Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Materials for

Direct Experimental Probing and Theoretical Analysis of the Reaction between the Simplest Criegee Intermediate CH_2OO and Isoprene

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EXPERIMENTAL

I. Time-Resolved Broadband Cavity-Enhanced Absorption Spectrometer

The TR-BB-CEAS instrument is a slow-flow chemical reactor integrated into a cavity-enhanced absorption spectrometer, capable of operating in the UV-VIS spectral range. Details of the setup have been published,[1] and a summary is given here, including a recent upgrade to operation at elevated temperatures. A schematic of the apparatus is shown in Fig. S1.

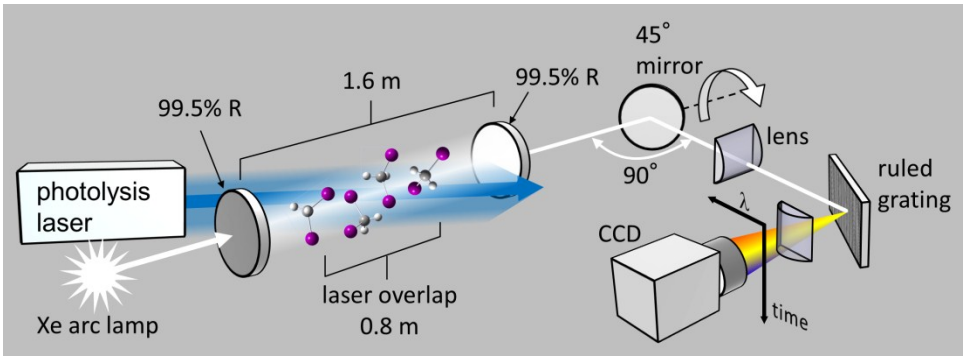

Figure S1. Schematic of the Time-Resolved Broadband Cavity-Enhanced Absorption Spectrometer.

The reactor is a 1.6 m-long Fused Silica tube with inner diameter of 3 cm, pumped by a large-capacity roots pump. Constant pressure is maintained by active feedback control using a downstream butterfly valve. Bath gas flows (He or N_2, both 99.9999%) are mixed prior to entering the reactor with O_2 (99.9999%), isoprene (99%) and CH_2I_2 (99%, entrained in bath gas using a glass bubbler kept at a constant temperature of 20°C). Individual flows of the sample mixture components are regulated by calibrated mass flow controllers; desired CH_2I_2 concentration is obtained by adjusting the total pressure in its bubbler and thus its dilution factor in the bath gas.

The multipass optical resonator (cavity) is incorporated directly into the reactor volume. A Xe arc lamp provides continuous broadband probe radiation that spans the 200 – 2000 nm range, and a BG-3 optical filter attenuates the wavelengths outside of the 300 – 450 nm range of interest for the present study. We measure the effective path length inside the cavity regularly with known concentrations of NO_2 and CH_2I_2.[2,3] The reaction $CH_2I + O_2$ is initiated by photodissociation of the CH_2I_2 precursor using a 266-nm laser pulse from the 4th harmonic of an Nd:YAG laser. The photolysis laser path and the optical cavity axis intersect at a 2° angle and overlap over a path length L = 80 cm, for a total absorption path length $L_{eff} \sim 40$ m.

The apparatus was recently outfitted with a heating jacket, consisting of four independent sections, that now allows operation at *T* up to 650 K. Heat transfer efficiency in our reactor varies depending on the experimental pressure, flow speed, and bath gas. In order to ensure uniform temperature profiles along the pump-probe overlap region, we characterized the heater performance at a wide range of experimental conditions using a thermocouple, translated along the length of the reactor. Based on these measurements, we developed parameterized relationships for the power requirements of each heater

section and have now demonstrated excellent temperature profiles at pressures up to 500 Torr of He or N_2, as shown in Fig. S2.

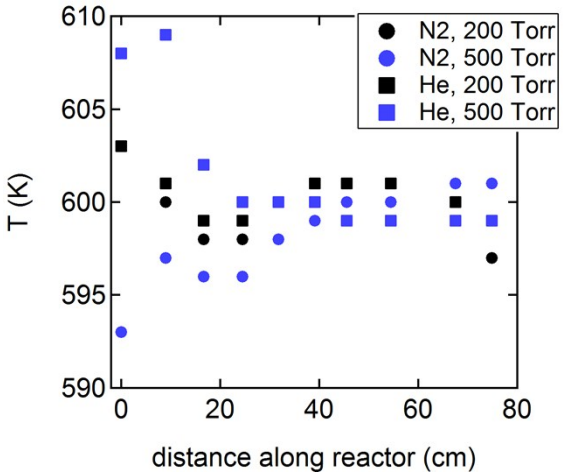

Figure S2. Temperature profiles along the pump-probe overlap region of the TR-BB-CEAS apparatus. The set point was 600 K, and four test conditions are shown, using He or N_2 bath gas at P = 200 and 500 Torr.

Transient absorption measurements are acquired by a custom spectrometer. The CW cavity output is spectrally dispersed horizontally by a ruled grating and focused onto a 1024x1024 pixel CCD camera. A phase-locked spinning mirror positioned before the grating sweeps the cavity output vertically, translating the probe spectrum with controlled speed over the CCD detector. The spectral and temporal information are thus mapped spatially along the x and y dimensions, respectively, of the CCD sensor. The firing of the photolysis laser is synchronized with the spinning mirror and therefore with the probe radiation sweep. The transient absorption is integrated directly on the CCD detector for many laser shots with the camera shutter open, and read out at the end of a "long exposure" mode, bypassing the need for fast data transfer electronics.

Our wavelength scale (resolution ~1.5 nm FWHM) is calibrated using atomic emission lines from a Hg(Ne) pencil lamp; kinetic time scale (resolution ~50 μs FWHM) is calibrated by varying the photolysis laser delay. Transient absorption is calculated using the difference between alternating "photolysis ON" and "photolysis OFF" images according to the Beer-Lambert equation:

$$OD = -ln(I/I_0) = C \cdot \sigma_{abs} \cdot L_{eff} \quad (1)$$

Here I and I_0 are the probe radiation intensity with and without the photolysis laser, respectively, C is the transient absorber concentration, σ_{abs} is the absorption cross-section, and L_{eff} is the effective optical path length in the reactor cavity. All transient images shown here have been smoothed with a 5-pixel Gaussian filter, which does not affect the stated experimental resolution.

II. Kinetic fits

The transient absorption traces (after subtraction of interfering signals) were fit to an expression for the concentration of CH_2OO as a function of time, convolved with the temporal response function of our instrument:

$$S(t) = OD(t) \otimes F_{\tau}(t')$$

Where $OD(t)$ is the transient absorption due to CH_2OO, determined by the kinetic model described by equation E2 in the main text:

$$OD(t) = \frac{S_0 \cdot k_1'}{(k_{decay}' - k_1')} \cdot \left(e^{-k_1' t} - e^{-k_{decay}' t}\right) + S_{\infty}$$

and $F_{\tau}(t')$ is the time response function, determined separately. The spectrometer works by mapping temporal information spatially onto the CCD detector; therefore its time response is governed by the spatial focusing of the probe radiation onto the detector. We measure this focusing directly by imaging the probe radiation spectrum at several fixed positions of the rotating mirror, and thus at several positions spanning the entire CCD area. The spatial resolution is a smooth Gaussian with FWHM ~7 pixels in the vertical (time) direction, independent of the wavelength, resulting in temporal resolution of ~50 μs at typical operating conditions. The experimental time response is therefore a Gaussian function:

$$F_{\tau}(t') = exp\left[-\left(\frac{t - t_0}{\omega}\right)^2\right]$$

Both t_0 and ω are allowed to vary during the fit, but the width of this function is always quite close to the independently measured resolution.

Kinetic fits are performed in batches: all time traces taken at the same T and P and on the same day are fit simultaneously. The parameters t_0 and ω are free but constrained to the same value for all traces in a single batch; k_1' is also constrained throughout the batch and is fixed according to $k_1' = k_1 \cdot [O_2]$. The long-time offset S_{∞} is free but constrained to the same value for all traces with isoprene present and a different value for all traces without isoprene. The remaining parameters for the amplitude (S_0) and signal decay (k_{decay}') are allowed to vary freely.

The following tables include detailed experimental conditions and the key fit parameters S_0, S_{∞}, k_1', and k_{decay}' for all data. Three distinct values are listed for k_{decay}' to represent three alternative treatments of interfering absorption signals: full subtraction of IO and isoprene signals (k_{decay}'-A), subtraction of IO contributions only (k_{decay}'-B), and no subtraction (k_{decay}'-C).

T = 295 K, P = 30 Torr

Exp't Type	[ISP]	$[CH_2I_2]$	$[O_2]$	[FA]	$[CH_2OO]$	S_0	S_∞	k_1'	$k_{decay\text{-}B}'$	$k_{decay\text{-}C}'$
	$/10^{16}$	$/10^{13}$	$/10^{16}$	$/10^{13}$	$/10^{11}$	$/10^{-4}$	$/10^{-6}$	$/\mu s^{-1}$	$/100\cdot ms^{-1}$	$/100\cdot ms^{-1}$
CI	0	2.94±0.16	1.63±0.09	0	5.47±0.43	3.48 ± 0.00	12.58 ± 0.19		1.3±0.2	1.2±0.2
CI+FA	0	2.94±0.16	1.63±0.09	14.2±0.8	4.21±0.33	3.34 ± 0.05			100±10	110±20
CI+ISP	3.25±0.20	2.92±0.16	1.62±0.09	0	5.24±0.41	3.14 ± 0.00			1.8±0.3	1.7±0.3
CI+ISP	6.49±0.37	2.92±0.16	1.62±0.09	0	5.10±0.40	3.14 ± 0.01			2.3±0.3	2.2±0.3
CI +ISP	38.95±2.16	2.92±0.16	1.62±0.09	0	5.27±0.41	3.26 ± 0.01			7.0±1.0	6.7±1.0
CI +ISP	9.74±0.55	2.94±0.16	1.62±0.09	0	5.30±0.42	3.54 ± 0.01			2.9±0.4	2.8±0.4
CI +ISP	35.82±1.99	2.94±0.16	1.63±0.09	0	4.94±0.39	3.28 ± 0.01			7.0±1.0	6.6±1.0
CI +ISP	12.98±0.73	2.93±0.16	1.62±0.09	0	4.92±0.39	3.46 ± 0.01		29.2	3.3±0.5	3.2±0.5
CI +ISP	32.56±1.81	2.94±0.16	1.63±0.09	0	4.68±0.37	3.32 ± 0.01	21.42 ± 0.15		6.3±1.0	6.3±0.9
CI +ISP	16.22±0.90	2.92±0.16	1.62±0.09	0	4.65±0.37	3.46 ± 0.01			3.9±0.6	3.8±0.6
CI +ISP	29.21±1.62	2.93±0.16	1.62±0.09	0	4.54±0.36	3.32 ± 0.01			5.8±0.9	5.7±0.9
CI +ISP	19.46±1.08	2.92±0.16	1.62±0.09	0	4.48±0.35	3.43 ± 0.01			4.4±0.7	4.3±0.7
CI +ISP	25.95±1.44	2.92±0.16	1.62±0.09	0	4.40±0.35	3.29 ± 0.01			5.1±0.8	5.0±0.8
CI +ISP	22.70±1.26	2.92±0.16	1.62±0.09	0	4.39±0.35	3.38 ± 0.01			4.6±0.7	4.6±0.7
CI +FA+ISP	6.48±0.37	2.92±0.16	1.62±0.09	14.1±0.8	4.09±0.32	3.21 ± 0.08			160±20	160±20

* No isoprene photolysis products were present at T = 295 K, hence no subtraction was needed

T = 350 K, P = 30 Torr

Exp't Type	[ISP]	$[CH_2I_2]$	$[O_2]$	[FA]	$[CH_2OO]$	S_0	S_∞	k_1'	$k_{decay\text{-}A}'$	$k_{decay\text{-}B}'$	$k_{decay\text{-}C}'$
	$/10^{16}$	$/10^{13}$	$/10^{16}$	$/10^{13}$	$/10^{11}$	$/10^{-4}$	$/10^{-6}$	$/\mu s^{-1}$	$/100\cdot ms^{-1}$	$/100\cdot ms^{-1}$	$/100\cdot ms^{-1}$
CI	0	9.69±0.56	1.64±0.10	0	5.58±0.51	2.86±0.01	9.08±0.22		1.6±0.2	1.6±0.2	1.4±0.2
CI+ISP	3.24±0.20	9.55±0.56	1.62±0.10	0	5.29±0.49	2.56±0.01	7.03±0.12	61.2	2.2±0.3	2.3±0.3	2.2±0.3
CI+ISP	29.64±1.73	9.80±0.57	1.65±0.10	0	4.75±0.46	2.03±0.01			9±1	9±1	9±1

CI+ISP	4.91±0.30	9.70±0.57	1.64±0.10	0	5.55±0.51	2.50±0.01			2.7±0.4	2.5±0.4	2.4±0.4
CI +ISP	36.31±2.11	9.58±0.56	1.65±0.10	0	4.36±0.43	2.05±0.01			9±1	10±1	10±1
CI +ISP	23.06±1.34	10.00±0.58	1.65±0.10	0	4.94±0.48	2.13±0.01			7±1	7±1	7±1
CI +ISP	13.18±0.77	10.01±0.58	1.65±0.10	0	5.08±0.49	2.31±0.01			4.4±0.7	4.2±0.6	4.2±0.6
CI +ISP	6.55±0.39	9.94±0.58	1.64±0.10	0	5.20±0.49	2.35±0.01			2.6±0.4	2.7±0.4	2.7±0.4
CI +ISP	19.79±1.15	9.93±0.58	1.65±0.10	0	4.93±0.47	2.12±0.01			5.5±0.8	5.6±0.8	5.6±0.8
CI +ISP+FA	3.28±0.21	9.71±0.57	1.64±0.10	8.08±0.47	5.55±0.51	2.38±0.03			44 ± 7	43±6	43±6
CI +ISP+FA	36.23±2.11	9.58±0.56	1.65±0.10	8.10±0.47	4.32±0.43	2.10±0.03			51 ± 8	48±7	48±7
CI+ISP+FA	19.84±1.16	9.97±0.58	1.65±0.10	8.13±0.48	4.76±0.46	2.18±0.03			58 ± 9	46±7	47±7
CI+FA	0	9.62±0.56	1.63±0.10	8.03±0.47	9.62±0.56	2.30±0.03	9.08±0.18		52 ± 8	53±8	55±8

T = 400K P = 30 Torr

Exp't Type	[ISP]	$[CH_2I_2]$	$[O_2]$	[FA]	$[CH_2OO]$	S_0	S_∞	k_1'	k_{decay}'-A	k_{decay}'-B	k_{decay}'-C
	$/10^{16}$	$/10^{13}$	$/10^{16}$	$/10^{13}$	$/10^{11}$	$/10^{-4}$	$/10^{-6}$	$/\mu s^{-1}$	$/100\cdot ms^{-1}$	$/100\cdot ms^{-1}$	$/100\cdot ms^{-1}$
CI	0	9.88±0.66	1.64±0.11	0	6.64±0.64	3.56±0.01	7.93±0.32		1.4±0.2	1.4±0.2	1.3±0.2
CI+ISP	3.26±0.23	9.83±0.65	1.63±0.11	0	6.34±0.61	3.34±0.01			2.5±0.4	2.5±0.4	2.3±0.4
CI+ISP	21.08±1.4	9.82±0.65	1.62±0.11	0	9.82±0.65	2.71±0.01			9±1	9±1	9±1
CI+ISP	4.90±0.34	9.92±0.66	1.63±0.11	0	9.92±0.66	3.14±0.01			3.1±0.5	3.0±0.4	2.9±0.4
CI +ISP	27.62±1.84	9.87±0.66	1.62±0.11	0	9.87±0.66	2.37±0.01			11.0±2	11.0±2	11.0±2
CI +ISP	13.07±0.87	9.91±0.66	1.63±0.11	0	9.91±0.66	2.96±0.01	2.28±0.23	29.3	6.0±0.9	5.9±0.9	5.8±0.9
CI +ISP	9.76±0.65	9.89±0.66	1.63±0.11	0	9.89±0.66	2.95±0.01			4.5±0.7	4.5±0.7	4.3±0.6
CI +ISP	6.53±0.44	9.93±0.66	1.63±0.11	0	9.93±0.66	3.11±0.01			3.6±0.5	3.5±0.5	3.4±0.5
CI +ISP	16.31±1.09	9.92±0.66	1.63±0.11	0	9.92±0.66	2.64±0.01			7.0±1.0	6.6±1.0	6.6±1.0
CI +ISP+FA	3.25±0.23	9.85±0.65	1.62±0.11	4.00±0.27	6.51±0.62	3.15±0.02			26±4	27±4	26±4
CI+FA	0	9.87±0.65	1.62±0.11	3.99±0.27	9.87±0.65	3.23±0.02	7.93±0.32		28±4	28±4	28±4

T = 450 K, P = 30 Torr

Exp't Type	[ISP]	$[CH_2I_2]$	$[O_2]$	[FA]	$[CH_2OO]$	S_0	S_∞	k_1'	k_{decay}'-A	k_{decay}'-B	k_{decay}'-C
	/10^{16}	/10^{13}	/10^{16}	/10^{13}	/10^{11}	/10^{-4}	/10^{-6}	/μs^{-1}	/100·ms^{-1}	/100·ms^{-1}	/100·ms^{-1}
CI	0.00	9.96±0.75	1.64±0.13	0.00	4.41±0.51	3.66±0.01	-0.13±0.38		1.6±0.2	1.6±0.2	1.5±0.2
CI+ISP	2.46±0.20	9.94±0.75	1.64±0.13	0.00	3.82±0.47	3.24±0.01			3.0±0.4	3.0±0.4	2.9±0.4
CI+ISP	14.74±1.12	9.93±0.75	1.64±0.12	0.00	2.73±0.4	2.33±0.02			9±1	9±1	9±1
CI+ISP	3.28±0.26	9.93±0.75	1.64±0.12	0.00	3.56±0.45	3.1±0.01			3.2±0.5	3.4±0.5	3.5±0.5
CI +ISP	9.85±0.75	9.97±0.75	1.64±0.13	0.00	2.93±0.41	2.67±0.01	-2.93±0.49	29.5	6.2±0.9	6.6±1	6.4±1.0
CI +ISP	12.23±0.93	9.91±0.75	1.63±0.12	0.00	2.75±0.4	2.38±0.01			8±1	7±1	8±1
CI +ISP	7.39±0.56	9.98±0.76	1.64±0.13	0.00	3.08±0.42	2.74±0.01			5.2±0.8	5.5±0.8	5.5±0.8
CI +ISP	4.07±0.32	9.91±0.75	1.63±0.12	0.00	3.24±0.43	2.88±0.01			3.8±0.6	3.9±0.6	3.8±0.6
CI +ISP	5.74±0.44	9.97±0.75	1.64±0.13	0.00	3.08±0.42	2.79±0.01			4.4±0.7	4.6±0.7	4.6±0.7
CI+FA	0.00	9.93±0.75	1.63±0.12	8.04±0.61	3.34±0.44	3.17±0.04	-0.13±0.38		40±6	40±6	41±6

T = 470 K, P = 30 Torr

Exp't Type	[ISP]	$[CH_2I_2]$	$[O_2]$	[FA]	$[CH_2OO]$	S_0	S_∞	k_1'	k_{decay}'-A	k_{decay}'-B	k_{decay}'-C
	/10^{16}	/10^{13}	/10^{16}	/10^{13}	/10^{11}	/10^{-4}	/10^{-6}	/μs^{-1}	/100·ms^{-1}	/100·ms^{-1}	/100·ms^{-1}
CI	0	27.34±2.02	1.53±0.11	0	6.17±0.57	6.13±0.01	16.63±0.31		2.2±0.3	2.1±0.3	1.9±3.0
CI+ISP	6.07±0.45	27.09±2.00	1.52±0.11	0	4.29±0.40	5.02±0.01			7±1	7±1	7±1
CI+ISP	9.07±0.67	26.96±1.99	1.51±0.11	0	3.84±0.36	4.55±0.01	-29.62±0.25	27.3	9±1	9±1	8±1
CI+ISP+FA	6.03±0.45	26.91±1.98	1.51±0.11	6.55±0.48	4.17±0.39	5.17±0.03			33±5	27±4	26±4
CI +FA	0	27.10±2.00	1.52±0.11	6.60±0.49	5.10±0.47	5.86±0.02	16.63±0.31		25±4	25±4	24±4

T = 500 K, P = 15 – 100 Torr

Exp't Type	P torr	[ISP] /10^{16}	[CH_2I_2] /10^{13}	[O_2] /10^{16}	[FA] /10^{13}	[CH_2OO] /10^{11}	S_0 /10^{-4}	S_∞ /10^{-6}	k_1' /μs^{-1}	k'_{decay}-A /100·ms^{-1}	k'_{decay}-B /100·ms^{-1}	k'_{decay}-C /100·ms^{-1}
CI	15	0	7.01±0.83	1.18±0.14	0	2.56±0.41	2.1±0.01	0.92±0.21		2.5±0.4	2.5±0.4	2.5±0.4
CI+ISP	15	1.18±0.15	6.99±0.83	1.18±0.14	0	2.43±0.39	2.07±0.01			4.5±0.7	4.9±0.7	4.8±0.7
CI+ISP	15	9.58±1.14	7.05±0.84	1.20±0.14	0	1.58±0.31	1.59±0.01	5.28±0.21	21.4	12±2	12±2	12±2
CI+ISP	15	4.16±0.50	7.00±0.83	1.19±0.14	0	2.03±0.35	1.97±0.01			8±1	7±1	7±1
CI+FA	15	0	7.05±0.84	1.19±0.14	5.85±0.70	2.52±0.4	2.06±0.02	0.92±0.18		32±5	32±5	32±5
CI	30	0	8.66±0.64	1.43±0.11	0	6.94±0.7	3.42±0.01	2.90±0.39		4.1±0.6	4.1±0.6	3.9±0.6
CI+ISP	30	2.88±0.22	8.72±0.65	1.44±0.11	0	5.44±0.57	3.33±0.01			7±1	8±1	8±1
CI+ISP	30	12.94±0.96	8.7±0.64	1.44±0.11	0	3.43±0.43	2.17±0.02			18±3	17±3	16±2
CI+ISP	30	1.44±0.13	8.7±0.64	1.44±0.11	0	5.86±0.61	3.53±0.01			5.2±0.8	5.5±0.8	5.6±0.8
CI +ISP	30	8.63±0.64	8.76±0.65	1.44±0.11	0	3.63±0.44	2.64±0.02			13±2	12±2	13±2
CI +ISP	30	2.16±0.17	8.65±0.64	1.44±0.11	0	13.11±1.23	4.03±0.01	-7.79±0.27	25.9	6.5±1	6.6±1	6.1±0.9
CI +ISP	30	6.47±0.48	8.65±0.64	1.44±0.11	0	3.85±0.45	3.11±0.02			11±2	10±2	10±2
CI +ISP	30	3.59±0.28	8.65±0.64	1.44±0.11	0	4.36±0.49	3.46±0.01			8±1	8±1	8±1
CI +ISP	30	5.04±0.38	8.69±0.64	1.44±0.11	0	3.98±0.46	3.1±0.02			9±1	9±1	9±1
CI+FA	30	0	8.65±0.64	1.44±0.11	7.06±0.52	4.87±0.53	3.75±0.04	2.90±0.39		35±5	35±5	36±5
CI	30	0	7.82±0.46	1.19±0.07	0	3.01±0.35	2.38±0.01	2.53±0.22		3.0±0.5	3.0±0.5	2.9±0.4
CI+ISP	30	1.19±0.09	7.84±0.47	1.19±0.07	0	7.84±0.47	2.27±0.01			5.0±0.8	5.6±0.8	5.4±0.8
CI+ISP	30	9.51±0.57	7.83±0.47	1.19±0.07	0	7.83±0.47	1.73±0.01	-3.12±0.25	21.4	13±2	12±2	13±2
CI+ISP	30	4.16±0.25	7.84±0.47	1.19±0.07	0	7.84±0.47	2.03±0.01			7±1	8±1	8±1
CI+FA	30	0	7.83±0.47	1.19±0.07	5.84±0.35	2.91±0.35	2.14±0.02	2.53±0.22		25±4	25±4	25±4
CI	50	0	6.95±0.25	1.19±0.04	0	2.29±0.27	1.99±0.01	4.01±0.23		3.5±0.5	3.5±0.5	3.4±0.5
CI+ISP	50	1.19±0.07	6.95±0.25	1.19±0.04	0	2.31±0.27	1.94±0.01			5.6±0.8	6.0±0.9	5.9±0.9
CI+ISP	50	9.55±0.35	6.94±0.25	1.19±0.04	0	1.58±0.25	1.55±0.01	-2.25±0.22	21.5	15±2	12±2	13±2
CI+ISP	50	4.16±0.16	6.92±0.25	1.19±0.04	0	1.86±0.26	1.70±0.02			8.0±1.0	9.0±1.0	9.0±1.0

CI+FA	50	0	6.96±0.25	1.19±0.04	5.88±0.22	2.38±0.28	1.91±0.01	4.01±0.23		28±4	28±4	29±4
CI	100	0	6.98±0.13	1.19±0.02	0	3.19±0.29	1.53±0.01	6.76±0.24		5.0±0.8	5.0±0.8	5.0±0.7
CI+ISP	100	1.19±0.06	6.97±0.13	1.19±0.02	0	2.75±0.28	1.12±0.01			8±1	8±1	8±1
CI+ISP	100	9.53±0.18	6.96±0.13	1.19±0.02	0	2.38±0.27	0.85±0.01	-0.89±0.22	24.7	15±2	12±2	13±2
CI+ISP	100	4.19±0.10	6.98±0.13	1.20±0.02	0	2.41±0.27	0.92±0.01			8±1	10±2	10±2
CI+FA	100	0	6.97±0.13	1.19±0.02	5.87±0.11	3.31±0.30	1.52±0.02	6.76±0.24		23±3	24±4	25±4

T = 540K, P = 30 Torr

Exp't Type	[ISP]	$[CH_2I_2]$	$[O_2]$	[FA]	$[CH_2OO]$	S_0	S_∞	k_1'	k_{decay}'-A	k_{decay}'-B
	/10^{16}	/10^{13}	/10^{16}	/10^{13}	/10^{11}	/10^{-4}	/10^{-6}	/μs^{-1}	/100·ms^{-1}	/100·ms^{-1}
CI	0	8.67±0.66	1.40±0.11	0	6.28±0.66	2.91±0.01	13.10±0.36		6.5±1.0	6.2±0.9
CI+ISP	2.81±0.22	8.70±0.66	1.40±0.11	0	5.28±0.58	2.62±0.01			12±2	13±2
CI+ISP	25.44±1.93	8.61±0.65	1.41±0.11	0	1.14±0.32	1.49±0.02			70±10	58±9
CI+ISP	4.20±0.33	8.66±0.66	1.40±0.11	0	4.73±0.53	2.41±0.01			14±2	14±2
CI +ISP	14.03±1.06	8.69±0.66	1.40±0.11	0	2.46±0.38	1.71±0.02	-10.07±0.08	2.53	43±6	39±6
CI +ISP	19.67±1.49	8.57±0.65	1.40±0.11	0	1.71±0.34	1.21±0.02			52±8	44±7
CI +ISP	11.27±0.86	8.60±0.65	1.41±0.11	0	2.94±0.40	1.75±0.02			29±4	27±4
CI +ISP	5.62±0.43	8.66±0.66	1.41±0.11	0	4.24±0.50	2.30±0.01			17±3	17±3
CI +ISP	16.9±1.28	8.70±0.66	1.41±0.11	0	2.07±0.36	1.46±0.02			51±8	44±7
CI+FA	0	8.59±0.65	1.40±0.11	0.69±0.07	6.33±0.66	3.00±0.01	13.10±0.36		8±1	8±1

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III. Cycloaddition reaction channels

Cycloaddition is the major pathway in the reaction of CH_2OO + isoprene, and we characterized in detail all 16 distinct cycloaddition channels, as described below:

Stationary point energies

Table S1. Computed energies in kcal/mol of isoprene conformers and the TS for internal CC-CC rotation

Compound	B3LYP[a]	CCSD(T)-F12/VDZ[b]	CCSD(T)-F12/VTZ[c]
s-trans-isoprene	0.00	0.00	0.00
s-gauche-isoprene	2.85	2.70	2.74
s-perp-isoprene (TS)	3.42	3.37	3.39
s-cis-isoprene (TS)	5.79	5.38	5.42

[a] B3LYP/6-311+G(2df,2p) geometries and ZPE corrections
[b] CCSD(T)-F12/cc-pVDZ-F12 single point energies on B3LYP geometries, with B3LYP ZPE corrections
[c] CCSD(T)-F12/cc-pVTZ-F12 single point energies on B3LYP geometries, with B3LYP ZPE corrections

Table S2. Computed energies in kcal/mol of reaction TS, relative to *s-trans*-isoprene + CH_2OO

TS	M06-2X[a]	CCSD(T)-F12/VTZ//M06-2X[b]	B3LYP[c]	CCSD(T)-F12/VDZ//B3LYP[d]	CCSD(T)-F12/VTZ//B3LYP[e]
cis-endo-1-2	-0.14		4.62	1.56	1.54
cis-endo-2-1	4.18		9.28	4.69	4.66
cis-endo-3-4	1.52		6.29	2.33	2.27
cis-endo-4-3	0.02	1.11	4.09	1.28	1.22
cis-exo-1-2	-0.16		4.35	1.33	1.33
cis-exo-2-1	3.53		9.16	4.19	4.16
cis-exo-3-4	1.66		6.18	2.42	2.34
cis-exo-4-3	-1.08	0.10	3.36	0.36 (0.43)	0.28 (0.36)
trans-endo-1-2	-0.33		3.64	0.73 (0.80)	0.70 (0.78)
trans-endo-2-1	1.80		7.07	2.44	2.39
trans-endo-3-4	0.24		5.04	1.06	0.96
trans-endo-4-3	0.22		3.93	1.14	1.09
trans-exo-1-2	-0.54		3.52	0.62 (0.71)	0.61 (0.70)
trans-exo-2-1	1.82		7.10	2.53	2.46
trans-exo-3-4	0.19		5.00	0.93	0.83
trans-exo-4-3	-0.65	0.39	3.26	0.50 (0.55)	0.44 (0.49)

[a] M06-2X/aug-cc-pVTZ geometries and ZPE corrections
[b] CCSD(T)-F12/cc-pVTZ-F12 single point energies on M06-2X geometries, with M06-2X ZPE corrections.
[c] B3LYP/6-311+G(2df,2p) geometries and ZPE corrections
[d] CCSD(T)-F12/cc-pVDZ-F12 single point energies on B3LYP geometries, with B3LYP ZPE corrections. Value in brackets is IRCMax value
[e] CCSD(T)-F12/cc-pVTZ-F12 single point energies on B3LYP geometries, with B3LYP ZPE corrections. Value in brackets is IRCMax value

Rate coefficients

Table S3. Calculated rate coefficients ($cm^3molecule^{-1}s^{-1}$) for sixteen possible CH_2OO + isoprene reaction channels

CH_2OO addition TS	250 K	300 K	350 K	400 K	450 K	500 K	550 K
cis-endo-1-2	1.07×10^{-16}	2.14×10^{-16}	3.66×10^{-16}	5.64×10^{-16}	8.08×10^{-16}	1.10×10^{-15}	1.43×10^{-15}
cis-endo-2-1	1.10×10^{-19}	5.99×10^{-19}	2.09×10^{-18}	5.50×10^{-18}	1.19×10^{-17}	2.25×10^{-17}	3.85×10^{-17}
cis-endo-3-4	1.39×10^{-17}	3.30×10^{-17}	6.37×10^{-17}	1.07×10^{-16}	1.64×10^{-16}	2.35×10^{-16}	3.20×10^{-16}
cis-endo-4-3	2.37×10^{-16}	4.14×10^{-16}	6.42×10^{-16}	9.21×10^{-16}	1.25×10^{-15}	1.62×10^{-15}	2.03×10^{-15}
cis-exo-1-2	1.73×10^{-16}	3.23×10^{-16}	5.27×10^{-16}	7.85×10^{-16}	1.09×10^{-15}	1.45×10^{-15}	1.86×10^{-15}
cis-exo-2-1	2.06×10^{-19}	9.30×10^{-19}	2.84×10^{-18}	6.78×10^{-18}	1.36×10^{-17}	2.42×10^{-17}	3.93×10^{-17}
cis-exo-3-4	1.25×10^{-17}	3.03×10^{-17}	5.92×10^{-17}	1.01×10^{-16}	1.55×10^{-16}	2.23×10^{-16}	3.05×10^{-16}
cis-exo-4-3	1.06×10^{-15}	1.41×10^{-15}	1.82×10^{-15}	2.26×10^{-15}	2.73×10^{-15}	3.24×10^{-15}	3.78×10^{-15}
trans-endo-1-2	3.35×10^{-16}	5.24×10^{-16}	7.52×10^{-16}	1.02×10^{-15}	1.31×10^{-15}	1.64×10^{-15}	2.00×10^{-15}
trans-endo-2-1	6.74×10^{-18}	1.64×10^{-17}	3.23×10^{-17}	5.51×10^{-17}	8.54×10^{-17}	1.23×10^{-16}	1.69×10^{-16}
trans-endo-3-4	1.51×10^{-16}	2.25×10^{-16}	3.11×10^{-16}	4.06×10^{-16}	5.11×10^{-16}	6.25×10^{-16}	7.46×10^{-16}
trans-endo-4-3	2.44×10^{-16}	4.04×10^{-16}	6.04×10^{-16}	8.40×10^{-16}	1.11×10^{-15}	1.41×10^{-15}	1.75×10^{-15}
trans-exo-1-2	4.21×10^{-16}	6.45×10^{-16}	9.15×10^{-16}	1.23×10^{-15}	1.57×10^{-15}	1.96×10^{-15}	2.37×10^{-15}
trans-exo-2-1	5.37×10^{-18}	1.33×10^{-17}	2.65×10^{-17}	4.56×10^{-17}	7.10×10^{-17}	1.03×10^{-16}	1.42×10^{-16}
trans-exo-3-4	1.99×10^{-16}	2.83×10^{-16}	3.77×10^{-16}	4.81×10^{-16}	5.93×10^{-16}	7.13×10^{-16}	8.40×10^{-16}
trans-exo-4-3	7.27×10^{-16}	1.00×10^{-15}	1.31×10^{-15}	1.66×10^{-15}	2.03×10^{-15}	2.42×10^{-15}	2.84×10^{-15}

Table S4. Calculated rate coefficients (s^{-1}) for isoprene isomerization

isoprene isomerization TS	250 K	300 K	350 K	400 K	450 K	500 K	550 K
trans → gauche (*perp*-TS)	$1.34\times10^{+08}$	$9.07\times10^{+08}$	$3.57\times10^{+09}$	$1.00\times10^{+10}$	$2.23\times10^{+10}$	$4.25\times10^{+10}$	$7.20\times10^{+10}$
gauche → trans (*perp*-TS)	$1.65\times10^{+10}$	$4.47\times10^{+10}$	$9.12\times10^{+10}$	$1.56\times10^{+11}$	$2.38\times10^{+11}$	$3.34\times10^{+11}$	$4.40\times10^{+11}$
gauche → gauche (*cis*-TS)	$9.88\times10^{+11}$	$1.35\times10^{+12}$	$1.69\times10^{+12}$	$2.01\times10^{+12}$	$2.31\times10^{+12}$	$2.58\times10^{+12}$	$2.83\times10^{+12}$

Internal rotation

Table S5. Potential energy for internal CC-CC rotation at the B3LYP/6-311+G(2df,2p) level of theory for isoprene and for two orientations (inner-facing and outer-facing) of the addition TS on the least-substituted (3,4) double bond of isoprene. The energies are in kcal/mol and are not ZPE-corrected. Plots are available in the main text.

