Supplementary Information for

Surprisingly long lifetime of methacrolein oxide, an isoprene derived Criegee intermediate, under humid conditions

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Supplementary Note 1: Experimental

The details of our experimental system have been described elsewhere.[1,2] We prepared MACRO following the method reported by Vansco et al.: $ICHC(CH_3)CH_2I$ (1,3-diiodo-2-methylprop-1-ene) + $h\nu \rightarrow CH_2=C(CH_3)CHI + I$, $CH_2=C(CH_3)CHI + O_2 \rightarrow CH_2=C(CH_3)CHOO + I$.[3] The 248 nm excimer (Coherent, CompExPro 205) was used as a photolysis light source, and coupled into and out of the reactor by two long-pass filters (Asahi Spectra Co., Ltd. UV 275 nm, 25 mm dia. F0201 & F0204). The laser power was measured by an energy meter (Gentec EO, UP25N-100H-H9-D0) after reflecting out of the reactor. Our reactor was a glass tube (80 cm long, 1.9 cm inner diameter) with anti-reflection SiO_2 windows (Edmunds, 65875). The windows were purged by N_2 flows to prevent contamination, and the effective sample length was thus reduced to 71 cm. The flow of $ICHC(CH_3)CH_2I/N_2/O_2$ was mixed with the flow of reactant (SO_2 or H_2O)/N_2 right before entering the reactor. All gas flows were controlled by mass flow controllers (Brooks, 5850E and Bronkhorst FG-201 CV). The gases in the reactor were set to be fully refreshed between consecutive laser pulses (laser repetition rate: 0.8–2.2 Hz). The probe light was from a broadband Xe lamp (Energetiq, EQ-99), and reflected six times through the reactor by a prism (Thorlabs, PS609, fused silica, right-angle, uncoated, 5 mm) and a spherical mirror (R = 1 m, Thorlabs, CM750-500-F01), extending the effective light path to 426 cm. The temperature of the reactor was 298.7±0.4 K.

[SO_2] and [$ICHC(CH_3)CH_2I$] measurements

The concentrations of $ICHC(CH_3)CH_2I$ ((*E*)-1,3-diiodo-2-methylprop-1-ene, Accela, 97.8 % by gas chromatography) and SO_2 (Matheson, 99.98 %) were measured separately in two glass cells (length = 90 cm and inner diameter = 1.2 cm for both cells) by mini-spectrometers (Ocean Optics, FLAME-S-XR1-ES for $ICHC(CH_3)CH_2I$; Ibsen FHW-380 for SO_2) before entering the reactor, and derived by Beer-Lambert law. Due to the lack of the absolute cross section of $ICHC(CH_3)CH_2I$, we report the relative concentration of $ICHC(CH_3)CH_2I$ by its absorbance at the reactor (L = 426 nm) at 236 nm. We diluted SO_2 in a ~2 L stainless steel cylinder by N_2 before the experiments, and [SO_2] was derived by comparing the integration of SO_2 absorbance and that of the reference cross section[4] within 200-350 nm.

Concentration of H_2O

The concentration of H_2O vapor (vaporized from Milli-Q water, 18 MΩ) was controlled by the flow ratio of dry N_2 and moisturized N_2. The temperature and humidity of H_2O/N_2 flow was measured by a humidity probe (Rotronic, HC2-S). The pressures at relevant locations were measured by diaphragm pressure gauges (INFICON, CDG025D 1000 Torr). The concentrations of the precursor and the reactants (SO_2 or H_2O) are derived by considering the flow, pressure, and temperature variations assuming the ideal gas behavior.

CMOS camera spectrometer

A grating spectrometer (Andor SR303i) and CMOS camera (Andor, Marana-4BU11) were used to obtain the time-resolved spectra of the reaction system. A series of spectra (exposure time 0.21 ms (or 0.43 ms) each) was recorded with each photolysis laser pulse. The spectrum taken 0.13-0.33 ms (or 0.36-0.79 ms) before the photolysis laser pulse was used as a reference spectrum; therefore, the change of absorbance caused by the photolysis laser pulse was recorded transiently. A spectrum with exposure time 0.21 ms each was obtained by accumulating 2560 laser pulses while that with exposure time 0.43 ms each was obtained by accumulating 256 or 512 laser pulses.

A background spectrum caused by the photolysis laser pulse and the long-pass filters that reflected the photolysis laser (other used optics might also contribute) was recorded in the experiments and all reported spectra have subtracted out the background spectrum.

Supplementary Table 1. Summary of experimental conditions and fitting results of the reaction of MACRO with SO_2 at 298 K. k_{SO2} = (1.5±0.4)x10^{-10} cm^3 s^{-1} (ave±1σ, considering all 8 data points from the two methods and 20% error in [SO_2]).

					Regular method[a]			SO_2 scavenge method[b]		
Exp #	P / Torr	P_{O2} / Torr	Abs_{pre}	I_{248nm} / mJ cm^{-2}	σL[MACRO]$_0$ / 10^{-3}	k_{SO2} / 10^{-10} cm^3 s^{-1}	k_0 / s^{-1}	σL[MACRO]$_0$ / 10^{-3}	k_{SO2} / 10^{-10} cm^3 s^{-1}	k_0 / s^{-1}
1	500.4[c]	12.0	0.280[d]	1.77[e]	1.24	1.7	389	1.14	1.8	408
2	500.1	11.9	0.279	1.74	1.29	1.5	393	1.21	1.7	427
3	150.6	10.5	0.347	1.88	1.00	1.0	341	0.81	1.4	332
4	150.4	10.4	0.342	1.87	0.96	1.1	318	0.77	1.8	281

[a] The fitting range is 0.18–10 ms.

[b] "SO_2 scavenge method" means the analysis in which the spectrum at the highest [SO_2] was subtracted from the spectra recorded at lower [SO_2]. The fitting range is 0.38–10 ms.

[c] Balanced by N_2.

[d] The concentration of the precursor is represented by its absorbance in the reactor (L = 71x6 = 426 cm) at 236 nm due to the lack of the absolute cross section.

[e] I_{248nm} represents the laser fluence.

Supplementary Table 2. Summary of experimental conditions and fitting results of the reaction of MACRO with H_2O at 298 K.

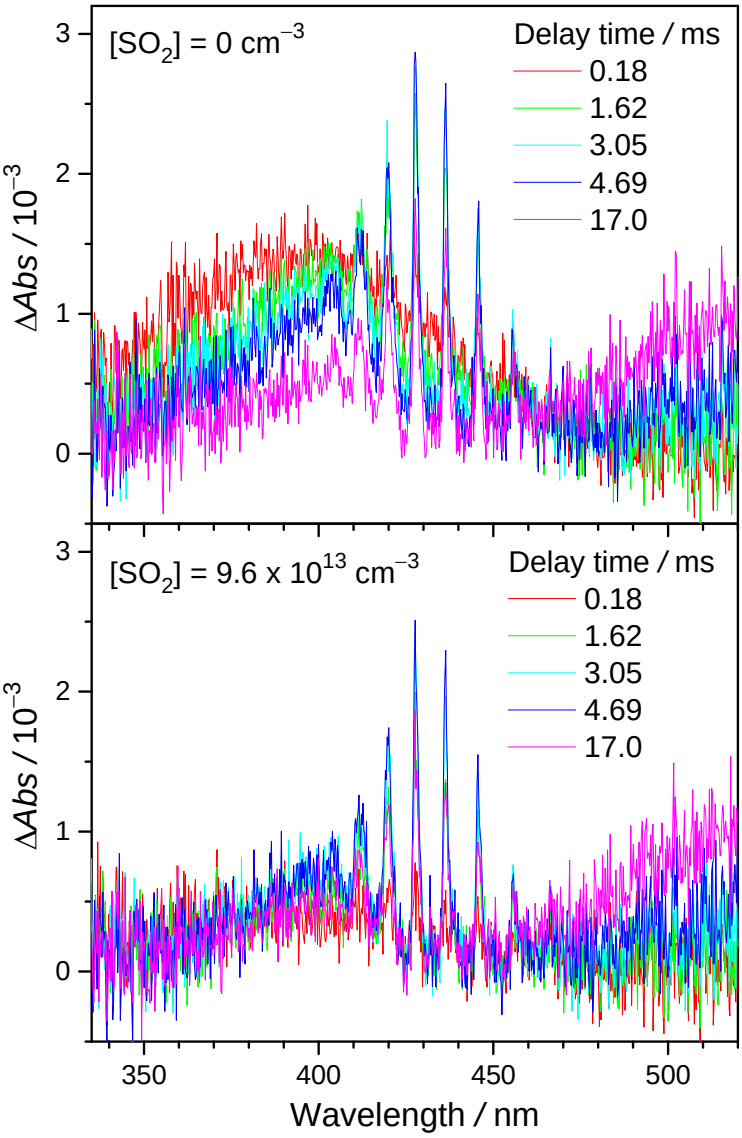
Exp #	P / Torr	P_{O2} / Torr	Abs_{pre}	I_{248nm} / mJ cm^{-2}	$k_{water\text{-}eff}$ / 10^{-17} cm^3 s^{-1}	k_0 / s^{-1}	# of points
5	501.2[a]	11.8	0.274[b]	1.79[c]	8.0±6.5[d]	370	14
6	150.6	10.5	0.379	1.81	13.3	262	10
7	301.0	11.4	0.485	3.64	−1.4	685	2
8	300.4	11.3	0.789	1.71	8.6	578	2
9	150.2	11.4	1.264	1.62	−5.1	621	2
10	150.0	11.3	0.454	3.62	8.9	469	2
11	500.3	11.8	0.795	1.71	2.6	641	2

[a] Balanced by N_2.

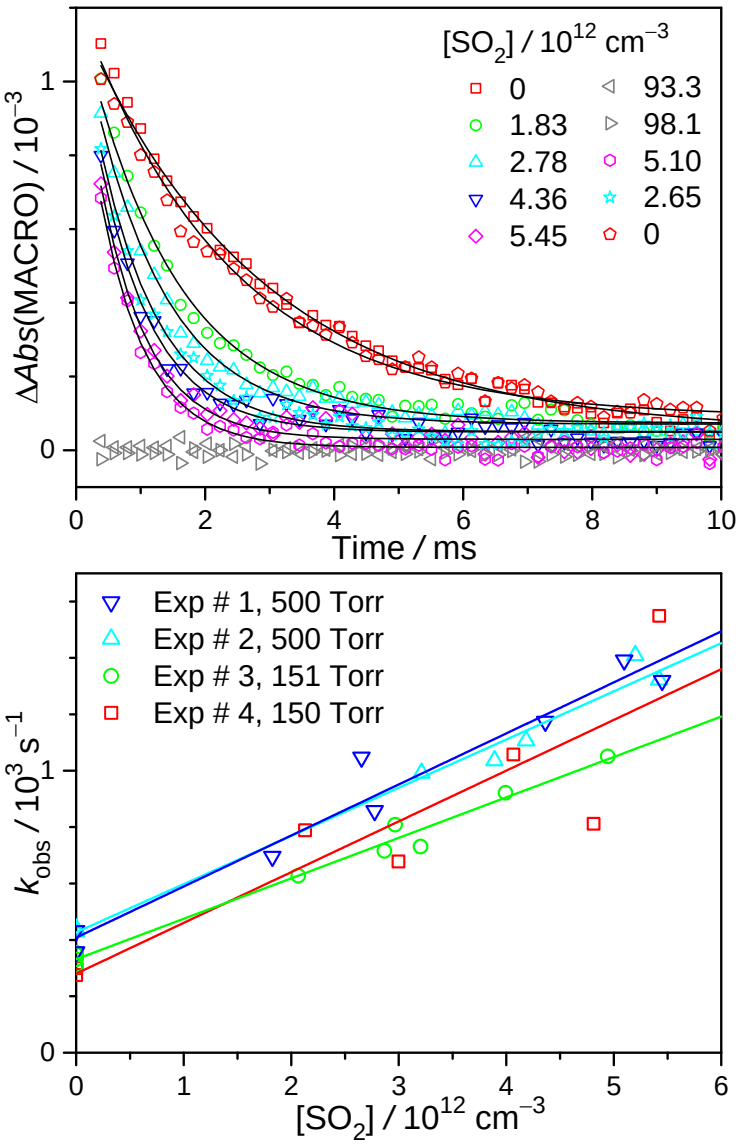
[b] The concentration of the precursor is represented by its absorbance in the reactor (L = 71x6 = 426 cm) at 236 nm due to the lack of the absolute cross section.

