 0.324031 | |
| C | 4.520888 | -0.724737 | -0.073687 | |
| H | -4.487241 | 0.032674 | 1.305961 | |
| H | -5.317230 | -0.686966 | -0.049872 | |
| H | -3.138771 | -1.810692 | 0.235072 | |
| H | -3.099706 | -0.908242 | -1.275588 | |
| H | -1.934048 | 0.990905 | -0.077413 | |
| H | -1.872307 | 0.015828 | 1.383085 | |
| H | -0.507194 | -1.719981 | 0.162665 | |
| H | -0.555680 | -0.729790 | -1.286065 | |
| H | 0.624429 | 1.118416 | -0.053674 | |
| H | 0.695562 | 0.114974 | 1.385161 | |
| H | 2.008061 | -1.615478 | 0.088690 | |
| H | 2.020982 | -0.546651 | -1.303606 | |
| C | 3.445922 | 1.557410 | -0.151069 | |
| H | 3.233072 | 0.113498 | 1.423379 | |
| H | 4.626001 | -0.770186 | -1.164811 | |
| H | 4.447317 | -1.753642 | 0.295584 | |
| H | 5.441900 | -0.289021 | 0.328827 | |
| H | 4.375224 | 1.995689 | 0.229014 | |
| H | 2.621368 | 2.193466 | 0.184912 | |
| H | 3.480828 | 1.607148 | -1.246724 | |
| Rotational constants (GHz): | 4.0070300 | 0.3303900 | 0.3138100 | |
| Vibrational harmonic frequencies (cm-1): | | | | |
| 32.3127 | 41.7486 | | 70.6704 | |
| 91.7833 | 110.4214 | | 148.9213 | |
| 156.5388 | 194.3851 | | 229.5290 | |
| 233.4056 | 257.7838 | | 317.6073 | |
| 361.3676 | 407.5532 | | 444.0938 | |
| 474.4994 | 488.3461 | | 543.4794 | |
| 737.3386 | 760.2986 | | 814.4537 | |
| 837.9495 | 901.8996 | | 927.2111 | |
| 933.3088 | 960.0081 | | 970.5796 | |
| 989.3174 | 1032.6513 | | 1048.4014 | |
| 1050.8714 | 1070.6064 | | 1094.4871 | |
| 1108.3050 | 1148.6848 | | 1194.9662 | |
| 1197.9580 | 1215.2211 | | 1255.0054 | |

| | | |
|-----------|-----------|-----------|
| 1275.4639 | 1305.1252 | 1320.3125 |
| 1335.3582 | 1340.2688 | 1347.7636 |
| 1364.0807 | 1369.4717 | 1377.9628 |
| 1393.2277 | 1412.4037 | 1416.3738 |
| 1419.9930 | 1435.9862 | 1492.4078 |
| 1494.4842 | 1499.9769 | 1503.6975 |
| 1508.5601 | 1513.1317 | 1519.4201 |
| 1524.2160 | 1526.5407 | 2881.7530 |
| 2935.7258 | 3002.1313 | 3007.8986 |
| 3012.0644 | 3015.6530 | 3022.8762 |
| 3030.4233 | 3032.5915 | 3037.9668 |
| 3040.0741 | 3044.2575 | 3062.0021 |
| 3072.1305 | 3085.2635 | 3098.1372 |
| 3103.6280 | 3109.2070 | 3118.7021 |

Zero-point correction (Hartree): 0.264866

C8H17O.1-8Hshift.8me

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -429.56382568

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 0.423298 | -1.537841 | -0.869609 |
| C | 1.482626 | -1.728041 | 0.029050 |
| C | 2.518689 | -0.597602 | 0.080525 |
| C | 1.948670 | 0.752550 | 0.546197 |
| C | 1.154001 | 1.534994 | -0.536145 |
| C | -0.217611 | 2.089024 | -0.082807 |
| C | -1.428257 | 1.217070 | -0.469977 |
| C | -1.516119 | -0.204335 | 0.089126 |
| C | -2.617537 | -1.023603 | -0.574932 |
| H | 1.105390 | -1.931958 | 1.047329 |
| H | 1.974766 | -2.661904 | -0.293541 |
| H | 2.980766 | -0.486663 | -0.909022 |
| H | 3.317388 | -0.915742 | 0.764981 |
| H | 2.772825 | 1.379730 | 0.906326 |
| H | 1.318259 | 0.577459 | 1.427522 |
| H | 1.002431 | 0.891916 | -1.408737 |
| H | 1.773836 | 2.370416 | -0.881564 |
| H | -0.381256 | 3.070562 | -0.544366 |
| H | -0.208274 | 2.275624 | 0.999087 |
| H | -1.466166 | 1.152774 | -1.565367 |
| H | -2.349121 | 1.745225 | -0.170053 |
| H | -0.496398 | -0.801063 | -0.323592 |
| C | -1.542872 | -0.313915 | 1.606816 |
| H | -2.503625 | -1.034403 | -1.663200 |
| H | -3.605652 | -0.599566 | -0.344613 |
| H | -2.607973 | -2.059826 | -0.223554 |
| H | -0.726505 | 0.231467 | 2.086778 |
| H | -1.491898 | -1.359068 | 1.929848 |
| H | -2.484718 | 0.100898 | 1.995495 |

Rotational constants (GHz): 1.5327900 1.0172100 0.7677900

Vibrational harmonic frequencies (cm-1):

| | | |
|------------|-----------|-----------|
| i1282.1740 | 76.5211 | 101.3630 |
| 119.5461 | 150.7268 | 181.4209 |
| 188.4422 | 214.1766 | 221.3399 |
| 305.9015 | 318.4626 | 331.8522 |
| 353.3684 | 366.6352 | 399.0071 |
| 493.0902 | 504.0501 | 563.7939 |
| 713.3494 | 769.7863 | 835.3020 |
| 842.5437 | 861.3102 | 888.5779 |
| 934.1317 | 946.2650 | 967.8713 |
| 991.2258 | 999.7339 | 1028.3370 |
| 1058.9333 | 1085.7692 | 1098.6675 |
| 1110.7331 | 1142.4408 | 1168.8200 |
| 1175.0829 | 1202.9136 | 1232.8282 |
| 1261.6996 | 1273.7231 | 1277.0917 |
| 1302.0347 | 1324.1324 | 1356.0041 |
| 1383.3934 | 1387.9529 | 1390.9222 |
| 1398.4002 | 1403.0719 | 1406.1470 |
| 1418.5456 | 1427.1848 | 1458.4469 |
| 1476.4325 | 1489.8413 | 1491.4553 |
| 1494.0574 | 1502.9570 | 1507.3325 |
| 1512.9900 | 1516.3853 | 1519.4977 |
| 2954.2119 | 2983.5997 | 2987.2033 |
| 3015.2139 | 3021.6541 | 3025.6038 |
| 3032.4523 | 3037.2617 | 3045.1406 |
| 3052.1412 | 3065.5589 | 3070.7186 |
| 3077.5657 | 3090.1515 | 3096.1388 |
| 3099.4852 | 3126.6263 | 3132.8696 |

Zero-point correction (Hartree): 0.261619

C8H17O.1-8Hshift.TBCd.8me.t

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -429.56715357

Electronic state : 2-A

```

Cartesian coordinates (Angs):
C      -2.520880      -0.653036      0.000438
C      -1.413545      -1.708033     -0.136218
O      -0.365785      -1.615084      0.793193
H       0.566889      -0.823388      0.344943
C       1.548342      -0.172789     -0.060787
C       1.015484       1.006344     -0.875192
C       0.140447       2.034390     -0.134485
C      -1.111990       1.463703      0.555297
C      -2.123114       0.776895     -0.402112
H      -3.363787      -0.979301     -0.625121
H      -2.880217      -0.662569      1.037780
H      -1.024925      -1.716450     -1.170537
H      -1.851701      -2.709674      0.016248
C       2.310253      -1.181468     -0.910860
C       2.278538       0.196085      1.224175
H       0.469715       0.609945     -1.741260
H       1.883387       1.536168     -1.301729
H      -0.163061       2.801456     -0.859867
H       0.748536       2.558202      0.613615
H      -1.611113       2.285844      1.082160
H      -0.808216       0.752149      1.327901
H      -1.721088       0.750598     -1.424133
H      -3.033001       1.385198     -0.467659
H       3.247664      -0.743165     -1.282890
H       1.727507      -1.496457     -1.783136
H       2.566207      -2.074183     -0.332289
H       2.568237      -0.701072      1.779756
H       1.667357       0.817754      1.883981
H       3.196670       0.757076      0.995148
Rotational constants (GHz):  1.5734000  1.0036300  0.7602000
Vibrational harmonic frequencies (cm-1):
11218.8774      67.7026      84.4713
 134.8383      189.6337     197.7655
 206.5802      219.6026     249.0792
 296.1896      316.1478     346.2485
 366.5681      380.2054     398.3432
 486.9651      520.6672     584.4237
 726.9185      760.6432     810.7344
 833.9023      875.7666     897.3142
 909.4363      942.8914     971.9800
 985.9414     1002.6155    1033.1884
1065.9023     1079.4183    1095.7332
1112.8333     1136.8688    1157.6879
1191.6687     1203.5024    1241.6121
1252.2601     1263.3611    1281.8489
1297.5685     1329.3978    1357.3644
1383.0652     1386.5486    1390.5327
1400.0512     1405.5478    1408.4461
1414.8282     1428.3122    1458.0650
1480.5313     1489.9186    1490.8820
1495.4495     1504.7742    1507.5117
1515.7430     1520.2860    1526.0468
2953.7125     2985.1106    2987.9001
3015.9006     3021.3775    3023.7331
3028.3414     3031.9810    3044.5947
3049.3106     3064.5314    3069.1678
3075.7425     3089.2719    3097.8309
3109.9299     3122.3248    3131.8906
Zero-point correction (Hartree): 0.261928
    
```

C8H17O.3oxo.pttttt

```

-----
E(UB+HF-LYP/6-31G(d,p)) (Hartree): -464.27907064
Electronic state : 2-A
Cartesian coordinates (Angs):
O       3.843682      -1.468278     -0.241026
C       3.911880      -0.210813      0.202233
C       2.519183       0.550787      0.010802
C       1.287292      -0.319139      0.057073
C      -0.029890       0.456728      0.028918
C      -1.255555      -0.465403      0.028316
C      -2.585344       0.298704      0.003233
C      -3.816478      -0.616355      0.000967
C      -5.140650       0.153700     -0.023816
H       3.988892      -0.167763      1.311921
H       4.692289       0.433706     -0.236476
O       2.535478       1.744195     -0.146000
H       1.377789      -1.009084     -0.794724
H       1.368249      -0.968182     -0.939350
H      -0.072191       1.130579      0.893573
H      -0.047261       1.103669     -0.856047
H      -1.206149      -1.137686     -0.840051
H      -1.226335      -1.114627      0.915087
H      -2.634345       0.970830      0.871833
    
```


| | | | |
|---|-----------|-----------|-----------|
| H | -2.614079 | 0.948139 | -0.883237 |
| H | -3.766633 | -1.287361 | -0.867390 |
| H | -3.786357 | -1.265280 | 0.886888 |
| H | -5.215067 | 0.785450 | -0.916312 |
| H | -5.235786 | 0.807091 | 0.850984 |
| H | -5.998925 | -0.526061 | -0.025550 |
| Rotational constants (GHz): | 3.9983100 | 0.3612800 | 0.3370400 |
| Vibrational harmonic frequencies (cm ⁻¹): | | | |
| 41.4302 | 54.4114 | | 63.0229 |
| 95.4871 | 102.2863 | | 131.1205 |
| 157.7423 | 158.6148 | | 215.0362 |
| 246.3592 | 282.5781 | | 375.2434 |
| 427.9049 | 457.3097 | | 492.0281 |
| 543.5475 | 724.8356 | | 739.3936 |
| 747.2025 | 784.0735 | | 837.3139 |
| 877.1660 | 903.8379 | | 931.4992 |
| 1002.0554 | 1016.3581 | | 1044.7675 |
| 1061.8571 | 1072.3525 | | 1098.8090 |
| 1134.4395 | 1149.8317 | | 1216.4956 |
| 1227.2109 | 1259.2476 | | 1275.1331 |
| 1279.9875 | 1316.5623 | | 1324.6518 |
| 1338.8765 | 1342.9630 | | 1377.2199 |
| 1409.9406 | 1418.5417 | | 1427.8138 |
| 1445.6112 | 1487.1983 | | 1499.4357 |
| 1500.4579 | 1507.4776 | | 1512.7457 |
| 1518.2655 | 1527.1267 | | 1849.7339 |
| 2870.4631 | 2996.3521 | | 3013.0187 |
| 3017.1454 | 3027.8819 | | 3034.3446 |
| 3037.7144 | 3039.6242 | | 3049.0306 |
| 3050.9051 | 3064.2185 | | 3070.3833 |
| 3094.4982 | 3107.4986 | | 3113.3767 |
| Zero-point correction (Hartree): | 0.217836 | | |

C8H17O.1-5Hshift.3oxo.ttt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -464.26051151

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -1.304421 | 1.686888 | 0.244081 |
| C | -2.621948 | 1.284459 | 0.082084 |
| C | -2.828247 | -0.253512 | -0.030186 |
| C | -1.582450 | -1.111999 | 0.222010 |
| C | -0.338674 | -0.490794 | -0.377696 |
| C | 0.986842 | -0.755186 | 0.310288 |
| C | 2.170037 | -0.004351 | -0.314344 |
| C | 3.506035 | -0.292170 | 0.381967 |
| C | 4.685776 | 0.454014 | -0.248899 |
| H | -3.211767 | 1.585593 | 0.963682 |
| H | -3.109250 | 1.718685 | -0.807327 |
| O | -3.917220 | -0.708199 | -0.289794 |
| H | -1.799692 | -2.115837 | -0.158015 |
| H | -1.468905 | -1.183304 | 1.313527 |
| H | -0.609427 | 0.747038 | -0.185748 |
| H | -0.295035 | -0.587726 | -1.468347 |
| H | 0.897708 | -0.491452 | 1.373235 |
| H | 1.189453 | -1.839066 | 0.285434 |
| H | 2.249162 | -0.272522 | -1.377400 |
| H | 1.968067 | 1.074837 | -0.285478 |
| H | 3.425868 | -0.020503 | 1.443228 |
| H | 3.701212 | -1.373131 | 0.359215 |
| H | 4.534048 | 1.538638 | -0.211069 |
| H | 4.814121 | 0.175409 | -1.301094 |
| H | 5.623343 | 0.231064 | 0.270514 |
| Rotational constants (GHz): | 3.4406200 | 0.4506400 | 0.4134800 |
| Vibrational harmonic frequencies (cm ⁻¹): | | | |
| i1459.3461 | 40.5025 | | 59.9076 |
| 65.8654 | 98.1750 | | 113.9483 |
| 144.8922 | 173.7123 | | 255.5123 |
| 261.6072 | 295.1687 | | 411.3696 |
| 443.5597 | 486.5197 | | 505.2664 |
| 557.4397 | 626.5456 | | 736.1815 |
| 757.7118 | 766.6133 | | 799.6973 |
| 868.2360 | 905.1076 | | 939.9378 |
| 988.8105 | 1022.5545 | | 1045.2665 |
| 1068.0673 | 1081.0743 | | 1111.6481 |
| 1121.2696 | 1136.6169 | | 1166.3872 |
| 1211.8966 | 1230.8312 | | 1242.0537 |
| 1249.9110 | 1264.3025 | | 1291.3111 |
| 1317.8691 | 1326.5650 | | 1339.9627 |
| 1352.7483 | 1397.4301 | | 1416.3793 |
| 1428.3480 | 1456.2934 | | 1483.2086 |
| 1490.1219 | 1500.4025 | | 1510.4055 |
| 1514.5248 | 1524.2893 | | 1559.4224 |
| 1832.5257 | 2974.8953 | | 2985.2753 |
| 3012.8392 | 3019.4231 | | 3026.9857 |

| | | |
|-----------|-----------|-----------|
| 3029.4392 | 3040.5240 | 3042.4388 |
| 3050.5986 | 3073.2690 | 3081.3575 |
| 3099.5737 | 3109.1425 | 3114.7682 |

Zero-point correction (Hartree): 0.213365

C8H17O.1-6Hshift.3oxo.catt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -464.25777075

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| C | 0.585690 | -1.513282 | 0.473126 |
| C | 1.484916 | -1.022579 | -0.693696 |
| C | 2.435925 | 0.080047 | -0.254673 |
| C | 1.832575 | 1.419195 | 0.206924 |
| O | 0.460930 | 1.578124 | 0.000800 |
| H | -0.122462 | 0.588976 | 0.569755 |
| C | -0.555133 | -0.558477 | 0.821175 |
| H | 1.214385 | -1.692210 | 1.352803 |
| H | 0.165024 | -2.489597 | 0.195368 |
| H | 2.101270 | -1.842554 | -1.069777 |
| H | 0.854381 | -0.651875 | -1.510666 |
| O | 3.641588 | -0.074493 | -0.218586 |
| H | 2.142854 | 1.579715 | 1.254173 |
| H | 2.330394 | 2.206552 | -0.380681 |
| C | -1.809000 | -0.662280 | -0.030287 |
| H | -0.778575 | -0.520679 | 1.893424 |
| C | -2.857617 | 0.416272 | 0.273982 |
| C | -4.125264 | 0.272929 | -0.573434 |
| H | -1.537090 | -0.620419 | -1.093762 |
| H | -2.251805 | -1.659945 | 0.128254 |
| H | -3.120411 | 0.372305 | 1.339663 |
| H | -2.409825 | 1.403503 | 0.107842 |
| H | -4.611468 | -0.694828 | -0.403852 |
| H | -3.896949 | 0.345169 | -1.642826 |
| H | -4.852417 | 1.055890 | -0.336127 |

Rotational constants (GHz): 2.7368600 0.5996300 0.5339200

Vibrational harmonic frequencies (cm-1):

| | | |
|------------|-----------|-----------|
| i1330.7765 | 30.2539 | 59.8099 |
| 77.2042 | 106.6574 | 127.1714 |
| 199.3824 | 217.0898 | 241.9605 |
| 272.0733 | 324.0479 | 403.3728 |
| 445.3349 | 483.7625 | 525.5129 |
| 557.4362 | 651.8109 | 721.2617 |
| 747.4118 | 814.6009 | 848.8532 |
| 892.9241 | 904.8296 | 929.7604 |
| 976.2132 | 981.3858 | 1046.9858 |
| 1066.5126 | 1083.7691 | 1105.3129 |
| 1119.0674 | 1124.8811 | 1183.4953 |
| 1195.8344 | 1226.7988 | 1256.3415 |
| 1266.6208 | 1286.6997 | 1300.2266 |
| 1334.6935 | 1342.2990 | 1349.9793 |
| 1360.8616 | 1365.8063 | 1406.1487 |
| 1424.7325 | 1435.0680 | 1439.6587 |
| 1476.3930 | 1484.8133 | 1502.6470 |
| 1506.6330 | 1512.5727 | 1522.0906 |
| 1811.9970 | 2974.5337 | 2986.0564 |
| 3026.7334 | 3027.8785 | 3031.1671 |
| 3039.3817 | 3047.2528 | 3058.4201 |
| 3072.9886 | 3077.4420 | 3086.9309 |
| 3108.2915 | 3116.2091 | 3130.6214 |

Zero-point correction (Hartree): 0.213836

C8H17O.1-6Hshift.3oxo.cett

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -464.25847001

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| C | 0.555996 | 1.522902 | -0.062284 |
| C | 1.946824 | 1.100578 | 0.476147 |
| C | 2.474575 | -0.155169 | -0.203092 |
| C | 1.608297 | -1.425687 | -0.155087 |
| O | 0.633051 | -1.465927 | 0.844455 |
| H | -0.136276 | -0.454452 | 0.660301 |
| C | -0.591041 | 0.699793 | 0.510095 |
| H | 0.555340 | 1.460885 | -1.158321 |
| H | 0.394716 | 2.582639 | 0.178232 |
| H | 2.687226 | 1.885816 | 0.306463 |
| H | 1.875983 | 0.917352 | 1.556097 |
| O | 3.524411 | -0.168508 | -0.817103 |
| H | 1.199897 | -1.586133 | -1.169609 |
| H | 2.288039 | -2.270494 | 0.031476 |
| C | -1.859465 | 0.602434 | -0.316109 |
| H | -0.785736 | 0.948637 | 1.561230 |
| C | -2.940968 | -0.289361 | 0.308619 |
| C | -4.213745 | -0.370299 | -0.539281 |

| | | | |
|--|-----------|-----------|-----------|
| H | -2.261796 | 1.619558 | -0.461069 |
| H | -1.613177 | 0.237265 | -1.323227 |
| H | -2.528633 | -1.295216 | 0.457830 |
| H | -3.187948 | 0.091421 | 1.308573 |
| H | -4.002962 | -0.782134 | -1.532781 |
| H | -4.661669 | 0.620080 | -0.680446 |
| H | -4.965536 | -1.010880 | -0.067620 |
| Rotational constants (GHz): | 2.6225600 | 0.5774000 | 0.5214100 |
| Vibrational harmonic frequencies (cm-1): | | | |
| i1274.1717 | 30.8479 | | 52.7308 |
| 76.2680 | 113.4432 | | 129.0582 |
| 200.9528 | 215.7118 | | 248.0750 |
| 301.4577 | 323.4977 | | 379.2067 |
| 422.2668 | 487.9337 | | 531.0169 |
| 538.9760 | 603.7656 | | 714.0435 |
| 740.8781 | 810.3091 | | 859.0004 |
| 893.6048 | 904.5693 | | 949.9948 |
| 963.1573 | 1019.0405 | | 1035.5654 |
| 1065.9998 | 1081.0903 | | 1101.6862 |
| 1117.3992 | 1131.5821 | | 1172.3736 |
| 1212.2135 | 1225.6791 | | 1262.8499 |
| 1279.4179 | 1280.6804 | | 1290.5254 |
| 1332.5099 | 1342.1496 | | 1352.6780 |
| 1353.6612 | 1388.7678 | | 1409.0670 |
| 1427.3763 | 1435.7152 | | 1443.3432 |
| 1476.2635 | 1483.4790 | | 1501.3411 |
| 1506.5496 | 1513.7873 | | 1522.2871 |
| 1811.5501 | 2959.1007 | | 2982.6726 |
| 3026.0183 | 3032.0016 | | 3037.3661 |
| 3038.0460 | 3041.2212 | | 3048.5299 |
| 3057.6079 | 3071.2895 | | 3075.7385 |
| 3108.4815 | 3116.8355 | | 3128.2950 |
| Zero-point correction (Hartree): | 0.213671 | | |

C8H17O.1-6Hshift.3oxo.tt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -464.25600029

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|--|-----------|-----------|-----------|
| O | 0.580147 | -1.557492 | -0.277611 |
| C | 1.833591 | -1.405551 | 0.336865 |
| C | 2.555645 | -0.092223 | -0.013983 |
| C | 1.894892 | 1.234753 | 0.360604 |
| C | 0.475524 | 1.481780 | -0.194791 |
| C | -0.580679 | 0.555475 | 0.383183 |
| C | -1.965516 | 0.623498 | -0.234104 |
| C | -2.958414 | -0.387500 | 0.355912 |
| C | -4.348977 | -0.300676 | -0.279905 |
| H | 1.779323 | -1.501034 | 1.437317 |
| H | 2.462304 | -2.224405 | -0.037096 |
| O | 3.659733 | -0.117294 | -0.524189 |
| H | 2.577323 | 2.020228 | 0.025600 |
| H | 1.857000 | 1.279405 | 1.459809 |
| H | 0.486653 | 1.386823 | -1.287488 |
| H | 0.199167 | 2.524812 | 0.018778 |
| H | -0.150638 | -0.582510 | 0.123289 |
| H | -0.601526 | 0.574799 | 1.481056 |
| H | -2.359031 | 1.645162 | -0.098646 |
| H | -1.885893 | 0.474954 | -1.319586 |
| H | -2.554697 | -1.399615 | 0.227160 |
| H | -3.038039 | -0.224488 | 1.439213 |
| H | -4.303970 | -0.493480 | -1.357667 |
| H | -4.789794 | 0.693085 | -0.139852 |
| H | -5.033623 | -1.032789 | 0.159836 |
| Rotational constants (GHz): | 2.8842200 | 0.5582900 | 0.4930300 |
| Vibrational harmonic frequencies (cm-1): | | | |
| i1232.6773 | 36.7503 | | 63.8817 |
| 67.8876 | 111.9077 | | 119.2629 |
| 188.8699 | 218.1299 | | 239.2620 |
| 248.2554 | 338.6296 | | 370.2242 |
| 392.3953 | 470.9694 | | 501.2766 |
| 600.4906 | 654.3337 | | 741.2971 |
| 779.9344 | 810.2660 | | 839.9278 |
| 878.7664 | 901.7817 | | 938.4555 |
| 986.9191 | 1030.6486 | | 1039.7921 |
| 1066.7884 | 1076.0521 | | 1092.5906 |
| 1122.9406 | 1138.0589 | | 1175.8463 |
| 1220.9837 | 1238.6380 | | 1258.3624 |
| 1264.6097 | 1286.9447 | | 1305.8201 |
| 1333.3159 | 1349.3654 | | 1353.9351 |
| 1370.0607 | 1394.3053 | | 1407.4229 |
| 1426.3682 | 1444.7616 | | 1458.0981 |
| 1478.9357 | 1482.2620 | | 1496.8898 |

| | | |
|-----------|-----------|-----------|
| 1506.2407 | 1513.0183 | 1522.2435 |
| 1807.9689 | 2948.3226 | 2984.5052 |
| 3015.8923 | 3018.6721 | 3030.7710 |
| 3039.9681 | 3044.4392 | 3054.7948 |
| 3061.4307 | 3072.2080 | 3077.3085 |
| 3108.8762 | 3116.5613 | 3117.1974 |

Zero-point correction (Hartree): 0.213815

C8H17O.4oxo.pttttt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -464.27816881

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 3.922849 | -0.407596 | 1.310579 |
| C | 3.879278 | -0.058236 | -0.009617 |
| C | 2.628369 | -0.552125 | -0.749922 |
| C | 1.380452 | 0.243247 | -0.359475 |
| C | 0.061973 | -0.508212 | -0.342257 |
| C | -1.165254 | 0.372599 | -0.107274 |
| C | -2.472987 | -0.425397 | -0.044889 |
| C | -3.708457 | 0.452224 | 0.192908 |
| C | -5.013546 | -0.347115 | 0.260436 |

| | | | |
|---|-----------|-----------|-----------|
| H | 3.857869 | 1.053049 | -0.009289 |
| H | 4.813486 | -0.336303 | -0.530632 |
| H | 2.765712 | -0.419004 | -1.833009 |
| H | 2.484498 | -1.624314 | -0.579910 |
| O | 1.462271 | 1.429365 | -0.096551 |
| H | -0.023128 | -1.072744 | -1.283104 |
| H | 0.148419 | -1.279406 | 0.439176 |
| H | -1.023642 | 0.936312 | 0.821976 |
| H | -1.224658 | 1.124754 | -0.903656 |
| H | -2.605492 | -0.989791 | -0.979616 |
| H | -2.405282 | -1.177815 | 0.754374 |
| H | -3.575248 | 1.016688 | 1.125572 |
| H | -3.778146 | 1.201895 | -0.606907 |
| H | -4.988413 | -1.079012 | 1.075941 |
| H | -5.190692 | -0.897522 | -0.670805 |
| H | -5.875222 | 0.307156 | 0.428204 |

Rotational constants (GHz): 4.3040800 0.3733400 0.3688700

Vibrational harmonic frequencies (cm⁻¹):

| | | |
|-----------|-----------|-----------|
| 22.6711 | 50.9785 | 59.1483 |
| 84.5486 | 98.0245 | 128.2585 |
| 137.6504 | 198.5144 | 253.7234 |
| 261.1385 | 267.7376 | 391.4685 |
| 421.4699 | 471.1630 | 493.7889 |
| 614.8974 | 713.7564 | 740.0263 |
| 761.8682 | 805.4294 | 866.4165 |
| 896.5542 | 918.5329 | 951.2960 |
| 984.3107 | 1019.6034 | 1050.0788 |
| 1069.5751 | 1083.2955 | 1088.1844 |
| 1104.6980 | 1144.6969 | 1169.6665 |
| 1203.9071 | 1235.6498 | 1271.2272 |
| 1295.8900 | 1317.6249 | 1330.7841 |
| 1338.1334 | 1346.4645 | 1379.5855 |
| 1382.5341 | 1406.9761 | 1418.0561 |
| 1428.4690 | 1460.5454 | 1465.6261 |
| 1498.3771 | 1502.4073 | 1514.2545 |
| 1514.6004 | 1525.9940 | 1807.0325 |
| 2901.1281 | 2965.8024 | 3008.6038 |
| 3012.6110 | 3027.4088 | 3033.8108 |
| 3036.8583 | 3039.1457 | 3039.6993 |
| 3051.2625 | 3063.8279 | 3094.4674 |
| 3099.2948 | 3107.0185 | 3113.2966 |

Zero-point correction (Hartree): 0.217705

C8H17O.4oxo.tttttt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -464.27909503

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 4.981229 | -0.403161 | -0.136845 |
| C | 3.805497 | 0.145898 | 0.275808 |
| C | 2.551955 | -0.651943 | -0.112823 |
| C | 1.283917 | 0.191854 | -0.032858 |
| C | -0.037975 | -0.555405 | 0.041456 |
| C | -1.273274 | 0.339042 | -0.072965 |
| C | -2.589251 | -0.438742 | 0.045486 |
| C | -3.831836 | 0.454273 | -0.065286 |
| C | -5.146621 | -0.322176 | 0.057054 |
| H | 3.815168 | 0.393987 | 1.353445 |
| H | 3.740465 | 1.138027 | -0.224130 |
| H | 2.662657 | -0.994165 | -1.151146 |
| H | 2.452813 | -1.557900 | 0.496581 |
| O | 1.343765 | 1.409115 | -0.044019 |

| | | | |
|--|-----------|-----------|-----------|
| H | -0.034917 | -1.335383 | -0.734091 |
| H | -0.043152 | -1.107881 | 0.993938 |
| H | -1.223173 | 1.113842 | 0.700670 |
| H | -1.240924 | 0.873981 | -1.030063 |
| H | -2.630954 | -1.213886 | -0.733552 |
| H | -2.613991 | -0.974633 | 1.005619 |
| H | -3.788971 | 1.228791 | 0.712210 |
| H | -3.807985 | 0.987528 | -1.025218 |
| H | -5.215784 | -0.835583 | 1.022988 |
| H | -5.232876 | -1.083100 | -0.727187 |
| H | -6.012793 | 0.341944 | -0.028379 |
| Rotational constants (GHz): | 6.2378100 | 0.3411800 | 0.3289200 |
| Vibrational harmonic frequencies (cm-1): | | | |
| 29.4057 | 35.9909 | | 62.3106 |
| 77.2403 | 93.2697 | | 118.9313 |
| 135.2419 | 176.6241 | | 232.4466 |
| 248.1396 | 270.4076 | | 386.1976 |
| 408.5497 | 465.2166 | | 480.3283 |
| 672.0073 | 705.4834 | | 734.1140 |
| 756.6533 | 816.5743 | | 867.8689 |
| 908.7921 | 928.3855 | | 964.3724 |
| 991.1690 | 1025.2877 | | 1053.9332 |
| 1068.9091 | 1075.5441 | | 1084.2617 |
| 1106.0610 | 1144.0625 | | 1159.3630 |
| 1196.3644 | 1233.8544 | | 1268.5851 |
| 1295.6392 | 1326.4940 | | 1330.5171 |
| 1338.2632 | 1348.8579 | | 1358.4063 |
| 1380.8076 | 1402.9478 | | 1416.1539 |
| 1427.6976 | 1460.3997 | | 1468.1035 |
| 1497.5036 | 1501.2411 | | 1513.2144 |
| 1513.7602 | 1524.6639 | | 1797.0162 |
| 2887.3686 | 2959.3625 | | 3009.1058 |
| 3014.2945 | 3027.6797 | | 3037.2503 |
| 3039.0386 | 3042.5529 | | 3044.9448 |
| 3051.6355 | 3063.8380 | | 3089.2361 |
| 3094.6894 | 3106.6762 | | 3113.5591 |
| Zero-point correction (Hartree): | 0.217485 | | |

C8H17O.1-5Hshift.4oxo.ttt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -464.26017439

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|--|-----------|-----------|-----------|
| O | -1.711184 | -1.890563 | -0.064439 |
| C | -2.852922 | -1.182112 | -0.478299 |
| C | -3.024044 | 0.122375 | 0.333430 |
| C | -1.747890 | 0.935152 | 0.169026 |
| C | -0.493745 | 0.176117 | 0.522733 |
| C | 0.799162 | 0.639617 | -0.112566 |
| C | 2.019852 | -0.204015 | 0.273659 |
| C | 3.324950 | 0.306207 | -0.350212 |
| C | 4.545529 | -0.534695 | 0.036340 |
| H | -2.826816 | -0.946077 | -1.554724 |
| H | -3.712165 | -1.845871 | -0.304650 |
| H | -3.162606 | -0.138547 | 1.390050 |
| H | -3.880927 | 0.707268 | -0.009110 |
| O | -1.724388 | 2.062440 | -0.296203 |
| H | -0.835678 | -0.990295 | 0.154167 |
| H | -0.425691 | -0.007463 | 1.602428 |
| H | 0.682892 | 0.663256 | -1.203188 |
| H | 0.953770 | 1.687917 | 0.185285 |
| H | 2.121630 | -0.218651 | 1.368261 |
| H | 1.853923 | -1.246711 | -0.030258 |
| H | 3.220779 | 0.320645 | -1.443541 |
| H | 3.486460 | 1.349656 | -0.047357 |
| H | 4.427253 | -1.576030 | -0.284115 |
| H | 4.696712 | -0.538992 | 1.121873 |
| H | 5.459680 | -0.146996 | -0.424662 |
| Rotational constants (GHz): | 2.4741400 | 0.5288300 | 0.4560000 |
| Vibrational harmonic frequencies (cm-1): | | | |
| i1544.9146 | 41.0619 | | 63.3571 |
| 82.6013 | 94.8065 | | 130.6000 |
| 171.8999 | 214.5422 | | 239.9562 |
| 252.2934 | 302.0682 | | 400.9594 |
| 443.0302 | 468.0816 | | 529.1921 |
| 588.9703 | 639.1836 | | 731.8140 |
| 769.2063 | 839.5881 | | 851.1563 |
| 870.7879 | 910.1868 | | 919.9098 |
| 959.1190 | 1018.8575 | | 1040.4801 |
| 1046.1117 | 1068.9580 | | 1082.8849 |
| 1134.6740 | 1136.0723 | | 1164.3468 |
| 1197.2597 | 1231.6567 | | 1238.5967 |
| 1243.1428 | 1266.9212 | | 1311.3178 |
| 1318.6766 | 1336.9813 | | 1340.9548 |
| 1382.6362 | 1392.2445 | | 1416.2438 |

| | | |
|-----------|-----------|-----------|
| 1428.4121 | 1472.2410 | 1477.9441 |
| 1500.4049 | 1507.8802 | 1510.5187 |
| 1513.8229 | 1524.2785 | 1538.6175 |
| 1784.7441 | 2984.9020 | 3013.8171 |
| 3017.9851 | 3028.5332 | 3036.3873 |
| 3040.5662 | 3045.9397 | 3056.8632 |
| 3061.2833 | 3071.3448 | 3081.2095 |
| 3108.8110 | 3114.6941 | 3136.0201 |