Isoprene		inner-facing exo-4-3		outer-facing exo-3-4	
0	3.808	0	2.379	0	5.432
15	3.576	15	3.021	15	6.096
30	3.194	30	3.909	30	7.151
37.4	3.126	45	5.021	45	8.848
45	3.206	60	6.077	60	10.906
60	3.837	75	6.854	75	12.169
75	4.899	90	7.293	90	12.064
90	5.947	105	7.278	105	10.637
103.3	6.366	120	6.652	120	8.530
120	5.561	135	5.403	135	6.272
135	3.806	150	3.894	150	4.333
150	1.891	165	2.641	165	3.378
165	0.500	180	1.920	169.0	3.319
180	0.002	187.4	1.827	180	3.592
195	0.500	195	1.929	195	4.880
210	1.891	210	2.702	210	6.864
225	3.806	225	4.118	225	9.089
240	5.561	240	5.959	240	10.815
256.7	6.366	255	7.767	255	11.299
270	5.947	270	8.557	270	10.460
285	4.899	285	7.310	285	8.666
300	3.837	300	5.059	300	6.649
315	3.206	315	3.189	315	5.194
322.6	3.126	330	2.217	330	4.679
330	3.194	341.6	2.029	331.3	4.676
345	3.576	345	2.042	345	4.917
360	3.808	360	2.379	360	5.432

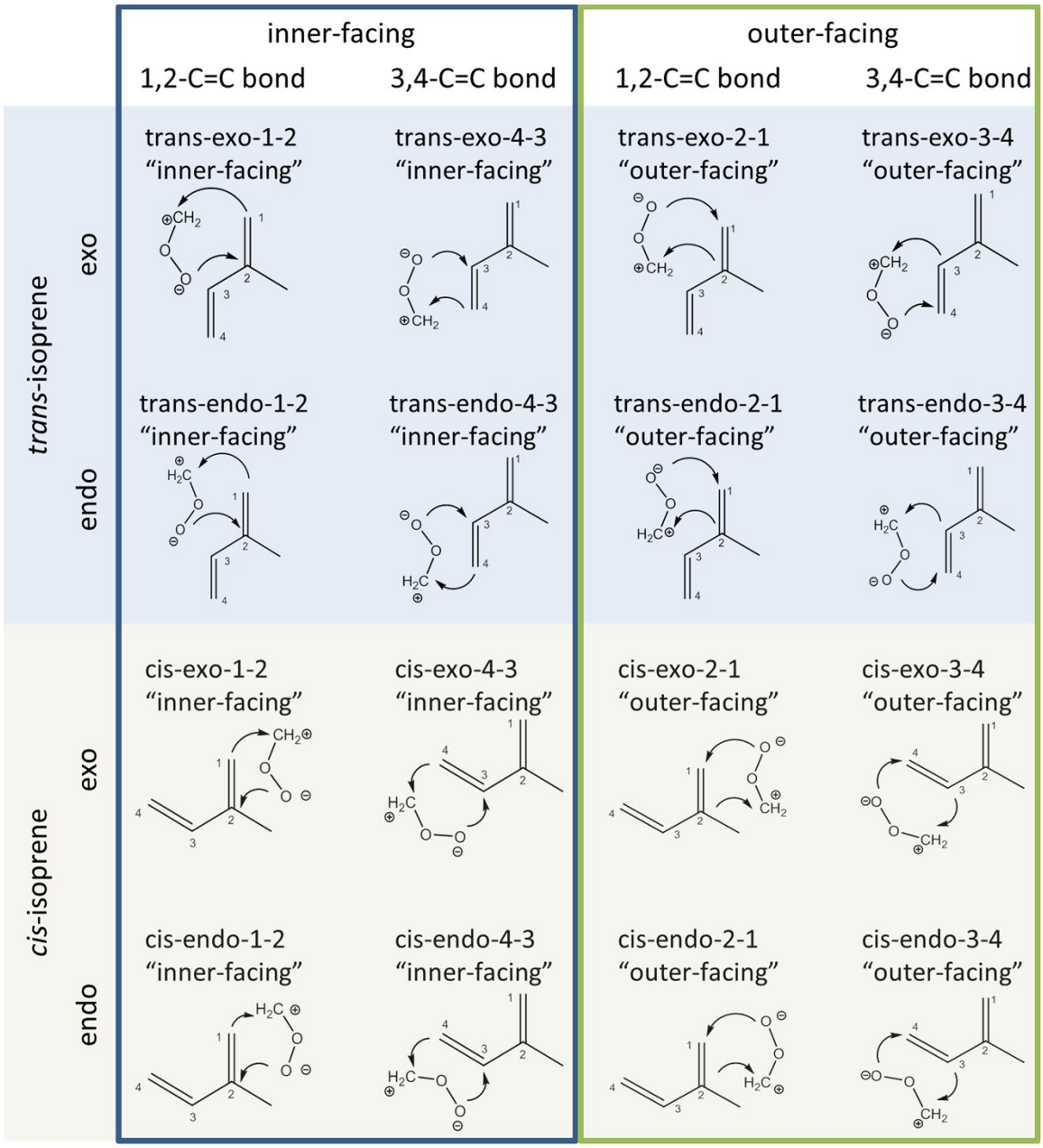


Figure S3. Schematic representation of the 16 distinct cycloaddition TS explored in this study

IV. Minor reaction channels

In our search for the source of the curvature in the Arrhenius plot for the $CH_2OO + C_5H_8$ rate coefficient measurements, we have examined four additional mechanisms, supplementing the chain addition discussed in detail in the main paper. All of these reaction combined comprise ≤ 0.2% of the reaction flux even at 550K, making them negligible under all atmospheric conditions. All quantum chemical calculations in this section were performed using Gaussian-09.[4]

a. H-abstraction

To our knowledge, H-abstraction reactions by carbonyl oxides from hydrocarbons have not been characterized yet. The reactions are expected to be energetically unfavorable, forming a pair of radicals on an overall singlet surface. The most easily abstracted H-atoms in isoprene are the methyl-H, forming a resonance-stabilized radical. The H-atom can be transferred to the C atom of CH_2OO or to the outer O-atom, forming CH_3OO and CH_2OOH, respectively. The table below gives the relative energies of the reactant and products for the H-abstraction channels, confirming that these channels are strongly endothermic and will not contribute significantly to the $CH_2OO+C_5H_8$ reaction.

It should be noted that the CH_2OOH fragment is not stable and was shown by Vereecken *et al*.[5] to decompose without a barrier to CH_2O + OH, which makes the overall reaction exothermic. However, this decomposition is only possible after the H-abstraction TS is passed, i.e. when the CH_2OOH moiety is formed and sufficiently detached from the isoprenyl radical. As such, this decomposition is not expected to not lower the H-abstraction barrier appreciably.

Table S6. Calculated relative energies of the reactants and products in the most favorable H-abstraction channel in the reaction of CH_2OO with isoprene

Compounds	E_{rel} (kcal/mol)[a]
$C_5H_8 + CH_2OO$	0.0
$^{\bullet}CH_2–C(=CH_2)-CH=CH_2 + CH_3OO^{\bullet}$	16.0
$^{\bullet}CH_2–C(=CH_2)-CH=CH_2 + {}^{\bullet}CH_2OOH$	28.1
$^{\bullet}CH_2–C(=CH_2)-CH=CH_2 + CH_2O + {}^{\bullet}OH$	-7.2

[a] ROHF-UCCSD(T)-F12/cc-pVTZ-F12//B3LYP level of theory

b. Chain addition

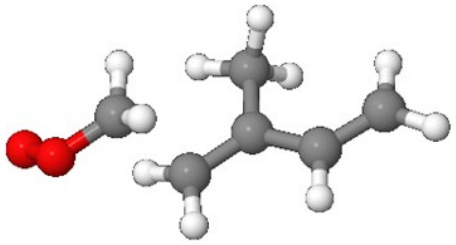


Figure S4. Representative chain-addition TS geometry (to the C1 atom of isoprene).

Chain addition of carbonyl oxides to alkenes was proposed indirectly by Crehuet *et al*.,[6] who found a high barrier of 21.6 kcal/mol for the attack of the outer O-atom of CH_2OO on $CH_2=CH_2$, forming CH_2O with a $^{\bullet}CH_2CH_2O^{\bullet}$ biradical coproduct. Our exploratory calculations likewise find very high barriers for the CI O-atom attack on alkenes, ≥ 40 kcal/mol. However, since the Crehuet *et al*. study we have learned[7] that radical reactions for carbonyl oxides typically proceed by C-atom attack (as shown schematically in Fig. S4), though later theoretical studies never

explored these channels.[7-9] Furthermore, O-atom radical sites tend to be more stable than C-atom sites, suggesting that C–C chain addition spearheaded by the CH_2OO carbon atom should be an energetically more favorable route, forming a singlet biradical species containing a peroxy radical moiety and an alkyl radical. Isoprene furthermore has a conjugated π-bonded system, allowing for resonance stabilization of the carbon-based free electron if the chain addition occurs on the outer carbon C_5H_8 atoms, which will additionally lower the barrier for chain addition.

We have characterized 18 distinct TS geometries for carbon-carbon CH_2OO chain addition on isoprene; the table below lists the lowest TS energies for each group of TS, i.e. for chain addition on each of the unsaturated carbon atoms. The calculations involved geometry optimization, vibrational frequency analysis and IRC reaction path verification at the B3LYP/6-311+G(2df,2pd) level of theory, where the energy of the lowest TS was refined at the UCCSD(T)/cc-pVTZ level of theory, using the broken symmetry approach by Noodleman[10] to allow convergence of the wavefunction to a singlet biradical with two separate radical centers. These TS have a high degree of multi-reference character in their wavefunction, with a T1 diagnostic exceeding 0.05, significantly higher than the ~0.03 values for cycloaddition, and higher than the recommendations for a maximum of 0.044. As such, the predicted energies carry a sizable uncertainty. Still, it is clear that the barrier heights are such that chain addition reactions are not competitive against the very low energy barriers of the cycloaddition channels, even though chain addition is entropically more favorable than cycloaddition due to the lower TS rigidity. We opted not to perform an exhaustive search for all chain addition TS structures, given the low importance of this channel.

The formation of the most stable chain adducts is exothermic by -11.5 kcal/mol; we expect that in all cases fast internal rotation will align the two radical centers, forming a new bond and thus recovering the same products formed in the cycloaddition pathways. In principle, one could also perform a 1,7-ring closure forming a peroxide with a 7-membered ring. This is entropically less favorable, and additionally will have a higher energy barrier as it will break the resonance stabilization of the hydrocarbon moiety free electron which is only effective if the allyl π-system remains mostly in-plane.

Table S7. Calculated energies of the most favorable TS geometry for each chain addition site of isoprene

Compound	Reaction product	E_{rel} (kcal/mol)[a]
$C_5H_8 + CH_2OO$		0.0
TS C–C chain addition on carbon 1	$^{\bullet}OOCH_2–CH_2–C^{\bullet}(CH_3)–CH=CH_2$	14.3
TS C–C chain addition on carbon 4	$CH_2=C(CH_3)–C^{\bullet}H–CH_2–CH_2OO^{\bullet}$	19.2
TS C–C chain addition on carbon 2	$^{\bullet}CH_2–C(CH_3)(CH_2OO^{\bullet})–CH=CH_2$	23.4
TS C–C chain addition on carbon 3	$CH_2=C(CH_3)–CH(CH_2OO^{\bullet})–C^{\bullet}H_2$	23.1

[a] UCCSD(T)/cc-pVTZ//B3LYP/6-311+G(2df,2pd) energies for the reactants and lowest chain addition TS; the energies of the remaining TS are based on B3LYP energies relative to this lowest TS.

c. Insertion into a vinylic C–H bond

The carbonyl oxide insertion reactions[7] in OH and NH bonds (e.g. CI + H_2O, ROH, NH_3) all proceed via an attack of the oxide outer O-atom on the H-atom, while the oxide moiety C-atom associates with a lone pair on the substrate O- or N-atom. CI insertion in C–H bonds in hydrocarbons has not been reported yet, to our knowledge, but the p-orbitals of the C atoms in olefinic π-bonds could lend themselves to make a partial bond

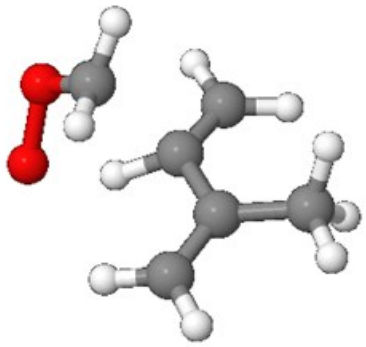


Figure S5. Lowest-energy TS for CH_2OO insertion into a C-H bond

with the CI carbon atom in the TS. This could allow CI insertion reactions into vinylic C–H bonds, forming a longer-chain hydroperoxide.

We have characterized four distinct transition states for insertion in a vinylic C–H bonds, using the same methodology as for the chain addition calculations. The lowest TS found involve the insertion in the C–H bond on carbon 3, as shown in Fig. S5. Even through the reaction involves formally the migration of an H-atom, the reaction rate will not be significantly enhanced by tunneling, as the effective mass of the reaction mode is rather high due to the concerted formation of the C–C bond. Similarly, since no radical intermediates are formed, no significant difference is expected between insertions on the outer or inner C-atoms. We conclude that this reaction channel is not competitive against the cycloaddition pathways across the entire temperature range considered in this study.

Table S8. Calculated energies for the most favorable C-H bond insertion channel, relative to the reactants

Compound	Reaction product	E_{rel} (kcal/mol)
$C_5H_8 + CH_2OO$		0.0[a]
TS Insertion in vinylic $=C_3–H$ bond	$CH_2=C(CH_3)–C(CH_2OOH)=CH_2$	12.4[a] (13.4[b])

[a] UCCSD(T)/cc-pVTZ//B3LYP/6-311+G(2df,2pd) energies
[b] ROHF-CCSD(T)-F12/cc-pVDZ-F12//B3LYP energy

d. Epoxidation

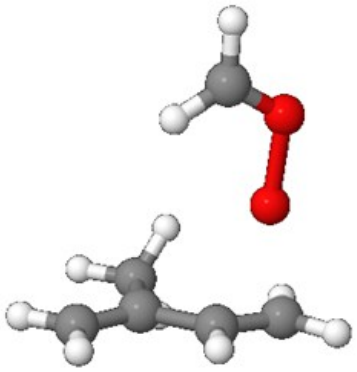
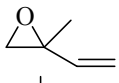
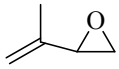


Figure S6. Representative geometry for epoxidation TS (3,4-epoxidation)

The epoxidation of alkenes by carbonyl oxides was studied by Crehuet *et al.*,[6] who found a barrier of ~11 kcal/mol for $C_2H_4 + CH_2OO$. Our calculations for the CH_2OO + isoprene epoxidation find similar barrier heights (see table S9), making this pathway not competitive with cycloaddition. Rate coefficient calculations show that, of the minor reactions considered here, it is the most important channel, comprising from ~0.000001% of the reaction flux at 250K to 0.2% at 550 K. A representative epoxidation TS geometry is shown in Fig. S6

Table S9. Most favorable TS energies for each possible epoxidation site (1,2- and 3,4-epoxidation)

Compound	Reaction product	E_{rel} (kcal/mol)
$C_5H_8 + CH_2OO$		0.0[a]
Epoxidation TS		10.4[a] (10.1[b])
		10.7[a]

[a] UCCSD(T)/cc-pVTZ//B3LYP/6-311+G(2df,2pd) energies
[b] ROHF-CCSD(T)-F12/cc-pVDZ-F12//B3LYP energy

References

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Quantum chemical data

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*******************************************
M06-2X/aug-cc-pVTZ geometries
*******************************************
C5H8
----
E(CCSD(T)-F12a/CC-PVTZ-F12) (Hartree): -195.02800094
E(CCSD(T)-F12b/CC-PVTZ-F12) (Hartree): -195.01489053
E(CCSD-F12a/CC-PVTZ-F12) (Hartree): -194.98623792
     T1 diagnostic:  0.011301
     D1 diagnostic:  0.034794
E(CCSD-F12b/CC-PVTZ-F12) (Hartree): -194.97312751
E(CCSD-T-F12a/CC-PVTZ-F12) (Hartree): -195.02762537
E(CCSD-T-F12b/CC-PVTZ-F12) (Hartree): -195.01451496
E(CCSD[T]-F12a/CC-PVTZ-F12) (Hartree): -195.02904540
E(CCSD[T]-F12b/CC-PVTZ-F12) (Hartree): -195.01593499
E(RHF/CC-PVTZ-F12) (Hartree): -194.04045366
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -194.95308144
E(CCSD/Aug-CC-pVTZ) (Hartree): -194.91177387
     T1 diagnostic:  0.010738
E(MP2/Aug-CC-pVTZ) (Hartree): -194.86924394
E(MP3/Aug-CC-pVTZ) (Hartree): -194.91028095
E(RHF/Aug-CC-pVTZ) (Hartree): -194.03019834
E(CCSD(T)/CC-pVTZ) (Hartree): -194.93993194
E(CCSD/CC-pVTZ) (Hartree): -194.89997766
     T1 diagnostic:  0.010668
E(MP2/CC-pVTZ) (Hartree): -194.85557294
E(MP3/CC-pVTZ) (Hartree): -194.89769767
E(RHF/CC-pVTZ) (Hartree): -194.02853961
E(RM062X/Aug-CC-pVTZ) (Hartree): -195.28212677
Point group : CS
Electronic state : 1-A'
Cartesian coordinates (Angs):
     C      -0.368704     -1.928823       0.000000
     C      -0.830697     -0.682072       0.000000
     C       0.000000      0.526691       0.000000
     C      -0.578674      1.727464       0.000000
     H       0.691409     -2.145767       0.000000
     H      -1.042457     -2.773898       0.000000
     H      -1.902623     -0.514483       0.000000
     C       1.491210      0.362196       0.000000
     H      -1.656359      1.828104       0.000000
     H       0.006379      2.637362       0.000000
     H       1.988209      1.329351       0.000000
     H       1.818316     -0.196700       0.878340
     H       1.818316     -0.196700      -0.878340
Rotational constants (GHz):    8.6160700    4.2289800    2.8870700
Vibrational harmonic frequencies (cm-1):
      163.4321 (  A")           225.6783 (  A")           295.3840 (  A')
      411.9327 (  A")           430.5408 (  A')           535.8969 (  A')
      653.7838 (  A")           797.8362 (  A")           807.5166 (  A')
      952.4082 (  A")           965.7746 (  A")           970.8205 (  A')
     1012.3737 (  A')          1038.6221 (  A")          1070.4720 (  A")
     1089.6268 (  A')          1324.7952 (  A')          1342.6578 (  A')
     1410.4354 (  A')          1440.0895 (  A')          1461.2737 (  A')
     1484.2287 (  A")          1504.3258 (  A')          1691.7210 (  A')
     1739.7854 (  A')          3060.3743 (  A')          3115.0837 (  A")
     3154.8567 (  A')          3165.3007 (  A')          3168.5198 (  A')
     3177.6847 (  A')          3251.5170 (  A')          3257.5925 (  A')
Zero-point correction (Hartree): 0.114301

C5H8.gauche
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E(RM062X/Aug-CC-pVTZ) (Hartree): -195.27708786
Electronic state : 1-A
Cartesian coordinates (Angs):
     C      -0.454174      0.111486      -0.063718
     C      -0.583840      1.434910      -0.093311
     H       0.262271      2.077136      -0.297968
     H      -1.543311      1.907216       0.071703
     C       0.850109     -0.549104      -0.261722
     C       2.009795     -0.102701       0.204032
     H       0.827045     -1.488087      -0.807939
     H       2.933056     -0.632656       0.015332
     H       2.064772      0.801034       0.797945
     C      -1.621567     -0.809898       0.150469
     H      -1.734311     -1.483502      -0.701672
     H      -1.463098     -1.434667       1.031180
     H      -2.548360     -0.254630       0.276917
Rotational constants (GHz):    8.8857600    3.9512900    2.8839400
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Vibrational harmonic frequencies (cm-1):
      118.6353                187.1349                275.1015
      364.7504                415.6711                550.7983
      667.7582                780.4727                814.0848
      952.6847                971.4950                976.9574
     1017.5353               1038.7405               1064.6931
     1102.0031               1273.8057               1334.6828
     1407.8430               1441.5425               1459.8313
     1483.6581               1497.0906               1715.2729
     1733.4651               3054.0731               3107.9627
     3150.0300               3151.8966               3165.6361
     3168.6374               3250.7213               3254.6317
Zero-point correction (Hartree): 0.113793

CH2O2
-----
E(CCSD(T)-F12a/CC-PVTZ-F12) (Hartree): -189.40471750
E(CCSD(T)-F12b/CC-PVTZ-F12) (Hartree): -189.39458673
E(CCSD-F12a/CC-PVTZ-F12) (Hartree): -189.37017675
     T1 diagnostic:  0.040930
     D1 diagnostic:  0.163610
E(CCSD-F12b/CC-PVTZ-F12) (Hartree): -189.36004598
E(CCSD-T-F12a/CC-PVTZ-F12) (Hartree): -189.40327427
E(CCSD-T-F12b/CC-PVTZ-F12) (Hartree): -189.39314350
E(CCSD[T]-F12a/CC-PVTZ-F12) (Hartree): -189.40956765
E(CCSD[T]-F12b/CC-PVTZ-F12) (Hartree): -189.39943688
E(RHF/CC-PVTZ-F12) (Hartree): -188.64649132
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -189.33060211
E(CCSD/Aug-CC-pVTZ) (Hartree): -189.29649796
     T1 diagnostic:  0.041955
E(MP2/Aug-CC-pVTZ) (Hartree): -189.28461070
E(MP3/Aug-CC-pVTZ) (Hartree): -189.28352041
E(RHF/Aug-CC-pVTZ) (Hartree): -188.63545695
E(CCSD(T)/CC-pVTZ) (Hartree): -189.31218211
E(CCSD/CC-pVTZ) (Hartree): -189.27975213
     T1 diagnostic:  0.043388
E(MP2/CC-pVTZ) (Hartree): -189.26562057
E(MP3/CC-pVTZ) (Hartree): -189.26599400
E(RHF/CC-pVTZ) (Hartree): -188.63062980
E(RM062X/Aug-CC-pVTZ) (Hartree): -189.57546386
Point group : CS
Electronic state : 1-A'
Cartesian coordinates (Angs):
     C       1.057244     -0.186665       0.000000
     O       0.000000      0.459010       0.000000
     O      -1.164498     -0.210115       0.000000
     H       1.006101     -1.269496       0.000000
     H       1.966418      0.398328       0.000000
Rotational constants (GHz):   81.1723800   12.6762200   10.9640300
Vibrational harmonic frequencies (cm-1):
      537.8612 (  A')           697.7926 (  A")           929.6060 (  A')
     1022.7616 (  A")          1261.0431 (  A')          1433.3312 (  A')
     1630.5789 (  A')          3141.0852 (  A')          3291.9601 (  A')
Zero-point correction (Hartree): 0.031771

