Supplementary Information: QM/MM Studies on Ozonolysis of α-Humulene and Criegee Reactions with Acids and Waters at Air-Water/Acetonitrile Interfaces

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I、Conformers of α-Humulene

Ground-state geometry optimizations of α-humulene conformers were done with the B3LYP functional and the 6-31G** basis set using Gaussian 09 program package. Considering the ε value of water-acetonitrile mixed solution (45.7) is very close to that of dimethyl sulfoxide (DMSO, 47.2), the keyword dimethylsulfoxide is used here in polarizable continuum model (PCM) of solvation calculations.

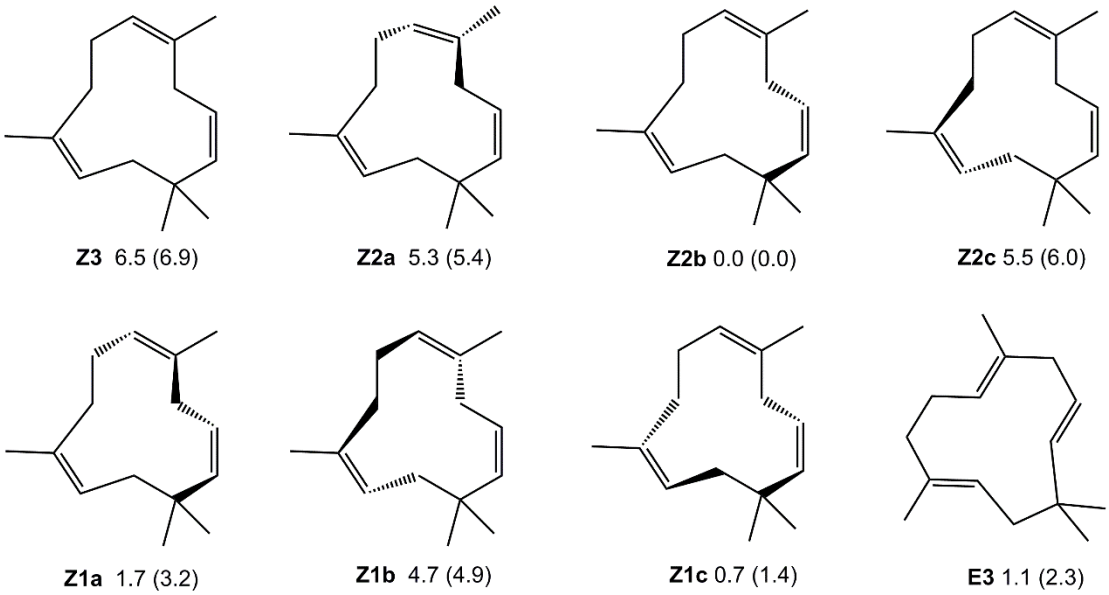

Figure S1: Possible ground-state conformers of α-humulene, along with free energy values (in kcal/mol) relative to the most stable Z2b conformer, at the B3LYP/6-31g** (B3LYP/6-31G**/PCM) calculation level.

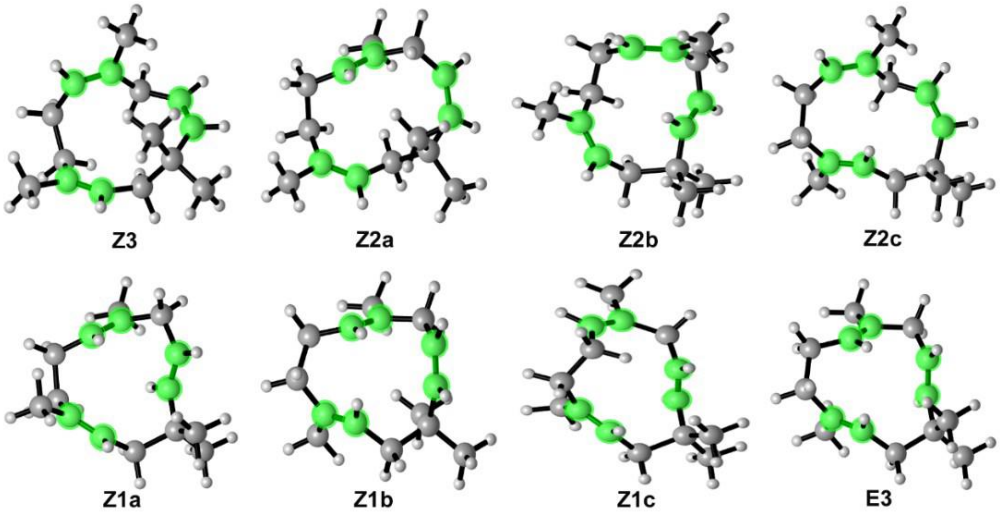

Figure S2: Optimized structures of α-humulene conformers at the B3LYP/6-31g** level. The double bond sites are colored in green.

II、QM/MM System Used in Stage II

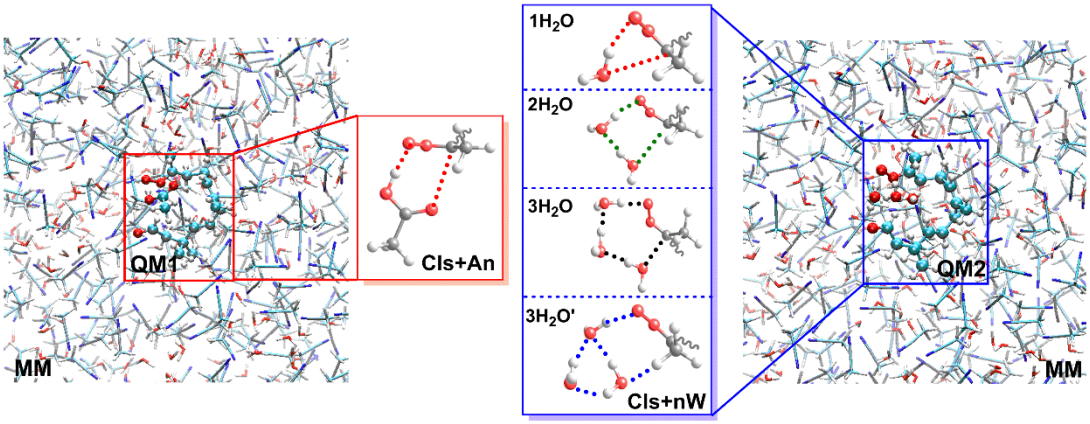

Figure S3: QM/MM system used to simulate Criegee reactions with acids and waters at the air-water/acetonitrile interface in stage II.

III、Tables

Table S1: QM(CASPT2(10,8)/6-31G*)/MM Calculated Key Electronic Configurations and Corresponding Weights of Initial Ozone-Substrate Structures **1a**, **1b**, **1c**, **1a'**, and **1b'** (u: spin up, d: spin down). See Active Spaces in Figs. S33-S37.

1a	22222000	0.56	2u222d00	0.12	20222200	0.08	22202002	0.02
1b	22222000	0.57	u2222d00	0.15	02222200	0.09	22202020	0.02
1c	22222000	0.57	u2222d00	0.12	02222200	0.08	22220020	0.01
1a'	22222000	0.55	2u222d00	0.12	20222200	0.08	22202002	0.01
1b'	22222000	0.71	02222200	0.14	22220002	0.09	22202020	0.01

Table S2: QM(CASPT2(10,8)/6-31G*)/MM Calculated Key Electronic Configurations and Corresponding Weights of Criegee Intermediates **3a1**, **3a2**, **3b1**, **3b2**, **3c1**, and **3c2** (u: Spin Up; d: Spin Down). See Active Spaces in Figs. S38-S43.

3a1	22222000	0.72	22u22d00	0.12	22022200	0.08	22220002	0.02
3a2	22222000	0.67	2222ud00	0.15	22220200	0.09	22ud20ud	0.02
3b1	22222000	0.71	222u2d00	0.12	22202200	0.08	22022020	0.01
3b2	22222000	0.71	22u22d00	0.12	22022200	0.08	222200ud	0.01
3c1	22222000	0.69	22u22d00	0.14	22022200	0.09	22220020	0.01
3c2	22222000	0.68	22u22d00	0.14	22022200	0.09	222ud0ud	0.03

Table S3: Energy Differences ($\Delta E = E_{UB3LYP} - E_{RB3LYP}$, in kcal/mol) of Initial Ozone-Substrate Complexes **1a**, **1b**, **1c**, **1a'**, and **1b'** and Criegee Intermediates **3a1**, **3a2**, **3b1**, **3b2**, **3c1**, and **3c2** at QM(UB3LYP/6-31G**, Guess = Mix)/MM and QM(B3LYP/6-31G**)/MM Calculation Levels.[a]

	ΔE		ΔE
1a	0.04	**3a1**	2.82
1b	0.03	**3a2**	2.21
1c	0.17	**3b1**	1.07
1a'	0.23	**3b2**	0.15
1b'	0.72	**3c1**	0.03
		3c2	0.09

[a]QM((U)B3LYP/6-31G**)/MM calculations in the Table were carried out using the locally developed modular program package Chemshell3.5 that interfaces with Gaussian09, the broken symmetry approach proposed by Noodleman (L. Noodleman, *J. Chem. Phys.*, 1981, **74**, 5737.) was used in unrestricted wavefunction calculations.

From Table S3, the unrestricted–restricted energy differences of initial ozone-substrate complexes and Criegee intermediates are all positive ($\Delta E > 0$). Energy differences of **1a**, **1b**, **1c**, **1a'**, and **1b'** are less than 0.8 kcal/mol, while these of Criegee intermediates range from 0.03 to the largest 2.82 kcal/mol. Positive ΔE values herein suggest that the restricted close-shell structures are slightly more stable than the unrestricted diradical ones. Then, the seprated ozone-substrate reactants and Criegee intermediates do not have significant singlet diradical characters but rather exhibit dominantly closed-shell characters at the air-water/acetonitrile interface.

Table S4: QM(B3LYP/def2-SVP)/MM Calculated Relative Energies (**R. E**, in kcal/mol) of Reactants, Transition States, Ozonides, and Criegee Intermediates in Stage I. The Energy of the Most Stable **1c** Conformer is Set as Zero Reference Point.

	R. E		R. E		R. E
1a	2.9	**TS1a**	3.4	**2a**	-54.4
1b	1.8	**TS1b**	1.81	**2b**	-55.1
1c	0.0	**TS1c**	0.3	**2c**	-59.2
1a'	1.4	**TS1a'**	6.5	**2a'**	-51.5
1b'	0.8	**TS1b'**	6.3	**2b'**	-52.3
2a	-54.4	**TS2a_1**	-44.1	**3a1**	-79.5
		TS2a_2	-39.0	**3a2**	-71.2
2b	-55.1	**TS2b_1**	-42.7	**3b1**	-73.7
		TS2b_2	-27.3	**3b2**	-73.0
2c	-59.2	**TS2c_1**	-42.6	**3c1**	-71.6
		TS2c_2	-40.6	**3c2**	-70.3
2a'	-51.5	**TS2a_1'**	-41.1	**3a1**	-79.5
		TS2a_2'	-35.6	**3a2**	-71.2
2b'	-52.3	**TS2b_1'**	-29.5	**3b1**	-73.7
		TS2b_2'	-39.0	**3b2**	-73.0

Table S5: QM(B3LYP/def2-SVP)/MM Calculated Relative Energies (**R. E**, in kcal/mol) of Transition States and Addition Products of Criegee with Waters or Acids in Stage II. The Energies of Complexed Criegee with Water or Acid Molecules are Set as Zero Reference Points.

TS	R. E	Pr	R. E	TS	R. E	Pr	R. E
TS3a1_1w	12.4	**4a1**	-23.2	**TS3a2_1w**	16.4	**4a2**	-16.5
TS3a1_2w	7.0	**4a1+1w**	-24.9	**TS3a2_2w**	4.0	**4a2+1w**	-22.6
TS3a1_3w	8.3	**4a1+2w**	-27.4	**TS3a2_3w**	6.0	**4a2+2w**	-21.4
TS3a1_3w'	5.2	**4a1+2w'**	-26.9	**TS3a2_3w'**	1.9	**4a2+2w'**	-20.7
TS3a1_R1	0.7	**5a1_R1**	-14.6	**TS3a2_R1**	0.4	**5a2_R1**	-13.7
TS3a1_ R2	0.9	**5a1_ R2**	-14.6	**TS3a2_ R2**	0.8	**5a2_ R2**	-13.5
TS3a1_ R3	1.0	**5a1_ R3**	-13.3	**TS3a2_ R3**	0.8	**5a2_ R3**	-12.0
TS3a1_ R4	1.5	**5a1_ R4**	-14.8	**TS3a2_ R4**	0.8	**5a2_ R4**	-12.1
TS3a1_ R5	1.7	**5a1_R5**	-15.6	**TS3a2_ R5**	0.9	**5a2_R5**	-12.2
TS3a1_ R6	2.0	**5a1_R6**	-15.1	**TS3a2_ R6**	1.2	**5a2_R6**	-9.6
TS3a1_ R7	2.8	**5a1_R7**	-15.9	**TS3a2_ R7**	1.2	**5a2_R7**	-15.8
TS3b1_1w	13.5	**4b1**	-22.4	**TS3b2_1w**	7.8	**4b2**	-33.0
TS3b1_2w	6.9	**4b1+1w**	-22.0	**TS3b2_2w**	3.2	**4b2+1w**	-26.9
TS3b1_3w	7.5	**4b1+2w**	-21.5	**TS3b2_3w**	6.0	**4b2+2w**	-24.4
TS3b1_3w'	4.8	**4b1+2w'**	-22.9	**TS3b2_3w'**	1.3	**4b2+2w'**	-28.7
TS3b1_R1	2.7	**5b1_R1**	-16.1	**TS3b2_R1**	0.0	**5b2_R1**	-19.0
TS3b1_ R2	2.5	**5b1_R2**	-13.9	**TS3b2_ R2**	0.1	**5b2_R2**	-19.3
TS3b1_ R3	2.4	**5b1_R3**	-10.5	**TS3b2_ R3**	0.1	**5b2_R3**	-19.5
TS3b1_ R4	2.6	**5b1_R4**	-12.9	**TS3b2_ R4**	0.0	**5b2_R4**	-19.5
TS3b1_ R5	4.5	**5b1_R5**	-11.3	**TS3b2_ R5**	0.0	**5b2_R5**	-20.2
TS3b1_ R6	4.6	**5b1_R6**	-10.3	**TS3b2_ R6**	0.0	**5b2_R6**	-20.3
TS3b1_ R7	4.8	**5b1_R7**	-12.3	**TS3b2_ R7**	0.0	**5b2_R7**	-20.7
TS3c1_1w	11.1	**4c1**	-28.8	**TS3c2_1w**	8.1	**4c2**	-29.9
TS3c1_2w	6.5	**4c1+1w**	-25.0	**TS3c2_2w**	4.4	**4c2+1w**	-25.7
TS3c1_3w	6.9	**4c1+2w**	-23.8	**TS3c2_3w**	5.7	**4c2+2w**	-26.7
TS3c1_3w'	4.5	**4c1+2w'**	-22.2	**TS3c2_3w'**	2.9	**4c2+2w'**	-28.6
TS3c1_R1	0.03	**5c1_R1**	-16.5	**TS3c2_R1**	1.2	**5c2_R1**	-20.8
TS3c1_ R2	0.04	**5c1_R2**	-15.4	**TS3c2_ R2**	1.0	**5c2_R2**	-19.9
TS3c1_ R3	0.09	**5c1_R3**	-15.0	**TS3c2_ R3**	0.9	**5c2_R3**	-20.4
TS3c1_ R4	0.04	**5c1_R4**	-15.1	**TS3c2_ R4**	2.0	**5c2_R4**	-19.7
TS3c1_ R5	0.07	**5c1_R5**	-15.1	**TS3c2_ R5**	1.0	**5c2_R5**	-20
TS3c1_ R6	0.15	**5c1_R6**	-15.1	**TS3c2_ R6**	1.0	**5c2_R6**	-20.3
TS3c1_ R7	0.11	**5c1_R7**	-15.9	**TS3c2_ R7**	2.8	**5c2_R7**	-18.2

IV、Two-Dimensional Potential Energy Surfaces

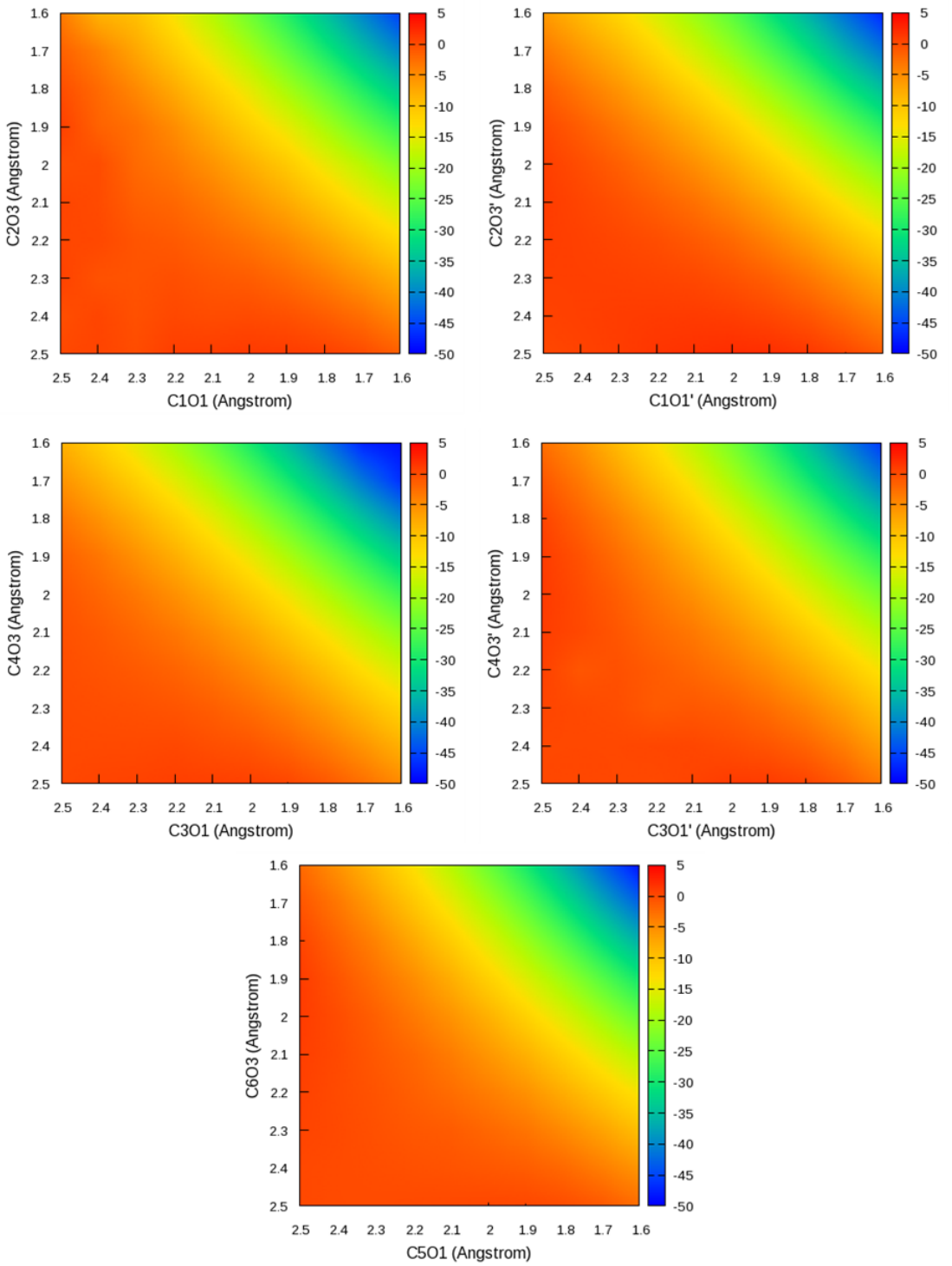

Figure S4: QM(B3LYP/def2-SVP)/MM computed two-dimensional potential energy surfaces (in kcal/mol) with respect to the two reaction coordinates related to the O1-C1 and O3-C2 bonds in **1a** (top-left) and **1a'** (top-right), the O1-C3 and O3-C4 bonds in **1b** (middle-left) and **1b'** (middle-right), and the O1-C5 and O3-C6 bonds in **1c** (bottom).