Zero-point correction (Hartree): 0.214012

C8H17O.1-6Hshift.4oxo.tt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -464.26167932

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 0.454445 | 1.846363 | 0.194113 |
| C | 1.769466 | 1.713946 | -0.272596 |
| C | 2.571367 | 0.584338 | 0.414559 |
| C | 2.089592 | -0.816099 | 0.049288 |
| C | 0.690531 | -1.227792 | 0.508244 |
| C | -0.407104 | -0.464544 | -0.230281 |
| C | -1.822523 | -0.636753 | 0.288445 |
| C | -2.860710 | 0.208897 | -0.462578 |
| C | -4.282756 | 0.024219 | 0.075176 |
| H | 1.814763 | 1.591621 | -1.367519 |
| H | 2.254375 | 2.674566 | -0.043422 |
| H | 2.494025 | 0.728639 | 1.499427 |
| H | 3.622951 | 0.650745 | 0.120825 |
| O | 2.783886 | -1.574346 | -0.602551 |
| H | 0.591330 | -1.044642 | 1.585966 |
| H | 0.588416 | -2.305468 | 0.331243 |
| H | -0.120425 | 0.747246 | -0.056519 |
| H | -0.332942 | -0.582489 | -1.318087 |
| H | -2.096101 | -1.702725 | 0.215474 |
| H | -1.848934 | -0.393079 | 1.359493 |
| H | -2.573694 | 1.265893 | -0.398493 |
| H | -2.833754 | -0.052174 | -1.528945 |
| H | -4.348082 | 0.311255 | 1.130803 |
| H | -4.606035 | -1.020043 | -0.004303 |
| H | -4.999717 | 0.637247 | -0.479983 |

Rotational constants (GHz): 2.2672200 0.6240300 0.5207600

Vibrational harmonic frequencies (cm-1):

| | | |
|------------|-----------|-----------|
| i1349.9376 | 52.2970 | 62.3002 |
| 80.7736 | 83.8521 | 137.9278 |
| 182.4591 | 236.8308 | 248.0556 |
| 250.1149 | 344.2693 | 368.5488 |
| 436.8883 | 455.1342 | 524.7030 |
| 593.4531 | 684.3938 | 742.5133 |
| 769.4064 | 799.5055 | 852.1509 |
| 891.4322 | 903.6714 | 931.4805 |
| 988.1705 | 1004.0690 | 1037.9569 |
| 1057.8476 | 1065.7625 | 1091.1731 |
| 1117.4378 | 1133.9884 | 1180.0378 |
| 1222.4730 | 1233.5837 | 1247.0114 |
| 1255.3906 | 1273.3982 | 1294.0426 |
| 1325.8750 | 1337.0918 | 1341.8854 |
| 1373.8782 | 1393.9048 | 1407.0104 |
| 1428.2477 | 1459.5826 | 1468.5045 |
| 1477.9868 | 1484.9689 | 1486.1753 |
| 1506.6215 | 1514.1034 | 1522.2944 |
| 1809.0471 | 2982.0348 | 2986.9311 |
| 3030.4980 | 3032.6502 | 3035.5594 |
| 3040.3135 | 3045.1493 | 3053.6755 |
| 3069.7857 | 3075.5791 | 3091.2285 |
| 3109.2449 | 3116.8484 | 3121.4000 |

Zero-point correction (Hartree): 0.214063

C8H17O.5oxo.pptttt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -464.28196541

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -3.532143 | -0.851178 | 1.233251 |
| C | -3.383488 | -0.689249 | -0.112296 |
| C | -2.855649 | 0.689255 | -0.548669 |
| C | -1.554732 | 1.070223 | 0.160420 |
| C | -0.340829 | 0.266219 | -0.289597 |
| C | 1.014380 | 0.739601 | 0.218749 |
| C | 2.173738 | -0.202302 | -0.109787 |
| C | 3.528959 | 0.322276 | 0.379914 |
| C | 4.688835 | -0.623358 | 0.052172 |
| O | -0.448157 | -0.706732 | -1.018175 |
| H | -2.626576 | -1.450475 | -0.406508 |
| H | -4.300671 | -0.972532 | -0.662691 |
| H | -2.709746 | 0.677181 | -1.634643 |

| | | | |
|---|-----------|-----------|-----------|
| H | -3.620393 | 1.443288 | -0.329717 |
| H | -1.330024 | 2.137526 | 0.038322 |
| H | -1.675602 | 0.913271 | 1.241526 |
| H | 0.934868 | 0.909427 | 1.302222 |
| H | 1.192247 | 1.737760 | -0.210350 |
| H | 1.973793 | -1.185887 | 0.332957 |
| H | 2.204252 | -0.366446 | -1.193153 |
| H | 3.722235 | 1.306965 | -0.068030 |
| H | 3.487310 | 0.487280 | 1.465482 |
| H | 4.776850 | -0.781470 | -1.028599 |
| H | 4.542993 | -1.604584 | 0.517712 |
| H | 5.643586 | -0.224025 | 0.409434 |
| Rotational constants (GHz): | 3.5988700 | 0.4304700 | 0.4231600 |
| Vibrational harmonic frequencies (cm ⁻¹): | | | |
| 26.6630 | 35.8505 | | 76.9758 |
| 84.6521 | 96.3801 | | 123.7603 |
| 183.0454 | 220.3775 | | 244.9870 |
| 259.6716 | 312.6604 | | 344.8636 |
| 454.1397 | 465.0180 | | 504.1480 |
| 657.0273 | 707.2923 | | 735.3381 |
| 780.9801 | 828.9684 | | 848.5632 |
| 895.3678 | 916.4704 | | 957.8960 |
| 971.7348 | 1010.0251 | | 1047.5374 |
| 1070.9915 | 1076.2249 | | 1102.4777 |
| 1113.0266 | 1143.0690 | | 1156.0671 |
| 1198.7526 | 1244.3755 | | 1269.3665 |
| 1293.7462 | 1306.0355 | | 1322.8173 |
| 1335.4770 | 1369.8536 | | 1381.9484 |
| 1391.1376 | 1402.5819 | | 1417.2447 |
| 1428.3709 | 1456.2956 | | 1467.6122 |
| 1488.3218 | 1499.5349 | | 1508.8303 |
| 1512.5806 | 1524.4040 | | 1795.1249 |
| 2880.8651 | 2952.5238 | | 3014.4952 |
| 3021.1100 | 3038.5256 | | 3040.7036 |
| 3046.2089 | 3049.0152 | | 3052.3123 |
| 3054.3030 | 3075.5771 | | 3093.0224 |
| 3100.2404 | 3110.3790 | | 3114.3216 |
| Zero-point correction (Hartree): | 0.218044 | | |

C8H17O.5oxo.pttttt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -464.27957519

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 4.187798 | -0.993796 | -0.790644 |
| C | 4.038798 | -0.085976 | 0.224942 |
| C | 2.695941 | 0.654136 | 0.250096 |
| C | 1.505823 | -0.302593 | 0.287408 |
| C | 0.158623 | 0.378648 | 0.075548 |
| C | -1.077158 | -0.483233 | 0.307024 |
| C | -2.389175 | 0.176807 | -0.119562 |
| C | -3.620374 | -0.688025 | 0.176237 |
| C | -4.932380 | -0.027843 | -0.259294 |
| H | 4.166901 | -0.690002 | 1.151736 |
| H | 4.895580 | 0.614330 | 0.246886 |
| H | 2.674760 | 1.330952 | 1.112661 |
| H | 2.617243 | 1.289483 | -0.637657 |
| H | 1.627235 | -1.060007 | -0.500025 |
| H | 1.472349 | -0.868128 | 1.229725 |
| O | 0.076347 | 1.545370 | -0.263156 |
| H | -0.931170 | -1.445733 | -0.204199 |
| H | -1.101916 | -0.734126 | 1.378948 |
| H | -2.480428 | 1.145828 | 0.384505 |
| H | -2.344375 | 0.404949 | -1.191806 |
| H | -3.515476 | -1.659274 | -0.327038 |
| H | -3.661232 | -0.908576 | 1.252058 |
| H | -4.935351 | 0.172716 | -1.336645 |
| H | -5.083458 | 0.928659 | 0.253758 |
| H | -5.794407 | -0.665179 | -0.036896 |
| Rotational constants (GHz): | 4.4375500 | 0.3787200 | 0.3628400 |
| Vibrational harmonic frequencies (cm ⁻¹): | | | |
| 21.4495 | 34.9486 | | 61.2762 |
| 76.8834 | 90.3227 | | 123.3878 |
| 148.3542 | 185.8426 | | 244.9681 |
| 250.0049 | 311.4262 | | 314.0544 |
| 459.0810 | 472.8997 | | 499.9635 |
| 615.1248 | 690.0276 | | 713.7217 |
| 750.8202 | 804.6419 | | 870.8560 |
| 893.8756 | 914.0774 | | 931.7026 |
| 970.2009 | 1018.1876 | | 1039.3083 |
| 1061.9664 | 1075.2433 | | 1093.0086 |
| 1109.8306 | 1143.7786 | | 1167.0692 |
| 1208.6639 | 1242.8217 | | 1282.0248 |
| 1303.4096 | 1310.1425 | | 1322.6996 |
| 1333.0077 | 1361.2117 | | 1369.7506 |

| | | |
|-----------|-----------|-----------|
| 1382.2146 | 1411.2269 | 1416.2765 |
| 1427.6202 | 1463.0763 | 1474.4572 |
| 1498.6741 | 1499.0701 | 1508.6164 |
| 1512.5747 | 1524.3478 | 1807.3191 |
| 2875.3360 | 2947.9241 | 3011.6182 |
| 3019.9858 | 3027.6179 | 3040.0314 |
| 3043.5691 | 3047.6568 | 3051.5412 |
| 3057.8241 | 3064.4051 | 3092.3576 |
| 3109.5198 | 3111.0440 | 3113.7742 |

Zero-point correction (Hartree): 0.217409

C8H17O.1-6Hshift.5oxo.tt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -464.26508738

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 0.828202 | -1.759578 | -0.501494 |
| C | 2.110090 | -1.646368 | 0.050987 |
| C | 2.807703 | -0.311205 | -0.239890 |
| C | 2.208856 | 0.899314 | 0.518019 |
| C | 0.783491 | 1.234798 | 0.087780 |
| C | -0.292778 | 0.267756 | 0.501484 |
| C | -1.695876 | 0.529677 | -0.003959 |
| C | -2.683079 | -0.599642 | 0.319750 |
| C | -4.097081 | -0.316401 | -0.196120 |
| H | 2.113710 | -1.852117 | 1.136659 |

| | | | |
|---|-----------|-----------|-----------|
| H | 2.685065 | -2.461252 | -0.419789 |
| H | 2.772686 | -0.123328 | -1.319111 |
| H | 3.864995 | -0.399370 | 0.039359 |
| H | 2.820185 | 1.787158 | 0.333758 |
| H | 2.224989 | 0.688733 | 1.596121 |
| O | 0.535650 | 2.211572 | -0.599150 |
| H | 0.123190 | -0.788651 | -0.013441 |
| H | -0.238128 | 0.022224 | 1.569773 |
| H | -2.052862 | 1.472852 | 0.436852 |
| H | -1.658323 | 0.709563 | -1.084575 |
| H | -2.312263 | -1.537581 | -0.112871 |
| H | -2.713363 | -0.756652 | 1.406722 |
| H | -4.102599 | -0.189226 | -1.284402 |
| H | -4.505166 | 0.600146 | 0.245165 |
| H | -4.780885 | -1.136033 | 0.046635 |

Rotational constants (GHz): 2.0019100 0.7092700 0.5608600

Vibrational harmonic frequencies (cm-1):

| | | |
|------------|-----------|-----------|
| i1297.4349 | 54.6126 | 67.3225 |
| 81.0902 | 93.6146 | 124.3447 |
| 212.7146 | 240.7721 | 249.4139 |
| 283.3548 | 302.2299 | 367.1758 |
| 445.9136 | 477.7463 | 558.6976 |
| 578.9309 | 659.0189 | 735.9132 |
| 799.6520 | 813.5161 | 850.2031 |
| 874.3326 | 906.0485 | 919.5742 |
| 954.8725 | 1000.4142 | 1041.7022 |
| 1044.8356 | 1077.3686 | 1093.3981 |
| 1115.9365 | 1138.9615 | 1164.7992 |
| 1211.7704 | 1220.1149 | 1231.5630 |
| 1260.0565 | 1274.7900 | 1290.6372 |
| 1329.6017 | 1348.0544 | 1362.6782 |
| 1379.2248 | 1400.1585 | 1406.2326 |
| 1427.5093 | 1449.5788 | 1467.0976 |
| 1481.0625 | 1486.7995 | 1491.7941 |
| 1505.8956 | 1513.3145 | 1522.3475 |
| 1787.8805 | 2957.0418 | 3002.2051 |
| 3014.4564 | 3027.8691 | 3035.6635 |
| 3040.9144 | 3047.4893 | 3061.8905 |
| 3067.0652 | 3086.4199 | 3096.3864 |
| 3109.9376 | 3115.9992 | 3116.2684 |

Zero-point correction (Hartree): 0.214048

C8H17O.6oxo.pttttt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -464.27895992

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 4.305501 | 0.675158 | 0.927997 |
| C | 4.110066 | -0.068015 | -0.205940 |
| C | 2.790591 | -0.848265 | -0.258333 |
| C | 1.564532 | 0.067470 | -0.191314 |
| C | 0.245412 | -0.701511 | -0.112333 |
| C | -0.993015 | 0.189870 | -0.148500 |
| C | -2.320356 | -0.480703 | 0.187551 |
| C | -3.547256 | 0.395605 | -0.071319 |
| C | -4.858496 | -0.290585 | 0.321925 |
| H | 4.158346 | 0.664570 | -1.041929 |
| H | 4.986687 | -0.722254 | -0.380910 |

| | | | |
|---|-----------|-----------|-----------|
| H | 2.774294 | -1.450069 | -1.177770 |
| H | 2.779877 | -1.558046 | 0.579478 |
| H | 1.660089 | 0.723851 | 0.680478 |
| H | 1.538720 | 0.728997 | -1.065034 |
| H | 0.156553 | -1.406967 | -0.953463 |
| H | 0.204426 | -1.328793 | 0.789214 |
| O | -0.923691 | 1.370871 | -0.435415 |
| H | -2.384192 | -1.428018 | -0.367530 |
| H | -2.275417 | -0.777383 | 1.247028 |
| H | -3.431190 | 1.336345 | 0.476961 |
| H | -3.571065 | 0.672700 | -1.131662 |
| H | -4.871916 | -0.545918 | 1.387986 |
| H | -5.010666 | -1.219180 | -0.240645 |
| H | -5.717894 | 0.358727 | 0.126716 |

Rotational constants (GHz): 4.7239200 0.3716800 0.3602400

| | | | |
|---|-----------|-----------|--|
| Vibrational harmonic frequencies (cm ⁻¹): | | | |
| 21.9626 | 36.2250 | 62.3035 | |
| 76.5979 | 88.5195 | 109.0276 | |
| 149.8100 | 185.5721 | 247.7172 | |
| 258.8548 | 297.0140 | 349.6462 | |
| 408.7384 | 470.2071 | 495.0058 | |
| 553.9241 | 682.0820 | 706.5175 | |
| 750.9378 | 806.5902 | 866.3976 | |
| 880.0903 | 907.1369 | 928.8143 | |
| 977.9921 | 1027.4286 | 1043.5114 | |
| 1053.6464 | 1077.6723 | 1094.6078 | |
| 1115.2175 | 1143.9920 | 1164.0268 | |
| 1200.0210 | 1254.0074 | 1279.6591 | |
| 1298.6174 | 1321.5880 | 1327.3287 | |
| 1334.1306 | 1361.3419 | 1365.9658 | |
| 1386.1143 | 1407.0772 | 1419.1787 | |
| 1427.5993 | 1461.6625 | 1472.0327 | |
| 1494.3211 | 1501.5045 | 1514.1239 | |
| 1514.4464 | 1520.9048 | 1809.0670 | |
| 2886.9976 | 2936.8200 | 3008.6181 | |
| 3015.8000 | 3027.3139 | 3037.2343 | |
| 3042.0088 | 3051.0568 | 3058.5059 | |
| 3059.4980 | 3066.1597 | 3088.2774 | |
| 3105.3703 | 3111.7735 | 3114.7010 | |

Zero-point correction (Hartree): 0.217152

C8H17O.1-5Hshift.6oxo.ttt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -464.26806591

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 2.023026 | 1.670049 | -0.240684 |
| C | 3.079028 | 0.820824 | -0.585757 |
| C | 3.186546 | -0.359583 | 0.399630 |
| C | 1.859713 | -1.137541 | 0.393454 |
| C | 0.684369 | -0.211739 | 0.647027 |
| C | -0.616423 | -0.537889 | -0.037571 |
| C | -1.852262 | 0.196439 | 0.463793 |
| C | -3.114101 | -0.072662 | -0.357493 |
| C | -4.338887 | 0.671472 | 0.181992 |
| H | 2.988342 | 0.442042 | -1.618300 |
| H | 4.000244 | 1.423740 | -0.527743 |
| H | 3.393070 | 0.037182 | 1.400812 |
| H | 4.023121 | -1.009648 | 0.119228 |
| H | 1.891447 | -1.930646 | 1.153000 |
| H | 1.707985 | -1.627495 | -0.574017 |
| H | 1.074994 | 0.855531 | 0.126315 |
| H | 0.558420 | 0.098087 | 1.689448 |
| O | -0.664857 | -1.337938 | -0.959248 |
| H | -2.005736 | -0.088004 | 1.516005 |
| H | -1.619774 | 1.271275 | 0.492327 |
| H | -2.928270 | 0.212108 | -1.399274 |
| H | -3.303280 | -1.151419 | -0.375135 |
| H | -4.183759 | 1.756573 | 0.174934 |
| H | -4.563491 | 0.377643 | 1.214038 |
| H | -5.226562 | 0.460218 | -0.422638 |

Rotational constants (GHz): 2.9054300 0.5343500 0.4944900

| | | | |
|---|-----------|-----------|--|
| Vibrational harmonic frequencies (cm ⁻¹): | | | |
| 11346.9398 | 37.3417 | 44.9286 | |
| 76.7926 | 92.8346 | 120.8284 | |
| 171.4769 | 247.5294 | 270.8066 | |
| 295.3010 | 317.0034 | 369.5241 | |
| 469.7030 | 486.8426 | 521.8463 | |
| 553.9103 | 701.1256 | 733.0791 | |
| 789.8522 | 845.2799 | 869.4016 | |
| 879.1763 | 902.5337 | 926.7604 | |
| 960.8473 | 971.9750 | 1041.4498 | |
| 1048.0613 | 1057.5079 | 1074.3808 | |
| 1120.3211 | 1142.5253 | 1151.8558 | |
| 1166.8646 | 1226.0930 | 1239.4173 | |

| | | |
|-----------|-----------|-----------|
| 1253.5560 | 1261.0102 | 1309.3939 |
| 1325.5561 | 1336.6094 | 1358.6768 |
| 1376.0568 | 1391.0320 | 1411.5710 |
| 1428.7837 | 1465.1977 | 1488.6454 |
| 1493.1772 | 1501.1081 | 1501.2960 |
| 1514.0833 | 1520.9183 | 1547.2409 |
| 1768.9877 | 2966.6098 | 3006.7672 |
| 3014.8986 | 3031.8934 | 3038.1749 |
| 3044.6182 | 3052.7462 | 3060.4170 |
| 3088.3834 | 3090.2075 | 3098.1098 |
| 3109.3313 | 3111.9180 | 3115.4355 |

Zero-point correction (Hartree): 0.214165

C8H17O.7oxo.pttttt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -464.27949447

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 4.471152 | -0.932968 | -0.633405 |
| C | 4.230483 | 0.105168 | 0.227920 |
| C | 2.863194 | 0.782402 | 0.077269 |
| C | 1.693841 | -0.189559 | 0.268277 |
| C | 0.325464 | 0.456272 | 0.024833 |
| C | -0.835720 | -0.522689 | 0.206296 |
| C | -2.210662 | 0.099321 | -0.017330 |
| C | -3.409288 | -0.838621 | 0.089878 |
| C | -4.752871 | -0.139736 | -0.106807 |
| H | 4.331543 | -0.339284 | 1.243411 |
| H | 5.063120 | 0.834145 | 0.179824 |
| H | 2.798127 | 1.608566 | 0.798332 |
| H | 2.809847 | 1.235215 | -0.921293 |
| H | 1.837403 | -1.038468 | -0.411953 |
| H | 1.729956 | -0.603564 | 1.287144 |
| H | 0.183231 | 1.307868 | 0.700458 |
| H | 0.284887 | 0.874034 | -0.988206 |
| H | -0.732816 | -1.382589 | -0.471558 |
| H | -0.825119 | -0.957634 | 1.217106 |
| O | -2.345513 | 1.283196 | -0.267007 |
| H | -3.271038 | -1.643067 | -0.646784 |
| H | -3.361376 | -1.339356 | 1.067369 |
| H | -4.804033 | 0.337073 | -1.089047 |
| H | -4.898497 | 0.644361 | 0.640948 |
| H | -5.576989 | -0.854473 | -0.024472 |

Rotational constants (GHz): 4.9996800 0.3547100 0.3406200

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 19.1581 | 39.4620 | 56.6755 |
| 70.9660 | 99.6205 | 117.6088 |
| 151.8266 | 193.2721 | 198.6175 |
| 242.3306 | 301.9921 | 352.2354 |
| 447.1576 | 467.3548 | 492.1358 |
| 543.9392 | 650.0019 | 707.5576 |
| 752.6332 | 807.5495 | 828.8130 |
| 884.9692 | 920.5630 | 985.4867 |
| 988.1742 | 1014.4055 | 1033.8748 |
| 1062.3733 | 1076.3806 | 1094.5122 |
| 1113.8024 | 1134.1744 | 1157.6758 |
| 1199.2030 | 1257.8411 | 1276.6384 |
| 1295.6768 | 1328.2214 | 1332.7547 |
| 1338.4966 | 1363.3779 | 1369.9384 |
| 1383.1233 | 1407.3134 | 1420.3542 |
| 1428.3504 | 1461.3253 | 1473.9812 |
| 1494.2433 | 1500.4961 | 1506.1207 |
| 1512.3026 | 1520.6273 | 1809.1593 |
| 2882.0396 | 2937.3048 | 3012.1006 |
| 3016.3633 | 3028.8343 | 3032.6918 |
| 3043.8601 | 3052.4346 | 3057.4102 |
| 3061.5015 | 3062.1243 | 3077.4826 |
| 3097.2907 | 3133.7321 | 3140.6344 |

Zero-point correction (Hartree): 0.217161

C8H17O.1-5Hshift.7oxo.ttt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -464.26348414

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 1.936152 | 1.609026 | 0.062418 |
| C | 3.108196 | 0.989011 | -0.390260 |
| C | 3.275017 | -0.416741 | 0.216642 |
| C | 2.036531 | -1.259377 | -0.131376 |
| C | 0.768031 | -0.557063 | 0.327434 |
| C | -0.493582 | -0.799328 | -0.472525 |
| C | -1.752051 | -0.196528 | 0.154788 |
| C | -2.919447 | 0.061974 | -0.786921 |
| C | -4.208478 | 0.462628 | -0.073448 |
| H | 3.140066 | 0.916587 | -1.493071 |

| | | | | |
|---|-----------|-----------|-----------|--|
| H | 3.953071 | 1.623190 | -0.077903 | |
| H | 3.370313 | -0.324978 | 1.305265 | |
| H | 4.191135 | -0.885421 | -0.160672 | |
| H | 2.113138 | -2.253357 | 0.333368 | |
| H | 2.005587 | -1.421150 | -1.217512 | |
| H | 1.116988 | 0.663041 | 0.197022 | |
| H | 0.589771 | -0.612172 | 1.404364 | |
| H | -0.384820 | -0.453595 | -1.508673 | |
| H | -0.683618 | -1.884963 | -0.550647 | |
| O | -1.815251 | 0.043045 | 1.345611 | |
| H | -2.596900 | 0.847582 | -1.486432 | |
| H | -3.063432 | -0.831053 | -1.411685 | |
| H | -4.050389 | 1.353780 | 0.538704 | |
| H | -4.550988 | -0.333247 | 0.593878 | |
| H | -5.002439 | 0.671729 | -0.796237 | |
| Rotational constants (GHz): | 3.0160600 | 0.5197800 | 0.4945100 | |
| Vibrational harmonic frequencies (cm ⁻¹): | | | | |
| i1464.2834 | 29.1175 | | 42.4474 | |
| 69.5349 | 96.7898 | | 122.8125 | |
| 183.9027 | 203.5439 | | 262.0366 | |
| 295.0806 | 312.7009 | | 381.7181 | |
| 451.8665 | 485.1143 | | 492.0942 | |
| 589.7766 | 653.9560 | | 724.5045 | |
| 788.2417 | 822.7845 | | 847.6510 | |
| 873.6659 | 908.0952 | | 944.7224 | |
| 981.0601 | 994.9631 | | 1028.7945 | |
| 1038.7582 | 1076.1215 | | 1096.3586 | |
| 1109.0784 | 1128.8115 | | 1150.4564 | |
| 1178.3214 | 1214.3368 | | 1222.5732 | |
| 1237.0338 | 1274.9285 | | 1290.4884 | |
| 1292.5369 | 1350.8942 | | 1369.5608 | |
| 1383.6971 | 1386.3198 | | 1407.2506 | |
| 1427.7610 | 1453.8594 | | 1466.9482 | |
| 1486.0465 | 1494.3416 | | 1506.7800 | |
| 1511.3530 | 1513.1077 | | 1560.5617 | |
| 1814.1056 | 2946.7517 | | 2974.9326 | |
| 3007.8487 | 3012.4427 | | 3022.8439 | |
| 3046.8622 | 3051.5872 | | 3058.2348 | |
| 3060.4554 | 3062.7974 | | 3098.8636 | |
| 3122.3294 | 3132.6859 | | 3144.0103 | |
| Zero-point correction (Hartree): | 0.213628 | | | |

C8H17O.1-6Hshift.7oxo.tt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -464.26760805

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | | |
|---|-----------|-----------|-----------|--|
| O | -1.105486 | 1.658751 | -0.424482 | |
| C | -2.412017 | 1.409551 | 0.018353 | |
| C | -2.957059 | 0.022813 | -0.354135 | |
| C | -2.331214 | -1.153544 | 0.415835 | |
| C | -0.851786 | -1.445012 | 0.101853 | |
| C | 0.092170 | -0.336178 | 0.523632 | |
| C | 1.498422 | -0.395548 | -0.014393 | |
| C | 2.503476 | 0.570295 | 0.599353 | |
| C | 3.868923 | 0.548483 | -0.083615 | |
| H | -2.518292 | 1.581542 | 1.104624 | |
| H | -3.018723 | 2.182656 | -0.481608 | |
| H | -2.825833 | -0.122632 | -1.433889 | |
| H | -4.037618 | 0.027807 | -0.160949 | |
| H | -2.909870 | -2.057258 | 0.190227 | |
| H | -2.451263 | -0.980149 | 1.495471 | |
| H | -0.716608 | -1.628259 | -0.969592 | |
| H | -0.553876 | -2.375447 | 0.604813 | |
| H | -0.346284 | 0.708626 | 0.025702 | |
| H | 0.060609 | -0.104025 | 1.595001 | |
| O | 1.799950 | -1.168532 | -0.909449 | |
| H | 2.057285 | 1.574428 | 0.574459 | |
| H | 2.593440 | 0.323563 | 1.667231 | |
| H | 3.782626 | 0.825916 | -1.137688 | |
| H | 4.308081 | -0.451732 | -0.046183 | |
| H | 4.555128 | 1.248049 | 0.402540 | |
| Rotational constants (GHz): | 2.4121700 | 0.6610200 | 0.5674900 | |
| Vibrational harmonic frequencies (cm ⁻¹): | | | | |
| i1232.1468 | 45.3579 | | 52.3648 | |
| 72.9240 | 115.7360 | | 171.0218 | |
| 192.5528 | 206.0652 | | 263.1789 | |
| 288.5222 | 337.4698 | | 399.9694 | |
| 422.7390 | 480.2353 | | 521.2123 | |
| 600.2280 | 665.6235 | | 735.0533 | |
| 789.9568 | 804.2667 | | 838.1726 | |
| 872.3067 | 898.8695 | | 950.6911 | |
| 982.8948 | 1009.1167 | | 1022.6822 | |
| 1043.2208 | 1072.8430 | | 1094.4485 | |
| 1104.7375 | 1130.5264 | | 1148.5914 | |

| | | |
|-----------|-----------|-----------|
| 1203.6855 | 1221.9569 | 1226.6334 |
| 1271.3382 | 1281.8895 | 1287.7822 |
| 1336.9103 | 1377.3035 | 1381.6990 |
| 1394.6737 | 1395.7751 | 1402.4365 |
| 1428.1601 | 1445.9157 | 1468.3334 |
| 1471.5952 | 1482.1208 | 1492.9674 |
| 1502.3960 | 1507.0538 | 1512.9175 |
| 1774.5789 | 2956.9891 | 3002.6223 |
| 3017.6026 | 3025.8678 | 3031.6526 |
| 3036.8233 | 3056.5600 | 3062.2825 |
| 3070.1510 | 3074.4451 | 3082.1562 |
| 3097.5477 | 3134.1147 | 3140.5241 |

Zero-point correction (Hartree): 0.214127

C8H17O.8oxo.pttttt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -464.27840853

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 4.478221 | 0.952083 | 0.736235 |
| C | 4.307770 | 0.014690 | -0.248213 |
| C | 3.010379 | -0.798572 | -0.163192 |
| C | 1.754761 | 0.076911 | -0.234256 |
| C | 0.451486 | -0.702415 | -0.021945 |
| C | -0.798827 | 0.180879 | -0.111088 |
| C | -2.096232 | -0.594714 | 0.119663 |
| C | -3.358009 | 0.252378 | -0.005575 |
| C | -4.676185 | -0.446539 | 0.287266 |
| H | 4.340507 | 0.591101 | -1.199681 |
| H | 5.203074 | -0.635093 | -0.306898 |
| H | 3.008094 | -1.542405 | -0.971803 |
| H | 3.019510 | -1.361762 | 0.779335 |
| H | 1.841387 | 0.867775 | 0.521026 |
| H | 1.720408 | 0.585041 | -1.208976 |
| H | 0.382875 | -1.510444 | -0.765058 |
| H | 0.483649 | -1.197365 | 0.959439 |
| H | -0.732961 | 0.995328 | 0.620115 |
| H | -0.845220 | 0.668452 | -1.091781 |
| H | -2.184749 | -1.429187 | -0.592743 |
| H | -2.100708 | -1.071082 | 1.111281 |
| O | -3.316702 | 1.426276 | -0.322623 |
| H | -4.706569 | -0.773425 | 1.333480 |
| H | -4.786609 | -1.345456 | -0.329881 |
| H | -5.505714 | 0.235956 | 0.097295 |

Rotational constants (GHz): 4.6005500 0.3350600 0.3221400

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 22.1658 | 41.1608 | 61.4602 |
| 69.4311 | 103.2056 | 110.2670 |
| 145.3796 | 156.2986 | 188.3759 |
| 231.4293 | 316.5566 | 386.2594 |
| 451.6229 | 474.4206 | 497.7652 |
| 553.6171 | 599.9421 | 724.6894 |
| 751.6669 | 810.6673 | 831.1774 |
| 894.0037 | 922.6946 | 947.0878 |
| 979.0374 | 1014.4570 | 1043.1769 |
| 1059.5294 | 1077.2625 | 1094.6254 |
| 1116.9276 | 1154.0813 | 1179.1003 |
| 1197.0128 | 1252.6840 | 1268.0594 |
| 1310.0789 | 1318.8587 | 1332.0441 |
| 1336.7593 | 1361.1839 | 1365.1256 |
| 1385.7036 | 1398.1694 | 1412.8119 |
| 1420.1168 | 1464.8480 | 1479.0472 |
| 1491.1323 | 1493.5435 | 1498.1401 |
| 1506.8304 | 1522.7135 | 1816.2203 |
| 2883.2124 | 2936.0913 | 3008.5620 |
| 3015.0289 | 3019.0425 | 3030.4439 |
| 3040.5408 | 3042.3222 | 3046.7142 |
| 3053.3884 | 3063.8572 | 3082.9472 |
| 3096.3051 | 3107.5153 | 3165.2985 |

Zero-point correction (Hartree): 0.216954

C8H17O.1-6Hshift.8oxo.tt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -464.26355870

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -0.990649 | 1.559896 | -0.479196 |
| C | -2.260161 | 1.467506 | 0.116423 |
| C | -3.033946 | 0.192125 | -0.245276 |
| C | -2.463062 | -1.109398 | 0.345296 |
| C | -1.073692 | -1.516771 | -0.183871 |
| C | 0.045008 | -0.590392 | 0.256412 |
| C | 1.378863 | -0.761278 | -0.439898 |
| C | 2.518080 | 0.035296 | 0.197134 |
| C | 3.738728 | 0.276898 | -0.670622 |

| | | | |
|--|-----------|-----------|-----------|
| H | -2.206913 | 1.578325 | 1.214068 |
| H | -2.810257 | 2.344473 | -0.259721 |
| H | -3.079441 | 0.113608 | -1.339448 |
| H | -4.066653 | 0.311141 | 0.108448 |
| H | -3.166296 | -1.923537 | 0.132004 |
| H | -2.420528 | -1.023023 | 1.440601 |
| H | -1.103614 | -1.563908 | -1.281278 |
| H | -0.844232 | -2.537809 | 0.158781 |
| H | -0.340181 | 0.563468 | -0.059014 |
| H | 0.157385 | -0.516878 | 1.342334 |
| H | 1.688541 | -1.821373 | -0.408012 |
| H | 1.303906 | -0.518497 | -1.507958 |
| O | 2.452066 | 0.439728 | 1.341783 |
| H | 3.489239 | 1.004642 | -1.452626 |
| H | 4.053149 | -0.641785 | -1.178394 |
| H | 4.555654 | 0.670233 | -0.064070 |
| Rotational constants (GHz): | 2.4129700 | 0.6259800 | 0.5620400 |
| Vibrational harmonic frequencies (cm-1): | | | |
| i1367.7209 | 36.2819 | | 49.3355 |
| 78.8939 | 125.3378 | | 134.6171 |
| 176.0740 | 210.3057 | | 271.3786 |
| 318.6871 | 337.6867 | | 378.6343 |
| 447.1348 | 467.6508 | | 502.1756 |
| 580.8613 | 617.1214 | | 779.2328 |
| 787.6738 | 807.8364 | | 826.9114 |
| 863.2327 | 908.2473 | | 949.9082 |
| 957.6848 | 993.4073 | | 1013.7018 |
| 1052.2592 | 1083.4184 | | 1102.3252 |
| 1108.7140 | 1139.5288 | | 1175.6857 |
| 1190.3564 | 1217.6571 | | 1225.6061 |
| 1266.9648 | 1283.7789 | | 1295.3788 |
| 1311.1378 | 1375.2148 | | 1385.4827 |
| 1394.8141 | 1396.1634 | | 1402.4570 |
| 1407.7585 | 1447.4622 | | 1462.3242 |
| 1476.8586 | 1479.2311 | | 1482.6526 |
| 1489.6709 | 1492.2218 | | 1502.8669 |
| 1819.7749 | 2962.8400 | | 2977.0724 |
| 3000.9564 | 3013.3633 | | 3022.4056 |
| 3033.2706 | 3044.8842 | | 3048.3062 |
| 3060.3431 | 3069.3847 | | 3077.4303 |
| 3106.9116 | 3107.2427 | | 3165.9596 |
| Zero-point correction (Hartree): | 0.213642 | | |