complex.CH2O2.H2C=CCH3CH=CH2
----------------------------
E(RM062X/Aug-CC-pVTZ) (Hartree): -384.86757192
Electronic state : 1-A
Cartesian coordinates (Angs):
     C      -2.085650     -1.210954      -0.450599
     C      -1.412504     -0.221846       0.143855
     C      -1.228728      1.056703      -0.554228
     C       1.295470     -1.068659      -0.858684
     O       1.947103     -0.060888      -0.560699
     O       2.407365      0.053337       0.710497
     H      -2.240249     -2.163740       0.038767
     H       1.130330     -1.832076      -0.106682
     H       0.927959     -1.111866      -1.874878
     H      -2.514325     -1.082307      -1.436721
     H      -1.774992      1.168927      -1.485519
     C      -0.439950      2.040899      -0.133775
     C      -0.821363     -0.369762       1.516252
     H       0.144401      1.959591       0.773943
     H      -0.337538      2.953420      -0.704350
     H      -1.016220     -1.363016       1.916421
     H       0.258055     -0.194977       1.511366
     H      -1.256811      0.368159       2.192336
Rotational constants (GHz):    2.5331100    1.3537200    1.2004400
Vibrational harmonic frequencies (cm-1):
       47.0678                 67.9365                 92.5091
```

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      108.0226                137.1198                162.0543
      180.2639                270.0955                311.0239
      422.6734                430.8947                536.7995
      539.8415                658.3864                700.7633
      798.4879                806.0491                901.5905
      945.7323                968.0841                988.8048
     1016.2070               1039.2725               1044.0247
     1080.8992               1093.7027               1256.0399
     1325.0806               1343.6296               1421.3010
     1435.4130               1441.5104               1465.7926
     1486.5560               1516.3236               1644.7412
     1685.4354               1732.1917               3045.5285
     3105.9814               3141.0948               3144.0147
     3158.8686               3162.3548               3174.7660
     3245.3842               3258.2586               3290.9959
Zero-point correction (Hartree): 0.147693

complex.CH2O2.H2C=CH3CCH=CH2
----------------------------
E(RM062X/Aug-CC-pVTZ) (Hartree): -384.86741408
Electronic state : 1-A
Cartesian coordinates (Angs):
     C       1.831514     -1.604209      -0.251906
     C       1.385535     -0.434434       0.212191
     C       1.677294      0.798686      -0.530957
     C      -1.460950     -0.638166      -1.021003
     O      -2.344982     -0.475172      -0.169665
     O      -2.429898      0.735718       0.433730
     H       2.420565     -1.659011      -1.158867
     H      -0.803490      0.190945      -1.262712
     H      -1.416221     -1.621347      -1.470288
     H       1.632584     -2.531367       0.269453
     H       2.358084      0.694215      -1.369889
     C       1.154718      1.990936      -0.256604
     C       0.580611     -0.327067       1.474503
     H       0.456711      2.136087       0.557987
     H       1.403487      2.857913      -0.852622
     H       0.403206     -1.310267       1.905316
     H       1.114363      0.281871       2.206682
     H      -0.382588      0.162113       1.305078
Rotational constants (GHz):    2.5288400    1.2288600    1.0547100
Vibrational harmonic frequencies (cm-1):
       31.4889                 59.0948                 75.0831
      112.8759                128.1886                161.7068
      201.6296                272.0828                317.3836
      420.1547                432.2132                538.0442
      540.1529                657.7643                710.5471
      798.5094                805.6434                905.6193
      949.0733                969.6676                983.1106
     1016.2939               1040.5468               1064.7087
     1077.8931               1091.8182               1259.9296
     1323.6001               1343.5234               1420.2476
     1437.8662               1441.4991               1465.3802
     1484.3008               1518.3386               1639.4824
     1686.9905               1733.6211               3047.4057
     3104.4612               3131.7872               3147.5137
     3160.4776               3164.2177               3175.7766
     3247.0699               3259.2492               3284.6821
Zero-point correction (Hartree): 0.147713

complex.CH2O2.H2C=CHCCH3=CH2
----------------------------
E(RM062X/Aug-CC-pVTZ) (Hartree): -384.86750343
Electronic state : 1-A
Cartesian coordinates (Angs):
     C      -1.077852      1.922679      -0.464010
     C      -0.646707      0.678450      -0.669222
     C      -1.289449     -0.532145      -0.147979
     C       1.771046      0.707547       1.030627
     O       2.042178     -0.386613       0.520715
     O       2.423980     -0.400087      -0.780095
     H      -0.551999      2.770807      -0.881696
     H       1.882988      1.606758       0.437214
     H       1.441304      0.680330       2.060697
     H      -1.974328      2.134063       0.104928
     H       0.253706      0.508060      -1.255856
     C      -0.717363     -1.715968      -0.372526
     C      -2.564550     -0.387157       0.630222
     H       0.211654     -1.788236      -0.925022
     H      -1.159506     -2.631657      -0.001420
     H      -2.935969     -1.358181       0.949466
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     H      -2.413760      0.232835       1.516467
     H      -3.334110      0.098378       0.027585
Rotational constants (GHz):    2.7861200    1.2287900    1.0356600
Vibrational harmonic frequencies (cm-1):
       53.2148                56.0785                85.9489
      116.0030               121.3923               209.5814
      218.9893               225.8220               292.8889
      425.9987               433.7055               534.1596
      538.2785               672.4615               696.5428
      806.3790               810.3588               909.5291
      962.9022               976.7331               988.8805
     1014.7759              1042.3443              1070.6378
     1091.7518              1094.4957              1256.2255
     1334.5317              1343.7630              1410.8930
     1436.8300              1444.0043              1465.3029
     1484.2047              1504.8775              1643.3593
     1685.7912              1733.0087              3055.0397
     3107.9905              3143.7028              3146.8540
     3151.5939              3157.7011              3168.2826
     3248.0862              3249.8063              3293.4098
Zero-point correction (Hartree): 0.147888

complex.CH2O2.H2C=HCCCH3=CH2
----------------------------
E(RM062X/Aug-CC-pVTZ) (Hartree): -384.86774891
Electronic state : 1-A
Cartesian coordinates (Angs):
     C       0.867936      1.908881      -0.517255
     C       0.603717      0.609719      -0.645154
     C       1.439551     -0.474226      -0.113900
     C      -1.746394      0.280845       1.168931
     O      -2.530467      0.239865       0.211628
     O      -2.366434     -0.749278      -0.700391
     H       1.756830      2.268075      -0.014125
     H      -0.980861     -0.482999       1.258317
     H      -1.898659      1.095929       1.864074
     H       0.203525      2.654570      -0.931919
     H      -0.294324      0.288190      -1.168163
     C       1.016310     -1.734583      -0.230130
     C       2.736362     -0.119101       0.552393
     H       0.068632     -1.957314      -0.705711
     H       1.602914     -2.561998       0.147904
     H       3.258383     -1.012670       0.886717
     H       3.385725      0.427895      -0.133166
     H       2.568138      0.526419       1.416868
Rotational constants (GHz):    2.9377800    1.1084800    0.9509500
Vibrational harmonic frequencies (cm-1):
       55.7156                58.3231                66.8223
      104.6767               128.3419               191.5579
      230.2438               232.1629               295.4126
      430.4762               432.6596               534.9572
      539.5310               671.9726               710.1551
      804.4247               811.3070               912.1714
      969.3832               975.9142               981.2052
     1015.4646              1060.1164              1071.5711
     1093.0947              1098.6665              1264.5705
     1336.2691              1342.7956              1410.9715
     1441.1544              1442.6875              1463.7135
     1485.2923              1504.5755              1640.8561
     1685.4976              1732.4713              3056.0579
     3109.8934              3133.6361              3145.6462
     3151.8546              3156.9671              3169.1891
     3247.2451              3252.2353              3284.0091
Zero-point correction (Hartree): 0.147930

complex.O2CH2.H2C=CCH3CH=CH2
----------------------------
E(RM062X/Aug-CC-pVTZ) (Hartree): -384.86603977
Electronic state : 1-A
Cartesian coordinates (Angs):
     C       0.023434      1.298259      -0.925972
     C      -0.951645      0.668694      -0.266474
     C      -1.434382     -0.632142      -0.745603
     O       2.766694      0.322865      -0.266228
     O       2.106226     -0.817611       0.036273
     C       1.313579     -0.787719       0.987197
     H      -0.952392     -1.006346      -1.643434
     H       1.218606      0.127213       1.559721
     H       0.772076     -1.703667       1.182665
     H       0.412765      2.251168      -0.594244
     H       0.479454      0.867567      -1.807327
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     C      -2.387998     -1.358574      -0.167915
     C      -1.576890      1.243955       0.971699
     H      -2.901859     -1.023326       0.723906
     H      -2.692615     -2.309954      -0.580653
     H      -1.123588      2.199126       1.227211
     H      -2.648620      1.394971       0.831860
     H      -1.463780      0.566382       1.822350
Rotational constants (GHz):    2.9185800    1.1595900    1.0284000
Vibrational harmonic frequencies (cm-1):
      i13.2377                  41.3532                  57.2945
       98.7047                 131.1710                 183.0172
      213.7397                 236.6638                 294.4473
      414.8752                 431.0139                 535.6270
      536.7814                 656.8407                 690.8820
      795.6482                 803.3699                 921.7132
      963.3671                 967.6061                 977.6728
     1007.7008                1034.1546                1045.4761
     1070.1415                1088.1074                1255.7338
     1322.4846                1339.5899                1411.6997
     1435.4349                1440.7122                1462.6133
     1482.8237                1506.0519                1638.1601
     1685.4125                1731.9506                3047.2504
     3102.1818                3143.9957                3151.5453
     3164.4747                3173.6886                3175.1380
     3256.9759                3258.9941                3290.8203
Zero-point correction (Hartree): 0.147341

complex.O2CH2.H2C=CH3CCH=CH2
----------------------------
E(RM062X/Aug-CC-pVTZ) (Hartree): -384.86747886
Electronic state : 1-A
Cartesian coordinates (Angs):
     C      -0.180099      1.335046      -0.869152
     C      -0.932445      0.285354      -0.524911
     C      -2.172084      0.491100       0.232669
     O       2.759342     -0.156322      -0.528969
     O       2.064960     -0.536202       0.574674
     C       1.596345      0.356543       1.291673
     H       1.803593      1.390760       1.045923
     H       1.013129      0.026486       2.141744
     H      -2.420285      1.523695       0.457045
     H      -0.481262      2.342491      -0.606540
     H       0.747604      1.205020      -1.414115
     C      -2.982940     -0.477425       0.648402
     C      -0.538994     -1.114220      -0.893573
     H      -2.778778     -1.519987       0.442028
     H      -3.882543     -0.253259       1.204107
     H       0.411954     -1.122379      -1.421298
     H      -0.442221     -1.739091      -0.002540
     H      -1.304303     -1.571932      -1.522650
Rotational constants (GHz):    3.5702600    1.0057300    0.9967300
Vibrational harmonic frequencies (cm-1):
       27.7872                  45.8499                  95.2719
      111.9916                 125.4933                 167.3006
      228.6659                 245.4173                 296.8658
      419.2178                 436.7668                 532.1481
      535.2562                 663.6214                 695.5287
      806.3380                 810.5106                 906.7762
      971.5037                 972.6581                 973.3735
     1019.3386                1039.2281                1044.1735
     1071.6006                1090.6326                1254.3007
     1326.0679                1346.6780                1412.2548
     1436.4702                1438.8158                1459.4811
     1484.6379                1502.7335                1643.6207
     1682.7891                1731.1610                3053.8119
     3108.2784                3144.1468                3146.3200
     3157.8526                3164.0289                3176.6706
     3237.8644                3258.8969                3289.4687
Zero-point correction (Hartree): 0.147602

complex.O2CH2.H2C=CHCCH3=CH2
----------------------------
E(RM062X/Aug-CC-pVTZ) (Hartree): -384.86777298
Electronic state : 1-A
Cartesian coordinates (Angs):
     C       0.094929      1.895835       0.332877
     C       0.949914      1.161426      -0.377162
     C       1.475449     -0.147100       0.034959
     O      -2.292549     -0.232199       0.817840
     O      -1.679595     -0.847923      -0.224967
     C      -1.581742     -0.218574      -1.284997
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     H       1.303511      1.530869     -1.335692
     H      -2.023377      0.768265     -1.349568
     H      -1.055937     -0.721705     -2.085849
     H      -0.251994      2.852847     -0.033349
     H      -0.296781      1.560471      1.283899
     C       2.238643     -0.842923     -0.809333
     C       1.130459     -0.646897      1.406843
     H       2.486929     -0.455004     -1.789677
     H       2.641729     -1.810230     -0.541073
     H       1.564545     -1.628923      1.579937
     H       1.512739      0.041497      2.163160
     H       0.049870     -0.707697      1.546105
Rotational constants (GHz):    2.5876200    1.3104600    1.2520400
Vibrational harmonic frequencies (cm-1):
       39.4275                   55.2120                   82.7094
      119.8775                  126.0132                  175.0741
      206.0322                  249.9650                  305.1654
      421.9177                  429.4295                  533.7547
      538.9737                  656.8723                  690.5086
      798.8952                  805.6681                  909.8475
      948.1911                  969.1827                  979.5145
     1016.8568                 1036.9578                 1043.1910
     1077.2993                 1092.9893                 1255.9522
     1323.0088                 1342.7561                 1418.2739
     1435.6433                 1440.7243                 1463.4428
     1485.0474                 1511.8329                 1645.3989
     1683.2551                 1732.4853                 3060.4526
     3120.7894                 3145.1555                 3150.9241
     3154.7452                 3161.5765                 3173.4875
     3247.3610                 3258.2344                 3291.6523
Zero-point correction (Hartree): 0.147652

complex.O2CH2.H2C=HCCCH3=CH2
----------------------------
E(RM062X/Aug-CC-pVTZ) (Hartree): -384.86813044
Electronic state : 1-A
Cartesian coordinates (Angs):
     C       0.069596      1.315287     -1.220275
     C       1.067006      1.162560     -0.351176
     C       1.644706     -0.129714      0.040331
     O      -2.232530     -0.952414     -0.463700
     O      -2.426309      0.078401      0.395958
     C      -1.543232      0.310332      1.230932
     H      -0.668467     -0.328920      1.278869
     H      -1.723619      1.155038      1.882943
     H       1.496762      2.036455      0.129138
     H      -0.406251      0.470554     -1.703793
     H      -0.314994      2.298895     -1.453892
     C       2.518301     -0.180240      1.047822
     C       1.211943     -1.354234     -0.711685
     H       2.822904      0.717934      1.570488
     H       2.958694     -1.115221      1.367652
     H       1.706290     -2.241613     -0.322784
     H       0.129780     -1.493856     -0.652669
     H       1.459695     -1.251112     -1.769705
Rotational constants (GHz):    2.8375200    1.1206400    1.0818800
Vibrational harmonic frequencies (cm-1):
       44.3681                   60.4114                   88.6134
      110.9876                  116.1718                  164.9147
      212.9074                  242.0918                  306.2866
      424.5294                  430.1904                  535.7753
      541.3197                  662.1090                  701.8117
      801.4604                  806.9508                  911.4039
      954.2996                  971.1368                  997.0637
     1018.6153                 1044.4354                 1051.7484
     1079.7354                 1095.3274                 1253.0863
     1325.0474                 1344.4635                 1420.1664
     1439.9934                 1442.9533                 1465.9133
     1484.8051                 1512.7511                 1645.1767
     1685.1404                 1732.4478                 3052.5720
     3110.3327                 3137.8092                 3151.7276
     3157.0723                 3161.8643                 3168.3593
     3247.7256                 3252.7859                 3284.2282
Zero-point correction (Hartree): 0.147742

TS.CH2O2.H2C=CCH3CH=CH2
-----------------------
E(CCSD(T)-F12a/CC-PVTZ-F12) (Hartree): -384.43412060
E(CCSD(T)-F12b/CC-PVTZ-F12) (Hartree): -384.41076800
E(CCSD-F12a/CC-PVTZ-F12) (Hartree): -384.35253028
     T1 diagnostic:  0.029028
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     D1 diagnostic:  0.176917
E(CCSD-F12b/CC-PVTZ-F12) (Hartree): -384.32917767
E(CCSD-T-F12a/CC-PVTZ-F12) (Hartree): -384.43234218
E(CCSD-T-F12b/CC-PVTZ-F12) (Hartree): -384.40898958
E(CCSD[T]-F12a/CC-PVTZ-F12) (Hartree): -384.44114759
E(CCSD[T]-F12b/CC-PVTZ-F12) (Hartree): -384.41779498
E(RHF/CC-PVTZ-F12) (Hartree): -382.66543567
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -384.28701559
E(CCSD/Aug-CC-pVTZ) (Hartree): -384.20623248
     T1 diagnostic:  0.029662
E(MP2/Aug-CC-pVTZ) (Hartree): -384.16159601
E(MP3/Aug-CC-pVTZ) (Hartree): -384.19256924
E(RHF/Aug-CC-pVTZ) (Hartree): -382.64458578
E(CCSD(T)/CC-pVTZ) (Hartree): -384.25418801
E(CCSD/CC-pVTZ) (Hartree): -384.17674526
     T1 diagnostic:  0.030324
E(MP2/CC-pVTZ) (Hartree): -384.12801898
E(MP3/CC-pVTZ) (Hartree): -384.16148752
E(RHF/CC-pVTZ) (Hartree): -382.63934607
E(RM062X/Aug-CC-pVTZ) (Hartree): -384.86064005
Electronic state : 1-A
Cartesian coordinates (Angs):
     C      -0.344724      1.214124      -0.994132
     C       0.598310      0.638965      -0.203781
     C       1.386558     -0.481412      -0.719696
     C      -2.215682      0.225225      -0.124717
     O      -1.818191     -0.966517      -0.047408
     O      -0.875360     -1.154960       0.910640
     H      -0.761357      2.180315      -0.738455
     H      -2.082694      0.868191       0.734583
     H      -2.935555      0.427027      -0.907589
     H      -0.494068      0.866416      -2.008212
     H       0.988611     -0.966286      -1.604572
     C       2.541723     -0.892326      -0.208329
     C       0.964270      1.228720       1.121954
     H       2.971575     -0.435579       0.673313
     H       3.090049     -1.708346      -0.656502
     H       0.237397      1.979096       1.428735
     H       1.008799      0.450818       1.881654
     H       1.942920      1.710388       1.063404
Rotational constants (GHz):    2.9599000    1.4711800    1.3038400
Vibrational harmonic frequencies (cm-1):
     i220.3280                  60.3873                 110.6131
      130.0221                 182.8542                 195.3640
      207.5227                 298.7588                 396.1719
      429.6567                 437.0897                 546.2509
      560.0978                 692.8447                 793.0860
      809.1888                 838.9707                 906.6003
      962.0089                 964.3904                 972.9594
     1012.9591                1028.9457                1054.2157
     1062.0855                1090.8433                1246.5664
     1323.6149                1348.1945                1399.0250
     1410.1136                1431.3188                1455.2461
     1482.5498                1497.1935                1569.7724
     1628.1946                1717.2019                3059.6164
     3125.5662                3146.6478                3154.1057
     3154.8156                3171.6615                3179.8490
     3241.5991                3261.0861                3282.2940
Zero-point correction (Hartree): 0.148150

TS.CH2O2.H2C=CH3CCH=CH2
-----------------------
E(RM062X/Aug-CC-pVTZ) (Hartree): -384.86055867
Electronic state : 1-A
Cartesian coordinates (Angs):
     C       0.318573      1.531080      -0.369975
     C      -0.593945      0.640427       0.102411
     C      -1.510220     -0.008786      -0.834312
     C       2.098484      0.132071      -0.678961
     O       1.962413     -0.628862       0.315360
     O       0.881015     -1.446306       0.211765
     H       0.308977      1.823181      -1.412827
     H       1.629203     -0.153227      -1.610225
     H       2.924843      0.829093      -0.623033
     H       0.867950      2.164862       0.313670
     H      -1.265807      0.103406      -1.885896
     C      -2.606923     -0.674341      -0.489006
     C      -0.794738      0.459762       1.576277
     H      -2.892062     -0.806088       0.546151
     H      -3.253366     -1.109931      -1.237486
     H       0.105890      0.745507       2.116791
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     H      -1.615458      1.096373       1.917586
     H      -1.024968     -0.573125       1.819664
Rotational constants (GHz):    3.0460000    1.4102800    1.3332600
Vibrational harmonic frequencies (cm-1):
     i227.2797                  59.0451                  93.0028
      126.2456                 181.7139                 189.6486
      230.0971                 304.4573                 397.9534
      433.3928                 447.4360                 544.0659
      560.0625                 696.4490                 793.3789
      807.1967                 845.9980                 899.1530
      958.8811                 972.1107                 975.7126
     1014.4742                1031.0740                1054.4514
     1064.1165                1090.2681                1246.2836
     1326.8942                1350.1935                1397.6075
     1410.3456                1428.3659                1455.7413
     1479.8700                1500.2941                1567.3188
     1623.9124                1718.9269                3054.0395
     3129.4904                3148.8694                3154.7632
     3164.4631                3172.3033                3180.0761
     3241.7693                3262.7241                3285.2474
Zero-point correction (Hartree): 0.148240

TS.CH2O2.H2C=CHCCH3=CH2
-----------------------
E(RM062X/Aug-CC-pVTZ) (Hartree): -384.85951719
Electronic state : 1-A
Cartesian coordinates (Angs):
     C       0.502011      1.602956      -0.189633
     C      -0.378976      0.736145      -0.746355
     C      -1.471046      0.075301      -0.029496
     C       2.305304      0.207742       0.044204
     O       1.704324     -0.824738       0.444930
     O       0.929715     -1.399864      -0.506084
     H       1.103629      2.246017      -0.817576
     H       2.464961      0.330702      -1.017519
     H       2.891006      0.724513       0.793609
     H       0.435861      1.868523       0.857062
     H      -0.371847      0.597744      -1.820830
     C      -2.484323     -0.445930      -0.719451
     C      -1.408857      0.038082       1.467855
     H      -2.496820     -0.421252      -1.801263
     H      -3.320919     -0.917427      -0.221917
     H      -2.247608     -0.522248       1.874031
     H      -0.482117     -0.439687       1.789967
     H      -1.433129      1.044154       1.890928
Rotational constants (GHz):    3.1458300    1.4018400    1.3023400
Vibrational harmonic frequencies (cm-1):
     i243.9794                  63.6898                  90.1510
      126.5684                 186.7914                 209.5375
      290.8647                 311.4169                 401.3617
      432.8958                 490.0235                 540.3300
      560.6631                 687.9273                 789.0781
      806.5531                 812.4536                 911.1328
      946.8134                 968.8663                 970.9910
     1012.1177                1031.3745                1051.1501
     1070.4980                1097.2929                1247.9193
     1311.6855                1336.7249                1403.2295
     1411.4925                1433.5724                1457.2861
     1487.4017                1502.0295                1567.8367
     1623.1242                1724.4304                3058.0726
     3116.4619                3151.0762                3153.9904
     3164.3535                3167.9003                3192.4923
     3249.5983                3253.6301                3287.7313
Zero-point correction (Hartree): 0.148451

TS.CH2O2.H2C=HCCCH3=CH2
-----------------------
E(RM062X/Aug-CC-pVTZ) (Hartree): -384.86052372
Electronic state : 1-A
Cartesian coordinates (Angs):
     C      -0.414222     -1.210138       1.011685
     C       0.339276     -0.084279       0.945549
     C       1.510964      0.077584       0.084304
     C      -1.995503     -0.626433      -0.535365
     O      -2.207701      0.555872      -0.150325
     O      -1.164150      1.388444      -0.376221
     H      -0.130862     -2.103943       0.469903
     H      -1.248337     -0.795071      -1.297660
     H      -2.788270     -1.331910      -0.322493
     H      -1.149915     -1.328602       1.794249
     H       0.136285      0.731645       1.624693
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     C       2.236983      1.191159       0.171057
     C       1.862074     -1.030639      -0.864992
     H       1.954994      1.987413       0.847244
     H       3.117131      1.341567      -0.439644
     H       2.742000     -0.773269      -1.449617
     H       2.062962     -1.960027      -0.329212
     H       1.041387     -1.225864      -1.558521
Rotational constants (GHz):    3.1509600    1.3696500    1.1860400
Vibrational harmonic frequencies (cm-1):
     i241.8150                 43.0559                  93.3872
      105.7919                 205.5809                 216.2019
      297.9482                 333.3920                 402.1746
      436.7098                 498.4465                 538.9440
      559.9704                 686.1700                 783.6699
      810.5373                 817.0389                 899.2534
      961.8716                 971.7462                 975.1884
     1010.1619                1026.1794                1049.7985
     1066.8754                1094.8093                1244.8868
     1311.6122                1339.1628                1402.3397
     1408.4411                1437.0095                1459.1106
     1485.5637                1501.1451                1562.3431
     1623.7637                1725.3763                3056.0787
     3108.5724                3152.6389                3154.0330
     3163.4357                3168.8850                3217.9770
     3252.5899                3255.8114                3287.3961
Zero-point correction (Hartree): 0.148544

TS.O2CH2.H2C=CCH3CH=CH2
-----------------------
E(RM062X/Aug-CC-pVTZ) (Hartree): -384.85729431
Electronic state : 1-A
Cartesian coordinates (Angs):
     C       0.438365      0.967609      -1.095982
     C      -0.563429      0.540485      -0.274108
     C      -1.336370     -0.653686      -0.651812
     O       2.384215      0.046791      -0.354208
     O       1.739491     -0.965034       0.270007
     C       0.910203     -0.548283       1.127517
     H      -0.888917     -1.267735      -1.427577
     H       1.072089      0.421910       1.576970
     H       0.279536     -1.307772       1.571527
     H       0.893038      1.938916      -0.967510
     H       0.683739      0.433869      -2.001417
     C      -2.504910     -1.016466      -0.130436
     C      -1.134997      1.446384       0.787903
     H      -2.995295     -0.434473       0.639428
     H      -3.014164     -1.906249      -0.471819
     H      -0.450982      2.265526       1.005220
     H      -2.081371      1.873779       0.451986
     H      -1.340487      0.911914       1.718301
Rotational constants (GHz):    3.1597700    1.4114200    1.2893500
Vibrational harmonic frequencies (cm-1):
     i343.6870                 76.2041                 119.8273
      181.7417                 225.0850                 241.4761
      262.6119                 300.3147                 419.8658
      427.9739                 440.7908                 540.6099
      574.0437                 697.9976                 772.6493
      792.5584                 808.8821                 948.2105
      957.0041                 982.1515                1000.5711
     1006.6904                1035.6625                1046.8686
     1083.3215                1086.3617                1244.6543
     1321.0611                1335.1743                1399.5664
     1410.1367                1427.6944                1461.6127
     1487.7139                1510.5153                1557.8056
     1612.5978                1711.8902                3048.7257
     3104.4534                3138.2979                3148.0739
     3161.8128                3174.0013                3190.3388
     3256.9322                3279.4765                3287.1549
Zero-point correction (Hartree): 0.148762

TS.O2CH2.H2C=CH3CCH=CH2
-----------------------
E(RM062X/Aug-CC-pVTZ) (Hartree): -384.85731131
Electronic state : 1-A
Cartesian coordinates (Angs):
     C      -0.420714      0.995533      -1.076396
     C       0.536841      0.544739      -0.215214
     C       1.565748     -0.387486      -0.701907
     O      -2.365318     -0.056232      -0.495291
     O      -1.858801     -0.488453       0.682904
     C      -0.802429     -1.166222       0.526742
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     H      -0.648084     -1.680245      -0.411173
     H      -0.288951     -1.448984       1.436825
     H      -1.018363      1.864866      -0.852441
     H      -0.490691      0.603534      -2.081636
     H       1.371867     -0.825740      -1.677098
     C       2.684592     -0.712166      -0.060543
     C       0.773071      1.257709       1.092658
     H       2.933512     -0.291724       0.905151
     H       3.397002     -1.397378      -0.497046
     H      -0.119798      1.802806       1.393180
     H       1.037636      0.569123       1.895917
     H       1.596172      1.968579       0.995384
Rotational constants (GHz):    3.3978100    1.3476700    1.2940300
Vibrational harmonic frequencies (cm-1):
     i345.3545                  81.4199                 110.1978
      165.3800                 217.6982                 226.9350
      254.0325                 300.5384                 417.5682
      442.1044                 448.6553                 537.0380
      573.7245                 693.9177                 783.3454
      790.1415                 810.7283                 950.5253
      959.3074                 978.9023                 998.5092
     1008.7399                1038.3383                1051.4288
     1083.0076                1084.6479                1238.0694
     1322.5491                1336.5785                1393.7592
     1410.1040                1426.6082                1460.1063
     1489.4472                1508.0742                1554.9350
     1611.6465                1713.8123                3056.6962
     3112.6479                3146.4948                3151.8832
     3152.9445                3175.5790                3187.6104
     3258.6960                3280.7425                3290.6157
Zero-point correction (Hartree): 0.148733

TS.O2CH2.H2C=CHCCH3=CH2
-----------------------
E(RM062X/Aug-CC-pVTZ) (Hartree): -384.85997583
Electronic state : 1-A
Cartesian coordinates (Angs):
     C      -0.546994     -0.951874       1.234500
     C       0.361390      0.039282       1.040260
     C       1.459771     -0.037600       0.058685
     O      -2.278229     -0.485432      -0.230128
     O      -1.552967      0.435724      -0.904786
     C      -1.102384      1.347951      -0.154661
     H       0.436700      0.832640       1.777279
     H      -1.622336      1.559911       0.769031
     H      -0.428807      2.048047      -0.631296
     H      -1.243447     -0.912660       2.058280
     H      -0.518830     -1.872897       0.674132
     C       2.443005      0.861782       0.068247
     C       1.408184     -1.156842      -0.939437
     H       2.467432      1.659343       0.800843
     H       3.254569      0.817925      -0.645117
     H       2.201395     -1.056874      -1.676426
     H       1.520715     -2.121239      -0.440383
     H       0.444358     -1.172728      -1.452592
Rotational constants (GHz):    3.2037700    1.3975000    1.3341800
Vibrational harmonic frequencies (cm-1):
     i322.6991                  67.4307                  94.5118
      134.9291                 230.4372                 244.0696
      304.4867                 365.7137                 407.7107
      445.0315                 524.7434                 540.6718
      570.7598                 676.1692                 763.1199
      787.5810                 806.5357                 931.5162
      948.6525                 961.0334                 993.5725
     1002.3896                1014.3224                1063.7853
     1072.4369                1091.2647                1249.0508
     1293.2536                1327.2480                1404.3424
     1410.8563                1430.1376                1459.4771
     1484.6420                1503.8565                1561.5910
     1614.9653                1724.6975                3056.8731