[c] I_{248nm} represents the laser fluence.

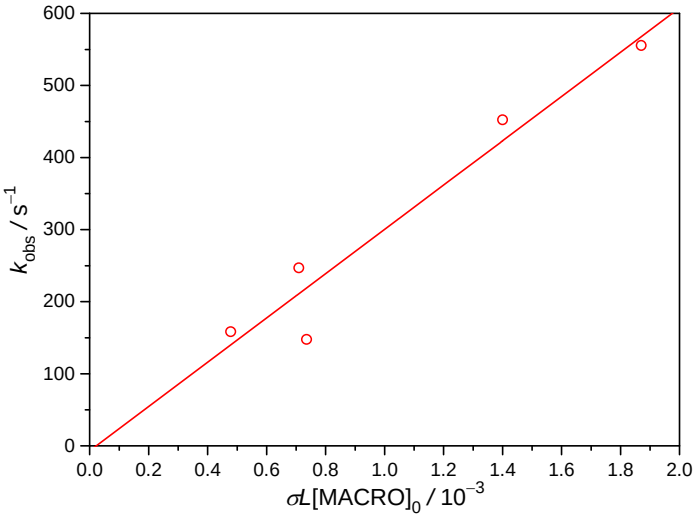
[d] error bar is $\pm 1\sigma$.



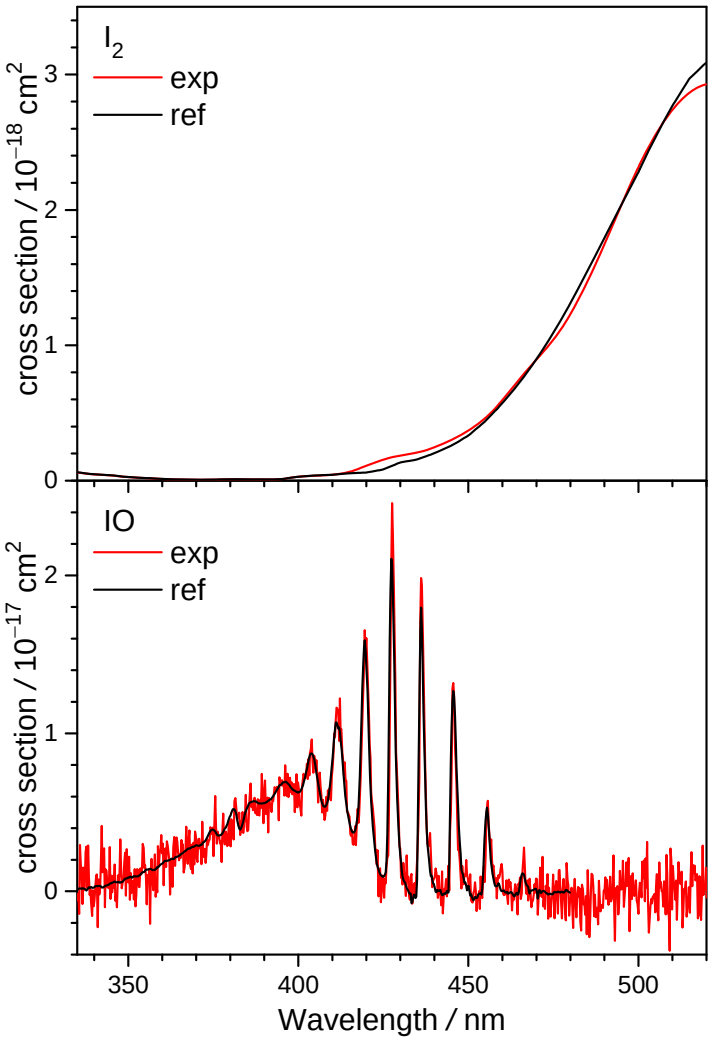
Supplementary Figure 1. Time-resolved difference absorption spectra recorded in the 1,3-diiodo-2- methylprop-1-ene/O_2 photolysis system at 298 K and 500 Torr at different delay times after the photolysis laser pulse. The data are from Exp # 1. Upper panel: The spectra recorded without adding SO_2. Lower panel: The spectra recorded at $[SO_2] = 9.6 \times 10^{13}$ cm^{-3}. Besides MACRO, byproducts IO and I_2 are also observed.



Supplementary Figure 2. Upper panel: MACRO time profiles obtained by fitting the spectra (Exp #1) obtained with the SO_2 scavenge method. The data points at 0.18 ms delay time are not included. Black curves show the fitting results of the exponential function. Lower panel: Pseudo-first-order plot for the reaction of MACRO with SO_2 at 298 K. The data points are from the exponential fitting of the MACRO time profiles.



Supplementary Figure 3. The observed decay rate coefficient k_{obs} plotted against the peak intensity of the MACRO absorption $\sigma L[MACRO]_0$ when no other reactant was added. Experimental condition: P = 299.6 Torr; P_{O2} = 10.7 Torr; T = 298 K; Abs_{pre} = 0.248-0.881; I_{248nm} = 0.90-1.72 mJ cm^{-2}. The intercept of this plot gives a preliminary estimation of the unimolecular decomposition rate coefficient of MACRO, which is < 50 s^{-1}.



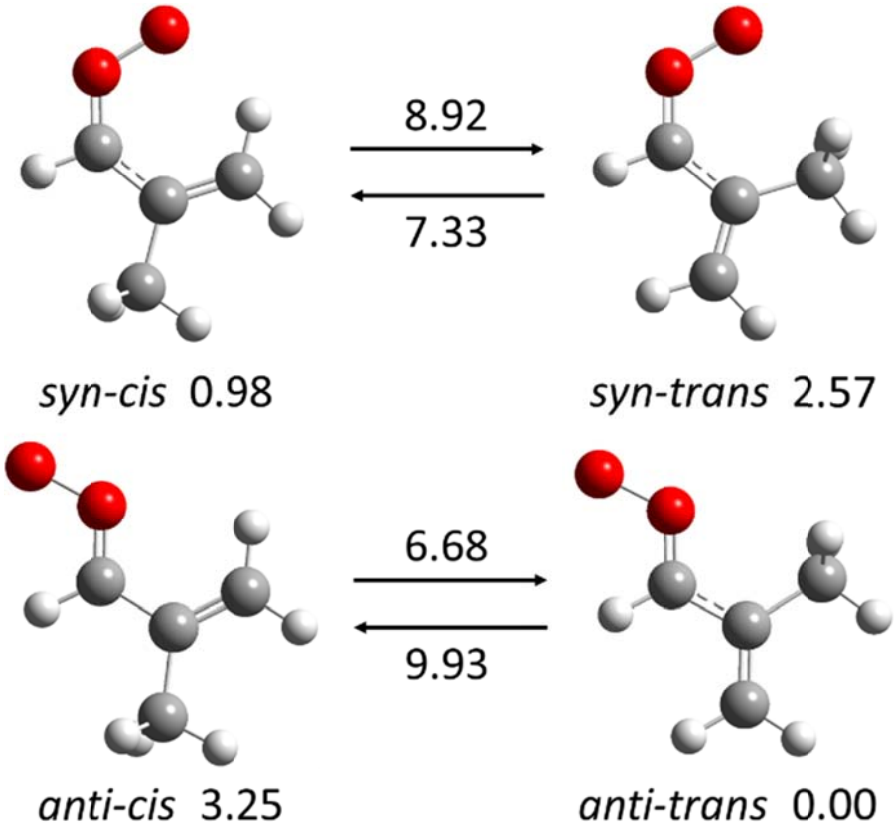
Supplementary Figure 4. The standard I_2 (upper panel) and IO (lower panel) spectra derived from our experimental spectra to include the instrumental functions (shown as red lines). They are consistent with the reported spectra in the literature (black lines).[5,6]

We used the *standardized* spectra of MACRO, IO, and I_2 in our analysis to extract their individual contributions. The standard MACRO spectrum is from the Gauss fit of our experimental results (see Figure 2). Supplementary Figure 4 shows the standard spectra of IO and I_2, which are derived from our experimental spectra to include the instrumental functions. This is important for IO, of which the shape of the sharp peaks depends on the resolution of the used spectrometer. We obtained the spectra of IO and I_2 at long photolysis-probe delay times (where the MACRO contribution is gone).

Supplementary Note 2: Theoretical Calculations

To obtain the rate coefficients for the unimolecular decomposition of MACRO and the reactions of MACRO with 1 and 2 water molecules, we optimized the reactant and transition state geometries on the singlet ground electronic state using Becke's three parameter hybrid functional (B3LYP)[7,8] with 6-311+G(2d,2p) basis set.[9] Using these geometries, we corrected the electronic energies by quadratic configuration interaction singles, and doubles with perturbative triples (QCISD(T)) method[10] with Dunning's Basis set[11] extrapolated to complete basis set (CBS) limit.[12] We used the aug-cc-pVXZ (X=D, T, Q) basis sets, and the Hartree−Fock energy was extrapolated using $E_{CBS} + Ae^{-BX}$. On the other hand, the correlation energy calculated by QCISD(T) was extrapolated using $E_{CBS} + Ae^{-(X-1)} + Be^{-(X-1)^2}$, where X is the cardinal number of the basis set and E_{CBS}, A, and B are optimization parameters. All density functional theory calculations were done with the Gaussian09 program[13] while all QCISD(T) calculations were performed using the MOLPRO[14] program. The rate coefficients were calculated using the conventional transition state theory method using rigid rotor harmonic oscillator approximations using the THERMO program in the Multiwell suite.[15,16] This method was used previously for shorter CIs and has shown good predictability.[17,18]

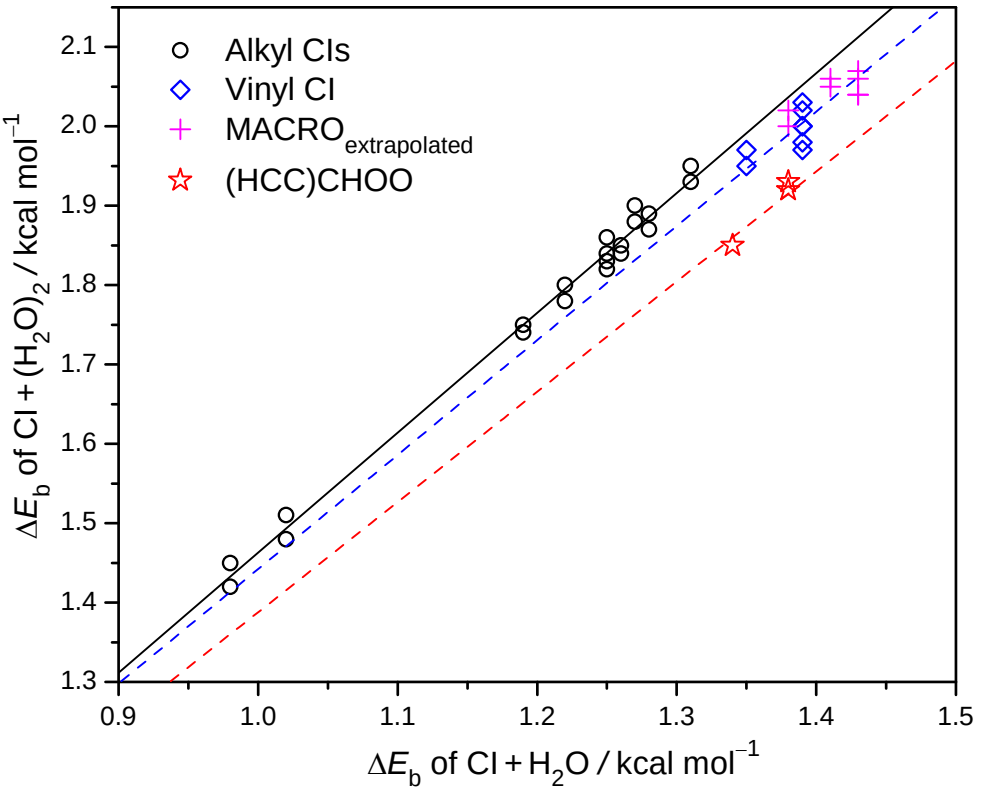
Supplementary Figure 5 shows the optimized geometries and relevant energies for the MACRO conformers. Our results are very similar to those of the previous works by Vereecken et al.[19] and Vansco et al.[3]



Supplementary Figure 5. Optimized structures of the four conformers of MACRO. The zero-point- corrected energies (in kcal mol^{-1}) from this work are shown below each structure. Energies are calculated using the electronic energies given at QCISD(T)/CBS//B3LYP/6-311+G(2d,2p) and harmonic zero-point correction at B3LYP/6-311+G(2d,2p). The double arrows indicate that the barrier between the *trans* and *cis* conformers within each *syn* or *anti* family is low, allowing rapid interconversion at room temperature, with the forward and backward barrier energies shown above and below the arrows.