C8H17O.4oh.mttttt.p

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -465.48612868

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|--|-----------|-----------|-----------|
| O | -4.179542 | 0.821641 | 0.018486 |
| C | -3.856041 | -0.485771 | 0.295148 |
| C | -2.494330 | -0.965004 | -0.227531 |
| C | -1.325720 | -0.056119 | 0.187656 |
| C | 0.032980 | -0.659649 | -0.173993 |
| C | 1.218842 | 0.208139 | 0.264051 |
| C | 2.577839 | -0.376864 | -0.138587 |
| C | 3.768157 | 0.484022 | 0.303263 |
| C | 5.123869 | -0.098681 | -0.108345 |
| H | -3.856270 | -0.513265 | 1.409762 |
| H | -4.683513 | -1.160074 | 0.007837 |
| H | -2.332905 | -1.985994 | 0.141700 |
| H | -2.526636 | -1.016405 | -1.322800 |
| O | -1.415352 | 1.209963 | -0.453469 |
| H | -1.363925 | 0.070278 | 1.288000 |
| H | 0.110320 | -1.655197 | 0.284215 |
| H | 0.063631 | -0.805144 | -1.262303 |
| H | 1.099563 | 1.207945 | -0.167746 |
| H | 1.187668 | 0.338068 | 1.355704 |
| H | 2.685366 | -1.386377 | 0.285319 |
| H | 2.609636 | -0.503610 | -1.230396 |
| H | 3.658981 | 1.492478 | -0.118092 |
| H | 3.738993 | 0.607891 | 1.394532 |
| H | 5.197553 | -0.200232 | -1.197268 |
| H | 5.276405 | -1.093821 | 0.325549 |
| H | 5.951450 | 0.537708 | 0.222280 |
| H | -2.330737 | 1.512482 | -0.346397 |
| Rotational constants (GHz): | 5.0002600 | 0.3658500 | 0.3515000 |
| Vibrational harmonic frequencies (cm-1): | | | |
| 42.0025 | 61.6861 | | 66.3109 |
| 92.6641 | 131.3416 | | 144.2718 |
| 183.9217 | 202.7353 | | 240.3547 |
| 249.5900 | 287.7615 | | 386.0407 |
| 398.2560 | 475.1413 | | 484.5547 |
| 500.5804 | 565.0275 | | 737.7471 |
| 741.1788 | 764.4811 | | 842.3535 |
| 858.7813 | 901.0314 | | 932.4967 |

| | | |
|-----------|-----------|-----------|
| 959.4078 | 999.0563 | 1013.4984 |
| 1033.9592 | 1056.8097 | 1069.7006 |
| 1083.4267 | 1095.2567 | 1109.5372 |
| 1151.9375 | 1182.9014 | 1232.7617 |
| 1237.5732 | 1260.0370 | 1281.8118 |
| 1298.4338 | 1328.2411 | 1334.5623 |
| 1336.7119 | 1347.7378 | 1365.9969 |
| 1378.1845 | 1398.7070 | 1407.0911 |
| 1415.4241 | 1427.5703 | 1463.9768 |
| 1480.3588 | 1490.4078 | 1500.3580 |
| 1504.7846 | 1513.2157 | 1517.4295 |
| 1526.8590 | 2864.0909 | 2916.6889 |
| 2962.7073 | 3007.9518 | 3017.6530 |
| 3024.1092 | 3026.8925 | 3037.0774 |
| 3038.5109 | 3042.7327 | 3062.0814 |
| 3064.0862 | 3089.6756 | 3096.0339 |
| 3105.0942 | 3110.4104 | 3744.1499 |

Zero-point correction (Hartree): 0.242178

C8H17O.4oh.mttttt.t

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -465.48035653

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| H | -2.517072 | -1.805416 | 0.835582 |
| C | -3.248039 | -1.095416 | 0.391353 |
| C | -2.779904 | 0.356989 | 0.550870 |
| C | -1.472022 | 0.690462 | -0.185088 |
| C | -0.231652 | 0.034295 | 0.438327 |
| C | 1.061812 | 0.313077 | -0.336865 |
| C | 2.308916 | -0.293242 | 0.317330 |
| C | 3.602407 | -0.010659 | -0.457514 |
| C | 4.846665 | -0.616095 | 0.199774 |
| O | -3.412938 | -1.521387 | -0.899800 |
| H | -4.171603 | -1.289079 | 0.971537 |
| H | -3.558530 | 1.019683 | 0.156879 |
| H | -2.679016 | 0.581050 | 1.623455 |
| O | -1.309468 | 2.107294 | -0.288792 |
| H | -1.577055 | 0.348343 | -1.221168 |
| H | -0.128248 | 0.393880 | 1.475086 |
| H | -0.386267 | -1.051006 | 0.509984 |
| H | 0.958059 | -0.079653 | -1.358115 |
| H | 1.182999 | 1.397598 | -0.441175 |
| H | 2.409665 | 0.094930 | 1.341614 |
| H | 2.178923 | -1.380678 | 0.419127 |
| H | 3.502445 | -0.398941 | -1.480210 |
| H | 3.731962 | 1.075477 | -0.558271 |
| H | 4.761940 | -1.705967 | 0.280599 |
| H | 4.992309 | -0.221519 | 1.212053 |
| H | 5.751687 | -0.395547 | -0.375747 |
| H | -1.202048 | 2.453117 | 0.608377 |

Rotational constants (GHz): 2.4851200 0.4256600 0.3884100

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 37.1539 | 55.5288 | 66.8519 |
| 87.5714 | 122.0556 | 136.6237 |
| 157.7920 | 201.4502 | 230.8989 |
| 250.0767 | 302.8783 | 323.4894 |
| 389.6889 | 396.5419 | 443.8400 |
| 481.1717 | 504.1788 | 563.6060 |
| 738.0661 | 764.7203 | 827.2825 |
| 848.9969 | 899.0671 | 909.9592 |
| 951.0691 | 1003.3407 | 1011.1631 |
| 1035.3193 | 1062.3223 | 1068.0424 |
| 1077.2361 | 1095.8000 | 1112.5499 |
| 1142.7753 | 1182.5218 | 1207.4193 |
| 1229.7890 | 1262.0390 | 1287.6772 |
| 1314.1802 | 1330.0000 | 1331.0471 |
| 1337.2562 | 1356.2539 | 1370.3152 |
| 1374.7964 | 1401.0618 | 1413.1481 |
| 1415.9086 | 1427.6492 | 1433.7386 |
| 1491.9199 | 1495.3007 | 1500.5440 |
| 1505.2018 | 1513.3887 | 1517.9866 |
| 1526.9908 | 2898.0104 | 2935.7560 |
| 2995.0651 | 3008.0252 | 3020.3683 |
| 3024.4618 | 3030.4390 | 3037.1416 |
| 3038.1770 | 3047.5629 | 3061.5282 |
| 3073.6343 | 3087.9653 | 3091.4738 |
| 3105.6174 | 3111.7571 | 3790.2131 |

Zero-point correction (Hartree): 0.241218

C8H17O.4oh.pttttt.m

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -465.48335643

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 4.054250 | -0.765525 | -0.625590 |
| C | 3.865215 | 0.342647 | 0.158011 |
| C | 2.495234 | 1.030128 | -0.008168 |
| C | 1.340737 | 0.021625 | -0.156175 |
| C | -0.021612 | 0.674758 | 0.072965 |
| C | -1.206074 | -0.251979 | -0.224351 |
| C | -2.567196 | 0.391865 | 0.065891 |
| C | -3.755898 | -0.531943 | -0.228713 |
| C | -5.112945 | 0.115071 | 0.066338 |
| H | 3.900172 | -0.077684 | 1.188211 |
| H | 4.702980 | 1.058122 | 0.092994 |
| H | 2.331693 | 1.674559 | 0.864807 |
| H | 2.522216 | 1.682342 | -0.889839 |
| O | 1.474882 | -1.048766 | 0.781889 |
| H | 1.372536 | -0.384931 | -1.178644 |
| H | -0.065338 | 1.008706 | 1.118796 |
| H | -0.086141 | 1.578655 | -0.548340 |
| H | -1.168257 | -0.561466 | -1.278994 |
| H | -1.091700 | -1.166004 | 0.369618 |
| H | -2.604363 | 0.702946 | 1.119918 |
| H | -2.671046 | 1.314073 | -0.524648 |
| H | -3.719839 | -0.843039 | -1.281775 |
| H | -3.651907 | -1.452109 | 0.362000 |
| H | -5.260527 | 1.018839 | -0.536175 |
| H | -5.192353 | 0.405835 | 1.120206 |
| H | -5.939892 | -0.568552 | -0.152589 |
| H | 2.163938 | -1.628998 | 0.429281 |

Rotational constants (GHz): 4.8178800 0.3680700 0.3568300

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 34.0095 | 52.6699 | 61.5973 |
| 84.0966 | 123.1765 | 132.8336 |
| 145.3737 | 195.9538 | 240.5837 |
| 250.5349 | 256.4212 | 377.7691 |
| 395.5930 | 462.8012 | 484.1293 |
| 498.3128 | 603.1227 | 736.3322 |
| 755.9277 | 764.1237 | 837.5774 |
| 885.6068 | 899.2668 | 918.4242 |
| 956.0239 | 996.0904 | 1019.3337 |
| 1030.1081 | 1053.1749 | 1068.3182 |
| 1077.3632 | 1106.6772 | 1122.4397 |
| 1144.8067 | 1158.1554 | 1227.0076 |
| 1227.6955 | 1236.9649 | 1264.2960 |
| 1285.8575 | 1318.1549 | 1328.5079 |
| 1333.5997 | 1346.7766 | 1364.4932 |
| 1394.7050 | 1402.9022 | 1413.6311 |
| 1419.2109 | 1425.3066 | 1438.1159 |
| 1485.6674 | 1494.6355 | 1499.3701 |
| 1504.3340 | 1513.0423 | 1516.9806 |
| 1526.1580 | 2876.3310 | 2985.0316 |
| 3000.2752 | 3008.5919 | 3017.4196 |
| 3024.3782 | 3027.4088 | 3037.4261 |
| 3038.6982 | 3041.8544 | 3060.4361 |
| 3063.1694 | 3087.2706 | 3091.3992 |
| 3105.5202 | 3111.0006 | 3798.6264 |

Zero-point correction (Hartree): 0.242103

C8H17O.4oh.pttttt.p

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -465.48355839

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 4.094550 | -0.360016 | 1.211712 |
| C | 3.880796 | -0.106292 | -0.114390 |
| C | 2.538741 | -0.626749 | -0.651906 |
| C | 1.350207 | 0.106657 | -0.018940 |
| C | -0.003923 | -0.488969 | -0.420874 |
| C | -1.199897 | 0.185216 | 0.262150 |
| C | -2.555142 | -0.361739 | -0.201793 |
| C | -3.751221 | 0.306437 | 0.488278 |
| C | -5.103437 | -0.235587 | 0.014366 |
| H | 3.866828 | 1.004039 | -0.184280 |
| H | 4.739925 | -0.427697 | -0.732272 |
| H | 2.514104 | -0.499472 | -1.744386 |
| H | 2.468548 | -1.703347 | -0.455668 |
| O | 1.419625 | 1.508826 | -0.312124 |
| H | 1.463091 | 0.052223 | 1.070486 |
| H | -0.111165 | -0.415048 | -1.515440 |
| H | 0.000358 | -1.563158 | -0.191970 |
| H | -1.107942 | 0.059184 | 1.350103 |
| H | -1.150727 | 1.265252 | 0.078609 |
| H | -2.647415 | -0.232068 | -1.290226 |
| H | -2.594402 | -1.446285 | -0.023734 |
| H | -3.662595 | 0.171339 | 1.574796 |
| H | -3.708464 | 1.390206 | 0.314229 |

| | | | |
|--|-----------|-----------|-----------|
| H | -5.189030 | -1.311228 | 0.207149 |
| H | -5.236253 | -0.082896 | -1.062954 |
| H | -5.935491 | 0.260290 | 0.524938 |
| H | 1.240475 | 1.614340 | -1.257418 |
| Rotational constants (GHz): | 4.2033200 | 0.3618500 | 0.3580400 |
| Vibrational harmonic frequencies (cm-1): | | | |
| 42.0879 | 59.4516 | 77.1460 | |
| 90.9501 | 121.5111 | 140.4587 | |
| 159.1286 | 198.3516 | 251.6679 | |
| 256.0223 | 263.1719 | 348.7206 | |
| 386.6204 | 422.6645 | 470.1999 | |
| 494.2479 | 565.0902 | 726.4419 | |
| 739.0572 | 765.1125 | 838.8683 | |
| 883.6786 | 896.8930 | 908.7911 | |
| 951.6888 | 1007.0746 | 1012.2507 | |
| 1048.9016 | 1064.7633 | 1070.6639 | |
| 1082.4377 | 1098.9316 | 1116.5777 | |
| 1141.9982 | 1150.3079 | 1201.5164 | |
| 1227.7160 | 1259.0396 | 1282.9247 | |
| 1294.1175 | 1324.0723 | 1327.9580 | |
| 1337.8301 | 1357.8353 | 1365.7805 | |
| 1386.3952 | 1397.8179 | 1411.9616 | |
| 1417.1804 | 1427.4686 | 1434.0485 | |
| 1483.7326 | 1496.2451 | 1500.1038 | |
| 1505.3126 | 1513.6259 | 1518.0368 | |
| 1526.9510 | 2888.3362 | 2956.8124 | |
| 2994.8322 | 3008.8866 | 3022.1349 | |
| 3024.3314 | 3030.6387 | 3037.5182 | |
| 3038.2632 | 3049.7765 | 3061.9087 | |
| 3068.7748 | 3083.3509 | 3088.6769 | |
| 3106.1426 | 3111.9474 | 3786.7933 | |
| Zero-point correction (Hartree): | 0.241961 | | |

C8H17O.4oh.pttttt.t

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -465.48391324
 Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 4.081935 | -0.243153 | 1.241937 |
| C | 3.880605 | -0.143214 | -0.106424 |
| C | 2.531361 | -0.689129 | -0.597605 |
| C | 1.354602 | 0.098418 | -0.026372 |
| C | -0.002548 | -0.524489 | -0.376977 |
| C | -1.202593 | 0.255426 | 0.174884 |
| C | -2.553541 | -0.399440 | -0.140161 |
| C | -3.756607 | 0.388038 | 0.394238 |
| C | -5.101033 | -0.275266 | 0.078526 |
| H | 3.896762 | 0.950550 | -0.308694 |
| H | 4.735094 | -0.555271 | -0.675090 |
| H | 2.501014 | -0.636494 | -1.693413 |
| H | 2.444449 | -1.744442 | -0.315017 |
| O | 1.478369 | 1.426295 | -0.556291 |
| H | 1.468743 | 0.124256 | 1.069202 |
| H | -0.082800 | -0.597005 | -1.469918 |
| H | -0.024479 | -1.551348 | 0.013052 |
| H | -1.098674 | 0.363521 | 1.264861 |
| H | -1.195274 | 1.272005 | -0.242280 |
| H | -2.652936 | -0.519144 | -1.228365 |
| H | -2.570013 | -1.415666 | 0.278895 |
| H | -3.654776 | 0.510323 | 1.481270 |
| H | -3.740793 | 1.402336 | -0.027567 |
| H | -5.160930 | -1.278002 | 0.516876 |
| H | -5.247412 | -0.379250 | -1.002703 |
| H | -5.938673 | 0.309686 | 0.472222 |
| H | 0.936784 | 2.016741 | -0.019152 |

| | | | |
|--|-----------|-----------|-----------|
| Rotational constants (GHz): | 4.2093800 | 0.3621600 | 0.3576700 |
| Vibrational harmonic frequencies (cm-1): | | | |
| 38.2925 | 50.3098 | 74.1128 | |
| 84.6049 | 115.8741 | 140.2890 | |
| 152.4176 | 193.0573 | 249.7453 | |
| 256.2475 | 261.4152 | 293.4695 | |
| 378.3270 | 418.3929 | 475.8324 | |
| 489.1589 | 559.4971 | 718.2822 | |
| 738.0050 | 763.0798 | 839.5335 | |
| 883.7021 | 897.3874 | 909.3740 | |
| 953.3236 | 1007.2954 | 1018.4387 | |
| 1042.1800 | 1056.9161 | 1069.2554 | |
| 1075.6422 | 1097.0525 | 1129.1140 | |
| 1138.2676 | 1166.8969 | 1210.8919 | |
| 1236.4629 | 1251.0067 | 1281.0122 | |
| 1296.6867 | 1315.6756 | 1325.7002 | |
| 1337.1175 | 1340.7998 | 1360.4310 | |
| 1382.1377 | 1395.7454 | 1412.4457 | |
| 1413.2275 | 1426.5277 | 1442.6710 | |
| 1478.5887 | 1489.5559 | 1498.8119 | |

| | | |
|-----------|-----------|-----------|
| 1503.7061 | 1513.4577 | 1516.6029 |
| 1525.7467 | 2890.5967 | 2956.3357 |
| 2997.0866 | 3007.3607 | 3014.1005 |
| 3023.9609 | 3027.5755 | 3036.5308 |
| 3039.3484 | 3046.9741 | 3048.5575 |
| 3065.1171 | 3077.1504 | 3098.2221 |
| 3107.2707 | 3112.8244 | 3840.3117 |

Zero-point correction (Hartree): 0.241666

C8H17O.1-5Hshift.4oh.tttR.m

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -465.46595789

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 1.534451 | 1.854920 | -0.241660 |
| C | 2.730697 | 1.169762 | -0.495698 |
| C | 2.941663 | 0.028975 | 0.516745 |
| C | 1.747685 | -0.942005 | 0.449412 |
| C | 0.453439 | -0.173573 | 0.671522 |
| C | -0.830226 | -0.723444 | 0.082907 |
| C | -2.037974 | 0.199784 | 0.293566 |
| C | -3.341096 | -0.369469 | -0.281024 |
| C | -4.543670 | 0.558416 | -0.081657 |
| H | 2.764096 | 0.758600 | -1.517444 |
| H | 3.551565 | 1.896941 | -0.395095 |
| H | 3.011662 | 0.444867 | 1.528935 |
| H | 3.882003 | -0.501240 | 0.313353 |
| O | 1.669867 | -1.587681 | -0.818782 |
| H | 1.856810 | -1.698182 | 1.249792 |
| H | 0.744280 | 0.943783 | 0.121997 |
| H | 0.355793 | 0.127942 | 1.720264 |
| H | -0.683285 | -0.921804 | -0.983498 |
| H | -1.034704 | -1.704716 | 0.543580 |
| H | -2.169387 | 0.394904 | 1.367696 |
| H | -1.831107 | 1.174360 | -0.169110 |
| H | -3.205431 | -0.568878 | -1.352559 |
| H | -3.547778 | -1.343125 | 0.184323 |
| H | -4.380731 | 1.527224 | -0.567322 |
| H | -4.724877 | 0.750015 | 0.982292 |
| H | -5.457647 | 0.125575 | -0.501517 |
| H | 2.511098 | -2.034847 | -0.976799 |

Rotational constants (GHz): 2.4917900 0.5271300 0.4714900

Vibrational harmonic frequencies (cm-1):

| | | |
|------------|-----------|-----------|
| 11461.4195 | 43.0221 | 64.8209 |
| 85.7803 | 108.0442 | 135.6681 |
| 190.3598 | 223.7133 | 246.7396 |
| 250.9505 | 291.7596 | 313.4589 |
| 394.7094 | 415.9309 | 477.5280 |
| 515.8048 | 581.0572 | 669.1080 |
| 734.7069 | 769.0450 | 829.9063 |
| 854.6985 | 888.1546 | 902.5831 |
| 921.7126 | 970.4253 | 1018.5985 |
| 1020.4001 | 1042.4700 | 1063.7271 |
| 1070.2081 | 1080.8069 | 1126.3271 |
| 1136.3630 | 1168.4634 | 1197.4521 |
| 1217.1940 | 1232.7747 | 1250.0932 |
| 1265.6518 | 1272.9921 | 1310.4440 |
| 1317.6277 | 1336.4465 | 1344.0885 |
| 1365.1689 | 1391.0635 | 1395.7313 |
| 1415.6016 | 1417.6343 | 1427.1146 |
| 1485.2112 | 1488.4227 | 1500.7089 |
| 1506.7772 | 1510.8962 | 1512.8263 |
| 1524.6374 | 1558.9859 | 2933.5643 |
| 2983.4470 | 2984.5517 | 3016.2738 |
| 3020.3295 | 3025.8696 | 3038.4169 |
| 3038.9801 | 3047.2266 | 3067.3516 |
| 3082.0436 | 3088.5593 | 3101.1029 |
| 3107.3989 | 3112.1068 | 3820.4477 |

Zero-point correction (Hartree): 0.237659

C8H17O.1-5Hshift.4oh.tttR.p

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -465.46599036

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 1.529586 | 1.857547 | -0.232416 |
| C | 2.720274 | 1.168035 | -0.514387 |
| C | 2.952574 | 0.024762 | 0.491160 |
| C | 1.762178 | -0.942200 | 0.454180 |
| C | 0.461766 | -0.171368 | 0.689744 |
| C | -0.816581 | -0.701134 | 0.069676 |
| C | -2.037408 | 0.196531 | 0.315321 |
| C | -3.327116 | -0.350056 | -0.309239 |
| C | -4.541135 | 0.552586 | -0.068192 |
| H | 2.731546 | 0.761831 | -1.537129 |

| | | | | |
|--|-----------|-----------|-----------|--|
| H | 3.543631 | 1.893923 | -0.425670 | |
| H | 3.040970 | 0.441483 | 1.500919 | |
| H | 3.876048 | -0.515532 | 0.258267 | |
| O | 1.804153 | -1.595410 | -0.811249 | |
| H | 1.888600 | -1.685414 | 1.264056 | |
| H | 0.756416 | 0.956123 | 0.157920 | |
| H | 0.346621 | 0.100624 | 1.745128 | |
| H | -0.668708 | -0.828909 | -1.010075 | |
| H | -1.026961 | -1.707255 | 0.475490 | |
| H | -2.182210 | 0.326010 | 1.397037 | |
| H | -1.830767 | 1.196981 | -0.087196 | |
| H | -3.177332 | -0.481768 | -1.389447 | |
| H | -3.529374 | -1.352131 | 0.093781 | |
| H | -4.382064 | 1.550792 | -0.491299 | |
| H | -4.736997 | 0.676093 | 1.003081 | |
| H | -5.445131 | 0.137648 | -0.525651 | |
| | | | | |
| H | 1.078494 | -2.230532 | -0.849459 | |
| Rotational constants (GHz): | 2.4830300 | 0.5266000 | 0.4710000 | |
| Vibrational harmonic frequencies (cm-1): | | | | |
| i1485.3436 | 40.8538 | | 59.8095 | |
| 83.9744 | 103.6922 | | 138.1472 | |
| 182.5758 | 224.2405 | | 245.6863 | |
| 249.1067 | 302.6602 | | 321.4934 | |
| 393.5174 | 417.5176 | | 475.3538 | |
| 517.9514 | 587.1592 | | 665.5855 | |
| 738.4334 | 772.2823 | | 827.6394 | |
| 853.2786 | 886.4285 | | 901.6571 | |
| 918.9447 | 977.2976 | | 1015.4425 | |
| 1021.2134 | 1032.6411 | | 1058.9292 | |
| 1069.1193 | 1079.1810 | | 1129.6357 | |
| 1147.1206 | 1171.8602 | | 1187.6087 | |
| 1234.7953 | 1239.1494 | | 1244.1504 | |
| 1248.9927 | 1271.3523 | | 1316.3969 | |
| 1331.0827 | 1337.0611 | | 1345.7788 | |
| 1365.1307 | 1379.3529 | | 1388.0651 | |
| 1404.2231 | 1416.3358 | | 1427.7967 | |
| 1480.1225 | 1495.3312 | | 1500.3718 | |
| 1510.2548 | 1511.6421 | | 1513.0897 | |
| 1524.4932 | 1549.9707 | | 2933.0152 | |
| 2959.7272 | 2992.5562 | | 3019.6918 | |
| 3026.6634 | 3029.8197 | | 3040.5455 | |
| 3048.4596 | 3056.9196 | | 3062.4117 | |
| 3075.5999 | 3084.5569 | | 3108.8563 | |
| 3113.1237 | 3114.1962 | | 3831.9517 | |
| Zero-point correction (Hartree): | 0.237684 | | | |

C8H17O.1-5Hshift.4oh.tttR.t

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -465.46612565

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | | |
|--|-----------|-----------|-----------|--|
| O | 1.551807 | 1.819264 | -0.280266 | |
| C | 2.785792 | 1.169599 | -0.426023 | |
| C | 2.938883 | -0.005274 | 0.561725 | |
| C | 1.742299 | -0.962511 | 0.417438 | |
| C | 0.449359 | -0.189534 | 0.663790 | |
| C | -0.847615 | -0.735828 | 0.102654 | |
| C | -2.043392 | 0.208579 | 0.286838 | |
| C | -3.357803 | -0.366902 | -0.254921 | |
| C | -4.547104 | 0.583261 | -0.083015 | |
| H | 2.941445 | 0.804022 | -1.458495 | |
| H | 3.578230 | 1.907590 | -0.228577 | |
| H | 2.967770 | 0.385958 | 1.585547 | |
| H | 3.875276 | -0.540313 | 0.372518 | |
| O | 1.753533 | -1.639420 | -0.836024 | |
| H | 1.835484 | -1.765308 | 1.163436 | |
| H | 0.753727 | 0.921835 | 0.108378 | |
| H | 0.365378 | 0.123103 | 1.710955 | |
| H | -0.720508 | -0.981088 | -0.957787 | |
| H | -1.059847 | -1.697437 | 0.599420 | |
| H | -2.162373 | 0.444875 | 1.353793 | |
| H | -1.829464 | 1.163186 | -0.212951 | |
| H | -3.233960 | -0.610189 | -1.318932 | |
| H | -3.572204 | -1.318722 | 0.250108 | |
| H | -4.377272 | 1.529394 | -0.609280 | |
| H | -4.716157 | 0.819966 | 0.973741 | |
| H | -5.469750 | 0.144671 | -0.476853 | |
| H | 1.658994 | -0.978639 | -1.535620 | |
| Rotational constants (GHz): | 2.4916300 | 0.5219300 | 0.4682000 | |
| Vibrational harmonic frequencies (cm-1): | | | | |
| i1457.6143 | 44.1773 | | 66.0804 | |
| 80.9371 | 91.0307 | | 131.5333 | |
| 188.5735 | 222.8579 | | 248.6948 | |
| 250.8645 | 298.5012 | | 303.5939 | |

| | | |
|-----------|-----------|-----------|
| 394.3940 | 413.6109 | 478.5463 |
| 522.3475 | 583.7315 | 658.0739 |
| 733.6832 | 767.7728 | 826.4481 |
| 847.6460 | 881.0512 | 901.1205 |
| 919.0892 | 968.4409 | 1012.7413 |
| 1019.3721 | 1043.2233 | 1064.9702 |
| 1072.2524 | 1079.2180 | 1122.7801 |
| 1147.7329 | 1162.4614 | 1194.0413 |
| 1219.7418 | 1238.9840 | 1247.5700 |
| 1257.4104 | 1283.5262 | 1300.7893 |
| 1315.4743 | 1336.9764 | 1343.4711 |
| 1361.4521 | 1379.6911 | 1395.1717 |
| 1415.2384 | 1416.9958 | 1427.9496 |
| 1482.5269 | 1484.6077 | 1500.7735 |
| 1510.7700 | 1513.1586 | 1524.6940 |
| 1526.1353 | 1558.6142 | 2937.3748 |
| 2987.9828 | 3014.7651 | 3018.4137 |
| 3021.0814 | 3027.0921 | 3039.8610 |
| 3046.9988 | 3058.4991 | 3065.1738 |
| 3076.5576 | 3088.5319 | 3108.0552 |
| 3110.9225 | 3113.4105 | 3804.1070 |

Zero-point correction (Hartree): 0.237618

C8H17O.1-5Hshift.4oh.tttS.m

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -465.46473244

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 1.438177 | -1.992344 | -0.238357 |
| C | 2.625735 | -1.517809 | 0.347594 |
| C | 2.945326 | -0.085213 | -0.102745 |
| C | 1.770005 | 0.833270 | 0.246398 |
| C | 0.479107 | 0.284061 | -0.353998 |
| C | -0.825987 | 0.578396 | 0.360487 |
| C | -2.051747 | -0.085958 | -0.280833 |
| C | -3.366168 | 0.236165 | 0.440675 |
| C | -4.584999 | -0.431425 | -0.203896 |
| H | 2.584187 | -1.560657 | 1.450633 |
| H | 3.433003 | -2.192579 | 0.024786 |
| H | 3.096547 | -0.060640 | -1.188112 |
| H | 3.862187 | 0.278119 | 0.373293 |
| O | 2.083229 | 2.135989 | -0.252911 |
| H | 1.665944 | 0.864343 | 1.344984 |
| H | 0.712544 | -0.967472 | -0.313042 |
| H | 0.441683 | 0.474779 | -1.432756 |
| H | -0.745298 | 0.271653 | 1.412478 |
| H | -0.983432 | 1.671838 | 0.381101 |
| H | -2.125592 | 0.227753 | -1.331489 |
| H | -1.899828 | -1.173532 | -0.297574 |
| H | -3.288733 | -0.078131 | 1.490408 |
| H | -3.512028 | 1.325124 | 0.460043 |
| H | -4.483366 | -1.522522 | -0.206408 |
| H | -4.709332 | -0.109623 | -1.244156 |
| H | -5.506707 | -0.184434 | 0.332824 |
| H | 1.339348 | 2.717897 | -0.048954 |

Rotational constants (GHz): 2.1720900 0.5276900 0.4446700

Vibrational harmonic frequencies (cm-1):

| | | |
|------------|-----------|-----------|
| 11491.4566 | 38.4611 | 65.5321 |
| 86.1882 | 103.0954 | 132.1956 |
| 173.0494 | 221.6655 | 252.8554 |
| 256.6954 | 284.1717 | 307.1126 |
| 384.2181 | 431.3457 | 457.8374 |
| 497.5964 | 524.9054 | 603.4201 |
| 735.7423 | 767.7943 | 848.8104 |
| 870.6896 | 895.1224 | 905.3706 |
| 943.9168 | 968.5980 | 1017.0324 |
| 1038.8196 | 1064.4726 | 1066.1741 |
| 1075.7670 | 1088.6639 | 1102.9439 |
| 1140.5236 | 1163.2469 | 1206.9070 |
| 1218.0462 | 1226.4944 | 1244.6667 |
| 1263.2747 | 1283.8613 | 1311.8637 |
| 1329.8128 | 1337.7894 | 1339.7302 |
| 1375.8368 | 1387.3473 | 1408.7935 |
| 1412.8847 | 1417.0306 | 1428.3116 |
| 1481.8225 | 1496.5443 | 1500.5233 |
| 1510.4216 | 1510.4785 | 1513.8694 |
| 1524.3645 | 1543.0475 | 2956.3934 |
| 2960.4356 | 2969.1104 | 3019.7115 |
| 3020.8229 | 3026.6458 | 3040.3753 |
| 3041.6553 | 3049.1037 | 3061.0995 |
| 3073.5676 | 3085.0000 | 3109.2269 |
| 3111.0724 | 3114.3085 | 3811.7151 |

Zero-point correction (Hartree): 0.237472

C8H17O.1-5Hshift.4oh.tttS.p

```

-----
E(UB+HF-LYP/6-31G(d,p)) (Hartree): -465.46460530
Electronic state : 2-A
Cartesian coordinates (Angs):
O      1.487541      -1.994460      -0.233945
C      2.666828      -1.493321       0.343381
C      2.945511      -0.054280      -0.115972
C      1.744480       0.839024       0.240951
C      0.470554       0.255251      -0.348282
C     -0.830183       0.538488       0.372786
C     -2.061991      -0.101209      -0.279682
C     -3.371958       0.226220       0.447722
C     -4.601086      -0.409540      -0.209265
H      2.633281      -1.530373       1.447107
H      3.487772      -2.150597       0.019534
H      3.088430      -0.030940      -1.202597
H      3.863006       0.323921       0.354179
O      1.883355       2.166003      -0.271134
H      1.645547       0.865529       1.340216
H      0.736741      -0.997098      -0.303137
H      0.424832       0.440602      -1.427150
H     -0.751385       0.212374       1.419309
H     -0.957670       1.633367       0.407655
H     -2.132735       0.232740      -1.324349
H     -1.926717      -1.190849      -0.316237
H     -3.299598      -0.109408       1.491292
H     -3.500294       1.316611       0.488224
H     -4.516707      -1.501948      -0.233580
H     -4.720324      -0.065319      -1.242967
H     -5.519097      -0.158888       0.332276
H      2.704828       2.534133       0.081018
Rotational constants (GHz):      2.1786200      0.5270800      0.4447300
Vibrational harmonic frequencies (cm-1):
i1508.6626          39.5542          65.8935
      86.8749          102.9710         133.6729
      173.3430         218.5019         251.9384
      257.8035         274.7355         295.5930
      387.7663         432.4508         455.3999
      496.0626         522.4596         604.1559
      735.3976         767.0752         851.3562
      869.6356         896.0872         906.7287
      945.6630         965.6616        1018.3744
     1049.5452        1062.6251        1067.8087
     1072.5906        1093.3457        1102.0660
     1143.5056        1162.9389        1212.0639
     1214.5560        1217.6447        1235.9594
     1258.9669        1283.4756        1315.9726
     1326.7597        1334.9380        1339.2459
     1380.8329        1385.9512        1391.6619
     1415.1304        1427.7530        1443.4880
     1481.9976        1494.6630        1500.7939
     1510.6198        1511.0439        1513.5587
     1524.4651        1548.3812        2954.7623
     2967.1608        2988.7824        3018.8091
     3021.4141        3026.6245        3038.7261
     3039.9968        3040.1151        3048.6670
     3071.9403        3089.7356        3095.2783
     3108.1955        3112.9152        3804.1520
Zero-point correction (Hartree): 0.237401
    
```