     3112.1766                3150.7249                3154.7443
     3158.2507                3161.9885                3203.1909
     3247.5678                3289.5803                3290.0897
Zero-point correction (Hartree): 0.148838

TS.O2CH2.H2C=HCCCH3=CH2
-----------------------
E(RM062X/Aug-CC-pVTZ) (Hartree): -384.86032889
Electronic state : 1-A
Cartesian coordinates (Angs):
     C       0.500238     -1.122314       0.982187
```

```
     C      -0.328691     -0.046567      0.940972
     C      -1.536792      0.031182      0.099818
     O       2.257595     -0.620407     -0.403857
     O       2.139486      0.703187     -0.156698
     C       1.018647      1.169775     -0.503210
     H       0.457330      0.670850     -1.280054
     H       0.836819      2.199338     -0.222987
     H      -0.234374      0.713666      1.708647
     H       0.331531     -1.997030      0.372119
     H       1.265005     -1.207002      1.737462
     C      -2.375632      1.061083      0.207872
     C      -1.764165     -1.077953     -0.885788
     H      -2.203033      1.851100      0.928453
     H      -3.263634      1.132940     -0.405125
     H      -2.626580     -0.870186     -1.514420
     H      -0.889229     -1.224095     -1.524476
     H      -1.932112     -2.023052     -0.366288
Rotational constants (GHz):    3.4296800    1.3093300    1.1753900
Vibrational harmonic frequencies (cm-1):
     i327.5963                  75.2499                  95.9911
      135.1283                 234.8531                 249.0435
      305.1954                 346.6877                 425.0563
      435.9655                 517.2217                 532.9085
      567.5301                 686.6224                 773.9931
      791.2266                 810.6249                 936.1709
      960.9663                 963.5876                 995.2297
     1009.0184                1013.9915                1062.4504
     1073.4886                1092.3252                1235.6791
     1299.6757                1327.4515                1402.2507
     1409.5353                1430.7713                1460.6098
     1482.1297                1504.2982                1558.0769
     1613.5281                1724.9439                3050.7306
     3104.4404                3154.2454                3155.9406
     3161.9990                3169.3025                3201.6669
     3248.8846                3287.8281                3293.5234
Zero-point correction (Hartree): 0.148919

ts_c_top_in_1_2
---------------
E(RM062X/Aug-CC-pVTZ) (Hartree): -384.85985759
Electronic state : 1-A
Cartesian coordinates (Angs):
     C      -0.650052      0.495395      0.395804
     C      -0.207558     -0.233924      1.448865
     H      -0.581166     -1.233334      1.631672
     H       0.338465      0.244534      2.251718
     C      -1.548250     -0.081223     -0.614592
     C      -2.454071     -1.024162     -0.377399
     H      -1.443073      0.326566     -1.612775
     H      -3.079092     -1.408873     -1.171113
     H      -2.614923     -1.423610      0.616036
     C      -0.317368      1.953910      0.278595
     H       0.661894      2.161589      0.707420
     H      -0.310345      2.272044     -0.759846
     H      -1.062139      2.541753      0.821426
     C       1.602551     -1.147156      0.385911
     O       2.051501     -0.171293     -0.268297
     O       1.256364      0.169129     -1.324312
     H       0.888967     -1.802933     -0.096742
     H       2.186982     -1.437467      1.249978
Rotational constants (GHz):    2.7065600    1.4955100    1.3888800
Vibrational harmonic frequencies (cm-1):
     i201.7061                  46.4706                  86.9906
      132.6024                 174.8385                 200.8432
      214.3128                 299.8270                 393.6614
      410.3348                 446.8322                 557.2637
      566.7021                 699.2114                 801.8495
      814.9654                 842.3785                 918.2694
      951.1754                 973.8871                 978.1405
     1028.4000                1041.1737                1059.9049
     1070.1427                1098.3532                1249.4431
     1280.6599                1335.5197                1401.7732
     1410.8403                1431.3505                1460.0595
     1481.5232                1488.0038                1572.0113
     1642.5737                1710.4925                3053.1813
     3124.3863                3138.4224                3154.9197
     3166.1752                3170.9377                3193.0444
     3241.6831                3253.4005                3276.0688
Zero-point correction (Hartree): 0.148183

ts_c_top_in_2_1
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---------------
E(RM062X/Aug-CC-pVTZ) (Hartree): -384.85316612
Electronic state : 1-A
Cartesian coordinates (Angs):
     C      -0.660489      0.574306       0.312147
     C       0.057538      0.143354       1.385857
     H      -0.173698     -0.788555       1.880443
     H       0.752625      0.797784       1.888566
     C      -1.829172     -0.183848      -0.184406
     C      -2.019458     -1.496185      -0.090942
     H      -2.588276      0.415650      -0.678791
     H      -2.920441     -1.958996      -0.466814
     H      -1.289451     -2.147857       0.376709
     C      -0.551490      2.014283      -0.140739
     H      -0.734664      2.119852      -1.210641
     H      -1.288886      2.633213       0.374510
     H       0.437257      2.414501       0.078679
     C       0.867706     -0.343865      -1.194859
     O       1.929341     -0.082206      -0.564330
     O       2.014628     -0.755064       0.606344
     H       0.709944      0.241272      -2.092604
     H       0.356022     -1.276973      -1.008518
Rotational constants (GHz):    2.6913400    1.5793300    1.3598700
Vibrational harmonic frequencies (cm-1):
     i336.9074                 55.1715                146.9827
      158.1334                 190.6176               209.5962
      221.0939                 305.3374               404.5550
      432.3107                 441.1650               518.0109
      573.9570                 693.6730               776.4389
      793.2480                 795.8728               958.6737
      964.7078                 979.9310               995.8259
     1024.9489                1041.3930              1045.2406
     1066.8601                1106.6144              1235.0245
     1268.7436                1338.1532              1402.0844
     1412.2734                1436.9666              1457.5519
     1492.3463                1506.4581              1562.7319
     1617.7543                1711.5030              3053.4660
     3110.2544                3141.2646              3149.1646
     3153.7876                3158.4810              3193.2886
     3251.8429                3280.7724              3291.9799
Zero-point correction (Hartree): 0.148369

ts_c_top_in_3_4
---------------
E(RM062X/Aug-CC-pVTZ) (Hartree): -384.85751068
Electronic state : 1-A
Cartesian coordinates (Angs):
     C       1.392827      0.036323       0.213523
     C       1.138081     -0.442009       1.429748
     H       0.181752     -0.281950       1.911467
     H       1.880823     -1.013987       1.969606
     C       0.397015      0.829699      -0.533321
     C      -0.540667      1.604184       0.061808
     H       0.563834      0.938929      -1.601053
     H      -1.198095      2.232832      -0.520373
     H      -0.568013      1.730667       1.133345
     C       2.688343     -0.222108      -0.501910
     H       2.508466     -0.748342      -1.443095
     H       3.184440      0.716627      -0.754990
     H       3.363956     -0.822509       0.103061
     C      -1.156096     -0.859300      -1.073552
     O      -1.609177     -0.956066       0.097803
     O      -2.302999      0.131474       0.498496
     H      -0.515951     -1.672920      -1.389101
     H      -1.620819     -0.163347      -1.757031
Rotational constants (GHz):    3.3853300    1.3355400    1.2965000
Vibrational harmonic frequencies (cm-1):
     i284.8517                 71.5867                 90.4236
      148.2995                 197.2013               216.9239
      294.5332                 330.7109               403.1666
      438.7308                 513.5649               549.1877
      567.8167                 686.9563               754.7699
      766.2393                 815.5493               939.7645
      956.2341                 973.4928               991.6079
     1002.3656                1019.6649              1044.2223
     1068.3713                1100.4764              1248.1315
     1267.8418                1305.0529              1407.3784
     1409.4559                1447.7329              1461.4041
     1483.5207                1497.9611              1568.9245
     1628.2333                1726.3131              3047.4416
     3100.6225                3150.5429              3151.4007
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     3154.3359                3164.1527                3193.2805
     3249.4060                3281.7568                3292.0764
Zero-point correction (Hartree): 0.148488

ts_c_top_in_4_3
---------------
E(CCSD(T)-F12a/CC-PVTZ-F12) (Hartree): -384.43326729
E(CCSD(T)-F12b/CC-PVTZ-F12) (Hartree): -384.40989773
E(CCSD-F12a/CC-PVTZ-F12) (Hartree): -384.35143547
     T1 diagnostic:  0.028087
     D1 diagnostic:  0.170512
E(CCSD-F12b/CC-PVTZ-F12) (Hartree): -384.32806592
E(CCSD-T-F12a/CC-PVTZ-F12) (Hartree): -384.43155636
E(CCSD-T-F12b/CC-PVTZ-F12) (Hartree): -384.40818681
E(CCSD[T]-F12a/CC-PVTZ-F12) (Hartree): -384.44001861
E(CCSD[T]-F12b/CC-PVTZ-F12) (Hartree): -384.41664905
E(RHF/CC-PVTZ-F12) (Hartree): -382.66231669
E(RM062X/Aug-CC-pVTZ) (Hartree): -384.85987791
Electronic state : 1-A
Cartesian coordinates (Angs):
     C       1.314405      0.270585       0.073030
     C       1.347085      0.763940       1.310791
     H       0.642254      1.506203       1.659634
     H       2.091165      0.429163       2.020460
     C       0.293598      0.666644      -0.903683
     C      -0.698351      1.559280      -0.686055
     H       0.376080      0.208525      -1.881107
     H      -1.338168      1.869915      -1.500147
     H      -0.724328      2.167400       0.208109
     C       2.289356     -0.766776      -0.399346
     H       1.743992     -1.675053      -0.658083
     H       2.815187     -0.423521      -1.292279
     H       3.024771     -0.999638       0.367314
     C      -2.183337      0.053780       0.258600
     O      -1.397813     -0.837700       0.678609
     O      -0.800213     -1.535844      -0.319492
     H      -2.576089     -0.038321      -0.743466
     H      -2.647197      0.658960       1.026598
Rotational constants (GHz):    2.8523100    1.5922800    1.3812000
Vibrational harmonic frequencies (cm-1):
     i210.6725                  59.3977                  93.5799
      132.1786                 189.0897                 208.3982
      309.2050                 322.6543                 412.3870
      434.8402                 482.2124                 522.0671
      560.3679                 682.6551                 771.4478
      795.2392                 817.3226                 903.2750
      942.5530                 963.1345                 972.7100
     1021.4625                1030.9796                1045.9242
     1073.2636                1105.0645                1244.9854
     1277.2576                1319.8284                1401.9215
     1405.0601                1442.7556                1461.7805
     1485.3615                1502.0819                1563.7915
     1646.0088                1722.5812                3059.1957
     3121.6339                3154.7660                3155.4752
     3169.1808                3176.8604                3201.1004
     3252.1353                3257.7672                3293.4705
Zero-point correction (Hartree): 0.148460

ts_c_top_out_1_2
----------------
E(RM062X/Aug-CC-pVTZ) (Hartree): -384.85981392
Electronic state : 1-A
Cartesian coordinates (Angs):
     C      -0.708532      0.602418       0.253565
     C      -0.146894      0.346821       1.460225
     H      -0.287283     -0.608366       1.947696
     H       0.241843      1.156914       2.064297
     C      -1.458071     -0.425944      -0.482374
     C      -2.070740     -1.466229       0.072781
     H      -1.507026     -0.286318      -1.554908
     H      -2.601830     -2.186327      -0.533582
     H      -2.075201     -1.625990       1.143250
     C      -0.684454      1.975714      -0.346084
     H      -0.449167      1.921028      -1.406690
     H      -1.665651      2.443882      -0.236268
     H       0.052875      2.610001       0.143436
     C       1.933991     -0.271244       0.695756
     O       1.642396     -0.899919      -0.353379
     O       1.194846     -0.087780      -1.351513
     H       2.262062     -0.880017       1.528560
     H       2.139641      0.787577       0.620130
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Rotational constants (GHz):    2.4563600    1.6272900    1.4512100
Vibrational harmonic frequencies (cm-1):
     i206.7431                  44.8401                  78.3166
      141.2298                 176.0607                 185.5728
      200.5739                 308.0610                 396.1698
      418.3678                 441.9655                 553.3330
      557.9621                 696.3233                 791.9227
      814.2509                 839.3104                 909.8666
      953.6924                 971.0074                 976.7786
     1020.4126                1037.0301                1054.7885
     1062.9658                1098.5013                1245.5232
     1285.0322                1341.5115                1401.5972
     1407.9574                1430.7343                1460.4773
     1479.1167                1491.3988                1572.5917
     1645.2779                1712.5776                3056.6662
     3124.9230                3148.9778                3157.2668
     3158.5613                3171.3566                3199.6186
     3245.2041                3257.2817                3284.8923
Zero-point correction (Hartree): 0.148099

ts_c_top_out_2_1
----------------
E(RM062X/Aug-CC-pVTZ) (Hartree): -384.85435923
Electronic state : 1-A
Cartesian coordinates (Angs):
     C       0.892340     -0.336441       0.302788
     C       0.075831     -0.422320       1.388454
     H      -0.187896      0.448890       1.966737
     H      -0.196354     -1.383156       1.802214
     C       1.383861      0.979013      -0.157152
     C       0.735027      2.129762      -0.013276
     H       2.344129      0.972489      -0.665221
     H       1.160797      3.058111      -0.366863
     H      -0.240923      2.174952       0.455403
     C       1.621826     -1.552743      -0.224247
     H       1.662315     -1.572812      -1.315206
     H       2.653544     -1.550233       0.131925
     H       1.153335     -2.473388       0.121260
     C      -0.877439     -0.578798      -1.150412
     O      -1.662386      0.252927      -0.616868
     O      -2.085405     -0.142336       0.606978
     H      -0.930379     -1.615956      -0.849277
     H      -0.424923     -0.254457      -2.078766
Rotational constants (GHz):    2.4967700    1.8022500    1.4549200
Vibrational harmonic frequencies (cm-1):
     i327.8263                  85.0432                 147.4288
      175.5631                 209.5890                 223.9047
      227.3793                 301.4248                 402.0954
      429.4266                 442.7634                 532.3754
      572.4712                 693.5290                 774.9333
      781.7403                 802.5177                 954.0228
      972.8803                 984.5535                 993.7682
     1016.5838                1032.3405                1038.6398
     1070.0349                1105.1125                1243.4598
     1266.0295                1339.6894                1402.9316
     1411.9261                1436.9597                1459.2162
     1489.1212                1507.8932                1561.2264
     1621.0483                1713.8613                3050.8541
     3106.1991                3137.0707                3148.0318
     3153.7874                3166.1817                3190.1692
     3254.7660                3282.7210                3286.3318
Zero-point correction (Hartree): 0.148536

ts_c_top_out_3_4
----------------
E(RM062X/Aug-CC-pVTZ) (Hartree): -384.85729165
Electronic state : 1-A
Cartesian coordinates (Angs):
     C      -1.518129     -0.128406       0.096774
     C      -1.463416     -0.686705       1.305481
     H      -0.568562     -1.188625       1.654957
     H      -2.315152     -0.666045       1.971558
     C      -0.381761     -0.174204      -0.846355
     C       0.505075     -1.197795      -0.905616
     H      -0.405670      0.537228      -1.665426
     H       1.221806     -1.269300      -1.708582
     H       0.407431     -2.061543      -0.264071
     C      -2.733036      0.608077      -0.391400
     H      -2.480566      1.642920      -0.634952
     H      -3.115195      0.152523      -1.306591
     H      -3.524093      0.612452       0.355010
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     C       1.129365      1.261937       0.356513
     O       2.202057      0.712649      -0.010397
     O       2.297515     -0.583938       0.352141
     H       0.561715      0.838591       1.173439
     H       0.993126      2.274678      -0.001682
Rotational constants (GHz):    3.6604800    1.1971300    1.1497700
Vibrational harmonic frequencies (cm-1):
     i307.7870                  61.6518                  81.3528
      157.5870                 193.0932                 218.8981
      286.2056                 316.9008                 411.3595
      422.4520                 506.0251                 551.0943
      568.0530                 699.7774                 765.1955
      779.3601                 814.6627                 944.7593
      955.0173                 967.2096                 993.1560
     1014.0954                1021.6801                1056.3567
     1069.5893                1102.1101                1243.4029
     1269.4340                1305.9964                1406.7560
     1417.2086                1442.2886                1458.9790
     1482.5934                1496.7265                1572.2509
     1621.3697                1721.1732                3050.8419
     3104.2272                3145.4362                3152.0287
     3156.8042                3164.2447                3193.9242
     3243.9491                3283.3276                3288.9834
Zero-point correction (Hartree): 0.148490

ts_c_top_out_4_3
----------------
E(CCSD(T)-F12a/CC-PVTZ-F12) (Hartree): -384.43490219
E(CCSD(T)-F12b/CC-PVTZ-F12) (Hartree): -384.41154333
E(CCSD-F12a/CC-PVTZ-F12) (Hartree): -384.35353221
     T1 diagnostic:  0.027801
     D1 diagnostic:  0.168596
E(CCSD-F12b/CC-PVTZ-F12) (Hartree): -384.33017335
E(CCSD-T-F12a/CC-PVTZ-F12) (Hartree): -384.43317498
E(CCSD-T-F12b/CC-PVTZ-F12) (Hartree): -384.40981612
E(CCSD[T]-F12a/CC-PVTZ-F12) (Hartree): -384.44159809
E(CCSD[T]-F12b/CC-PVTZ-F12) (Hartree): -384.41823923
E(RHF/CC-PVTZ-F12) (Hartree): -382.66564123
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -384.28771786
E(CCSD/Aug-CC-pVTZ) (Hartree): -384.20715301
     T1 diagnostic:  0.028429
E(MP2/Aug-CC-pVTZ) (Hartree): -384.16278131
E(MP3/Aug-CC-pVTZ) (Hartree): -384.19410818
E(RHF/Aug-CC-pVTZ) (Hartree): -382.64476331
E(CCSD(T)/CC-pVTZ) (Hartree): -384.25461327
E(CCSD/CC-pVTZ) (Hartree): -384.17746885
     T1 diagnostic:  0.028957
E(MP2/CC-pVTZ) (Hartree): -384.12907892
E(MP3/CC-pVTZ) (Hartree): -384.16289290
E(RHF/CC-pVTZ) (Hartree): -382.63960287
E(RM062X/Aug-CC-pVTZ) (Hartree): -384.86165586
Electronic state : 1-A
Cartesian coordinates (Angs):
     C       1.429833     -0.129673       0.022213
     C       1.863911     -1.007834      -0.882427
     H       1.464403     -2.010845      -0.953159
     H       2.659983     -0.749908      -1.567580
     C       0.329545     -0.432674       0.950773
     C      -0.522159     -1.474761       0.846136
     H       0.211695      0.254655       1.778149
     H      -1.255948     -1.661697       1.617410
     H      -0.369451     -2.263311       0.119494
     C       2.025248      1.239940       0.158361
     H       1.252860      1.992030      -0.002662
     H       2.416161      1.380801       1.168062
     H       2.835505      1.393606      -0.550782
     C      -1.863417     -0.448541      -0.726456
     O      -2.106034      0.639664      -0.143752
     O      -1.031668      1.464971      -0.065557
     H      -2.694182     -1.141478      -0.770178
     H      -0.997176     -0.509685      -1.375881
Rotational constants (GHz):    2.9227300    1.5120000    1.2357600
Vibrational harmonic frequencies (cm-1):
     i191.9686                  55.5285                  98.9151
      132.6795                 187.2766                 208.0664
      317.4862                 331.3912                 398.3909
      424.1181                 475.5003                 523.5441
      560.1695                 687.0362                 778.8492
      803.0652                 817.1126                 920.5023
      946.5432                 969.2704                 970.5921
     1018.6033                1030.6332                1069.3107
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     1074.0640                1104.4332                1252.6630
     1278.1126                1322.3362                1405.4107
     1411.7714                1442.5452                1462.4349
     1481.7189                1501.0687                1571.9371
     1648.6523                1720.4309                3059.8166
     3121.9510                3126.4016                3155.8080
     3161.5807                3172.9932                3206.5277
     3250.2723                3254.6397                3268.6971
Zero-point correction (Hartree): 0.148493

TS.chainaddition
----------------
E(CCSD(T)/CC-pVTZ) (Hartree): -384.23234691
E(CCSD/CC-pVTZ) (Hartree): -384.16056632
     T1 diagnostic:  0.047166
E(MP2/CC-pVTZ) (Hartree): -384.07119127
E(MP3/CC-pVTZ) (Hartree): -384.12699545
E(PMP2/CC-pVTZ) (Hartree): -384.19604711
E(PMP3/CC-pVTZ) (Hartree): -384.24798818
E(PUHF/CC-pVTZ) (Hartree): -382.78494169
E(UHF/CC-pVTZ) (Hartree): -382.65778620
E(UM062X/Aug-CC-pVTZ) (Hartree): -384.85068057
Electronic state : 1-A
Cartesian coordinates (Angs):
     O      -2.548871     -0.627470      0.242520
     O      -3.031403      0.524664     -0.270748
     C      -1.379403     -0.489708      0.787666
     C      -0.237413     -0.273122     -0.808725
     C       0.977767      0.177079     -0.351622
     C       2.095282     -0.733816     -0.235660
     C       3.285926     -0.419249      0.284528
     C       1.113891      1.581780      0.140704
     H      -1.175276      0.474378      1.237817
     H      -1.016495     -1.395144      1.256778
     H      -0.292281     -1.267745     -1.235462
     H      -0.995524      0.436190     -1.149193
     H       1.929968     -1.739490     -0.607533
     H       3.499096      0.570854      0.665383
     H       4.082078     -1.147799      0.337686
     H       1.945491      2.087863     -0.352319
     H       0.203607      2.148596     -0.042683
     H       1.325224      1.596957      1.213999
Rotational constants (GHz):    4.9053700    0.9130800    0.8449400
Vibrational harmonic frequencies (cm-1):
    i1105.9217                  52.3112                  68.7261
      118.0277                 169.9217                 198.7638
      201.7484                 300.4909                 371.7985
      442.9778                 455.1308                 542.4831
      568.7127                 681.1353                 745.3028
      818.3177                 854.5221                 969.0559
      970.3104                 988.9642                1016.4019
     1030.5312                1035.3583                1068.7682
     1089.8760                1150.7898                1232.0424
     1278.0692                1323.4528                1359.8351
     1402.0731                1422.4805                1454.6609
     1481.0999                1486.1155                1505.8426
     1584.9455                1667.1733                3043.1377
     3047.5240                3103.2611                3130.3025
     3151.5055                3171.0485                3179.0026
     3201.6117                3256.7067                3264.3345
Zero-point correction (Hartree): 0.147299

*********************************************
B3LYP/6-311+G(2df,2p) geometries
*********************************************
ci
--
E(RHF-RMP2/CC-PVTZ-F12) (Hartree): -189.31212903
     T1 diagnostic:  0.000011
E(RHF-UCCSD(T)-F12a/CC-PVTZ-F12) (Hartree): -189.40530640
E(RHF-UCCSD(T)-F12b/CC-PVTZ-F12) (Hartree): -189.39515305
E(RHF-UCCSD-F12a/CC-PVTZ-F12) (Hartree): -189.37004041
     T1 diagnostic:  0.042251
     D1 diagnostic:  0.169069
E(RHF-UCCSD-F12b/CC-PVTZ-F12) (Hartree): -189.35988705
E(RHF-UCCSD-T-F12a/CC-PVTZ-F12) (Hartree): -189.40377529
E(RHF-UCCSD-T-F12b/CC-PVTZ-F12) (Hartree): -189.39362193
E(RHF-UCCSD[T]-F12a/CC-PVTZ-F12) (Hartree): -189.41044981
E(RHF-UCCSD[T]-F12b/CC-PVTZ-F12) (Hartree): -189.40029645
E(RHF/CC-PVTZ-F12) (Hartree): -188.64470100
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -189.33145151
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E(CCSD/Aug-CC-pVTZ) (Hartree): -189.29662075
     T1 diagnostic:  0.043285
E(MP2/Aug-CC-pVTZ) (Hartree): -189.28496868
E(MP3/Aug-CC-pVTZ) (Hartree): -189.28306020
E(RHF/Aug-CC-pVTZ) (Hartree): -188.63374831
E(CCSD(T)/CC-pVTZ) (Hartree): -189.31304228
E(CCSD/CC-pVTZ) (Hartree): -189.27988032
     T1 diagnostic:  0.044741
E(MP2/CC-pVTZ) (Hartree): -189.26594166
E(MP3/CC-pVTZ) (Hartree): -189.26551404
E(RHF/CC-pVTZ) (Hartree): -188.62891361
E(RB3LYP/6-311+G(2df,2p)) (Hartree): -189.65490404
Electronic state : 1-A
Cartesian coordinates (Angs):
     C       1.068675      0.200813      -0.000033
     O       0.001877     -0.457173       0.000040
     O      -1.178525      0.194450      -0.000023
     H       1.975727     -0.386329      -0.000082
     H       1.025411      1.283233       0.000149
Rotational constants (GHz):   81.3293200   12.4071400   10.7649100
Vibrational harmonic frequencies (cm-1):
      529.9236                674.3864                922.3590
      951.5504               1244.2629               1404.0130
     1544.7014               3120.9900               3271.0156
Zero-point correction (Hartree): 0.031127

t_isp
-----
E(RHF-RMP2/CC-PVTZ-F12) (Hartree): -194.89364594
     T1 diagnostic:  0.000003
E(RHF-UCCSD(T)-F12a/CC-PVTZ-F12) (Hartree): -195.02808630
E(RHF-UCCSD(T)-F12b/CC-PVTZ-F12) (Hartree): -195.01497516
E(RHF-UCCSD-F12a/CC-PVTZ-F12) (Hartree): -194.98617780
     T1 diagnostic:  0.011373
     D1 diagnostic:  0.035246
E(RHF-UCCSD-F12b/CC-PVTZ-F12) (Hartree): -194.97306667
E(RHF-UCCSD-T-F12a/CC-PVTZ-F12) (Hartree): -195.02770613
E(RHF-UCCSD-T-F12b/CC-PVTZ-F12) (Hartree): -195.01459500
E(RHF-UCCSD[T]-F12a/CC-PVTZ-F12) (Hartree): -195.02914325
E(RHF-UCCSD[T]-F12b/CC-PVTZ-F12) (Hartree): -195.01603211
E(RHF/CC-PVTZ-F12) (Hartree): -194.04023095
E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -194.95328892
E(CCSD/Aug-CC-pVTZ) (Hartree): -194.91183346
     T1 diagnostic:  0.010804
E(MP2/Aug-CC-pVTZ) (Hartree): -194.86931372
E(MP3/Aug-CC-pVTZ) (Hartree): -194.91029152
E(RHF/Aug-CC-pVTZ) (Hartree): -194.02999474
E(CCSD(T)/CC-pVTZ) (Hartree): -194.94012721
E(CCSD/CC-pVTZ) (Hartree): -194.90002953
     T1 diagnostic:  0.010733
E(MP2/CC-pVTZ) (Hartree): -194.85562453
E(MP3/CC-pVTZ) (Hartree): -194.89769218
E(RHF/CC-pVTZ) (Hartree): -194.02832478
E(RB3LYP/6-311+G(2df,2p)) (Hartree): -195.38219886
Electronic state : 1-A
Cartesian coordinates (Angs):
     C      -1.979533      0.009453      -0.000044
     C      -0.833392     -0.673729      -0.000037
     H      -2.009863      1.090596      -0.000017
     H      -2.932818     -0.500084      -0.000079
     H      -0.874503     -1.758202      -0.000067
     C       0.513895     -0.100640       0.000007
     C       1.578704     -0.911898      -0.000001
     H       2.589002     -0.525921       0.000032
     H       1.466413     -1.988300      -0.000041
     C       0.664847      1.396500       0.000065
     H       0.190087      1.840241      -0.877553
     H       0.190054      1.840177       0.877697
     H       1.714495      1.683372       0.000095
Rotational constants (GHz):    8.5696700    4.1850600    2.8613000
Vibrational harmonic frequencies (cm-1):
      162.7463                203.0958                280.2186
      412.2008                429.3150                538.2837
      647.3041                788.5430                791.5500
      933.7868                944.0811                961.9230
     1015.1723               1032.5903               1072.1358
     1092.3929               1329.7855               1331.5020
     1415.7865               1433.4989               1464.5382
     1486.5265               1506.4261               1656.2052
     1693.5547               3028.0368               3072.3587
     3112.8073               3133.6780               3139.6155
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     3149.1728                3218.5512                3225.7495
Zero-point correction (Hartree): 0.113232

g_isp
-----
E(RHF-RMP2/CC-PVTZ-F12) (Hartree): -194.88873648
     T1 diagnostic:  0.000003
E(RHF-UCCSD(T)-F12a/CC-PVTZ-F12) (Hartree): -195.02329190
E(RHF-UCCSD(T)-F12b/CC-PVTZ-F12) (Hartree): -195.01016932
E(RHF-UCCSD-F12a/CC-PVTZ-F12) (Hartree): -194.98162652
     T1 diagnostic:  0.011152
     D1 diagnostic:  0.033322
E(RHF-UCCSD-F12b/CC-PVTZ-F12) (Hartree): -194.96850394
E(RHF-UCCSD-T-F12a/CC-PVTZ-F12) (Hartree): -195.02290748
E(RHF-UCCSD-T-F12b/CC-PVTZ-F12) (Hartree): -195.00978490
E(RHF-UCCSD[T]-F12a/CC-PVTZ-F12) (Hartree): -195.02434108
E(RHF-UCCSD[T]-F12b/CC-PVTZ-F12) (Hartree): -195.01121850
E(RHF/CC-PVTZ-F12) (Hartree): -194.03582424
E(RB3LYP/6-311+G(2df,2p)) (Hartree): -195.37721647
Electronic state : 1-A
Cartesian coordinates (Angs):
     C      -0.453816      0.111064      -0.059699
     C      -0.599360      1.437745      -0.089944
     H       0.235605      2.095469      -0.288339
     H      -1.563767      1.901917       0.068004
     C       0.853376     -0.543417      -0.252644
     C       2.025740     -0.099771       0.195925
     H       0.828173     -1.490121      -0.785926
     H       2.942029     -0.639696       0.000641
     H       2.105622      0.807685       0.780397
     C      -1.623171     -0.817218       0.145694
     H      -1.728329     -1.499932      -0.701434
     H      -1.479883     -1.437990       1.033196
     H      -2.556061     -0.267747       0.257467
Rotational constants (GHz):    8.8694700    3.9126600    2.8551200
Vibrational harmonic frequencies (cm-1):
      112.8388                 181.4839                 269.9880
      368.1142                 414.4641                 549.9103
      660.6454                 771.0039                 801.6497
      932.3562                 956.2144                 964.4379
     1017.7596                1033.2010                1065.9479
     1104.8216                1264.6455                1334.0689
     1414.6225                1442.6962                1461.7628
     1484.6177                1499.1483                1671.3937
     1697.7146                3020.6167                3062.9458
     3109.8622                3117.2651                3139.6961
     3141.6682                3219.8168                3221.5115
Zero-point correction (Hartree): 0.112790

p_isp
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E(CCSD(T)-F12a/CC-PVTZ-F12) (Hartree): -195.01853168
E(CCSD(T)-F12b/CC-PVTZ-F12) (Hartree): -195.00540062
E(CCSD-F12a/CC-PVTZ-F12) (Hartree): -194.97720493
     T1 diagnostic:  0.011160
     D1 diagnostic:  0.031374
E(CCSD-F12b/CC-PVTZ-F12) (Hartree): -194.96407387
E(CCSD-T-F12a/CC-PVTZ-F12) (Hartree): -195.01814841
E(CCSD-T-F12b/CC-PVTZ-F12) (Hartree): -195.00501735
E(CCSD[T]-F12a/CC-PVTZ-F12) (Hartree): -195.01958837
E(CCSD[T]-F12b/CC-PVTZ-F12) (Hartree): -195.00645731
E(RHF/CC-PVTZ-F12) (Hartree): -194.03171144
E(RB3LYP/6-311+G(2df,2p)) (Hartree): -195.37205390
Electronic state : 1-A
Cartesian coordinates (Angs):
     C       0.490940      0.129452       0.081237
     C       1.183303      1.240901      -0.156604
     H       0.726150      2.219265      -0.092559
     H       2.230724      1.204854      -0.427714
     C      -0.945053      0.180763       0.475436
     C      -1.964263     -0.085393      -0.332268
     H      -1.148502      0.442302       1.510606
     H      -2.987084     -0.038499       0.016603
     H      -1.814199     -0.349496      -1.371981
     C       1.106658     -1.242940       0.001141
     H       1.014499     -1.766752       0.955882
     H       0.587438     -1.855865      -0.738949
     H       2.161464     -1.192508      -0.265544
Rotational constants (GHz):    8.0478800    3.9784700    2.9876700
Vibrational harmonic frequencies (cm-1):
     i136.2430                 203.3385                 264.3566
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      309.2173                409.9516                563.7336
      689.8768                729.2720                791.0214
      936.5406                956.3082                963.9249
     1017.0519               1032.5294               1051.6830
     1104.0582               1281.9374               1320.6859
     1411.7532               1433.9874               1461.8745
     1480.3225               1495.5979               1675.9708
     1710.9374               3020.4878               3064.7450
     3104.1854               3114.6980               3133.0788
     3134.1527               3213.2594               3213.4200
Zero-point correction (Hartree): 0.112300

c_isp
-----
E(RHF-RMP2/CC-PVTZ-F12) (Hartree): -194.88714484
     T1 diagnostic:  0.000004
E(RHF-UCCSD(T)-F12a/CC-PVTZ-F12) (Hartree): -195.02206695
E(RHF-UCCSD(T)-F12b/CC-PVTZ-F12) (Hartree): -195.00893880
E(RHF-UCCSD-F12a/CC-PVTZ-F12) (Hartree): -194.98021168
     T1 diagnostic:  0.011236
     D1 diagnostic:  0.033903
E(RHF-UCCSD-F12b/CC-PVTZ-F12) (Hartree): -194.96708353
E(RHF-UCCSD-T-F12a/CC-PVTZ-F12) (Hartree): -195.02167727
E(RHF-UCCSD-T-F12b/CC-PVTZ-F12) (Hartree): -195.00854912
E(RHF-UCCSD[T]-F12a/CC-PVTZ-F12) (Hartree): -195.02312351
E(RHF-UCCSD[T]-F12b/CC-PVTZ-F12) (Hartree): -195.00999536
E(RHF/CC-PVTZ-F12) (Hartree): -194.03387134
E(RB3LYP/6-311+G(2df,2p)) (Hartree): -195.37612960
Electronic state : 1-A
Cartesian coordinates (Angs):
     C      -0.453158      0.112665      -0.000036
     C      -0.556480      1.444096      -0.000065
     H       0.309012      2.092236      -0.000185