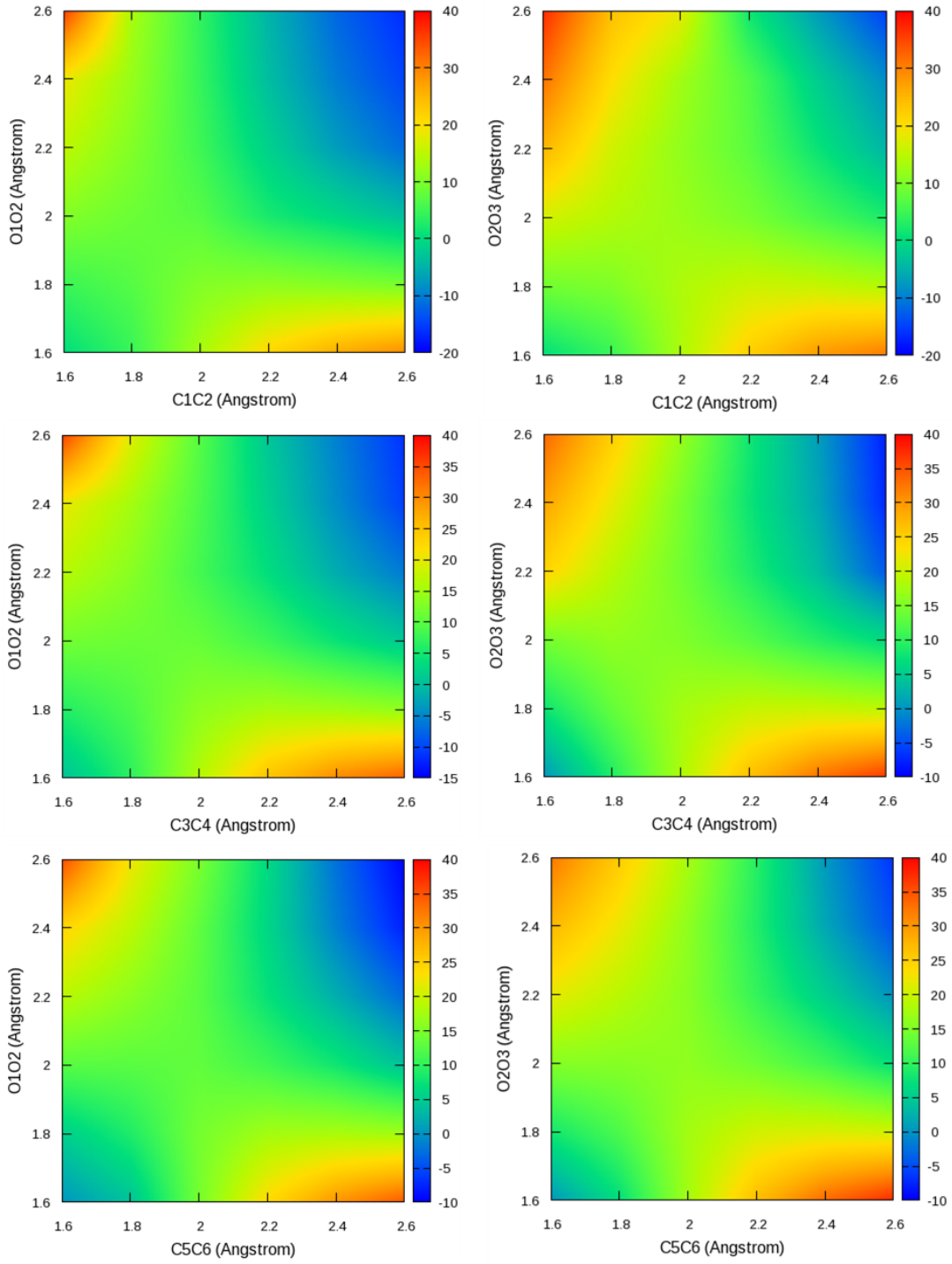

Figure S5: QM(B3LYP/def2-SVP)/MM computed two-dimensional potential energy surfaces (in kcal/mol) with respect to the two reaction coordinates related to (top-left) O1-O2 and C1-C2 bonds and (top-right) O2-O3 and C1-C2 bonds in **2a**, (middle-left) O1-O2 and C3-C4 bonds and (middle-right) O2-O3 and C3-C4 bonds in **2b**, and (bottom-left) O1-O2 and C5-C6 bonds and (bottom-right) O2-O3 and C5-C6 bonds in **2c**.

V、Minimum Energy Paths

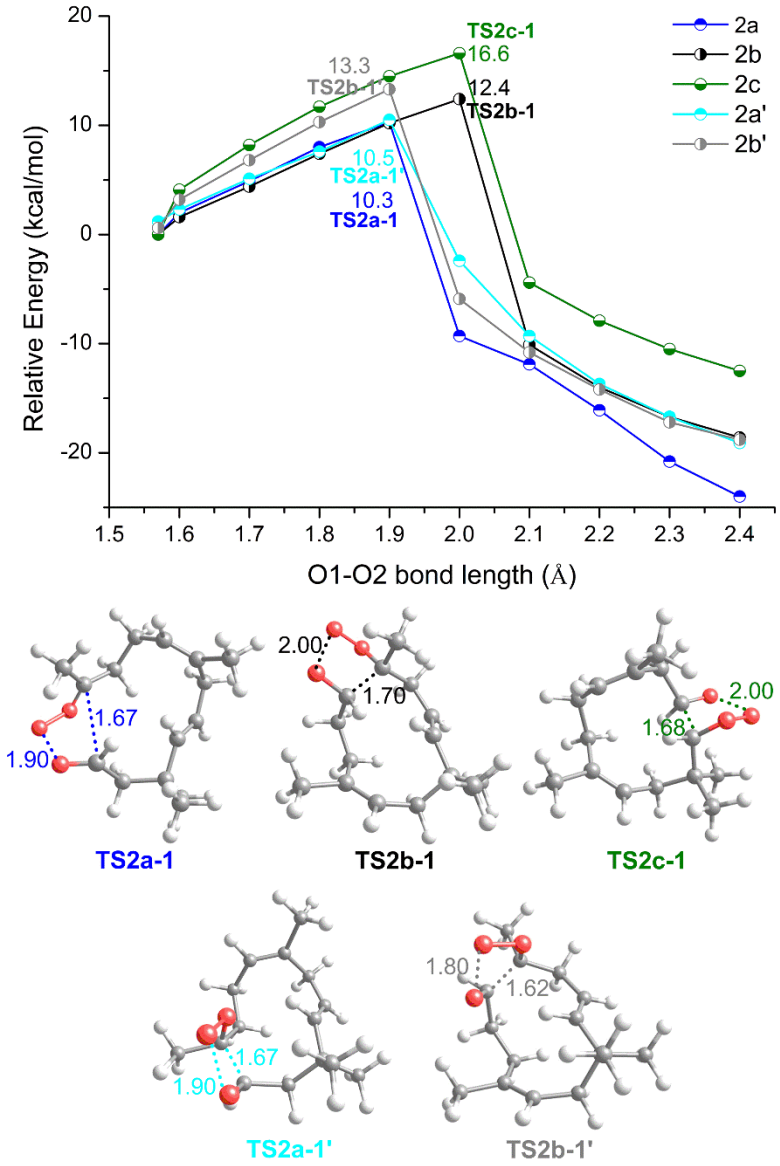

Figure S6: QM(B3LYP/def2-SVP)/MM calculated minimum-energy paths (in kcal/mol) of O1-O2 and C-C bonds cleavage in **2a**, **2a'**, **2b**, **2b'**, and **2c**.The selected bond lengths are in Å.

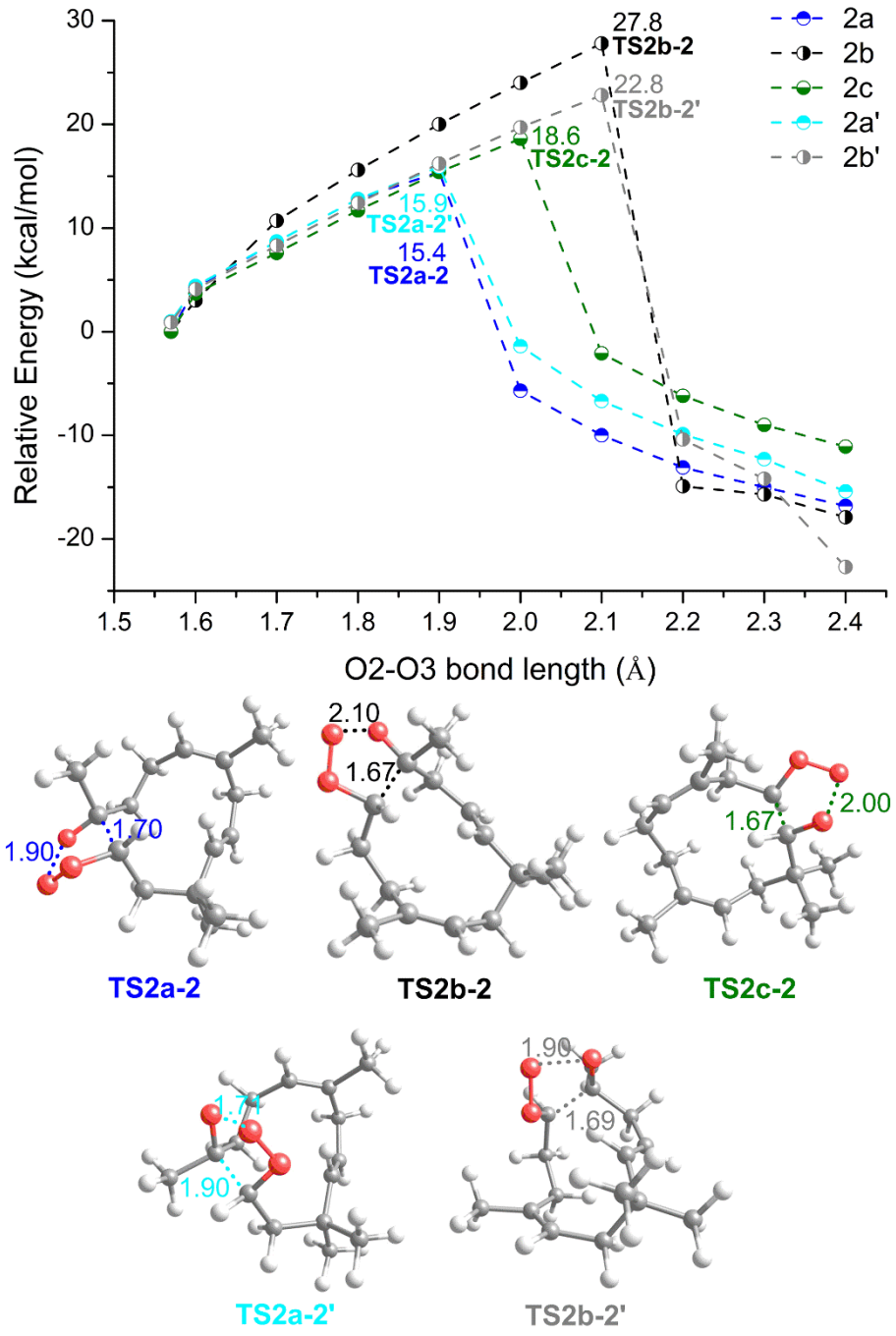

Figure S7: QM(B3LYP/def2-SVP)/MM calculated minimum-energy paths (in kcal/mol) of O2-O3 and C-C bonds cleavage in **2a**, **2a'**, **2b**, **2b'**, and **2c**. Also shown are selected bond lengths in Å.

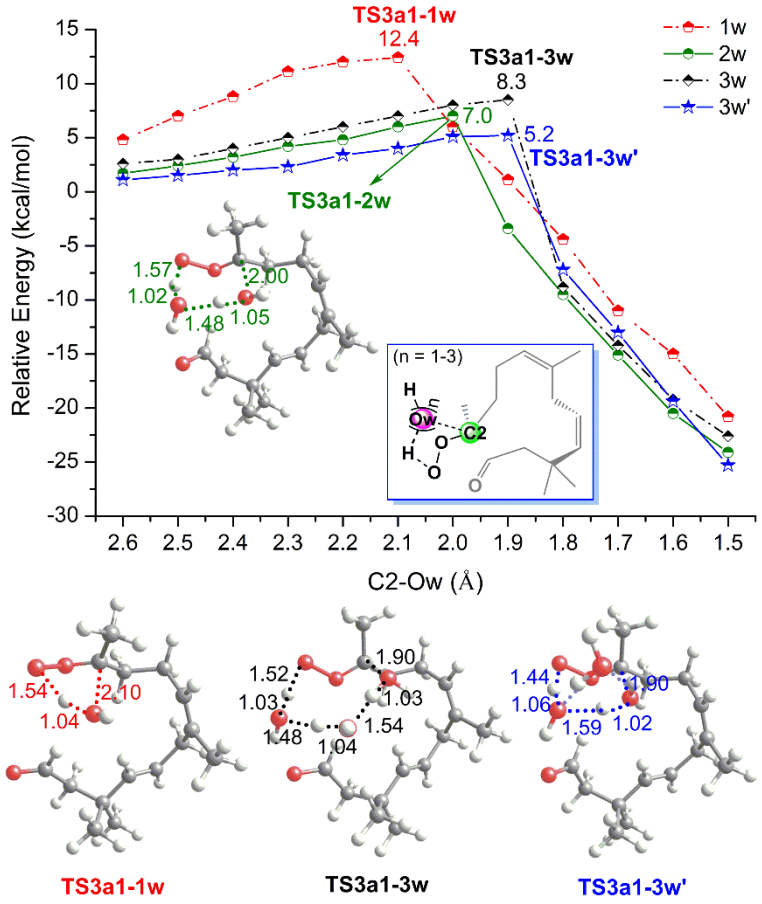

Figure S8: QM(B3LYP/def2-SVP)/MM calculated minimum-energy paths (in kcal/mol) for addition reactions of waters on Criegee intermediate **3a1**. Also shown are selected bond lengths in Å.

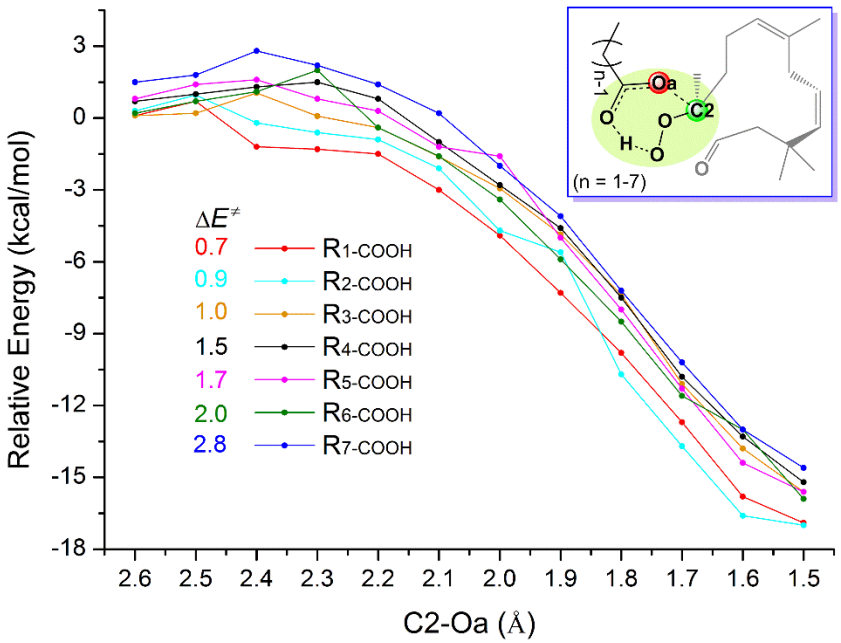

Figure S9: QM(B3LYP/def2-SVP)/MM calculated minimum-energy paths (in kcal/mol) for addition reactions of different acids on Criegee intermediate **3a1**.

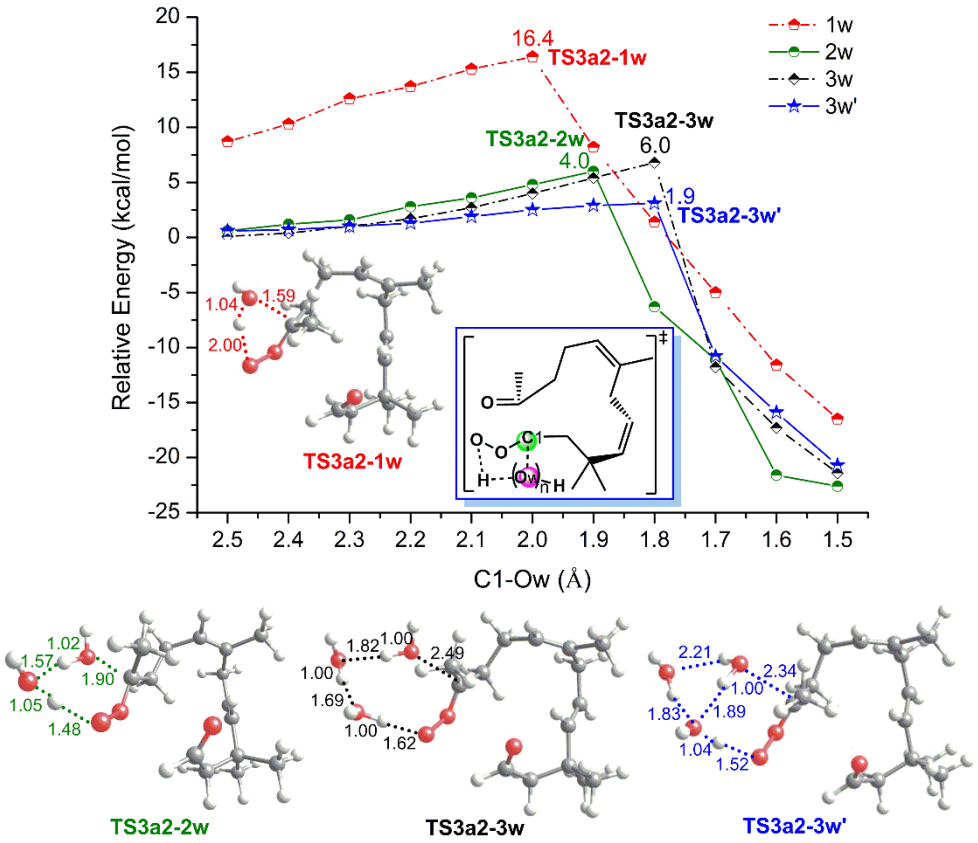

Figure S10: QM(B3LYP/def2-SVP)/MM calculated minimum-energy paths (in kcal/mol) for addition reactions of waters on Criegee intermediate **3a2**. Also shown are selected bond lengths in Å.