C8H17O.1-5Hshift.4oh.tttS.t

```

-----
E(UB+HF-LYP/6-31G(d,p)) (Hartree): -465.46529473
Electronic state : 2-A
Cartesian coordinates (Angs):
O      1.542733      -1.992651      -0.238396
C      2.711666      -1.464551       0.339804
C      2.957301      -0.016356      -0.110415
C      1.736935       0.845156       0.248828
C      0.468804       0.230217      -0.334405
C     -0.837312       0.519691       0.375404
C     -2.068677      -0.117653      -0.280127
C     -3.379417       0.211993       0.445084
C     -4.608717      -0.421023      -0.214154
H      2.680271      -1.506572       1.443068
H      3.545253      -2.103920       0.012783
H      3.105247       0.001197      -1.199388
H      3.859003       0.391969       0.358240
O      1.892707       2.213918      -0.135270
H      1.643917       0.879145       1.341846
H      0.754829      -1.013126      -0.276538
H      0.413496       0.382139      -1.420835
H     -0.763818       0.195885       1.422910
H     -0.960058       1.614929       0.409027
H     -2.137546       0.216696      -1.325079
    
```

| | | | |
|--|-----------|-----------|-----------|
| H | -1.935773 | -1.207536 | -0.317308 |
| H | -3.309151 | -0.124469 | 1.488425 |
| H | -3.505505 | 1.302592 | 0.486340 |
| H | -4.526457 | -1.513567 | -0.238977 |
| H | -4.726204 | -0.075911 | -1.247796 |
| H | -5.526849 | -0.168951 | 0.326416 |
| H | 2.022334 | 2.234537 | -1.093914 |
| Rotational constants (GHz): | 2.1731900 | 0.5234700 | 0.4421200 |
| Vibrational harmonic frequencies (cm-1): | | | |
| i1510.7865 | 40.6067 | | 67.4164 |
| 86.0505 | 105.1768 | | 134.2692 |
| 176.0461 | 217.9494 | | 251.5762 |
| 256.6070 | 275.5764 | | 306.6220 |
| 389.2993 | 431.6137 | | 460.3300 |
| 490.4077 | 520.5952 | | 597.2226 |
| 735.5392 | 767.9052 | | 850.7870 |
| 867.7492 | 894.0290 | | 906.8533 |
| 938.7854 | 967.7347 | | 1018.0685 |
| 1043.1386 | 1064.9850 | | 1065.7339 |
| 1078.5777 | 1097.7927 | | 1110.4646 |
| 1137.3038 | 1144.0057 | | 1208.8063 |
| 1219.2537 | 1227.7217 | | 1242.3516 |
| 1256.6431 | 1291.0158 | | 1312.7428 |
| 1326.3125 | 1337.7818 | | 1358.6800 |
| 1375.8480 | 1389.5748 | | 1401.9015 |
| 1415.4963 | 1427.9162 | | 1428.2987 |
| 1483.0220 | 1492.6599 | | 1500.6896 |
| 1510.4520 | 1510.6217 | | 1513.5798 |
| 1524.4131 | 1544.4847 | | 2960.5201 |
| 2991.0672 | 3017.6050 | | 3020.5561 |
| 3026.3894 | 3034.6169 | | 3038.8278 |
| 3039.9628 | 3045.9387 | | 3049.8734 |
| 3061.8475 | 3072.5658 | | 3101.2098 |
| 3108.0780 | 3113.4562 | | 3793.0158 |
| Zero-point correction (Hartree): | 0.237550 | | |

C8H17O.5oh.pmpptttt.m

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -465.48594440

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|--|-----------|-----------|-----------|
| O | -3.175786 | -1.497188 | 0.174953 |
| C | -3.641456 | -0.248209 | -0.152505 |
| C | -2.850723 | 0.950318 | 0.402640 |
| C | -1.452500 | 1.219396 | -0.182183 |
| C | -0.338102 | 0.227578 | 0.200648 |
| O | -0.499289 | -1.028915 | -0.442256 |
| H | -1.317809 | -1.428957 | -0.103709 |
| H | -3.596421 | -0.237770 | -1.265366 |
| H | -4.716342 | -0.165491 | 0.088082 |
| H | -3.479937 | 1.833006 | 0.228267 |
| H | -2.787024 | 0.835033 | 1.492868 |
| H | -1.507551 | 1.261697 | -1.278589 |
| H | -1.149968 | 2.219548 | 0.154435 |
| C | 1.043009 | 0.758148 | -0.197506 |
| H | -0.354201 | 0.100887 | 1.299894 |
| C | 2.195507 | -0.162331 | 0.219510 |
| C | 3.571656 | 0.353063 | -0.219429 |
| C | 4.721840 | -0.567663 | 0.200906 |
| H | 1.055543 | 0.892544 | -1.288083 |
| H | 1.182923 | 1.753025 | 0.246417 |
| H | 2.185813 | -0.282605 | 1.312938 |
| H | 2.017730 | -1.158435 | -0.200435 |
| H | 3.580677 | 0.473457 | -1.311485 |
| H | 3.736795 | 1.357074 | 0.196358 |
| H | 4.602954 | -1.569019 | -0.228241 |
| H | 4.761338 | -0.679908 | 1.290618 |
| H | 5.690691 | -0.177060 | -0.128040 |
| Rotational constants (GHz): | 3.5738900 | 0.4436600 | 0.4094700 |
| Vibrational harmonic frequencies (cm-1): | | | |
| 45.8057 | 52.7870 | | 69.4230 |
| 91.1556 | 109.7870 | | 147.5550 |
| 191.1728 | 229.5059 | | 244.3244 |
| 266.1093 | 314.4545 | | 334.6051 |
| 435.6965 | 460.8387 | | 482.3414 |
| 536.1331 | 552.6381 | | 741.9011 |
| 778.1336 | 789.5333 | | 801.4069 |
| 890.4539 | 898.8474 | | 914.1162 |
| 935.3840 | 993.6535 | | 1022.6514 |
| 1041.6490 | 1051.0978 | | 1072.1623 |
| 1085.3851 | 1102.3180 | | 1116.4678 |
| 1148.7376 | 1171.7476 | | 1212.5075 |
| 1237.9171 | 1250.3804 | | 1280.2762 |
| 1312.6532 | 1318.0475 | | 1334.8509 |
| 1340.3026 | 1359.1696 | | 1383.4340 |

| | | |
|-----------|-----------|-----------|
| 1388.8374 | 1401.0574 | 1406.0482 |
| 1416.1297 | 1426.4739 | 1466.0857 |
| 1481.5773 | 1488.7458 | 1492.2083 |
| 1502.8116 | 1512.2801 | 1513.7175 |
| 1526.2244 | 2876.1918 | 2934.9890 |
| 2971.2143 | 3015.0025 | 3018.0180 |
| 3023.6365 | 3029.7243 | 3033.9832 |
| 3037.8812 | 3050.1697 | 3060.5238 |
| 3070.5324 | 3076.9234 | 3094.4073 |
| 3106.7585 | 3110.0801 | 3695.9664 |

Zero-point correction (Hartree): 0.242346

C8H17O.5oh.pttttt.m

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -465.48175755

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 4.231418 | -0.740963 | -0.917543 |
| C | 4.017635 | -0.246842 | 0.342153 |
| C | 2.692202 | 0.496856 | 0.546073 |
| C | 1.471081 | -0.363374 | 0.208855 |
| C | 0.144083 | 0.390903 | 0.303223 |
| C | -1.060159 | -0.523064 | 0.031953 |
| C | -2.417197 | 0.186662 | 0.119574 |
| C | -3.611724 | -0.751555 | -0.098179 |
| C | -4.964111 | -0.036073 | -0.023704 |
| H | 4.059041 | -1.145736 | 0.998666 |
| H | 4.885445 | 0.357969 | 0.670480 |
| H | 2.644907 | 0.841403 | 1.588754 |
| H | 2.684595 | 1.392007 | -0.084123 |
| H | 1.583987 | -0.752009 | -0.809878 |
| H | 1.426648 | -1.231751 | 0.880425 |
| H | 0.045466 | 0.803817 | 1.324077 |
| O | 0.214744 | 1.462466 | -0.641662 |
| H | -0.940296 | -0.966529 | -0.965303 |
| H | -1.038258 | -1.351353 | 0.753643 |
| H | -2.515807 | 0.672937 | 1.101870 |
| H | -2.460544 | 0.988886 | -0.631116 |
| H | -3.509140 | -1.243238 | -1.074735 |
| H | -3.578978 | -1.554525 | 0.650569 |
| H | -5.039752 | 0.749218 | -0.784657 |
| H | -5.109476 | 0.437304 | 0.954192 |
| H | -5.794155 | -0.732197 | -0.182041 |
| H | -0.543833 | 2.040697 | -0.496875 |

Rotational constants (GHz): 4.1534100 0.3730500 0.3621900

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 36.2216 | 49.8107 | 69.4735 |
| 80.1202 | 105.5969 | 141.8839 |
| 152.6378 | 191.1640 | 247.6620 |
| 258.2823 | 287.2989 | 309.0055 |
| 311.6512 | 437.9951 | 454.8940 |
| 511.2786 | 554.9729 | 597.0406 |
| 740.9122 | 783.5407 | 799.3535 |
| 879.1846 | 899.4122 | 919.5634 |
| 940.6552 | 986.4253 | 1022.1367 |
| 1036.8816 | 1050.9214 | 1070.2179 |
| 1084.5884 | 1097.9667 | 1124.3421 |
| 1144.0603 | 1174.5133 | 1207.8120 |
| 1247.3817 | 1265.5245 | 1288.2495 |
| 1299.8788 | 1317.4480 | 1334.9484 |
| 1342.2477 | 1345.3666 | 1368.9170 |
| 1369.9746 | 1399.4892 | 1408.6762 |
| 1419.1440 | 1427.5286 | 1441.7785 |
| 1484.5017 | 1494.1928 | 1500.2474 |
| 1507.2748 | 1511.3424 | 1513.6907 |
| 1523.8756 | 2873.4195 | 2938.0319 |
| 2947.9536 | 3004.3446 | 3022.6573 |
| 3028.6461 | 3032.1335 | 3034.6251 |
| 3036.0292 | 3038.9145 | 3061.7009 |
| 3076.1951 | 3088.5615 | 3106.4997 |
| 3107.5395 | 3113.4958 | 3835.0976 |

Zero-point correction (Hartree): 0.241297

C8H17O.5oh.pttttt.p

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -465.48111433

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 4.252811 | -0.821483 | -0.849788 |
| C | 4.012447 | -0.244504 | 0.368316 |
| C | 2.692850 | 0.528745 | 0.484739 |
| C | 1.465037 | -0.346547 | 0.213741 |
| C | 0.128448 | 0.408498 | 0.277558 |
| C | -1.063483 | -0.510263 | 0.003557 |
| C | -2.423870 | 0.175448 | 0.174840 |

| | | | |
|--|-----------|-----------|-----------|
| C | -3.609924 | -0.741900 | -0.147052 |
| C | -4.967530 | -0.053098 | 0.025141 |
| H | 4.037810 | -1.082538 | 1.099567 |
| H | 4.881889 | 0.377920 | 0.659369 |
| H | 2.637159 | 0.974994 | 1.488152 |
| H | 2.726261 | 1.356993 | -0.234845 |
| H | 1.570204 | -0.801866 | -0.777784 |
| H | 1.437121 | -1.167344 | 0.944402 |
| H | 0.014684 | 0.837600 | 1.289652 |
| O | 0.071919 | 1.455129 | -0.696741 |
| H | -0.966992 | -0.892537 | -1.021580 |
| H | -0.996152 | -1.379076 | 0.671969 |
| H | -2.519043 | 0.540745 | 1.208185 |
| H | -2.454216 | 1.061976 | -0.468919 |
| H | -3.513720 | -1.107574 | -1.178448 |
| H | -3.567793 | -1.633174 | 0.494644 |
| H | -5.052616 | 0.820938 | -0.630549 |
| H | -5.108278 | 0.293696 | 1.055471 |
| H | -5.794623 | -0.730030 | -0.213269 |
| H | 0.666618 | 2.161832 | -0.418826 |
| Rotational constants (GHz): | 4.1220100 | 0.3726500 | 0.3609800 |
| Vibrational harmonic frequencies (cm-1): | | | |
| 45.6092 | 49.1937 | | 68.4746 |
| 82.9903 | 108.5683 | | 135.2701 |
| 156.6674 | 192.8357 | | 248.5676 |
| 254.9324 | 270.1473 | | 307.3961 |
| 315.6950 | 427.8413 | | 439.6648 |
| 459.7837 | 510.0874 | | 582.6945 |
| 741.3386 | 782.3374 | | 798.9923 |
| 878.1014 | 899.5436 | | 915.4822 |
| 930.6141 | 983.6596 | | 1022.3200 |
| 1036.3457 | 1060.6216 | | 1073.1724 |
| 1080.7236 | 1095.8125 | | 1121.8105 |
| 1146.4178 | 1173.8934 | | 1213.0093 |
| 1235.0146 | 1274.0551 | | 1290.0019 |
| 1303.7261 | 1320.4821 | | 1333.1156 |
| 1340.7377 | 1355.0773 | | 1361.1311 |
| 1380.1707 | 1399.2729 | | 1409.4269 |
| 1417.0792 | 1427.3452 | | 1440.4765 |
| 1484.3583 | 1492.4070 | | 1502.8498 |
| 1503.7734 | 1512.9665 | | 1513.9811 |
| 1526.6095 | 2887.0922 | | 2932.4596 |
| 2953.1002 | 3014.9440 | | 3020.7961 |
| 3021.8366 | 3024.7576 | | 3032.5859 |
| 3038.3947 | 3051.8247 | | 3065.4752 |
| 3066.9354 | 3089.3568 | | 3094.3725 |
| 3106.8639 | 3111.4846 | | 3837.4028 |
| Zero-point correction (Hartree): | 0.240994 | | |

C8H17O.5oh.pttttt.t

```

-----
E(UB+HF-LYP/6-31G(d,p)) (Hartree): -465.48307041
Electronic state : 2-A
Cartesian coordinates (Angs):
O      -4.189775    -0.690225    0.964780
C      -4.017727    -0.230280   -0.314589
C      -2.690906     0.490511   -0.580238
C      -1.470452    -0.385843   -0.284920
C      -0.140520     0.380521   -0.319917
C       1.065806    -0.536191   -0.071990
C       2.416403     0.180955   -0.178622
C       3.613593    -0.716546   -0.157159
C       4.959367     0.005881    0.038374
H      -4.098645    -1.140585   -0.950696
H      -4.889979     0.379856   -0.620151
H      -2.677387     0.830063   -1.624869
H      -2.644069     1.390355    0.042498
H      -1.597353    -0.838839    0.708604
H      -1.422668    -1.219208   -0.999658
H      -0.027660     0.854054   -1.304868
O      -0.154965     1.482368    0.593836
H       0.961958    -0.986163    0.928081
H       1.029390    -1.372612   -0.783582
H       2.534070     0.577308   -1.197495
H       2.406403     1.053718    0.485298
H       3.497650    -1.108230    1.177230
H       3.609650    -1.593947   -0.504529
H       5.006728     0.867702    0.713803
H       5.120839     0.377400   -0.980049
H       5.794300    -0.657785   -0.286267
H      -0.258703     1.115722    1.483643
Rotational constants (GHz): 4.1463200 0.3737400 0.3647900
Vibrational harmonic frequencies (cm-1):
42.8601 52.7489 74.6289
82.0054 113.1132 146.3981

```

| | | |
|-----------|-----------|-----------|
| 169.4285 | 187.8546 | 248.5728 |
| 260.9727 | 307.4293 | 310.8389 |
| 342.4088 | 435.0699 | 460.9814 |
| 507.9798 | 550.0113 | 602.2593 |
| 740.8488 | 782.7499 | 798.7086 |
| 876.5399 | 900.8807 | 915.6029 |
| 935.3039 | 981.6787 | 1024.5084 |
| 1031.0287 | 1065.4235 | 1074.5103 |
| 1084.1830 | 1096.3180 | 1115.5758 |
| 1147.9075 | 1154.5049 | 1201.5211 |
| 1235.5942 | 1267.9993 | 1296.0279 |
| 1297.4193 | 1315.6915 | 1332.3363 |
| 1342.4435 | 1364.4542 | 1369.7166 |
| 1373.5580 | 1395.4377 | 1414.6862 |
| 1416.0041 | 1427.5433 | 1428.9373 |
| 1489.4309 | 1498.0671 | 1502.2374 |
| 1510.4366 | 1513.1584 | 1514.3947 |
| 1526.6754 | 2877.1580 | 2939.8109 |
| 3001.1669 | 3018.2465 | 3019.7216 |
| 3025.7722 | 3035.8700 | 3038.7589 |
| 3039.4978 | 3047.9838 | 3049.5263 |
| 3065.4923 | 3083.7865 | 3100.1717 |
| 3107.6415 | 3112.2157 | 3786.6197 |

Zero-point correction (Hartree): 0.241497

C8H17O.1-5Hshift.5oh.ttt.m

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -465.47500559

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 1.865334 | 1.643344 | 0.171858 |
| C | 2.963712 | 1.063118 | -0.473832 |
| C | 3.086092 | -0.438934 | -0.147193 |
| C | 1.769476 | -1.147527 | -0.497626 |
| C | 0.569032 | -0.455070 | 0.158381 |
| C | -0.791567 | -0.741801 | -0.451759 |
| C | -1.925320 | 0.130048 | 0.104041 |
| C | -3.294956 | -0.215380 | -0.492898 |
| C | -4.425961 | 0.660212 | 0.055857 |
| H | 2.922282 | 1.200052 | -1.569814 |
| H | 3.863442 | 1.588654 | -0.114734 |
| H | 3.309352 | -0.559938 | 0.920753 |
| H | 3.924506 | -0.877472 | -0.700141 |
| H | 1.791782 | -2.197766 | -0.177810 |
| H | 1.631011 | -1.137161 | -1.585870 |
| H | 0.897995 | 0.731387 | -0.000146 |
| O | 0.512143 | -0.619543 | 1.548752 |
| H | -0.718018 | -0.618261 | -1.539324 |
| H | -1.023748 | -1.804022 | -0.274370 |
| H | -1.954512 | 0.019669 | 1.193763 |
| H | -1.696531 | 1.186541 | -0.093062 |
| H | -3.252778 | -0.115477 | -1.586449 |
| H | -3.520807 | -1.272158 | -0.294197 |
| H | -4.246220 | 1.719696 | -0.159361 |
| H | -4.514562 | 0.555759 | 1.143146 |
| H | -5.391519 | 0.390442 | -0.384476 |
| H | 1.255464 | -0.128359 | 1.927383 |

Rotational constants (GHz): 2.7070500 0.5238500 0.4982900

Vibrational harmonic frequencies (cm-1):

| | | |
|------------|-----------|-----------|
| i1129.4227 | 47.4251 | 53.1082 |
| 90.6000 | 102.9343 | 130.0580 |
| 165.0021 | 235.8644 | 243.9099 |
| 286.2787 | 299.5350 | 322.1837 |
| 383.0107 | 434.6321 | 461.5713 |
| 515.7842 | 539.4712 | 611.5429 |
| 738.7127 | 793.7608 | 815.4923 |
| 862.5642 | 903.2786 | 907.9334 |
| 921.6517 | 970.2344 | 1004.6056 |
| 1023.1134 | 1052.5737 | 1064.9613 |
| 1073.3289 | 1089.1860 | 1110.1028 |
| 1140.2110 | 1183.0149 | 1201.7260 |
| 1227.5952 | 1247.6770 | 1269.8343 |
| 1285.3265 | 1315.3014 | 1329.4372 |
| 1337.2089 | 1353.6693 | 1369.8395 |
| 1382.7096 | 1391.2558 | 1402.0481 |
| 1414.0099 | 1427.3451 | 1475.4118 |
| 1483.7220 | 1497.0060 | 1502.1214 |
| 1503.3015 | 1511.8912 | 1512.6876 |
| 1525.6880 | 1608.8546 | 2951.3454 |
| 3001.4562 | 3003.6457 | 3019.9218 |
| 3032.0976 | 3033.6288 | 3039.8209 |
| 3043.7357 | 3051.1150 | 3064.2042 |
| 3080.4555 | 3093.2631 | 3095.3059 |
| 3108.6560 | 3112.3767 | 3792.0324 |

Zero-point correction (Hartree): 0.238470

C8H17O.1-5Hshift.5oh.ttt.p

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -465.47435131

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 1.804622 | 1.639708 | 0.477566 |
| C | 2.930396 | 1.200002 | -0.225856 |
| C | 3.088053 | -0.331980 | -0.163458 |
| C | 1.810661 | -0.995772 | -0.701881 |
| C | 0.598481 | -0.528510 | 0.094730 |
| C | -0.740089 | -0.520712 | -0.643259 |
| C | -1.920000 | 0.014376 | 0.179487 |
| C | -3.233930 | 0.064294 | -0.611801 |
| C | -4.415814 | 0.577673 | 0.216375 |
| H | 2.910782 | 1.520070 | -1.284968 |
| H | 3.812724 | 1.669643 | 0.240696 |
| H | 3.243306 | -0.638509 | 0.876428 |
| H | 3.966352 | -0.639027 | -0.742939 |
| H | 1.880533 | -2.089298 | -0.639811 |
| H | 1.672640 | -0.730642 | -1.757270 |
| H | 0.918345 | 0.639089 | 0.317733 |
| O | 0.580058 | -1.213745 | 1.317465 |
| H | -0.624270 | 0.085608 | -1.549786 |
| H | -0.957701 | -1.547978 | -0.974393 |
| H | -2.073919 | -0.619195 | 1.065630 |
| H | -1.680159 | 1.021078 | 0.549588 |
| H | -3.096759 | 0.704330 | -1.493471 |
| H | -3.461984 | -0.938981 | -0.996180 |
| H | -4.229718 | 1.592198 | 0.586504 |
| H | -4.598481 | -0.063245 | 1.086526 |
| H | -5.336260 | 0.603509 | -0.375642 |
| H | -0.129416 | -0.852573 | 1.865090 |

Rotational constants (GHz): 2.5718700 0.5306900 0.4995400

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| i961.4888 | 39.6673 | 58.8165 |
| 90.8956 | 112.1663 | 136.5957 |
| 145.1976 | 241.9884 | 262.7602 |
| 280.8665 | 299.9286 | 315.9458 |
| 381.5559 | 427.3645 | 479.3065 |
| 507.1844 | 537.4211 | 642.8882 |
| 742.9827 | 794.6151 | 827.3571 |
| 860.4870 | 901.5411 | 909.9230 |
| 931.5734 | 974.1072 | 1002.4251 |
| 1023.8899 | 1056.2619 | 1061.2198 |
| 1075.3246 | 1087.3845 | 1124.8893 |
| 1139.5950 | 1182.2307 | 1191.4708 |
| 1220.5913 | 1244.8945 | 1259.1969 |
| 1277.5668 | 1296.1394 | 1315.8314 |
| 1334.9710 | 1345.0308 | 1358.5581 |
| 1375.1546 | 1386.5140 | 1390.4651 |
| 1416.0464 | 1426.4676 | 1476.5787 |
| 1482.3181 | 1492.2085 | 1500.8343 |
| 1509.3059 | 1510.7396 | 1512.6565 |
| 1524.0142 | 1626.1178 | 2935.6133 |
| 2990.0929 | 3005.3507 | 3007.6179 |
| 3028.7995 | 3037.6977 | 3040.2324 |
| 3044.3263 | 3058.0168 | 3064.5823 |
| 3077.9168 | 3085.5350 | 3108.5974 |
| 3110.0967 | 3115.2869 | 3816.0691 |

Zero-point correction (Hartree): 0.238424

C8H17O.1-5Hshift.5oh.ttt.t

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -465.47435131

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 1.804615 | 1.639702 | 0.477573 |
| C | 2.930393 | 1.200006 | -0.225851 |
| C | 3.088056 | -0.331976 | -0.163463 |
| C | 1.810663 | -0.995771 | -0.701882 |
| C | 0.598483 | -0.528512 | 0.094731 |
| C | -0.740085 | -0.520700 | -0.643262 |
| C | -1.920000 | 0.014375 | 0.179488 |
| C | -3.233930 | 0.064289 | -0.611799 |
| C | -4.415813 | 0.577674 | 0.216374 |
| H | 2.910780 | 1.520080 | -1.284960 |
| H | 3.812719 | 1.669646 | 0.240705 |
| H | 3.243317 | -0.638511 | 0.876420 |
| H | 3.966352 | -0.639017 | -0.742952 |
| H | 1.880538 | -2.089297 | -0.639811 |
| H | 1.672639 | -0.730643 | -1.757271 |
| H | 0.918352 | 0.639086 | 0.317739 |
| O | 0.580055 | -1.213752 | 1.317461 |
| H | -0.624262 | 0.085637 | -1.549777 |

| | | | | |
|--|-----------|-----------|-----------|--|
| H | -0.957696 | -1.547960 | -0.974416 | |
| H | -2.073916 | -0.619203 | 1.065627 | |
| H | -1.680164 | 1.021076 | 0.549596 | |
| H | -3.096758 | 0.704321 | -1.493473 | |
| H | -3.461984 | -0.938988 | -0.996173 | |
| H | -4.229718 | 1.592204 | 0.586491 | |
| H | -4.598477 | -0.063235 | 1.086531 | |
| H | -5.336260 | 0.603501 | -0.375643 | |
| H | -0.129438 | -0.852602 | 1.865076 | |
| Rotational constants (GHz): | 2.5718700 | 0.5306900 | 0.4995400 | |
| Vibrational harmonic frequencies (cm-1): | | | | |
| i961.5209 | 39.6656 | | 58.8161 | |
| 90.8946 | 112.1651 | | 136.5954 | |
| 145.1971 | 241.9887 | | 262.7604 | |
| 280.8656 | 299.9278 | | 315.9451 | |
| 381.5574 | 427.3638 | | 479.3038 | |
| 507.1843 | 537.4223 | | 642.8856 | |
| 742.9821 | 794.6144 | | 827.3571 | |
| 860.4870 | 901.5413 | | 909.9228 | |
| 931.5731 | 974.1072 | | 1002.4254 | |
| 1023.8906 | 1056.2624 | | 1061.2196 | |
| 1075.3245 | 1087.3853 | | 1124.8890 | |
| 1139.5951 | 1182.2312 | | 1191.4713 | |
| 1220.5908 | 1244.8950 | | 1259.1971 | |
| 1277.5673 | 1296.1387 | | 1315.8308 | |
| 1334.9706 | 1345.0309 | | 1358.5583 | |
| 1375.1547 | 1386.5142 | | 1390.4653 | |
| 1416.0471 | 1426.4678 | | 1476.5788 | |
| 1482.3180 | 1492.2086 | | 1500.8340 | |
| 1509.3072 | 1510.7392 | | 1512.6565 | |
| 1524.0141 | 1626.1120 | | 2935.6124 | |
| 2990.0941 | 3005.3494 | | 3007.6168 | |
| 3028.7994 | 3037.6976 | | 3040.2323 | |
| 3044.3267 | 3058.0165 | | 3064.5823 | |
| 3077.9167 | 3085.5347 | | 3108.5971 | |
| 3110.0961 | 3115.2870 | | 3816.0682 | |
| Zero-point correction (Hartree): | 0.238424 | | | |

C8H17O.1-6Hshift.5oh.ttr.m

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -465.46601515

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | | |
|--|-----------|-----------|-----------|--|
| O | -0.667933 | 1.755816 | -0.489223 | |
| C | -1.992969 | 1.719256 | -0.021963 | |
| C | -2.701255 | 0.373612 | -0.233146 | |
| C | -2.208273 | -0.774580 | 0.666156 | |
| C | -0.798670 | -1.305255 | 0.353741 | |
| C | 0.295952 | -0.274856 | 0.612280 | |
| C | 1.676188 | -0.550943 | 0.043590 | |
| C | 2.701592 | 0.546000 | 0.363847 | |
| C | 4.081551 | 0.270963 | -0.240380 | |
| H | -2.063544 | 2.018573 | 1.040319 | |
| H | -2.515986 | 2.495694 | -0.602062 | |
| H | -2.600202 | 0.081958 | -1.283377 | |
| H | -3.770953 | 0.522109 | -0.036527 | |
| H | -2.899104 | -1.619225 | 0.567187 | |
| H | -2.236352 | -0.463863 | 1.719553 | |
| O | -0.826843 | -1.765591 | -0.994150 | |
| H | -0.608759 | -2.160623 | 1.031595 | |
| H | -0.089835 | 0.784404 | 0.043368 | |
| H | 0.325030 | 0.004874 | 1.672571 | |
| H | 2.044197 | -1.516516 | 0.434159 | |
| H | 1.601720 | -0.665547 | -1.046121 | |
| H | 2.318130 | 1.505329 | -0.004100 | |
| H | 2.789851 | 0.648260 | 1.453678 | |
| H | 4.028531 | 0.198964 | -1.332638 | |
| H | 4.500607 | -0.670610 | 0.133446 | |
| H | 4.788906 | 1.069471 | 0.005002 | |
| H | 0.021273 | -2.180234 | -1.193823 | |
| Rotational constants (GHz): | 1.9853500 | 0.7037400 | 0.5802100 | |
| Vibrational harmonic frequencies (cm-1): | | | | |
| i1381.1577 | 55.7635 | | 76.8231 | |
| 86.3920 | 115.9717 | | 144.3870 | |
| 201.5151 | 246.5358 | | 255.8953 | |
| 274.8696 | 279.1663 | | 304.2766 | |
| 363.9008 | 440.1295 | | 459.5826 | |
| 512.2784 | 581.7250 | | 623.4761 | |
| 746.5671 | 786.3307 | | 811.3342 | |
| 860.4934 | 867.4751 | | 909.4173 | |
| 924.4391 | 960.2200 | | 996.6066 | |
| 1019.6368 | 1048.0680 | | 1065.4818 | |
| 1082.9177 | 1093.6670 | | 1119.0109 | |
| 1136.6008 | 1159.6980 | | 1197.1512 | |

| | | |
|-----------|-----------|-----------|
| 1225.9350 | 1241.5339 | 1266.0004 |
| 1273.6418 | 1277.9836 | 1295.0516 |
| 1335.7703 | 1354.4129 | 1370.1689 |
| 1379.4409 | 1397.6627 | 1402.0009 |
| 1406.9057 | 1421.6394 | 1429.2882 |
| 1453.5180 | 1482.5442 | 1484.2337 |
| 1490.9468 | 1493.0068 | 1507.2458 |
| 1514.2953 | 1522.8332 | 2916.6853 |
| 2945.6683 | 2967.2841 | 3013.1097 |
| 3032.7671 | 3034.4193 | 3039.0515 |
| 3045.1953 | 3046.4821 | 3070.5178 |
| 3077.5796 | 3085.5483 | 3108.1111 |
| 3109.2588 | 3115.8925 | 3832.5126 |

Zero-point correction (Hartree): 0.237554

C8H17O.1-6Hshift.5oh.ttR.p

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -465.46617772

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -0.685112 | 1.755303 | -0.515046 |
| C | -1.992249 | 1.715887 | -0.005416 |
| C | -2.709089 | 0.372812 | -0.208852 |
| C | -2.199051 | -0.777618 | 0.676893 |
| C | -0.783209 | -1.297558 | 0.346825 |
| C | 0.301345 | -0.264774 | 0.594588 |
| C | 1.689872 | -0.564127 | 0.061068 |
| C | 2.700155 | 0.559222 | 0.330338 |
| C | 4.094896 | 0.251549 | -0.222611 |
| H | -2.030474 | 2.002666 | 1.062140 |
| H | -2.533910 | 2.498831 | -0.559154 |
| H | -2.618858 | 0.088877 | -1.263027 |
| H | -3.776271 | 0.520205 | 0.001248 |
| H | -2.894113 | -1.624758 | 0.588788 |
| H | -2.225565 | -0.478061 | 1.734012 |
| O | -0.684448 | -1.720473 | -1.011462 |
| H | -0.578058 | -2.155887 | 1.016022 |
| H | -0.080536 | 0.777325 | -0.000358 |
| H | 0.303006 | 0.046263 | 1.646183 |
| H | 2.049490 | -1.500098 | 0.522265 |
| H | 1.622910 | -0.767031 | -1.012949 |
| H | 2.323946 | 1.490569 | -0.110872 |
| H | 2.765466 | 0.738842 | 1.412339 |
| H | 4.065204 | 0.101855 | -1.307763 |
| H | 4.508861 | -0.659825 | 0.224602 |
| H | 4.794250 | 1.068901 | -0.018786 |
| H | -1.354891 | -2.399672 | -1.159626 |

Rotational constants (GHz): 1.9976800 0.7030000 0.5808100

Vibrational harmonic frequencies (cm-1):

| | | |
|------------|-----------|-----------|
| 11349.2057 | 55.9271 | 74.1948 |
| 85.9978 | 110.3143 | 147.3544 |
| 208.2278 | 247.4677 | 256.9229 |
| 273.2077 | 288.5134 | 302.2945 |
| 364.3454 | 439.9621 | 461.8773 |
| 506.3406 | 582.7436 | 625.4938 |
| 740.3836 | 789.3609 | 811.3969 |
| 864.4664 | 865.4182 | 908.8821 |
| 918.6303 | 968.8112 | 995.8110 |
| 1019.8663 | 1047.9507 | 1065.2662 |
| 1085.1695 | 1101.4570 | 1118.3439 |
| 1125.5843 | 1161.8493 | 1212.1246 |
| 1226.8919 | 1238.5118 | 1240.7769 |
| 1270.4715 | 1288.2283 | 1293.4424 |
| 1332.2884 | 1339.7891 | 1369.9596 |
| 1382.4941 | 1402.0905 | 1402.9398 |
| 1413.2870 | 1427.1605 | 1431.0605 |
| 1460.1682 | 1480.7040 | 1484.0570 |
| 1486.4547 | 1496.4664 | 1506.7439 |
| 1513.6095 | 1522.7865 | 2919.9287 |
| 2944.0922 | 2979.6927 | 3012.2946 |
| 3016.8727 | 3027.6783 | 3038.5373 |
| 3043.6948 | 3054.6113 | 3067.2087 |
| 3071.8962 | 3094.9834 | 3099.2157 |
| 3107.8739 | 3113.6432 | 3818.1086 |

Zero-point correction (Hartree): 0.237505

C8H17O.1-6Hshift.5oh.ttR.t

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -465.47121105

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|----------|-----------|-----------|
| O | 0.790599 | 1.531123 | 0.647366 |
| C | 2.009942 | 1.614356 | -0.063767 |
| C | 2.818778 | 0.312007 | -0.055068 |
| C | 2.144563 | -0.883943 | -0.751611 |

| | | | |
|---|-----------|-----------|-----------|
| C | 0.759496 | -1.273589 | -0.180159 |
| C | -0.340661 | -0.303687 | -0.602184 |
| C | -1.737575 | -0.570366 | -0.076010 |
| C | -2.741191 | 0.553164 | -0.368975 |
| C | -4.147869 | 0.246598 | 0.153806 |
| H | 1.843234 | 1.962602 | -1.096752 |
| H | 2.580207 | 2.406444 | 0.445363 |
| H | 3.034971 | 0.043094 | 0.985707 |
| H | 3.786554 | 0.501285 | -0.536664 |
| H | 2.807092 | -1.751168 | -0.654441 |
| H | 2.041898 | -0.685517 | -1.827502 |
| O | 0.796840 | -1.406373 | 1.237150 |
| H | 0.503822 | -2.275053 | -0.557517 |
| H | 0.047036 | 0.760153 | -0.052019 |
| H | -0.314558 | -0.069082 | -1.673449 |
| H | -2.099060 | -1.509750 | -0.528520 |
| H | -1.681675 | -0.762199 | 1.001390 |
| H | -2.375593 | 1.485540 | 0.079909 |
| H | -2.782387 | 0.731361 | -1.452233 |
| H | -4.141907 | 0.095929 | 1.239153 |
| H | -4.552553 | -0.663857 | -0.303186 |
| H | -4.841447 | 1.064908 | -0.064712 |
| H | 0.851966 | -0.499929 | 1.583152 |