     H      -1.522450      1.929947       0.000021
     C       0.833759     -0.612943      -0.000143
     C       2.063046     -0.099432       0.000114
     H       0.742854     -1.694960      -0.000454
     H       2.932457     -0.741572      -0.000006
     H       2.250747      0.966335       0.000458
     C      -1.677451     -0.766606       0.000094
     H      -1.688338     -1.419080      -0.876768
     H      -1.688181     -1.419044       0.876985
     H      -2.594397     -0.180543       0.000163
Rotational constants (GHz):    9.1865900    3.8810600    2.7748300
Vibrational harmonic frequencies (cm-1):
     i106.0847                190.7870                290.3291
      399.6894                411.5337                522.4736
      645.6422                748.9903                796.6910
      926.6206                953.2934                957.9972
     1024.4055               1036.8883               1072.5475
     1103.5985               1262.5103               1349.0735
     1415.8342               1446.2677               1463.8452
     1485.5561               1500.4676               1666.0206
     1704.7115               3018.6246               3059.9472
     3111.4313               3127.2776               3142.9989
     3147.0364               3219.8959               3223.7784
Zero-point correction (Hartree): 0.112602

ts_t_top_in_1_2
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IRC pathway available
E(RHF-RMP2/CC-PVTZ-F12) (Hartree): -384.21046422
     T1 diagnostic:  0.000010
E(RHF-UCCSD(T)-F12a/CC-PVTZ-F12) (Hartree): -384.43431057
E(RHF-UCCSD(T)-F12b/CC-PVTZ-F12) (Hartree): -384.41093252
E(RHF-UCCSD-F12a/CC-PVTZ-F12) (Hartree): -384.35187776
     T1 diagnostic:  0.030348
     D1 diagnostic:  0.185605
E(RHF-UCCSD-F12b/CC-PVTZ-F12) (Hartree): -384.32849971
E(RHF-UCCSD-T-F12a/CC-PVTZ-F12) (Hartree): -384.43240597
E(RHF-UCCSD-T-F12b/CC-PVTZ-F12) (Hartree): -384.40902792
E(RHF-UCCSD[T]-F12a/CC-PVTZ-F12) (Hartree): -384.44177726
E(RHF-UCCSD[T]-F12b/CC-PVTZ-F12) (Hartree): -384.41839921
E(RHF/CC-PVTZ-F12) (Hartree): -382.66442035
E(RB3LYP/6-311+G(2df,2p)) (Hartree): -385.03334741
Electronic state : 1-A
Cartesian coordinates (Angs):
     C      -2.633580     -0.748604       0.462545
     C      -1.540724     -0.077141       0.829734
     H      -2.932924     -0.845484      -0.571681
     H      -3.264092     -1.229140       1.197039
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     H      -1.299592     -0.016455      1.885954
     C      -0.634485      0.637449     -0.062066
     C       0.291261      1.492105      0.472796
     H       0.819106      2.191523     -0.160550
     H       0.282141      1.713137      1.532161
     C      -0.854950      0.586504     -1.547821
     H      -1.066444     -0.422317     -1.890623
     H      -1.699606      1.226557     -1.820300
     H       0.022098      0.948107     -2.080834
     C       2.143514      0.125689      0.687376
     O       2.023121     -0.587792     -0.360256
     O       0.957445     -1.445367     -0.317224
     H       1.705585     -0.228600      1.608127
     H       2.962986      0.831930      0.665166
Rotational constants (GHz):    3.0058100    1.3543200    1.2817400
Vibrational harmonic frequencies (cm-1):
     i236.2488                 66.1029                  89.3918
      130.7248                161.3505                 186.9687
      203.4683                289.2757                 385.8995
      428.2794                440.2546                 537.1792
      547.9889                690.0386                 765.4092
      791.4101                832.0270                 870.7807
      923.6385                952.3948                 968.6834
     1007.3044               1018.1639                1024.7689
     1062.8601               1091.3696                1227.2626
     1329.8138               1339.3231                1360.1969
     1404.1527               1418.1525                1459.5220
     1484.1852               1502.2904                1514.7256
     1579.6762               1675.3702                3020.7014
     3096.9098               3127.8765                3132.0187
     3135.8199               3137.3138                3153.7541
     3214.9514               3232.0337                3264.6713
Zero-point correction (Hartree): 0.146433

ts_t_top_in_2_1
---------------
E(RHF-RMP2/CC-PVTZ-F12) (Hartree): -384.21196859
     T1 diagnostic:  0.000011
E(RHF-UCCSD(T)-F12a/CC-PVTZ-F12) (Hartree): -384.43213219
E(RHF-UCCSD(T)-F12b/CC-PVTZ-F12) (Hartree): -384.40875554
E(RHF-UCCSD-F12a/CC-PVTZ-F12) (Hartree): -384.34822352
     T1 diagnostic:  0.028019
     D1 diagnostic:  0.166672
E(RHF-UCCSD-F12b/CC-PVTZ-F12) (Hartree): -384.32484688
E(RHF-UCCSD-T-F12a/CC-PVTZ-F12) (Hartree): -384.43053347
E(RHF-UCCSD-T-F12b/CC-PVTZ-F12) (Hartree): -384.40715683
E(RHF-UCCSD[T]-F12a/CC-PVTZ-F12) (Hartree): -384.43905763
E(RHF-UCCSD[T]-F12b/CC-PVTZ-F12) (Hartree): -384.41568098
E(RHF/CC-PVTZ-F12) (Hartree): -382.65412633
E(RB3LYP/6-311+G(2df,2p)) (Hartree): -385.02837802
Electronic state : 1-A
Cartesian coordinates (Angs):
     C       2.723432     -0.731723     -0.077349
     C       1.576158     -0.421042     -0.683315
     H       3.014394     -0.302905      0.871962
     H       3.420633     -1.422200     -0.530153
     H       1.360499     -0.880232     -1.643859
     C       0.550779      0.514831     -0.198299
     C      -0.403430      0.968815     -1.080711
     H      -0.973678      1.861567     -0.883388
     H      -0.461039      0.577225     -2.085131
     C       0.810254      1.284909      1.078804
     H       1.136831      0.641373      1.895830
     H       1.596947      2.027563      0.924612
     H      -0.087103      1.809572      1.402099
     C      -0.866039     -1.150701      0.617467
     O      -1.935204     -0.449122      0.669877
     O      -2.346049     -0.046840     -0.570536
     H      -0.439671     -1.399246      1.580080
     H      -0.664714     -1.735546     -0.266356
Rotational constants (GHz):    3.3574700    1.3104100    1.2652200
Vibrational harmonic frequencies (cm-1):
     i314.9368                 82.0901                 108.5730
      165.2549                202.1852                 219.8092
      244.9722                288.8182                 413.9300
      430.1160                443.4813                 540.1648
      557.9575                687.0988                 748.7817
      770.3591                797.3030                 928.5566
      947.4153                952.1936                 970.8735
      998.9427               1010.7409                1038.8308
     1071.5494               1085.4594                1217.8781
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     1320.2215                1326.0594                1345.7455
     1400.7059                1418.6635                1462.9937
     1493.6680                1505.7432                1511.9974
     1566.7071                1676.0700                3027.0536
     3076.9101                3111.6178                3122.8114
     3134.5879                3149.2528                3170.0555
     3226.4365                3259.0539                3271.4409
Zero-point correction (Hartree): 0.146944

ts_t_top_in_3_4
---------------
E(RHF-RMP2/CC-PVTZ-F12) (Hartree): -384.21328226
     T1 diagnostic:  0.000011
E(RHF-UCCSD(T)-F12a/CC-PVTZ-F12) (Hartree): -384.43449262
E(RHF-UCCSD(T)-F12b/CC-PVTZ-F12) (Hartree): -384.41111091
E(RHF-UCCSD-F12a/CC-PVTZ-F12) (Hartree): -384.35114626
     T1 diagnostic:  0.028165
     D1 diagnostic:  0.167623
E(RHF-UCCSD-F12b/CC-PVTZ-F12) (Hartree): -384.32776454
E(RHF-UCCSD-T-F12a/CC-PVTZ-F12) (Hartree): -384.43286876
E(RHF-UCCSD-T-F12b/CC-PVTZ-F12) (Hartree): -384.40948704
E(RHF-UCCSD[T]-F12a/CC-PVTZ-F12) (Hartree): -384.44141036
E(RHF-UCCSD[T]-F12b/CC-PVTZ-F12) (Hartree): -384.41802864
E(RHF/CC-PVTZ-F12) (Hartree): -382.65881120
E(RB3LYP/6-311+G(2df,2p)) (Hartree): -385.03170668
Electronic state : 1-A
Cartesian coordinates (Angs):
     C      -0.537736      0.967772       1.198914
     C       0.360958     -0.044537       0.995010
     H      -0.494174      1.894402       0.651098
     H      -1.212050      0.945723       2.039815
     H       0.424469     -0.824929       1.745828
     C       1.496417      0.020012       0.056171
     C       2.484828     -0.878608       0.128049
     H       3.332698     -0.843471      -0.541893
     H       2.479998     -1.668750       0.868399
     C       1.510527      1.126623      -0.964047
     H       0.593024      1.132847      -1.555574
     H       1.582238      2.104206      -0.482034
     H       2.357015      1.022046      -1.639510
     C      -1.153570     -1.348374      -0.192211
     O      -1.658552     -0.411392      -0.901394
     O      -2.326134      0.514781      -0.151568
     H      -1.624507     -1.604187       0.745001
     H      -0.529769     -2.042327      -0.738759
Rotational constants (GHz):    3.2365300    1.3330300    1.2699300
Vibrational harmonic frequencies (cm-1):
     i295.4435                  73.0019                  86.7929
      127.7538                 204.2357                 223.8608
      289.0424                 364.3691                 405.0767
      441.3598                 522.9341                 542.1931
      557.2927                 675.7908                 737.0000
      767.7240                 790.4092                 911.6794
      927.7196                 951.5407                 954.5922
      982.9603                1013.7915                1030.9643
     1072.3586                1094.1398                1227.4718
     1287.3387                1316.9052                1353.2729
     1412.4529                1420.4966                1461.4171
     1486.8955                1505.8305                1513.3729
     1574.6603                1680.4952                3028.6012
     3074.4467                3115.3667                3129.1119
     3133.3294                3136.5898                3183.8972
     3215.4710                3267.8411                3268.4879
Zero-point correction (Hartree): 0.147038

ts_t_top_in_4_3
---------------
E(RHF-RMP2/CC-PVTZ-F12) (Hartree): -384.21034939
     T1 diagnostic:  0.000010
E(RHF-UCCSD(T)-F12a/CC-PVTZ-F12) (Hartree): -384.38847657
E(RHF-UCCSD(T)-F12b/CC-PVTZ-F12) (Hartree): -384.35235271
E(RHF-UCCSD-F12a/CC-PVTZ-F12) (Hartree): -384.31772102
     T1 diagnostic:  0.029999
     D1 diagnostic:  0.182824
E(RHF-UCCSD-F12b/CC-PVTZ-F12) (Hartree): -384.28159716
E(RHF-UCCSD-T-F12a/CC-PVTZ-F12) (Hartree): -384.38665288
E(RHF-UCCSD-T-F12b/CC-PVTZ-F12) (Hartree): -384.35052902
E(RHF-UCCSD[T]-F12a/CC-PVTZ-F12) (Hartree): -384.39581420
E(RHF-UCCSD[T]-F12b/CC-PVTZ-F12) (Hartree): -384.35969034
E(RHF/CC-PVTZ-F12) (Hartree): -382.66254394
E(RB3LYP/6-311+G(2df,2p)) (Hartree): -385.03303187
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Electronic state : 1-A
Cartesian coordinates (Angs):
     C      -0.464140      1.504397       0.584862
     C       0.403156      0.498439       0.892170
     H      -0.370365      2.064075      -0.335083
     H      -1.053880      1.964380       1.365069
     H       0.370897      0.076051       1.887955
     C       1.506867      0.040895       0.053026
     C       2.472605     -0.710154       0.596783
     H       3.326456     -1.039833       0.021108
     H       2.428964     -1.022119       1.631675
     C       1.547497      0.459903      -1.391198
     H       0.655443      0.116130      -1.917239
     H       1.590719      1.546481      -1.493824
     H       2.418480      0.041309      -1.891124
     C      -2.343677      0.290589      -0.060867
     O      -1.770240     -0.684715      -0.645230
     O      -1.062149     -1.493334       0.196567
     H      -2.569181      0.206050       0.991080
     H      -2.872271      0.967457      -0.718966
Rotational constants (GHz):    3.0853300    1.3362500    1.2418200
Vibrational harmonic frequencies (cm-1):
     i239.9333                 54.6429                   78.7158
      112.9788                165.2259                  190.3827
      281.8678                305.3625                  391.5243
      433.1553                487.6696                  539.2734
      544.9053                676.6677                  759.1598
      793.9872                799.1515                  879.7018
      931.8803                933.3722                  958.9332
     1002.9687               1007.1150                 1021.1975
     1071.2699               1098.8161                 1228.6310
     1303.4590               1331.2125                 1363.1075
     1413.5807               1423.3139                 1459.9963
     1489.6610               1505.3937                 1515.9846
     1585.5046               1673.8862                 3029.2844
     3078.3127               3115.0243                 3131.1658
     3142.2659               3143.6424                 3172.7397
     3223.3370               3224.8620                 3267.2636
Zero-point correction (Hartree): 0.146581

ts_t_top_out_1_2
----------------
IRC pathway available
E(RHF-RMP2/CC-PVTZ-F12) (Hartree): -384.21052435
     T1 diagnostic:  0.000010
E(RHF-UCCSD(T)-F12a/CC-PVTZ-F12) (Hartree): -384.43433943
E(RHF-UCCSD(T)-F12b/CC-PVTZ-F12) (Hartree): -384.41095915
E(RHF-UCCSD-F12a/CC-PVTZ-F12) (Hartree): -384.35193335
     T1 diagnostic:  0.030397
     D1 diagnostic:  0.186365
E(RHF-UCCSD-F12b/CC-PVTZ-F12) (Hartree): -384.32855307
E(RHF-UCCSD-T-F12a/CC-PVTZ-F12) (Hartree): -384.43242160
E(RHF-UCCSD-T-F12b/CC-PVTZ-F12) (Hartree): -384.40904132
E(RHF-UCCSD[T]-F12a/CC-PVTZ-F12) (Hartree): -384.44183234
E(RHF-UCCSD[T]-F12b/CC-PVTZ-F12) (Hartree): -384.41845206
E(RHF/CC-PVTZ-F12) (Hartree): -382.66437853
E(RB3LYP/6-311+G(2df,2p)) (Hartree): -385.03341714
Electronic state : 1-A
Cartesian coordinates (Angs):
     C       2.555815     -0.956480      -0.218129
     C       1.410459     -0.491654      -0.720356
     H       3.005080     -0.547899       0.676424
     H       3.078498     -1.774951      -0.691991
     H       1.013813     -0.944028      -1.622585
     C       0.642663      0.632728      -0.194360
     C      -0.312557      1.217403      -0.978965
     H      -0.701205      2.195966      -0.730914
     H      -0.462708      0.882719      -1.996516
     C       1.034968      1.241100       1.120728
     H       1.071512      0.486887       1.904337
     H       2.024592      1.699662       1.048273
     H       0.332172      2.016125       1.421451
     C      -2.254758      0.256264      -0.170056
     O      -1.874701     -0.951939      -0.046482
     O      -0.962917     -1.143251       0.953611
     H      -2.952539      0.433729      -0.977735
     H      -2.167808      0.917137       0.679058
Rotational constants (GHz):    2.9079300    1.4135700    1.2563400
Vibrational harmonic frequencies (cm-1):
     i231.2955                 62.8770                  104.1012
      122.2595                156.2652                  174.2542
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      199.3468                286.0967                382.9443
      427.5719                431.7861                538.6799
      548.6040                686.9105                764.1337
      792.4494                826.5144                878.0666
      927.0072                943.6320                966.0204
     1002.6952               1019.3662               1023.6473
     1061.5143               1091.6213               1228.3204
     1328.7238               1339.0945               1361.2009
     1405.2456               1417.9676               1459.0387
     1484.9255               1500.2974               1516.2481
     1583.0303               1673.6911               3029.3180
     3090.7841               3121.6904               3128.1458
     3132.9164               3143.9694               3153.4317
     3214.7808               3230.8465               3263.7770
Zero-point correction (Hartree): 0.146317

ts_t_top_out_2_1
----------------
E(RHF-RMP2/CC-PVTZ-F12) (Hartree): -384.21174463
     T1 diagnostic:  0.000011
E(RHF-UCCSD(T)-F12a/CC-PVTZ-F12) (Hartree): -384.43203396
E(RHF-UCCSD(T)-F12b/CC-PVTZ-F12) (Hartree): -384.40865975
E(RHF-UCCSD-F12a/CC-PVTZ-F12) (Hartree): -384.34819809
     T1 diagnostic:  0.028004
     D1 diagnostic:  0.166298
E(RHF-UCCSD-F12b/CC-PVTZ-F12) (Hartree): -384.32482388
E(RHF-UCCSD-T-F12a/CC-PVTZ-F12) (Hartree): -384.43044766
E(RHF-UCCSD-T-F12b/CC-PVTZ-F12) (Hartree): -384.40707345
E(RHF-UCCSD[T]-F12a/CC-PVTZ-F12) (Hartree): -384.43891870
E(RHF-UCCSD[T]-F12b/CC-PVTZ-F12) (Hartree): -384.41554449
E(RHF/CC-PVTZ-F12) (Hartree): -382.65419697
E(RB3LYP/6-311+G(2df,2p)) (Hartree): -385.02835524
Electronic state : 1-A
Cartesian coordinates (Angs):
     C       2.556433     -1.003204      -0.143211
     C       1.369631     -0.646317      -0.637865
     H       3.056318     -0.440936       0.634049
     H       3.073547     -1.875520      -0.516767
     H       0.932895     -1.253475      -1.424685
     C       0.570111      0.522869      -0.240850
     C      -0.424881      0.960885      -1.085524
     H      -0.861630      1.940907      -0.973380
     H      -0.641959      0.445023      -2.007092
     C       1.127506      1.452778       0.815262
     H       1.382492      0.931543       1.739849
     H       2.043692      1.929201       0.459444
     H       0.416150      2.241913       1.055519
     C      -0.955546     -0.611092       1.130295
     O      -1.800497     -0.966244       0.238374
     O      -2.372165      0.105523      -0.387328
     H      -1.089985      0.335594       1.631398
     H      -0.389745     -1.424002       1.564662
Rotational constants (GHz):    3.1354200    1.3778000    1.2605700
Vibrational harmonic frequencies (cm-1):
     i314.8393                78.0763                116.4698
      179.5015                211.5119                225.2922
      243.7176                290.6072                416.0027
      418.7311                439.4479                542.5159
      558.8210                689.1411                740.2388
      773.5265                798.0224                924.8506
      944.8204                953.4093                970.2842
      998.6004               1009.2381               1036.9140
     1072.5716               1085.7049               1223.3913
     1318.9300               1325.5624               1351.1204
     1401.6419               1418.3138               1463.1226
     1492.3638               1510.1437               1513.5806
     1567.0500               1674.9072               3024.9246
     3069.7566               3102.3767               3131.1900
     3132.4629               3147.7229               3172.0511
     3224.6542               3258.4351               3268.4161
Zero-point correction (Hartree): 0.146965

ts_t_top_out_3_4
----------------
E(RHF-RMP2/CC-PVTZ-F12) (Hartree): -384.21353164
     T1 diagnostic:  0.000011
E(RHF-UCCSD(T)-F12a/CC-PVTZ-F12) (Hartree): -384.43476011
E(RHF-UCCSD(T)-F12b/CC-PVTZ-F12) (Hartree): -384.41138699
E(RHF-UCCSD-F12a/CC-PVTZ-F12) (Hartree): -384.35139793
     T1 diagnostic:  0.028133
     D1 diagnostic:  0.167225
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E(RHF-UCCSD-F12b/CC-PVTZ-F12) (Hartree): -384.32802480
E(RHF-UCCSD-T-F12a/CC-PVTZ-F12) (Hartree): -384.43316958
E(RHF-UCCSD-T-F12b/CC-PVTZ-F12) (Hartree): -384.40979646
E(RHF-UCCSD[T]-F12a/CC-PVTZ-F12) (Hartree): -384.44160811
E(RHF-UCCSD[T]-F12b/CC-PVTZ-F12) (Hartree): -384.41823499
E(RHF/CC-PVTZ-F12) (Hartree): -382.65907833
E(RB3LYP/6-311+G(2df,2p)) (Hartree): -385.03181378
Electronic state : 1-A
Cartesian coordinates (Angs):
     C       0.495645     -1.101350       0.980798
     C      -0.328100     -0.010276       0.897129
     H       0.314724     -2.000256       0.413365
     H       1.239683     -1.175122       1.756161
     H      -0.232304      0.757089       1.656632
     C      -1.561294      0.046495       0.091580
     C      -2.412137      1.070268       0.224478
     H      -3.326298      1.126445      -0.350106
     H      -2.225498      1.874244       0.925170
     C      -1.834517     -1.078278      -0.871545
     H      -0.999272     -1.234356      -1.558378
     H      -1.979652     -2.021304      -0.339952
     H      -2.728613     -0.880259      -1.458853
     C       1.089852      1.179656      -0.528801
     O       2.203555      0.673142      -0.158768
     O       2.264535     -0.675914      -0.366985
     H       0.962170      2.223109      -0.273212
     H       0.533645      0.713503      -1.326642
Rotational constants (GHz):    3.4456400    1.2666600    1.1355400
Vibrational harmonic frequencies (cm-1):
     i300.0566                 76.5503                 84.1998
      129.4742                213.1062                230.7180
      286.6205                345.8810                417.9957
      435.9817                519.3824                534.4272
      553.0161                682.2150                746.6208
      771.5837                795.3107                916.4384
      934.8698                947.2834                955.4891
      991.6475               1011.3723               1029.3447
     1071.3804               1092.4129               1216.4633
     1289.4174               1316.8532               1354.9110
     1411.9729               1421.6958               1462.2429
     1485.0040               1505.6460               1509.4035
     1573.0981               1680.9545               3025.2472
     3067.3379               3115.1300               3135.4670
     3136.7819               3144.2477               3183.4396
     3216.5483               3267.8653               3273.0384
Zero-point correction (Hartree): 0.147092

ts_t_top_out_4_3
----------------
IRC pathway available
E(RHF-RMP2/CC-PVTZ-F12) (Hartree): -384.21147226
     T1 diagnostic:  0.000010
E(RHF-UCCSD(T)-F12a/CC-PVTZ-F12) (Hartree): -384.43497364
E(RHF-UCCSD(T)-F12b/CC-PVTZ-F12) (Hartree): -384.41158488
E(RHF-UCCSD-F12a/CC-PVTZ-F12) (Hartree): -384.35225044
     T1 diagnostic:  0.030030
     D1 diagnostic:  0.183629
E(RHF-UCCSD-F12b/CC-PVTZ-F12) (Hartree): -384.32886169
E(RHF-UCCSD-T-F12a/CC-PVTZ-F12) (Hartree): -384.43308998
E(RHF-UCCSD-T-F12b/CC-PVTZ-F12) (Hartree): -384.40970122
E(RHF-UCCSD[T]-F12a/CC-PVTZ-F12) (Hartree): -384.44241480
E(RHF-UCCSD[T]-F12b/CC-PVTZ-F12) (Hartree): -384.41902604
E(RHF/CC-PVTZ-F12) (Hartree): -382.66362953
E(CCSD(T)/CC-pVTZ) (Hartree): -384.25505245
E(CCSD/CC-pVTZ) (Hartree): -384.17652366
     T1 diagnostic:  0.031314
E(MP2/CC-pVTZ) (Hartree): -384.12791061
E(MP3/CC-pVTZ) (Hartree): -384.16059584
E(RHF/CC-pVTZ) (Hartree): -382.63741583
E(RB3LYP/6-311+G(2df,2p)) (Hartree): -385.03419138
Electronic state : 1-A
Cartesian coordinates (Angs):
     C       0.391932     -1.192250       1.014936
     C      -0.372332     -0.066897       0.919300
     H       0.112844     -2.105869       0.507529
     H       1.109372     -1.291588       1.816186
     H      -0.163450      0.760663       1.581573
     C      -1.554066      0.083021       0.076340
     C      -2.300923      1.188752       0.186431
     H      -3.197747      1.329439      -0.401299
     H      -2.025245      1.987856       0.861050
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     C      -1.922102     -1.021256      -0.878425
     H      -1.127015     -1.197581      -1.606063
     H      -2.094388     -1.963693      -0.354284
     H      -2.826462     -0.772052      -1.429528
     C       2.066792     -0.660746      -0.495733
     O       2.274084      0.543126      -0.131241
     O       1.242781      1.391136      -0.416223
     H       1.362949     -0.851886      -1.290852
     H       2.858419     -1.353133      -0.241702
Rotational constants (GHz):    3.1629500    1.2957400    1.1305600
Vibrational harmonic frequencies (cm-1):
     i236.4506                  52.5359                  85.2496
       97.0888                 187.9254                 191.6024
      282.5366                 319.1057                 389.4160
      434.7883                 495.7795                 538.9201
      540.3766                 677.3266                 757.4443
      793.4687                 805.7098                 868.0931
      934.4246                 945.4110                 961.8858
     1001.0864                1006.1259                1018.6191
     1068.4361                1097.6527                1226.1426
     1303.0396                1333.4230                1357.2433
     1413.8219                1426.7044                1462.2062
     1488.6560                1504.3055                1512.9342
     1586.8369                1675.3762                3027.0272
     3070.2696                3114.0605                3132.7656
     3142.8760                3143.9294                3192.3818
     3225.6949                3227.5119                3267.4551
Zero-point correction (Hartree): 0.146681

ts_c_top_in_1_2
---------------
E(RHF-RMP2/CC-PVTZ-F12) (Hartree): -384.20879207
     T1 diagnostic:  0.000010
E(RHF-UCCSD(T)-F12a/CC-PVTZ-F12) (Hartree): -384.43285635
E(RHF-UCCSD(T)-F12b/CC-PVTZ-F12) (Hartree): -384.40948713
E(RHF-UCCSD-F12a/CC-PVTZ-F12) (Hartree): -384.35124610
     T1 diagnostic:  0.029541
     D1 diagnostic:  0.180036
E(RHF-UCCSD-F12b/CC-PVTZ-F12) (Hartree): -384.32787689
E(RHF-UCCSD-T-F12a/CC-PVTZ-F12) (Hartree): -384.43099788
E(RHF-UCCSD-T-F12b/CC-PVTZ-F12) (Hartree): -384.40762867
E(RHF-UCCSD[T]-F12a/CC-PVTZ-F12) (Hartree): -384.44001465
E(RHF-UCCSD[T]-F12b/CC-PVTZ-F12) (Hartree): -384.41664544
E(RHF/CC-PVTZ-F12) (Hartree): -382.66553156
E(RB3LYP/6-311+G(2df,2p)) (Hartree): -385.03164757
Electronic state : 1-A
Cartesian coordinates (Angs):
     C      -0.692530      0.481587       0.386341
     C      -0.188045     -0.230914       1.432792
     H      -0.521169     -1.240263       1.631941
     H       0.334530      0.273136       2.234428
     C      -1.602022     -0.117388      -0.597751
     C      -2.456785     -1.114243      -0.366629
     H      -1.571840      0.329236      -1.584459
     H      -3.093383     -1.495566      -1.152825
     H      -2.564951     -1.568287       0.609849
     C      -0.447253      1.961819       0.272858
     H       0.473910      2.253321       0.774242
     H      -0.386483      2.277401      -0.765334
     H      -1.272777      2.504852       0.744081
     C       1.724867     -1.093346       0.419321
     O       2.108946     -0.105631      -0.282139
     O       1.286328      0.164907      -1.345748
     H       1.063966     -1.821193      -0.027937
     H       2.346612     -1.311937       1.277518
Rotational constants (GHz):    2.6824400    1.4295700    1.3269800
Vibrational harmonic frequencies (cm-1):
     i213.0455                  59.8038                  83.6106
      132.3656                 154.4606                 181.6341
      189.6167                 288.4135                 382.3631
      404.1927                 439.0477                 538.0481
      562.7570                 690.9986                 767.4257
      801.4522                 825.3886                 884.6136
      918.3012                 956.6842                 965.3684
     1009.4825                1025.5991                1035.8153
     1061.1657                1097.4953                1230.4853
     1273.2611                1334.2972                1364.1272
     1412.3865                1426.5849                1460.5067
     1483.7897                1492.2569                1517.8651
     1594.5528                1675.8127                3015.0249
     3090.7576                3125.0701                3132.6077
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     3134.6443                3141.3960                3158.1989
     3215.6636                3222.7309                3261.7928
Zero-point correction (Hartree): 0.146304

ts_c_top_in_2_1
---------------
E(RHF-RMP2/CC-PVTZ-F12) (Hartree): -384.20721886
     T1 diagnostic:  0.000011
E(RHF-UCCSD(T)-F12a/CC-PVTZ-F12) (Hartree): -384.42814123
E(RHF-UCCSD(T)-F12b/CC-PVTZ-F12) (Hartree): -384.40475077
E(RHF-UCCSD-F12a/CC-PVTZ-F12) (Hartree): -384.34432587
     T1 diagnostic:  0.028004
     D1 diagnostic:  0.165943
E(RHF-UCCSD-F12b/CC-PVTZ-F12) (Hartree): -384.32093541
E(RHF-UCCSD-T-F12a/CC-PVTZ-F12) (Hartree): -384.42655209
E(RHF-UCCSD-T-F12b/CC-PVTZ-F12) (Hartree): -384.40316163
E(RHF-UCCSD[T]-F12a/CC-PVTZ-F12) (Hartree): -384.43498534
E(RHF-UCCSD[T]-F12b/CC-PVTZ-F12) (Hartree): -384.41159488
E(RHF/CC-PVTZ-F12) (Hartree): -382.65012773
E(RB3LYP/6-311+G(2df,2p)) (Hartree): -385.02448655
Electronic state : 1-A
Cartesian coordinates (Angs):
     C      -0.659682      0.565599       0.292654
     C       0.056777      0.122662       1.376799
     H      -0.170829     -0.814489       1.859596
     H       0.711416      0.786786       1.917165
     C      -1.819832     -0.185357      -0.231405
     C      -2.090818     -1.482889      -0.080596
     H      -2.513413      0.410008      -0.818055
     H      -2.983786     -1.916478      -0.507461
     H      -1.447718     -2.152534       0.476958
     C      -0.576927      2.028481      -0.105306
     H      -0.757437      2.176679      -1.170633
     H      -1.329038      2.614682       0.429472
     H       0.399156      2.447885       0.133665
     C       0.929614     -0.333118      -1.230360
     O       1.983273     -0.095484      -0.548975
     O       1.993826     -0.758812       0.645780
     H       0.844423      0.249393      -2.138722
     H       0.395638     -1.259823      -1.087150
Rotational constants (GHz):    2.6611200    1.5341300    1.3321700
Vibrational harmonic frequencies (cm-1):
     i301.7560                  62.0014                 102.9092
      158.1764                 184.1250                 201.1043
      216.4618                 297.9425                 403.3045
      419.8453                 444.1827                 519.9979
      558.4831                 687.1506                 745.0122
      780.0632                 782.2328                 934.9108
      945.9945                 950.6635                 971.9759
      998.7430                1024.3870                1036.6966
     1065.7106                1098.2139                1217.3723
     1255.5145                1340.6479                1355.2303
     1415.9429                1426.6372                1457.7118
     1495.5416                1506.5873                1515.3497
     1571.8843                1676.2881                3020.6573
     3069.7195                3107.6732                3124.7532
     3125.6007                3139.2365                3176.3528
     3220.8392                3260.4781                3266.6836
Zero-point correction (Hartree): 0.146570

ts_c_top_in_3_4
---------------
E(RHF-RMP2/CC-PVTZ-F12) (Hartree): -384.21082732
     T1 diagnostic:  0.000012
E(RHF-UCCSD(T)-F12a/CC-PVTZ-F12) (Hartree): -384.43207535
E(RHF-UCCSD(T)-F12b/CC-PVTZ-F12) (Hartree): -384.40869846
E(RHF-UCCSD-F12a/CC-PVTZ-F12) (Hartree): -384.34902488
     T1 diagnostic:  0.027906
     D1 diagnostic:  0.165970
E(RHF-UCCSD-F12b/CC-PVTZ-F12) (Hartree): -384.32564800
E(RHF-UCCSD-T-F12a/CC-PVTZ-F12) (Hartree): -384.43044555
E(RHF-UCCSD-T-F12b/CC-PVTZ-F12) (Hartree): -384.40706867
E(RHF-UCCSD[T]-F12a/CC-PVTZ-F12) (Hartree): -384.43889630
E(RHF-UCCSD[T]-F12b/CC-PVTZ-F12) (Hartree): -384.41551941
E(RHF/CC-PVTZ-F12) (Hartree): -382.65694266
E(RB3LYP/6-311+G(2df,2p)) (Hartree): -385.02937215
Electronic state : 1-A
Cartesian coordinates (Angs):
     C       1.430759      0.128536       0.162812
     C       1.268670      0.307185       1.477108
     H       0.351825      0.700149       1.894007
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     H       2.054328      0.054751       2.176089
     C       0.389569      0.475620      -0.824360
     C      -0.552460      1.445645      -0.645084
     H       0.543095      0.098883      -1.830298
     H      -1.196836      1.749535      -1.454875
     H      -0.567095      2.064613       0.237641
     C       2.694010     -0.462791      -0.408420
     H       2.480944     -1.375679      -0.972056
     H       3.171044      0.230151      -1.105703
     H       3.410181     -0.708133       0.373357
     C      -1.196151     -1.291034      -0.519660
     O      -1.689398     -0.792254       0.545058
     O      -2.339306      0.388833       0.338498
     H      -0.597917     -2.178799      -0.367531
     H      -1.626320     -1.027055      -1.473460
Rotational constants (GHz):    3.3641300    1.2845500    1.2489100
Vibrational harmonic frequencies (cm-1):
     i255.8354                  64.6678                  84.1679
      129.7012                 185.8239                 209.5241
      289.0864                 331.3647                 400.4004
      431.0440                 511.9465                 547.4718
      554.7151                 683.3819                 727.0625
      746.7039                 803.2470                 911.2780
      927.1690                 948.4961                 960.1860
      986.8925                1006.9446                1021.2000
     1070.0639                1103.5016                1226.6751
     1259.3245                1293.6461                1360.0907
     1415.4633                1447.8130                1456.8697
     1485.2757                1499.9289                1513.3276
     1583.0206                1685.8062                3015.4390
     3056.4201                3111.2507                3129.2306
     3137.0639                3145.1698                3175.5665
     3224.3527                3260.9599                3273.5552
Zero-point correction (Hartree): 0.146696

ts_c_top_in_4_3
---------------
E(RHF-RMP2/CC-PVTZ-F12) (Hartree): -384.20987862
     T1 diagnostic:  0.000009
E(RHF-UCCSD(T)-F12a/CC-PVTZ-F12) (Hartree): -384.43351987
E(RHF-UCCSD(T)-F12b/CC-PVTZ-F12) (Hartree): -384.41013098
E(RHF-UCCSD-F12a/CC-PVTZ-F12) (Hartree): -384.35135375
     T1 diagnostic:  0.029304
     D1 diagnostic:  0.178803
E(RHF-UCCSD-F12b/CC-PVTZ-F12) (Hartree): -384.32796485
E(RHF-UCCSD-T-F12a/CC-PVTZ-F12) (Hartree): -384.43167810
E(RHF-UCCSD-T-F12b/CC-PVTZ-F12) (Hartree): -384.40828920
E(RHF-UCCSD[T]-F12a/CC-PVTZ-F12) (Hartree): -384.44065447
E(RHF-UCCSD[T]-F12b/CC-PVTZ-F12) (Hartree): -384.41726558
E(RHF/CC-PVTZ-F12) (Hartree): -382.66329267
E(RB3LYP/6-311+G(2df,2p)) (Hartree): -385.03265402
Electronic state : 1-A
Cartesian coordinates (Angs):
     C      -1.431641      0.186403      -0.013026
     C      -1.784963      0.926661      -1.071032
     H      -1.304642      1.864997      -1.310295
     H      -2.584272      0.613524      -1.728330
     C      -0.348154      0.578548       0.895356
     C       0.569310      1.556906       0.682132
     H      -0.323969      0.057384       1.843612
     H       1.198532      1.895972       1.492749
     H       0.524815      2.195544      -0.189285
     C      -2.148263     -1.092121       0.327875
     H      -1.451706     -1.929373       0.278649