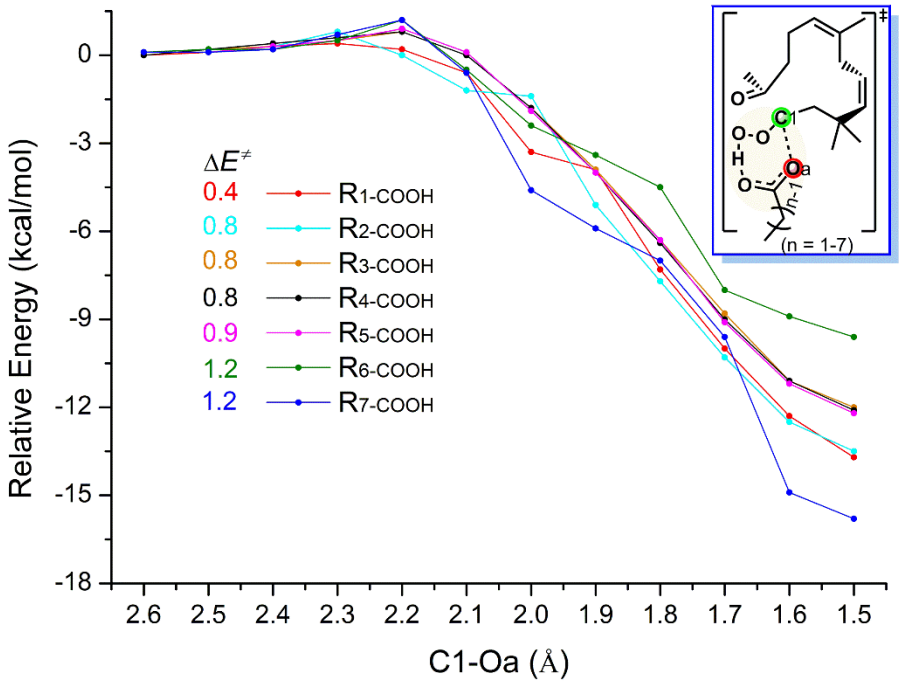

Figure S11: QM(B3LYP/def2-SVP)/MM calculated minimum-energy paths (in kcal/mol) for addition reactions of different acids on Criegee intermediate **3a2**.

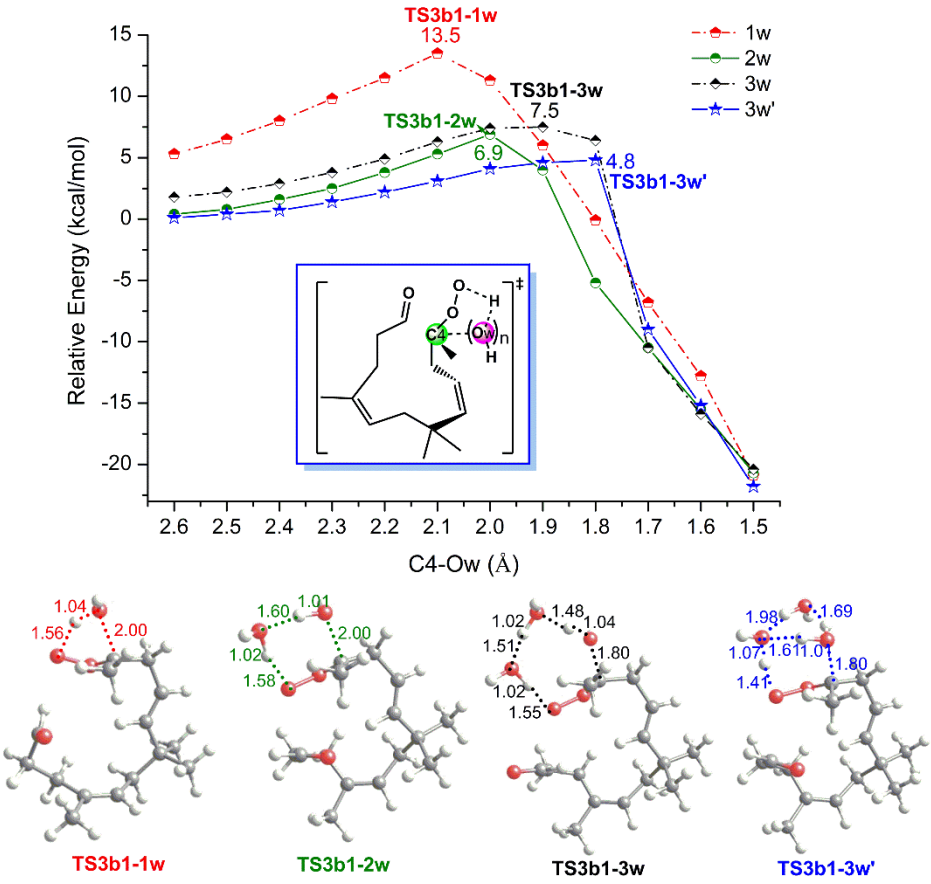

Figure S12: QM(B3LYP/def2-SVP)/MM calculated minimum-energy paths (in kcal/mol) for addition reactions of waters on Criegee intermediate **3b1**. Also shown are selected bond lengths in Å.

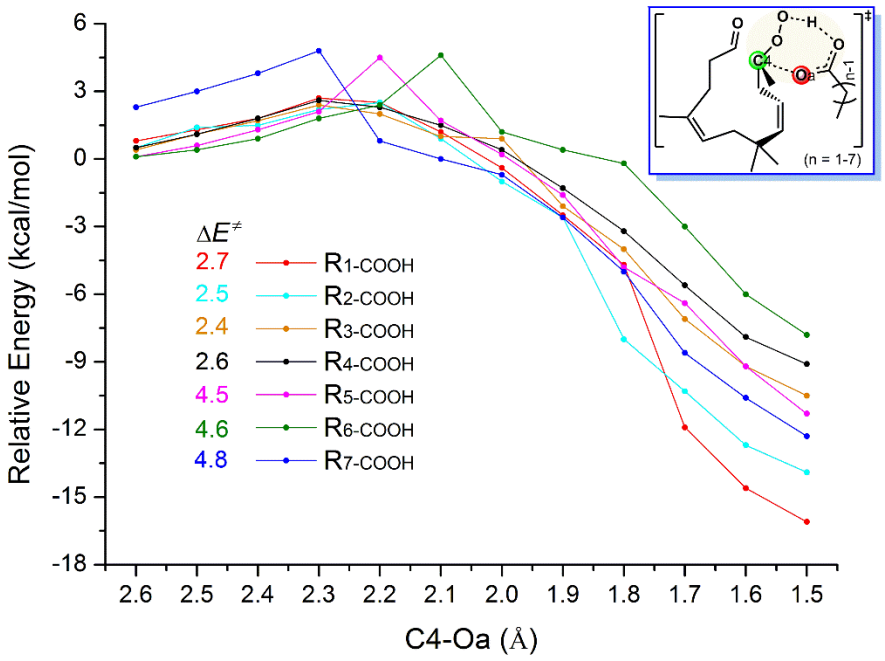

Figure S13: QM(B3LYP/def2-SVP)/MM calculated minimum-energy paths for addition reactions of different acids on Criegee intermediate **3b1**.

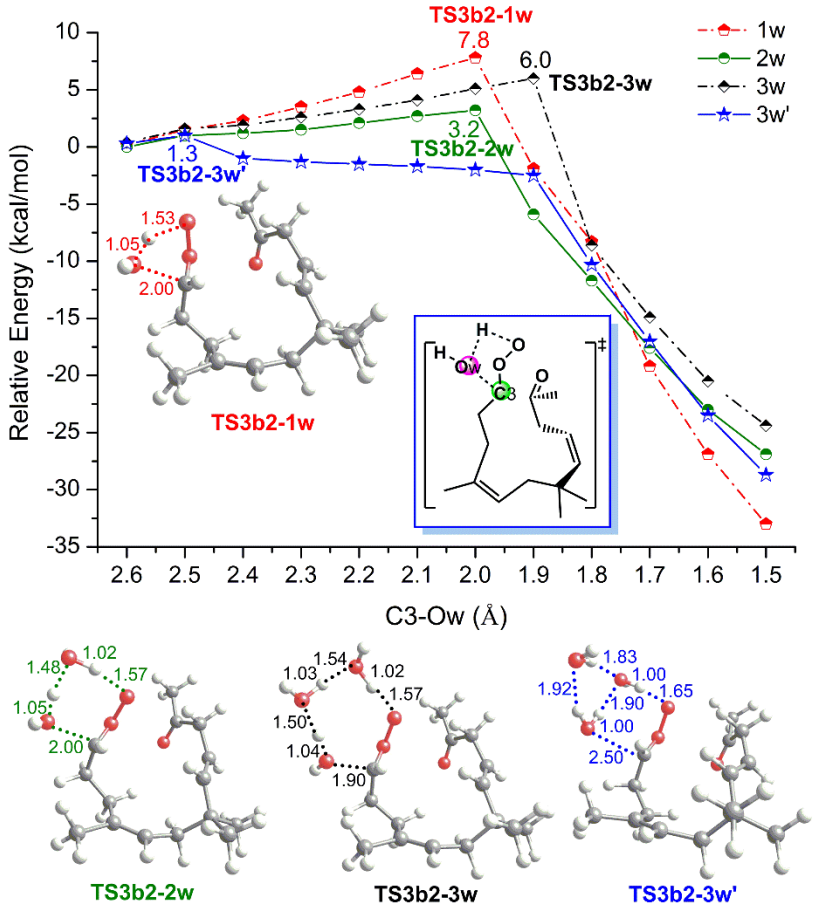

Figure S14: QM(B3LYP/def2-SVP)/MM calculated minimum-energy paths (in kcal/mol) for addition reactions of waters on Criegee intermediate **3b2**. Also shown are selected bond lengths in Å.

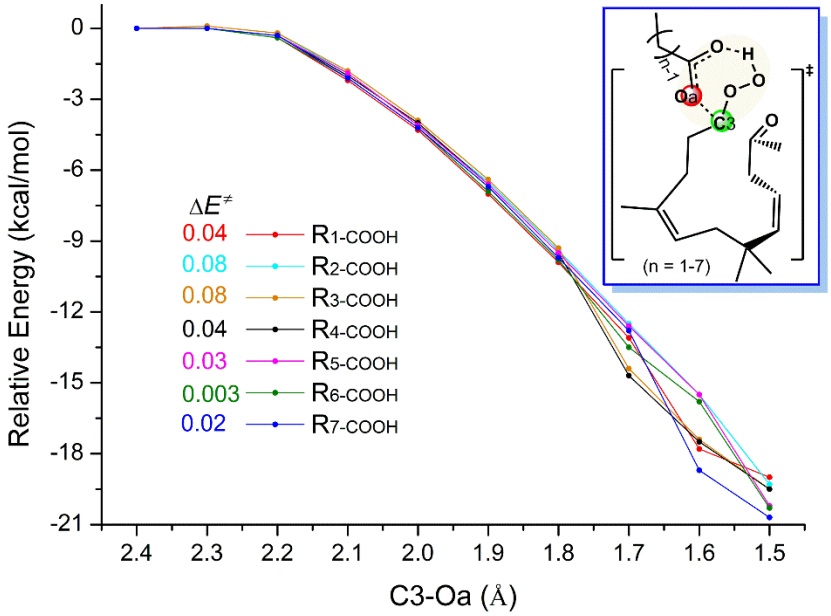

Figure S15: QM(B3LYP/def2-SVP)/MM calculated minimum-energy paths (in kcal/mol) for addition reactions of different acids on Criegee intermediate **3b2**.

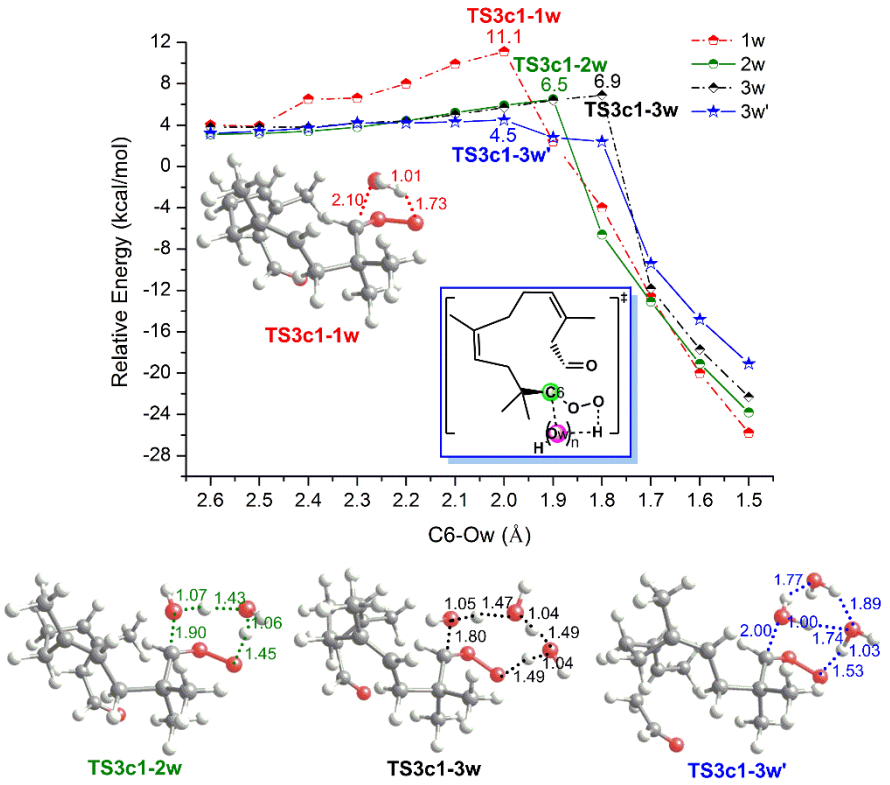

Figure S16: QM(B3LYP/def2-SVP)/MM calculated minimum-energy paths (in kcal/mol) for addition reactions of waters on Criegee intermediate **3c1**. Also shown are selected bond lengths in Å.

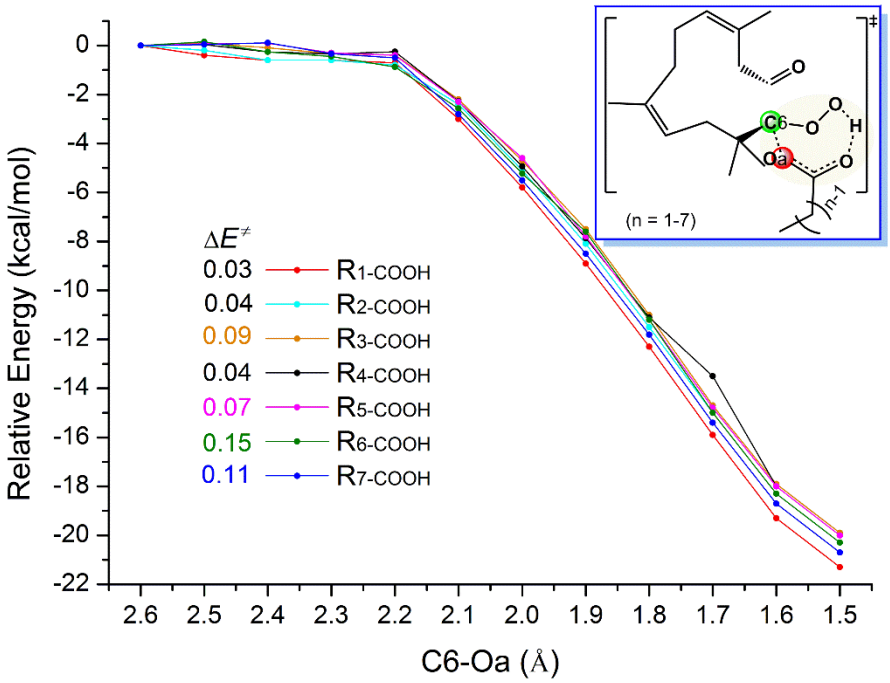

Figure S17: QM(B3LYP/def2-SVP)/MM calculated minimum-energy paths (in kcal/mol) for addition reactions of different acids on Criegee intermediate **3c1**.

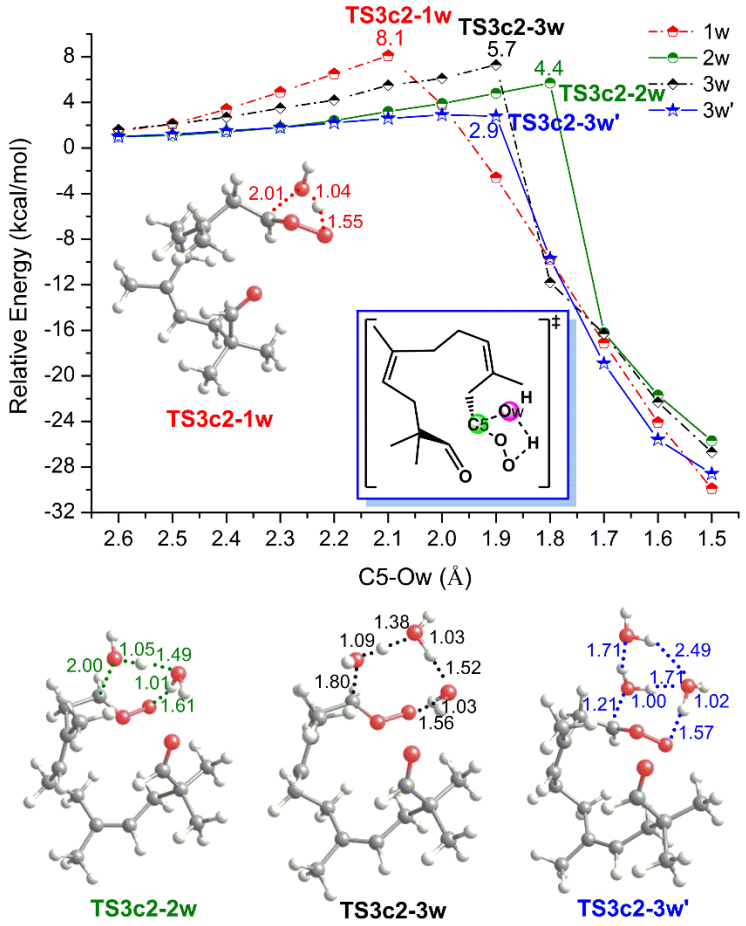

Figure S18: QM(B3LYP/def2-SVP)/MM calculated minimum-energy paths (in kcal/mol) for addition reactions of waters on Criegee intermediate **3c2**. Also shown are selected bond lengths in Å.