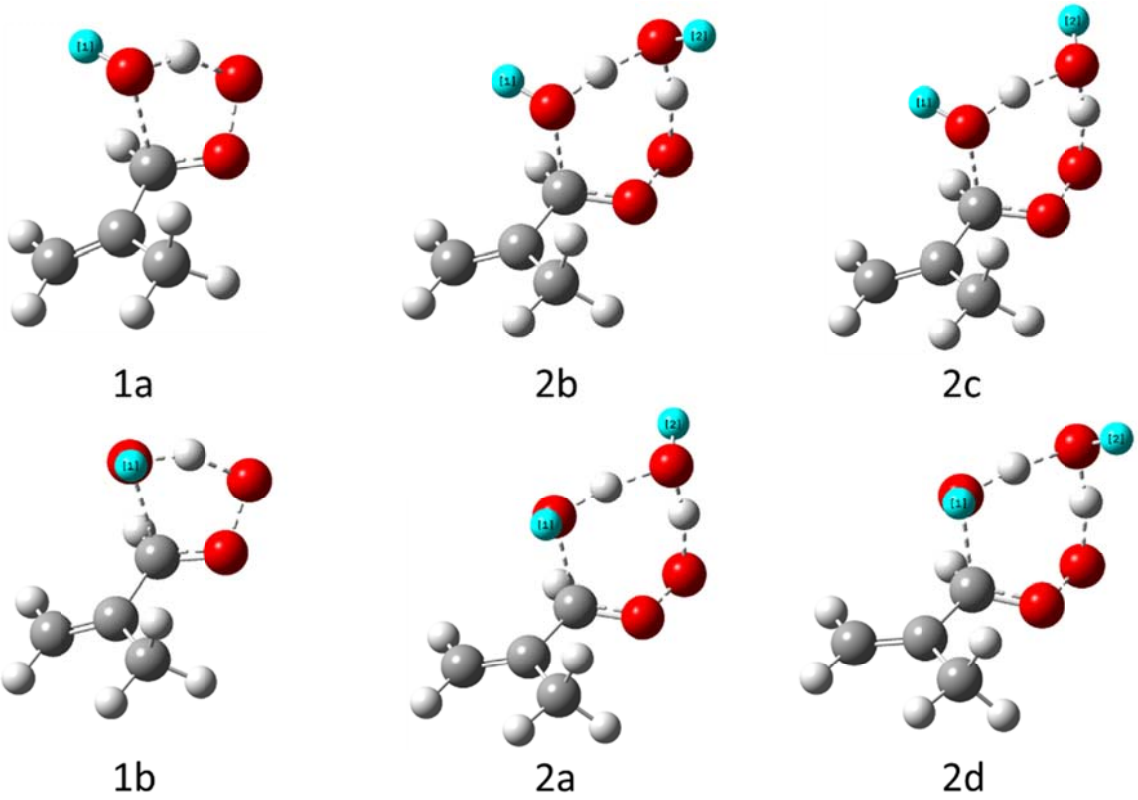
For calculating the rate coefficients of the reactions of Criegee intermediate with water monomer and dimer, it is important to calculate the reaction barrier energies using high level quantum chemistry methods including basis set extrapolation. However, due to the limitation of our computational resource, we were not able to perform the QCISD(T)/aug-cc-pVQZ calculation for the MACRO+$(H_2O)_2$ reaction, which is required to obtain the CBS energy. On the other hand, we noticed there is a strong correlation between the H_2O versus $(H_2O)_2$ reactions in the differences between the QCISD(T)/aug-cc-pVTZ and QCISD(T)/CBS energies for the alkyl substituted C1 to C3 CIs calculated previously.[18] The difference of the

reaction barrier (from the free reactants to the transition state) calculated at aug-cc-pVTZ (AVTZ) and CBS levels for the water monomer reaction and the water dimer reaction shows a linear relation for the alkyl Criegee intermediates as shown in Supplementary Figure 6 and Supplementary Table 3.



Supplementary Figure 6. Horizontal coordinate: energy difference between QCISD(T)/CBS and QCISD(T)/AVTZ, ΔE_b = E_b(CBS) – E_b(AVTZ), for the transition state of CI+H_2O reaction; Vertical coordinate: ΔE_b for the transition state of CI+$(H_2O)_2$ reaction. The black solid line is a linear fit to all the alkyl CI data points (listed in Supplementary Table 3). The dashed blue and red lines are through the origin and fitted to the data of the vinyl CI and (HC≡C)CHOO, respectively.

The pairing used to plot Supplementary Figure 6 and calculate the extrapolated CBS values is based on the orientation of the free OH bond of the H_2O molecule that is bonded to the carbonyl carbon of the CI, as shown in Supplementary Figure 7. The 1a channel in the water monomer reaction is paired with the 2b and 2c channels in the water dimer reaction, while the 1b channel is paired with the 2a and 2d channels.



Supplementary Figure 7. Optimized transition state structures of the reaction channels of *anti-trans* MACRO; 1a and 1b are for the water monomer reactions and 2a, 2b, 2c, and 2d for the water dimer reactions.

We also noticed the similarity in geometry between *anti*-$(CH_2{=}CH)CHOO$ (a vinyl CI) and *anti*-MACRO. The only difference is that *anti*-MARCO has a CH_3 group, which is mainly a spectator in the reaction with water molecule(s). The QCISD(T)/CBS reaction barrier heights (transition state energy relative to the free reactants) of *anti*-$(CH_2{=}CH)CHOO+H_2O$ and *anti*-$MACRO+H_2O$ are also very close to each other (see Supplementary Table 3), further confirming the idea that we can estimate the CBS value of *anti*-$MACRO+(H_2O)_2$ by the following strategy:

(i) We used B3LYP geometries to perform single point calculation with QCISD(T)/AVTZ for all the stationary points of *anti*-$CH_2CHCHOO$, *anti*-MACRO, H_2O, $(H_2O)_2$, *anti*-$CH_2CHCHOO+H_2O$, *anti*-$CH_2CHCHOO+(H_2O)_2$, *anti*-$MACRO+H_2O$, and *anti*-$MACRO+(H_2O)_2$.

(ii) For the stationary points of *anti*-$CH_2CHCHOO$, *anti*-MACRO, H_2O, $(H_2O)_2$, *anti*-$CH_2CHCHOO+H_2O$, *anti*-$CH_2CHCHOO+(H_2O)_2$, and *anti*-$MACRO+H_2O$, we performed QCISD(T)/aug-cc-pVQZ calculations and obtained the CBS energy using the

equation given above.

(iii) We obtained the energy difference between the QCISD(T)/CBS and QCISD(T)/aug-cc-pVTZ energies, $\Delta E_b = E_b(\mathrm{CBS}) - E_b(\mathrm{AVTZ})$, for the reaction barrier for *anti*-$CH_2CHCHOO+H_2O$, *anti*-$CH_2CHCHOO+(H_2O)_2$, and *anti*-$MACRO+H_2O$. Then, the approximate reaction barrier of CBS energy of the $MACRO+(H_2O)_2$ is obtained by the following equation and plotted in Supplementary Figure 6.

$$\Delta E_b^i(\mathrm{MACRO}) = \frac{\Delta E_b^i(\mathrm{vinyl\,CI})}{\Delta E_b^j(\mathrm{vinyl\,CI})}\Delta E_b^j(\mathrm{MACRO})$$

When i = 2a or 2d, j = 1b; when i = 2b or 2c, j = 1a. Similar strategy was used to estimate the barriers for the reaction involving *syn*-MACRO by using the results of *syn*-$CH_2CHCHOO$.

Supplementary Table 3. Zero-point corrected energies for the transition state, in kcal mol^{-1}, relative to the free reactants. Harmonic zero-point correction are from B3LYP/6-311+G(2d,2p). Electronic energies are from QCISD(T)/AVTZ//B3LYP/6-311+G(2d,2p) and QCISD(T)/CBS// B3LYP/6-311+G(2d,2p). We also listed the difference between CBS and AVTZ barrier energies, which is used to plot Supplementary Figure 6. The values with parentheses are estimated by the extrapolation method mentioned above.

Criegee intermediates	H_2O	Eb(AVTZ)	Eb(CBS)	ΔE_b	$(H_2O)_2$	Eb(AVTZ)	Eb(CBS)	ΔE_b
CH_2OO	1a	2.67	3.69	1.02	2a	-8.03	-6.60	1.42
	1b	1.83	2.81	0.98	2b	-8.00	-6.51	1.48
					2c	-6.85	-5.34	1.51
					2d	-7.84	-6.39	1.45
anti	1a	-0.25	0.97	1.22	2a	-9.19	-7.45	1.74
CH_3CHOO	1b	-0.84	0.35	1.19	2b	-9.50	-7.72	1.78
					2c	-8.30	-6.51	1.80
					2d	-8.96	-7.20	1.75
anti_Syn	1a	-0.91	0.40	1.31	2a	-9.49	-7.61	1.87
CH_3CH_2CHOO	1b	-1.27	0.01	1.28	2b	-10.07	-8.14	1.93
					2c	-8.92	-6.97	1.95
					2d	-9.21	-7.32	1.89
anti_Gauche	1a	-0.65	0.62	1.27	2a	-9.30	-7.47	1.84