Rotational constants (GHz): 2.2113000 0.6722900 0.5900400

Vibrational harmonic frequencies (cm-1):

| | | |
|------------|-----------|-----------|
| i1342.5501 | 59.5296 | 71.7602 |
| 95.4596 | 120.4806 | 151.5126 |
| 220.0008 | 248.1602 | 264.2385 |
| 280.0357 | 302.8869 | 346.2306 |
| 457.4629 | 466.6163 | 497.0243 |
| 565.3765 | 607.4709 | 679.4446 |
| 746.8815 | 798.8918 | 818.8479 |
| 861.7712 | 874.7084 | 905.9960 |
| 920.8708 | 959.5223 | 984.2183 |
| 1018.3828 | 1040.3669 | 1054.4314 |
| 1088.9179 | 1099.1770 | 1119.9013 |
| 1149.3871 | 1156.3567 | 1213.2647 |
| 1223.6421 | 1247.5680 | 1264.8118 |
| 1285.5902 | 1303.9293 | 1328.0615 |
| 1330.9219 | 1334.1025 | 1365.9284 |
| 1381.3042 | 1399.2078 | 1404.9362 |
| 1409.0240 | 1425.4137 | 1433.5669 |
| 1450.0491 | 1477.2125 | 1487.4677 |
| 1491.0245 | 1499.8292 | 1506.4610 |
| 1513.4211 | 1522.4959 | 2979.8743 |
| 2981.4272 | 3012.7793 | 3024.3351 |
| 3028.1548 | 3032.7697 | 3040.0070 |
| 3046.2009 | 3062.8467 | 3068.5123 |
| 3081.9373 | 3087.7579 | 3090.9804 |
| 3108.8501 | 3115.2076 | 3724.7199 |

Zero-point correction (Hartree): 0.238793

C8H17O.1-6Hshift.5oh.ttS.m

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -465.46749082

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 0.722181 | -1.933175 | -0.256075 |
| C | 2.028808 | -1.781931 | 0.236010 |
| C | 2.761935 | -0.548912 | -0.308998 |
| C | 2.222001 | 0.799172 | 0.200331 |
| C | 0.801208 | 1.169641 | -0.262170 |
| C | -0.274501 | 0.281663 | 0.336942 |
| C | -1.669880 | 0.409927 | -0.240891 |
| C | -2.692684 | -0.541235 | 0.394488 |
| C | -4.095380 | -0.394549 | -0.202901 |
| H | 2.056967 | -1.779240 | 1.340388 |
| H | 2.559834 | -2.690293 | -0.089101 |
| H | 2.719080 | -0.579052 | -1.405436 |
| H | 3.820716 | -0.627187 | -0.030202 |
| H | 2.899209 | 1.593832 | -0.143743 |
| H | 2.248554 | 0.828156 | 1.297992 |
| H | 0.753539 | 1.080159 | -1.361255 |
| O | 0.474018 | 2.507054 | 0.133597 |
| H | 0.109042 | -0.896623 | 0.069190 |
| H | -0.253154 | 0.314933 | 1.433164 |
| H | -1.995032 | 1.453234 | -0.106807 |
| H | -1.631046 | 0.241698 | -1.326370 |
| H | -2.344762 | -1.575043 | 0.274384 |
| H | -2.733012 | -0.355376 | 1.476248 |
| H | -4.092682 | -0.610626 | -1.277389 |
| H | -4.478086 | 0.624167 | -0.071990 |
| H | -4.804820 | -1.080313 | 0.271471 |
| H | 1.107014 | 3.103887 | -0.287589 |

Rotational constants (GHz): 1.7326800 0.7270300 0.5385100

Vibrational harmonic frequencies (cm-1):

| | | |
|------------|-----------|-----------|
| i1396.1871 | 53.2315 | 65.5485 |
| 80.1079 | 118.1683 | 144.9949 |
| 211.6885 | 224.9667 | 246.3947 |
| 247.0410 | 302.4058 | 312.1808 |
| 368.1345 | 412.3721 | 428.7091 |
| 498.3004 | 523.4206 | 632.0893 |
| 740.9239 | 803.5936 | 811.8907 |
| 860.4217 | 895.6236 | 912.3455 |
| 930.3975 | 959.0618 | 1005.4310 |
| 1044.7658 | 1053.3979 | 1083.9212 |
| 1088.5178 | 1089.5019 | 1101.3169 |
| 1126.1122 | 1157.3217 | 1203.3211 |
| 1229.2695 | 1234.8123 | 1252.9808 |
| 1266.6262 | 1281.4091 | 1299.5148 |
| 1332.1326 | 1350.7545 | 1357.4927 |
| 1381.3212 | 1396.0473 | 1404.1314 |
| 1408.3452 | 1425.3461 | 1434.7623 |
| 1458.0643 | 1482.0892 | 1484.4470 |
| 1486.9021 | 1499.2102 | 1506.4008 |
| 1512.9810 | 1522.3998 | 2959.6141 |
| 2970.6541 | 3007.0974 | 3014.7006 |
| 3017.4236 | 3031.2391 | 3037.8226 |
| 3038.9068 | 3043.8345 | 3061.4942 |
| 3069.8878 | 3075.9913 | 3080.6490 |
| 3107.8328 | 3113.6764 | 3803.5239 |

Zero-point correction (Hartree): 0.237338

C8H17O.1-6Hshift.5oh.ttS.p

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -465.46808907

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 0.675718 | -1.930326 | -0.236575 |
| C | 1.993483 | -1.800456 | 0.231584 |
| C | 2.740141 | -0.580260 | -0.325009 |
| C | 2.237301 | 0.779334 | 0.188827 |
| C | 0.827891 | 1.176577 | -0.264837 |
| C | -0.266417 | 0.314532 | 0.348346 |
| C | -1.667849 | 0.444975 | -0.222439 |
| C | -2.674700 | -0.542839 | 0.385237 |
| C | -4.081220 | -0.403446 | -0.204226 |
| H | 2.041046 | -1.799166 | 1.335360 |
| H | 2.502978 | -2.717778 | -0.103541 |
| H | 2.685580 | -0.611282 | -1.420818 |
| H | 3.800149 | -0.678557 | -0.057672 |
| H | 2.914076 | 1.568965 | -0.156498 |
| H | 2.269684 | 0.802215 | 1.286680 |
| H | 0.773906 | 1.089259 | -1.363277 |
| O | 0.662468 | 2.546761 | 0.124603 |
| H | 0.092977 | -0.868099 | 0.088288 |
| H | -0.242671 | 0.363518 | 1.443856 |
| H | -2.035270 | 1.471978 | -0.052906 |
| H | -1.631282 | 0.310290 | -1.312706 |
| H | -2.305392 | -1.564003 | 0.230829 |
| H | -2.713470 | -0.391885 | 1.472212 |
| H | -4.077579 | -0.583368 | -1.285288 |
| H | -4.485708 | 0.601701 | -0.037413 |
| H | -4.774554 | -1.119397 | 0.248484 |
| H | -0.171742 | 2.863623 | -0.244704 |

Rotational constants (GHz): 1.7128200 0.7318900 0.5389200

Vibrational harmonic frequencies (cm-1):

| | | |
|------------|-----------|-----------|
| i1368.9340 | 53.5036 | 67.9027 |
| 80.4639 | 114.3972 | 143.4556 |
| 212.0314 | 225.0149 | 246.5873 |
| 295.0040 | 299.5548 | 315.2636 |
| 366.6345 | 412.9008 | 431.9802 |
| 500.0917 | 524.6073 | 629.9068 |
| 744.5691 | 802.7476 | 811.9918 |
| 861.8152 | 895.1781 | 917.8806 |
| 932.1487 | 953.2565 | 1001.1477 |
| 1039.2808 | 1053.1932 | 1074.4080 |
| 1086.6687 | 1099.4299 | 1107.8089 |
| 1125.7533 | 1158.5099 | 1200.2981 |
| 1232.3784 | 1237.1282 | 1248.6952 |
| 1279.1539 | 1287.0885 | 1295.2685 |
| 1333.7675 | 1349.9543 | 1361.5461 |
| 1381.7171 | 1399.3150 | 1405.2596 |
| 1410.3889 | 1419.2863 | 1426.0983 |
| 1453.7660 | 1482.0352 | 1484.4965 |
| 1487.4724 | 1502.4829 | 1506.1285 |
| 1513.1090 | 1521.7781 | 2958.6741 |
| 2971.5712 | 2977.5691 | 3012.4569 |
| 3033.1442 | 3035.7907 | 3038.1400 |
| 3038.2646 | 3042.6108 | 3073.4291 |

3078.0702 3079.0979 3088.9863
3108.0072 3115.4217 3819.9809
Zero-point correction (Hartree): 0.237556

C8H17O.1-6Hshift.5oh.ttS.t

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -465.46882837

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 0.742847 | -1.943562 | -0.229347 |
| C | 2.051246 | -1.767879 | 0.246162 |
| C | 2.765513 | -0.533234 | -0.320393 |
| C | 2.221341 | 0.817532 | 0.179212 |
| C | 0.797072 | 1.175168 | -0.276130 |
| C | -0.275246 | 0.277640 | 0.323921 |
| C | -1.671548 | 0.391024 | -0.258449 |
| C | -2.697507 | -0.535711 | 0.407024 |
| C | -4.097133 | -0.412359 | -0.202758 |
| H | 2.092260 | -1.752528 | 1.350581 |
| H | 2.591384 | -2.673223 | -0.073471 |
| H | 2.709940 | -0.573561 | -1.415653 |
| H | 3.828253 | -0.598710 | -0.053643 |
| H | 2.878311 | 1.621942 | -0.171187 |
| H | 2.258442 | 0.840260 | 1.279999 |
| H | 0.746954 | 1.104206 | -1.369765 |
| O | 0.505960 | 2.551523 | 0.002641 |
| H | 0.119934 | -0.893927 | 0.074683 |
| H | -0.263645 | 0.313775 | 1.423137 |
| H | -1.996714 | 1.438721 | -0.166695 |
| H | -1.629520 | 0.183492 | -1.336793 |
| H | -2.348631 | -1.573104 | 0.327694 |
| H | -2.743899 | -0.310128 | 1.481264 |
| H | -4.088579 | -0.669993 | -1.267881 |
| H | -4.480484 | 0.610656 | -0.113861 |
| H | -4.809011 | -1.079292 | 0.294196 |
| H | 0.582115 | 2.674630 | 0.959498 |

Rotational constants (GHz): 1.7212700 0.7239800 0.5365800

Vibrational harmonic frequencies (cm-1):

| | | |
|------------|-----------|-----------|
| i1351.2227 | 53.5753 | 66.4817 |
| 79.7331 | 120.9323 | 145.3339 |
| 211.2785 | 222.7157 | 247.5228 |
| 297.6208 | 311.7118 | 319.1745 |
| 365.5970 | 412.7180 | 442.5831 |
| 497.7298 | 520.6784 | 630.7017 |
| 741.5105 | 803.5026 | 812.7407 |
| 860.9241 | 894.5379 | 913.5907 |
| 929.8276 | 953.0001 | 1010.3346 |
| 1036.0583 | 1048.8658 | 1075.1748 |
| 1088.4477 | 1100.8922 | 1115.5685 |
| 1130.5372 | 1147.9322 | 1196.5500 |
| 1230.2799 | 1237.1283 | 1246.5731 |
| 1278.6471 | 1280.4477 | 1304.0619 |
| 1329.8207 | 1346.3401 | 1375.2577 |
| 1386.9400 | 1396.8800 | 1402.3097 |
| 1408.3950 | 1423.8055 | 1426.1962 |
| 1445.8145 | 1480.7204 | 1486.3222 |
| 1487.3339 | 1500.4007 | 1506.2926 |
| 1513.2198 | 1522.5377 | 2953.3011 |
| 3002.5386 | 3008.2542 | 3011.3361 |
| 3028.2421 | 3032.4458 | 3037.9927 |
| 3039.5928 | 3047.6506 | 3060.9799 |
| 3071.9582 | 3078.6385 | 3083.1694 |
| 3108.4061 | 3114.3335 | 3789.6165 |

Zero-point correction (Hartree): 0.237591

C8H17O.6oh.fold.pmmppmtt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -465.48535983

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 2.739801 | -1.268936 | 0.203474 |
| C | 3.153549 | -0.150295 | -0.480614 |
| C | 2.029373 | 0.766331 | -0.991696 |
| C | 1.276786 | 1.484045 | 0.144400 |
| C | 0.628709 | 0.576976 | 1.205513 |
| C | -0.520371 | -0.347843 | 0.755138 |
| O | -0.122850 | -1.260684 | -0.265159 |
| H | 0.776421 | -1.568012 | -0.062517 |
| H | 3.920930 | 0.405927 | 0.088655 |
| H | 3.688987 | -0.572653 | -1.360378 |
| H | 2.484813 | 1.515086 | -1.652553 |
| H | 1.333516 | 0.170047 | -1.586317 |
| H | 1.976820 | 2.157229 | 0.658608 |
| H | 0.515336 | 2.132885 | -0.305285 |

| | | | |
|--|-----------|-----------|-----------|
| H | 1.407637 | -0.052939 | 1.663220 |
| H | 0.251354 | 1.208590 | 2.020823 |
| C | -1.750847 | 0.404291 | 0.239383 |
| H | -0.831900 | -0.913776 | 1.652850 |
| C | -2.936198 | -0.518877 | -0.069817 |
| C | -4.160435 | 0.234207 | -0.598777 |
| H | -2.048109 | 1.148949 | 0.990961 |
| H | -1.476798 | 0.958581 | -0.667988 |
| H | -2.612998 | -1.270755 | -0.797205 |
| H | -3.209480 | -1.069445 | 0.841099 |
| H | -3.928387 | 0.765521 | -1.529171 |
| H | -4.516656 | 0.977941 | 0.124112 |
| H | -4.990482 | -0.449223 | -0.806617 |
| Rotational constants (GHz): | 2.6771900 | 0.5855600 | 0.5531500 |
| Vibrational harmonic frequencies (cm-1): | | | |
| 43.9275 | 81.7455 | | 90.6725 |
| 121.4605 | 135.0264 | | 159.8818 |
| 205.8807 | 237.6603 | | 246.5036 |
| 321.0576 | 337.4443 | | 360.4818 |
| 401.7171 | 469.4023 | | 492.7878 |
| 603.3628 | 615.1402 | | 752.3068 |
| 766.1730 | 808.5620 | | 835.2002 |
| 857.5424 | 867.2547 | | 908.5427 |
| 939.0412 | 976.6780 | | 1001.9063 |
| 1033.2975 | 1051.6385 | | 1064.4892 |
| 1087.6797 | 1105.1349 | | 1117.8481 |
| 1130.1374 | 1161.4080 | | 1198.3391 |
| 1228.5107 | 1263.4552 | | 1299.4782 |
| 1306.7194 | 1327.0178 | | 1336.2126 |
| 1346.8686 | 1369.8407 | | 1374.7093 |
| 1391.6862 | 1402.8038 | | 1411.9942 |
| 1416.3146 | 1425.3323 | | 1469.1475 |
| 1486.5508 | 1489.2913 | | 1493.2842 |
| 1502.4149 | 1507.5307 | | 1512.8669 |
| 1522.7744 | 2879.0016 | | 2937.5737 |
| 2963.5939 | 2995.2189 | | 3022.9868 |
| 3025.2539 | 3030.0473 | | 3035.2570 |
| 3047.3713 | 3053.9532 | | 3065.0836 |
| 3073.6410 | 3087.3955 | | 3108.5348 |
| 3110.4804 | 3131.4736 | | 3710.6358 |
| Zero-point correction (Hartree): | 0.243194 | | |

C8H17O.6oh.fold.pmmpttt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -465.48669319

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|--|-----------|-----------|-----------|
| O | -1.953246 | -1.644581 | -0.601737 |
| C | -3.030624 | -0.870197 | -0.240727 |
| C | -2.706343 | 0.339536 | 0.650854 |
| C | -1.912203 | 1.434252 | -0.086406 |
| C | -0.576117 | 1.002931 | -0.714760 |
| C | 0.533453 | 0.576313 | 0.260857 |
| O | 0.150776 | -0.534918 | 1.071853 |
| H | -0.342779 | -1.156308 | 0.509748 |
| H | -3.635983 | -0.591633 | -1.123034 |
| H | -3.667450 | -1.574969 | 0.339729 |
| H | -3.657265 | 0.759963 | 1.002515 |
| H | -2.146990 | -0.007046 | 1.522717 |
| H | -2.544965 | 1.851427 | -0.882105 |
| H | -1.730110 | 2.256992 | 0.617715 |
| H | -0.748987 | 0.179346 | -1.426376 |
| H | -0.196681 | 1.837174 | -1.319030 |
| C | 1.851760 | 0.287217 | -0.477033 |
| H | 0.708948 | 1.399777 | 0.969654 |
| C | 3.005884 | -0.076835 | 0.463378 |
| C | 4.298826 | -0.430777 | -0.277586 |
| H | 1.681657 | -0.536153 | -1.186905 |
| H | 2.126370 | 1.164346 | -1.080491 |
| H | 3.193195 | 0.764373 | 1.145430 |
| H | 2.688704 | -0.914923 | 1.092981 |
| H | 4.647635 | 0.404284 | -0.896686 |
| H | 4.153574 | -1.292174 | -0.939870 |
| H | 5.103074 | -0.683111 | 0.421616 |
| Rotational constants (GHz): | 2.6963100 | 0.5683400 | 0.5294600 |
| Vibrational harmonic frequencies (cm-1): | | | |
| 43.8099 | 85.7912 | | 90.1426 |
| 121.7560 | 144.1013 | | 156.8370 |
| 191.0275 | 242.7119 | | 251.7283 |
| 293.6255 | 333.6601 | | 353.6457 |
| 410.8368 | 462.1162 | | 494.8563 |
| 561.0762 | 578.1431 | | 752.6312 |
| 773.9253 | 804.0519 | | 840.4439 |
| 858.0034 | 867.2742 | | 908.2075 |
| 940.1361 | 989.9350 | | 1000.9254 |

| | | |
|-----------|-----------|-----------|
| 1040.4335 | 1050.6417 | 1056.5560 |
| 1092.9025 | 1104.4162 | 1120.3184 |
| 1132.5245 | 1156.8276 | 1195.5840 |
| 1203.2828 | 1259.9366 | 1290.1364 |
| 1305.9272 | 1320.2100 | 1334.4173 |
| 1350.3728 | 1372.8065 | 1382.6036 |
| 1393.8242 | 1405.1911 | 1410.1103 |
| 1413.7022 | 1425.8514 | 1447.8645 |
| 1482.7211 | 1486.7074 | 1497.0466 |
| 1497.8468 | 1509.2306 | 1513.5245 |
| 1524.7098 | 2878.8392 | 2961.8716 |
| 2988.0705 | 3005.9257 | 3014.3198 |
| 3021.2308 | 3027.9470 | 3035.7270 |
| 3047.3544 | 3048.3289 | 3059.4895 |
| 3064.4142 | 3085.9868 | 3107.8274 |
| 3109.8043 | 3132.9923 | 3701.6081 |

Zero-point correction (Hartree): 0.242901

C8H17O.6oh.fold.t

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -465.48460235

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 1.818273 | -1.589477 | -0.670003 |
| C | 2.814725 | -1.107400 | 0.135525 |
| C | 3.051168 | 0.412002 | -0.194024 |
| C | 1.916774 | 1.350480 | 0.234404 |
| C | 0.578235 | 1.155950 | -0.516309 |
| C | -0.553150 | 0.602674 | 0.367958 |
| C | -1.840068 | 0.359931 | -0.434921 |
| C | -3.018351 | -0.104617 | 0.428535 |
| C | -4.274739 | -0.421611 | -0.388090 |
| H | 2.575915 | -1.194891 | 1.206536 |
| H | 3.765032 | -1.618651 | -0.095062 |
| H | 3.242842 | 0.493428 | -1.269436 |
| H | 3.978250 | 0.677213 | 0.328205 |
| H | 2.281137 | 2.373953 | 0.080782 |
| H | 1.752575 | 1.238349 | 1.312101 |
| H | 0.723631 | 0.473669 | -1.366520 |
| H | 0.245045 | 2.106151 | -0.951020 |
| O | -0.144808 | -0.569029 | 1.069770 |
| H | -0.767462 | 1.339895 | 1.155881 |

| | | | |
|---|-----------|-----------|-----------|
| H | -2.110328 | 1.282262 | -0.969147 |
| H | -1.630979 | -0.393816 | -1.208925 |
| H | -2.704303 | -0.985885 | 0.998226 |
| H | -3.248778 | 0.672605 | 1.170326 |
| H | -4.083468 | -1.218647 | -1.116107 |
| H | -4.621568 | 0.456091 | -0.946319 |
| H | -5.097418 | -0.751348 | 0.255177 |
| H | 0.264591 | -1.166788 | 0.418701 |

Rotational constants (GHz): 2.6902800 0.5730800 0.5256400

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 47.2328 | 75.1931 | 85.6705 |
| 109.2020 | 127.4470 | 158.6037 |
| 191.4676 | 249.1463 | 261.4932 |
| 285.0702 | 323.2876 | 337.2617 |
| 387.0795 | 461.9476 | 493.7897 |
| 550.8867 | 621.1469 | 741.7614 |
| 755.0930 | 783.4681 | 819.9586 |
| 858.0326 | 881.0846 | 908.6165 |
| 942.9971 | 983.3261 | 1000.3705 |
| 1015.5032 | 1050.7370 | 1082.1140 |
| 1090.1226 | 1100.8501 | 1144.5597 |
| 1152.5864 | 1186.4362 | 1207.7355 |
| 1244.8066 | 1257.9614 | 1280.9553 |
| 1295.1017 | 1320.0490 | 1325.1194 |
| 1341.6600 | 1366.6387 | 1376.7028 |
| 1390.0978 | 1404.6498 | 1410.8609 |
| 1425.5491 | 1455.4081 | 1484.5288 |
| 1488.9731 | 1490.8126 | 1502.6248 |
| 1508.5174 | 1513.0598 | 1523.6929 |
| 1528.1585 | 2959.5197 | 3006.7891 |
| 3011.0768 | 3023.2143 | 3027.2038 |
| 3029.5777 | 3035.5007 | 3037.8520 |
| 3048.3625 | 3053.5693 | 3071.7457 |
| 3084.1932 | 3085.9371 | 3106.8674 |
| 3106.9733 | 3109.5537 | 3667.8012 |

Zero-point correction (Hartree): 0.243474

C8H17O.6oh.pttttt.m

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -465.48187618

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -4.340593 | 0.966405 | -0.272968 |
| C | -4.134105 | -0.295944 | 0.217640 |
| C | -2.792015 | -0.936017 | -0.159418 |
| C | -1.588728 | -0.098146 | 0.285406 |
| C | -0.242463 | -0.669921 | -0.174379 |
| C | 0.971104 | 0.157802 | 0.275961 |
| C | 2.294413 | -0.461923 | -0.175903 |
| C | 3.533288 | 0.276569 | 0.345062 |
| C | 4.846278 | -0.336608 | -0.150935 |
| H | -4.208849 | -0.182537 | 1.322568 |
| H | -4.992063 | -0.948277 | -0.036831 |
| H | -2.745915 | -1.941503 | 0.280626 |
| H | -2.766646 | -1.070193 | -1.248520 |
| H | -1.724523 | 0.914662 | -0.113879 |
| H | -1.594722 | -0.008932 | 1.382475 |
| H | -0.130791 | -1.693011 | 0.210451 |
| H | -0.226870 | -0.737768 | -1.270195 |
| O | 0.932445 | 1.479977 | -0.267802 |
| H | 0.968159 | 0.209661 | 1.380259 |
| H | 2.319974 | -1.509766 | 0.152423 |
| H | 2.307077 | -0.474605 | -1.274334 |
| H | 3.469120 | 1.326006 | 0.039319 |
| H | 3.519599 | 0.273343 | 1.444029 |
| H | 4.903539 | -0.317776 | -1.245359 |
| H | 4.945265 | -1.381775 | 0.165578 |
| H | 5.713059 | 0.209821 | 0.235327 |
| H | 0.183139 | 1.946724 | 0.121629 |
| Rotational constants (GHz): 4.4213200 0.3731800 0.3546600 | | | |
| Vibrational harmonic frequencies (cm ⁻¹): | | | |
| 36.0897 | 52.3480 | 70.0360 | |
| 89.7843 | 106.8344 | 141.1904 | |
| 152.1623 | 189.2611 | 244.7256 | |
| 257.5180 | 288.5364 | 302.4032 | |
| 334.6826 | 394.3575 | 480.7507 | |
| 515.3208 | 554.2090 | 562.4875 | |
| 747.8880 | 760.6561 | 832.2053 | |
| 858.5136 | 900.9056 | 920.3952 | |
| 935.6493 | 991.4838 | 1010.8424 | |
| 1044.0190 | 1052.0858 | 1076.4708 | |
| 1092.8836 | 1094.2750 | 1104.4101 | |
| 1154.8140 | 1174.1341 | 1208.9341 | |
| 1244.5825 | 1258.4802 | 1296.9357 | |
| 1308.5863 | 1313.6934 | 1334.2431 | |
| 1343.9018 | 1346.8033 | 1365.8606 | |
| 1371.6796 | 1399.3161 | 1408.9656 | |
| 1418.9423 | 1426.5758 | 1442.5057 | |
| 1483.7001 | 1492.8893 | 1495.6995 | |
| 1508.8511 | 1513.0248 | 1519.0017 | |
| 1524.0183 | 2880.1246 | 2940.5539 | |
| 2949.2874 | 3009.1509 | 3021.5166 | |
| 3026.1478 | 3030.7025 | 3033.7421 | |
| 3037.2571 | 3057.9303 | 3064.2368 | |
| 3071.9136 | 3085.5742 | 3088.4313 | |
| 3109.8187 | 3111.1389 | 3834.1204 | |
| Zero-point correction (Hartree): 0.241265 | | | |

C8H17O.6oh.pttttt.p

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -465.48237322

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -4.338378 | 0.985938 | -0.292921 |
| C | -4.133434 | -0.272825 | 0.207486 |
| C | -2.797455 | -0.921597 | -0.173950 |
| C | -1.587957 | -0.120021 | 0.317484 |
| C | -0.246988 | -0.684485 | -0.163219 |
| C | 0.966641 | 0.135469 | 0.298355 |
| C | 2.296384 | -0.475116 | -0.167269 |
| C | 3.531733 | 0.275454 | 0.344231 |
| C | 4.848478 | -0.299454 | -0.186069 |
| H | -4.207605 | -0.159595 | 1.311984 |
| H | -4.996899 | -0.919492 | -0.045382 |
| H | -2.774912 | -1.943755 | 0.229093 |
| H | -2.763913 | -1.017481 | -1.267414 |
| H | -1.685986 | 0.917449 | -0.017554 |
| H | -1.594116 | -0.088937 | 1.416908 |
| H | -0.127314 | -1.719746 | 0.185105 |
| H | -0.241394 | -0.733774 | -1.263609 |
| O | 0.853750 | 1.504828 | -0.101527 |
| H | 0.964363 | 0.179129 | 1.396190 |
| H | 2.339155 | -1.525329 | 0.153278 |
| H | 2.306278 | -0.495310 | -1.268891 |
| H | 3.441025 | 1.331232 | 0.066278 |
| H | 3.535858 | 0.250641 | 1.442490 |
| H | 4.889100 | -0.256064 | -1.280768 |

| | | | |
|---|-----------|-----------|-----------|
| H | 4.973320 | -1.348872 | 0.105573 |
| H | 5.709786 | 0.256129 | 0.199092 |
| H | 0.845866 | 1.523100 | -1.069080 |
| Rotational constants (GHz): | 4.3951100 | 0.3732700 | 0.3550700 |
| Vibrational harmonic frequencies (cm ⁻¹): | | | |
| 35.2946 | 48.5587 | 71.6496 | |
| 90.7484 | 109.7895 | 143.7368 | |
| 156.5220 | 187.2159 | 246.7848 | |
| 259.1596 | 297.4615 | 311.2295 | |
| 346.8585 | 393.1289 | 446.1643 | |
| 479.2088 | 543.1987 | 570.4693 | |
| 749.3283 | 758.0026 | 827.4409 | |
| 856.3946 | 901.7551 | 917.4408 | |
| 926.9517 | 984.1420 | 1012.2663 | |
| 1045.6643 | 1050.8742 | 1080.4320 | |
| 1093.7324 | 1098.6977 | 1118.9846 | |
| 1124.0892 | 1159.7915 | 1201.1738 | |
| 1247.0080 | 1258.5343 | 1290.6016 | |
| 1303.6926 | 1319.5486 | 1326.9894 | |
| 1348.4671 | 1362.6887 | 1370.3982 | |
| 1373.6973 | 1396.6463 | 1411.9273 | |
| 1418.6206 | 1426.5792 | 1428.3215 | |
| 1488.4755 | 1494.0748 | 1498.9311 | |
| 1508.8981 | 1513.3427 | 1521.2521 | |
| 1524.6697 | 2884.9655 | 2933.7229 | |
| 2996.2696 | 3002.5651 | 3020.2663 | |
| 3027.6025 | 3032.6381 | 3036.3869 | |
| 3038.2097 | 3044.2445 | 3059.0737 | |
| 3065.9514 | 3083.5243 | 3104.8770 | |
| 3107.3414 | 3112.0381 | 3788.9841 | |

Zero-point correction (Hartree): 0.241067

C8H17O.6oh.pttttt.t

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -465.48237320

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -4.338626 | 0.985773 | -0.292304 |
| C | -4.133481 | -0.273092 | 0.207756 |
| C | -2.797451 | -0.921601 | -0.174011 |
| C | -1.587985 | -0.119908 | 0.317277 |
| C | -0.247021 | -0.684103 | -0.163778 |
| C | 0.966641 | 0.135702 | 0.298071 |
| C | 2.296339 | -0.475068 | -0.167364 |
| C | 3.531701 | 0.275345 | 0.344376 |
| C | 4.848519 | -0.299827 | -0.185431 |
| H | -4.207351 | -0.159967 | 1.312293 |
| H | -4.996874 | -0.919883 | -0.044995 |
| H | -2.774677 | -1.943801 | 0.228912 |
| H | -2.764125 | -1.017368 | -1.267494 |
| H | -1.686229 | 0.917588 | -0.017573 |
| H | -1.593939 | -0.088967 | 1.416706 |
| H | -0.127229 | -1.719477 | 0.184159 |
| H | -0.241466 | -0.732998 | -1.264188 |
| O | 0.854153 | 1.505053 | -0.102042 |
| H | 0.964121 | 0.179376 | 1.395906 |
| H | 2.338839 | -1.525273 | 0.153207 |
| H | 2.306412 | -0.495306 | -1.268999 |
| H | 3.441151 | 1.331070 | 0.066199 |
| H | 3.535513 | 0.250707 | 1.442640 |
| H | 4.889616 | -0.256397 | -1.280109 |
| H | 4.973010 | -1.349288 | 0.106215 |
| H | 5.709789 | 0.255545 | 0.200119 |
| H | 0.845646 | 1.523144 | -1.069607 |

Rotational constants (GHz): 4.3951500 0.3732600 0.3550600

Vibrational harmonic frequencies (cm⁻¹):

| | | |
|-----------|-----------|-----------|
| 35.2942 | 48.5569 | 71.6463 |
| 90.7480 | 109.8198 | 143.7409 |
| 156.4805 | 187.2110 | 246.7525 |
| 259.1558 | 297.4551 | 311.3772 |
| 346.9104 | 393.1402 | 447.2535 |
| 479.2737 | 543.2625 | 570.4622 |
| 749.3190 | 757.9918 | 827.4281 |
| 856.4092 | 901.7518 | 917.4493 |
| 926.9549 | 984.1905 | 1012.2647 |
| 1045.6625 | 1050.8704 | 1080.3998 |
| 1093.7333 | 1098.6859 | 1118.9447 |
| 1124.1031 | 1159.7337 | 1201.1578 |
| 1247.0099 | 1258.4982 | 1290.5800 |
| 1303.6858 | 1319.5334 | 1326.9818 |
| 1348.4096 | 1362.7420 | 1370.3969 |
| 1373.5963 | 1396.6310 | 1411.9246 |
| 1418.6135 | 1426.5298 | 1428.3187 |
| 1488.4721 | 1494.0835 | 1498.9274 |
| 1508.8990 | 1513.3359 | 1521.2447 |

| | | |
|-----------|-----------|-----------|
| 1524.6637 | 2884.8876 | 2933.8292 |
| 2996.2028 | 3002.5271 | 3020.2761 |
| 3027.6017 | 3032.6428 | 3036.4005 |
| 3038.2237 | 3044.2672 | 3059.0967 |
| 3065.9499 | 3083.5599 | 3104.9797 |
| 3107.3546 | 3112.0304 | 3788.7919 |

Zero-point correction (Hartree): 0.241070

C8H17O.1-5Hshift.6oh.m.tttR.t

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -465.47231140

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| C | -0.691326 | -0.712956 | -0.823532 |
| C | -2.014775 | -1.305664 | -0.351368 |
| C | -2.802731 | -0.339502 | 0.556061 |
| C | -2.863809 | 1.049672 | -0.103672 |
| O | -1.575830 | 1.539641 | -0.408331 |
| C | 0.490970 | -0.682190 | 0.141923 |
| H | -0.404027 | -1.019593 | -1.834046 |
| H | -1.830816 | -2.244716 | 0.191064 |
| H | -2.624105 | -1.558907 | -1.227346 |
| H | -2.301672 | -0.260232 | 1.523935 |
| H | -3.819596 | -0.711580 | 0.727343 |
| H | -3.317180 | 1.770293 | 0.593446 |
| H | -3.496485 | 1.014850 | -1.006313 |
| H | -1.009402 | 0.525273 | -0.913264 |
| O | 0.169138 | 0.024196 | 1.337911 |
| H | 0.696873 | -1.716286 | 0.464935 |
| H | -0.259435 | 0.850542 | 1.051397 |
| C | 1.760172 | -0.119149 | -0.520036 |
| C | 2.981558 | -0.136553 | 0.405543 |

| | | | |
|---|----------|-----------|-----------|
| C | 4.226171 | 0.488292 | -0.231817 |
| H | 1.974439 | -0.695800 | -1.431237 |
| H | 1.557360 | 0.911591 | -0.845653 |
| H | 2.724080 | 0.390534 | 1.330312 |
| H | 3.198803 | -1.174139 | 0.695225 |
| H | 4.051603 | 1.537537 | -0.496708 |
| H | 4.513926 | -0.038775 | -1.149111 |
| H | 5.081796 | 0.456997 | 0.450769 |