     H      -2.545003     -1.053987       1.345431
     H      -2.977259     -1.278439      -0.352310
     C       2.301583      0.238178      -0.240217
     O       1.622151     -0.706463      -0.752636
     O       1.016901     -1.516323       0.166621
     H       2.648165      0.138507       0.776687
     H       2.755694      0.910703      -0.955325
Rotational constants (GHz):    2.8580700    1.4721700    1.2278200
Vibrational harmonic frequencies (cm-1):
     i200.6711                  40.1395                  75.8290
      124.9792                 171.0151                 178.4475
      298.1630                 308.7645                 389.4403
      421.2128                 474.1213                 527.4234
      541.1120                 670.3545                 748.9284
      781.5537                 805.3433                 880.6872
      928.0576                 931.9637                 963.3148
      996.3129                1005.9377                1031.7848
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     1071.6659                1109.2818                1228.5576
     1267.3760                1312.7710                1366.8410
     1408.6978                1444.2943                1456.4709
     1484.3674                1506.0016                1516.8252
     1602.4069                1677.7787                3027.2415
     3083.7144                3115.7781                3134.3737
     3141.3390                3148.1333                3170.8491
     3221.3158                3225.7030                3272.3597
Zero-point correction (Hartree): 0.146461

ts_c_top_out_1_2
----------------
E(RHF-RMP2/CC-PVTZ-F12) (Hartree): -384.20920297
     T1 diagnostic:  0.000010
E(RHF-UCCSD(T)-F12a/CC-PVTZ-F12) (Hartree): -384.43312749
E(RHF-UCCSD(T)-F12b/CC-PVTZ-F12) (Hartree): -384.40975823
E(RHF-UCCSD-F12a/CC-PVTZ-F12) (Hartree): -384.35144653
     T1 diagnostic:  0.029577
     D1 diagnostic:  0.180424
E(RHF-UCCSD-F12b/CC-PVTZ-F12) (Hartree): -384.32807727
E(RHF-UCCSD-T-F12a/CC-PVTZ-F12) (Hartree): -384.43126742
E(RHF-UCCSD-T-F12b/CC-PVTZ-F12) (Hartree): -384.40789816
E(RHF-UCCSD[T]-F12a/CC-PVTZ-F12) (Hartree): -384.44028839
E(RHF-UCCSD[T]-F12b/CC-PVTZ-F12) (Hartree): -384.41691913
E(RHF/CC-PVTZ-F12) (Hartree): -382.66536242
E(RB3LYP/6-311+G(2df,2p)) (Hartree): -385.03201112
Electronic state : 1-A
Cartesian coordinates (Angs):
     C      -0.751668      0.585526       0.247988
     C      -0.150103      0.349610       1.447438
     H      -0.259496     -0.601648       1.948343
     H       0.214439      1.172885       2.047227
     C      -1.500435     -0.453652      -0.468580
     C      -2.078609     -1.521555       0.082571
     H      -1.599027     -0.299724      -1.535971
     H      -2.614581     -2.237991      -0.523942
     H      -2.048803     -1.713310       1.147012
     C      -0.787937      1.965950      -0.346026
     H      -0.552404      1.938455      -1.408156
     H      -1.790061      2.391210      -0.238191
     H      -0.085144      2.636247       0.146102
     C       2.003268     -0.218943       0.705562
     O       1.729894     -0.863859      -0.354057
     O       1.243033     -0.079609      -1.366138
     H       2.362584     -0.823264       1.527811
     H       2.181987      0.843267       0.637603
Rotational constants (GHz):    2.4458700    1.5485300    1.3855200
Vibrational harmonic frequencies (cm-1):
     i208.7653                  56.0071                  80.1649
      150.1468                 154.6657                 169.5949
      179.4190                 295.5247                 383.0328
      408.9625                 436.2170                 538.8825
      553.0749                 689.3334                 758.0867
      801.9050                 820.2553                 877.2651
      919.3704                 952.5324                 966.5336
      999.2985                1021.0425                1030.6770
     1062.1203                1098.3487                1226.9433
     1276.2009                1338.0617                1364.9667
     1410.5031                1425.7886                1461.2300
     1482.6920                1493.8784                1519.0992
     1597.5366                1675.9295                3021.7160
     3086.8885                3121.4188                3131.1200
     3136.5347                3144.1698                3163.4013
     3218.4471                3225.0428                3267.5949
Zero-point correction (Hartree): 0.146239

ts_c_top_out_2_1
----------------
E(RHF-RMP2/CC-PVTZ-F12) (Hartree): -384.20837929
     T1 diagnostic:  0.000011
E(RHF-UCCSD(T)-F12a/CC-PVTZ-F12) (Hartree): -384.42898980
E(RHF-UCCSD(T)-F12b/CC-PVTZ-F12) (Hartree): -384.40559820
E(RHF-UCCSD-F12a/CC-PVTZ-F12) (Hartree): -384.34517102
     T1 diagnostic:  0.028059
     D1 diagnostic:  0.167411
E(RHF-UCCSD-F12b/CC-PVTZ-F12) (Hartree): -384.32177942
E(RHF-UCCSD-T-F12a/CC-PVTZ-F12) (Hartree): -384.42734941
E(RHF-UCCSD-T-F12b/CC-PVTZ-F12) (Hartree): -384.40395781
E(RHF-UCCSD[T]-F12a/CC-PVTZ-F12) (Hartree): -384.43593406
E(RHF-UCCSD[T]-F12b/CC-PVTZ-F12) (Hartree): -384.41254245
E(RHF/CC-PVTZ-F12) (Hartree): -382.65051830
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E(RB3LYP/6-311+G(2df,2p)) (Hartree): -385.02473736
Electronic state : 1-A
Cartesian coordinates (Angs):
     C       0.845571     -0.416734       0.277487
     C       0.026441     -0.409468       1.377679
     H      -0.138864      0.484860       1.954951
     H      -0.312958     -1.333341       1.820483
     C       1.498337      0.822667      -0.192362
     C       1.080284      2.072692       0.007784
     H       2.405287      0.672305      -0.771138
     H       1.641954      2.913053      -0.374960
     H       0.170043      2.299999       0.546878
     C       1.454701     -1.718791      -0.210172
     H       1.545222     -1.757977      -1.297369
     H       2.462987     -1.837362       0.194052
     H       0.870554     -2.579165       0.114393
     C      -0.995380     -0.452470      -1.195821
     O      -1.705555      0.417526      -0.589126
     O      -2.095288      0.002990       0.653018
     H      -1.118405     -1.496299      -0.950052
     H      -0.578800     -0.117573      -2.135939
Rotational constants (GHz):    2.4544200    1.7284400    1.4075100
Vibrational harmonic frequencies (cm-1):
     i294.7474                  79.8994                 111.0932
      161.6121                 192.1653                 211.4605
      222.3148                 296.9362                 400.0669
      421.5641                 435.8589                 527.8676
      558.5969                 684.0655                 736.3353
      768.4554                 786.2159                 936.5634
      945.0128                 950.1366                 969.7604
      986.8996                1020.2300                1032.0983
     1066.7512                1098.7072                1223.7038
     1253.3926                1341.1467                1355.5041
     1417.2494                1427.1767                1459.5997
     1492.7806                1508.1131                1512.9796
     1574.6493                1679.0991                3021.1864
     3064.9001                3100.6117                3121.8328
     3132.2036                3145.3440                3173.8969
     3224.9719                3261.4466                3269.5186
Zero-point correction (Hartree): 0.146627

ts_c_top_out_3_4
----------------
E(RHF-RMP2/CC-PVTZ-F12) (Hartree): -384.21040911
     T1 diagnostic:  0.000011
E(RHF-UCCSD(T)-F12a/CC-PVTZ-F12) (Hartree): -384.43206164
E(RHF-UCCSD(T)-F12b/CC-PVTZ-F12) (Hartree): -384.40869325
E(RHF-UCCSD-F12a/CC-PVTZ-F12) (Hartree): -384.34902576
     T1 diagnostic:  0.027875
     D1 diagnostic:  0.164419
E(RHF-UCCSD-F12b/CC-PVTZ-F12) (Hartree): -384.32565736
E(RHF-UCCSD-T-F12a/CC-PVTZ-F12) (Hartree): -384.43050806
E(RHF-UCCSD-T-F12b/CC-PVTZ-F12) (Hartree): -384.40713966
E(RHF-UCCSD[T]-F12a/CC-PVTZ-F12) (Hartree): -384.43872957
E(RHF-UCCSD[T]-F12b/CC-PVTZ-F12) (Hartree): -384.41536118
E(RHF/CC-PVTZ-F12) (Hartree): -382.65747803
E(RB3LYP/6-311+G(2df,2p)) (Hartree): -385.02965128
Electronic state : 1-A
Cartesian coordinates (Angs):
     C      -1.533520     -0.138736       0.079195
     C      -1.554675     -0.786984       1.248643
     H      -0.707931     -1.360467       1.602368
     H      -2.430231     -0.770728       1.882846
     C      -0.370690     -0.154668      -0.831734
     C       0.529669     -1.177956      -0.924945
     H      -0.392386      0.569689      -1.638296
     H       1.228926     -1.226858      -1.743370
     H       0.434889     -2.069701      -0.324687
     C      -2.707882      0.681402      -0.389517
     H      -2.417753      1.722609      -0.555012
     H      -3.087990      0.308166      -1.343377
     H      -3.521454      0.666749       0.333066
     C       1.136417      1.259235       0.423468
     O       2.227183      0.726190       0.033353
     O       2.310899     -0.606478       0.316513
     H       0.577838      0.817295       1.234595
     H       1.015521      2.291793       0.122282
Rotational constants (GHz):    3.6015700    1.1858400    1.1250600
Vibrational harmonic frequencies (cm-1):
     i268.5962                  62.4265                  82.7979
      143.9771                 185.3117                 216.3404
```

```
      282.4317                317.2849                408.8261
      424.2044                509.8495                547.4894
      555.2652                693.2177                742.3977
      756.9791                803.7094                919.4971
      931.3562                944.1933                957.8024
     1001.6674               1015.9895               1021.5156
     1070.0378               1103.8002               1223.3459
     1258.1538               1297.0362               1365.6778
     1415.2806               1445.1049               1455.8183
     1484.8135               1499.0456               1519.8180
     1577.0493               1682.0536               3018.3764
     3059.9425               3112.0008               3124.1021
     3138.7256               3141.4161               3174.7840
     3218.4163               3261.4989               3265.3531
Zero-point correction (Hartree): 0.146796

ts_c_top_out_4_3
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IRC pathway available
E(RHF-RMP2/CC-PVTZ-F12) (Hartree): -384.21123562
     T1 diagnostic:  0.000010
E(RHF-UCCSD(T)-F12a/CC-PVTZ-F12) (Hartree): -384.43505637
E(RHF-UCCSD(T)-F12b/CC-PVTZ-F12) (Hartree): -384.41167419
E(RHF-UCCSD-F12a/CC-PVTZ-F12) (Hartree): -384.35325834
     T1 diagnostic:  0.029077
     D1 diagnostic:  0.177413
E(RHF-UCCSD-F12b/CC-PVTZ-F12) (Hartree): -384.32987617
E(RHF-UCCSD-T-F12a/CC-PVTZ-F12) (Hartree): -384.43319959
E(RHF-UCCSD-T-F12b/CC-PVTZ-F12) (Hartree): -384.40981742
E(RHF-UCCSD[T]-F12a/CC-PVTZ-F12) (Hartree): -384.44214570
E(RHF-UCCSD[T]-F12b/CC-PVTZ-F12) (Hartree): -384.41876353
E(RHF/CC-PVTZ-F12) (Hartree): -382.66615400
E(CCSD(T)/CC-pVTZ) (Hartree): -384.25521567
E(CCSD/CC-pVTZ) (Hartree): -384.17762995
     T1 diagnostic:  0.030297
E(MP2/CC-pVTZ) (Hartree): -384.12789348
E(MP3/CC-pVTZ) (Hartree): -384.16203681
E(RHF/CC-pVTZ) (Hartree): -382.64014115
E(RB3LYP/6-311+G(2df,2p)) (Hartree): -385.03387017
Electronic state : 1-A
Cartesian coordinates (Angs):
     C      -1.514058      0.078588       0.025610
     C      -2.106247      0.969800      -0.778813
     H      -1.800437      2.006173      -0.819296
     H      -2.939239      0.687271      -1.407782
     C      -0.377119      0.427555       0.887084
     C       0.429648      1.509271       0.753463
     H      -0.192663     -0.247365       1.711999
     H       1.150351      1.751081       1.521214
     H       0.230651      2.279503       0.019533
     C      -1.996342     -1.343369       0.123154
     H      -1.198213     -2.031400      -0.156172
     H      -2.280158     -1.581826       1.151094
     H      -2.859137     -1.517530      -0.517015
     C       1.998596      0.517672      -0.702537
     O       2.224771     -0.562762      -0.073641
     O       1.182862     -1.446967      -0.080142
     H       2.809597      1.233270      -0.678768
     H       1.211313      0.541556      -1.442302
Rotational constants (GHz):    2.9853000    1.3960900    1.1293000
Vibrational harmonic frequencies (cm-1):
     i183.3971                47.9747                79.2634
      110.3106               178.8072               181.4492
      298.5897               311.5498               379.2484
      416.7291               471.2909               529.0858
      538.9931               676.3289               755.4748
      781.5751               806.5146               890.0182
      929.4938               933.0379               963.1926
      999.7415              1011.8992              1030.5326
     1071.0941              1108.7446              1231.6248
     1267.7846              1315.8091              1368.9297
     1412.6380              1443.8939              1459.5460
     1482.5399              1503.2821              1518.3942
     1605.8099              1678.4573              3029.3719
     3084.6618              3116.8922              3124.1906
     3136.1459              3145.3764              3178.8365
     3220.6788              3224.0606              3261.4454
Zero-point correction (Hartree): 0.146512

cycCH2CCH3OOCH2_CHCH2.mc
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E(RB3LYP/6-311+G(2df,2p)) (Hartree): -385.11148567
Electronic state : 1-A
Cartesian coordinates (Angs):

O	1.721902	-0.682562	0.731995
C	0.788216	0.306866	1.145398
C	-0.283710	0.396625	0.010694
C	0.393448	-0.498792	-1.049672
O	1.774616	-0.492318	-0.710894
H	1.292946	1.266665	1.283244
H	0.382706	-0.038789	2.095294
C	-0.405381	1.850864	-0.481207
H	0.018176	-1.522585	-1.026058
H	0.325603	-0.098038	-2.060136
C	-1.637531	-0.077359	0.479614
C	-2.389484	-1.048381	-0.023004
H	-2.033504	0.490741	1.317669
H	-2.085444	-1.656392	-0.864074
H	-3.358918	-1.271868	0.400962
H	-1.128436	1.926552	-1.293214
H	0.559478	2.214364	-0.836305
H	-0.738094	2.509443	0.322878

Rotational constants (GHz): 3.1051500 1.6721500 1.5331800
Vibrational harmonic frequencies (cm-1):

59.8853	90.6255	243.0257
274.3928	286.5997	323.5795
366.9949	404.3163	500.7375
577.1048	657.1365	714.7645
787.0922	855.1397	903.6677
940.3778	958.1748	964.8726
980.3352	1006.5123	1024.7069
1043.1137	1067.5129	1171.8846
1186.6295	1235.5896	1253.2015
1276.9510	1339.4384	1356.3582
1382.4704	1414.1039	1464.4907
1492.1758	1502.8210	1504.4208
1507.5283	1699.8757	3018.3420
3029.6045	3045.7805	3091.0999
3098.3386	3103.8339	3108.4452
3113.0744	3146.6151	3219.9777

Zero-point correction (Hartree): 0.152167

cycCH2CCH3OOCH2_CHCH2.mt

E(RB3LYP/6-311+G(2df,2p)) (Hartree): -385.11130224
Electronic state : 1-A
Cartesian coordinates (Angs):

O	1.490494	-1.188807	0.292146
C	0.382294	-0.639477	0.999303
C	-0.273431	0.399590	0.052025
C	0.800518	0.431491	-1.073424
O	1.988282	-0.049671	-0.467595
H	0.725782	-0.161360	1.919753
H	-0.255459	-1.484664	1.245912
C	-0.381872	1.770105	0.745671
H	0.517959	-0.210361	-1.911603
H	1.021918	1.437565	-1.428343
C	-1.620688	0.025455	-0.518488
C	-2.422820	-0.972862	-0.173938
H	-1.959858	0.698141	-1.302820
H	-2.179586	-1.688609	0.599572
H	-3.374739	-1.111897	-0.667824
H	-0.833117	2.509869	0.083194
H	0.605310	2.128987	1.038976
H	-1.002420	1.704347	1.639884

Rotational constants (GHz): 3.1295800 1.7129000 1.4866500
Vibrational harmonic frequencies (cm-1):

48.6356	73.9826	243.6246
271.4968	299.6971	325.7764
377.6855	390.1222	503.7458
563.8879	684.5396	694.6864
791.5943	852.1996	891.4445
949.8763	955.8757	962.7883
981.6544	1002.1789	1029.3610
1041.0844	1075.8313	1158.0260
1199.5786	1218.8974	1254.5687
1276.6976	1344.9876	1350.7323
1378.9962	1415.2570	1461.5111
1492.9588	1502.7845	1505.1260
1508.9601	1703.4728	3023.7530
3026.2448	3031.3112	3093.8895
3098.1140	3101.3572	3109.1890

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     3120.2233                3146.3076                3218.8454
Zero-point correction (Hartree): 0.152076

cycCH2CCH3OOCH2_CHCH2.pc
------------------------
E(RB3LYP/6-311+G(2df,2p)) (Hartree): -385.11130225
Electronic state : 1-A
Cartesian coordinates (Angs):
     O       1.988159     -0.049677      0.467710
     C       0.800256      0.431197      1.073578
     C      -0.273423      0.399513     -0.051991
     C       0.382261     -0.639566     -0.999299
     O       1.490567     -1.188740     -0.292120
     H       1.021510      1.437188      1.428834
     H       0.517766     -0.210972      1.911537
     C      -0.381327      1.770168     -0.745631
     H      -0.255472     -1.484803     -1.245759
     H       0.725713     -0.161521     -1.919778
     C      -1.620962      0.025805      0.518089
     C      -2.422877     -0.972826      0.173912
     H      -1.960533      0.699031      1.301783
     H      -2.179205     -1.689143     -0.598930
     H      -3.375019     -1.111540      0.667447
     H      -1.001757      1.704643     -1.639936
     H       0.606034      2.128696     -1.038728
     H      -0.832414      2.510006     -0.083136
Rotational constants (GHz):    3.1296700    1.7129300    1.4866600
Vibrational harmonic frequencies (cm-1):
       48.6009                  73.9840                 243.6256
      271.4874                 299.7009                 325.7844
      377.7349                 390.1283                 503.7717
      563.9038                 684.5572                 694.6613
      791.6184                 852.3760                 891.4820
      949.8666                 955.8691                 962.8186
      981.5514                1002.1781                1029.2907
     1041.0838                1075.8102                1158.0406
     1199.5718                1218.8725                1254.5848
     1276.6875                1344.9903                1350.6859
     1378.9839                1415.1999                1461.5050
     1492.9580                1502.7882                1505.1194
     1508.9571                1703.4528                3023.7652
     3026.3708                3031.3895                3093.9377
     3098.1806                3101.3548                3109.2055
     3120.3023                3146.3291                3218.8776
Zero-point correction (Hartree): 0.152077

cycCH2CCH3OOCH2_CHCH2.pw
------------------------
E(RB3LYP/6-311+G(2df,2p)) (Hartree): -385.11148573
Electronic state : 1-A
Cartesian coordinates (Angs):
     O       1.774572     -0.492598      0.710896
     C       0.393286     -0.498820      1.049665
     C      -0.283728      0.396678     -0.010527
     C       0.788495      0.307335     -1.145168
     O       1.721880     -0.682375     -0.732088
     H       0.325545     -0.098228      2.060181
     H       0.017993     -1.522608      1.025860
     C      -0.405845      1.850853      0.481367
     H       0.383209     -0.038007     -2.095248
     H       1.293325      1.267154     -1.282408
     C      -1.637316     -0.077549     -0.479837
     C      -2.389233     -1.048605      0.022754
     H      -2.033153      0.490459     -1.318018
     H      -2.085160     -1.656583      0.863848
     H      -3.358595     -1.272258     -0.401280
     H      -0.738320      2.509403     -0.322837
     H       0.558818      2.214557      0.836827
     H      -1.129221      1.926538      1.293093
Rotational constants (GHz):    3.1049200    1.6722700    1.5332100
Vibrational harmonic frequencies (cm-1):
       59.9093                  90.5981                 243.0883
      274.3526                 286.6168                 323.6016
      366.9979                 404.2476                 500.7535
      577.1321                 657.1131                 714.7740
      787.0935                 855.0560                 903.6755
      940.2521                 958.1939                 964.9040
      980.3719                1006.5358                1024.6853
     1043.1183                1067.5063                1171.7923
     1186.6866                1235.6263                1253.2223
     1276.9514                1339.4260                1356.3783
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     1382.5048                1414.1417                1464.5009
     1492.1552                1502.8189                1504.3780
     1507.5068                1699.8935                3018.4353
     3029.5921                3045.7654                3091.0691
     3098.5096                3103.7944                3108.5699
     3113.0963                3146.5882                3219.9438
Zero-point correction (Hartree): 0.152168

cycCH2CH2CCH3OO_CHCH2.mc
------------------------
E(RB3LYP/6-311+G(2df,2p)) (Hartree): -385.11994928
Electronic state : 1-A
Cartesian coordinates (Angs):
     C       1.991956     -0.608738       0.341164
     C       0.657869     -0.560711       1.094707
     C      -0.291869      0.124345       0.063820
     O       0.502336      0.138701      -1.152779
     O       1.860997      0.361115      -0.691470
     H       2.850605     -0.303334       0.937941
     H       2.177022     -1.594651      -0.092962
     H       0.718537      0.033255       2.004263
     H       0.314764     -1.557508       1.364045
     C      -0.630858      1.555224       0.464691
     C      -1.477102     -0.742705      -0.268289
     C      -2.754914     -0.432470      -0.099356
     H      -1.209366     -1.712646      -0.674320
     H      -3.075497      0.522182       0.294443
     H      -3.534682     -1.138009      -0.351015
     H       0.289993      2.123532       0.583454
     H      -1.173517      1.582428       1.410054
     H      -1.235007      2.036564      -0.302337
Rotational constants (GHz):    3.9664600    1.5176000    1.4629900
Vibrational harmonic frequencies (cm-1):
       78.6092                  92.3383                 254.3348
      271.6362                 283.9296                 316.5303
      381.1844                 426.8998                 460.6908
      633.0992                 652.8828                 687.2203
      782.8184                 847.1504                 879.1095
      908.4174                 941.7318                 969.9930
      972.0264                 988.8280                1010.7815
     1037.0619                1062.9679                1124.8227
     1183.1312                1207.0068                1245.0664
     1305.2196                1309.8628                1336.8818
     1366.8858                1409.1762                1455.6772
     1496.4208                1499.6952                1505.2259
     1514.0084                1704.4762                3021.4335
     3044.2466                3072.1188                3095.2893
     3109.2918                3116.8913                3123.2153
     3139.3370                3151.1608                3225.5362
Zero-point correction (Hartree): 0.151959

cycCH2CH2CCH3OO_CHCH2.mw
------------------------
E(RB3LYP/6-311+G(2df,2p)) (Hartree): -385.11945931
Electronic state : 1-A
Cartesian coordinates (Angs):
     C       1.773751     -0.723008       0.523888
     C       0.743009      0.168943       1.215351
     C      -0.288135      0.425880       0.071322
     O       0.194807     -0.385731      -1.021569
     O       1.635758     -0.411945      -0.857786
     H       2.806364     -0.496154       0.785608
     H       1.573339     -1.784330       0.690634
     H       1.183398      1.107532       1.546834
     H       0.289764     -0.321501       2.073834
     C      -0.307205      1.895949      -0.355902
     C      -1.672474     -0.052941       0.423207
     C      -2.293806     -1.108313      -0.084707
     H      -2.175329      0.564483       1.161039
     H      -1.828999     -1.738570      -0.829089
     H      -3.294624     -1.365919       0.233680
     H       0.692414      2.206654      -0.656980
     H      -0.635452      2.534262       0.466027
     H      -0.986241      2.035890      -1.195708
Rotational constants (GHz):    3.1121200    1.7757900    1.5944900
Vibrational harmonic frequencies (cm-1):
       56.6905                 102.5065                 230.7907
      257.7453                 278.5327                 307.9865
      347.0809                 443.1202                 523.7327
      588.8246                 647.6049                 702.7683
      774.9900                 861.3250                 891.7315
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      920.5347                 938.6049                 970.5888
      974.6643                 993.1291                1018.3187
     1035.0786                1049.6526                1160.9561
     1170.2151                1204.4822                1245.4113
     1281.0805                1313.2055                1334.6146
     1368.9352                1406.6497                1450.2246
     1491.4233                1495.8067                1500.3983
     1511.4313                1700.7486                3025.1586
     3036.3971                3069.3089                3099.9409
     3101.9046                3116.5034                3120.0354
     3132.9950                3151.7518                3233.8400
Zero-point correction (Hartree): 0.151816

cycCH2CH2CCH3OO_CHCH2.pc
------------------------
E(RB3LYP/6-311+G(2df,2p)) (Hartree): -385.11962827
Electronic state : 1-A
Cartesian coordinates (Angs):
     C       2.025512     -0.127170      0.527897
     C       0.700802      0.264782      1.187949
     C      -0.287004      0.287899     -0.018205
     O       0.584164      0.085533     -1.167078
     O       1.642405     -0.776196     -0.679787
     H       2.643819      0.745610      0.303093
     H       2.606595     -0.854740      1.092700
     H       0.759209      1.236675      1.674338
     H       0.386649     -0.467701      1.928191
     C      -0.938543      1.645205     -0.239687
     C      -1.249523     -0.871606      0.043571
     C      -2.565461     -0.810602      0.196685
     H      -0.765265     -1.837302     -0.056846
     H      -3.100064      0.124210      0.299393
     H      -3.163857     -1.711055      0.223348
     H      -0.172391      2.415348     -0.310672
     H      -1.599034      1.892259      0.590417
     H      -1.522913      1.650944     -1.158297
Rotational constants (GHz):    3.5344500    1.6145400    1.5049100
Vibrational harmonic frequencies (cm-1):
       68.7798                  96.9426                 239.7722
      249.8685                 287.4032                 336.4224
      359.3873                 425.9322                 450.3956
      636.2670                 655.8079                 708.6423
      773.7560                 860.1871                 875.7021
      887.2123                 927.3167                 959.8178
      974.2843                 999.1997                1024.7019
     1042.0250                1054.6381                1134.2410
     1183.4867                1208.4374                1245.3751
     1302.5136                1312.3363                1336.7038
     1365.4916                1412.7789                1457.5259
     1494.8209                1499.0827                1505.7011
     1513.5118                1701.2050                3023.0553
     3049.4524                3071.8043                3098.8418
     3116.4916                3117.3662                3121.9310
     3140.2365                3149.0638                3218.7632
Zero-point correction (Hartree): 0.151896

cycCH2CH2CCH3OO_CHCH2.pw
------------------------
E(RB3LYP/6-311+G(2df,2p)) (Hartree): -385.11997226
Electronic state : 1-A
Cartesian coordinates (Angs):
     C       1.942134     -0.332463      0.354579
     C       0.900521      0.568309      1.026433
     C      -0.289141      0.508099      0.022276
     O       0.258008     -0.188004     -1.113768
     O       1.196008     -1.140870     -0.548256
     H       2.688459      0.249293     -0.192958
     H       2.440213     -1.020900      1.035637
     H       1.270860      1.584120      1.153341
     H       0.603952      0.187937      2.001507
     C      -0.709898      1.880499     -0.503202
     C      -1.472687     -0.227143      0.610733
     C      -2.007989     -1.338237      0.128669
     H      -1.893951      0.236750      1.498258
     H      -1.602071     -1.822605     -0.748394
     H      -2.863266     -1.797488      0.604900
     H       0.153272      2.422971     -0.887232
     H      -1.165092      2.465244      0.296122
     H      -1.442137      1.771292     -1.301915
Rotational constants (GHz):    2.8367300    2.0026400    1.6129700
Vibrational harmonic frequencies (cm-1):
```

```
       70.7237                106.8808                216.9253
      237.5068                302.9643                327.9870
      336.1904                401.1058                557.6538
      585.0486                670.0710                702.5122
      787.0321                855.5299                883.9965
      898.3546                922.9310                975.4650
      976.2323               1004.7748               1028.0755
     1030.2368               1047.3034               1151.1193
     1186.9899               1205.7129               1249.8342
     1266.7645               1314.8790               1328.8246
     1368.9664               1410.4330               1444.8181
     1488.5268               1497.2966               1502.0939
     1513.3756               1704.2197               3019.2375
     3041.5590               3068.6548               3097.7446
     3109.2037               3114.2595               3117.7929
     3123.1315               3149.4677               3231.3100
Zero-point correction (Hartree): 0.151798

cycCH2CH2CHOO_CCH2CH3.mc
------------------------
E(RB3LYP/6-311+G(2df,2p)) (Hartree): -385.12186237
Electronic state : 1-A
Cartesian coordinates (Angs):
     C      -2.086572      0.247046       0.576320
     C      -0.815199     -0.369536       1.172812
     C       0.060988     -0.590269      -0.088576
     O      -0.629252      0.123718      -1.128075
     O      -2.031836     -0.073146      -0.810860
     H      -3.011306     -0.190443       0.949689
     H      -2.111627      1.331604       0.708992
     H      -1.007924     -1.320188       1.665102
     H      -0.345709      0.296315       1.893508
     H       0.073311     -1.651861      -0.344572
     C       1.473759     -0.067989      -0.010720
     C       2.492261     -0.922958      -0.052378
     C       1.662176      1.417649       0.121791
     H       2.336119     -1.986222      -0.178850
     H       3.516648     -0.587285       0.040397
     H       1.127786      1.818775       0.985898
     H       1.270873      1.934469      -0.754981
     H       2.716059      1.666596       0.230804
Rotational constants (GHz):    4.1160900    1.3662100    1.3594300
Vibrational harmonic frequencies (cm-1):
       62.1261                73.6602                169.7996
      207.9502               259.4072                320.4438
      381.9585               514.5576                539.3582
      643.5115               686.1938                735.2789
      797.0350               872.3383                886.4748
      935.4450               947.8477                957.1330
      988.6778              1020.7727               1023.5060
     1050.4863              1077.5581               1108.2694
     1222.0877              1239.8696               1297.8985
     1312.5276              1329.9926               1359.3084
     1370.1294              1417.8877               1458.0899
     1480.7437              1498.5367               1501.7646
     1514.8410              1708.1181               3022.6574
     3031.8186              3032.5401               3076.2275
     3081.3460              3099.0253               3114.2861
     3121.5557              3137.5484               3215.8293
Zero-point correction (Hartree): 0.152419

cycCH2CH2CHOO_CCH2CH3.mw
------------------------
E(RB3LYP/6-311+G(2df,2p)) (Hartree): -385.12076419
Electronic state : 1-A
Cartesian coordinates (Angs):
     C       2.081603      0.474612       0.562029
     C       0.732660      1.178771       0.367001
     C      -0.045957      0.133741      -0.480407
     O       0.761971     -1.044299      -0.430175
     O       2.118035     -0.530175      -0.447810
     H       2.946740      1.111607       0.384533
     H       2.157624      0.014285       1.549791
     H       0.834170      2.118800      -0.171228
     H       0.242923      1.374249       1.318798
     H      -0.090584      0.476696      -1.520540
     C      -1.440857     -0.167503       0.003756
     C      -1.759557     -1.303034       0.616757
     C      -2.440185      0.921765      -0.273911
     H      -1.029765     -2.078764       0.793711
     H      -2.772515     -1.484235       0.951219
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     H      -2.531701      1.106005      -1.347445
     H      -2.139705      1.868451       0.182745
     H      -3.423479      0.658593       0.110937
Rotational constants (GHz):    4.1536700    1.4505100    1.2305300
Vibrational harmonic frequencies (cm-1):
       56.4327                77.0000                179.9525
      201.0320                257.9723                339.2613
      359.4741                494.7732                543.7388
      640.4241                678.1757                744.2329
      813.9271                881.7763                906.8342
      932.2419                952.2654                960.5912
      986.4935               1009.5863               1038.5682
     1056.7327               1076.0194               1115.1941
     1227.0637               1243.5055               1266.6132
     1301.6575               1330.3038               1369.3656
     1391.7583               1417.8575               1447.2140
     1485.7444               1497.7327               1498.5211
     1513.5570               1710.6864               2988.1678
     3018.7104               3028.6857               3058.2957
     3070.9344               3099.6278               3111.9861
     3119.7382               3146.6701               3234.6808
Zero-point correction (Hartree): 0.152368

cycCH2CH2CHOO_CCH2CH3.pc
------------------------
E(RB3LYP/6-311+G(2df,2p)) (Hartree): -385.12160255
Electronic state : 1-A
Cartesian coordinates (Angs):
     C      -2.109998     -0.178915       0.462418
     C      -0.844236     -0.937942       0.860397
     C       0.094877     -0.662307      -0.341786
     O      -0.682924      0.169633      -1.232421
     O      -1.640695      0.862091      -0.381395
     H      -2.816908     -0.814442      -0.078005
     H      -2.613205      0.310041       1.295622
     H      -1.023046     -2.002588       0.994020
     H      -0.418106     -0.547456       1.781908
     H       0.273499     -1.574343      -0.911422
     C       1.418410     -0.026376       0.012973
     C       2.544795     -0.711594      -0.168916
     C       1.395048      1.376305       0.551007