CH_3CH_2CHOO	1b	-1.04	0.21	1.25	2b	-9.96	-8.08	1.88
					2c	-8.78	-6.88	1.90
					2d	-9.09	-7.24	1.86
	1a'	-0.35	0.90	1.26	2a'	-9.76	-7.94	1.82
	1b'	-1.02	0.23	1.25	2b'	-9.98	-8.14	1.84
					2c'	-8.78	-6.93	1.85
					2d'	-9.53	-7.70	1.83
anti_syn	1a	2.54	3.92	1.39	2a	-6.69	-4.74	1.95
$CH_2CHCHOO$	1b	1.57	2.92	1.35	2b	-5.89	-3.88	2.02
(vinyl CI)					2c	-4.59	-2.56	2.03
					2d	-6.47	-4.50	1.97
anti_anti	1a	3.59	4.98	1.39	2a	-4.70	-2.73	1.97
$CH_2CHCHOO$	1b	2.55	3.94	1.39	2b	-4.67	-2.67	2.00
(vinyl CI)					2c	-3.39	-1.39	2.00
					2d	-4.42	-2.44	1.98
anti	1a	4.41	5.79	1.38	2a	-4.91	-3.06	1.85
CHCCHOO	1b	3.19	4.53	1.34	2b	-4.25	-2.33	1.92
					2c	-2.95	-1.02	1.93
					2d	-4.65	-2.80	1.85
anti-cis	1a	1.84	3.25	1.41	2a	-7.21	(-5.21)	(2.00)
MARCO	1b	0.36	1.75	1.38	2b	-6.56	(-4.51)	(2.05)
					2c	-5.47	(-3.41)	(2.06)
					2d	-7.19	(-5.17)	(2.02)
anti-trans	1a	2.75	4.18	1.43	2a	-4.75	(-2.71)	(2.04)
MACRO	1b	2.36	3.79	1.43	2b	-5.32	(-3.26)	(2.07)
					2c	-4.28	(-2.22)	(2.06)
					2d	-4.38	(-2.33)	(2.04)
syn_syn	1a	9.58	10.95	1.37	2a	-0.39	1.67	2.06
$CH_2CHCHOO$	1b	9.18	10.55	1.37	2b	-0.64	1.38	2.02
(vinyl CI)					2c	0.69	2.70	2.01
					2d	-0.23	1.90	2.13
syn_anti	1a	6.60	7.97	1.37	2a	-2.06	0.02	2.08
$CH_2CHCHOO$	1b	6.59	7.99	1.40	2b	-3.47	-1.47	2.01

(vinyl CI)					2c	-2.04	-0.04	2.00
					2d	-2.21	-0.08	2.14
syn-cis	1a	8.46	9.87	1.41	2a	-1.47	(0.66)	(2.13)
MARCO	1b	7.49	8.91	1.42	2b	-1.14	(0.95)	(2.08)
					2c	-0.03	(2.04)	(2.07)
					2d	-1.35	(0.85)	(2.20)
syn-trans	1a	5.30	6.69	1.39	2a	-2.88	(-0.79)	(2.09)
MACRO	1b	5.20	6.61	1.41	2b	-4.11	(-2.09)	(2.03)
					2c	-2.30	(-0.29)	(2.01)
					2d	-3.11	(-0.96)	(2.15)

Supplementary Table 4 Theoretical rate coefficients for MACRO+H_2O and MACRO+$(H_2O)_2$. The last two columns are the total water monomer and dimer reaction rate coefficients estimated by the Boltzmann distributions of the fast-interconverting *cis* and *trans* conformers.

Temp (K)	*anti-trans-* MACRO + H_2O (10^{-17} cm^3 s^{-1})	*anti-trans-* MACRO + $(H_2O)_2$ (10^{-14} cm^3 s^{-1})	*anti-cis-* MACRO + H_2O (10^{-15} cm^3 s^{-1})	*anti-cis-* MACRO + $(H_2O)_2$ (10^{-13} cm^3 s^{-1})	*anti-* MACRO + H_2O (10^{-17} cm^3 s^{-1})	*anti-* MACRO + $(H_2O)_2$ (10^{-14} cm^3 s^{-1})
273.15	2.78	3.99	1.27	5.45	3.10	4.12
278.15	3.05	3.25	1.30	4.32	3.41	3.36
283.15	3.35	2.68	1.34	3.47	3.75	2.78
288.15	3.66	2.22	1.37	2.79	4.12	2.30
293.15	3.99	1.85	1.41	2.27	4.50	1.93
298.15	**4.34**	**1.55**	**1.45**	**1.86**	**4.92**	**1.62**
303.15	4.71	1.31	1.49	1.53	5.36	1.37
308.15	5.10	1.11	1.54	1.27	5.83	1.17

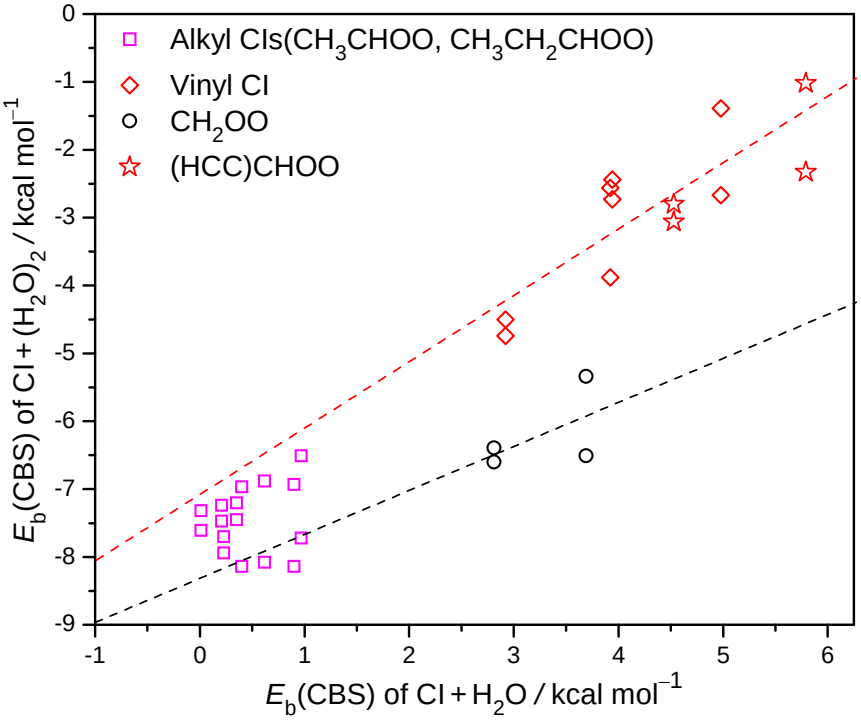
Temp (K)	*syn-trans-* MACRO + H_2O (10^{-19} cm^3 s^{-1})	*syn-trans-* MACRO + $(H_2O)_2$ (10^{-15} cm^3 s^{-1})	*syn-cis-* MACRO + H_2O (10^{-20} cm^3 s^{-1})	*syn-cis-* MACRO + $(H_2O)_2$ (10^{-17} cm^3 s^{-1})	*syn-* MACRO + H_2O (10^{-20} cm^3 s^{-1})	*syn-* MACRO + $(H_2O)_2$ (10^{-17} cm^3 s^{-1})
273.15	3.87	1.81	0.86	4.89	0.96	5.33
278.15	4.05	1.63	0.86	4.55	0.97	4.99
283.15	4.37	1.47	0.91	4.27	1.05	4.71
288.15	4.69	1.33	0.96	4.01	1.12	4.45
293.15	5.20	1.21	1.05	3.80	1.24	4.24
298.15	**5.78**	**1.10**	**1.18**	**3.62**	**1.41**	**4.06**
303.15	6.41	1.01	1.31	3.44	1.59	3.88
308.15	7.23	0.93	1.51	3.30	1.86	3.74

Supplementary Table 5 Theoretical rate coefficients of the unimolecular reactions for MACRO conformers. The last two columns are the total reaction rate coefficients estimated by the Boltzmann distributions of the fast-interconverting *cis* and *trans* conformers.

Temp (K)	*anti-trans-* MARCO (s^{-1})	*anti-cis-* MARCO (s^{-1})	*syn-trans-* MARCO (s^{-1})	*syn-cis-* MARCO (s^{-1})	*anti-* MARCO (s^{-1})	*syn-* MARCO (s^{-1})
273.15	2	104	0	398	2	378
278.15	3	166	1	605	3	573
283.15	5	260	1	908	6	857
288.15	8	401	2	1342	10	1264
293.15	13	610	4	1959	16	1839
298.15	**21**	**916**	**6**	**2824**	**25**	**2644**
303.15	34	1356	9	4022	40	3755
308.15	52	1983	15	5666	62	5274

Before ending this section, we comment on using the E_b values of the water monomer reactions to estimate the E_b values of the water dimer reactions, which was used in previous

studies.[19] As given in Supplementary Figure 8, we can see a correlation between them. However, one important aspect is that the trend for the simplest CI CH_2OO (black dashed line) is quite different from the correlation involving unsaturated CIs (red dashed line). In addition, the standard deviation from the linear fit is much larger than in the case when we use ΔE_b, as given in Supplementary Figure 6. Therefore, we think it is more efficient to use the ΔE_b strategy to approximate the QCISD(T)/CBS energies for the MACRO+$(H_2O)_2$ reaction.



Supplementary Figure 8. Horizontal coordinate: QCISD(T)/CBS E_b for the transition state of CI+H_2O reaction; Vertical coordinate: QCISD(T)/CBS E_b for the transition state of CI+$(H_2O)_2$ reaction. The dashed black and red lines are fitted to the data of the simplest CI CH_2OO and unsaturated CIs ((HC≡C)CHOO, (CH_2=CH)CHOO), respectively.

XYZ geometries

Below are the optimized geometries for the MACRO, pre-reactive complex (PC), transition state (TS), and product (Prod), obtained at B3LYP/6-311+G(2d,2p). Unit: Angstrom.

anti-trans MACRO

C	0.375031	0.463072	-0.122636
H	0.862698	1.415131	-0.302750
O	1.083326	-0.578965	-0.251465
O	2.393647	-0.425442	-0.603750
C	-1.008133	0.339304	0.247147
C	-1.719333	1.474059	0.371659
H	-1.270955	2.443050	0.200896
H	-2.763935	1.455285	0.646848
C	-1.580294	-1.033381	0.472496
H	-1.486947	-1.645172	-0.425153
H	-1.042555	-1.552746	1.266136
H	-2.631026	-0.969914	0.745113

anti-cis MARCO

C	-0.501703	-0.151632	-0.111266
H	-1.359465	-0.797339	-0.271354
O	-0.707442	1.090188	-0.238500
O	-1.965872	1.507333	-0.560184
C	0.809248	-0.664878	0.228798
C	1.858640	0.149076	0.423139
H	2.829317	-0.252066	0.676293
H	1.768884	1.221676	0.333906
C	0.899038	-2.166412	0.345306
H	0.223114	-2.543418	1.115055
H	0.624053	-2.651958	-0.592858
H	1.910024	-2.473361	0.602151

syn-trans MACRO

C	0.705602	0.523428	-0.323289
H	1.679657	0.784897	-0.719776
O	-0.015937	1.557410	-0.175532
O	-1.287490	1.469299	0.311958
C	0.407282	-0.861907	-0.046651
C	1.412487	-1.716768	-0.322135
H	1.304655	-2.778879	-0.155363
H	2.359375	-1.375963	-0.717900
C	-0.913235	-1.329483	0.504375
H	-1.124804	-0.858259	1.461268
H	-1.731292	-1.051028	-0.155715
H	-0.895117	-2.411791	0.626598

syn-cis MARCO

C	0.605348	0.589698	-0.240335
H	1.575463	0.949754	-0.563343
O	-0.205511	1.566955	-0.111794
O	-1.487642	1.355426	0.285894
C	0.400246	-0.812654	-0.025261
C	-0.776390	-1.339116	0.376155
H	-0.857113	-2.409438	0.518132
H	-1.630584	-0.711226	0.555769
C	1.619841	-1.671793	-0.285749
H	1.962223	-1.574975	-1.317487
H	2.451426	-1.389746	0.362328
H	1.393804	-2.719907	-0.104348

anti-trans MACRO 1a PC

C	-0.062688	-0.113837	-0.063083
O	-0.270391	1.086070	0.282283
O	0.744596	2.009202	0.126718
C	-1.119805	-1.075601	0.105088
C	-0.853288	-2.336535	-0.277822
H	0.108402	-2.607628	-0.690933
H	-1.591637	-3.120204	-0.185122
O	2.753009	0.599607	-1.159418
H	3.263394	1.058843	-1.829734
H	2.174099	1.270010	-0.739184
C	-2.433425	-0.632052	0.686173
H	-2.295277	-0.212985	1.683221
H	-2.884559	0.149741	0.074523