Rotational constants (GHz): 2.8129200 0.5876100 0.5604300

Vibrational harmonic frequencies (cm-1):

| | | |
|------------|-----------|-----------|
| 11454.6753 | 51.0308 | 87.6572 |
| 96.6577 | 132.4449 | 148.7829 |
| 189.0566 | 253.8293 | 265.8653 |
| 283.9531 | 331.5012 | 363.7943 |
| 471.4408 | 472.2644 | 527.9506 |
| 554.7547 | 633.1148 | 690.0068 |
| 756.1552 | 809.4452 | 846.8202 |
| 858.1997 | 867.3929 | 904.6174 |
| 921.8354 | 961.6118 | 989.9998 |
| 1026.9715 | 1041.1668 | 1052.5386 |
| 1070.4561 | 1088.2148 | 1111.5765 |
| 1145.7223 | 1160.5409 | 1188.5554 |
| 1216.7807 | 1238.6376 | 1256.8879 |
| 1272.0085 | 1285.2780 | 1318.9138 |
| 1341.4507 | 1347.9025 | 1353.0699 |
| 1372.4963 | 1388.0280 | 1393.8016 |
| 1408.7686 | 1429.2849 | 1463.8880 |
| 1481.1540 | 1494.6718 | 1497.3734 |
| 1501.8414 | 1509.6403 | 1514.7014 |
| 1524.9979 | 1534.3782 | 2977.8677 |
| 2986.8113 | 3013.7405 | 3017.1341 |
| 3029.1153 | 3029.3254 | 3037.4045 |
| 3054.1324 | 3063.9817 | 3067.4047 |
| 3087.4149 | 3099.6939 | 3109.3811 |
| 3111.7933 | 3129.0718 | 3679.3513 |

Zero-point correction (Hartree): 0.239197

C8H17O.1-5Hshift.6oh.tttR.m

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -465.46519117

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -1.812112 | 1.690805 | 0.203367 |
| C | -2.954918 | 0.965593 | 0.567669 |
| C | -3.197903 | -0.215611 | -0.390187 |
| C | -1.953523 | -1.120929 | -0.393763 |
| C | -0.705577 | -0.314454 | -0.714846 |
| C | 0.640092 | -0.786474 | -0.174970 |
| C | 1.730267 | 0.277892 | -0.331952 |
| C | 3.133641 | -0.222700 | 0.027818 |
| C | 4.202903 | 0.867274 | -0.092115 |
| H | -2.895485 | 0.591714 | 1.605535 |

| | | | | |
|--|-----------|-----------|-----------|--|
| H | -3.808283 | 1.659906 | 0.514602 | |
| H | -3.378261 | 0.176165 | -1.398585 | |
| H | -4.089927 | -0.775518 | -0.085713 | |
| H | -2.085900 | -1.940404 | -1.115827 | |
| H | -1.850872 | -1.576276 | 0.599290 | |
| H | -1.010569 | 0.809434 | -0.171884 | |
| H | -0.640968 | -0.037234 | -1.772784 | |
| O | 0.583144 | -1.127063 | 1.210344 | |
| H | 0.940362 | -1.677161 | -0.762186 | |
| H | 1.715828 | 0.642897 | -1.367428 | |
| H | 1.461532 | 1.129489 | 0.306372 | |
| H | 3.112971 | -0.617591 | 1.049088 | |
| H | 3.395829 | -1.066728 | -0.625951 | |
| H | 3.985816 | 1.709234 | 0.574926 | |
| H | 4.258841 | 1.262387 | -1.113259 | |
| H | 5.194400 | 0.483555 | 0.169876 | |
| H | 0.156526 | -1.987363 | 1.298317 | |
| Rotational constants (GHz): | 2.6050700 | 0.5528700 | 0.5079500 | |
| Vibrational harmonic frequencies (cm-1): | | | | |
| i1509.3454 | 39.7143 | | 59.6329 | |
| 82.7438 | 104.4559 | | 112.8368 | |
| 189.7708 | 227.8973 | | 251.1325 | |
| 271.5972 | 303.2507 | | 315.9024 | |
| 362.5528 | 445.3518 | | 475.1045 | |
| 506.9130 | 520.5653 | | 627.3871 | |
| 750.3512 | 791.9331 | | 854.5382 | |
| 858.4014 | 885.2485 | | 904.3111 | |
| 920.8150 | 959.6380 | | 986.0209 | |
| 1026.3496 | 1047.0236 | | 1057.1403 | |
| 1073.4865 | 1082.5233 | | 1122.7573 | |
| 1140.8088 | 1165.4657 | | 1186.1724 | |
| 1220.5871 | 1235.5209 | | 1241.1010 | |
| 1255.4967 | 1284.9536 | | 1302.1512 | |
| 1320.6591 | 1340.8575 | | 1350.8510 | |
| 1363.0254 | 1381.6552 | | 1388.2091 | |
| 1412.1648 | 1424.3538 | | 1428.1630 | |
| 1482.9822 | 1488.2871 | | 1494.4635 | |
| 1509.0193 | 1509.3426 | | 1513.6404 | |
| 1524.2111 | 1559.6527 | | 2914.1059 | |
| 2957.2556 | 3010.9403 | | 3012.1120 | |
| 3024.2365 | 3034.7821 | | 3039.1481 | |
| 3048.1989 | 3063.1200 | | 3073.1731 | |
| 3086.6490 | 3090.4389 | | 3096.9144 | |
| 3110.9773 | 3112.3333 | | 3840.6271 | |
| Zero-point correction (Hartree): | 0.237513 | | | |

C8H17O.1-5Hshift.6oh.tttR.p

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -465.46614544

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | | |
|--|-----------|-----------|-----------|--|
| O | -1.841127 | 1.679684 | 0.190435 | |
| C | -2.963075 | 0.926833 | 0.565693 | |
| C | -3.195188 | -0.248590 | -0.401740 | |
| C | -1.939291 | -1.137602 | -0.423650 | |
| C | -0.699071 | -0.309692 | -0.722197 | |
| C | 0.623929 | -0.767687 | -0.139731 | |
| C | 1.750524 | 0.249047 | -0.383496 | |
| C | 3.124822 | -0.210800 | 0.119385 | |
| C | 4.236522 | 0.804043 | -0.166343 | |
| H | -2.878973 | 0.544975 | 1.598265 | |
| H | -3.830080 | 1.605531 | 0.530955 | |
| H | -3.391864 | 0.153284 | -1.403477 | |
| H | -4.076708 | -0.824244 | -0.095680 | |
| H | -2.058976 | -1.932934 | -1.174473 | |
| H | -1.814817 | -1.622501 | 0.549729 | |
| H | -1.026132 | 0.811100 | -0.186901 | |
| H | -0.602071 | -0.030182 | -1.776230 | |
| O | 0.419789 | -1.012539 | 1.251849 | |
| H | 0.898968 | -1.716772 | -0.644073 | |
| H | 1.809289 | 0.451379 | -1.461659 | |
| H | 1.473009 | 1.192043 | 0.103955 | |
| H | 3.077471 | -0.387629 | 1.202831 | |
| H | 3.380633 | -1.174492 | -0.343729 | |
| H | 4.020949 | 1.767969 | 0.307452 | |
| H | 4.342222 | 0.981269 | -1.242496 | |
| H | 5.203216 | 0.455113 | 0.210818 | |
| H | 1.209535 | -1.444375 | 1.598914 | |
| Rotational constants (GHz): | 2.6737800 | 0.5480200 | 0.5103700 | |
| Vibrational harmonic frequencies (cm-1): | | | | |
| i1510.9918 | 42.8544 | | 57.0173 | |
| 86.0756 | 103.1723 | | 108.9115 | |
| 187.3404 | 244.3760 | | 252.9860 | |
| 272.6804 | 303.3524 | | 317.0431 | |
| 356.6969 | 458.4768 | | 475.6000 | |

| | | |
|-----------|-----------|-----------|
| 512.5883 | 523.1032 | 609.7570 |
| 751.9811 | 793.0750 | 854.1148 |
| 858.8005 | 893.4337 | 906.6639 |
| 915.7625 | 958.0256 | 986.0916 |
| 1030.3345 | 1049.9544 | 1052.3745 |
| 1075.6111 | 1098.6671 | 1118.1443 |
| 1149.6360 | 1171.4429 | 1181.4547 |
| 1216.1214 | 1227.9093 | 1235.0335 |
| 1267.7900 | 1273.1852 | 1290.0835 |
| 1323.4590 | 1335.5726 | 1356.6834 |
| 1369.2892 | 1386.2451 | 1394.6705 |
| 1404.1789 | 1427.1788 | 1430.0142 |
| 1487.8652 | 1488.6486 | 1494.8684 |
| 1506.2956 | 1506.8249 | 1513.1423 |
| 1522.0096 | 1555.0316 | 2901.3322 |
| 2963.4749 | 3010.7562 | 3012.4526 |
| 3014.6234 | 3031.4681 | 3042.5459 |
| 3046.7405 | 3047.1178 | 3082.6252 |
| 3085.9386 | 3093.6045 | 3108.8056 |
| 3112.1370 | 3115.8319 | 3838.1142 |

Zero-point correction (Hartree): 0.237561

C8H17O.1-5Hshift.6oh.tttR.t

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -465.47097327

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -1.604767 | 1.516933 | -0.455054 |
| C | -2.785239 | 1.071175 | 0.176170 |
| C | -3.157135 | -0.358283 | -0.258073 |
| C | -1.971601 | -1.299177 | 0.035360 |
| C | -0.696863 | -0.773695 | -0.614130 |
| C | 0.544574 | -0.672116 | 0.265068 |
| C | 1.775550 | -0.173466 | -0.506901 |
| C | 3.043696 | -0.113884 | 0.351813 |
| C | 4.251296 | 0.455645 | -0.398164 |
| H | -2.686160 | 1.103908 | 1.272958 |
| H | -3.593368 | 1.760400 | -0.114272 |
| H | -3.380410 | -0.358190 | -1.332078 |
| H | -4.061577 | -0.682940 | 0.268741 |
| H | -2.202007 | -2.308950 | -0.328685 |
| H | -1.822930 | -1.357092 | 1.118974 |
| H | -1.008527 | 0.441669 | -0.785307 |
| H | -0.507125 | -1.150858 | -1.624143 |
| O | 0.266125 | 0.141237 | 1.404071 |
| H | 0.768568 | -1.669569 | 0.677442 |
| H | 1.940885 | -0.828602 | -1.374086 |
| H | 1.554283 | 0.825168 | -0.911473 |
| H | 2.832461 | 0.488776 | 1.241667 |
| H | 3.279268 | -1.123669 | 0.715696 |
| H | 4.058226 | 1.478600 | -0.741400 |
| H | 4.495926 | -0.146520 | -1.281183 |
| H | 5.140166 | 0.482978 | 0.240666 |
| H | -0.124220 | 0.962335 | 1.057484 |

Rotational constants (GHz): 2.8769000 0.5686200 0.5403600

Vibrational harmonic frequencies (cm-1):

| | | |
|------------|-----------|-----------|
| 11365.3556 | 50.2561 | 67.1533 |
| 82.8693 | 122.0909 | 128.9464 |
| 160.4356 | 246.1485 | 253.7431 |
| 300.7530 | 313.3849 | 356.6962 |
| 450.7569 | 488.5472 | 521.0826 |
| 567.2252 | 592.7419 | 649.1434 |
| 754.9808 | 805.7279 | 851.8286 |
| 858.8555 | 895.6903 | 908.8148 |
| 919.2401 | 955.4150 | 984.0575 |
| 1026.4057 | 1047.7126 | 1050.6655 |
| 1069.3007 | 1093.6891 | 1110.4593 |
| 1144.5988 | 1160.9275 | 1186.2847 |
| 1217.0770 | 1222.5450 | 1256.4686 |
| 1265.5458 | 1278.1576 | 1314.2137 |
| 1318.3421 | 1339.9129 | 1356.4225 |
| 1371.3468 | 1383.0696 | 1394.6965 |
| 1409.3021 | 1427.8883 | 1451.6187 |
| 1481.4055 | 1494.6212 | 1495.1630 |
| 1508.5101 | 1513.2280 | 1513.3568 |
| 1524.7228 | 1540.5957 | 2982.1801 |
| 2992.4403 | 3013.4594 | 3020.7797 |
| 3029.8981 | 3034.8079 | 3037.0988 |
| 3050.9043 | 3053.5029 | 3085.2650 |
| 3087.4016 | 3097.0687 | 3106.6692 |
| 3108.4566 | 3111.4386 | 3703.6472 |

Zero-point correction (Hartree): 0.238683

C8H17O.1-5Hshift.6oh.tttS.m

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -465.46565216

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 1.903664 | -1.760748 | -0.087356 |
| C | 3.027603 | -1.110295 | 0.443497 |
| C | 3.228123 | 0.278926 | -0.190291 |
| C | 1.955841 | 1.117171 | 0.026561 |
| C | 0.734695 | 0.377191 | -0.492146 |
| C | -0.587204 | 0.613950 | 0.211590 |
| C | -1.702737 | -0.302650 | -0.308370 |
| C | -3.052796 | -0.097813 | 0.390483 |
| C | -4.139250 | -1.053265 | -0.113544 |
| H | 2.964517 | -1.007417 | 1.541877 |
| H | 3.900909 | -1.743326 | 0.220500 |
| H | 3.416859 | 0.154676 | -1.263621 |
| H | 4.104979 | 0.770623 | 0.246597 |
| H | 2.050119 | 2.090038 | -0.473499 |
| H | 1.834418 | 1.325383 | 1.097470 |
| H | 1.092476 | -0.840968 | -0.288313 |
| H | 0.639238 | 0.404745 | -1.583102 |
| O | -0.896872 | 2.002073 | 0.012390 |
| H | -0.444393 | 0.420777 | 1.289336 |
| H | -1.817796 | -0.132925 | -1.387206 |
| H | -1.381082 | -1.344988 | -0.181107 |
| H | -2.926342 | -0.228602 | 1.474707 |
| H | -3.389000 | 0.936688 | 0.237027 |
| H | -3.854285 | -2.097972 | 0.053449 |
| H | -4.309464 | -0.925131 | -1.188294 |
| H | -5.091863 | -0.881220 | 0.397851 |
| H | -1.629273 | 2.229735 | 0.599376 |

Rotational constants (GHz): 2.3370900 0.5675100 0.4786800

Vibrational harmonic frequencies (cm-1):

| | | |
|------------|-----------|-----------|
| 11512.7767 | 41.8353 | 63.5529 |
| 89.3969 | 95.3166 | 115.3301 |
| 174.4753 | 246.9501 | 251.4038 |
| 273.0043 | 296.3045 | 318.1961 |
| 334.4550 | 393.5437 | 481.0083 |
| 520.1485 | 527.1768 | 606.0604 |
| 754.6668 | 804.9601 | 850.6058 |
| 860.2019 | 896.5906 | 900.9214 |
| 940.2514 | 958.3474 | 978.2361 |
| 1035.9568 | 1046.7296 | 1062.6706 |
| 1083.4030 | 1092.6855 | 1099.3306 |
| 1143.0455 | 1165.5568 | 1174.3014 |
| 1215.2958 | 1216.1583 | 1244.7160 |
| 1264.2193 | 1275.1511 | 1297.0746 |
| 1322.5444 | 1340.2250 | 1358.3539 |
| 1373.0480 | 1384.3911 | 1390.4689 |
| 1407.5361 | 1427.7053 | 1446.3496 |
| 1484.0320 | 1488.8589 | 1495.1391 |
| 1507.8082 | 1510.7618 | 1513.6931 |
| 1522.8213 | 1553.3120 | 2953.7138 |
| 2964.7542 | 3010.8532 | 3016.3661 |
| 3030.4637 | 3031.0552 | 3042.3574 |
| 3047.7085 | 3048.8622 | 3069.0589 |
| 3078.1251 | 3090.6956 | 3098.3142 |
| 3111.8766 | 3115.1645 | 3817.6472 |

Zero-point correction (Hartree): 0.237484

C8H17O.1-5Hshift.6oh.tttS.p

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -465.46651526

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 1.907208 | -1.763046 | -0.120459 |
| C | 3.026500 | -1.123229 | 0.429958 |
| C | 3.228968 | 0.277216 | -0.176402 |
| C | 1.954989 | 1.111704 | 0.051498 |
| C | 0.731396 | 0.379983 | -0.483674 |
| C | -0.600680 | 0.616531 | 0.211645 |
| C | -1.710578 | -0.298526 | -0.303016 |
| C | -3.044613 | -0.122200 | 0.432467 |
| C | -4.148742 | -1.031793 | -0.114906 |
| H | 2.958135 | -1.040703 | 1.530015 |
| H | 3.902946 | -1.749759 | 0.200822 |
| H | 3.417730 | 0.174559 | -1.251701 |
| H | 4.103877 | 0.763000 | 0.270933 |
| H | 2.065354 | 2.093637 | -0.430184 |
| H | 1.838172 | 1.293299 | 1.129933 |
| H | 1.085784 | -0.835481 | -0.295960 |
| H | 0.641986 | 0.434344 | -1.574037 |
| O | -1.029170 | 1.969078 | -0.017503 |
| H | -0.471406 | 0.447217 | 1.294272 |
| H | -1.848530 | -0.100315 | -1.374641 |
| H | -1.367834 | -1.337511 | -0.214048 |

| | | | | |
|---|-----------|-----------|-----------|-----------|
| H | -2.896690 | -0.328952 | 1.501641 | |
| H | -3.351483 | 0.926558 | 0.360465 | |
| H | -3.874580 | -2.089662 | -0.028390 | |
| H | -4.341285 | -0.827305 | -1.174359 | |
| H | -5.089316 | -0.887190 | 0.426697 | |
| H | -0.420595 | 2.557899 | 0.446805 | |
| Rotational constants (GHz): | 2.3449200 | | 0.5656300 | 0.4777900 |
| Vibrational harmonic frequencies (cm ⁻¹): | | | | |
| i1466.9003 | | 42.6091 | | 64.9722 |
| 84.0973 | | 96.7885 | | 115.4138 |
| 176.6222 | | 250.6315 | | 271.5706 |
| 293.1627 | | 305.3654 | | 318.7195 |
| 335.7034 | | 392.4014 | | 480.8139 |
| 521.5145 | | 522.8775 | | 603.5293 |
| 751.5785 | | 811.4852 | | 851.0666 |
| 857.4661 | | 897.6749 | | 900.3563 |
| 944.8164 | | 961.3267 | | 982.1792 |
| 1036.9477 | | 1038.6853 | | 1072.0026 |
| 1073.4808 | | 1087.7256 | | 1108.6919 |
| 1139.0023 | | 1162.5155 | | 1181.5999 |
| 1214.8464 | | 1225.3138 | | 1244.4146 |
| 1254.5940 | | 1285.8873 | | 1301.6918 |
| 1321.6646 | | 1339.4512 | | 1356.2669 |
| 1370.7650 | | 1385.6605 | | 1397.4766 |
| 1405.4983 | | 1427.1921 | | 1437.2317 |
| 1488.7822 | | 1489.2594 | | 1495.6421 |
| 1508.7817 | | 1510.9563 | | 1513.8348 |
| 1523.9587 | | 1559.9172 | | 2950.9639 |
| 2974.6441 | | 3008.6448 | | 3010.5914 |
| 3026.2167 | | 3033.8120 | | 3038.9069 |
| 3043.0008 | | 3055.9862 | | 3071.1027 |
| 3088.9714 | | 3092.1757 | | 3098.8477 |
| 3110.4690 | | 3112.6146 | | 3821.4670 |
| Zero-point correction (Hartree): | 0.237688 | | | |

C8H17O.1-5Hshift.6oh.tttS.t

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -465.46739944

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | | |
|---|-----------|-----------|-----------|-----------|
| O | 1.929040 | -1.758971 | -0.125248 | |
| C | 3.041593 | -1.107249 | 0.426435 | |
| C | 3.229868 | 0.295768 | -0.179691 | |
| C | 1.949688 | 1.118962 | 0.050016 | |
| C | 0.733464 | 0.373684 | -0.478546 | |
| C | -0.595421 | 0.600783 | 0.224701 | |
| C | -1.711610 | -0.311193 | -0.296928 | |
| C | -3.045358 | -0.133838 | 0.438503 | |
| C | -4.164813 | -1.009977 | -0.131397 | |
| H | 2.970823 | -1.026336 | 1.526138 | |
| H | 3.923702 | -1.725813 | 0.197045 | |
| H | 3.422596 | 0.193305 | -1.254698 | |
| H | 4.100610 | 0.788308 | 0.268442 | |
| H | 2.041287 | 2.101992 | -0.430450 | |
| H | 1.824878 | 1.308317 | 1.123837 | |
| H | 1.097073 | -0.838945 | -0.295504 | |
| H | 0.644406 | 0.413210 | -1.572214 | |
| O | -0.956876 | 1.989580 | 0.142989 | |
| H | -0.461438 | 0.425571 | 1.299775 | |
| H | -1.851926 | -0.116827 | -1.372382 | |
| H | -1.375729 | -1.353869 | -0.220035 | |
| H | -2.900799 | -0.368266 | 1.501823 | |
| H | -3.335021 | 0.922209 | 0.398510 | |
| H | -3.908207 | -2.073926 | -0.072235 | |
| H | -4.355469 | -0.776203 | -1.185374 | |
| H | -5.102195 | -0.863555 | 0.415009 | |
| H | -1.136371 | 2.184316 | -0.788174 | |
| Rotational constants (GHz): | 2.3532300 | | 0.5630700 | 0.4770500 |
| Vibrational harmonic frequencies (cm ⁻¹): | | | | |
| i1472.5991 | | 44.0116 | | 61.8800 |
| 85.1620 | | 97.6238 | | 118.0434 |
| 177.4529 | | 251.0657 | | 270.9146 |
| 289.4424 | | 309.4651 | | 326.2667 |
| 355.1875 | | 391.6268 | | 479.4398 |
| 519.5312 | | 530.4244 | | 610.1897 |
| 752.2773 | | 808.3524 | | 850.6981 |
| 854.5009 | | 895.0710 | | 900.4885 |
| 941.2989 | | 953.1753 | | 976.3798 |
| 1036.6674 | | 1044.6244 | | 1070.6530 |
| 1083.4747 | | 1089.7458 | | 1100.6982 |
| 1133.7331 | | 1158.1591 | | 1176.6257 |
| 1212.9425 | | 1227.3980 | | 1240.6248 |
| 1253.3033 | | 1281.0273 | | 1299.3642 |
| 1324.9435 | | 1345.5836 | | 1356.7621 |

| | | |
|-----------|-----------|-----------|
| 1370.6596 | 1384.9517 | 1401.8139 |
| 1418.0728 | 1419.5566 | 1428.6603 |
| 1485.4580 | 1493.9860 | 1494.9655 |
| 1508.4797 | 1510.1609 | 1513.8412 |
| 1524.5399 | 1557.5242 | 2954.5086 |
| 2999.5460 | 3010.0169 | 3030.3911 |
| 3034.9941 | 3038.7377 | 3047.0995 |
| 3048.3436 | 3055.0024 | 3062.8877 |
| 3076.2389 | 3082.9345 | 3097.0996 |
| 3107.8721 | 3113.6285 | 3785.1804 |

Zero-point correction (Hartree): 0.237712

C8H17O.1-6Hshift.6oh.tt.m

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -465.47503751

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -0.961306 | 1.768111 | -0.181918 |
| C | -2.216612 | 1.408653 | 0.308931 |
| C | -2.876794 | 0.232593 | -0.429406 |
| C | -2.248380 | -1.146928 | -0.162670 |
| C | -0.791105 | -1.321549 | -0.634618 |
| C | 0.237820 | -0.488187 | 0.133497 |
| C | 1.637178 | -0.486061 | -0.469443 |
| C | 2.628799 | 0.433164 | 0.255958 |
| C | 4.022312 | 0.413635 | -0.379190 |
| H | -2.196013 | 1.208544 | 1.398456 |
| H | -2.842503 | 2.308754 | 0.182048 |
| H | -2.849564 | 0.449013 | -1.504906 |
| H | -3.934652 | 0.192044 | -0.137742 |
| H | -2.859121 | -1.911128 | -0.657640 |
| H | -2.329903 | -1.377073 | 0.912388 |
| H | -0.726607 | -1.051459 | -1.695216 |
| H | -0.503888 | -2.379382 | -0.554141 |
| H | -0.156212 | 0.635469 | 0.042463 |
| O | 0.330642 | -0.830216 | 1.492988 |
| H | 2.014826 | -1.520137 | -0.463542 |
| H | 1.551661 | -0.185771 | -1.521130 |
| H | 2.232788 | 1.456591 | 0.252288 |
| H | 2.691327 | 0.130008 | 1.306281 |
| H | 3.989564 | 0.741450 | -1.424793 |
| H | 4.453270 | -0.594301 | -0.363059 |
| H | 4.711003 | 1.076737 | 0.154304 |
| H | -0.559964 | -0.954446 | 1.847015 |

Rotational constants (GHz): 2.2133500 0.6734700 0.6005600

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| i391.0009 | 59.2124 | 77.5624 |
| 93.4558 | 104.5616 | 153.7413 |
| 217.8601 | 247.5989 | 257.2971 |
| 312.0103 | 332.9859 | 346.4845 |
| 350.2465 | 421.5569 | 484.4030 |
| 491.2241 | 557.0317 | 751.6327 |
| 772.7746 | 788.7148 | 861.1869 |
| 884.1059 | 896.1004 | 913.7089 |
| 918.4879 | 968.6305 | 1009.4745 |
| 1037.4201 | 1050.9761 | 1085.6103 |
| 1096.8078 | 1099.5037 | 1108.6576 |
| 1154.8204 | 1179.4181 | 1207.1304 |
| 1238.1983 | 1259.8980 | 1273.1612 |
| 1289.6729 | 1297.7812 | 1330.6149 |
| 1348.6840 | 1375.1954 | 1378.6685 |
| 1390.2963 | 1400.8176 | 1408.2443 |
| 1419.1951 | 1427.8429 | 1467.9511 |
| 1476.0859 | 1483.0165 | 1490.4887 |
| 1508.7143 | 1509.0727 | 1513.7211 |
| 1523.6805 | 1548.6366 | 2922.6842 |
| 2986.6543 | 2990.6796 | 3009.3347 |
| 3027.2280 | 3033.6076 | 3037.0709 |
| 3048.7189 | 3066.9465 | 3069.3767 |
| 3079.2933 | 3084.9786 | 3089.9866 |
| 3110.9491 | 3113.8477 | 3811.2308 |

Zero-point correction (Hartree): 0.239514

C8H17O.1-6Hshift.6oh.tt.p

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -465.47503756

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -0.960466 | 1.767911 | -0.180246 |
| C | -2.216545 | 1.409026 | 0.309099 |
| C | -2.876456 | 0.233314 | -0.430046 |
| C | -2.248555 | -1.146374 | -0.162992 |
| C | -0.791359 | -1.321482 | -0.634960 |
| C | 0.237771 | -0.488827 | 0.133670 |
| C | 1.636999 | -0.486102 | -0.469552 |

| | | | |
|--|-----------|-----------|-----------|
| C | 2.628440 | 0.433291 | 0.255880 |
| C | 4.021875 | 0.414315 | -0.379454 |
| H | -2.197415 | 1.208833 | 1.398635 |
| H | -2.841824 | 2.309441 | 0.181440 |
| H | -2.848311 | 0.449919 | -1.505486 |
| H | -3.934551 | 0.192998 | -0.139218 |
| H | -2.859610 | -1.910558 | -0.657593 |
| H | -2.329987 | -1.376068 | 0.912172 |
| H | -0.726644 | -1.050943 | -1.695427 |
| H | -0.504569 | -2.379458 | -0.554897 |
| H | -0.156294 | 0.634828 | 0.043696 |
| O | 0.330949 | -0.832140 | 1.492802 |
| H | 2.014972 | -1.520060 | -0.463901 |
| H | 1.551196 | -0.185650 | -1.521166 |
| H | 2.232104 | 1.456591 | 0.252463 |
| H | 2.691208 | 0.129937 | 1.306135 |
| H | 3.988873 | 0.742233 | -1.425016 |
| H | 4.453185 | -0.593473 | -0.363489 |
| H | 4.710406 | 1.077600 | 0.154020 |
| H | -0.559622 | -0.955298 | 1.847300 |
| Rotational constants (GHz): | | | 2.2127500 |
| Vibrational harmonic frequencies (cm-1): | | | 0.6735800 |
| i390.7832 | | | 0.6006100 |
| 93.4579 | 59.2166 | | 77.5661 |
| 217.8217 | 104.5737 | | 153.7309 |
| 312.0803 | 247.5705 | | 257.3295 |
| 350.2437 | 333.0872 | | 346.6797 |
| 491.2708 | 421.5162 | | 484.4292 |
| 772.9034 | 557.0458 | | 751.6219 |
| 884.1398 | 788.7019 | | 861.1789 |
| 918.4853 | 896.1373 | | 913.8088 |
| 1037.4407 | 968.6656 | | 1009.4898 |
| 1096.8433 | 1050.9845 | | 1085.5842 |
| 1154.7745 | 1099.4438 | | 1108.6555 |
| 1238.1766 | 1179.4404 | | 1207.1213 |
| 1289.6485 | 1259.8648 | | 1273.1408 |
| 1348.6991 | 1297.7921 | | 1330.5559 |
| 1390.2729 | 1375.1689 | | 1378.6390 |
| 1419.2433 | 1400.8158 | | 1408.2461 |
| 1476.0743 | 1427.8517 | | 1468.0144 |
| 1508.7215 | 1483.0070 | | 1490.4889 |
| 1523.6812 | 1509.0842 | | 1513.7167 |
| 2986.6619 | 1548.5303 | | 2922.6886 |
| 3027.2691 | 2990.6708 | | 3009.3552 |
| 3048.7295 | 3033.6094 | | 3037.0721 |
| 3079.2868 | 3066.9757 | | 3069.4161 |
| 3110.9477 | 3084.9981 | | 3089.9853 |
| | 3113.8410 | | 3811.2041 |
| Zero-point correction (Hartree): | | | 0.239516 |

C8H17O.1-6Hshift.6oh.tt.t

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -465.47655030
 Electronic state : 2-A
 Cartesian coordinates (Angs):

| | | | |
|--|-----------|-----------|-----------|
| O | -0.927738 | 1.761329 | -0.221966 |
| C | -2.187901 | 1.419006 | 0.281939 |
| C | -2.860119 | 0.238393 | -0.437197 |
| C | -2.257743 | -1.145732 | -0.132934 |
| C | -0.805816 | -1.358137 | -0.601230 |
| C | 0.213087 | -0.497753 | 0.133490 |
| C | 1.628778 | -0.530203 | -0.446295 |
| C | 2.623597 | 0.407793 | 0.251996 |
| C | 4.005969 | 0.404900 | -0.408675 |
| H | -2.158409 | 1.230005 | 1.370490 |
| H | -2.802571 | 2.324736 | 0.141347 |
| H | -2.828785 | 0.434920 | -1.517080 |
| H | -3.919382 | 0.221831 | -0.147559 |
| H | -2.884037 | -1.908063 | -0.612266 |
| H | -2.310045 | -1.335274 | 0.945773 |
| H | -0.724583 | -1.142085 | -1.673487 |
| H | -0.529019 | -2.412828 | -0.463164 |
| H | -0.168594 | 0.631879 | -0.022443 |
| O | 0.149100 | -0.804405 | 1.503599 |
| H | 1.999461 | -1.565802 | -0.402617 |
| H | 1.564260 | -0.260682 | -1.507504 |
| H | 2.215863 | 1.426855 | 0.254691 |
| H | 2.739796 | 0.112295 | 1.305052 |
| H | 3.943321 | 0.734197 | -1.451690 |
| H | 4.445917 | -0.598665 | -0.403723 |
| H | 4.697365 | 1.075253 | 0.111506 |
| H | 0.789433 | -0.253566 | 1.973044 |
| Rotational constants (GHz): | | | 2.2061300 |
| Vibrational harmonic frequencies (cm-1): | | | 0.6799300 |
| i523.4678 | | | 0.6055400 |
| 89.7459 | 59.4001 | | 72.0651 |
| | 106.4263 | | 144.3627 |

| | | |
|-----------|-----------|-----------|
| 217.7223 | 241.1783 | 253.5814 |
| 319.2078 | 326.8546 | 345.4940 |
| 370.0237 | 424.1785 | 480.1275 |
| 485.4321 | 557.8161 | 752.5221 |
| 756.7128 | 789.1887 | 858.1116 |
| 863.1733 | 899.0121 | 901.3692 |
| 923.9067 | 960.6027 | 1005.9127 |
| 1038.3102 | 1051.8771 | 1081.1871 |
| 1086.4199 | 1101.0030 | 1116.9643 |
| 1145.8123 | 1178.8989 | 1203.8929 |
| 1239.3934 | 1269.9380 | 1273.9655 |
| 1284.5183 | 1305.7461 | 1328.6109 |
| 1338.5518 | 1360.0114 | 1380.1707 |
| 1397.1594 | 1398.5502 | 1407.8723 |
| 1416.0892 | 1428.3029 | 1466.1406 |
| 1475.4497 | 1482.5290 | 1489.0597 |
| 1504.2428 | 1507.1203 | 1512.3021 |
| 1515.0302 | 1521.8844 | 2952.8099 |
| 2990.2660 | 3009.9034 | 3011.7922 |
| 3025.5513 | 3028.7621 | 3042.7460 |
| 3045.1531 | 3059.6633 | 3069.7909 |
| 3073.1398 | 3080.2591 | 3091.9872 |
| 3112.0395 | 3117.9212 | 3816.7603 |

Zero-point correction (Hartree): 0.239298

C8H17O.7oh.pttttt.m

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -465.48187094

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 4.543302 | -1.100665 | -0.325372 |
| C | 4.287876 | 0.139260 | 0.198345 |
| C | 2.931808 | 0.746525 | -0.180798 |
| C | 1.748430 | -0.120983 | 0.260710 |
| C | 0.388674 | 0.414345 | -0.203748 |
| C | -0.792804 | -0.446548 | 0.260864 |
| C | -2.160952 | 0.051821 | -0.228233 |
| C | -3.309484 | -0.828232 | 0.268590 |
| C | -4.676369 | -0.414674 | -0.283771 |
| H | 4.356146 | 0.003795 | 1.300868 |
| H | 5.128506 | 0.823217 | -0.031359 |
| H | 2.860043 | 1.749799 | 0.261452 |
| H | 2.908578 | 0.882576 | -1.270078 |
| H | 1.899966 | -1.136290 | -0.126142 |
| H | 1.748965 | -0.205856 | 1.357084 |
| H | 0.261730 | 1.438891 | 0.173764 |
| H | 0.384517 | 0.482763 | -1.301837 |
| H | -0.649653 | -1.477450 | -0.090448 |
| H | -0.810150 | -0.483503 | 1.358287 |
| O | -2.430723 | 1.378509 | 0.237301 |
| H | -2.164337 | 0.039897 | -1.333324 |
| H | -3.090756 | -1.868924 | -0.001917 |
| H | -3.320548 | -0.781868 | 1.365284 |
| H | -4.704694 | -0.501968 | -1.376364 |
| H | -4.894866 | 0.624158 | -0.024349 |
| H | -5.473496 | -1.046799 | 0.120534 |
| H | -1.843654 | 1.985713 | -0.228650 |