     H       2.540775     -1.710779      -0.586000
     H       3.509923     -0.298097       0.092556
     H       0.831305      1.444263       1.483895
     H       0.906574      2.047170      -0.156210
     H       2.404757      1.737418       0.737604
Rotational constants (GHz):    3.8774100    1.5171700    1.4120400
Vibrational harmonic frequencies (cm-1):
       66.6016                76.0894                180.4918
      208.8832               260.1752                324.3175
      381.7907               498.7032                560.5250
      639.4762               728.6743                753.2284
      779.3229               850.9464                892.9082
      933.4848               936.5713                941.4862
      974.3379              1007.6243               1030.1809
     1042.7607              1072.7686               1116.3076
     1214.5761              1240.6625               1286.2564
     1308.0616              1313.9621               1347.8245
     1367.5828              1417.8801               1456.7485
     1481.1908              1496.7480               1498.8844
     1512.4241              1703.8404               3019.1213
     3032.9458              3065.3463               3076.7783
     3083.1101              3100.0308               3114.1615
     3122.0800              3132.6941               3209.8434
Zero-point correction (Hartree): 0.152319

cycCH2CH2CHOO_CCH2CH3.pw
------------------------
E(RB3LYP/6-311+G(2df,2p)) (Hartree): -385.12056765
Electronic state : 1-A
Cartesian coordinates (Angs):
     C       2.071846     -0.537753      -0.412555
     C       0.745005     -1.270248      -0.203483
     C      -0.058610     -0.237840       0.637462
     O       0.854063      0.843467       0.860169
     O       1.739595      0.837412      -0.296622
     H       2.813959     -0.811833       0.342277
     H       2.492259     -0.665256      -1.409099
     H       0.878331     -2.217180       0.315738
     H       0.246256     -1.462834      -1.150806
     H      -0.259190     -0.631925       1.638090
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     C      -1.365584      0.184960       0.001200
     C      -1.555792      1.408467      -0.477723
     C      -2.426053     -0.881684      -0.017702
     H      -0.777841      2.156238      -0.433251
     H      -2.499899      1.691120      -0.924321
     H      -2.661919     -1.217396       0.996256
     H      -2.102408     -1.766781      -0.571631
     H      -3.343697     -0.516599      -0.474824
Rotational constants (GHz):    3.8087600    1.5929100    1.3107600
Vibrational harmonic frequencies (cm-1):
       68.9364                  79.0115                 178.1285
      211.6038                 262.5171                 323.9630
      379.2036                 517.0967                 533.0280
      642.2299                 720.4541                 754.4658
      808.1255                 851.0083                 904.7662
      928.0413                 949.9830                 954.3878
      980.5447                 999.8446                1027.6060
     1047.0723                1066.7929                1119.6850
     1216.7346                1241.5078                1264.2775
     1282.8325                1314.3632                1361.6179
     1382.4528                1417.0673                1443.9865
     1486.2601                1494.6035                1496.9784
     1509.9112                1715.5389                3014.3922
     3018.7464                3023.3835                3053.1532
     3072.7221                3100.6958                3110.2283
     3120.0804                3146.1501                3233.6406
Zero-point correction (Hartree): 0.152250

cycCH2CHOOCH2_CCH2CH3.mn
------------------------
E(RB3LYP/6-311+G(2df,2p)) (Hartree): -385.11582670
Electronic state : 1-A
Cartesian coordinates (Angs):
     O       1.894273      0.579356       0.753358
     C       0.719889      1.201247       0.240012
     C      -0.045084      0.083232      -0.532316
     C       0.992123     -1.048958      -0.477770
     O       2.236571     -0.390204      -0.276894
     H       0.989406      2.031143      -0.416914
     H       0.176441      1.573110       1.107361
     H      -0.148100      0.411476      -1.569186
     H       0.809584     -1.742553       0.343347
     H       1.083532     -1.596209      -1.414522
     C      -1.436114     -0.197041      -0.007974
     C      -1.795961     -1.308123       0.630106
     C      -2.430719      0.900914      -0.283044
     H      -1.115121     -2.121088       0.833295
     H      -2.811934     -1.439479       0.978455
     H      -2.543691      1.060367      -1.358731
     H      -2.101938      1.853896       0.139560
     H      -3.409732      0.668496       0.131535
Rotational constants (GHz):    4.0225500    1.4183800    1.2111500
Vibrational harmonic frequencies (cm-1):
       32.5866                  83.2815                 186.3989
      210.3777                 299.4469                 339.4649
      366.0090                 487.2199                 537.9779
      614.5686                 680.5369                 754.5477
      810.9955                 855.1218                 923.1405
      937.4566                 951.5568                 977.3169
     1004.1588                1010.0580                1036.2109
     1061.9971                1094.8259                1114.3190
     1235.6407                1251.7489                1255.7381
     1300.2018                1337.2524                1361.7635
     1402.7615                1419.9906                1456.9731
     1487.0585                1493.7657                1500.7208
     1506.4227                1707.1916                3017.5599
     3021.0230                3036.1854                3051.2601
     3057.8505                3101.9197                3110.7775
     3113.7705                3148.4303                3225.7463
Zero-point correction (Hartree): 0.152572

cycCH2CHOOCH2_CCH2CH3.mw
------------------------
E(RB3LYP/6-311+G(2df,2p)) (Hartree): -385.11595330
Electronic state : 1-A
Cartesian coordinates (Angs):
     O      -1.989773      0.680187      -0.294626
     C      -1.006486      0.949396       0.701590
     C       0.053435     -0.163315       0.565233
     C      -0.707946     -1.155148      -0.358776
     O      -2.072288     -0.772420      -0.274771
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     H      -1.465809      0.927023       1.692446
     H      -0.636633      1.950349       0.496545
     H       0.193907     -0.629895       1.542401
     H      -0.353127     -1.073872      -1.389412
     H      -0.665054     -2.190879      -0.025965
     C       1.421990      0.194829       0.023101
     C       1.721242      1.348316      -0.566849
     C       2.447286     -0.898311       0.174689
     H       1.004340      2.145740      -0.699132
     H       2.714409      1.531284      -0.954894
     H       2.128728     -1.813933      -0.331181
     H       2.587507     -1.157086       1.227564
     H       3.411102     -0.605478      -0.237120
Rotational constants (GHz):    3.9560600    1.4665000    1.2174500
Vibrational harmonic frequencies (cm-1):
       33.0610                  71.0117                 191.7098
      214.0027                 306.7566                 340.6819
      377.5720                 480.4286                 543.8740
      626.7390                 713.7232                 732.7978
      795.3020                 853.1699                 917.3885
      934.8052                 952.2285                 962.7990
     1006.0163                1019.3990                1042.1266
     1055.7288                1088.4232                1108.3584
     1235.4683                1241.6621                1255.4957
     1290.2825                1336.6773                1374.5493
     1391.5071                1418.3303                1451.1495
     1486.6838                1495.3703                1498.4073
     1513.8421                1710.8630                3016.1023
     3021.9939                3026.4341                3042.9931
     3056.1536                3107.6687                3111.1463
     3126.2731                3146.8237                3220.7081
Zero-point correction (Hartree): 0.152511

cycCH2CHOOCH2_CCH2CH3.pn
------------------------
E(RB3LYP/6-311+G(2df,2p)) (Hartree): -385.11595333
Electronic state : 1-A
Cartesian coordinates (Angs):
     O       2.072470     -0.773392      -0.272744
     C       0.707923     -1.154627      -0.358609
     C      -0.053330     -0.162064       0.564527
     C       1.006546      0.951276       0.699117
     O       1.991377      0.679252      -0.294794
     H       0.663379     -2.190374      -0.026048
     H       0.354482     -1.072727      -1.389685
     H      -0.192606     -0.627566       1.542399
     H       0.637044      1.951615       0.490497
     H       1.464178      0.931830       1.690813
     C      -1.422514      0.194653       0.023234
     C      -1.723653      1.348219      -0.565623
     C      -2.446395     -0.899862       0.174664
     H      -1.007944      2.146749      -0.697565
     H      -2.717300      1.530145      -0.952936
     H      -2.585416     -1.159787       1.227404
     H      -2.127181     -1.814615      -0.332357
     H      -3.410871     -0.607727      -0.236078
Rotational constants (GHz):    3.9568900    1.4661700    1.2167100
Vibrational harmonic frequencies (cm-1):
       32.9705                  71.0073                 191.6882
      213.9015                 307.0790                 340.6495
      377.4011                 480.3531                 543.8434
      626.3781                 713.5650                 732.6142
      795.5375                 853.2083                 917.3297
      934.7710                 952.3566                 962.9478
     1006.0867                1019.4547                1042.3060
     1055.6048                1088.2914                1108.3897
     1235.4217                1241.7323                1255.5196
     1290.4102                1336.6816                1374.4736
     1391.4846                1418.3158                1451.1508
     1486.6759                1495.3787                1498.3502
     1513.8668                1710.8303                3016.1546
     3021.8694                3026.3817                3042.8834
     3056.2321                3107.6608                3111.2150
     3126.2774                3146.8683                3220.7906
Zero-point correction (Hartree): 0.152510

cycCH2CHOOCH2_CCH2CH3.pw
------------------------
E(RB3LYP/6-311+G(2df,2p)) (Hartree): -385.11582668
Electronic state : 1-A
Cartesian coordinates (Angs):
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     O      -2.236600      0.390161      0.276534
     C      -0.992213      1.048784      0.478259
     C       0.045102     -0.083366      0.532500
     C      -0.719925     -1.201394     -0.239713
     O      -1.893829     -0.579177     -0.753807
     H      -1.083966      1.595482      1.415301
     H      -0.809404      1.742890     -0.342361
     H       0.148404     -0.411697      1.569322
     H      -0.176330     -1.573830     -1.106713
     H      -0.990111     -2.030873      0.417450
     C       1.436012      0.197093      0.007936
     C       1.795671      1.308193     -0.630212
     C       2.430806     -0.900721      0.282914
     H       1.114748      2.121083     -0.833418
     H       2.811605      1.439642     -0.978651
     H       2.102127     -1.853738     -0.139693
     H       2.543889     -1.060200      1.358586
     H       3.409749     -0.668159     -0.131745
Rotational constants (GHz):    4.0222500    1.4184500    1.2112600
Vibrational harmonic frequencies (cm-1):
       32.5280                83.3212                186.3831
      210.4310               299.5456                339.4799
      366.0329               487.2245                537.9499
      614.6708               680.5249                754.5846
      810.9050               855.0558                923.1423
      937.4757               951.5579                977.2625
     1004.1300              1010.0572               1036.2050
     1061.9957              1094.7996               1114.2931
     1235.6792              1251.7244               1255.7333
     1300.1600              1337.2686               1361.7925
     1402.7514              1419.9926               1456.9814
     1487.0591              1493.7748               1500.7328
     1506.3610              1707.2072               3017.5521
     3021.0416              3036.1811               3051.2873
     3057.8396              3102.0387               3110.7851
     3113.7618              3148.4137               3225.7299
Zero-point correction (Hartree): 0.152572

CH3OO
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E(RHF-RMP2/CC-PVTZ-F12) (Hartree): -189.93299175
     T1 diagnostic:  0.000999
E(RHF-UCCSD(T)-F12a/CC-PVTZ-F12) (Hartree): -190.03451503
E(RHF-UCCSD(T)-F12b/CC-PVTZ-F12) (Hartree): -190.02444813
E(RHF-UCCSD-F12a/CC-PVTZ-F12) (Hartree): -190.00717918
     T1 diagnostic:  0.035848
     D1 diagnostic:  0.146313
E(RHF-UCCSD-F12b/CC-PVTZ-F12) (Hartree): -189.99711228
E(RHF-UCCSD-T-F12a/CC-PVTZ-F12) (Hartree): -190.03424102
E(RHF-UCCSD-T-F12b/CC-PVTZ-F12) (Hartree): -190.02417412
E(RHF-UCCSD[T]-F12a/CC-PVTZ-F12) (Hartree): -190.03743401
E(RHF-UCCSD[T]-F12b/CC-PVTZ-F12) (Hartree): -190.02736711
E(ROHF/CC-PVTZ-F12) (Hartree): -189.28439542
E(UB3LYP/6-311+G(2df,2p)) (Hartree): -190.29004259
Electronic state : 2-A
Cartesian coordinates (Angs):
     C      -1.095229      0.182491     -0.000000
     O       0.156642     -0.541040     -0.000004
     O       1.186083      0.277069      0.000002
     H      -1.870815     -0.578840      0.000265
     H      -1.149920      0.797650     -0.895183
     H      -1.149692      0.798016      0.894939
Rotational constants (GHz):   53.1762300   11.2928900    9.9043000
Vibrational harmonic frequencies (cm-1):
      132.0629                492.1116                915.2217
     1127.3381               1157.1925               1221.2884
     1446.1937               1475.0728               1485.7601
     3054.1280               3142.2956               3155.9074
Zero-point correction (Hartree): 0.042840

CH2OOH
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E(RHF-RMP2/CC-PVTZ-F12) (Hartree): -189.91988435
     T1 diagnostic:  0.000630
E(RHF-UCCSD(T)-F12a/CC-PVTZ-F12) (Hartree): -190.01288807
E(RHF-UCCSD(T)-F12b/CC-PVTZ-F12) (Hartree): -190.00274350
E(RHF-UCCSD-F12a/CC-PVTZ-F12) (Hartree): -189.98468091
     T1 diagnostic:  0.019931
     D1 diagnostic:  0.064339
E(RHF-UCCSD-F12b/CC-PVTZ-F12) (Hartree): -189.97453633
E(RHF-UCCSD-T-F12a/CC-PVTZ-F12) (Hartree): -190.01241851
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E(RHF-UCCSD-T-F12b/CC-PVTZ-F12) (Hartree): -190.00227393
E(RHF-UCCSD[T]-F12a/CC-PVTZ-F12) (Hartree): -190.01430030
E(RHF-UCCSD[T]-F12b/CC-PVTZ-F12) (Hartree): -190.00415572
E(ROHF/CC-PVTZ-F12) (Hartree): -189.25465377
E(UB3LYP/6-311+G(2df,2p)) (Hartree): -190.26522525
Electronic state : 2-A
Cartesian coordinates (Angs):
     C      -1.134746      0.272473       0.095897
     O      -0.078195     -0.566220      -0.081865
     O       1.148597      0.223553      -0.072223
     H       1.392953      0.148841       0.866516
     H      -2.060368     -0.288477       0.173816
     H      -1.087323      1.246135      -0.383002
Rotational constants (GHz):   52.3915500   11.1742100    9.6201300
Vibrational harmonic frequencies (cm-1):
      269.5809                326.1683                 491.5701
      719.7893                839.9592                1114.3207
     1190.3111               1383.1402                1439.6241
     3079.2235               3216.5981                3685.0362
Zero-point correction (Hartree): 0.040450

CH2O+OH
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E(RHF-RMP2/CC-PVTZ-F12) (Hartree): -189.97271238
     T1 diagnostic:  0.000326
E(RHF-UCCSD(T)-F12a/CC-PVTZ-F12) (Hartree): -190.06626516
E(RHF-UCCSD(T)-F12b/CC-PVTZ-F12) (Hartree): -190.05617107
E(RHF-UCCSD-F12a/CC-PVTZ-F12) (Hartree): -190.04169426
     T1 diagnostic:  0.016834
     D1 diagnostic:  0.046339
E(RHF-UCCSD-F12b/CC-PVTZ-F12) (Hartree): -190.03160017
E(RHF-UCCSD-T-F12a/CC-PVTZ-F12) (Hartree): -190.06575640
E(RHF-UCCSD-T-F12b/CC-PVTZ-F12) (Hartree): -190.05566231
E(RHF-UCCSD[T]-F12a/CC-PVTZ-F12) (Hartree): -190.06771974
E(RHF-UCCSD[T]-F12b/CC-PVTZ-F12) (Hartree): -190.05762565
E(ROHF/CC-PVTZ-F12) (Hartree): -189.34070898
E(UB3LYP/6-311+G(2df,2p)) (Hartree): -190.31884172
Electronic state : 2-A
Cartesian coordinates (Angs):
     C      -1.225882      0.382435      -0.000002
     O      -0.590711     -0.638782       0.000001
     O       1.660208      0.225790       0.000006
     H      -0.736915      1.367623      -0.000025
     H      -2.329304      0.364352       0.000017
     H       1.865537     -0.722647      -0.000040
Rotational constants (GHz):   44.0796900    6.5336500    5.6902200
Vibrational harmonic frequencies (cm-1):
       81.4362                 119.4448                 185.4392
      191.9373                 389.1694                1206.2882
     1257.2272                1516.4274                1799.5223
     2921.3913                3007.1635                3760.8307
Zero-point correction (Hartree): 0.037445

isoprene_5yl
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E(RHF-RMP2/CC-PVTZ-F12) (Hartree): -194.23789902
     T1 diagnostic:  0.001458
E(RHF-UCCSD(T)-F12a/CC-PVTZ-F12) (Hartree): -194.37099273
E(RHF-UCCSD(T)-F12b/CC-PVTZ-F12) (Hartree): -194.35836283
E(RHF-UCCSD-F12a/CC-PVTZ-F12) (Hartree): -194.32913744
     T1 diagnostic:  0.024246
     D1 diagnostic:  0.091397
E(RHF-UCCSD-F12b/CC-PVTZ-F12) (Hartree): -194.31650753
E(RHF-UCCSD-T-F12a/CC-PVTZ-F12) (Hartree): -194.37102922
E(RHF-UCCSD-T-F12b/CC-PVTZ-F12) (Hartree): -194.35839932
E(RHF-UCCSD[T]-F12a/CC-PVTZ-F12) (Hartree): -194.37206260
E(RHF-UCCSD[T]-F12b/CC-PVTZ-F12) (Hartree): -194.35943270
E(ROHF/CC-PVTZ-F12) (Hartree): -193.40756400
E(UB3LYP/6-311+G(2df,2p)) (Hartree): -194.72853259
Point group : CS
Electronic state : 2-A"
Cartesian coordinates (Angs):
     C       0.024676     -1.994590       0.000000
     C      -0.608430     -0.824242       0.000000
     H       1.103170     -2.077403       0.000000
     H      -0.528237     -2.923361       0.000000
     H      -1.693236     -0.828568       0.000000
     C       0.000000      0.524837      -0.000000
     C      -0.856442      1.612155      -0.000000
     H      -0.475732      2.623490      -0.000000
     H      -1.929241      1.483551      -0.000000
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     C       1.381636      0.705756      -0.000000
     H       2.073126     -0.122262       0.000000
     H       1.801512      1.701059      -0.000000
Rotational constants (GHz):    9.6936100    4.1389200    2.9004800
Vibrational harmonic frequencies (cm-1):
       32.7372 (  A")          302.5670 (  A')          426.5897 (  A")
      432.5327 (  A')          499.7667 (  A")          527.8990 (  A')
      560.2157 (  A")          734.5347 (  A")          774.0074 (  A")
      816.0815 (  A')          828.7145 (  A")          950.9861 (  A")
      986.0333 (  A')         1030.5063 (  A")         1032.4560 (  A')
     1077.4077 (  A')         1303.2702 (  A')         1353.2278 (  A')
     1365.7390 (  A')         1462.5316 (  A')         1498.4760 (  A')
     1532.7262 (  A')         1688.5947 (  A')         3137.9171 (  A')
     3148.1497 (  A')         3148.5584 (  A')         3160.6368 (  A')
     3224.0982 (  A')         3239.5244 (  A')         3250.3508 (  A')
Zero-point correction (Hartree): 0.099161

TS.chainaddition.1dm
--------------------
E(UB3LYP/6-311+G(2df,2p)) (Hartree): -385.02710830
Electronic state : 1-A
Cartesian coordinates (Angs):
     C      -2.273320     -1.633501      -0.215288
     C      -1.182589     -0.996685       0.239108
     C      -1.015797      0.435685       0.308954
     C       0.193878      0.945023       0.744549
     H      -3.146106     -1.106536      -0.576149
     H      -2.319203     -2.712989      -0.231589
     H      -0.340650     -1.585274       0.585279
     H       0.251572      2.009368       0.938978
     H       0.856821      0.316013       1.342209
     C      -2.113555      1.345749      -0.155764
     H      -2.364863      1.165700      -1.204236
     H      -3.028777      1.179599       0.416944
     H      -1.833556      2.391338      -0.046974
     C       1.577254      0.781369      -0.688718
     O       2.000000     -0.448921      -0.624629
     O       2.689626     -0.734090       0.528736
     H       2.203465      1.534476      -0.225761
     H       1.089069      1.006548      -1.628601
Rotational constants (GHz):    3.1904600    1.1796300    0.9722400
Vibrational harmonic frequencies (cm-1):
     i755.0375                47.8535                68.7549
      104.4584               147.8700               176.3502
      186.5324               283.2348               373.5861
      430.6277               467.9805               527.2299
      554.6754               684.2352               720.3356
      804.0739               877.4447               898.9015
      952.5139               957.6944               992.6638
     1036.7313              1041.4294              1068.5641
     1101.8708              1135.4214              1217.3053
     1258.5654              1329.5266              1352.8035
     1397.6075              1416.0760              1459.7546
     1475.2422              1482.8499              1503.1867
     1563.5576              1637.9160              3018.8850
     3022.9414              3063.8265              3100.4043
     3115.1005              3150.5571              3156.9461
     3167.0479              3220.1512              3233.4952
Zero-point correction (Hartree): 0.145768

TS.chainaddition.1gp
--------------------
E(UB3LYP/6-311+G(2df,2p)) (Hartree): -385.02830605
Electronic state : 1-A
Cartesian coordinates (Angs):
     C       3.249785     -0.035817       0.415996
     C       2.159866     -0.611241      -0.114573
     C       0.906303      0.048357      -0.398498
     C      -0.163350     -0.683882      -0.872570
     H       3.279130      1.011273       0.683349
     H       4.149944     -0.606703       0.593292
     H       2.202197     -1.666981      -0.361977
     H      -0.988467     -0.171858      -1.372382
     H       0.019202     -1.707821      -1.178582
     C       0.723522      1.501852      -0.089636
     H       0.675556      1.660464       0.992442
     H       1.558611      2.097242      -0.460730
     H      -0.200283      1.882241      -0.517412
     C      -1.470951     -0.951829       0.623290
     O      -2.125472      0.168047       0.713686
     O      -2.909085      0.436160      -0.384327
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     H      -1.957097     -1.760854       0.091421
     H      -0.893389     -1.175304       1.511657
Rotational constants (GHz):    4.5729100    0.9898700    0.9222100
Vibrational harmonic frequencies (cm-1):
     i754.8248                  29.8273                  66.8015
       92.9216                 120.6479                 174.8799
      198.1085                 292.7791                 370.8532
      436.3249                 476.8490                 536.0861
      548.2436                 682.5010                 718.5598
      802.7805                 876.0981                 910.0209
      952.0667                 959.8708                 986.2293
     1023.5354                1037.3172                1070.8104
     1097.8231                1135.0261                1218.4299
     1256.4969                1325.7865                1355.6772
     1398.7304                1415.8523                1454.5571
     1477.0974                1485.2003                1502.6457
     1568.0115                1637.6105                3013.7348
     3019.0679                3074.1207                3099.8844
     3131.7793                3136.8459                3154.5293
     3161.6700                3219.8311                3235.6169
Zero-point correction (Hartree): 0.145666

TS.chainaddition.1tm
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IRC pathway available
E(CCSD(T)/CC-pVTZ) (Hartree): -384.23197655
E(CCSD/CC-pVTZ) (Hartree): -384.15958109
     T1 diagnostic:  0.050204
E(MP2/CC-pVTZ) (Hartree): -384.06615898
E(MP3/CC-pVTZ) (Hartree): -384.12304260
E(PMP2/CC-pVTZ) (Hartree): -384.20692529
E(PMP3/CC-pVTZ) (Hartree): -384.25975261
E(PUHF/CC-pVTZ) (Hartree): -382.80088809
E(UHF/CC-pVTZ) (Hartree): -382.65774361
E(UB3LYP/6-311+G(2df,2p)) (Hartree): -385.02855337
Electronic state : 1-A
Cartesian coordinates (Angs):
     C       3.331885     -0.492056       0.249369
     C       2.106279     -0.743545      -0.235905
     C       1.017556      0.202335      -0.320087
     C      -0.213973     -0.208699      -0.783218
     H       3.614298      0.477862       0.634801
     H       4.092118     -1.259689       0.266770
     H       1.893281     -1.739377      -0.610536
     H      -0.951041      0.521785      -1.115899
     H      -0.292000     -1.188180      -1.238672
     C       1.205686      1.606386       0.171830
     H       1.452308      1.625630       1.237246
     H       2.032351      2.094707      -0.348336
     H       0.309249      2.202416       0.016812
     C      -1.451209     -0.495546       0.797591
     O      -2.598618     -0.644370       0.205542
     O      -3.122221      0.519677      -0.286705
     H      -1.273039      0.457545       1.277513
     H      -1.088166     -1.408405       1.252121
Rotational constants (GHz):    4.8287600    0.8750400    0.8081200
Vibrational harmonic frequencies (cm-1):
     i723.1462                  53.6493                  64.5282
      111.9782                 144.1484                 168.6314
      201.5907                 286.8795                 359.8123
      440.3860                 446.8443                 531.3850
      556.0313                 685.1996                 789.5260
      802.9933                 828.6161                 945.4001
      947.8786                 959.6810                 983.7419
     1024.5491                1027.8687                1064.8872
     1092.5979                1123.9130                1221.5523
     1255.6875                1325.0528                1349.3625
     1399.7079                1415.8193                1457.5349
     1476.9932                1487.3423                1505.9432
     1567.3078                1636.3096                3019.8826
     3048.2261                3065.6321                3110.9736
     3120.6239                3138.3751                3153.7757
     3178.0484                3234.6623                3234.7339
Zero-point correction (Hartree): 0.145908

TS.chainaddition.1tp
--------------------
E(UB3LYP/6-311+G(2df,2p)) (Hartree): -385.02800582
Electronic state : 1-A
Cartesian coordinates (Angs):
     C       2.803637     -1.309310       0.291013
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     C       1.581250     -0.981302      -0.155890
     C       1.073489      0.360575      -0.324633
     C      -0.235149      0.538085      -0.726271
     H       3.535535     -0.566094       0.576067
     H       3.105852     -2.343253       0.375786
     H       0.898979     -1.779507      -0.428951
     H      -0.562465      1.532505      -1.000283
     H      -0.774650     -0.277925      -1.204870
     C       1.942282      1.535954       0.012152
     H       2.260414      1.512039       1.057857
     H       2.853072      1.534662      -0.590914
     H       1.422214      2.474968      -0.164262
     C      -1.471593      0.263753       0.854658
     O      -2.640065      0.263535       0.281802
     O      -2.924161     -0.885325      -0.401907
     H      -1.080825     -0.696944       1.161477
     H      -1.307819      1.137342       1.472758
Rotational constants (GHz):    3.7792600    0.9545300    0.8369900
Vibrational harmonic frequencies (cm-1):
     i721.2513                  49.3144                  77.9484
       94.6132                 153.2415                 169.4273
      201.2685                 281.8467                 357.5374
      438.0891                 442.6541                 528.2608
      557.2164                 695.5768                 789.4181
      804.7650                 822.3069                 941.7018
      950.6482                 957.3715                 986.0210
     1030.5544                1032.2792                1066.5072
     1093.4519                1120.7065                1220.2246
     1252.4314                1325.4606                1347.4099
     1397.2812                1416.4162                1458.3731
     1477.9821                1483.5325                1505.7073
     1563.5606                1636.0949                3021.0977
     3060.4218                3063.1271                3111.5834
     3116.1996                3141.7365                3153.2315
     3186.6449                3234.2896                3235.5439
Zero-point correction (Hartree): 0.145919

TS.chainaddition.2mm
--------------------
E(UB3LYP/6-311+G(2df,2p)) (Hartree): -384.99945264
Electronic state : 1-A
Cartesian coordinates (Angs):
     C      -1.383840      1.980171      -0.062533
     C      -0.693078      1.016502       0.540243
     C      -0.768830     -0.435753       0.227946
     C      -0.638011     -1.302020       1.326168
     H      -2.081044      1.787632      -0.866683
     H      -1.272297      3.011121       0.242139
     H      -0.009694      1.280899       1.338514
     H      -0.920626     -2.343222       1.252973
     H      -0.140998     -0.984170       2.231629
     C      -1.753350     -0.861916      -0.852622
     H      -2.772040     -0.631175      -0.539526
     H      -1.577211     -0.350129      -1.798334
     H      -1.694900     -1.935140      -1.029529
     C       0.901086     -0.661348      -0.800991
     O       1.999422     -0.433933      -0.074902
     O       2.367835      0.854717       0.017506
     H       0.700009      0.088607      -1.555876
     H       0.846888     -1.704512      -1.085409
Rotational constants (GHz):    2.5549100    1.5755200    1.2625600
Vibrational harmonic frequencies (cm-1):
     i720.0055                  46.9563                 102.7698
      145.2077                 204.8446                 226.6608
      240.5551                 275.6931                 318.6394
      382.2883                 417.9119                 472.7997
      519.6908                 541.3674                 675.4612
      741.2118                 784.9669                 834.4893
      913.8496                 947.9872                 948.2050
     1005.0054                1016.2849                1029.1231
     1067.0700                1093.9238                1200.3880
     1257.1771                1298.8640                1312.4651
     1358.6747                1415.5014                1455.9931
     1458.8462                1492.3138                1505.0884
     1516.7633                1680.5748                3039.7344
     3097.6392                3102.8534                3107.9807
     3142.3228                3147.4483                3158.9993
     3223.2008                3225.9719                3236.8942
Zero-point correction (Hartree): 0.144410

TS.chainaddition.2pp
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E(UB3LYP/6-311+G(2df,2p)) (Hartree): -385.00031270
Electronic state : 1-A
Cartesian coordinates (Angs):
     C      -2.510069     -1.088830      -0.175557
     C      -1.798891     -0.019140      -0.519547
     C      -0.600667      0.512927       0.188797
     C      -0.401253      1.898042       0.056252
     H      -2.275197     -1.690252       0.691846
     H      -3.371573     -1.390584      -0.754729
     H      -2.097820      0.544589      -1.398097
     H       0.316943      2.419497       0.672620
     H      -0.870162      2.456694      -0.742343
     C      -0.256083     -0.103431       1.535644
     H      -1.035245      0.145853       2.257413
     H      -0.172877     -1.186929       1.488498
     H       0.692615      0.277673       1.907047
     C       0.766062     -0.313462      -0.968598
     O       2.012601      0.023388      -0.616887
     O       2.560434     -0.728171       0.353278
     H       0.506180     -1.345979      -0.771913
     H       0.528271      0.091066      -1.943416
Rotational constants (GHz):    3.1214600    1.2859000    1.2245200
Vibrational harmonic frequencies (cm-1):
     i721.5542                45.2095               102.4949
      143.7877               196.1389               221.1611
      246.7701               282.4572               305.9581
      398.3142               419.2450               474.6195
      525.9823               533.0015               671.7604
      745.7009               783.3043               842.4192
      910.9221               959.0386               961.7338
     1008.8819              1017.5099              1036.0959
     1067.6086              1087.5654              1201.0937
     1252.8474              1296.1086              1310.8880
     1356.1182              1421.6499              1452.4558
     1458.2380              1487.9494              1502.5376
     1512.7274              1684.7915              3044.1438
     3106.7406              3108.4914              3127.4922
     3127.5373              3142.6103              3150.6831
     3227.6251              3228.6765              3236.8803
Zero-point correction (Hartree): 0.144495

TS.chainaddition.2tm
--------------------
E(UB3LYP/6-311+G(2df,2p)) (Hartree): -385.00242289
Electronic state : 1-A
Cartesian coordinates (Angs):
     C      -1.283654      1.983299      -0.009418
     C      -1.354529      0.762393       0.509224
     C      -0.826913     -0.484106      -0.109784
     C      -1.471431     -1.672489       0.278818
     H      -0.812379      2.184539      -0.961188
     H      -1.700708      2.832266       0.513906
     H      -1.837091      0.628325       1.472589
     H      -1.320670     -2.593903      -0.266118
     H      -2.038258     -1.726590       1.198495
     C      -0.347851     -0.394401      -1.548123
     H      -1.173210     -0.070397      -2.183590
     H       0.470562      0.310511      -1.671264
     H      -0.006729     -1.365404      -1.903613
     C       0.870980     -0.687815       0.858524
     O       1.648202      0.378204       0.619167
     O       2.489468      0.253513      -0.420802
     H       1.259627     -1.612268       0.451077
     H       0.537884     -0.682105       1.887350
Rotational constants (GHz):    2.5249500    1.5996500    1.3487200
Vibrational harmonic frequencies (cm-1):
     i703.1351                43.8129               101.4934
      171.6979               217.4784               231.4688