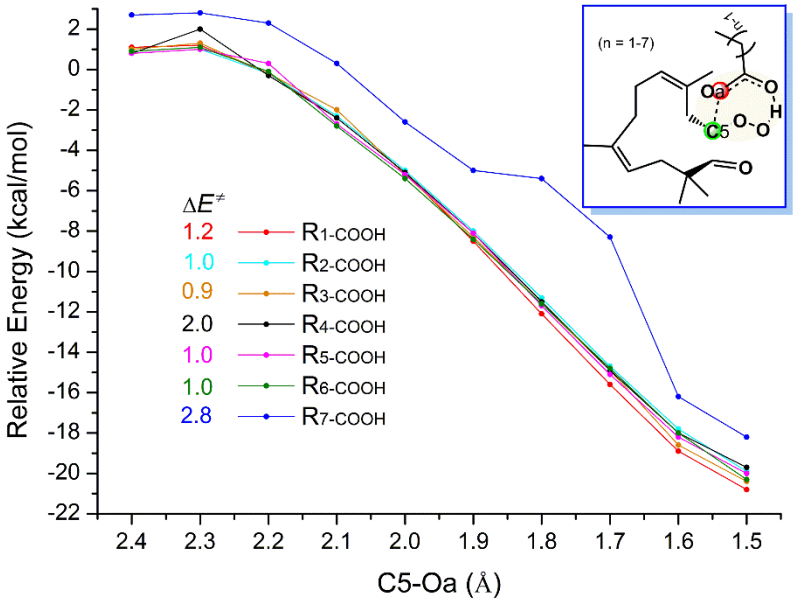

Figure S19: QM(B3LYP/def2-SVP)/MM calculated minimum-energy paths (in kcal/mol) for addition reactions of different acids on Criegee intermediate **3c2**.

VI、QM(CASPT2)/MM Computed Energy Profiles

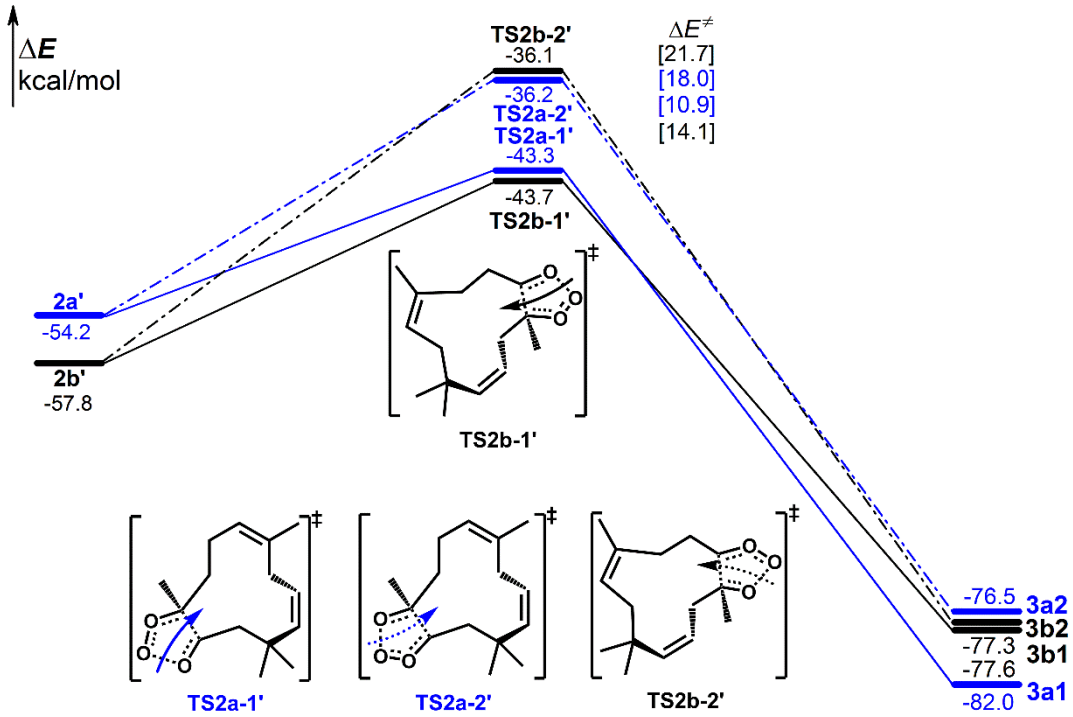

Figure S20: QM(CASPT2)/MM computed energy profiles (in kcal/mol) for ring-cleavage reactions of the ozonides **2a'**, **2b'**.

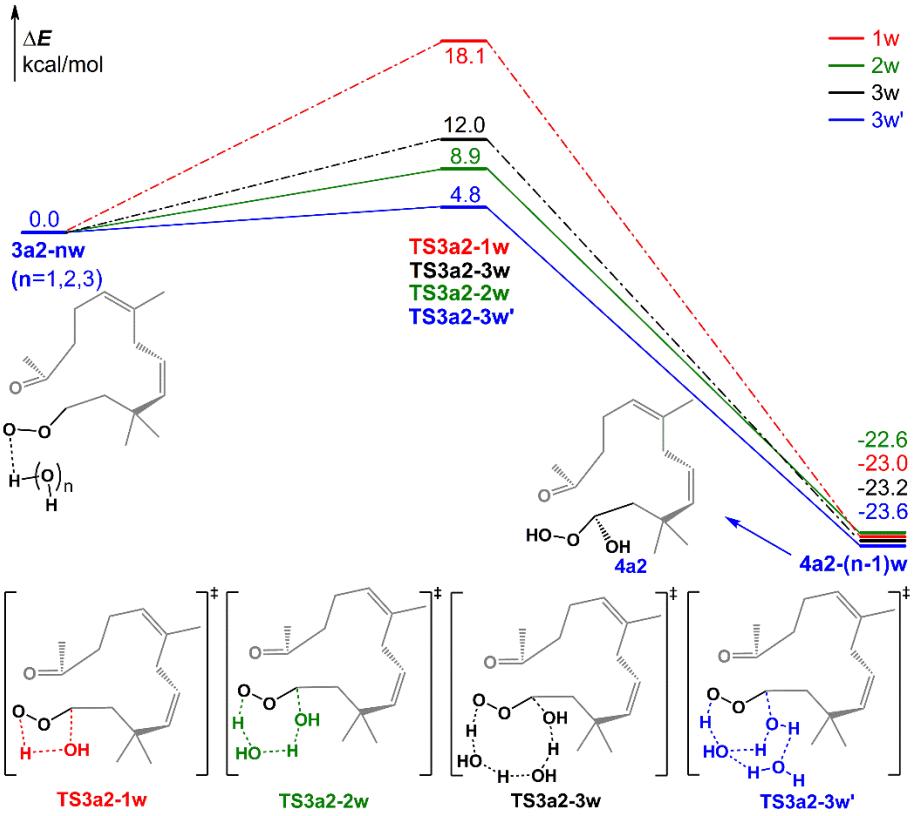

Figure S21: QM(CASPT2)/MM computed energy profiles (in kcal/mol) for addition reactions of waters on Criegee intermediate **3a2**.

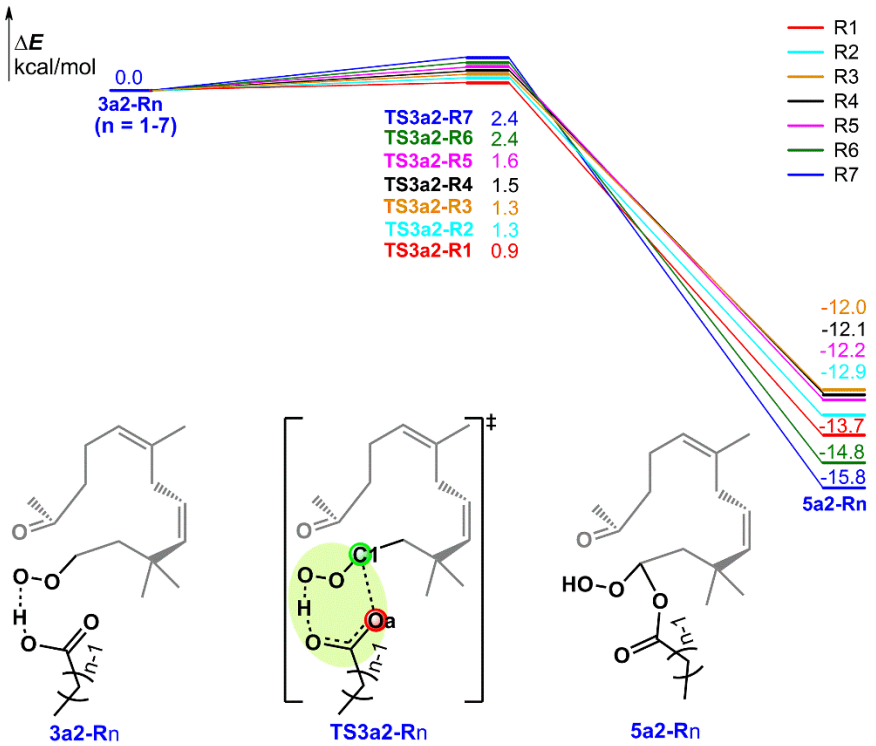

Figure S22: QM(CASPT2)/MM computed energy profiles (in kcal/mol) for addition reactions of different acids on Criegee intermediate **3a2**.

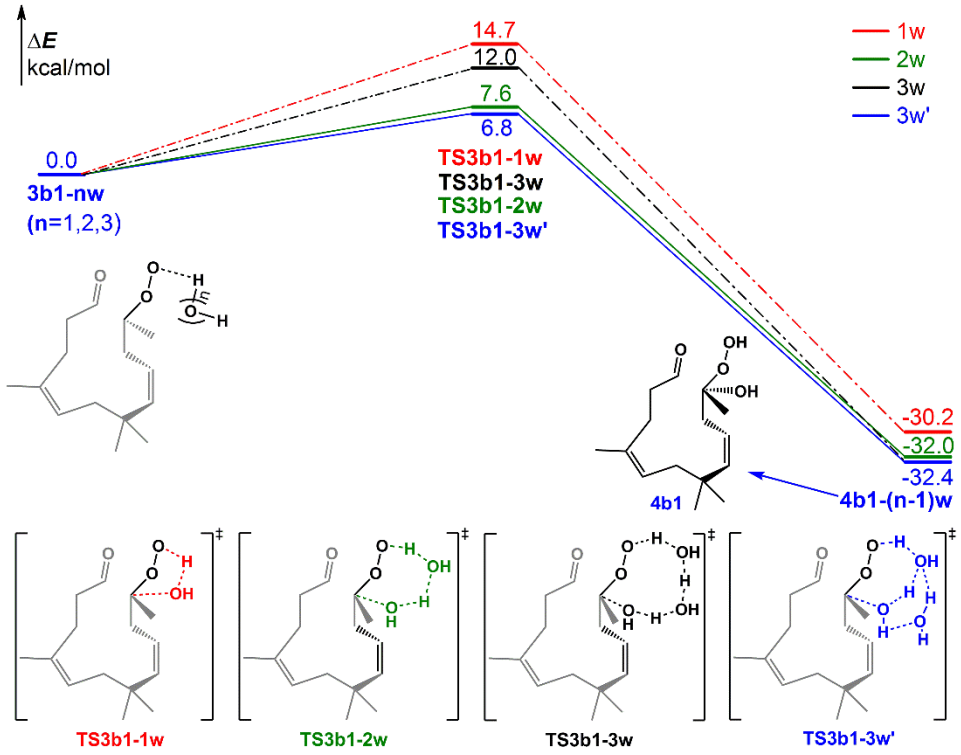

Figure S23: QM(CASPT2)/MM computed energy profiles (in kcal/mol) for addition reactions of waters on Criegee intermediate **3b1**.

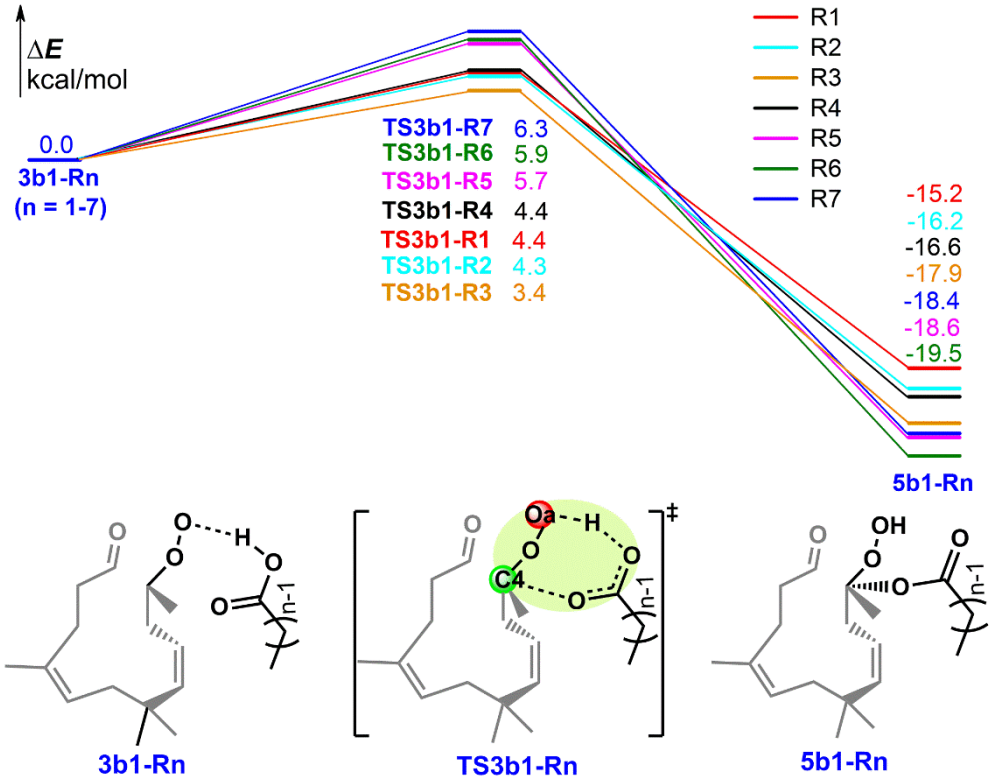

Figure S24: QM(CASPT2)/MM computed energy profiles (in kcal/mol) for addition reactions of different acids on Criegee intermediate **3b1**.

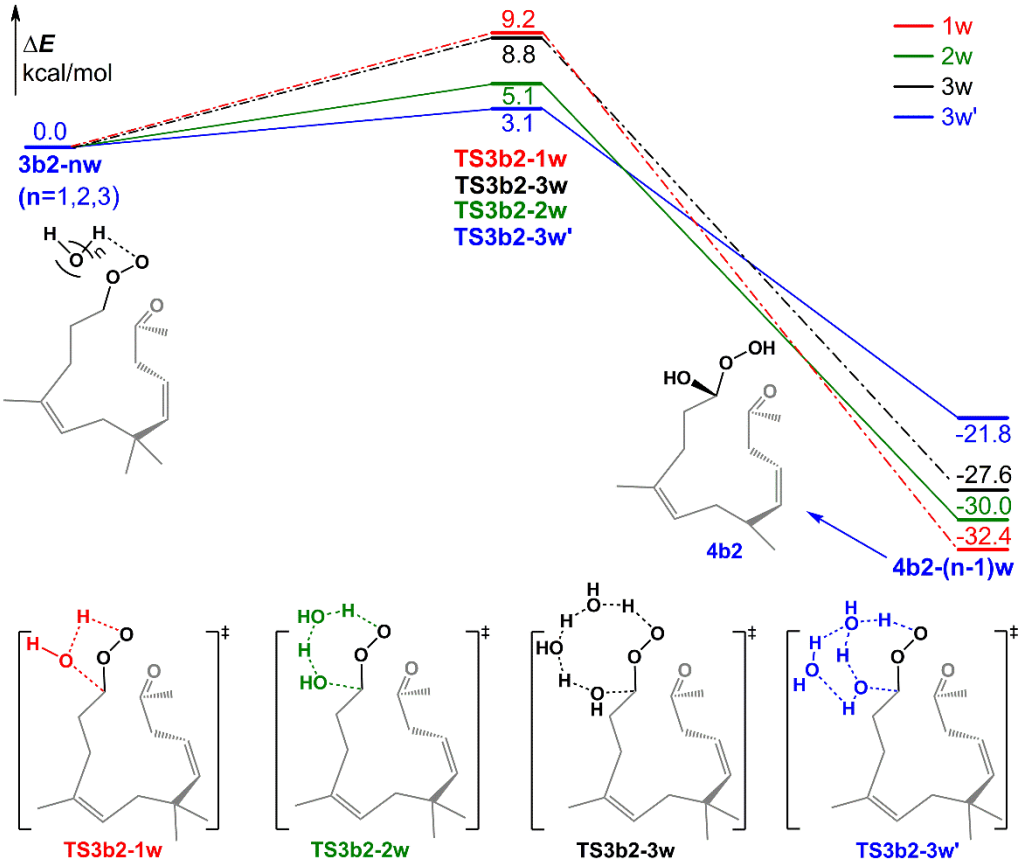

Figure S25: QM(CASPT2)/MM computed energy profiles (in kcal/mol) for addition reactions of waters on Criegee intermediate **3b2**.

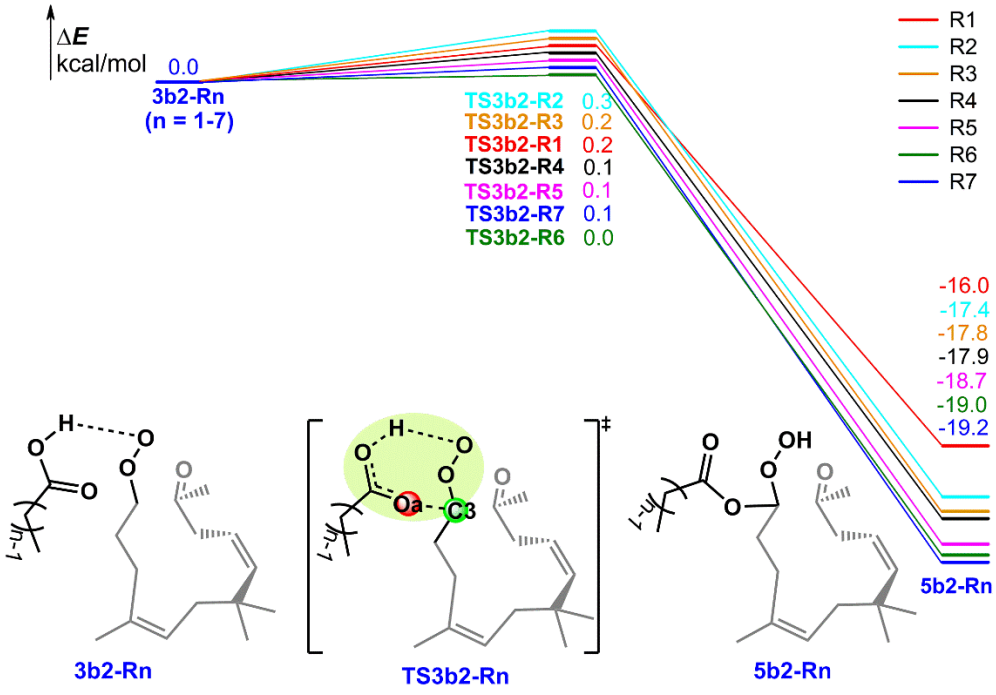

Figure S26: QM(CASPT2)/MM computed energy profiles (in kcal/mol) for addition reactions of different acids on Criegee intermediate **3b2**.