Rotational constants (GHz): 4.4187400 0.3502900 0.3341900

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 35.1657 | 46.3707 | 71.0725 |
| 99.0286 | 118.0938 | 130.0981 |
| 160.5202 | 195.3762 | 220.2212 |
| 246.2257 | 278.8405 | 304.4620 |
| 343.5159 | 425.3214 | 465.9172 |
| 475.9392 | 525.1540 | 554.5384 |
| 746.7978 | 777.8244 | 791.0745 |
| 862.3853 | 898.1812 | 927.1960 |
| 958.1874 | 993.2797 | 1019.1802 |
| 1038.5248 | 1050.6609 | 1068.6395 |
| 1088.5471 | 1094.4740 | 1106.4961 |
| 1153.4861 | 1173.3124 | 1200.2864 |
| 1250.8327 | 1260.7140 | 1287.8251 |
| 1310.8837 | 1322.1881 | 1337.8562 |
| 1343.8642 | 1351.0761 | 1363.2509 |
| 1374.4220 | 1398.0075 | 1407.2651 |
| 1417.9450 | 1421.1630 | 1440.6100 |
| 1484.1410 | 1493.0908 | 1496.0741 |
| 1506.1088 | 1508.6673 | 1522.4851 |
| 1524.0414 | 2883.5201 | 2936.0406 |
| 2952.9730 | 3006.4131 | 3019.8598 |
| 3027.1443 | 3030.8688 | 3038.3175 |
| 3040.2471 | 3044.5017 | 3063.1023 |
| 3070.6461 | 3079.2249 | 3087.0582 |

3109.4420 3139.3778 3835.9165
Zero-point correction (Hartree): 0.241102

C8H17O.7oh.pttttt.p

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -465.48215328

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -4.566663 | -1.098012 | 0.221945 |
| C | -4.286984 | 0.176372 | -0.196825 |
| C | -2.929702 | 0.733460 | 0.247868 |
| C | -1.747698 | -0.106794 | -0.246976 |
| C | -0.391234 | 0.389125 | 0.266632 |
| C | 0.787623 | -0.452226 | -0.236826 |
| C | 2.151337 | 0.059483 | 0.229130 |
| C | 3.299501 | -0.865509 | -0.201972 |
| C | 4.683410 | -0.375074 | 0.236736 |
| H | -4.338606 | 0.128192 | -1.307686 |
| H | -5.122902 | 0.851767 | 0.072650 |
| H | -2.840603 | 1.768385 | -0.109965 |
| H | -2.919895 | 0.781004 | 1.344807 |
| H | -1.910236 | -1.147630 | 0.060687 |
| H | -1.741214 | -0.109163 | -1.346979 |
| H | -0.233052 | 1.430506 | -0.035989 |
| H | -0.396840 | 0.383986 | 1.366344 |
| H | 0.671871 | -1.492713 | 0.094174 |
| H | 0.788748 | -0.467911 | -1.335235 |
| O | 2.304329 | 1.372678 | -0.319297 |
| H | 2.146434 | 0.117821 | 1.332940 |
| H | 3.116315 | -1.864586 | 0.214179 |
| H | 3.271817 | -0.964973 | -1.294506 |
| H | 4.743020 | -0.263863 | 1.326308 |
| H | 4.925900 | 0.592271 | -0.217688 |
| H | 5.466951 | -1.076200 | -0.066147 |
| H | 3.073454 | 1.782754 | 0.094325 |

Rotational constants (GHz): 4.4735500 0.3506400 0.3346200

Vibrational harmonic frequencies (cm-1):

| | | |
|-----------|-----------|-----------|
| 38.2495 | 48.3745 | 68.3908 |
| 102.3351 | 118.9530 | 127.9573 |
| 160.2275 | 197.7886 | 231.6996 |
| 241.1016 | 293.7238 | 312.6613 |
| 343.9547 | 426.5764 | 465.0646 |
| 481.2669 | 519.2552 | 549.4256 |
| 744.6163 | 777.2353 | 790.4567 |
| 865.5164 | 894.5754 | 921.3373 |
| 963.6616 | 995.7601 | 1013.7782 |
| 1036.7914 | 1047.0233 | 1071.2352 |
| 1092.8031 | 1094.9584 | 1109.5011 |
| 1144.4852 | 1164.8634 | 1199.9290 |
| 1250.9414 | 1269.3828 | 1291.9759 |
| 1304.1398 | 1319.1262 | 1335.0474 |
| 1339.7977 | 1350.0139 | 1363.4285 |
| 1372.1135 | 1399.1921 | 1406.3369 |
| 1418.4752 | 1424.9456 | 1442.5228 |
| 1484.2015 | 1493.2719 | 1495.9407 |
| 1506.6959 | 1514.7987 | 1523.2567 |
| 1525.9309 | 2881.1934 | 2933.9857 |
| 2951.2083 | 3012.9940 | 3020.3172 |
| 3028.3522 | 3032.3598 | 3036.3694 |
| 3038.4301 | 3058.1269 | 3064.9885 |
| 3074.2170 | 3077.5059 | 3095.6041 |
| 3104.9597 | 3117.2180 | 3833.7785 |

Zero-point correction (Hartree): 0.241141

C8H17O.7oh.pttttt.t

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -465.48269443

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 4.564688 | -1.100695 | -0.198045 |
| C | 4.285191 | 0.183510 | 0.189517 |
| C | 2.926015 | 0.728114 | -0.264909 |
| C | 1.747203 | -0.106823 | 0.246579 |
| C | 0.388949 | 0.374775 | -0.275595 |
| C | -0.789627 | -0.465414 | 0.229870 |
| C | -2.158314 | 0.058633 | -0.227731 |
| C | -3.315267 | -0.841687 | 0.229200 |
| C | -4.684128 | -0.368967 | -0.267972 |
| H | 4.341657 | 0.164194 | 1.300995 |
| H | 5.119388 | 0.852339 | -0.100639 |
| H | 2.833944 | 1.769627 | 0.072479 |
| H | 2.914668 | 0.754167 | -1.362428 |
| H | 1.913037 | -1.152317 | -0.042436 |
| H | 1.742325 | -0.090316 | 1.346763 |
| H | 0.223710 | 1.420480 | 0.009940 |

| | | | | |
|--|-----------|-----------|-----------|-----------|
| H | 0.396053 | 0.358235 | -1.374690 | |
| H | -0.675758 | -1.506008 | -0.102960 | |
| H | -0.777282 | -0.497139 | 1.331120 | |
| O | -2.360496 | 1.414277 | 0.187792 | |
| H | -2.167063 | 0.113208 | -1.325032 | |
| H | -3.122212 | -1.866929 | -0.112164 | |
| H | -3.310628 | -0.883125 | 1.329313 | |
| H | -4.738522 | -0.404379 | -1.361945 | |
| H | -4.867567 | 0.664603 | 0.037496 | |
| H | -5.489658 | -0.996084 | 0.126898 | |
| H | -2.369750 | 1.417932 | 1.155566 | |
| Rotational constants (GHz): | 4.4470000 | | 0.3501300 | 0.3343500 |
| Vibrational harmonic frequencies (cm-1): | | | | |
| 34.8115 | 47.5240 | | | 68.8041 |
| 102.9514 | 122.8139 | | | 129.4399 |
| 161.2269 | 198.9416 | | | 223.8807 |
| 244.5627 | 303.9372 | | | 313.1571 |
| 348.0954 | 425.2319 | | | 460.9392 |
| 479.8605 | 527.9030 | | | 558.7185 |
| 744.5014 | 780.2222 | | | 791.1394 |
| 860.3842 | 893.7762 | | | 921.3755 |
| 963.3576 | 992.5873 | | | 1018.3795 |
| 1032.6123 | 1049.0102 | | | 1073.4716 |
| 1093.5179 | 1095.5503 | | | 1116.1190 |
| 1128.2713 | 1154.4782 | | | 1199.5980 |
| 1248.2904 | 1263.9167 | | | 1283.9954 |
| 1305.9058 | 1321.5825 | | | 1334.0004 |
| 1348.5574 | 1362.2411 | | | 1368.1079 |
| 1374.0156 | 1395.7960 | | | 1410.6549 |
| 1418.1991 | 1418.8072 | | | 1430.7886 |
| 1488.4990 | 1494.4416 | | | 1499.9591 |
| 1506.9339 | 1509.4381 | | | 1523.1425 |
| 1523.9605 | 2881.3354 | | | 2934.8914 |
| 2997.5217 | 3008.5142 | | | 3011.6271 |
| 3026.1391 | 3032.9294 | | | 3038.9938 |
| 3047.7060 | 3050.6620 | | | 3058.9176 |
| 3065.8219 | 3074.5028 | | | 3090.8621 |
| 3113.0911 | 3134.9138 | | | 3787.1811 |
| Zero-point correction (Hartree): | 0.241139 | | | |

C8H17O.1-6Hshift.7oh.Rt.mm

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -465.46470901

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | | |
|--|-----------|-----------|-----------|-----------|
| O | -1.698142 | -1.660450 | -0.095578 | |
| C | -2.830586 | -0.916560 | -0.463686 | |
| C | -3.001496 | 0.399436 | 0.308949 | |
| C | -1.988613 | 1.502590 | -0.044686 | |
| C | -0.522479 | 1.199149 | 0.323783 | |
| C | 0.081455 | 0.051124 | -0.467296 | |
| C | 1.471290 | -0.448364 | -0.075028 | |
| C | 2.587359 | 0.506464 | -0.555627 | |
| C | 3.991257 | -0.037893 | -0.276834 | |
| H | -2.861435 | -0.718841 | -1.551031 | |
| H | -3.683244 | -1.577882 | -0.243623 | |
| H | -2.950891 | 0.177173 | 1.382759 | |
| H | -4.011301 | 0.781788 | 0.109482 | |
| H | -2.287452 | 2.424983 | 0.468044 | |
| H | -2.051110 | 1.719164 | -1.120999 | |
| H | -0.467374 | 0.967297 | 1.395854 | |
| H | 0.074455 | 2.110961 | 0.167289 | |
| H | -0.705151 | -0.916411 | -0.269649 | |
| H | 0.006626 | 0.205785 | -1.550733 | |
| O | 1.583105 | -0.719306 | 1.319307 | |
| H | 1.631700 | -1.422079 | -0.555535 | |
| H | 2.459030 | 0.690433 | -1.629676 | |
| H | 2.458237 | 1.480339 | -0.061222 | |
| H | 4.168123 | -0.967590 | -0.829081 | |
| H | 4.115457 | -0.257575 | 0.786789 | |
| H | 4.760626 | 0.681153 | -0.575565 | |
| H | 1.534885 | 0.123677 | 1.789626 | |
| Rotational constants (GHz): | 2.5564600 | | 0.6096200 | 0.5554700 |
| Vibrational harmonic frequencies (cm-1): | | | | |
| i1400.4080 | 47.1486 | | | 66.5790 |
| 88.6296 | 131.3895 | | | 184.9712 |
| 201.7534 | 233.5673 | | | 242.6226 |
| 273.8855 | 308.2025 | | | 338.2078 |
| 366.8825 | 409.4540 | | | 467.8439 |
| 482.0418 | 582.6983 | | | 673.2470 |
| 770.0622 | 783.9899 | | | 793.5806 |
| 828.4691 | 868.2782 | | | 904.9772 |
| 941.2574 | 960.3999 | | | 995.4846 |
| 1019.6248 | 1036.8501 | | | 1065.2407 |
| 1077.3727 | 1097.2913 | | | 1100.9019 |

| | | |
|-----------|-----------|-----------|
| 1141.6413 | 1148.1577 | 1200.5715 |
| 1226.6344 | 1245.1258 | 1258.4733 |
| 1274.9921 | 1292.2711 | 1317.6935 |
| 1329.1530 | 1346.0788 | 1376.4613 |
| 1383.2562 | 1395.3060 | 1401.2190 |
| 1406.1328 | 1418.3996 | 1431.8995 |
| 1468.7132 | 1480.6443 | 1482.5028 |
| 1492.6988 | 1497.9347 | 1503.8020 |
| 1507.4727 | 1521.6771 | 2949.8057 |
| 3000.1266 | 3013.2597 | 3019.8978 |
| 3020.6592 | 3033.8060 | 3047.8053 |
| 3049.1837 | 3051.2594 | 3065.3738 |
| 3069.0258 | 3074.6475 | 3079.3042 |
| 3114.7711 | 3136.3383 | 3808.4529 |

Zero-point correction (Hartree): 0.237899

C8H17O.1-6Hshift.7oh.Rt.mp

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -465.47135670

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 1.418959 | -1.568596 | 0.362824 |
| C | 2.703842 | -1.003419 | 0.242199 |
| C | 2.771420 | 0.265399 | -0.618806 |
| C | 2.020522 | 1.485396 | -0.054020 |
| C | 0.481552 | 1.389039 | -0.121868 |
| C | -0.121803 | 0.348808 | 0.809408 |
| C | -1.399215 | -0.349077 | 0.343019 |
| C | -2.597543 | 0.602940 | 0.215316 |
| C | -3.886297 | -0.125563 | -0.178962 |
| H | 3.142370 | -0.802882 | 1.234705 |
| H | 3.316575 | -1.790172 | -0.225183 |
| H | 2.397521 | 0.034650 | -1.624834 |
| H | 3.832467 | 0.525409 | -0.726832 |
| H | 2.330791 | 2.370840 | -0.621635 |
| H | 2.339411 | 1.662528 | 0.983479 |
| H | 0.184584 | 1.147557 | -1.148532 |
| H | 0.053616 | 2.373710 | 0.112198 |
| H | 0.660385 | -0.613951 | 0.807030 |
| H | -0.154786 | 0.658359 | 1.860792 |
| O | -1.192114 | -0.958029 | -0.926534 |
| H | -1.655257 | -1.117507 | 1.094041 |
| H | -2.732783 | 1.121982 | 1.172810 |
| H | -2.356942 | 1.366498 | -0.533851 |
| H | -4.169383 | -0.864945 | 0.578995 |
| H | -3.752425 | -0.651498 | -1.127222 |
| H | -4.717787 | 0.578665 | -0.286211 |
| H | -0.367975 | -1.467372 | -0.857786 |

Rotational constants (GHz): 2.5149200 0.6790200 0.5958000

Vibrational harmonic frequencies (cm-1):

| | | |
|------------|-----------|-----------|
| i1189.6850 | 53.5300 | 83.2693 |
| 107.1826 | 127.3070 | 194.8000 |
| 221.9314 | 235.4020 | 270.7057 |
| 283.4557 | 339.0148 | 358.8992 |
| 393.3226 | 469.4404 | 493.5855 |
| 546.8156 | 657.1961 | 666.9213 |
| 776.7084 | 785.9203 | 823.0063 |
| 838.1684 | 879.1443 | 917.2234 |
| 948.1148 | 957.4163 | 992.6389 |
| 1013.6748 | 1047.8253 | 1059.1319 |
| 1077.5925 | 1085.9489 | 1131.2552 |
| 1136.7137 | 1164.2757 | 1206.3989 |
| 1219.0865 | 1270.1932 | 1282.8189 |
| 1289.7686 | 1313.5024 | 1326.2678 |
| 1340.0568 | 1353.7612 | 1374.3695 |
| 1378.1596 | 1389.2142 | 1394.2564 |
| 1404.2809 | 1419.2548 | 1426.9180 |
| 1469.5212 | 1482.6160 | 1486.3423 |
| 1491.1350 | 1496.9677 | 1502.0624 |
| 1508.6828 | 1523.3591 | 2957.5101 |
| 2971.5555 | 3016.6272 | 3019.5323 |
| 3025.6349 | 3035.6217 | 3040.8941 |
| 3046.5865 | 3069.7622 | 3073.6720 |
| 3078.0062 | 3083.5955 | 3093.4129 |
| 3111.6145 | 3143.2124 | 3731.6321 |

Zero-point correction (Hartree): 0.239174

C8H17O.1-6Hshift.7oh.Rt.mt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -465.46496551

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -1.692221 | -1.659448 | -0.149103 |
| C | -2.838285 | -0.906420 | -0.450320 |
| C | -2.977745 | 0.390573 | 0.360198 |

| | | | |
|---|-----------|-----------|-----------|
| C | -1.984061 | 1.505452 | -0.012674 |
| C | -0.506361 | 1.214346 | 0.314404 |
| C | 0.080504 | 0.071913 | -0.496712 |
| C | 1.456455 | -0.445112 | -0.107908 |
| C | 2.587276 | 0.501956 | -0.568665 |
| C | 3.983796 | -0.015462 | -0.209140 |
| H | -2.913850 | -0.681057 | -1.530343 |
| H | -3.681616 | -1.573790 | -0.211896 |
| H | -2.879738 | 0.144290 | 1.425314 |
| H | -3.996896 | 0.771999 | 0.212383 |
| H | -2.277292 | 2.420476 | 0.516430 |
| H | -2.083301 | 1.730675 | -1.084989 |
| H | -0.397654 | 0.982799 | 1.379208 |
| H | 0.080445 | 2.127866 | 0.134074 |
| H | -0.707327 | -0.891600 | -0.311770 |
| H | 0.012789 | 0.236490 | -1.578789 |
| O | 1.470815 | -0.621684 | 1.307603 |
| H | 1.608201 | -1.416345 | -0.609591 |
| H | 2.510805 | 0.634173 | -1.655343 |
| H | 2.429067 | 1.486039 | -0.112336 |
| H | 4.171434 | -1.002000 | -0.650226 |
| H | 4.107726 | -0.097354 | 0.876117 |
| H | 4.761831 | 0.662313 | -0.573434 |
| H | 2.217152 | -1.189388 | 1.532108 |
| Rotational constants (GHz): | 2.5727700 | 0.6146800 | 0.5597600 |
| Vibrational harmonic frequencies (cm ⁻¹): | | | |
| 11368.0150 | 51.3875 | | 66.0390 |
| 92.2447 | 127.7171 | | 185.0266 |
| 198.9137 | 215.7595 | | 238.1321 |
| 268.7846 | 281.0463 | | 337.7001 |
| 370.2613 | 408.9980 | | 464.5911 |
| 483.8038 | 583.1159 | | 659.5689 |
| 767.9657 | 781.5480 | | 791.4709 |
| 835.4439 | 870.3056 | | 905.5074 |
| 941.6820 | 959.5952 | | 997.8103 |
| 1017.8175 | 1037.7126 | | 1060.9627 |
| 1077.9034 | 1095.8319 | | 1116.0030 |
| 1138.3990 | 1161.4896 | | 1187.0812 |
| 1226.8608 | 1244.3995 | | 1247.1836 |
| 1282.2174 | 1290.0317 | | 1300.8293 |
| 1329.9325 | 1344.9415 | | 1379.8838 |
| 1383.7250 | 1395.3721 | | 1404.7423 |
| 1406.6115 | 1416.7732 | | 1436.3177 |
| 1468.9009 | 1481.4472 | | 1482.7894 |
| 1491.0059 | 1495.9633 | | 1503.9558 |
| 1513.4362 | 1525.7111 | | 2946.4726 |
| 2969.0632 | 3006.3937 | | 3009.5606 |
| 3017.3049 | 3032.7516 | | 3038.7183 |
| 3041.8367 | 3065.2161 | | 3070.8373 |
| 3077.8881 | 3084.3516 | | 3098.6684 |
| 3110.1086 | 3118.2875 | | 3844.8654 |
| Zero-point correction (Hartree): | 0.237756 | | |

C8H17O.1-6Hshift.7oh.Rt.pm

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -465.46802117

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 1.025171 | -1.597807 | -0.325629 |
| C | 2.391102 | -1.306868 | -0.151881 |
| C | 2.812105 | 0.085920 | -0.643639 |
| C | 2.294527 | 1.269945 | 0.194613 |
| C | 0.769545 | 1.496855 | 0.140516 |
| C | -0.021127 | 0.383255 | 0.803161 |
| C | -1.531656 | 0.289842 | 0.614428 |
| C | -1.979921 | 0.216047 | -0.854668 |
| C | -3.499159 | 0.104095 | -1.007024 |
| H | 2.708344 | -1.446284 | 0.896905 |
| H | 2.916641 | -2.072706 | -0.743536 |
| H | 2.486641 | 0.198632 | -1.686110 |
| H | 3.909496 | 0.119545 | -0.648265 |
| H | 2.790519 | 2.182703 | -0.156767 |
| H | 2.606396 | 1.137801 | 1.240683 |
| H | 0.465574 | 1.608336 | -0.906984 |
| H | 0.530252 | 2.451165 | 0.633987 |
| H | 0.407845 | -0.672040 | 0.288005 |
| H | 0.237409 | 0.256795 | 1.861031 |
| O | -2.037701 | -0.809865 | 1.372508 |
| H | -1.994163 | 1.176597 | 1.077804 |
| H | -1.620042 | 1.105874 | -1.385342 |
| H | -1.482330 | -0.643301 | -1.324708 |
| H | -4.002635 | 0.991830 | -0.606934 |
| H | -3.878606 | -0.763336 | -0.461269 |
| H | -3.783546 | 0.004673 | -2.059216 |

| | | | | |
|--|-----------|-----------|-----------|-----------|
| H | -1.610049 | -1.609456 | 1.032644 | |
| Rotational constants (GHz): | 2.0786400 | | 0.6809800 | 0.6316900 |
| Vibrational harmonic frequencies (cm-1): | | | | |
| i1253.0586 | 48.7030 | | | 57.8380 |
| 90.9748 | 138.1949 | | | 168.7982 |
| 196.6946 | 232.3625 | | | 263.0496 |
| 280.1338 | 339.9560 | | | 349.7025 |
| 395.5165 | 431.5502 | | | 475.6311 |
| 490.8234 | 568.3715 | | | 616.3062 |
| 772.9291 | 788.0286 | | | 792.0603 |
| 828.4053 | 878.3043 | | | 908.6751 |
| 946.4830 | 989.1181 | | | 992.4261 |
| 1022.4808 | 1049.8457 | | | 1067.9223 |
| 1078.3994 | 1097.6424 | | | 1106.9225 |
| 1132.5579 | 1161.0777 | | | 1211.2418 |
| 1215.9852 | 1231.3754 | | | 1264.6714 |
| 1278.5796 | 1287.7951 | | | 1306.8328 |
| 1324.9624 | 1341.2701 | | | 1379.9661 |
| 1388.3171 | 1392.2870 | | | 1397.2726 |
| 1408.4846 | 1416.2179 | | | 1429.4578 |
| 1455.2003 | 1481.0095 | | | 1483.2809 |
| 1491.5143 | 1501.9048 | | | 1504.0958 |
| 1510.5565 | 1524.2256 | | | 2962.4225 |
| 2993.8444 | 3008.7153 | | | 3015.3137 |
| 3024.1136 | 3034.5794 | | | 3034.9169 |
| 3047.7242 | 3063.0583 | | | 3071.1483 |
| 3076.5201 | 3077.4354 | | | 3085.4388 |
| 3112.8116 | 3139.1646 | | | 3783.8426 |
| Zero-point correction (Hartree): | 0.238104 | | | |

C8H17O.1-6Hshift.7oh.Rt.pp

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -465.46503236

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 1.081131 | -1.632374 | -0.128005 |
| C | 2.433643 | -1.298914 | 0.056803 |
| C | 2.861664 | 0.014775 | -0.612196 |
| C | 2.291704 | 1.291433 | 0.030558 |
| C | 0.764466 | 1.461489 | -0.089023 |
| C | -0.027613 | 0.440210 | 0.708907 |
| C | -1.539836 | 0.389295 | 0.509898 |
| C | -1.969436 | -0.119031 | -0.871046 |
| C | -3.486270 | -0.080432 | -1.076642 |
| H | 2.710176 | -1.281310 | 1.126688 |
| H | 2.991495 | -2.133552 | -0.395723 |
| H | 2.576720 | -0.026972 | -1.671524 |
| H | 3.957880 | 0.069204 | -0.579436 |
| H | 2.772082 | 2.159428 | -0.437033 |
| H | 2.577999 | 1.320928 | 1.092075 |
| H | 0.481742 | 1.410010 | -1.147785 |
| H | 0.489354 | 2.471890 | 0.251037 |
| H | 0.409648 | -0.696896 | 0.355759 |
| H | 0.235233 | 0.469107 | 1.775806 |
| O | -2.159145 | -0.464586 | 1.467791 |
| H | -1.921699 | 1.424895 | 0.629073 |
| H | -1.474508 | 0.487282 | -1.638217 |
| H | -1.593847 | -1.142091 | -0.985110 |
| H | -3.871254 | 0.943689 | -1.003050 |
| H | -3.992930 | -0.684426 | -0.320256 |
| H | -3.756167 | -0.467064 | -2.064490 |
| H | -1.937743 | -0.141390 | 2.350332 |

| | | | |
|-----------------------------|-----------|-----------|-----------|
| Rotational constants (GHz): | 2.1045200 | 0.6628800 | 0.6252100 |
|-----------------------------|-----------|-----------|-----------|

| | | | |
|--|-----------|--|-----------|
| Vibrational harmonic frequencies (cm-1): | | | |
| i1428.2782 | 43.5663 | | 60.9648 |
| 81.4566 | 135.5890 | | 179.6590 |
| 199.9966 | 225.3699 | | 255.2219 |
| 275.1584 | 281.9243 | | 336.3103 |
| 388.6806 | 417.3081 | | 473.2349 |
| 497.5097 | 563.3990 | | 595.5991 |
| 775.4008 | 783.4949 | | 795.5282 |
| 836.9489 | 877.2543 | | 910.9131 |
| 947.0336 | 988.9403 | | 998.4154 |
| 1022.0931 | 1054.1617 | | 1071.0558 |
| 1076.4264 | 1099.4374 | | 1100.7677 |
| 1124.1179 | 1158.0508 | | 1207.2603 |
| 1223.1870 | 1246.9599 | | 1259.2551 |
| 1270.7322 | 1291.7434 | | 1316.6476 |
| 1323.6787 | 1334.2811 | | 1371.8712 |
| 1384.2191 | 1394.3276 | | 1399.6419 |
| 1407.5862 | 1421.1099 | | 1432.1325 |
| 1460.6914 | 1481.2484 | | 1483.6354 |
| 1490.6611 | 1494.6086 | | 1502.8249 |
| 1507.8154 | 1522.9892 | | 2892.3006 |
| 2954.4558 | 3003.4055 | | 3014.6352 |

| | | |
|-----------|-----------|-----------|
| 3020.4521 | 3033.8865 | 3037.7536 |
| 3044.0337 | 3056.6210 | 3066.0532 |
| 3072.7476 | 3079.8733 | 3096.5500 |
| 3112.2131 | 3142.6979 | 3819.0441 |

Zero-point correction (Hartree): 0.237628

C8H17O.1-6Hshift.7oh.Rt.pt

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -465.46517821

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 1.048775 | -1.631027 | -0.033259 |
| C | 2.407605 | -1.314541 | 0.134441 |
| C | 2.859655 | -0.047473 | -0.604975 |
| C | 2.306161 | 1.272055 | -0.038783 |
| C | 0.781693 | 1.456593 | -0.171927 |
| C | -0.024089 | 0.504357 | 0.693042 |
| C | -1.528130 | 0.454119 | 0.484980 |
| C | -1.945758 | -0.152484 | -0.866636 |
| C | -3.463463 | -0.199691 | -1.073322 |
| H | 2.683325 | -1.244169 | 1.201994 |
| H | 2.949558 | -2.183172 | -0.271462 |
| H | 2.579704 | -0.144467 | -1.662146 |
| H | 3.956490 | -0.008208 | -0.568831 |
| H | 2.800151 | 2.104357 | -0.554751 |
| H | 2.589874 | 1.359135 | 1.020021 |
| H | 0.499848 | 1.341565 | -1.226233 |
| H | 0.522033 | 2.490810 | 0.101973 |
| H | 0.399306 | -0.654426 | 0.419587 |
| H | 0.210640 | 0.598834 | 1.759046 |
| O | -2.053825 | -0.284637 | 1.585626 |
| H | -1.903798 | 1.497972 | 0.524034 |
| H | -1.493675 | 0.439852 | -1.671041 |
| H | -1.521665 | -1.159932 | -0.938414 |
| H | -3.914485 | 0.796601 | -0.989485 |
| H | -3.952577 | -0.856719 | -0.344479 |
| H | -3.710975 | -0.591582 | -2.064361 |
| H | -3.015406 | -0.298743 | 1.504690 |

Rotational constants (GHz): 2.0902000 0.6678600 0.6311700

Vibrational harmonic frequencies (cm-1):

| | | |
|------------|-----------|-----------|
| i1402.1721 | 47.7148 | 62.9665 |
| 80.6167 | 135.0571 | 183.2783 |
| 200.8299 | 231.9850 | 257.7131 |
| 273.5369 | 309.8187 | 338.3748 |
| 387.0608 | 419.2541 | 476.6458 |
| 500.3560 | 556.3099 | 601.0061 |
| 772.5701 | 791.0826 | 795.8602 |
| 836.6985 | 875.2072 | 910.7315 |
| 948.0214 | 989.4604 | 999.1021 |
| 1015.8709 | 1047.9258 | 1068.2079 |
| 1078.8526 | 1096.6690 | 1111.5205 |
| 1145.6641 | 1157.8629 | 1208.9932 |
| 1214.4284 | 1230.6695 | 1270.7032 |
| 1284.0440 | 1290.8318 | 1305.6302 |
| 1324.0063 | 1334.3191 | 1381.1062 |
| 1385.4562 | 1396.8129 | 1398.0526 |
| 1406.8699 | 1415.8399 | 1433.5566 |
| 1461.6952 | 1482.0127 | 1484.0749 |
| 1491.5965 | 1495.0920 | 1503.7136 |
| 1512.6084 | 1526.3822 | 2893.3889 |
| 2959.1273 | 3004.2615 | 3013.1534 |
| 3022.8924 | 3032.9465 | 3034.7707 |
| 3052.9407 | 3062.1744 | 3069.5711 |
| 3077.2165 | 3088.2371 | 3089.4229 |
| 3111.0158 | 3118.0463 | 3830.6599 |

Zero-point correction (Hartree): 0.237846

C8H17O.1-6Hshift.7oh.Rt.tm

 E(UB+HF-LYP/6-31G(d,p)) (Hartree): -465.46837440

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 1.191894 | -1.705102 | -0.233716 |
| C | 2.474619 | -1.380290 | 0.242313 |
| C | 3.044520 | -0.067650 | -0.314750 |
| C | 2.360618 | 1.214803 | 0.193187 |
| C | 0.896569 | 1.400943 | -0.248184 |
| C | -0.054719 | 0.380284 | 0.349287 |
| C | -1.470410 | 0.339707 | -0.211432 |
| C | -2.303056 | -0.813924 | 0.360263 |
| C | -3.705743 | -0.904587 | -0.246572 |
| H | 2.511919 | -1.367147 | 1.346657 |
| H | 3.112045 | -2.217829 | -0.081852 |
| H | 2.993058 | -0.106675 | -1.410660 |

| | | | |
|---|-----------|-----------|-----------|
| H | 4.108643 | -0.023418 | -0.047501 |
| H | 2.939578 | 2.076853 | -0.159773 |
| H | 2.416229 | 1.242477 | 1.291485 |
| H | 0.836375 | 1.350195 | -1.343770 |
| H | 0.553951 | 2.407663 | 0.026526 |
| H | 0.447450 | -0.742110 | 0.071848 |
| H | -0.045273 | 0.386404 | 1.448912 |
| O | -2.110971 | 1.609852 | -0.011404 |
| H | -1.414827 | 0.237242 | -1.302484 |
| H | -1.754640 | -1.750431 | 0.201606 |
| H | -2.373503 | -0.684560 | 1.451464 |
| H | -3.655558 | -1.119229 | -1.319868 |
| H | -4.243124 | 0.039848 | -0.123536 |
| H | -4.291048 | -1.699665 | 0.225553 |
| H | -2.243054 | 1.716668 | 0.941686 |
| Rotational constants (GHz): | 2.2072400 | 0.6665100 | 0.5384500 |
| Vibrational harmonic frequencies (cm ⁻¹): | | | |
| i1370.3005 | 55.9621 | | 61.6981 |
| 95.9558 | 118.5040 | | 187.0112 |
| 197.2306 | 225.5262 | | 255.4282 |
| 290.0790 | 331.8759 | | 338.8942 |
| 375.9839 | 408.7287 | | 455.4181 |
| 482.2171 | 534.5861 | | 633.6835 |
| 773.9912 | 786.0658 | | 794.8409 |
| 862.5705 | 877.7698 | | 900.3221 |
| 949.2642 | 980.0072 | | 993.1650 |
| 1021.4201 | 1053.5910 | | 1064.9357 |
| 1086.9144 | 1093.8334 | | 1111.3046 |
| 1124.3495 | 1153.9665 | | 1185.7925 |
| 1220.2849 | 1237.0477 | | 1261.1696 |
| 1265.7831 | 1283.1246 | | 1306.1604 |
| 1333.6400 | 1358.0643 | | 1380.6324 |
| 1393.6223 | 1396.3969 | | 1406.0541 |
| 1411.1190 | 1416.5978 | | 1427.8188 |
| 1453.4233 | 1480.4836 | | 1482.4473 |
| 1492.7389 | 1499.1963 | | 1503.2426 |
| 1510.9374 | 1523.7410 | | 2956.3393 |
| 3007.9625 | 3013.6045 | | 3017.5026 |
| 3025.8988 | 3033.4754 | | 3035.1014 |
| 3049.4241 | 3057.0974 | | 3065.5765 |
| 3069.0551 | 3076.0535 | | 3078.1129 |
| 3115.9089 | 3132.9242 | | 3785.2552 |
| Zero-point correction (Hartree): | 0.237900 | | |

C8H17O.1-6Hshift.7oh.Rt.tp

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -465.46756992

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 1.181009 | -1.698016 | -0.258551 |
| C | 2.468572 | -1.392058 | 0.215852 |
| C | 3.041223 | -0.071741 | -0.319361 |
| C | 2.364675 | 1.202490 | 0.216905 |
| C | 0.897991 | 1.403130 | -0.213392 |
| C | -0.058914 | 0.377946 | 0.370562 |
| C | -1.470645 | 0.334085 | -0.202219 |
| C | -2.308957 | -0.799849 | 0.386896 |
| C | -3.700747 | -0.912149 | -0.241157 |
| H | 2.513399 | -1.400368 | 1.319787 |
| H | 3.099554 | -2.225942 | -0.129298 |
| H | 2.984671 | -0.089561 | -1.415622 |
| H | 4.106564 | -0.034645 | -0.056153 |
| H | 2.944694 | 2.069933 | -0.120755 |
| H | 2.421474 | 1.208130 | 1.314931 |
| H | 0.837233 | 1.376411 | -1.310999 |
| H | 0.578309 | 2.410157 | 0.094531 |
| H | 0.445186 | -0.741723 | 0.079212 |
| H | -0.065075 | 0.385618 | 1.467409 |
| O | -2.152758 | 1.562744 | 0.095960 |
| H | -1.405214 | 0.200271 | -1.295025 |
| H | -1.753708 | -1.736602 | 0.259469 |
| H | -2.398588 | -0.627034 | 1.467255 |
| H | -3.634395 | -1.136125 | -1.312266 |
| H | -4.251442 | 0.024968 | -0.126386 |
| H | -4.280541 | -1.712403 | 0.229415 |
| H | -1.767315 | 2.259966 | -0.449280 |
| Rotational constants (GHz): | 2.2149100 | 0.6667500 | 0.5388100 |
| Vibrational harmonic frequencies (cm ⁻¹): | | | |
| i1369.0666 | 53.8464 | | 61.8376 |
| 93.5438 | 113.4466 | | 183.3979 |
| 195.4096 | 223.8983 | | 256.4613 |
| 286.8741 | 299.0703 | | 339.0770 |
| 374.5790 | 404.3545 | | 456.5330 |
| 479.0459 | 526.6552 | | 632.9042 |
| 775.2563 | 786.3043 | | 794.4587 |

| | | |
|-----------|-----------|-----------|
| 864.8401 | 881.1384 | 903.5213 |
| 949.9833 | 978.6414 | 995.7518 |
| 1023.7477 | 1053.5699 | 1072.5097 |
| 1073.6156 | 1096.2840 | 1105.7115 |
| 1134.0991 | 1158.8736 | 1193.0874 |
| 1220.1225 | 1242.9233 | 1257.2024 |
| 1266.3456 | 1287.4562 | 1310.8128 |
| 1327.8279 | 1355.2440 | 1380.2879 |
| 1382.6143 | 1396.1453 | 1406.5153 |
| 1407.7462 | 1422.5439 | 1428.5751 |
| 1455.9974 | 1481.0302 | 1483.1958 |
| 1493.4377 | 1494.3213 | 1503.5559 |
| 1510.7046 | 1524.1424 | 2958.4178 |
| 2981.1953 | 3001.5420 | 3014.9238 |
| 3021.9318 | 3033.9491 | 3041.4659 |
| 3043.5340 | 3046.7534 | 3069.0596 |
| 3074.3412 | 3078.6807 | 3086.3680 |
| 3112.1227 | 3138.5279 | 3826.9207 |