H	-3.125358	-1.468342	0.751078
H	0.906074	-0.368624	-0.483265

anti-cis MARCO 1a PC

C	0.009435	-0.108878	0.199699
O	-0.179666	1.111387	0.464754
O	0.884325	1.983735	0.340377
C	-1.074021	-1.067507	0.309461
C	-2.299788	-0.695686	0.707868
H	-2.527469	0.329438	0.960764
H	-3.098510	-1.419068	0.786916
O	2.280562	0.744296	-1.689315
H	2.467051	1.272250	-2.468595
H	1.911036	1.360329	-1.022260
C	-0.712166	-2.485339	-0.054584
H	-0.346693	-2.544973	-1.080999
H	0.079702	-2.867542	0.592047
H	-1.574970	-3.140196	0.040575
H	1.002795	-0.399660	-0.125567

syn-trans MACRO 1a PC

C	-0.818056	-0.772157	0.478222
O	-1.427478	0.336533	0.506241
O	-0.725740	1.527181	0.464786
C	0.593713	-1.071325	0.427721
C	0.863755	-2.392321	0.427674
H	0.080059	-3.136914	0.454275
H	1.881620	-2.753829	0.397056
O	0.050216	1.498935	-2.185784
H	-0.370191	2.155888	-2.744778
H	-0.284862	1.667614	-1.281681
C	1.677385	-0.029282	0.379883
H	1.623054	0.537590	-0.547812
H	1.571965	0.683464	1.193361
H	2.649486	-0.516331	0.443822
H	-1.522681	-1.595925	0.511873

syn-cis MARCO 1a PC

C	-0.520068	-0.911533	-0.012712
O	-0.884962	0.224295	-0.457157
O	0.043912	1.199362	-0.695900
C	0.786404	-1.407232	0.309549
C	1.911564	-0.673737	0.174476
H	1.875653	0.337853	-0.187783
H	2.865627	-1.114491	0.434120
O	-1.433885	3.174020	-2.137376
H	-1.532343	3.913852	-1.534214
H	-0.921017	2.510607	-1.640815
C	0.807687	-2.834096	0.815806
H	0.215073	-2.942431	1.725677
H	0.400636	-3.524854	0.075601
H	1.825633	-3.143792	1.039565
H	-1.384621	-1.553400	0.116082

anti-trans MACRO 2a PC

C	0.263481	-0.128793	-0.585659
O	-0.454920	-1.138641	-0.833623
O	-1.831739	-0.949180	-0.916970
C	1.688953	-0.287501	-0.480292
C	2.375026	0.819080	-0.141977
H	1.863930	1.753491	0.046680
H	3.450281	0.798581	-0.031292
O	-2.608547	0.769397	1.014168
H	-2.896074	0.269872	1.781384
H	-2.393259	0.106701	0.309417
O	-0.610196	2.650191	0.750624
H	-0.981690	3.499697	0.501606
H	-1.377059	2.085112	0.977814
C	2.309018	-1.633587	-0.729968
H	1.919173	-2.376427	-0.033313
H	2.076700	-1.989375	-1.734194
H	3.389590	-1.584117	-0.618045
H	-0.213459	0.836896	-0.445698

anti-trans MACRO 2b PC

C	0.563822	-0.545182	0.418110
O	-0.384832	-1.069945	-0.222701
O	-1.508278	-1.443776	0.523754
C	1.772697	-0.181175	-0.273587
C	2.783070	0.274181	0.483297
H	2.683160	0.375179	1.554976

H	3.728524	0.561826	0.045946
O	-3.023355	0.779925	0.333983
H	-3.583256	0.737805	-0.444707
H	-2.574528	-0.099867	0.392897
O	-0.582087	2.069548	0.320598
H	-0.603836	2.865702	0.856268
H	-1.506800	1.744175	0.297543
C	1.829120	-0.323177	-1.767486
H	1.618237	-1.348136	-2.073159
H	1.077365	0.314009	-2.234090
H	2.809781	-0.039969	-2.142439
H	0.433349	-0.416437	1.485905

anti-cis MARCO 2a PC

C	0.396328	-0.581625	0.286884
O	-0.478222	-1.192499	-0.380992
O	-1.703055	-1.431241	0.250231
C	1.717468	-0.327173	-0.259446
C	2.071252	-0.812222	-1.457875
H	1.391294	-1.402292	-2.054754
H	3.056221	-0.624682	-1.860980
O	-2.871147	1.007839	0.197374
H	-3.524811	1.057972	0.898863
H	-2.551928	0.071059	0.189520
O	-0.392147	2.163874	0.481673
H	-0.297603	2.853462	-0.179863
H	-1.325978	1.868244	0.413089
C	2.625900	0.493474	0.617378
H	2.160285	1.450262	0.853461
H	2.823055	-0.016413	1.562611
H	3.578737	0.672871	0.124797
H	0.123383	-0.276730	1.290134

anti-cis MARCO 2b PC

C	0.427693	-0.350779	0.347284
O	0.028056	-1.477349	-0.055459
O	-1.280535	-1.843908	0.243906
C	1.775692	0.106430	0.062256
C	2.630584	-0.652511	-0.639912
H	2.350649	-1.626536	-1.013820
H	3.631163	-0.304447	-0.853028
O	-2.843672	0.154040	-0.678550
H	-3.071434	-0.036510	-1.591312
H	-2.340761	-0.632297	-0.349206
O	-1.313581	2.257375	0.235044
H	-1.850475	2.902412	0.700858
H	-1.946289	1.619709	-0.155556
C	2.113409	1.472758	0.600963
H	1.381213	2.208245	0.266994
H	2.095714	1.475829	1.692627
H	3.104612	1.780060	0.275788
H	-0.276593	0.271474	0.891040

syn-trans MACRO 2a PC

C	-0.832441	-0.422226	0.893001
O	0.332694	-0.859775	1.103325
O	1.100150	-1.336047	0.045715
O	2.912174	0.688328	0.055272
H	3.495544	0.633283	-0.705050
H	2.385710	-0.146962	0.055927
O	0.557531	2.189604	0.012448
H	0.675507	3.076533	0.359217
H	1.450386	1.789565	0.005911
C	-1.588860	-0.313537	-0.332437
C	-2.876769	0.030364	-0.143797
H	-3.281746	0.210670	0.842427
H	-3.554107	0.139467	-0.978764
C	-1.001474	-0.529798	-1.698617
H	-0.177085	0.161349	-1.860107
H	-0.602136	-1.534646	-1.803204
H	-1.766041	-0.355161	-2.454496
H	-1.298982	-0.110969	1.820865

syn-trans MACRO 2b PC

C	-0.768833	-0.334984	0.841610
O	0.374867	-0.810244	1.080337
O	1.116332	-1.394197	0.052105
O	2.745315	0.732012	-0.342085
H	3.547123	0.669848	0.182329
H	2.272123	-0.126213	-0.215174

O	0.565739	2.254791	0.517923
H	0.506785	3.069828	0.014594
H	1.403167	1.834228	0.235062
C	-1.538382	-0.315866	-0.381472
C	-2.783301	0.172880	-0.228463
H	-3.144562	0.525322	0.727585
H	-3.466796	0.233387	-1.063487
C	-1.014526	-0.787879	-1.709705
H	-0.128606	-0.224565	-1.994175
H	-0.715275	-1.831733	-1.665873
H	-1.783022	-0.657969	-2.470710
H	-1.203702	0.095218	1.735960

syn-cis MARCO 2a PC

C	1.024142	-0.519105	-0.021850
O	0.328966	-1.309383	-0.729890
O	-0.927244	-1.708414	-0.295879
C	0.770714	0.052672	1.273057
C	-0.265236	-0.318956	2.049745
H	-0.975562	-1.053214	1.713277
H	-0.378209	0.123150	3.031467
O	-2.130546	0.368759	-1.657963
H	-2.977030	0.600463	-1.268859
H	-1.843452	-0.457838	-1.208459
O	0.125656	1.992019	-1.267826
H	0.332014	2.421434	-2.101382
H	-0.711591	1.511316	-1.428106
C	1.773590	1.101194	1.694341
H	2.793871	0.714086	1.669981
H	1.722200	1.956877	1.020422
H	1.566889	1.443816	2.705596
H	1.950309	-0.278730	-0.530787

syn-cis MARCO 2b PC

C	-0.576815	0.128811	0.979777
O	0.300346	-0.752321	1.229952
O	0.484195	-1.816037	0.357593
O	2.562224	-0.560923	-0.927964
H	3.402331	-0.813323	-0.537112
H	1.889322	-1.143918	-0.508622
O	1.423444	1.906422	-0.201317
H	1.618079	2.566266	-0.870655
H	1.904034	1.102355	-0.484475
C	-1.530116	0.227062	-0.091284
C	-1.710712	-0.741588	-1.010103
H	-1.120600	-1.640469	-0.992442
H	-2.465094	-0.613042	-1.775916
C	-2.323127	1.513990	-0.096190
H	-2.874979	1.648676	0.835821
H	-1.657957	2.370219	-0.213792
H	-3.038654	1.519458	-0.915102
H	-0.551596	0.904449	1.736472

anti-trans MACRO 1a TS

C	1.679190	-0.146783	-0.011276
O	1.426474	1.046658	0.413400
O	2.673219	1.787142	0.349785
C	0.546290	-0.991791	-0.379915
C	0.734966	-2.314568	-0.344851
H	1.685589	-2.742802	-0.056903
H	-0.055990	-3.004519	-0.603637
O	2.561606	0.533693	-1.672716
H	3.341615	0.004685	-1.867169
H	2.840019	1.293118	-0.859984
C	-0.735517	-0.321325	-0.779222
H	-1.116869	0.303775	0.028428
H	-0.565929	0.332194	-1.635526
H	-1.491600	-1.058555	-1.039816
H	2.612490	-0.599679	0.299677

anti-trans MACRO 1b TS

C	1.656063	-0.118930	-0.038790
O	1.406341	1.086915	0.360766
O	2.643431	1.833548	0.245824
C	0.512725	-0.980185	-0.329284
C	0.743916	-2.295105	-0.397599
H	1.735237	-2.701031	-0.250983
H	-0.049895	-2.997034	-0.612016
O	2.658556	0.430597	-1.681808
H	2.039084	0.779271	-2.332227

H	2.850678	1.268227	-0.909523
C	-0.833908	-0.344691	-0.532771
H	-1.135679	0.221017	0.348917
H	-0.812239	0.360121	-1.365189
H	-1.587679	-1.101423	-0.738109
H	2.602787	-0.559764	0.242732

anti-cis MARCO 1a TS

C	1.686019	-0.140412	0.083961
O	1.442534	1.066735	0.471997
O	2.661431	1.828764	0.271268
C	0.560920	-1.039561	-0.175759
C	-0.666391	-0.536496	-0.332014
H	-0.845289	0.527713	-0.293915
H	-1.514980	-1.183566	-0.504947
O	2.476455	0.452661	-1.669996
H	3.277204	-0.043226	-1.869409
H	2.764082	1.264772	-0.921550
C	0.892365	-2.504490	-0.259773
H	1.604757	-2.694268	-1.065332
H	1.344629	-2.864619	0.666366
H	-0.000657	-3.094169	-0.453758
H	2.654115	-0.550335	0.344886

anti-cis MARCO 1b TS

C	0.077495	0.015569	0.602572
O	-0.422622	-0.979209	-0.051450
O	-1.864306	-0.798806	-0.043364
C	1.506284	0.317428	0.463152
C	2.228332	-0.283842	-0.486702
H	1.780250	-0.985640	-1.174911
H	3.287212	-0.090040	-0.586165
O	-1.021701	1.434977	-0.285281
H	-0.686054	1.537124	-1.183111
H	-1.671136	0.517343	-0.283768
C	2.056707	1.317223	1.442545
H	1.511791	2.260282	1.374932
H	1.955920	0.958935	2.468996
H	3.109598	1.511453	1.251217
H	-0.450723	0.336083	1.491678

syn-trans MACRO 1a TS

C	1.947650	-0.089673	-0.321111
O	1.326828	0.873111	0.286669
O	2.150327	2.067988	0.187154
C	3.313379	-0.554951	-0.022629
C	3.609499	-1.784878	-0.462572
H	2.905629	-2.369353	-1.039922
H	4.566807	-2.240718	-0.252174
O	2.237026	0.985149	-1.956967
H	3.127413	0.818168	-2.282205
H	2.305410	1.740511	-1.153590
C	4.259813	0.259740	0.814830
H	4.635603	1.124354	0.271412
H	3.754873	0.654099	1.694474
H	5.099803	-0.359980	1.125696
H	1.258186	-0.846328	-0.682820

syn-trans MACRO 1b TS

C	1.939370	-0.063795	-0.388820
O	1.267185	0.863533	0.225781
O	2.033867	2.097689	0.163967
C	3.316282	-0.486290	-0.099986
C	3.600151	-1.748676	-0.443862
H	2.879909	-2.381322	-0.944636
H	4.567109	-2.182904	-0.232440
O	2.350083	1.069959	-1.981839
H	1.531792	1.161539	-2.483361
H	2.286255	1.803988	-1.141763
C	4.297749	0.405689	0.604146
H	4.610915	1.224171	-0.041435
H	3.851075	0.860485	1.485583
H	5.174348	-0.171223	0.895492
H	1.283883	-0.845433	-0.763508

syn-cis MARCO 1a TS

C	1.960263	-0.053768	-0.160272
O	1.552959	0.975883	0.507158
O	2.435629	2.098787	0.212901
C	3.311481	-0.647962	-0.163912
C	4.306761	-0.135772	0.563655