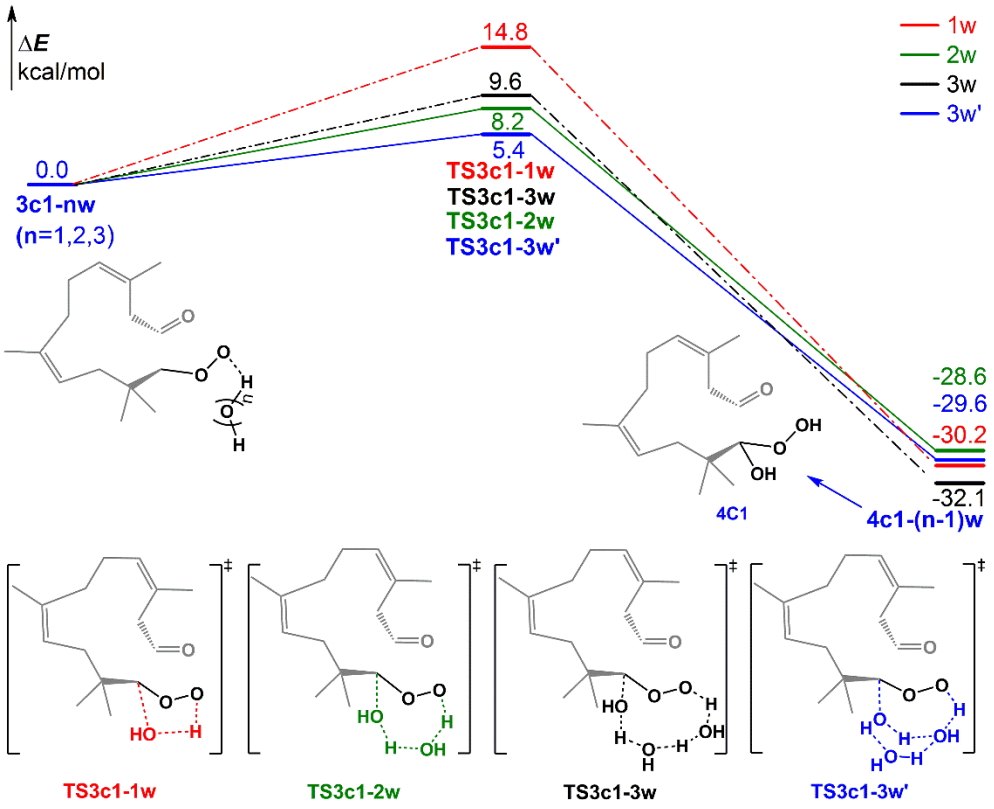

Figure S27: QM(CASPT2)/MM computed energy profiles (in kcal/mol) for addition reactions of waters on Criegee intermediate **3c1**.

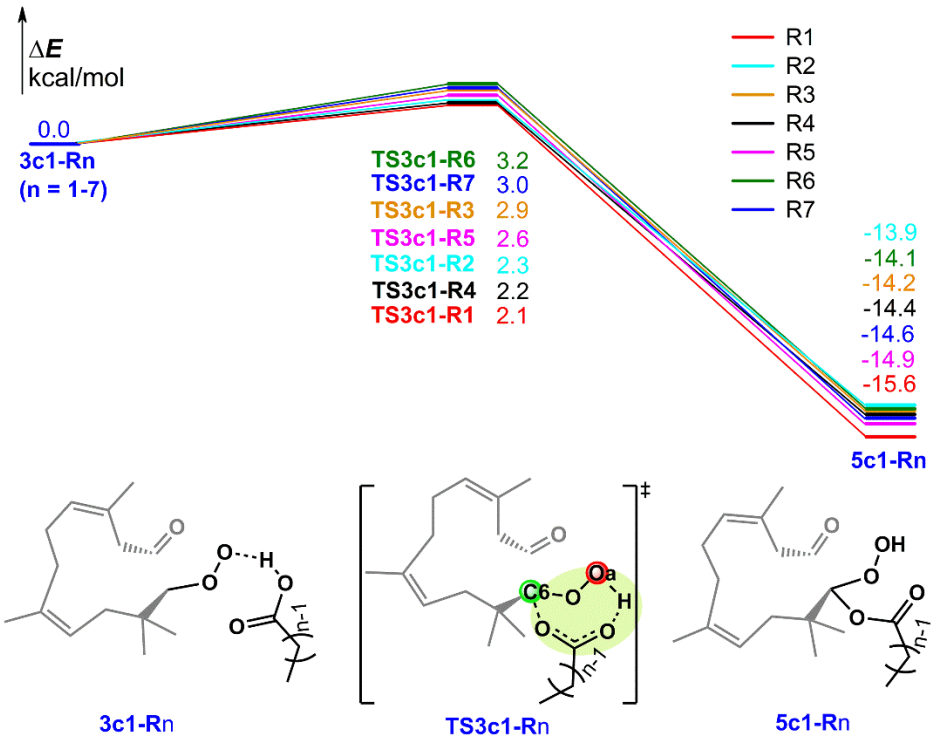

Figure S28: QM(CASPT2)/MM computed energy profiles (in kcal/mol) for addition reactions of different acids on Criegee intermediate **3c1**.

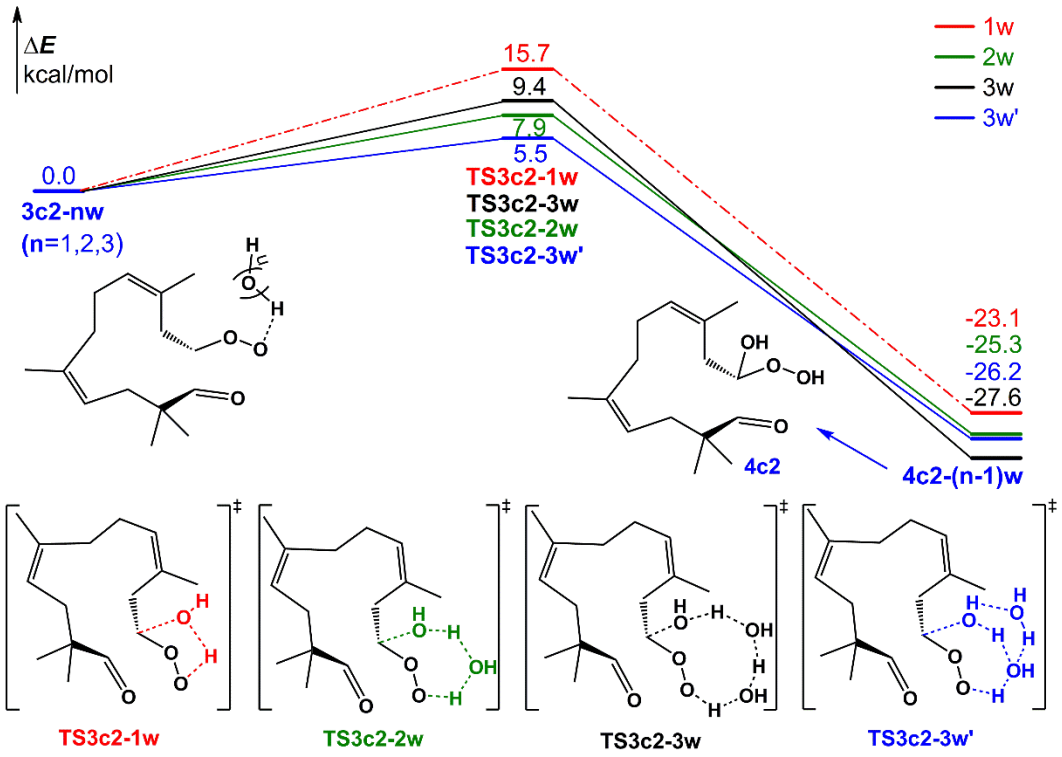

Figure S29: QM(CASPT2)/MM computed energy profiles (in kcal/mol) for addition reactions of waters on Criegee intermediate **3c2**.

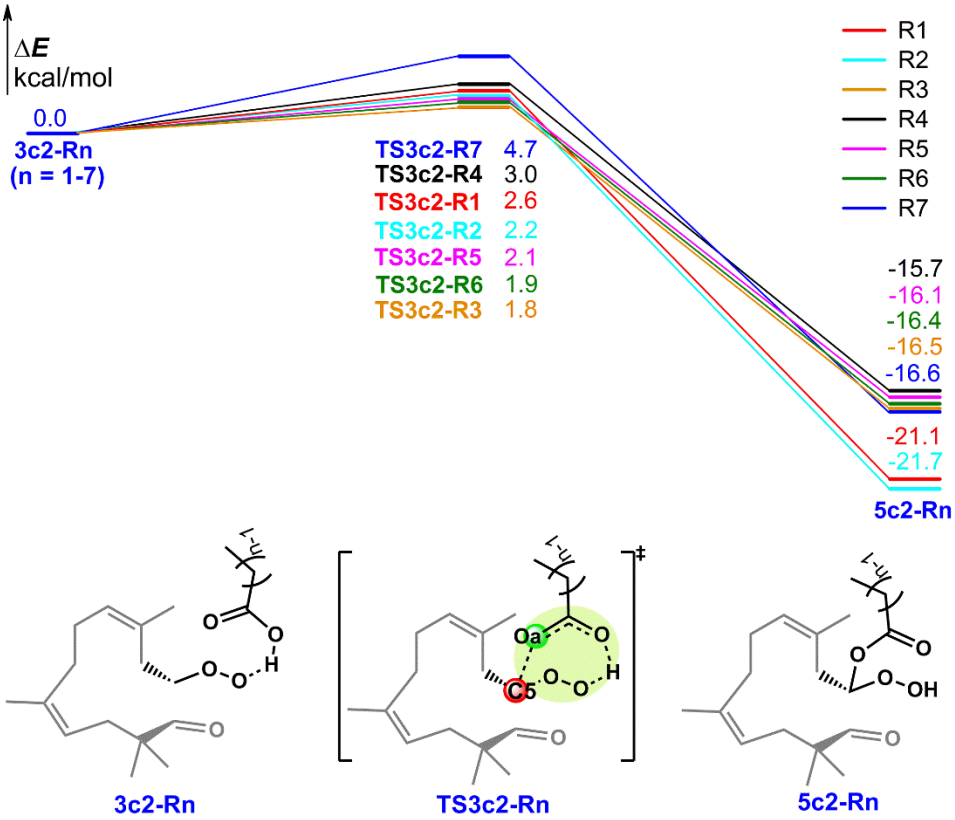

Figure S30: QM(CASPT2)/MM computed energy profiles (in kcal/mol) for addition reactions of different acids on Criegee intermediate **3c2**.

VII、QM/MM Computed Structures in Addition of Acids and Waters on 3a1

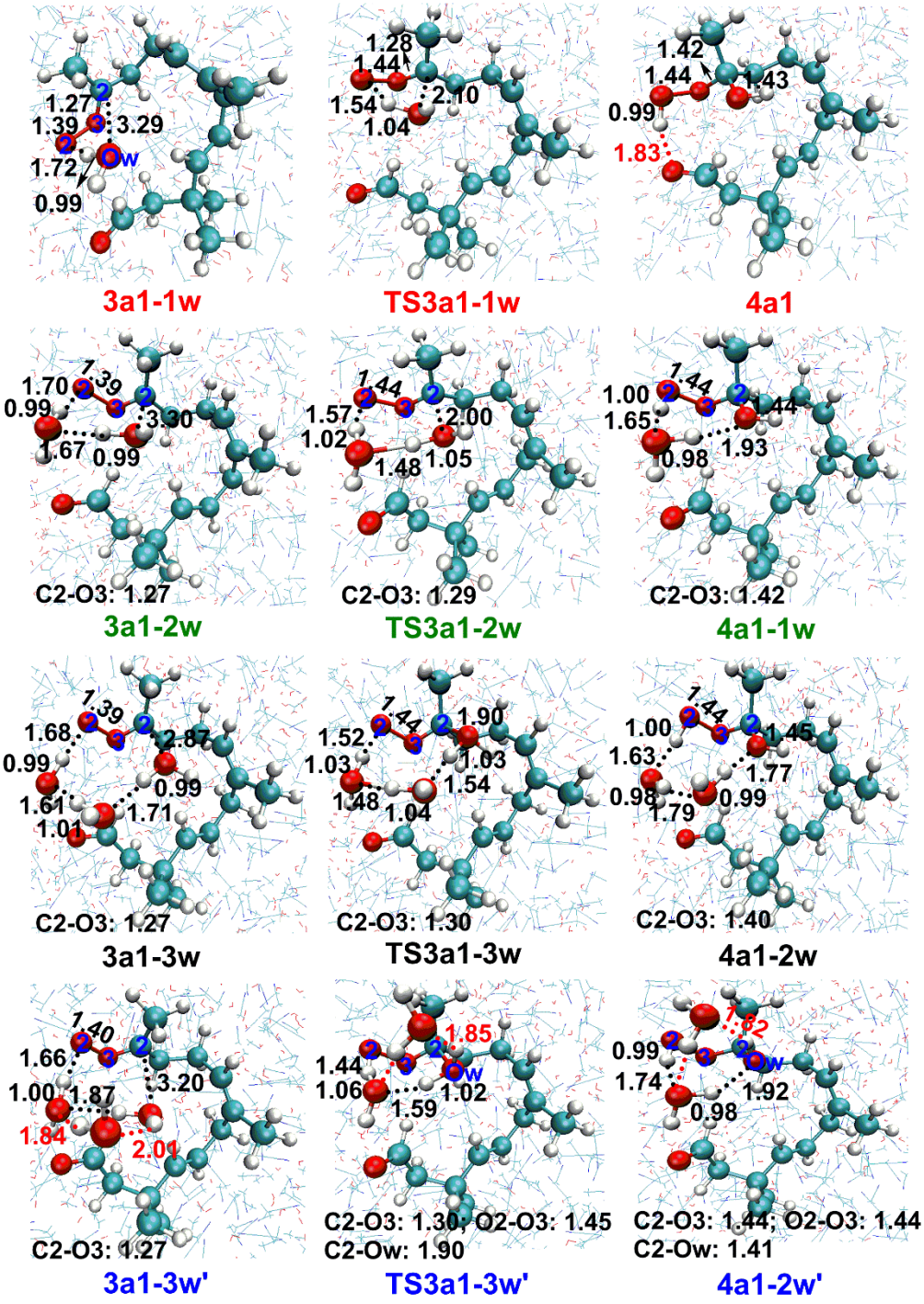

Figure S31: QM/MM computed transition states and minimum-energy structures relevant to the addition of waters on Criegee **3a1**. Also shown are selected bond lengths in Å.

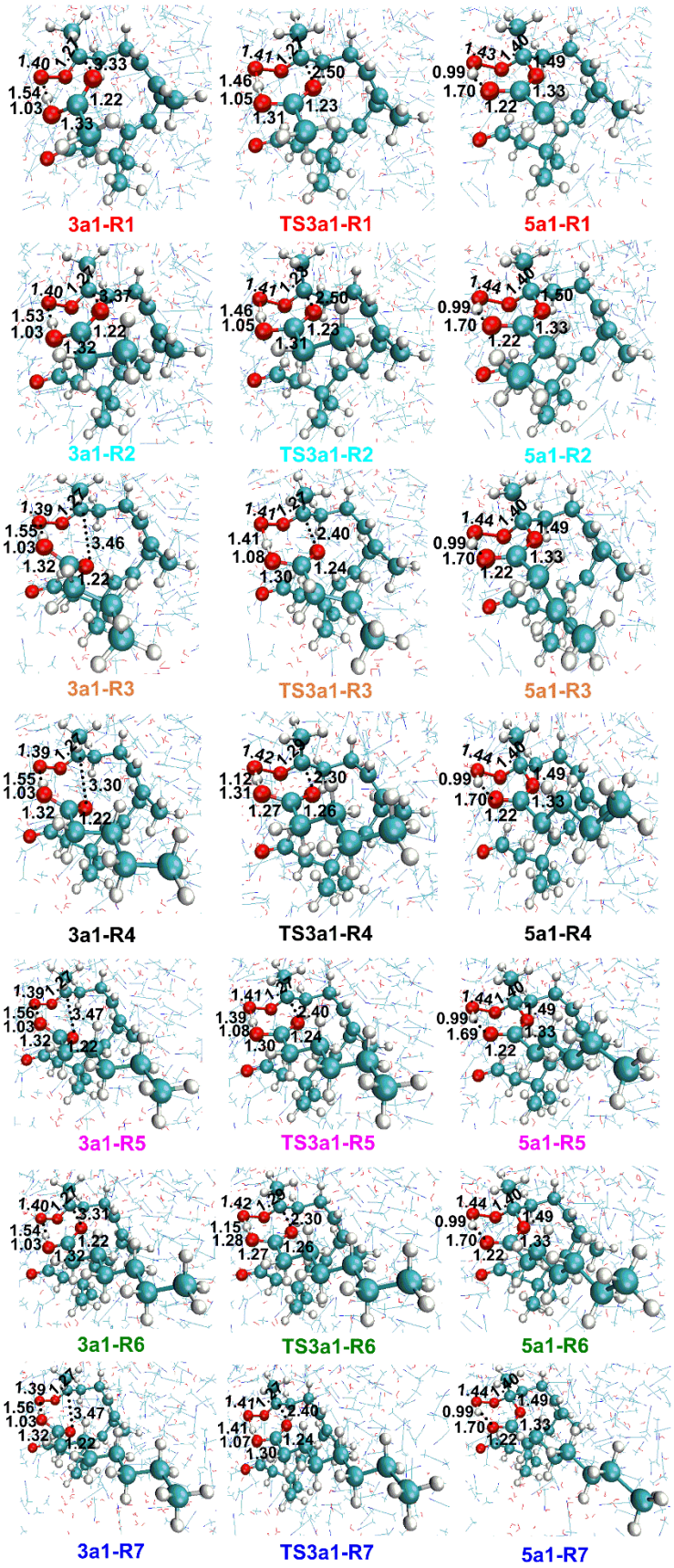

Figure S32: QM/MM computed transition states and minimum-energy structures relevant to the addition of different acids on Criegee **3a1**. Also shown are selected bond lengths in Å.

VIII、Active Orbitals in QM(CASPT2)/MM Computations

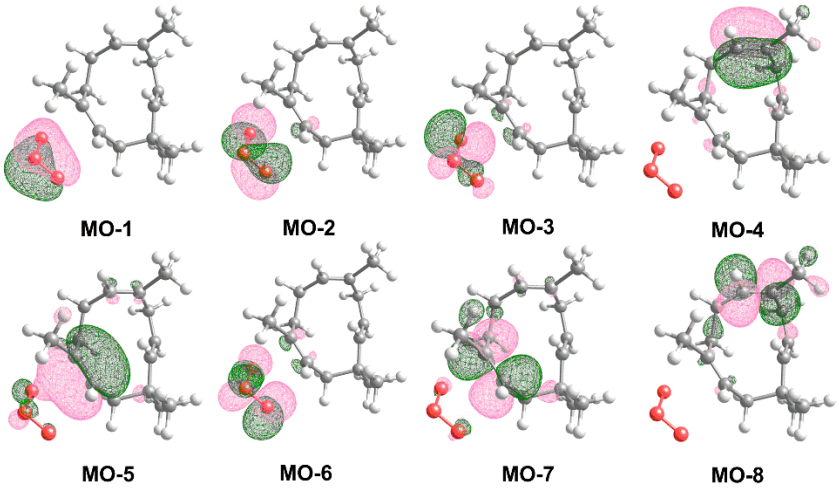

Figure S33: Active space of 10 electrons in 8 orbitals in QM(CASPT2)/MM calculations for **1a**.