      242.7869               287.9728               301.7037
      409.1801               422.3749               483.2458
      516.2539               533.4297               691.3485
      744.3657               779.5980               862.4549
      931.1082               960.8158               968.5443
     1008.5001              1019.0305              1030.2805
     1074.9677              1089.9958              1205.1752
     1265.1120              1303.5541              1309.6727
     1356.6953              1423.8364              1452.5586
     1457.7286              1488.2127              1504.8540
     1516.8496              1691.6225              3043.3404
     3103.2745              3113.3698              3127.1523
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     3128.3435                3139.5867                3153.1116
     3230.3716                3231.6339                3232.8985
Zero-point correction (Hartree): 0.144898

TS.chainaddition.2tp
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E(UB3LYP/6-311+G(2df,2p)) (Hartree): -385.00287127
Electronic state : 1-A
Cartesian coordinates (Angs):
     C      -0.076526      2.160538       0.058752
     C       0.457805      1.159064      -0.633964
     C       1.017943     -0.091822      -0.070044
     C       1.974555     -0.758465      -0.854615
     H      -0.154762      2.148980       1.136462
     H      -0.466974      3.033551      -0.444397
     H       0.490031      1.231261      -1.716160
     H       2.568882     -1.563778      -0.446003
     H       2.066033     -0.561515      -1.914013
     C       1.199610     -0.155614       1.438018
     H       1.924285      0.595570       1.754318
     H       0.267052      0.030302       1.967094
     H       1.575464     -1.132185       1.741578
     C      -0.539148     -1.286535      -0.316748
     O      -1.560592     -0.824391       0.413398
     O      -2.391555      0.012900      -0.230630
     H      -0.705380     -1.253149      -1.384978
     H      -0.152888     -2.200115       0.115558
Rotational constants (GHz):    2.5293100    1.7145000    1.3757200
Vibrational harmonic frequencies (cm-1):
     i663.7285                 67.2921                  87.1132
      155.4759                 227.8292                 233.9526
      249.9191                 287.7616                 311.6231
      412.5304                 425.1317                 488.0458
      523.3655                 531.5793                 682.1895
      746.2301                 768.9010                 857.3147
      932.1988                 958.6856                 975.9002
     1009.8738                1012.8506                1025.3794
     1070.7092                1087.4931                1204.6854
     1262.1108                1305.4266                1311.6961
     1358.9128                1416.1151                1453.6573
     1458.6226                1491.1098                1506.8609
     1517.3926                1681.5563                3041.5226
     3099.7520                3114.9875                3118.1622
     3134.9147                3141.1217                3157.1373
     3232.2556                3234.2372                3234.7457
Zero-point correction (Hartree): 0.144906

TS.chainaddition.3dm
--------------------
E(UB3LYP/6-311+G(2df,2p)) (Hartree): -385.00317892
Electronic state : 1-A
Cartesian coordinates (Angs):
     C       0.941433     -2.005410      -0.349048
     C       0.647293     -0.933199       0.500877
     C       1.075542      0.456665       0.179888
     C       1.273845      1.331065       1.167735
     H       1.141892     -1.865783      -1.400724
     H       0.859798     -3.023641       0.003715
     H       0.716020     -1.168146       1.560630
     H       1.590098      2.345653       0.969548
     H       1.119180      1.063849       2.205443
     C       1.283764      0.820058      -1.262709
     H       2.120881      0.264274      -1.691809
     H       0.399316      0.590907      -1.858951
     H       1.493029      1.882251      -1.366186
     C      -1.309278     -0.792678       0.596504
     O      -1.810306     -0.116826      -0.441038
     O      -1.929229      1.210536      -0.249532
     H      -1.389604     -0.267013       1.540193
     H      -1.609917     -1.831042       0.563223
Rotational constants (GHz):    2.3061300    1.7466100    1.3695700
Vibrational harmonic frequencies (cm-1):
     i702.3461                 41.5608                  95.0457
      118.0875                 190.3654                 206.4254
      236.4183                 287.0843                 368.3001
      415.7267                 432.7045                 512.8263
      539.1192                 576.1735                 699.3545
      760.3762                 788.0883                 845.9092
      888.9266                 934.9229                 956.9629
     1007.2601                1012.8826                1074.0628
     1082.1935                1139.3372                1206.0381
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     1241.7329                1264.3851                1304.0374
     1386.3920                1419.0871                1455.1531
     1459.2267                1487.0932                1501.5839
     1514.9121                1685.2852                3028.4071
     3078.9815                3090.0260                3108.3951
     3121.1397                3137.7453                3153.4224
     3218.9167                3225.5604                3244.1986
Zero-point correction (Hartree): 0.144759

TS.chainaddition.4dm
--------------------
E(UB3LYP/6-311+G(2df,2p)) (Hartree): -385.02548482
Electronic state : 1-A
Cartesian coordinates (Angs):
     C      -0.315779     -1.099619      0.873059
     C       0.960369     -1.068468      0.348752
     C       1.718262      0.110173      0.014444
     C       2.911032     -0.041675     -0.598856
     H      -0.741272     -0.220428      1.353861
     H      -0.657998     -2.050140      1.263108
     H       1.436980     -2.014963      0.115185
     H       3.526942      0.807388     -0.860526
     H       3.294951     -1.022027     -0.848432
     C       1.186775      1.472253      0.377957
     H       0.217926      1.665680     -0.080034
     H       1.045616      1.555565      1.457330
     H       1.878529      2.251875      0.065926
     C      -1.697421     -0.908851     -0.568344
     O      -1.866592      0.371938     -0.752556
     O      -2.487967      1.010416      0.286219
     H      -2.453150     -1.410957      0.022922
     H      -1.291481     -1.403701     -1.440717
Rotational constants (GHz):    3.4396100    1.1628700    1.0076100
Vibrational harmonic frequencies (cm-1):
     i763.9578                  34.7599                  83.3127
       93.9011                 154.6732                 172.2377
      260.9710                 290.4930                 398.6753
      430.4644                 494.9492                 526.6465
      548.5170                 668.6773                 711.1417
      803.0146                 848.8262                 874.6951
      934.1442                 942.8268                 970.7021
     1012.5245                1042.2326                1069.9638
     1120.8458                1124.6707                1216.6547
     1256.2123                1298.7066                1336.5786
     1414.8055                1428.9191                1458.3650
     1472.5727                1489.9750                1507.1437
     1563.7647                1622.7177                3041.0636
     3064.2067                3098.6910                3106.4201
     3125.1891                3135.5050                3143.3013
     3178.9509                3227.5103                3228.9180
Zero-point correction (Hartree): 0.145871

TS.chainaddition.4gp
--------------------
E(UB3LYP/6-311+G(2df,2p)) (Hartree): -385.02491736
Electronic state : 1-A
Cartesian coordinates (Angs):
     C       0.337291      0.450135     -0.700022
     C      -0.652343     -0.474395     -0.454321
     C      -2.006203     -0.191316     -0.052552
     C      -2.844006     -1.217832      0.201001
     H       0.061739      1.496429     -0.752872
     H       1.204582      0.169876     -1.301983
     H      -0.388410     -1.524992     -0.517856
     H      -3.871908     -1.054311      0.493298
     H      -2.515385     -2.244750      0.114049
     C      -2.466252      1.239018      0.067357
     H      -1.875904      1.787000      0.804223
     H      -2.364205      1.767573     -0.882041
     H      -3.509669      1.287678      0.370902
     C       1.635722      0.471106      0.829205
     O       2.505906     -0.458761      0.548059
     O       3.272692     -0.178305     -0.550208
     H       1.928557      1.491592      0.614063
     H       1.076564      0.260134      1.731403
Rotational constants (GHz):    4.8592200    0.8257800    0.7813500
Vibrational harmonic frequencies (cm-1):
     i764.4801                  56.9900                  62.7071
       89.4462                 143.5594                 182.7943
      252.8226                 281.9946                 420.6931
      435.2305                 488.9984                 533.8773
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      549.5949                675.3181                728.2826
      803.1759                860.3209                886.4346
      935.0363                954.6005                965.8947
     1011.3529               1037.4280               1069.0917
     1115.8960               1139.1222               1215.8124
     1253.8780               1306.8203               1337.3379
     1412.3574               1425.9488               1458.8481
     1475.3730               1489.5407               1506.1614
     1571.3969               1624.7068               3013.1514
     3032.9516               3079.0209               3104.0414
     3118.0990               3140.6080               3145.8876
     3170.8562               3225.8921               3229.4482
Zero-point correction (Hartree): 0.145846

TS.chainaddition.4tm
--------------------
E(UB3LYP/6-311+G(2df,2p)) (Hartree): -385.02626831
Electronic state : 1-A
Cartesian coordinates (Angs):
     C       0.343396     -0.052638      -0.705534
     C      -0.813117     -0.714478      -0.368781
     C      -2.078307     -0.107753      -0.037340
     C      -3.108162     -0.893846       0.336615
     H       0.304572      1.009392      -0.909307
     H       1.148396     -0.584515      -1.210590
     H      -0.775544     -1.796255      -0.287722
     H      -4.077907     -0.483106       0.580671
     H      -3.000416     -1.968466       0.399339
     C      -2.231105      1.388842      -0.128332
     H      -1.530389      1.902734       0.532334
     H      -2.033540      1.743948      -1.141205
     H      -3.237967      1.694501       0.147379
     C       1.595114     -0.009485       0.887250
     O       2.667230      0.507761       0.356513
     O       3.361665     -0.353223      -0.441369
     H       1.612741     -1.074327       1.074029
     H       1.111970      0.655932       1.590650
Rotational constants (GHz):    5.2060500    0.7875000    0.7487200
Vibrational harmonic frequencies (cm-1):
     i730.7700                 54.6251                 70.2396
       84.4411                137.9212                180.8455
      269.7694                300.1252                364.3878
      436.0101                493.6119                536.6502
      549.7326                674.1970                791.8753
      801.8588                832.2226                886.2268
      935.0041                956.2559                967.7039
     1007.9597               1037.8851               1069.0877
     1107.4776               1124.0006               1214.5430
     1248.5229               1305.1708               1336.7965
     1411.9731               1424.8618               1456.1983
     1479.5791               1489.1775               1506.1624
     1568.5794               1626.4800               3033.9300
     3060.2395               3080.0725               3116.9056
     3118.4626               3135.3941               3144.5749
     3188.7574               3228.4311               3240.7296
Zero-point correction (Hartree): 0.145998

TS.chainaddition.4tp
--------------------
E(UB3LYP/6-311+G(2df,2p)) (Hartree): -385.02642466
Electronic state : 1-A
Cartesian coordinates (Angs):
     C      -0.308966     -0.817701       0.869501
     C       0.992902     -0.978872       0.449946
     C       1.867484      0.078625       0.007652
     C       3.070003     -0.240421      -0.514184
     H      -0.671702      0.161571       1.173927
     H      -0.799537     -1.659995       1.338499
     H       1.392643     -1.984954       0.377906
     H       3.763991      0.518228      -0.848245
     H       3.384663     -1.270953      -0.612307
     C       1.434431      1.513778       0.165245
     H       0.476710      1.710264      -0.317961
     H       1.304077      1.762496       1.220256
     H       2.175306      2.191197      -0.253780
     C      -1.518064     -0.679549      -0.744979
     O      -2.625316     -0.226316      -0.225185
     O      -2.589626      1.100661       0.090315
     H      -0.927815      0.025385      -1.313272
     H      -1.605531     -1.703161      -1.085147
Rotational constants (GHz):    3.9623600    0.9949100    0.8831100
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Vibrational harmonic frequencies (cm-1):
     i735.8961                39.0993                74.1784
       98.0196               160.3671               173.3641
      283.1372               290.4373               362.2389
      431.8610               498.3904               528.5529
      565.4259               669.9237               778.6352
      791.3943               828.0314               886.6441
      936.1301               959.1347               966.1419
     1011.4102              1039.5505              1069.3042
     1110.9250              1125.0908              1214.8067
     1248.4195              1298.6913              1335.7439
     1413.5367              1429.6949              1455.7717
     1478.6637              1490.8597              1506.0857
     1564.9926              1624.3354              3037.3009
     3074.4990              3085.6398              3118.5544
     3120.0110              3138.4777              3144.1336
     3194.0528              3227.6323              3241.1029
Zero-point correction (Hartree): 0.146077

TS.chainaddition.1mtm
---------------------
E(UB3LYP/6-311+G(2df,2p)) (Hartree): -385.02733922
Electronic state : 1-A
Cartesian coordinates (Angs):
     C       0.142289     -0.731137      -0.693960
     C       1.345347     -0.254677      -0.222968
     C       0.595277      2.097350       0.103828
     C       1.537440      1.139115       0.127690
     H      -0.561028     -0.045306      -1.171346
     H       0.097253     -1.760325      -1.026008
     H       2.535626      1.407841       0.458012
     H       0.843540      3.109931       0.390725
     H      -0.428387      1.909144      -0.197886
     C       2.502791     -1.175602       0.029526
     H       3.380133     -0.848648      -0.534892
     H       2.794655     -1.161688       1.083682
     H       2.277814     -2.201307      -0.253810
     C      -1.194404     -0.738054       0.806732
     O      -2.320013     -0.668129       0.169175
     O      -2.507531      0.552837      -0.448164
     H      -0.834558      0.176453       1.264164
     H      -1.057143     -1.685733       1.314176
Rotational constants (GHz):    3.0642400    1.2860700    0.9986000
Vibrational harmonic frequencies (cm-1):
     i331.2114                61.4678                95.9830
      127.3087               163.2695               188.6929
      206.8572               306.0701               396.8107
      433.2945               473.7514               543.4419
      553.1386               702.8713               816.7997
      838.6117               883.1391               937.1828
      980.4620              1011.9266              1023.3781
     1033.2083              1047.8362              1069.8726
     1110.7454              1157.1996              1241.9661
     1286.1348              1311.9665              1350.0211
     1411.2763              1424.6717              1472.0781
     1480.5058              1490.5084              1501.9714
     1579.9860              1649.3230              3009.8296
     3015.7079              3055.5035              3087.1222
     3118.8224              3126.9589              3136.1564
     3178.1437              3211.3725              3222.3619
Zero-point correction (Hartree): 0.147000

TS.chainaddition.1pdm
---------------------
E(UB3LYP/6-311+G(2df,2p)) (Hartree): -385.02860795
Electronic state : 1-A
Cartesian coordinates (Angs):
     C       0.296997     -0.847517       0.798346
     C       1.326221     -0.138924       0.222582
     C       0.127545      2.032331       0.015306
     C       1.218114      1.260621      -0.128390
     H      -0.509926     -0.339250       1.328465
     H       0.505158     -1.859564       1.122160
     H       2.103254      1.700167      -0.576821
     H       0.154469      3.064595      -0.307094
     H      -0.798926      1.682056       0.449542
     C       2.617756     -0.817414      -0.135171
     H       2.825745     -0.726059      -1.204691
     H       3.453878     -0.339031       0.381519
     H       2.613519     -1.872494       0.129221
     C      -1.130893     -1.175977      -0.619925
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     O      -1.837400     -0.094977      -0.633294
     O      -2.532344      0.117463       0.552263
     H      -1.512012     -2.006485      -0.038803
     H      -0.611653     -1.362544      -1.551738
Rotational constants (GHz):    3.0887500    1.3986300    1.0976700
Vibrational harmonic frequencies (cm-1):
     i323.0591                  82.3005                 115.5010
      127.2814                 145.2259                 190.6894
      210.1527                 302.1726                 401.1366
      445.1434                 471.1418                 533.8652
      555.4222                 702.5495                 801.9506
      855.4959                 868.6763                 894.5474
      960.5381                1008.1249                1023.3854
     1036.4601                1040.8354                1065.3177
     1106.7803                1136.0504                1226.7714
     1283.8891                1313.4421                1351.8001
     1411.3582                1430.5894                1477.4233
     1481.3413                1488.9819                1498.6646
     1587.8610                1653.0052                3018.8634
     3030.0432                3059.4506                3104.5055
     3118.0731                3132.4580                3141.0803
     3173.7925                3224.5901                3229.4907
Zero-point correction (Hartree): 0.146983

TS.chainaddition.1ppp
---------------------
E(UB3LYP/6-311+G(2df,2p)) (Hartree): -385.02442265
Electronic state : 1-A
Cartesian coordinates (Angs):
     C      -0.114685     -0.525828       0.795165
     C      -0.902256      0.451944       0.234244
     C      -3.027612     -0.848371       0.001618
     C      -2.259172      0.221282      -0.240318
     H      -0.548974     -1.488713       1.032540
     H       0.755230     -0.229168       1.383273
     H      -2.682647      1.022979      -0.836245
     H      -4.026513     -0.915735      -0.404902
     H      -2.700048     -1.675301       0.617158
     C      -0.296227      1.794038      -0.024762
     H       0.337364      1.741726      -0.919993
     H      -1.049179      2.562890      -0.188827
     H       0.369998      2.095196       0.782577
     C       1.246630     -1.050300      -0.610056
     O       2.100168     -0.077578      -0.635494
     O       2.830913      0.043160       0.532156
     H       1.516503     -1.928552      -0.036451
     H       0.699545     -1.166567      -1.537771
Rotational constants (GHz):    4.0187800    1.0807300    0.9563900
Vibrational harmonic frequencies (cm-1):
     i743.4388                  38.7947                  63.1775
       83.6679                 103.2107                 146.0305
      183.4584                 305.4745                 378.3927
      438.3867                 467.5759                 522.2052
      555.4088                 678.9127                 700.4936
      802.9804                 867.9606                 893.2580
      941.5811                 963.0845                1009.7893
     1021.7799                1039.2079                1055.5988
     1098.4593                1128.5402                1217.3067
     1258.5092                1286.2307                1342.9880
     1409.2198                1420.7153                1454.7020
     1471.1555                1485.6053                1489.8430
     1577.5916                1657.2263                2990.3187
     3028.7346                3074.3371                3099.6012
     3121.8355                3139.1170                3150.3540
     3177.2699                3219.6055                3231.9750
Zero-point correction (Hartree): 0.145328

TS.chainaddition.1ptm
---------------------
E(UB3LYP/6-311+G(2df,2p)) (Hartree): -385.02436392
Electronic state : 1-A
Cartesian coordinates (Angs):
     C      -0.016057     -0.072434      -0.721875
     C       1.110928      0.523759      -0.210797
     C       2.573268     -1.505951      -0.073006
     C       2.338972     -0.196491       0.088439
     H       0.038265     -1.084258      -1.099943
     H      -0.808054      0.537295      -1.151696
     H       3.142525      0.411112       0.492314
     H       3.531070     -1.932659       0.187660
     H       1.832753     -2.188683      -0.467422
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     C       1.087558      1.978482       0.158684
     H       1.205728      2.110374       1.239312
     H       1.922647      2.507539      -0.306939
     H       0.162204      2.461416      -0.146797
     C      -1.316311     -0.411894       0.825356
     O      -2.386541     -0.772694       0.190249
     O      -3.057406      0.262068      -0.407207
     H      -1.302115      0.593489       1.224492
     H      -0.843588     -1.223436       1.363867
Rotational constants (GHz):    3.4516900    1.0193900    0.8583500
Vibrational harmonic frequencies (cm-1):
     i718.6254                  40.3555                  50.0535
       85.1511                 111.3836                 141.3792
      161.0225                 306.2613                 356.8082
      430.0159                 438.2371                 529.7563
      535.3714                 682.2022                 775.3273
      808.0411                 822.4353                 928.2707
      949.8030                 957.1868                 987.0068
     1021.3381                1034.7628                1055.2476
     1097.5449                1114.6886                1220.8879
     1256.7714                1278.8581                1342.6340
     1411.4559                1417.1633                1461.5529
     1477.4634                1484.1946                1499.7770
     1572.4825                1655.5698                3008.9995
     3055.0802                3071.8659                3109.2582
     3121.3809                3134.8806                3150.2765
     3193.2525                3231.7794                3235.0617
Zero-point correction (Hartree): 0.145371

TS.chainaddition.3pdm
---------------------
E(UB3LYP/6-311+G(2df,2p)) (Hartree): -385.00067755
Electronic state : 1-A
Cartesian coordinates (Angs):
     C       0.993965     -0.708439       1.384579
     C       1.140118     -0.287358       0.128461
     C       0.547667      2.152873       0.463225
     C       0.600552      1.017475      -0.345365
     H       0.464264     -0.132452       2.130102
     H       1.380019     -1.666968       1.701319
     H       0.820022      1.227020      -1.390482
     H       0.336741      3.122790       0.035456
     H       0.625746      2.094415       1.538774
     C       1.822802     -1.124627      -0.918800
     H       1.143048     -1.353366      -1.744092
     H       2.680059     -0.599686      -1.347685
     H       2.170618     -2.069036      -0.505619
     C      -1.271684      0.523464      -0.849250
     O      -1.924465     -0.043596       0.159587
     O      -1.813508     -1.383538       0.234505
     H      -1.042037     -0.146058      -1.669373
     H      -1.675220      1.500080      -1.078238
Rotational constants (GHz):    2.3107400    1.7083300    1.3363000
Vibrational harmonic frequencies (cm-1):
     i683.8018                  44.4791                  69.4781
      107.9107                 174.3631                 201.7757
      225.5431                 279.1755                 354.6546
      412.8059                 418.6200                 518.6353
      539.3987                 570.7512                 695.0899
      755.8819                 795.6977                 823.8408
      871.8750                 939.1931                 957.2699
     1004.2810                1021.7375                1071.1852
     1088.3165                1127.8907                1206.9208
     1237.7233                1252.3630                1264.2539
     1417.2705                1429.6874                1446.6184
     1461.7998                1485.9887                1496.2751
     1515.9693                1687.6062                3017.2855
     3057.9283                3082.9559                3108.2703
     3115.0383                3148.9983                3152.2399
     3228.3642                3228.8945                3241.2549
Zero-point correction (Hartree): 0.144330

TS.insertion.3gp
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E(UB3LYP/6-311+G(2df,2p)) (Hartree): -385.00956190
Electronic state : 1-A
Cartesian coordinates (Angs):
     C       0.183010      1.762566      -0.515291
     C       0.154509      0.432071      -0.272033
     C       1.381293     -0.368411      -0.046778
     C       1.308821     -1.702626      -0.092612
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     H       1.100238      2.329078      -0.615276
     H      -0.740288      2.313411      -0.643197
     H      -0.740904     -0.209784      -0.786106
     H       2.183183     -2.320803       0.060980
     H       0.375595     -2.210692      -0.296968
     C       2.682319      0.342262       0.216829
     H       2.982813      0.952961      -0.637717
     H       2.603284      1.014285       1.074476
     H       3.481568     -0.369739       0.412451
     C      -1.290506      0.147674       1.049781
     O      -2.342562      0.134806       0.272237
     O      -2.103805     -0.801861      -0.740555
     H      -0.880668     -0.802999       1.369868
     H      -1.310562      0.959509       1.768656
Rotational constants (GHz):    3.3849500    1.3218200    1.1005000
Vibrational harmonic frequencies (cm-1):
     i706.4873                 67.5276                103.8907
      166.0856                208.1417                232.1043
      290.1211                341.2454                375.5203
      433.0618                474.6422                564.3923
      584.7864                666.3027                791.4006
      794.2586                874.5358                918.5784
      960.4660                967.5745                980.7605
     1021.8927               1048.9256               1071.2892
     1130.5904               1178.4341               1227.1346
     1282.0989               1312.8375               1408.5902
     1416.0325               1440.4052               1462.4628
     1486.5471               1501.9297               1510.2599
     1586.3427               1648.8891               1693.4880
     3023.7997               3066.1575               3097.6166
     3112.6499               3132.8037               3139.2094
     3207.6596               3213.0190               3221.8766
Zero-point correction (Hartree): 0.144523

TS.insertion.3tm
----------------
E(UB3LYP/6-311+G(2df,2p)) (Hartree): -385.00957393
Electronic state : 1-A
Cartesian coordinates (Angs):
     C       0.557336      1.900878      -0.499174
     C       0.200107      0.607230      -0.322549
     C       1.194924     -0.466122      -0.088395
     C       0.850024     -1.743393      -0.277761
     H       1.586582      2.233989      -0.518064
     H      -0.193176      2.668042      -0.643430
     H      -0.789063      0.217188      -0.890676
     H       1.560434     -2.542365      -0.110490
     H      -0.140174     -2.020037      -0.610138
     C       2.582704     -0.081883       0.356072
     H       2.558619      0.529235       1.261522
     H       3.182499     -0.967137       0.557596
     H       3.101835      0.502606      -0.407191
     C      -1.311106      0.586359       0.935666
     O      -1.908659     -0.521103       0.569742
     O      -2.171374     -0.415676      -0.795378
     H      -1.760992      1.512910       0.599793
     H      -0.910234      0.541393       1.943012
Rotational constants (GHz):    3.0500300    1.4832400    1.1891000
Vibrational harmonic frequencies (cm-1):
     i641.9879                 58.8906                120.7985
      162.1724                206.3179                226.5220
      315.0648                335.5881                406.1866
      425.5887                495.8773                562.1742
      610.0567                671.6100                757.5840
      785.3411                867.5532                940.5594
      959.4751                973.8752                976.9842
     1022.4960               1057.1778               1071.2200
     1148.2895               1198.5370               1256.5096
     1298.8605               1321.3308               1347.6235
     1415.7891               1431.0136               1463.9827
     1486.6242               1492.0832               1505.8181
     1612.1006               1682.0001               1692.9823
     3021.6826               3063.0527               3092.9285
     3111.8540               3135.2739               3143.9325
     3206.2530               3213.8668               3232.6228
Zero-point correction (Hartree): 0.144855

TS.insertion.3mdm
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E(UB3LYP/6-311+G(2df,2p)) (Hartree): -385.00833355
Electronic state : 1-A
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Cartesian coordinates (Angs):
     C       2.322993     -0.605452       0.706668
     C       1.439434      0.128465       0.028391
     C       0.040499     -1.625643      -1.037530
     C       0.131250     -0.430630      -0.407504
     H       2.125596     -1.637205       0.966802
     H       3.269182     -0.192644       1.030524
     H      -0.669222      0.404124      -0.707717
     H      -0.926458     -2.036748      -1.300843
     H       0.914630     -2.200688      -1.317216
     C       1.673546      1.577086      -0.307051
     H       1.673730      1.727008      -1.389290
     H       0.869991      2.202365       0.088573
     H       2.622327      1.931833       0.090877
     C      -1.215169     -0.379709       0.998562
     O      -2.288616     -0.033072       0.333843
     O      -1.991214      1.130581      -0.379855
     H      -0.691570      0.392259       1.552735
     H      -1.304885     -1.355075       1.464434
Rotational constants (GHz):    3.0337000    1.3700300    1.1638400
Vibrational harmonic frequencies (cm-1):
     i576.8281                 61.2356                   98.6649
      142.7070                194.0522                  215.6272
      265.0603                290.5767                  373.2475
      437.7519                500.4152                  567.9503
      585.2793                669.6803                  771.9527
      802.7858                887.2418                  917.3108
      939.2098                958.3683                  988.0084
     1026.5403               1066.2218                 1085.1947
     1144.1004               1177.8929                 1221.0510
     1266.2363               1294.0368                 1391.8779
     1420.1690               1448.6446                 1481.3312
     1488.8631               1501.0239                 1502.6964
     1623.6354               1688.0094                 1754.9237
     3025.1984               3069.2044                 3089.1695
     3113.8892               3126.6054                 3136.3902
     3198.9914               3212.6733                 3215.0398
Zero-point correction (Hartree): 0.144520

TS.insertion.3phm
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E(UB3LYP/6-311+G(2df,2p)) (Hartree): -385.00832818
Electronic state : 1-A
Cartesian coordinates (Angs):
     C       2.216847      0.130285       0.854817
     C       1.265073     -0.276326       0.013488
     C       0.441916      1.900473      -0.849361
     C       0.174294      0.643156      -0.421560
     H       2.227919      1.132198       1.264182
     H       3.009284     -0.534412       1.171625
     H      -0.744447      0.084732      -0.915438
     H      -0.356963      2.576392      -1.129751
     H       1.452786      2.277896      -0.934967
     C       1.209336     -1.678725      -0.528938
     H       0.264204     -2.156710      -0.268554
     H       1.262491     -1.673008      -1.620312
     H       2.030421     -2.282166      -0.146484
     C      -1.283053      0.677620       0.854365
     O      -1.738113     -0.546537       0.719232
     O      -2.083083     -0.719707      -0.616258
     H      -1.867574      1.460841       0.385693
     H      -0.855029      0.865293       1.833344
Rotational constants (GHz):    2.6761600    1.5730000    1.2840400
Vibrational harmonic frequencies (cm-1):
     i523.5243                 62.1412                  113.6745
      144.7064                188.5016                  208.6620
      286.4037                297.3253                  404.7107
      437.6715                504.7044                  566.2086
      613.7531                682.4079                  764.8169
      770.8545                870.0721                  934.8910
      942.5968                957.6693                  979.2774
     1029.0424               1067.3877                 1086.1255
     1158.6603               1199.9709                 1261.3138
     1266.5809               1298.9672                 1337.3635
     1419.8047               1443.6300                 1454.5925
     1480.9912               1491.5754                 1498.4939
     1608.7400               1688.4969                 1895.5464
     3029.0206               3081.5955                 3091.2699
     3116.3964               3128.5879                 3135.9440
     3205.7301               3213.1520                 3214.4965
Zero-point correction (Hartree): 0.144970
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