H	4.187082	0.797872	1.090970
H	5.253609	-0.654516	0.633348
O	2.017957	0.951987	-1.870094
H	2.826204	0.739683	-2.348175
H	2.297886	1.715172	-1.113764
C	3.426579	-1.930376	-0.948494
H	2.724164	-2.683654	-0.584775
H	3.200747	-1.774101	-2.005519
H	4.431313	-2.339635	-0.873476
H	1.143782	-0.752260	-0.333166

syn-cis MARCO 1b TS

C	0.034599	0.309289	0.817918
O	0.672178	-0.815249	0.768819
O	0.827765	-1.196215	-0.632224
O	1.167065	1.198552	-0.571689
H	2.038364	1.349741	-0.186903
H	1.150372	0.131800	-0.876196
C	-1.253589	0.638803	0.185324
C	-1.985466	-0.308812	-0.403190
H	-1.601614	-1.307332	-0.543331
H	-2.982523	-0.086522	-0.758606
C	-1.704633	2.062577	0.363012
H	-1.689625	2.361484	1.413955
H	-1.041473	2.738261	-0.177983
H	-2.716810	2.195397	-0.012201
H	0.256339	0.850417	1.737287

anti-trans MACRO 2a TS

C	0.560344	-0.319354	0.217092
O	-0.258641	-1.145358	-0.342750
O	-1.440502	-1.369893	0.471531
C	1.890293	-0.219442	-0.416519
C	2.905910	0.202140	0.337760
H	2.764191	0.485711	1.371447
H	3.908283	0.276073	-0.060567
O	-2.485926	0.724237	-0.151415
H	-3.064324	1.066692	0.534446
H	-2.115061	-0.318399	0.155243
O	-0.164526	1.429397	-0.026759
H	0.123727	1.759289	-0.884746
H	-1.263741	1.226236	-0.089162
C	2.020441	-0.633538	-1.855750
H	1.733622	-1.677178	-1.985601
H	1.361322	-0.048924	-2.500254
H	3.044194	-0.504173	-2.199512
H	0.469700	-0.196433	1.287490

anti-trans MACRO 2b TS

C	0.568046	-0.278979	0.152398
O	-0.237259	-1.092745	-0.438724
O	-1.378312	-1.422352	0.403200
C	1.879895	-0.074000	-0.487369
C	2.919862	0.169326	0.311469
H	2.810034	0.229483	1.385966
H	3.915053	0.305960	-0.088037
O	-2.528610	0.684225	0.097101
H	-3.062303	0.714311	-0.700649
H	-2.100614	-0.368284	0.225866
O	-0.232619	1.435071	-0.151527
H	0.008266	2.042430	0.556447
H	-1.323423	1.205361	-0.067269
C	1.956586	-0.177879	-1.981785
H	1.620692	-1.158369	-2.320069
H	1.305464	0.563854	-2.445411
H	2.975591	-0.017529	-2.326829
H	0.487397	-0.230295	1.231143

anti-trans MACRO 2c TS

C	0.533897	0.141753	0.682699
H	0.130695	0.560633	1.596299
O	0.074469	-1.011780	0.337780
O	-1.216011	-1.277270	0.953863
C	1.931911	0.424719	0.309915
C	2.641785	1.197827	1.132831
H	2.212137	1.615192	2.033685
H	3.678939	1.427666	0.932470
O	-2.423546	0.050336	-0.671552
H	-3.243592	0.410358	-0.325899
H	-1.965688	-0.658234	0.107029

O	-0.383486	1.353452	-0.473921
H	-0.487869	2.204464	-0.035527
H	-1.388280	0.873791	-0.599561
C	2.459233	-0.193118	-0.951035
H	2.390585	-1.280318	-0.908035
H	1.867121	0.132695	-1.806724
H	3.497747	0.087549	-1.111878

anti-trans MACRO 2d TS

C	-0.141705	0.957174	0.500102
O	0.268275	-0.033834	1.220059
O	0.112001	-1.304263	0.529655
O	1.925738	-0.987636	-1.039773
H	2.778755	-1.257567	-0.691838
H	1.108411	-1.254140	-0.282807
O	1.224086	1.322767	-0.774586
H	1.882097	1.884159	-0.351280
H	1.670444	0.311301	-0.941540
C	-0.279746	2.244035	1.211663
C	-1.120681	3.145573	0.703919
H	-1.666714	2.958870	-0.210361
H	-1.284356	4.097206	1.190261
C	0.503156	2.439438	2.480106
H	0.238981	1.682647	3.218853
H	1.576688	2.342381	2.306463
H	0.310327	3.423969	2.900207
H	-0.822762	0.720139	-0.305764

anti-cis MARCO 2a TS

C	0.511227	-0.382689	0.085060
O	-0.319851	-1.053543	-0.633668
O	-1.536726	-1.373725	0.099324
C	1.894722	-0.225049	-0.425686
C	2.230877	-0.714496	-1.619336
H	1.513497	-1.225667	-2.244148
H	3.243083	-0.624162	-1.988191
O	-2.437366	0.883878	0.050499
H	-2.943883	1.088351	0.840214
H	-2.140912	-0.205474	0.075906
O	-0.063214	1.435000	0.076130
H	0.150728	1.760706	-0.806411
H	-1.160929	1.302523	0.101090
C	2.855256	0.465287	0.503480
H	2.508418	1.467799	0.754307
H	2.949877	-0.085080	1.442250
H	3.842601	0.537871	0.052893
H	0.352752	-0.425850	1.155753

anti-cis MARCO 2b TS

C	0.556456	0.019586	0.556120
O	0.073473	-0.946111	-0.141742
O	-1.140900	-1.484629	0.457759
C	1.918548	0.490343	0.222160
C	2.663988	-0.194594	-0.644477
H	2.287986	-1.075943	-1.141673
H	3.676612	0.113136	-0.864983
O	-2.528119	0.297617	-0.409430
H	-2.760506	0.180474	-1.333777
H	-1.983564	-0.629326	-0.038908
O	-0.490083	1.550352	0.039520
H	-0.675979	2.104296	0.806227
H	-1.458286	1.062760	-0.231812
C	2.399587	1.711155	0.955848
H	1.853981	2.598120	0.632556
H	2.256400	1.609201	2.034080
H	3.458623	1.876701	0.771478
H	0.215625	0.070571	1.583876

anti-cis MARCO 2c TS

C	0.562184	0.016421	0.578094
H	0.233194	0.073263	1.609383
O	0.072657	-0.954444	-0.108585
O	-1.153421	-1.464273	0.487473
C	1.921176	0.483061	0.227072
C	2.644641	-0.188040	-0.668452
H	2.253214	-1.056518	-1.176279
H	3.653583	0.119968	-0.904843
O	-2.437036	0.261137	-0.617858
H	-3.281881	0.456500	-0.206193
H	-1.959483	-0.644476	-0.103567

O	-0.487436	1.546112	0.072327
H	-0.691754	2.066103	0.857382
H	-1.445514	1.060777	-0.253867
C	2.421779	1.689227	0.971916
H	1.866815	2.581759	0.681284
H	2.308784	1.565564	2.051538
H	3.475188	1.859708	0.761608

anti-cis MARCO 2d TS

C	0.497466	0.041652	0.540903
O	0.097576	-0.987400	-0.122569
O	-1.158060	-1.515588	0.394754
C	1.893355	0.498251	0.333027
C	2.680733	-0.125576	-0.543548
H	2.327522	-0.964041	-1.125371
H	3.707044	0.184524	-0.682334
O	-2.574133	0.361277	-0.206021
H	-3.018385	0.253265	-1.050179
H	-2.004388	-0.583890	0.038443
O	-0.449678	1.553398	-0.129389
H	-0.094411	1.677269	-1.017294
H	-1.459708	1.118024	-0.238744
C	2.338158	1.644642	1.199075
H	1.710019	2.521649	1.043695
H	2.264950	1.381895	2.256755
H	3.371585	1.909442	0.986765
H	0.042688	0.182958	1.514131

syn-trans MACRO 2a TS

C	-0.610062	-0.096480	0.633930
O	0.317217	-0.888969	1.065919
O	1.089895	-1.550843	0.028531
O	2.418159	0.439156	-0.373230
H	2.754085	0.506686	-1.269919
H	1.910566	-0.568988	-0.230127
O	0.284648	1.506825	0.136771
H	0.404868	2.007563	0.951508
H	1.287208	1.127185	-0.144544
C	-1.445134	-0.284418	-0.578565
C	-2.757713	-0.145233	-0.376838
H	-3.168711	0.108016	0.591032
H	-3.464231	-0.297839	-1.180780
C	-0.859165	-0.612833	-1.920976
H	-0.118877	0.133469	-2.208447
H	-0.353501	-1.574292	-1.896261
H	-1.646058	-0.624220	-2.673585
H	-1.141188	0.322794	1.482065

syn-trans MACRO 2b TS

C	-0.600317	-0.117787	0.657426
O	0.347958	-0.910746	1.035715
O	1.111939	-1.516589	-0.042414
O	2.354324	0.502598	-0.535956
H	3.135478	0.615590	0.010979
H	1.887811	-0.512923	-0.317235
O	0.304329	1.516090	0.305602
H	-0.141291	1.992885	-0.403246
H	1.286720	1.167207	-0.073219
C	-1.453071	-0.259845	-0.549546
C	-2.735650	0.072407	-0.366920
H	-3.109381	0.420772	0.586396
H	-3.453510	-0.011728	-1.170997
C	-0.925266	-0.748997	-1.869444
H	-0.064212	-0.166874	-2.195499
H	-0.581111	-1.776819	-1.787371
H	-1.706879	-0.679705	-2.625007
H	-1.108223	0.271207	1.531555

syn-trans MACRO 2c TS

C	-0.595321	-0.121018	0.628333
O	0.364493	-0.915717	0.977647
O	1.137159	-1.460505	-0.127100
O	2.462722	0.567453	-0.250004
H	2.868795	0.722322	-1.105699
H	1.970001	-0.452541	-0.243027
O	0.271390	1.506055	0.258722
H	-0.154941	1.928251	-0.494680
H	1.298748	1.198862	-0.030758
C	-1.487530	-0.273880	-0.550659
C	-2.756280	0.095055	-0.345126