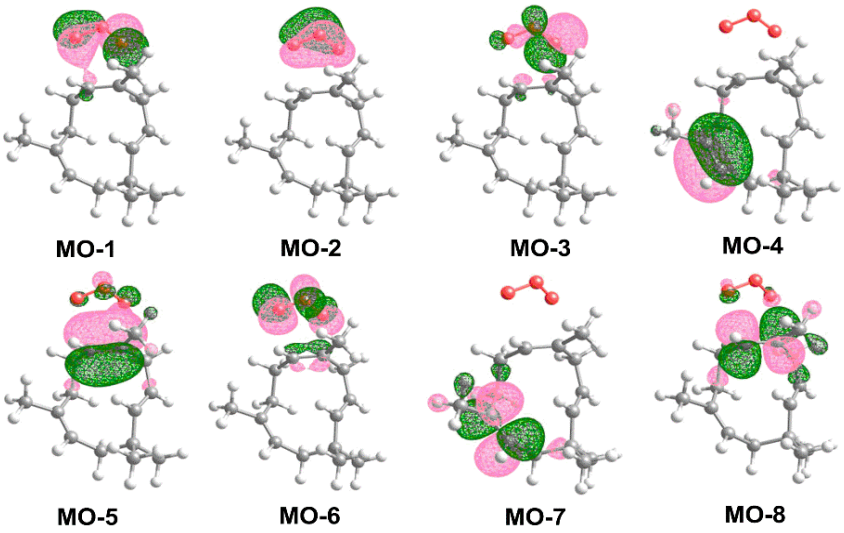

Figure S34: Active space of 10 electrons in 8 orbitals in QM(CASPT2)/MM calculations for **1b**.

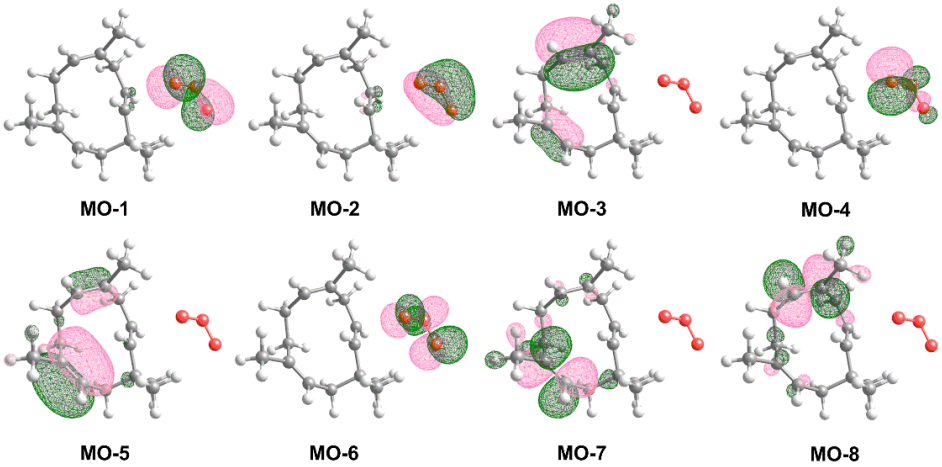

Figure S35: Active space of 10 electrons in 8 orbitals in QM(CASPT2)/MM calculations for **1c**.

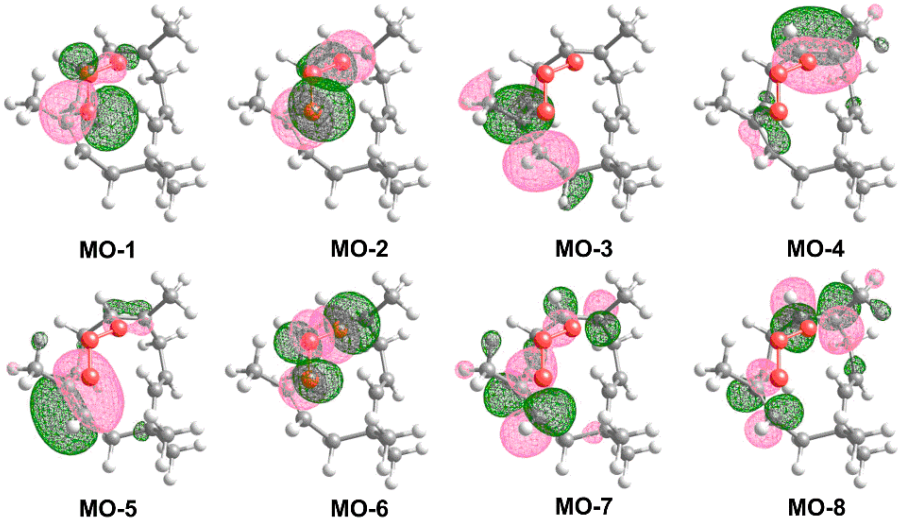

Figure S36: Active space of 10 electrons in 8 orbitals in QM(CASPT2)/MM calculations for **1a'**.

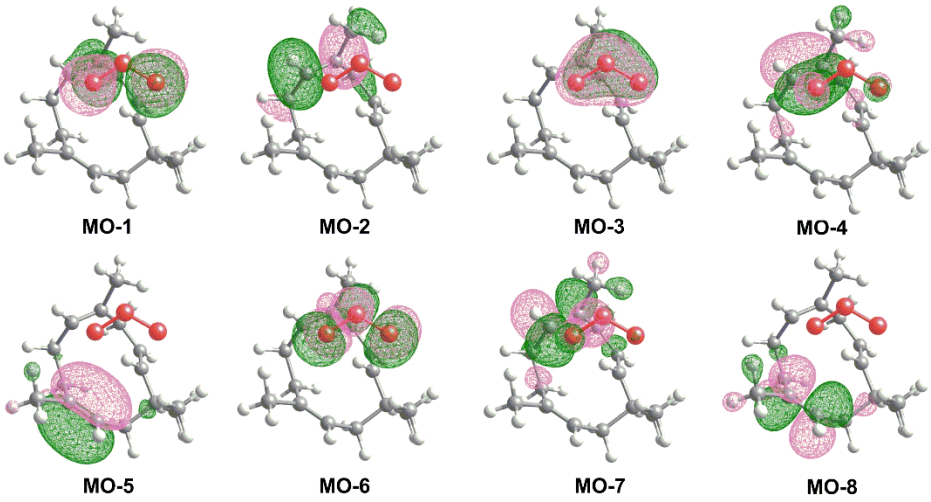

Figure S37: Active space of 10 electrons in 8 orbitals in QM(CASPT2)/MM calculations for **1b'**.

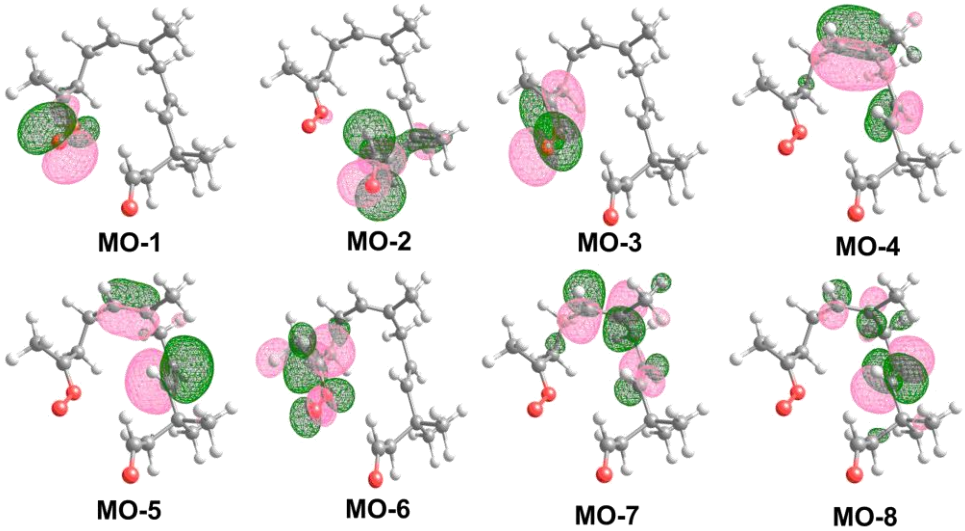

Figure S38: Active space of 10 electrons in 8 orbitals in QM(CASPT2)/MM calculations for **3a1**.

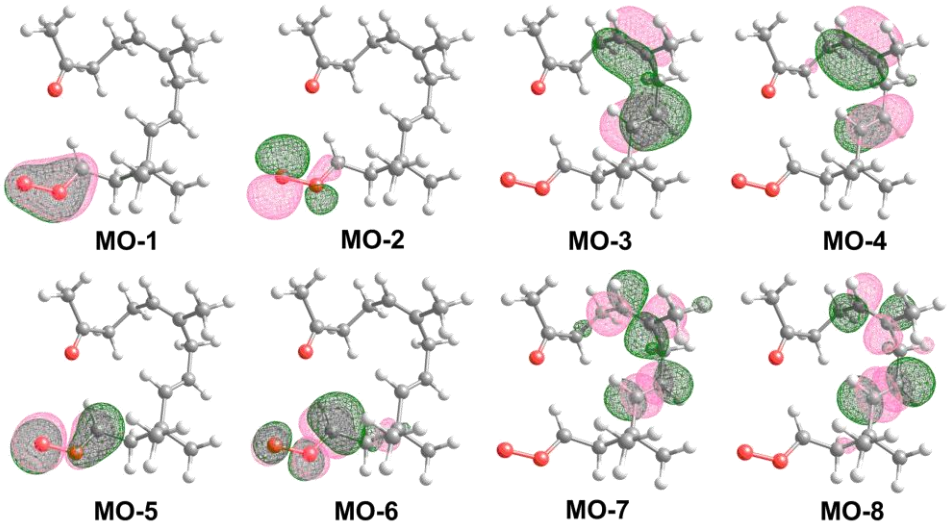

Figure S39: Active space of 10 electrons in 8 orbitals in QM(CASPT2)/MM calculations for **3a2**.

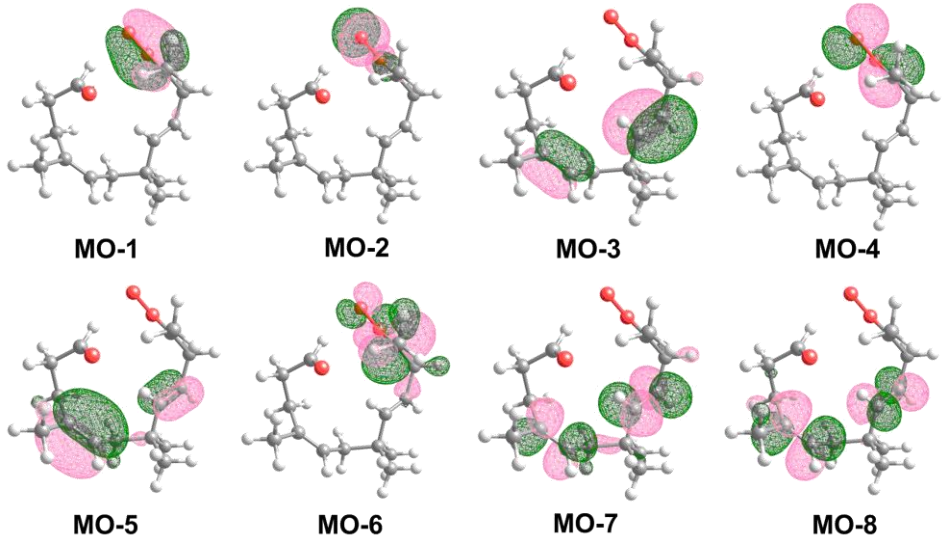

Figure S40: Active space of 10 electrons in 8 orbitals in QM(CASPT2)/MM calculations for **3b1**.

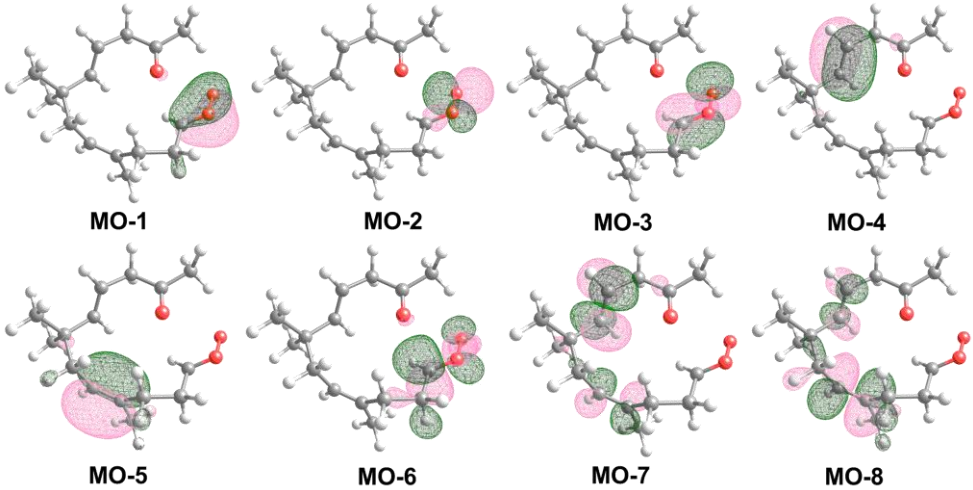

Figure S41: Active space of 10 electrons in 8 orbitals in QM(CASPT2)/MM calculations for **3b2**.

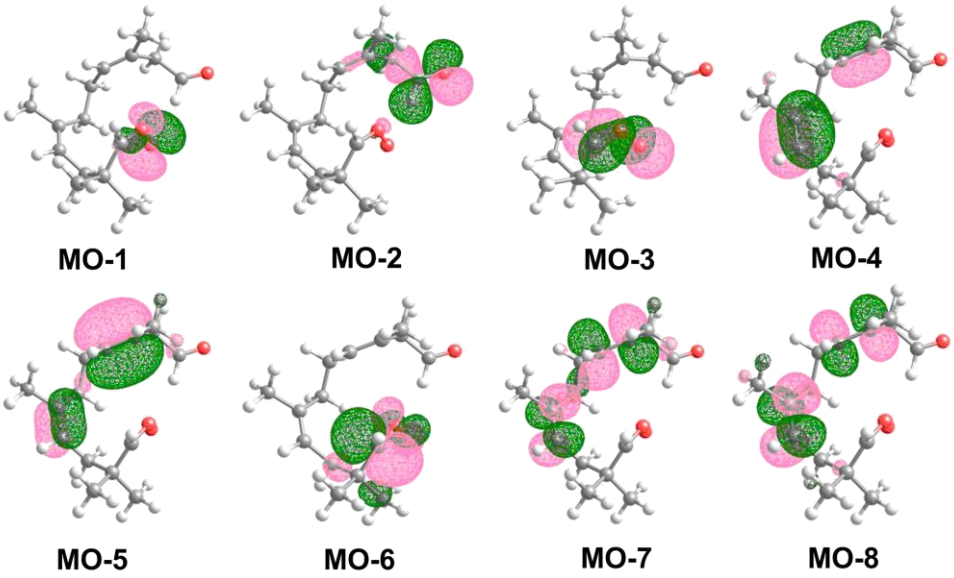

Figure S42: Active space of 10 electrons in 8 orbitals in QM(CASPT2)/MM calculations for **3c1**.

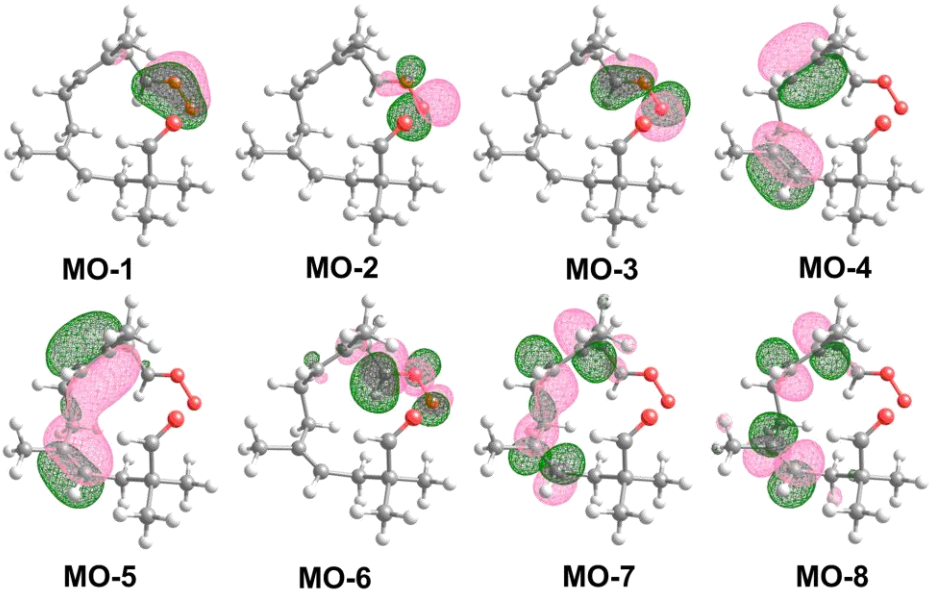

Figure S43: Active space of 10 electrons in 8 orbitals in QM(CASPT2)/MM calculations for **3c2**.

IX、Energy Profiles in Gas Phase

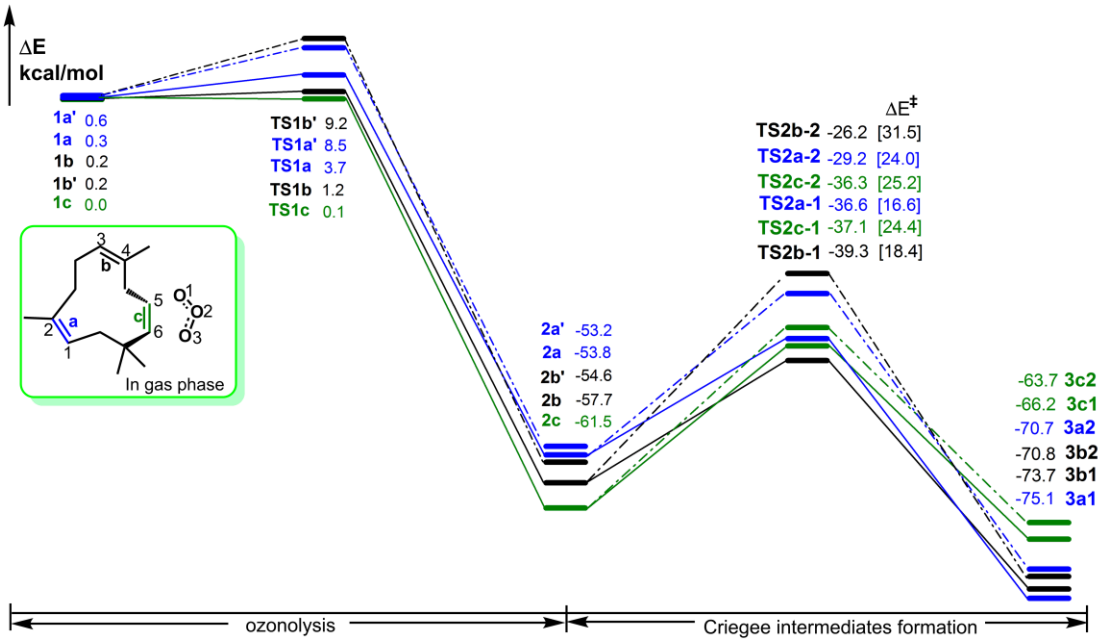

Figure S44: CASPT2(10,8)/6-31G*//B3LYP/def2-SVP computed energy profiles (in kcal/mol) for 1,3-cycloaddition reactions of ozone with α-humulene substrate and the following ring-cleavage reactions of the ozonides 2a, 2b, and 2c.