Zero-point correction (Hartree): 0.237820

C8H17O.1-6Hshift.7oh.Rt.tt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -465.46664929

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 1.179396 | -1.694266 | -0.264623 |
| C | 2.467600 | -1.387716 | 0.211776 |
| C | 3.041126 | -0.065874 | -0.318795 |
| C | 2.365123 | 1.207923 | 0.220452 |
| C | 0.899764 | 1.409649 | -0.210405 |
| C | -0.052693 | 0.382693 | 0.370058 |
| C | -1.457593 | 0.337060 | -0.205011 |
| C | -2.288534 | -0.816489 | 0.373479 |
| C | -3.702815 | -0.902031 | -0.208909 |
| H | 2.509911 | -1.399687 | 1.315657 |
| H | 3.097263 | -2.221906 | -0.134881 |
| H | 2.984861 | -0.080608 | -1.415157 |
| H | 4.106634 | -0.032911 | -0.055355 |
| H | 2.946424 | 2.075266 | -0.115332 |
| H | 2.424504 | 1.210909 | 1.318681 |
| H | 0.835236 | 1.385393 | -1.306883 |
| H | 0.559479 | 2.408590 | 0.093724 |
| H | 0.450757 | -0.739808 | 0.073849 |
| H | -0.055758 | 0.373848 | 1.466988 |
| O | -2.047644 | 1.614253 | 0.080013 |
| H | -1.377244 | 0.203035 | -1.297764 |
| H | -1.752203 | -1.755150 | 0.187798 |
| H | -2.342959 | -0.687931 | 1.461932 |
| H | -3.680692 | -1.033873 | -1.297403 |
| H | -4.281888 | 0.001792 | 0.012962 |
| H | -4.253533 | -1.747552 | 0.213922 |
| H | -2.856674 | 1.689403 | -0.441722 |

Rotational constants (GHz): 2.2130200 0.6702200 0.5404700

Vibrational harmonic frequencies (cm-1):

| | | |
|------------|-----------|-----------|
| i1416.2333 | 52.6913 | 60.7929 |
| 94.0984 | 111.5644 | 182.9569 |
| 194.8017 | 209.8852 | 257.1724 |
| 265.6485 | 291.2540 | 338.5436 |
| 375.7080 | 407.3570 | 454.3679 |
| 480.3618 | 525.1393 | 634.0585 |
| 769.7968 | 781.7141 | 794.2291 |
| 862.8606 | 876.8785 | 900.9760 |
| 949.3255 | 983.4589 | 986.7936 |
| 1021.7648 | 1048.9972 | 1068.4661 |
| 1086.7594 | 1091.5832 | 1106.0530 |
| 1130.9775 | 1159.5222 | 1191.8768 |
| 1213.4339 | 1233.4963 | 1261.3690 |
| 1274.1399 | 1285.8211 | 1302.0783 |
| 1320.8596 | 1349.2857 | 1380.6910 |
| 1387.8377 | 1394.3010 | 1402.4713 |
| 1406.4917 | 1420.4607 | 1439.9087 |
| 1457.5167 | 1480.6199 | 1482.5068 |
| 1491.3765 | 1492.4174 | 1503.4359 |
| 1514.6624 | 1525.1999 | 2959.7142 |
| 2969.2425 | 3015.3071 | 3019.8030 |
| 3025.3573 | 3033.3010 | 3037.0642 |
| 3041.8824 | 3059.9013 | 3068.3195 |
| 3073.7582 | 3078.2755 | 3081.4044 |
| 3106.3306 | 3118.5708 | 3821.7460 |

Zero-point correction (Hartree): 0.237565

C8H17O.1-6Hshift.7oh.St.mm

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -465.46901368

Electronic state : 2-A

```

Cartesian coordinates (Angs):
O      -1.538105      1.584954      -0.284647
C      -2.766248      1.023860      0.108956
C      -2.994510     -0.408976     -0.395076
C      -2.101563     -1.487936      0.245884
C      -0.601710     -1.408524     -0.110093
C       0.088134     -0.178728      0.451375
C       1.422444      0.250073     -0.143324
C       2.573038     -0.691281      0.240263
C       3.908101     -0.289376     -0.394702
H      -2.903056      1.064076      1.204297
H      -3.530069      1.686285     -0.327884
H      -2.864558     -0.418437     -1.485130
H      -4.043142     -0.667768     -0.197964
H      -2.475151     -2.471086     -0.064734
H      -2.216666     -1.450716      1.338701
H      -0.489017     -1.423948     -1.202786
H      -0.101538     -2.313476      0.264270
H      -0.653455      0.767828      0.145447
H       0.101953     -0.145964      1.547648
O       1.777834      1.549633      0.323149
H       1.327332      0.253011     -1.243900
H       2.661325     -0.689502      1.333991
H       2.305209     -1.711708     -0.059545
H       4.180948      0.727231     -0.102432
H       3.850470     -0.321534     -1.488814
H       4.709070     -0.967285     -0.082288
H       1.056406      2.151624      0.093418
Rotational constants (GHz):      2.4274600      0.6425600      0.5364400
Vibrational harmonic frequencies (cm-1):
i1183.8411      47.8655      67.5186

      85.3890      110.1664      189.6389
      208.2766      216.5027      243.9936
      276.3385      334.6641      378.7431
      391.9228      403.1812      469.2564
      492.6222      520.9406      669.2918
      773.5726      787.0577      791.3267
      856.6642      867.3827      918.6388
      944.3181      992.9212     1001.2410
      1019.4510     1050.5428     1069.5956
      1075.0175     1102.8198     1103.7942
      1139.8422     1159.3138     1199.1048
      1222.3170     1244.7031     1268.9508
      1269.5662     1285.6627     1312.6231
      1327.6072     1349.9655     1379.8000
      1382.1013     1390.8943     1396.2230
      1406.1288     1416.0372     1417.7301

      1462.2252     1480.5646     1482.2400
      1489.7274     1493.2311     1501.1231
      1507.7904     1522.5346     2960.1627
      2961.4355     3013.4903     3014.0093
      3023.0163     3034.4352     3041.7997
      3046.8337     3053.5844     3070.8483
      3075.0115     3079.7146     3083.3552
      3111.3928     3143.8844     3802.1192
Zero-point correction (Hartree): 0.238032

```

C8H17O.1-6Hshift.7oh.St.mp

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -465.46541459

Electronic state : 2-A

```

Cartesian coordinates (Angs):
O      -1.639691      1.576950      -0.354849
C      -2.811235      0.978371      0.135271
C      -3.026508     -0.467638     -0.332006
C      -2.056300     -1.497390      0.271531
C      -0.579057     -1.340259     -0.141293
C       0.077664     -0.075451      0.384418
C       1.446245      0.299452     -0.168066
C       2.541318     -0.710386      0.238645
C       3.911930     -0.365027     -0.350827
H      -2.870955      1.028505      1.238058
H      -3.628438      1.608635     -0.249208
H      -2.960368     -0.490692     -1.427513
H      -4.051310     -0.760823     -0.068243
H      -2.388269     -2.500635     -0.022112
H      -2.129350     -1.462881      1.368344
H      -0.503800     -1.357757     -1.237248
H      -0.022393     -2.218063      0.218108
H      -0.680068      0.875241      0.029501
H       0.047843     -0.015175      1.482408
O       1.811467      1.627217      0.203679
H       1.388259      0.327685     -1.264035

```

| | | | | |
|--|-----------|-----------|-----------|-----------|
| H | 2.598698 | -0.735662 | 1.337093 | |
| H | 2.239965 | -1.716712 | -0.076673 | |
| H | 4.207869 | 0.648078 | -0.067442 | |
| H | 3.890846 | -0.410463 | -1.445470 | |
| H | 4.678920 | -1.063535 | -0.001314 | |
| H | 1.784004 | 1.680895 | 1.169064 | |
| Rotational constants (GHz): | 2.4317600 | | 0.6338500 | 0.5300400 |
| Vibrational harmonic frequencies (cm-1): | | | | |
| i1437.2430 | | 38.5115 | | 70.9363 |
| 97.6497 | | 112.5625 | | 190.4923 |
| 206.6326 | | 222.7928 | | 243.3035 |
| 268.8822 | | 279.5267 | | 338.7477 |
| 383.0722 | | 405.7851 | | 465.4239 |
| 483.2140 | | 524.6649 | | 627.7374 |
| 770.5000 | | 786.1918 | | 796.6868 |
| 852.7037 | | 867.2780 | | 916.8416 |
| 945.4593 | | 990.3428 | | 998.4965 |
| 1023.8692 | | 1054.0278 | | 1064.1386 |
| 1081.6571 | | 1096.6704 | | 1101.7230 |
| 1128.0073 | | 1143.4851 | | 1186.0592 |
| 1225.6529 | | 1244.4128 | | 1255.1832 |
| 1276.2851 | | 1287.4810 | | 1310.6886 |
| 1333.0069 | | 1357.4898 | | 1378.0192 |
| 1382.3383 | | 1396.6558 | | 1400.3478 |
| 1407.6605 | | 1416.7185 | | 1425.9972 |
| 1446.0736 | | 1480.4165 | | 1482.3923 |
| 1492.0148 | | 1496.3489 | | 1502.7689 |
| 1507.5468 | | 1522.7993 | | 2950.8863 |
| 3011.1652 | | 3013.1489 | | 3015.7852 |
| 3020.1662 | | 3028.2226 | | 3034.0503 |
| 3048.2093 | | 3049.1966 | | 3059.3029 |
| 3069.2602 | | 3074.0040 | | 3078.8400 |
| 3113.7650 | | 3139.3294 | | 3796.1430 |
| Zero-point correction (Hartree): | 0.237599 | | | |

C8H17O.1-6Hshift.7oh.St.mt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -465.46506949

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | | |
|--|-----------|-----------|-----------|-----------|
| O | -1.624694 | 1.563950 | -0.412275 | |
| C | -2.814015 | 0.992857 | 0.067273 | |
| C | -3.021395 | -0.470736 | -0.345655 | |
| C | -2.059822 | -1.475238 | 0.312143 | |
| C | -0.576072 | -1.330288 | -0.082711 | |
| C | 0.073344 | -0.058998 | 0.433228 | |
| C | 1.430677 | 0.321513 | -0.128501 | |
| C | 2.504418 | -0.759251 | 0.122125 | |
| C | 3.889189 | -0.357043 | -0.395777 | |
| H | -2.904988 | 1.090228 | 1.164286 | |
| H | -3.616914 | 1.608943 | -0.367628 | |
| H | -2.937468 | -0.537494 | -1.438298 | |
| H | -4.050380 | -0.754318 | -0.087251 | |
| H | -2.386412 | -2.489106 | 0.050547 | |
| H | -2.149795 | -1.399849 | 1.405457 | |
| H | -0.486804 | -1.370011 | -1.177277 | |
| H | -0.027424 | -2.202437 | 0.301649 | |
| H | -0.680942 | 0.882987 | 0.067389 | |
| H | 0.059027 | 0.022490 | 1.526879 | |
| O | 1.790876 | 1.554654 | 0.494950 | |
| H | 1.330022 | 0.460973 | -1.218881 | |
| H | 2.552933 | -0.953692 | 1.200854 | |
| H | 2.189844 | -1.692167 | -0.360670 | |
| H | 4.257404 | 0.537400 | 0.117177 | |
| H | 3.869298 | -0.150579 | -1.472883 | |
| H | 4.619947 | -1.153785 | -0.226410 | |
| H | 2.475255 | 1.974689 | -0.039084 | |
| Rotational constants (GHz): | 2.4324800 | | 0.6354900 | 0.5343300 |
| Vibrational harmonic frequencies (cm-1): | | | | |
| i1399.9778 | | 47.4704 | | 71.6464 |
| 99.6893 | | 109.5130 | | 194.2273 |
| 206.9217 | | 211.2482 | | 230.0993 |
| 269.0247 | | 294.8186 | | 338.7189 |
| 391.7348 | | 406.5276 | | 462.5066 |
| 487.7492 | | 520.5541 | | 638.7370 |
| 773.6097 | | 794.1514 | | 796.9122 |
| 853.7943 | | 865.5345 | | 919.8998 |
| 945.8633 | | 994.1403 | | 996.0030 |
| 1019.6061 | | 1044.8729 | | 1071.8620 |
| 1085.5172 | | 1100.1797 | | 1107.8671 |
| 1121.1720 | | 1153.0631 | | 1190.6376 |
| 1225.6793 | | 1247.9218 | | 1263.3553 |
| 1282.1530 | | 1289.4048 | | 1309.7538 |
| 1322.5463 | | 1341.0910 | | 1380.8518 |
| 1383.6957 | | 1391.3398 | | 1397.1551 |

| | | |
|-----------|-----------|-----------|
| 1409.0917 | 1416.1036 | 1429.1401 |
| 1452.5214 | 1480.1006 | 1482.3815 |
| 1491.2224 | 1493.3283 | 1502.7805 |
| 1512.6775 | 1526.8937 | 2956.7180 |
| 2970.3981 | 3010.9132 | 3011.2994 |
| 3021.5092 | 3032.2555 | 3039.2362 |
| 3042.4555 | 3050.6727 | 3068.1536 |
| 3074.8420 | 3078.7293 | 3084.1736 |
| 3110.5792 | 3120.2081 | 3843.2229 |

Zero-point correction (Hartree): 0.237755

C8H17O.1-6Hshift.7oh.St.pm

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -465.46641259

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -1.284036 | -1.630778 | -0.506825 |
| C | -2.594329 | -1.121643 | -0.467711 |
| C | -2.842272 | -0.078117 | 0.630908 |
| C | -2.145693 | 1.278392 | 0.418391 |
| C | -0.607084 | 1.242735 | 0.497819 |
| C | 0.036889 | 0.484694 | -0.649774 |
| C | 1.533474 | 0.184568 | -0.578836 |
| C | 1.952889 | -0.641407 | 0.638445 |
| C | 3.415213 | -1.091904 | 0.573710 |
| H | -2.903821 | -0.714435 | -1.447130 |
| H | -3.229488 | -2.001604 | -0.280279 |
| H | -2.532705 | -0.506781 | 1.592973 |
| H | -3.925368 | 0.091857 | 0.692287 |
| H | -2.514551 | 1.978248 | 1.178024 |
| H | -2.453072 | 1.694642 | -0.552355 |
| H | -0.309939 | 0.795801 | 1.454045 |
| H | -0.213624 | 2.268324 | 0.506585 |
| H | -0.524194 | -0.644624 | -0.670980 |
| H | -0.245251 | 0.906159 | -1.624821 |
| O | 2.276038 | 1.414222 | -0.528552 |
| H | 1.809911 | -0.376933 | -1.486172 |
| H | 1.795463 | -0.037614 | 1.539737 |
| H | 1.284294 | -1.506951 | 0.711418 |
| H | 4.079874 | -0.228688 | 0.481781 |
| H | 3.590288 | -1.746636 | -0.287995 |
| H | 3.696338 | -1.647040 | 1.474193 |
| H | 2.165307 | 1.864811 | -1.376009 |

Rotational constants (GHz): 2.0928600 0.6902400 0.5932800

Vibrational harmonic frequencies (cm-1):

| | | |
|------------|-----------|-----------|
| i1378.0553 | 49.3010 | 67.6669 |
| 93.4149 | 147.4897 | 177.7309 |
| 194.2238 | 221.9450 | 258.4064 |
| 285.5921 | 310.7433 | 337.3326 |
| 351.4417 | 404.5352 | 462.5176 |
| 481.8090 | 593.9917 | 666.4082 |
| 777.9979 | 782.6380 | 793.3125 |
| 830.3642 | 880.7142 | 893.8074 |
| 951.5733 | 976.0672 | 980.6190 |
| 1018.5661 | 1046.8778 | 1068.1168 |
| 1077.3987 | 1098.1982 | 1110.4716 |
| 1123.1369 | 1153.0480 | 1205.0676 |
| 1219.4071 | 1244.4445 | 1260.6517 |
| 1275.0612 | 1287.5951 | 1322.7243 |
| 1331.0426 | 1348.8580 | 1379.3331 |
| 1386.5817 | 1393.4068 | 1398.9111 |
| 1406.8375 | 1422.8513 | 1443.9680 |
| 1453.4292 | 1480.0675 | 1484.0052 |
| 1492.4735 | 1498.4483 | 1503.6889 |
| 1510.7804 | 1524.3883 | 2956.8163 |
| 2984.0200 | 3013.7019 | 3017.4377 |
| 3031.0311 | 3033.7639 | 3040.5823 |
| 3045.5381 | 3052.6694 | 3067.7422 |
| 3074.9144 | 3082.2746 | 3093.9483 |
| 3113.0963 | 3135.5321 | 3814.1047 |

Zero-point correction (Hartree): 0.238065

C8H17O.1-6Hshift.7oh.St.pp

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -465.46639286

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | -1.260049 | -1.631076 | -0.481040 |
| C | -2.579198 | -1.145685 | -0.446107 |
| C | -2.837926 | -0.083202 | 0.631430 |
| C | -2.159476 | 1.277045 | 0.388875 |
| C | -0.619182 | 1.264606 | 0.467477 |
| C | 0.036023 | 0.496604 | -0.669546 |
| C | 1.532186 | 0.190822 | -0.588949 |
| C | 1.940895 | -0.651142 | 0.627120 |

| | | | |
|--|-----------|-----------|-----------|
| C | 3.407203 | -1.090259 | 0.576738 |
| H | -2.900840 | -0.764850 | -1.431919 |
| H | -3.198263 | -2.031759 | -0.235487 |
| H | -2.522000 | -0.487828 | 1.601916 |
| H | -3.922652 | 0.076076 | 0.691571 |
| H | -2.536979 | 1.988899 | 1.132891 |
| H | -2.469283 | 1.667823 | -0.591059 |
| H | -0.318629 | 0.843309 | 1.435114 |
| H | -0.258350 | 2.304214 | 0.452373 |
| H | -0.521181 | -0.634588 | -0.675050 |
| H | -0.228783 | 0.916189 | -1.646965 |
| O | 2.284521 | 1.411148 | -0.672383 |
| H | 1.810869 | -0.356103 | -1.497570 |
| H | 1.763194 | -0.069839 | 1.543486 |
| H | 1.277132 | -1.521966 | 0.686104 |
| H | 4.067093 | -0.224226 | 0.471902 |
| H | 3.589872 | -1.751469 | -0.277724 |
| H | 3.690947 | -1.632285 | 1.484183 |
| H | 2.158925 | 1.885087 | 0.161391 |
| Rotational constants (GHz): | 2.0787600 | 0.6926600 | 0.5936000 |
| Vibrational harmonic frequencies (cm-1): | | | |
| i1367.0160 | 52.8483 | | 67.6613 |
| 94.1748 | 149.5379 | | 180.6802 |
| 194.4887 | 222.5634 | | 259.2261 |
| 287.2908 | 325.5815 | | 338.2464 |
| 358.2909 | 405.6663 | | 468.5443 |
| 483.7025 | 594.5010 | | 661.5608 |
| 774.6078 | 784.2254 | | 793.4258 |
| 825.9882 | 878.5202 | | 895.1321 |
| 950.9779 | 977.2598 | | 983.2081 |
| 1018.5040 | 1049.9241 | | 1064.9523 |
| 1077.7616 | 1097.7439 | | 1098.6839 |
| 1139.7753 | 1157.3823 | | 1204.4454 |
| 1220.4515 | 1241.5270 | | 1261.7944 |
| 1276.4717 | 1291.4471 | | 1319.7747 |
| 1335.9817 | 1349.3996 | | 1381.6894 |
| 1394.8820 | 1396.7417 | | 1406.5868 |
| 1409.1156 | 1420.0767 | | 1431.1266 |
| 1449.6667 | 1479.8410 | | 1484.4885 |
| 1494.3007 | 1502.9499 | | 1504.7666 |
| 1510.7200 | 1524.4963 | | 2960.1423 |
| 3004.7303 | 3014.8648 | | 3021.0982 |
| 3023.8292 | 3034.2741 | | 3047.9495 |
| 3058.6611 | 3061.7911 | | 3070.3467 |
| 3077.1392 | 3080.6995 | | 3084.7298 |
| 3115.3940 | 3130.4160 | | 3800.3792 |
| Zero-point correction (Hartree): | 0.238278 | | |

C8H17O.1-6Hshift.7oh.St.pt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -465.46499640

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|--|-----------|-----------|-----------|
| O | -1.267216 | -1.625633 | -0.502377 |
| C | -2.583691 | -1.129396 | -0.460935 |
| C | -2.837184 | -0.082114 | 0.632741 |
| C | -2.152681 | 1.279070 | 0.411078 |
| C | -0.613324 | 1.256268 | 0.486432 |
| C | 0.031699 | 0.499799 | -0.659925 |
| C | 1.522311 | 0.193305 | -0.587677 |
| C | 1.928092 | -0.663806 | 0.620505 |
| C | 3.403421 | -1.077174 | 0.595042 |
| H | -2.899533 | -0.730600 | -1.441411 |
| H | -3.208403 | -2.015100 | -0.266639 |
| H | -2.522164 | -0.503206 | 1.596497 |
| H | -3.921616 | 0.078696 | 0.695575 |
| H | -2.525471 | 1.980277 | 1.167503 |
| H | -2.464937 | 1.687214 | -0.561291 |
| H | -0.310423 | 0.821062 | 1.446317 |
| H | -0.227767 | 2.285049 | 0.480322 |
| H | -0.528548 | -0.634407 | -0.676728 |
| H | -0.238463 | 0.922584 | -1.634371 |
| O | 2.187550 | 1.465547 | -0.589318 |
| H | 1.788414 | -0.361947 | -1.503189 |
| H | 1.724019 | -0.101343 | 1.538548 |
| H | 1.289651 | -1.555169 | 0.641135 |
| H | 4.066867 | -0.205092 | 0.635303 |
| H | 3.645009 | -1.645185 | -0.311304 |
| H | 3.652218 | -1.706533 | 1.454798 |
| H | 3.126613 | 1.308682 | -0.751078 |
| Rotational constants (GHz): | 2.0834800 | 0.6956100 | 0.5961800 |
| Vibrational harmonic frequencies (cm-1): | | | |
| i1413.7433 | 45.0102 | | 59.0251 |
| 83.7998 | 142.8055 | | 172.6087 |
| 194.4476 | 204.5691 | | 258.2900 |

| | | |
|-----------|-----------|-----------|
| 260.2202 | 288.7128 | 337.9816 |
| 347.8620 | 406.6758 | 464.8772 |
| 481.8969 | 592.0843 | 657.9937 |
| 768.1422 | 778.0917 | 792.9510 |
| 828.0350 | 879.2988 | 892.2501 |
| 950.4665 | 973.5355 | 985.7057 |
| 1015.9356 | 1046.0202 | 1065.6916 |
| 1076.0857 | 1095.4634 | 1103.5002 |
| 1141.1345 | 1163.1622 | 1202.3486 |
| 1212.0418 | 1227.5878 | 1262.8693 |
| 1278.3574 | 1287.4140 | 1302.6354 |
| 1332.5107 | 1347.6905 | 1382.2078 |
| 1393.4774 | 1396.7966 | 1406.3512 |
| 1409.0698 | 1423.3028 | 1438.1889 |
| 1451.4838 | 1480.3570 | 1483.4365 |
| 1490.3540 | 1496.7929 | 1504.1285 |
| 1514.3572 | 1523.6034 | 2960.7872 |
| 2972.5921 | 3015.6776 | 3019.9840 |
| 3030.5814 | 3033.7149 | 3036.1929 |
| 3051.4248 | 3067.3141 | 3070.7232 |
| 3076.3036 | 3084.4802 | 3088.2587 |
| 3108.6575 | 3117.5559 | 3819.3253 |

Zero-point correction (Hartree): 0.237739

C8H17O.1-6Hshift.7oh.St.tm

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -465.46576770

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 1.042377 | 1.606351 | 0.476213 |
| C | 2.344515 | 1.448840 | -0.027285 |
| C | 2.987137 | 0.091352 | 0.292712 |
| C | 2.398062 | -1.109307 | -0.469171 |
| C | 0.931312 | -1.445710 | -0.136212 |
| | | | |
| C | -0.054790 | -0.377186 | -0.571447 |
| C | -1.514884 | -0.547898 | -0.163048 |
| C | -2.350016 | 0.705359 | -0.442770 |
| C | -3.844607 | 0.504607 | -0.181290 |
| H | 2.393500 | 1.639898 | -1.114965 |
| H | 2.928770 | 2.247865 | 0.455222 |
| H | 2.909164 | -0.079087 | 1.374293 |
| H | 4.057504 | 0.158269 | 0.056885 |
| H | 3.012380 | -1.992071 | -0.253922 |
| H | 2.489716 | -0.931369 | -1.550468 |
| H | 0.838838 | -1.601668 | 0.946689 |
| H | 0.666840 | -2.401625 | -0.616935 |
| H | 0.356949 | 0.682184 | -0.010088 |
| H | 0.031192 | -0.141063 | -1.639378 |
| O | -1.666558 | -0.851277 | 1.221275 |
| H | -1.926001 | -1.379900 | -0.771394 |
| H | -1.959976 | 1.515676 | 0.184180 |
| H | -2.183214 | 1.004110 | -1.485219 |
| H | -4.014533 | 0.198221 | 0.853851 |
| H | -4.262126 | -0.270373 | -0.835240 |
| H | -4.402360 | 1.428709 | -0.362867 |
| H | -1.323560 | -1.738709 | 1.380520 |

Rotational constants (GHz): 2.3098700 0.6610600 0.5779900

Vibrational harmonic frequencies (cm-1):

| | | |
|------------|-----------|-----------|
| i1424.1117 | 47.7070 | 67.8643 |
| 93.4637 | 115.9635 | 180.2103 |
| 193.7652 | 232.5930 | 262.7845 |
| 274.0741 | 289.4034 | 340.0379 |
| 390.0842 | 407.4509 | 466.0834 |
| 483.8886 | 577.2656 | 609.7271 |
| 771.4040 | 787.6033 | 794.4070 |
| 840.8279 | 877.8354 | 907.9188 |
| 943.9215 | 959.6562 | 1003.3850 |
| 1021.3264 | 1041.7264 | 1063.4920 |
| 1078.6342 | 1096.8031 | 1109.7470 |
| 1142.6492 | 1165.1392 | 1202.3741 |
| 1222.9813 | 1234.9811 | 1255.8258 |
| 1271.5510 | 1290.5417 | 1304.4157 |
| 1327.9984 | 1337.8587 | 1376.5116 |
| 1381.6461 | 1395.6296 | 1398.1162 |
| 1408.9786 | 1422.1069 | 1428.6661 |
| 1466.0854 | 1481.2537 | 1483.7782 |
| 1491.5384 | 1495.8415 | 1504.4622 |
| 1509.6390 | 1524.2239 | 2899.3179 |
| 2952.5303 | 2989.9459 | 3014.3840 |
| 3020.7159 | 3034.2103 | 3044.2161 |
| 3046.4704 | 3051.2314 | 3067.7372 |
| 3071.4166 | 3079.3397 | 3088.9137 |
| 3111.5109 | 3140.2636 | 3836.2172 |

Zero-point correction (Hartree): 0.237623

C8H17O.1-6Hshift.7oh.St.tp

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -465.47210085

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 0.771918 | 1.569475 | -0.082207 |
| C | 2.172608 | 1.489387 | -0.223084 |
| C | 2.813642 | 0.244562 | 0.405617 |
| C | 2.433978 | -1.095680 | -0.250812 |
| C | 0.987210 | -1.559047 | 0.016920 |
| C | -0.079145 | -0.709202 | -0.654550 |
| C | -1.417727 | -0.599076 | 0.072623 |
| C | -2.440864 | 0.243828 | -0.705158 |
| C | -3.799188 | 0.323354 | -0.004763 |
| H | 2.468184 | 1.565639 | -1.283336 |
| H | 2.557957 | 2.388690 | 0.282088 |
| H | 2.562829 | 0.216054 | 1.473973 |
| H | 3.901755 | 0.373316 | 0.338386 |
| H | 3.114683 | -1.867359 | 0.128035 |
| H | 2.614409 | -1.036349 | -1.334052 |
| H | 0.802267 | -1.552826 | 1.096845 |
| H | 0.875621 | -2.599788 | -0.319919 |
| H | 0.313400 | 0.470511 | -0.578886 |
| H | -0.173745 | -0.884653 | -1.732447 |
| O | -1.217470 | -0.102125 | 1.394034 |
| H | -1.827680 | -1.613845 | 0.207579 |
| H | -2.026773 | 1.252066 | -0.840042 |
| H | -2.557335 | -0.182899 | -1.710752 |
| H | -3.680694 | 0.711326 | 1.010240 |
| H | -4.264577 | -0.666477 | 0.069444 |
| H | -4.488713 | 0.976596 | -0.548676 |
| H | -0.650258 | 0.682437 | 1.306144 |

Rotational constants (GHz): 2.3445600 0.7026500 0.6247300

Vibrational harmonic frequencies (cm-1):

| | | |
|------------|-----------|-----------|
| 11235.3877 | 56.0456 | 74.0954 |
| 104.7880 | 135.8741 | 182.7227 |
| 208.9783 | 234.2340 | 276.1935 |
| 300.9659 | 339.9071 | 382.5715 |
| 399.3209 | 482.1431 | 491.7898 |
| 523.3080 | 562.5293 | 665.2958 |
| 785.8745 | 787.5673 | 814.4704 |
| 853.0265 | 883.3399 | 918.0257 |
| 949.3362 | 961.9812 | 1000.3201 |
| 1006.5341 | 1045.5975 | 1064.5970 |
| 1084.1351 | 1099.0883 | 1125.5234 |
| 1138.6454 | 1154.8346 | 1206.4065 |
| 1213.2693 | 1266.3070 | 1269.3053 |
| 1282.2844 | 1288.9710 | 1311.5377 |
| 1327.6173 | 1354.8650 | 1379.2625 |
| 1388.2312 | 1394.3760 | 1402.6813 |
| 1405.0132 | 1419.6623 | 1424.9458 |
| 1461.6525 | 1481.9736 | 1485.9212 |
| 1497.6436 | 1499.0177 | 1503.0144 |
| 1509.5210 | 1524.1950 | 2973.2354 |
| 2988.7531 | 3016.9453 | 3018.7864 |
| 3023.4056 | 3026.7904 | 3036.3062 |
| 3045.6109 | 3066.5119 | 3070.4781 |
| 3076.4985 | 3078.8534 | 3094.2690 |
| 3111.2920 | 3137.3641 | 3720.9491 |

Zero-point correction (Hartree): 0.238928

C8H17O.1-6Hshift.7oh.St.tt

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -465.46612252

Electronic state : 2-A

Cartesian coordinates (Angs):

| | | | |
|---|-----------|-----------|-----------|
| O | 1.021338 | 1.621513 | 0.427332 |
| C | 2.335490 | 1.451383 | -0.039716 |
| C | 2.968099 | 0.099041 | 0.320452 |
| C | 2.404425 | -1.112665 | -0.444095 |
| C | 0.937525 | -1.466028 | -0.133466 |
| C | -0.049956 | -0.402662 | -0.576130 |
| C | -1.497056 | -0.569406 | -0.150289 |
| C | -2.359199 | 0.646319 | -0.529550 |
| C | -3.834685 | 0.494279 | -0.147287 |
| H | 2.412365 | 1.621857 | -1.129492 |
| H | 2.908516 | 2.258872 | 0.442673 |
| H | 2.855795 | -0.056373 | 1.401141 |
| H | 4.045244 | 0.166028 | 0.117213 |
| H | 3.025249 | -1.986873 | -0.212705 |
| H | 2.517139 | -0.938663 | -1.524607 |
| H | 0.811204 | -1.638511 | 0.940446 |
| H | 0.684865 | -2.415762 | -0.631306 |
| H | 0.355947 | 0.664213 | -0.031746 |

| | | | | |
|---|-----------|-----------|-----------|--|
| H | 0.021502 | -0.171149 | -1.645507 | |
| O | -1.507470 | -0.817158 | 1.253729 | |
| H | -1.895991 | -1.456854 | -0.684486 | |
| H | -1.934104 | 1.533607 | -0.046572 | |
| H | -2.276397 | 0.801623 | -1.612990 | |
| H | -3.961740 | 0.408273 | 0.938175 | |
| H | -4.283059 | -0.391372 | -0.613932 | |
| H | -4.415414 | 1.364947 | -0.466062 | |
| H | -2.409923 | -1.040278 | 1.511749 | |
| Rotational constants (GHz): | 2.3059400 | 0.6656700 | 0.5839600 | |
| Vibrational harmonic frequencies (cm ⁻¹): | | | | |
| i1407.4259 | 55.9367 | | 64.2732 | |
| 90.2754 | 115.2264 | | 182.0624 | |
| 193.0901 | 227.2972 | | 257.4546 | |
| 279.6588 | 290.6507 | | 339.4663 | |
| 391.0643 | 408.4377 | | 468.3352 | |
| 487.1719 | 578.6084 | | 590.7554 | |
| 767.6329 | 786.0464 | | 792.7046 | |
| 844.1145 | 876.9235 | | 905.9561 | |
| 944.9947 | 961.4351 | | 1003.9095 | |
| 1019.0733 | 1039.3169 | | 1064.6446 | |
| 1090.9140 | 1095.4174 | | 1122.1101 | |
| 1138.2354 | 1166.3800 | | 1184.9381 | |
| 1216.9468 | 1226.5476 | | 1263.3762 | |
| 1276.1783 | 1295.8891 | | 1297.1674 | |
| 1308.7726 | 1348.8403 | | 1380.5237 | |
| 1386.4526 | 1395.1669 | | 1402.9357 | |
| 1407.7381 | 1416.6405 | | 1432.2886 | |
| 1466.1850 | 1481.6818 | | 1484.0136 | |
| 1492.2475 | 1495.6604 | | 1504.4009 | |
| 1513.9566 | 1524.9536 | | 2896.0026 | |
| 2949.0513 | 2997.8298 | | 3011.4005 | |
| 3016.3023 | 3033.1766 | | 3035.0744 | |
| 3042.4389 | 3065.1134 | | 3073.1455 | |
| 3077.9748 | 3084.6668 | | 3099.7018 | |
| 3106.2895 | 3118.2710 | | 3835.5761 | |
| Zero-point correction (Hartree): | 0.237579 | | | |