H	-3.095158	0.481534	0.606505
H	-3.497598	0.005345	-1.127040
C	-1.012632	-0.824448	-1.866299
H	-0.174433	-0.250371	-2.259561
H	-0.649878	-1.842289	-1.748371
H	-1.827245	-0.801645	-2.589237
H	-1.086342	0.252229	1.519173

syn-trans MACRO 2d TS

C	-0.587413	-0.137305	0.630109
O	0.339805	-0.949886	1.025785
O	1.126428	-1.552097	-0.036736
O	2.299264	0.478345	-0.631490
H	3.139356	0.591725	-0.181267
H	1.853155	-0.546254	-0.361432
O	0.300464	1.522214	0.301020
H	0.476569	1.889130	1.174404
H	1.269611	1.165516	-0.098699
H	-1.144924	0.212822	1.492064
C	-1.381200	-0.230231	-0.619244
C	-2.697955	-0.084412	-0.448709
H	-3.136643	0.108230	0.520954
H	-3.379818	-0.168511	-1.283398
C	-0.756146	-0.474136	-1.962698
H	0.037235	0.245228	-2.161335
H	-0.303922	-1.461696	-2.003766
H	-1.512945	-0.381525	-2.740123

syn-cis MARCO 2a TS

C	0.189951	0.017247	0.340917
O	-0.350635	-0.980807	-0.284974
O	-1.723380	-1.295205	0.070872
C	-0.022093	0.435356	1.745725
C	-0.809294	-0.247380	2.579158
H	-1.411349	-1.071007	2.232862
H	-0.842700	0.024556	3.626223
O	-2.667124	0.727414	-0.887008
H	-3.352506	1.100832	-0.327448
H	-2.332883	-0.268641	-0.447393
O	-0.422858	1.594199	-0.540719
H	-0.006726	1.580535	-1.410589
H	-1.493256	1.306288	-0.710308
C	0.822991	1.603131	2.186023
H	1.881005	1.433818	1.971046
H	0.529375	2.512593	1.663149
H	0.719120	1.764868	3.256651
H	1.211777	0.133900	-0.010021

syn-cis MARCO 2b TS

C	-0.555892	0.504165	0.766567
O	0.109976	-0.537717	1.156759
O	0.378291	-1.528975	0.127145
O	2.237361	-0.230433	-0.725495
H	3.030102	-0.322911	-0.191201
H	1.456970	-0.956448	-0.353570
O	0.727579	1.578644	-0.110599
H	0.359113	1.883409	-0.947487
H	1.505525	0.817554	-0.388505
C	-1.694508	0.552277	-0.181549
C	-2.078999	-0.492406	-0.917568
H	-1.522343	-1.414594	-0.907211
H	-2.969388	-0.418075	-1.528742
C	-2.446560	1.862455	-0.163989
H	-2.854533	2.070052	0.827862
H	-1.804793	2.707875	-0.420581
H	-3.272616	1.838976	-0.870906
H	-0.641175	1.186419	1.606490

syn-cis MARCO 2c TS

C	-0.559764	0.502796	0.752164
O	0.096074	-0.550372	1.129268
O	0.375358	-1.514977	0.077274
O	2.339810	-0.215170	-0.492102
H	2.672018	-0.347483	-1.383019
H	1.512421	-0.955183	-0.285648
O	0.709382	1.564223	-0.139694
H	0.335283	1.799100	-0.996069
H	1.525388	0.821856	-0.354621
C	-1.710910	0.563412	-0.182599
C	-2.119623	-0.483563	-0.901707

H	-1.574843	-1.413094	-0.887941
H	-3.017763	-0.405276	-1.500986
C	-2.445000	1.883387	-0.164436
H	-2.838184	2.101349	0.831165
H	-1.794578	2.718663	-0.431868
H	-3.279890	1.867210	-0.861215
H	-0.634183	1.177742	1.599395

syn-cis MARCO 2d TS

C	-0.534706	0.629706	0.722739
O	0.001122	-0.390396	1.319156
O	0.280367	-1.547490	0.487252
O	1.878443	-0.476967	-0.984746
H	2.791008	-0.671201	-0.757763
H	1.179427	-1.077144	-0.297971
O	0.909506	1.571777	-0.107771
H	1.444479	1.884716	0.630461
H	1.457155	0.696288	-0.551556
H	-0.704379	1.410664	1.458809
C	-1.497279	0.630686	-0.400369
C	-1.982141	-0.497034	-0.923407
H	-1.609168	-1.461850	-0.623088
H	-2.768208	-0.446529	-1.665459
C	-1.974089	1.999284	-0.814522
H	-2.344427	2.570217	0.040575
H	-1.161790	2.573101	-1.259026
H	-2.781139	1.916143	-1.538978

anti-trans MACRO 1a Prod

C	0.505435	-0.120407	-0.073973
O	0.216270	0.910400	0.872924
O	1.423814	1.717901	0.985463
C	-0.723528	-0.997043	-0.105263
C	-0.657343	-2.222749	0.404345
H	0.253282	-2.607912	0.842826
H	-1.515505	-2.881118	0.398416
O	0.745187	0.402821	-1.354372
H	1.616138	0.811280	-1.347066
H	1.094991	2.565370	0.658283
C	-1.959247	-0.411452	-0.727003
H	-2.276933	0.484045	-0.190610
H	-1.767054	-0.115071	-1.758504
H	-2.775375	-1.131261	-0.714190
H	1.378394	-0.667844	0.286804

anti-trans MACRO 1b Prod

C	0.498458	-0.102610	-0.083617
O	0.197472	0.994041	0.766707
O	1.415705	1.750693	0.960385
C	-0.712763	-1.007456	-0.048420
C	-0.570397	-2.266032	0.353900
H	0.387541	-2.655812	0.669861
H	-1.409885	-2.947750	0.379486
O	0.837668	0.355545	-1.378428
H	0.038900	0.660614	-1.822046
H	1.529054	2.163627	0.090992
C	-2.029505	-0.423585	-0.485111
H	-2.303957	0.429893	0.135819
H	-1.998412	-0.072164	-1.520727
H	-2.819988	-1.168477	-0.421654
H	1.388840	-0.606407	0.285020

anti-cis MARCO 1a Prod

C	0.425056	-0.038116	0.080984
O	0.010803	1.263403	0.467120
O	1.224308	2.042248	0.641113
C	-0.793163	-0.933290	0.015290
C	-2.051039	-0.452663	0.098698
H	-2.257027	0.599757	0.222759
H	-2.900384	-1.121312	0.047194
O	1.056746	-0.038829	-1.178291
H	1.948518	0.302605	-1.061284
H	1.120909	2.684869	-0.073220
C	-0.469127	-2.392238	-0.159098
H	0.098305	-2.556699	-1.076056
H	0.143134	-2.761371	0.667886
H	-1.378824	-2.987853	-0.201033
H	1.124366	-0.400185	0.842270

anti-cis MARCO 1b Prod

C	-0.323960	0.113433	0.260658

O	-0.734732	-1.036564	-0.448196
O	-2.146685	-1.216961	-0.197806
C	1.186335	0.204614	0.217789
C	1.917579	-0.526512	-0.618849
H	1.472079	-1.249458	-1.285432
H	2.994307	-0.424394	-0.643152
O	-0.938643	1.276755	-0.274029
H	-0.493270	1.490501	-1.102488
H	-2.529376	-0.487224	-0.708406
C	1.772721	1.201268	1.180261
H	1.342366	2.193429	1.035399
H	1.560650	0.912686	2.212760
H	2.852130	1.269354	1.060775
H	-0.694506	0.046678	1.283911

syn-trans MACRO 1a Prod

C	-0.488492	-0.247434	-0.613127
O	-1.451822	0.332633	0.278219
O	-0.866025	1.511989	0.894924
C	0.676739	-0.898863	0.107713
C	0.697181	-2.225448	0.203920
H	-0.092097	-2.838469	-0.210455
H	1.503237	-2.743243	0.706157
O	-0.109718	0.647941	-1.617998
H	0.534493	1.264489	-1.256232
H	-1.386427	2.202998	0.464703
C	1.770349	-0.032754	0.672871
H	2.235157	0.586888	-0.099124
H	1.387064	0.639066	1.439942
H	2.555673	-0.648783	1.106685
H	-1.095958	-1.014916	-1.091559

syn-trans MACRO 1b Prod

C	-0.484555	-0.274213	-0.630861
O	-1.538903	0.191213	0.211247
O	-1.033127	1.192181	1.129714
C	0.710068	-0.852177	0.098148
C	0.719993	-2.159561	0.342681
H	-0.093346	-2.804263	0.036593
H	1.540490	-2.626774	0.869923
O	-0.052928	0.741850	-1.505794
H	-0.768516	0.939618	-2.117989
H	-1.076311	1.991178	0.586105
C	1.832401	0.064916	0.494343
H	2.209725	0.610836	-0.370428
H	1.490966	0.803460	1.219137
H	2.650522	-0.504142	0.932439
H	-1.009840	-1.067092	-1.170174

syn-cis MARCO 1a Prod

C	-0.700556	-0.186870	-0.108933
O	-0.978692	0.863368	0.811702
O	-0.104829	1.985421	0.504563
C	0.627929	-0.886316	0.116515
C	1.452468	-0.539750	1.099289
H	1.229851	0.277747	1.767268
H	2.379444	-1.075060	1.256553
O	-0.880870	0.223215	-1.439322
H	-0.105358	0.735094	-1.694765
H	-0.755868	2.610417	0.159074
C	0.898125	-2.038770	-0.814833
H	0.085425	-2.769231	-0.778614
H	0.971026	-1.710610	-1.852439
H	1.822969	-2.545141	-0.545792
H	-1.520934	-0.877319	0.106280

syn-cis MARCO 1b Prod

C	0.420151	0.188748	0.584025
O	0.926507	-1.132022	0.512554
O	0.977550	-1.561377	-0.871742
O	1.273448	1.086879	-0.100698
H	2.092267	1.166856	0.398815
H	1.673857	-0.988358	-1.225770
C	-1.003371	0.386379	0.106243
C	-1.810037	-0.648234	-0.098622
H	-1.464946	-1.666066	-0.003526
H	-2.842852	-0.494310	-0.380424
C	-1.447744	1.818042	-0.019392
H	-1.260939	2.374315	0.903148
H	-0.898654	2.331112	-0.808977

H	-2.512095	1.871399	-0.239939
H	0.468572	0.367830	1.665463

anti-trans MACRO 2a Prod

C	0.350779	0.084738	0.402446
O	-0.390332	-1.036610	-0.019863
O	-1.513221	-1.218132	0.875689
C	1.734445	-0.056218	-0.191175
C	2.793280	-0.010215	0.610426
H	2.691425	0.113905	1.679818
H	3.798408	-0.097462	0.220306
O	-3.094736	0.941425	-0.025590
H	-3.689334	1.337794	0.616491
H	-2.197396	-0.644681	0.472407
O	-0.284443	1.309246	0.014721
H	-0.156732	1.430633	-0.932827
H	-2.227414	1.358816	0.107429
C	1.832399	-0.243875	-1.681482
H	1.301553	-1.143211	-1.995135
H	1.394417	0.593686	-2.232774
H	2.872281	-0.325398	-1.990837
H	0.375944	0.111702	1.488089

anti-trans MACRO 2b Prod

C	0.486310	0.083358	0.641170
O	-0.348121	-0.993255	0.264262
O	-1.449737	-1.042025	1.208443
C	1.690747	0.027491	-0.267187
C	2.883586	-0.238936	0.254527
H	3.013861	-0.421871	1.312545
H	3.770154	-0.284393	-0.363397
O	-2.847540	0.722873	-0.475583
H	-3.106586	0.458065	-1.362109
H	-2.147307	-0.598857	0.682732
O	-0.181728	1.332059	0.469907
H	-0.631277	1.541324	1.294332
H	-1.946314	1.073925	-0.548797
C	1.455742	0.286731	-1.728417
H	0.765877	-0.447872	-2.146825
H	1.013667	1.272616	-1.879809
H	2.390033	0.238509	-2.284193
H	0.766574	-0.035441	1.687987

anti-trans MACRO 2c Prod

C	0.225666	0.313255	0.538527
H	0.077365	0.603212	1.579600
O	-0.210027	-0.995678	0.347180
O	-1.471025	-1.171069	1.040432
C	1.684327	0.367026	0.145718
C	2.568217	0.842409	1.018831
H	2.273580	1.161284	2.010019
H	3.618394	0.920817	0.771850
O	-2.858412	-0.265441	-1.213449
H	-3.701124	0.189756	-1.141945
H	-2.105086	-1.030659	0.305467
O	-0.567175	1.176597	-0.307647
H	-0.517084	2.073157	0.036824
H	-2.172168	0.415778	-1.122121
C	2.037274	-0.104345	-1.235974
H	1.797214	-1.161887	-1.353767
H	1.464095	0.438347	-1.988569
H	3.097986	0.036075	-1.434618

anti-trans MACRO 2d Prod

C	-0.407230	0.256894	-0.214472
O	-0.232902	-0.856733	0.630816
O	-0.514933	-2.062374	-0.119465
O	1.822847	-2.121066	-1.642234
H	2.710401	-2.244621	-1.296391
H	0.353059	-2.260798	-0.530860
O	0.747053	0.471871	-1.041039
H	1.401194	0.958813	-0.528935
H	1.657116	-1.163500	-1.638030
C	-0.700951	1.446765	0.670453
C	-1.772304	2.193168	0.423416
H	-2.449126	1.964389	-0.388257
H	-2.007342	3.057699	1.029621
C	0.254327	1.720243	1.801712
H	0.293832	0.873221	2.487214
H	1.276587	1.890901	1.450244