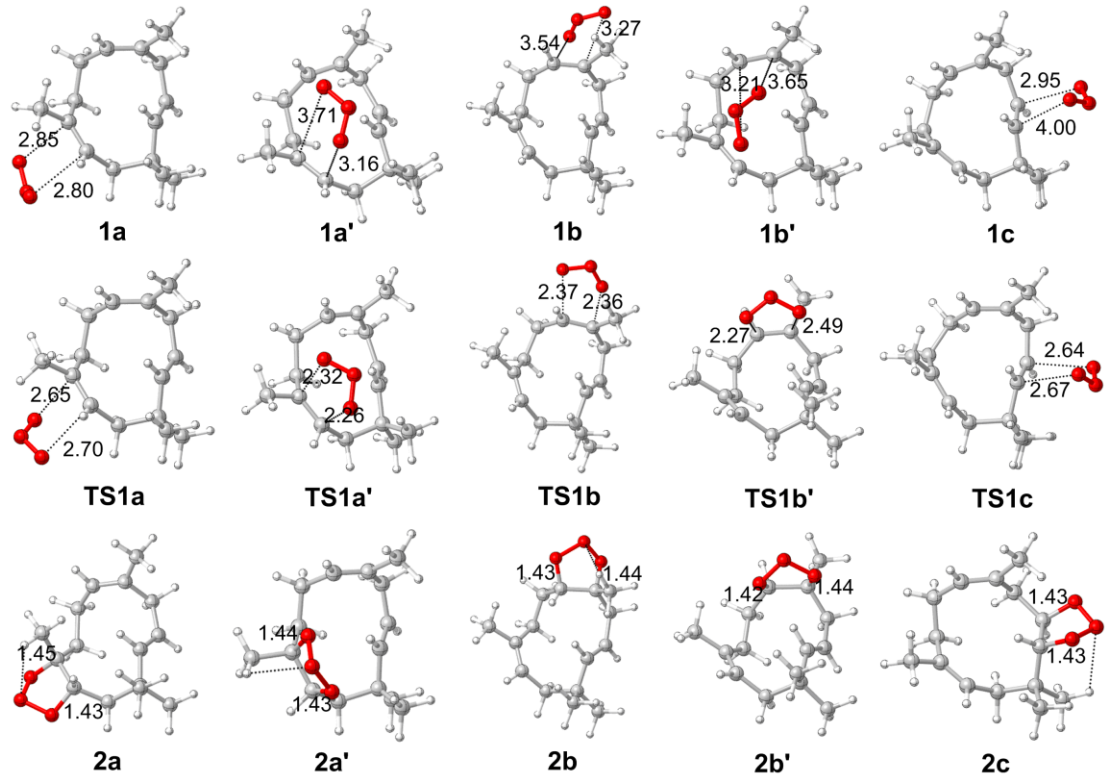

Figure S45: B3LYP/def2-SVP computed structures of transition states and intermediates relevant to the 1,3-cycloaddition reactions of ozone with α-humulene in gas phase in Fig. S44. Also shown are selected bond lengths in Å.

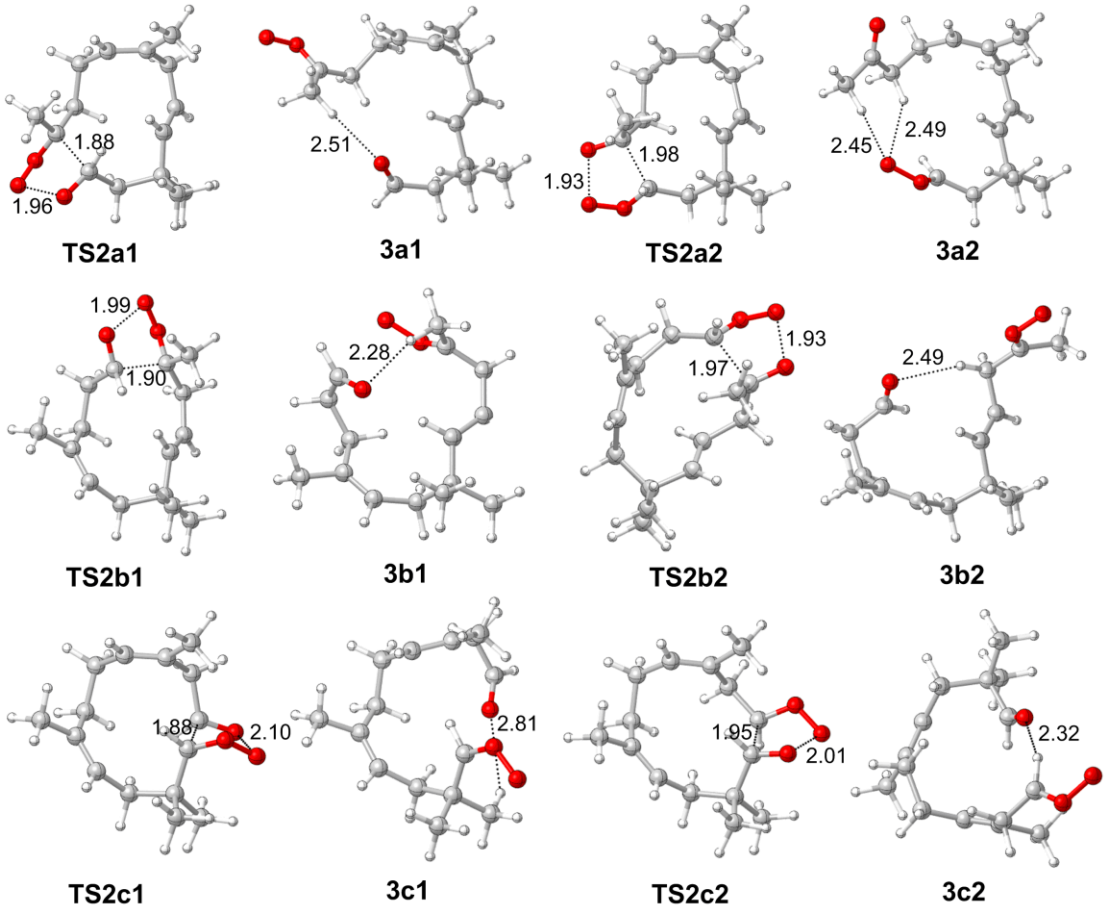

Figure S46: B3LYP/def2-SVP computed structures of transition states and intermediates relevant to the ring-cleavage reactions of the ozonides 2a, 2b, and 2c in gas phase in Fig. S44. Also shown are selected bond lengths in Å.

X、Cartesian Coordinates of Optimized Structures in QM Region

1) Conformers of α-Humulene Optimized in Gas Phase

Z3

	Symbol	X	Y	Z
1	C	-0.3855220	2.0583080	0.2754600
2	C	-1.6360990	1.6151970	0.4841450
3	H	-2.0521140	1.8166930	1.4711980
4	C	-2.6077120	0.9525990	-0.4770030
5	H	-2.8173550	1.6310720	-1.3158520
6	H	-3.5621760	0.8447840	0.0494660
7	C	0.3592590	1.9193280	-1.0448670
8	H	0.3400790	2.9036420	-1.5345790
9	H	-0.1895870	1.2530400	-1.7131540
10	C	1.8248330	1.5063440	-0.9576550
11	H	2.5138800	2.2786110	-1.2981080
12	C	2.4160860	0.3748970	-0.5421280
13	H	3.5063070	0.3958710	-0.5912860

14	C	-2.2340000	-0.4266200	-1.0883870
15	H	-3.1260010	-0.7887080	-1.6195730
16	H	-1.4720080	-0.2918780	-1.8575840
17	C	1.8756280	-0.9285850	0.0501610
18	C	0.6666210	-1.5070990	-0.7923200
19	C	-0.5397460	-1.9469070	-0.0069170
20	H	-0.3565120	-2.7367540	0.7224470
21	C	-1.7976860	-1.4862880	-0.1007710
22	C	-2.8889930	-2.0358050	0.7877230
23	H	-2.5128960	-2.8151830	1.4561750
24	H	-3.3338090	-1.2492120	1.4109580
25	H	-3.7088200	-2.4620010	0.1940560
26	C	0.3401280	2.8396490	1.3457690
27	H	1.3032590	2.3835380	1.5960970
28	H	0.5590680	3.8580080	0.9954460
29	H	-0.2545570	2.9195930	2.2597430
30	C	3.0216260	-1.9649360	0.0197530
31	H	2.6852720	-2.9266310	0.4219430
32	H	3.3756640	-2.1337350	-1.0034870
33	H	3.8753860	-1.6312480	0.6206640
34	C	1.5070870	-0.6773520	1.5326070
35	H	2.3478820	-0.2045230	2.0514900
36	H	0.6330440	-0.0311280	1.6242960
37	H	1.2872450	-1.6180150	2.0485570
38	H	1.0474600	-2.3726930	-1.3517020
39	H	0.3822340	-0.7795280	-1.5506270

Z2a

Symbol		X	Y	Z
1	C	0.1724490	2.1187390	0.2837680
2	C	-0.9072100	1.5562920	0.8483270
3	H	-0.7583060	1.0077980	1.7760480
4	C	-2.3023680	1.4729920	0.2805110
5	H	-2.5917070	2.4069770	-0.2153910
6	H	-3.0198110	1.3259340	1.0964820
7	C	2.5138450	1.1648900	-0.0246300
8	H	3.3023860	1.7819450	-0.4548180
9	C	2.5173170	-0.1216690	-0.4098680
10	H	3.3109310	-0.3889520	-1.1095190
11	C	-2.4498170	0.3182490	-0.7538440
12	H	-3.4780770	0.3386890	-1.1399940
13	H	-1.8001420	0.5419840	-1.6047510
14	C	1.5871820	-1.2868720	-0.0669670
15	C	0.2801530	-1.1631170	-0.9550240
16	C	-0.9830190	-1.7092020	-0.3444800

17	H	-0.9238630	-2.7280540	0.0409970
18	C	-2.1642330	-1.0779820	-0.2231810
19	C	-3.3342160	-1.7556900	0.4518360
20	H	-3.0651480	-2.7406680	0.8435250
21	H	-3.7142110	-1.1545670	1.2886150
22	H	-4.1752300	-1.8831550	-0.2428600
23	C	0.1394990	2.9240820	-0.9918920
24	H	0.5977140	3.9094790	-0.8346180
25	H	0.7220610	2.4331100	-1.7809450
26	H	-0.8730920	3.0819010	-1.3683830
27	C	2.3107670	-2.6008010	-0.4373860
28	H	1.6548010	-3.4642150	-0.2817960
29	H	2.6196090	-2.6005300	-1.4887920
30	H	3.2065470	-2.7464340	0.1767080
31	C	1.2793030	-1.3460860	1.4450230
32	H	2.2094570	-1.2847740	2.0193330
33	H	0.6194580	-0.5441730	1.7706380
34	H	0.7895970	-2.2904000	1.7019630
35	H	0.4849400	-1.6837090	-1.9021490
36	H	0.1344170	-0.1147810	-1.2073340
37	C	1.5549390	1.9200530	0.8911950
38	H	2.0022930	2.9008750	1.1017530
39	H	1.4578180	1.4124520	1.8549590

Z2b

Symbol		X	Y	Z
1	C	2.0304890	-1.4304040	0.2409410
2	C	2.4639220	-0.1599020	0.1909230
3	H	2.9883560	0.2103630	1.0722000
4	C	2.3438380	0.8330680	-0.9480150
5	H	2.6254220	0.3501670	-1.8933010
6	H	3.0914820	1.6173320	-0.7843680
7	C	1.2277750	-2.0851780	-0.8661570
8	H	1.4071400	-3.1698360	-0.8650840
9	H	1.5778560	-1.7333560	-1.8479430
10	C	-0.2670450	-1.8106510	-0.7952440
11	H	-0.8600730	-2.2672980	-1.5868780
12	C	-0.8261360	-0.9871390	0.0930330
13	H	-0.1730920	-0.5543610	0.8463260
14	C	0.9604550	1.5100970	-1.1973290
15	H	1.1357610	2.2957420	-1.9491280
16	H	0.2949780	0.7807050	-1.6580900
17	C	-2.2112330	-0.3820550	0.1000530
18	C	-2.0362040	1.0975570	-0.4113910
19	C	-1.0166190	1.9491710	0.3138640

20	H	-1.3936360	2.4768310	1.1903690
21	C	0.2783280	2.1431160	0.0010870
22	C	1.1289250	3.0818860	0.8240260
23	H	0.5487690	3.5610700	1.6172890
24	H	1.9709750	2.5581150	1.2929470
25	H	1.5638280	3.8724650	0.1974740
26	C	2.2539950	-2.2837860	1.4656670
27	H	1.2989080	-2.6443190	1.8688440
28	H	2.8463120	-3.1759350	1.2221880
29	H	2.7741780	-1.7367970	2.2570340
30	C	-2.7664460	-0.3819610	1.5392470
31	H	-2.9010620	-1.4055960	1.9047160
32	H	-2.0874370	0.1314050	2.2276210
33	H	-3.7380860	0.1234170	1.5836610
34	C	-3.1968330	-1.1044030	-0.8301520
35	H	-4.1788470	-0.6195740	-0.8016670
36	H	-2.8543610	-1.0938450	-1.8701990
37	H	-3.3290090	-2.1489920	-0.5289040
38	H	-3.0152530	1.5912640	-0.3400080
39	H	-1.7963800	1.0445290	-1.4784070

Z2c

Symbol		X	Y	Z
1	C	-1.6475910	1.6987350	-0.1120120
2	C	-2.6367710	0.8953370	0.3080420
3	H	-3.3022610	1.3110340	1.0670680
4	C	-2.9966650	-0.5117390	-0.1077430
5	H	-2.7495940	-0.6871790	-1.1612370
6	H	-4.0860920	-0.6121760	-0.0327980
7	C	-0.5955100	1.3141970	-1.1551360
8	H	-0.8872150	1.7724250	-2.1138860
9	H	-0.5906700	0.2372070	-1.3045980
10	C	0.7848370	1.8523210	-0.8199110
11	H	0.8639240	2.9231810	-1.0136570
12	C	1.9030740	1.3169640	-0.3136210
13	H	2.7088360	2.0455420	-0.1841410
14	C	-2.3286140	-1.6248080	0.7603090
15	H	-2.9662680	-2.5171190	0.7541810
16	H	-2.2685030	-1.2822100	1.7987060
17	C	2.3933870	-0.0562130	0.1420040
18	C	1.4638320	-1.2684500	-0.1058990
19	C	0.1127700	-1.2311410	0.5654900
20	H	-0.0231030	-0.4850250	1.3464000
21	C	-0.9564470	-1.9562560	0.2146460
22	C	-0.9350990	-3.0321490	-0.8451740

23	H	0.0452850	-3.1567000	-1.3090650
24	H	-1.2222790	-3.9974980	-0.4089260
25	H	-1.6640550	-2.8265600	-1.6408270
26	C	-1.5517500	3.1088860	0.4277430
27	H	-0.6110710	3.2721570	0.9655920
28	H	-1.5770520	3.8453230	-0.3867860
29	H	-2.3785540	3.3322720	1.1070520
30	C	3.7092900	-0.3304830	-0.6298800
31	H	4.1687090	-1.2660400	-0.2922720
32	H	3.5239750	-0.4112150	-1.7056570
33	H	4.4352990	0.4742260	-0.4742850
34	C	2.7364100	0.0491200	1.6489730
35	H	3.4500700	0.8597180	1.8294250
36	H	1.8499730	0.2497790	2.2570880
37	H	3.1900720	-0.8830060	2.0052240
38	H	2.0239980	-2.1579980	0.2203390
39	H	1.3356480	-1.3860740	-1.1899360

Z1a

Symbol		X	Y	Z
1	C	2.2201430	-0.2659010	0.2205900
2	C	1.7094170	1.0959240	0.8233560
3	C	0.9969510	-1.1334150	0.0319270
4	C	3.1517300	-0.9185930	1.2670170
5	C	2.9984850	-0.0360850	-1.0829250
6	C	0.8343340	1.9508120	-0.0601430
7	C	-0.4867030	2.1998810	0.0126980
8	C	-1.4440250	1.6053030	1.0306560
9	C	0.5454930	-1.7681650	-1.0515430
10	C	-2.5976190	0.7416420	0.4201970
11	C	-0.8522490	-2.3812310	-1.1246750
12	C	-1.8423320	-1.6341670	-0.2255730
13	C	-2.0268250	-0.3278940	-0.4639410
14	C	-1.1231810	3.1601690	-0.9684720
15	C	-2.4219950	-2.4007440	0.9340630
16	H	2.5986720	1.6851680	1.0903190
17	H	1.2027840	0.8689410	1.7680460
18	H	0.3541990	-1.1410130	0.9120910
19	H	4.0057710	-0.2691980	1.4921150
20	H	2.6206810	-1.1114820	2.2058630
21	H	3.5377540	-1.8747610	0.8995070
22	H	3.8514400	0.6299970	-0.9105850
23	H	3.3909400	-0.9799760	-1.4759050
24	H	2.3670160	0.4120000	-1.8552700
25	H	1.3741370	2.4655890	-0.8558200

26	H	-0.9016370	0.9865180	1.7501980
27	H	-1.9055660	2.4250960	1.6010300
28	H	1.1407650	-1.8043850	-1.9622010
29	H	-3.2731600	1.3936810	-0.1486920
30	H	-3.1870230	0.3293060	1.2453890
31	H	-1.1884430	-2.3457230	-2.1690430
32	H	-0.8253920	-3.4485400	-0.8641420
33	H	-1.5202690	0.0700040	-1.3429620
34	H	-0.3831820	3.5991940	-1.6429280
35	H	-1.6312040	3.9798800	-0.4428040
36	H	-1.8866050	2.6684440	-1.5844090
37	H	-1.6288670	-2.7976660	1.5823410
38	H	-2.9907760	-3.2699520	0.5782600
39	H	-3.0917780	-1.7963370	1.5502100

Z1b

	Symbol	X	Y	Z
1	C	-2.1006080	-0.1925340	0.1143970
2	C	-1.5937700	-1.6345810	-0.2796490
3	C	-1.8083500	0.7749790	-1.0275300
4	C	-1.4922390	0.2061060	1.4682660
5	C	-3.6373720	-0.2687810	0.2769760
6	C	-0.1777770	-1.6722840	-0.7850490
7	C	0.9673570	-1.9318700	-0.1330850
8	C	2.2866020	-1.6324010	-0.8233310
9	C	-1.0026780	1.8410550	-1.1638030
10	C	2.8157930	-0.1966920	-0.5009000
11	C	-0.0470200	2.4991660	-0.1833600
12	C	1.2614190	1.7593680	0.1051590
13	C	1.7228640	0.8131600	-0.7231100
14	C	1.0621570	-2.3989920	1.2972350
15	C	1.9316880	2.1782720	1.3903540
16	H	-2.2566730	-2.0213490	-1.0653170
17	H	-1.7393210	-2.2831930	0.5921720
18	H	-2.3822560	0.5196270	-1.9217840
19	H	-1.8551290	1.1861420	1.7926490
20	H	-1.7875340	-0.5198050	2.2343390
21	H	-0.4022790	0.2303310	1.4292370
22	H	-3.9101820	-1.0179560	1.0290390
23	H	-4.0458650	0.6957810	0.5958040
24	H	-4.1259380	-0.5452970	-0.6638200
25	H	-0.0797280	-1.3502070	-1.8209590
26	H	3.0564020	-2.3643790	-0.5469980
27	H	2.1521800	-1.7080860	-1.9086080
28	H	-1.0272560	2.3117990	-2.1465790