H	-0.049519	2.605958	2.355661
H	-1.219137	0.053200	-0.906154

anti-cis MARCO 2a Prod

C	0.299750	-0.127053	0.310778
O	-0.520915	-0.931235	-0.490350
O	-1.675964	-1.330290	0.284678
C	1.713626	-0.138824	-0.233385
C	2.020401	-0.718130	-1.390525
H	1.280129	-1.231236	-1.985124
H	3.036196	-0.700980	-1.762273
O	-3.024083	1.144015	0.229384
H	-3.589378	1.353064	0.977437
H	-2.297461	-0.588875	0.128186
O	-0.195966	1.221364	0.385425
H	-0.011999	1.639276	-0.464962
H	-2.123948	1.411325	0.480524
C	2.725676	0.553028	0.640000
H	2.452351	1.592582	0.825454
H	2.790671	0.066113	1.616378
H	3.712597	0.529240	0.182396
H	0.260989	-0.490235	1.336957

anti-cis MARCO 2b Prod

C	0.285730	-0.032083	0.591393
O	-0.211438	-1.136009	-0.123849
O	-1.404873	-1.589854	0.562201
C	1.622446	0.372083	0.010244
C	2.208172	-0.319672	-0.961880
H	1.751064	-1.194689	-1.397337
H	3.175634	-0.020192	-1.341889
O	-2.831800	0.161572	-1.102402
H	-2.861540	0.002319	-2.049562
H	-2.090010	-1.197175	-0.018252
O	-0.607382	1.079001	0.513677
H	-1.259875	0.979645	1.214427
H	-2.031068	0.684937	-0.942509
C	2.238414	1.587591	0.646450
H	1.615506	2.468691	0.491670
H	2.340891	1.457084	1.726983
H	3.226266	1.778909	0.232221
H	0.393464	-0.317621	1.642312

anti-cis MARCO 2c Prod

C	0.280516	-0.021255	0.618320
H	0.395729	-0.289883	1.673218
O	-0.223452	-1.136037	-0.074932
O	-1.426233	-1.559851	0.615245
C	1.612166	0.373390	0.021398
C	2.159977	-0.295670	-0.987665
H	1.674276	-1.145429	-1.441833
H	3.123162	-0.001199	-1.382197
O	-2.714261	0.073137	-1.277172
H	-3.504493	0.616019	-1.330371
H	-2.100934	-1.223449	-0.007718
O	-0.611029	1.090440	0.530874
H	-1.286091	0.965434	1.205679
H	-1.989108	0.664693	-1.026028
C	2.263792	1.557442	0.681060
H	1.648395	2.451328	0.576119
H	2.397853	1.387176	1.752596
H	3.240820	1.751922	0.243275

anti-cis MARCO 2d Prod

C	0.215006	0.056608	0.368912
O	-0.151569	-1.102874	-0.326989
O	-1.307141	-1.688141	0.319148
C	1.689754	0.337525	0.166049
C	2.434331	-0.375472	-0.674302
H	2.027510	-1.205714	-1.231074
H	3.483307	-0.148013	-0.809317
O	-3.199906	0.162212	-0.558448
H	-3.479891	0.288193	-1.468613
H	-2.049671	-1.210041	-0.108073
O	-0.569580	1.189307	-0.050726
H	-0.215613	1.478915	-0.900080
H	-2.450554	0.764525	-0.415518
C	2.231785	1.473799	0.991589
H	1.695267	2.403921	0.799809
H	2.120659	1.262590	2.058130

H	3.288204	1.632795	0.784967
H	-0.028667	-0.072803	1.422195

syn-trans MACRO 2a Prod

C	-0.562384	0.386594	0.713901
O	0.211758	-0.623511	1.331317
O	0.944470	-1.385349	0.338466
O	2.900833	0.573983	-0.319741
H	3.337696	0.530034	-1.174178
H	1.774782	-0.875074	0.264102
O	0.253396	1.470727	0.271123
H	0.608016	1.903439	1.055251
H	2.064737	1.045221	-0.459921
C	-1.446434	-0.070364	-0.427630
C	-2.684238	-0.461021	-0.138898
H	-3.062589	-0.457328	0.874747
H	-3.356577	-0.813104	-0.909212
C	-0.900949	-0.049874	-1.827559
H	-0.557557	0.949739	-2.096655
H	-0.052636	-0.727317	-1.920598
H	-1.668709	-0.351945	-2.537642
H	-1.179674	0.712256	1.553892

syn-trans MACRO 2b Prod

C	-0.455501	0.372724	0.547074
O	0.388270	-0.670730	1.017425
O	1.117368	-1.246684	-0.097538
O	3.087107	0.713227	0.285340
H	3.575896	0.748079	1.111855
H	1.972226	-0.778656	0.001608
O	0.300393	1.414054	-0.045296
H	0.394871	1.230086	-0.985818
H	2.278231	1.229633	0.427763
C	-1.609421	-0.094930	-0.317515
C	-2.828176	-0.107264	0.215737
H	-3.006587	0.201916	1.236930
H	-3.688578	-0.436446	-0.351059
C	-1.346535	-0.523963	-1.736434
H	-0.876031	0.268946	-2.326145
H	-0.679228	-1.383444	-1.768782
H	-2.280992	-0.777284	-2.233531
H	-0.841306	0.769850	1.485243

syn-trans MACRO 2c Prod

C	-0.484850	0.381317	0.487358
O	0.374887	-0.658392	0.937232
O	1.131941	-1.180381	-0.186302
O	3.041846	0.771463	0.495669
H	3.708845	1.270252	0.017813
H	1.988561	-0.736553	-0.027479
O	0.251505	1.437668	-0.102982
H	0.388099	1.224073	-1.031977
H	2.234156	1.307524	0.482938
C	-1.639510	-0.092917	-0.372238
C	-2.859599	-0.092018	0.158092
H	-3.038685	0.232186	1.174497
H	-3.720459	-0.424424	-0.406193
C	-1.374635	-0.545646	-1.783346
H	-0.895245	0.234627	-2.382390
H	-0.713840	-1.410759	-1.800369
H	-2.308948	-0.800283	-2.280090
H	-0.866896	0.765580	1.432066

syn-trans MACRO 2d Prod

C	-0.556841	0.348532	0.762471
O	0.237670	-0.684686	1.309307
O	0.926336	-1.415043	0.263387
O	2.822511	0.510625	-0.493074
H	3.559429	0.908014	-0.022467
H	1.747067	-0.894281	0.152735
O	0.239079	1.484623	0.407286
H	0.512728	1.908091	1.226944
H	2.056094	1.087172	-0.345423
H	-1.185642	0.604063	1.617538
C	-1.421537	-0.042830	-0.417521
C	-2.643398	-0.503332	-0.166383
H	-3.020954	-0.601840	0.842833
H	-3.301762	-0.813618	-0.966106
C	-0.876153	0.121505	-1.807695
H	-0.581945	1.155397	-1.991233

H	0.005778	-0.500708	-1.955516
H	-1.627919	-0.158251	-2.543513

syn-cis MARCO 2a Prod

C	0.878559	-0.108547	-0.224769
O	0.279758	-1.294143	-0.691552
O	-1.123903	-1.342969	-0.326764
C	0.823432	0.148650	1.266362
C	0.477198	-0.808437	2.119287
H	0.144361	-1.777981	1.783786
H	0.510682	-0.632077	3.185979
O	-2.247408	0.720732	-1.938514
H	-3.087909	1.056089	-1.615678
H	-1.546391	-0.849010	-1.056167
O	0.386170	1.039523	-0.916902
H	0.680034	0.974487	-1.832072
H	-1.557386	1.165855	-1.423131
C	1.291959	1.510130	1.704283
H	2.279612	1.740747	1.296230
H	0.620101	2.292631	1.351091
H	1.350506	1.563572	2.789660
H	1.921670	-0.278227	-0.519016

syn-cis MARCO 2b Prod

C	-0.192306	0.399880	0.572630
O	0.336365	-0.873833	0.884654
O	0.647680	-1.574414	-0.349492
O	3.179085	-0.364297	-0.299259
H	3.776619	-0.509038	0.439122
H	1.614249	-1.419609	-0.385543
O	0.720992	1.164597	-0.202282
H	0.603447	0.903826	-1.123700
H	2.607902	0.376923	-0.043493
C	-1.585735	0.402269	-0.025279
C	-2.250505	-0.723464	-0.262017
H	-1.813599	-1.691402	-0.072764
H	-3.257357	-0.696126	-0.657042
C	-2.173239	1.770254	-0.256693
H	-2.171511	2.358027	0.665260
H	-1.598566	2.340975	-0.987625
H	-3.199871	1.694890	-0.609314
H	-0.213892	0.877721	1.555868

syn-cis MARCO 2c Prod

C	-0.197442	0.395569	0.553564
O	0.324114	-0.882380	0.857270
O	0.647652	-1.569180	-0.382048
O	3.193142	-0.399433	-0.090216
H	3.888656	-0.142312	-0.700344
H	1.618958	-1.456617	-0.378382
O	0.717613	1.159616	-0.221082
H	0.611332	0.875588	-1.136875
H	2.618383	0.374391	0.014488
C	-1.590654	0.406484	-0.045293
C	-2.255818	-0.716274	-0.295173
H	-1.820296	-1.686305	-0.113107
H	-3.261827	-0.684432	-0.692073
C	-2.176156	1.777396	-0.263157
H	-2.178188	2.353709	0.666011
H	-1.596909	2.356093	-0.984099
H	-3.201278	1.707526	-0.621342
H	-0.215058	0.869007	1.538715

syn-cis MARCO 2d Prod

C	-0.245495	0.503085	0.741363
O	0.156954	-0.720981	1.305876
O	0.472291	-1.693053	0.276138
O	2.780286	-0.677034	-0.967735
H	3.678248	-0.453876	-0.710542
H	1.401079	-1.482141	0.057877
O	0.855565	1.192998	0.138831
H	1.427196	1.491996	0.853211
H	2.256276	0.133485	-0.876450
H	-0.549668	1.053605	1.639803
C	-1.406415	0.466759	-0.230268
C	-2.209389	-0.588355	-0.302667
H	-2.019533	-1.489655	0.258480
H	-3.077652	-0.574162	-0.947494
C	-1.643775	1.734088	-1.006214
H	-1.702636	2.602077	-0.344265

H	-0.828614	1.929160	-1.703229		H	-2.574047	1.668872	-1.567111

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