29	H	3.6824220	-0.0048780	-1.1497120
30	H	3.1861130	-0.1600300	0.5286700
31	H	0.1810560	3.5115620	-0.5471460
32	H	-0.5464050	2.6572460	0.7794120
33	H	1.1544890	0.6502240	-1.6359810
34	H	0.0857290	-2.5767470	1.7520880
35	H	1.5906820	-1.6658370	1.9207150
36	H	1.6394510	-3.3308080	1.3588910
37	H	1.2805620	2.0023340	2.2570140
38	H	2.1421510	3.2562210	1.3771320
39	H	2.8789390	1.6634760	1.5643160

Z1c

	Symbol	X	Y	Z
1	C	2.3780420	-0.5461250	0.0132050
2	C	2.2877060	0.9521710	0.5098540
3	C	1.0353750	-1.2078530	0.2643590
4	C	3.4604840	-1.2628560	0.8464620
5	C	2.7879280	-0.5857760	-1.4698380
6	C	1.1658420	1.7039490	-0.1457150
7	C	-0.0587390	1.9431680	0.3505130
8	C	-1.1693820	2.3543780	-0.5982810
9	C	0.0593340	-1.4327770	-0.6197290
10	C	-1.8073120	1.1240530	-1.3127370
11	C	-1.2949730	-1.9874500	-0.2526920
12	C	-2.4716520	-1.0345560	-0.0148280
13	C	-2.6465860	0.2300290	-0.4361620
14	C	-0.4686600	1.7241770	1.7846510
15	C	-3.5637370	-1.6964310	0.8010510
16	H	3.2563100	1.4268580	0.3004110
17	H	2.1739680	0.9435000	1.5987820
18	H	0.8367080	-1.4417020	1.3133390
19	H	4.4292950	-0.7612820	0.7436010
20	H	3.1999000	-1.2724700	1.9108410
21	H	3.5822120	-2.3019740	0.5223660
22	H	3.7697490	-0.1190550	-1.6053040
23	H	2.8535320	-1.6187120	-1.8270390
24	H	2.0801400	-0.0554620	-2.1122610
25	H	1.3210940	1.9386700	-1.1998560
26	H	-1.9518360	2.9169450	-0.0725520
27	H	-0.7703180	3.0168560	-1.3755980
28	H	0.2266400	-1.2099450	-1.6707670
29	H	-2.4632760	1.5091840	-2.1072220
30	H	-1.0101980	0.5679030	-1.8078650
31	H	-1.6126910	-2.7191850	-1.0122120

32	H	-1.1830220	-2.5721190	0.6705080
33	H	-3.5771080	0.7035270	-0.1155440
34	H	0.3568550	1.4073020	2.4248630
35	H	-1.2618200	0.9709030	1.8500740
36	H	-0.8800210	2.6519340	2.2040350
37	H	-3.2009410	-1.9796570	1.7981160
38	H	-3.9039320	-2.6244400	0.3218880
39	H	-4.4332610	-1.0461870	0.9267170

E3

	Symbol	X	Y	Z
1	C	-2.4032990	0.1841310	0.0428340
2	C	-1.9306720	-1.2942890	0.3315100
3	C	-1.2405130	1.1016370	0.3653070
4	C	-3.5834820	0.4948660	0.9889500
5	C	-2.8814620	0.3206180	-1.4118160
6	C	-0.6722700	-1.6929590	-0.3932030
7	C	0.5423890	-1.9658250	0.1145430
8	C	1.7343290	-2.1185970	-0.8151040
9	C	-0.5292190	1.8705430	-0.4634130
10	C	2.6971060	-0.8864370	-0.7745400
11	C	0.7947030	2.4890890	-0.0590390
12	C	1.9422470	1.4672740	-0.0454780
13	C	1.8885610	0.3811920	-0.8290470
14	C	0.8641570	-2.0396410	1.5862950
15	C	3.0475760	1.7645600	0.9358690
16	H	-2.7598810	-1.9598120	0.0495020
17	H	-1.8049720	-1.4018800	1.4137730
18	H	-0.8961580	1.0233890	1.4002470
19	H	-4.3993730	-0.2231470	0.8466870
20	H	-3.2739510	0.4464000	2.0388870
21	H	-3.9785790	1.4990190	0.8030990
22	H	-3.7209280	-0.3566660	-1.6022740
23	H	-3.2228820	1.3409130	-1.6157820
24	H	-2.0918310	0.0852490	-2.1308070
25	H	-0.7533630	-1.6842010	-1.4805030
26	H	2.3100460	-3.0225010	-0.5731760
27	H	1.3722200	-2.2384920	-1.8427340
28	H	-0.8234600	1.9638910	-1.5068900
29	H	3.3884180	-0.9720730	-1.6250760
30	H	3.3151130	-0.9223920	0.1284290
31	H	1.0444290	3.3456820	-0.7008720
32	H	0.7101940	2.8992680	0.9565340
33	H	1.0479590	0.3191520	-1.5157480
34	H	-0.0203360	-1.9818680	2.2232430

35	H	1.5394770	-1.2261350	1.8799800
36	H	1.3825040	-2.9786620	1.8194150
37	H	2.6640530	1.8350800	1.9625760
38	H	3.5075530	2.7367220	0.7124470
39	H	3.8428420	1.0160880	0.9170290

2) QM/MM Computed Transition States and Minimum-energy Structures in Stage I

1a

	Symbol	X	Y	Z
1	C	23.0810000	23.8650000	87.0930000
2	C	22.2820000	24.7940000	86.5330000
3	C	21.8980000	24.9610000	85.0760000
4	C	23.6760000	22.7010000	86.3260000
5	C	22.7430000	21.5090000	86.1780000
6	C	21.4500000	21.5330000	86.5180000
7	C	20.8030000	24.0410000	84.4550000
8	C	20.3390000	20.5690000	86.1710000
9	C	19.4250000	21.3070000	85.1200000
10	C	18.9280000	22.6790000	85.5070000
11	C	19.5040000	23.8930000	85.2250000
12	C	18.8930000	25.1550000	85.7780000
13	C	23.3740000	23.8760000	88.5720000
14	C	19.5230000	20.2450000	87.4390000
15	C	20.8390000	19.2620000	85.5390000
16	H	21.8720000	25.5520000	87.2140000
17	H	22.7940000	24.8350000	84.4430000
18	H	21.5780000	26.0060000	84.9370000
19	H	24.6170000	22.3760000	86.8060000
20	H	23.9640000	23.0260000	85.3090000
21	H	23.1800000	20.6230000	85.7020000
22	H	21.0850000	22.4390000	87.0130000
23	H	20.5580000	24.4700000	83.4680000
24	H	21.2320000	23.0520000	84.2600000
25	H	18.0390000	22.7000000	86.1440000
26	H	17.8750000	24.9730000	86.1510000
27	H	19.4970000	25.5440000	86.6160000
28	H	18.8520000	25.9520000	85.0190000
29	H	23.0700000	22.9230000	89.0410000
30	H	24.4580000	23.9840000	88.7570000
31	H	22.8550000	24.6950000	89.0930000
32	H	20.1440000	19.7020000	88.1700000
33	H	19.1550000	21.1600000	87.9310000
34	H	18.6490000	19.6160000	87.1980000
35	H	19.9920000	18.6040000	85.2830000

36	H	21.3990000	19.4480000	84.6100000
37	H	21.5120000	18.7220000	86.2240000
38	H	18.5550000	20.6600000	84.9270000
39	H	19.9830000	21.3610000	84.1730000
40	O	17.8410000	24.3180000	83.1360000
41	O	17.4100000	23.1460000	82.9410000
42	O	16.8150000	22.6090000	83.9260000

1b

	Symbol	X	Y	Z
1	C	22.9090000	23.4480000	88.9860000
2	C	22.1160000	24.4360000	88.4530000
3	C	22.0060000	24.8680000	87.0130000
4	C	23.6740000	22.4480000	88.1470000
5	C	22.8270000	21.2790000	87.6750000
6	C	21.5000000	21.2060000	87.8220000
7	C	21.1100000	24.0270000	86.0560000
8	C	20.5060000	20.2960000	87.1380000
9	C	19.7940000	21.1860000	86.0520000
10	C	19.1610000	22.4790000	86.5150000
11	C	19.6970000	23.7200000	86.5160000
12	C	18.8780000	24.9160000	86.9410000
13	C	22.8640000	23.1650000	90.4650000
14	C	19.4780000	19.7810000	88.1660000
15	C	21.1620000	19.1030000	86.4300000
16	H	21.4400000	24.9390000	89.1530000
17	H	23.0150000	24.9060000	86.5700000
18	H	21.6450000	25.9080000	87.0120000
19	H	24.5520000	22.0800000	88.7050000
20	H	24.0910000	22.9480000	87.2540000
21	H	23.3670000	20.5070000	87.1150000
22	H	21.0130000	21.9980000	88.4010000
23	H	21.0450000	24.6030000	85.1140000
24	H	21.6280000	23.0950000	85.8080000
25	H	18.1250000	22.3900000	86.8710000
26	H	17.8370000	24.6400000	87.1710000
27	H	19.3000000	25.4050000	87.8370000
28	H	18.8740000	25.6940000	86.1560000
29	H	22.5390000	22.1260000	90.6520000
30	H	23.8690000	23.2670000	90.9100000
31	H	22.1810000	23.8430000	90.9990000
32	H	19.9660000	19.1510000	88.9280000
33	H	18.9800000	20.6140000	88.6890000
34	H	18.6970000	19.1770000	87.6740000
35	H	20.3940000	18.4940000	85.9240000

36	H	21.8790000	19.4280000	85.6590000
37	H	21.7040000	18.4580000	87.1400000
38	H	19.0170000	20.5670000	85.5710000
39	H	20.5410000	21.3980000	85.2730000
40	O	24.9200000	24.9250000	88.9670000
41	O	24.3970000	25.8690000	89.6420000
42	O	23.4320000	26.4670000	89.0670000

1c

	Symbol	X	Y	Z
1	C	23.8890000	24.0640000	88.3340000
2	C	22.7990000	24.8410000	88.1780000
3	C	21.8970000	24.9670000	86.9660000
4	C	24.3350000	23.0450000	87.3060000
5	C	23.6040000	21.7160000	87.3980000
6	C	22.5670000	21.4790000	88.2080000
7	C	20.8290000	23.8680000	86.6850000
8	C	21.5680000	20.3430000	88.1830000
9	C	20.2330000	20.9450000	87.5980000
10	C	19.7160000	22.1990000	88.2530000
11	C	19.9210000	23.4960000	87.8400000
12	C	19.3410000	24.6350000	88.6410000
13	C	24.7140000	24.1100000	89.5960000
14	C	21.3390000	19.8260000	89.6180000
15	C	21.9980000	19.1760000	87.2840000
16	H	22.5490000	25.5000000	89.0210000
17	H	22.5190000	25.0230000	86.0560000
18	H	21.3820000	25.9390000	87.0330000
19	H	25.4250000	22.8780000	87.3850000
20	H	24.1810000	23.4430000	86.2850000
21	H	23.9180000	20.9510000	86.6790000
22	H	22.2950000	22.2710000	88.9120000
23	H	20.2020000	24.2460000	85.8590000
24	H	21.3220000	22.9720000	86.2970000
25	H	19.1590000	22.0620000	89.1870000
26	H	18.5060000	24.3060000	89.2780000
27	H	20.1090000	25.0730000	89.3020000
28	H	18.9870000	25.4480000	87.9870000
29	H	24.7950000	23.1060000	90.0510000
30	H	25.7450000	24.4390000	89.3740000
31	H	24.2910000	24.7950000	90.3470000
32	H	22.2590000	19.3760000	90.0220000
33	H	21.0360000	20.6390000	90.2980000
34	H	20.5490000	19.0560000	89.6380000
35	H	21.2230000	18.3920000	87.2810000

36	H	22.1460000	19.4990000	86.2420000
37	H	22.9330000	18.7170000	87.6420000
38	H	19.4510000	20.1710000	87.6790000
39	H	20.3810000	21.1260000	86.5230000
40	O	25.3250000	20.2300000	89.4100000
41	O	24.1810000	20.4150000	89.9310000
42	O	25.5530000	20.8960000	88.3510000

1a'

Symbol		X	Y	Z
1	C	23.7520000	23.4590000	87.2490000
2	C	23.0200000	24.4510000	86.7030000
3	C	22.5790000	24.6210000	85.2660000
4	C	24.1920000	22.2290000	86.4830000
5	C	23.1470000	21.1240000	86.4220000
6	C	21.8880000	21.2820000	86.8450000
7	C	21.3780000	23.7780000	84.7410000
8	C	20.6670000	20.4280000	86.5950000
9	C	19.7840000	21.2300000	85.5650000
10	C	19.4290000	22.6590000	85.9000000
11	C	20.0950000	23.7890000	85.5470000
12	C	19.5230000	25.1470000	85.8650000
13	C	24.1170000	23.4700000	88.7120000
14	C	19.8910000	20.2280000	87.9120000
15	C	21.0030000	19.0630000	85.9810000
16	H	22.7140000	25.2540000	87.3840000
17	H	23.4240000	24.4040000	84.5910000
18	H	22.3480000	25.6850000	85.1120000
19	H	25.1290000	21.8330000	86.9180000
20	H	24.4470000	22.5010000	85.4420000
21	H	23.4660000	20.1950000	85.9370000
22	H	21.6430000	22.2310000	87.3290000
23	H	21.1380000	24.1810000	83.7390000
24	H	21.7100000	22.7440000	84.5880000
25	H	18.4920000	22.7970000	86.4520000
26	H	18.5490000	25.0690000	86.3680000
27	H	20.1870000	25.7320000	86.5210000
28	H	19.4040000	25.7460000	84.9450000
29	H	23.7710000	22.5450000	89.2090000
30	H	25.2140000	23.5020000	88.8460000
31	H	23.6760000	24.3260000	89.2420000
32	H	20.4940000	19.6570000	88.6360000
33	H	19.6260000	21.1900000	88.3770000
34	H	18.9550000	19.6720000	87.7340000
35	H	20.0820000	18.4850000	85.7970000

36	H	21.5260000	19.1690000	85.0180000
37	H	21.6580000	18.4780000	86.6470000
38	H	18.8490000	20.6640000	85.4160000
39	H	20.3130000	21.1990000	84.6000000
40	O	21.0310000	25.1010000	89.2370000
41	O	20.4280000	24.0270000	89.4950000
42	O	19.4210000	23.7380000	88.8010000

1b'

Symbol		X	Y	Z
1	C	23.8170000	23.4730000	87.2390000
2	C	23.0640000	24.4480000	86.6910000
3	C	22.5830000	24.5940000	85.2610000
4	C	24.2300000	22.2220000	86.4940000
5	C	23.1820000	21.1180000	86.4890000
6	C	21.9340000	21.2850000	86.9390000
7	C	21.3950000	23.7250000	84.7570000
8	C	20.7090000	20.4250000	86.7310000
9	C	19.8300000	21.1820000	85.6650000
10	C	19.4630000	22.6190000	85.9560000
11	C	20.1140000	23.7400000	85.5710000
12	C	19.5330000	25.1040000	85.8550000
13	C	24.2560000	23.5360000	88.6800000
14	C	19.9410000	20.2960000	88.0620000
15	C	21.0350000	19.0290000	86.1840000
16	H	22.7960000	25.2750000	87.3590000
17	H	23.4240000	24.3990000	84.5720000
18	H	22.3250000	25.6520000	85.1100000
19	H	25.1790000	21.8400000	86.9100000
20	H	24.4530000	22.4670000	85.4380000
21	H	23.4880000	20.1790000	86.0130000
22	H	21.6990000	22.2390000	87.4190000
23	H	21.1480000	24.1050000	83.7480000
24	H	21.7380000	22.6920000	84.6240000
25	H	18.5320000	22.7600000	86.5220000
26	H	18.5650000	25.0330000	86.3760000
27	H	20.2020000	25.7280000	86.4690000
28	H	19.3850000	25.6720000	84.9190000
29	H	23.9780000	22.6120000	89.2160000
30	H	25.3560000	23.6220000	88.7490000
31	H	23.8030000	24.3830000	89.2140000
32	H	20.5340000	19.7270000	88.7960000
33	H	19.7310000	21.2840000	88.5020000
34	H	18.9820000	19.7700000	87.9190000
35	H	20.1100000	18.4500000	86.0330000

36	H	21.5530000	19.0830000	85.2130000
37	H	21.6870000	18.4720000	86.8760000
38	H	18.9000000	20.6040000	85.5250000
39	H	20.3670000	21.1230000	84.7050000
40	O	21.0070000	25.6820000	88.9890000
41	O	20.3910000	24.6020000	89.1530000
42	O	21.0240000	23.6310000	89.6270000

TS1a'

	Symbol	X	Y	Z
1	C	23.7680000	23.2020000	87.5450000
2	C	23.0630000	24.2100000	86.9990000
3	C	22.5690000	24.3800000	85.5760000
4	C	24.1280000	21.9300000	86.8080000
5	C	23.0300000	20.8790000	86.7790000
6	C	21.7650000	21.1160000	87.1520000
7	C	21.4510000	23.4450000	85.0300000
8	C	20.5400000	20.2630000	86.9190000
9	C	19.6330000	20.9860000	85.8510000
10	C	19.2550000	22.4520000	85.8930000
11	C	20.0310000	23.5620000	85.5500000
12	C	19.3000000	24.8380000	85.2040000
13	C	24.1670000	23.2320000	89.0000000
14	C	19.7810000	20.0710000	88.2490000
15	C	20.8830000	18.8790000	86.3450000
16	H	22.8030000	25.0320000	87.6730000
17	H	23.4210000	24.2620000	84.8810000
18	H	22.2390000	25.4220000	85.4510000
19	H	25.0460000	21.4920000	87.2380000
20	H	24.3870000	22.1640000	85.7570000
21	H	23.3210000	19.9150000	86.3460000
22	H	21.5320000	22.0910000	87.5920000
23	H	21.3740000	23.6830000	83.9540000
24	H	21.7860000	22.4050000	85.0960000
25	H	18.1770000	22.6300000	85.9030000
26	H	18.3850000	24.9510000	85.8070000
27	H	19.9180000	25.7340000	85.3470000
28	H	19.0030000	24.8050000	84.1390000
29	H	23.7690000	22.3500000	89.5350000
30	H	25.2670000	23.1980000	89.1140000
31	H	23.7990000	24.1350000	89.5090000
32	H	20.4080000	19.5110000	88.9610000
33	H	19.5110000	21.0340000	88.6980000
34	H	18.8540000	19.4930000	88.0910000
35	H	19.9640000	18.2900000	86.1810000

36	H	21.4090000	18.9560000	85.3800000
37	H	21.5320000	18.3210000	87.0380000
38	H	18.6940000	20.4140000	85.7940000
39	H	20.1280000	20.8340000	84.8770000
40	O	18.6750000	23.0340000	88.1440000
41	O	19.1320000	24.2350000	88.0710000
42	O	20.3670000	24.2800000	87.7110000

TS1b'

	Symbol	X	Y	Z
1	C	23.8230000	23.2230000	87.7110000
2	C	23.0010000	24.2440000	87.2690000
3	C	22.1830000	24.4080000	86.0030000
4	C	23.9780000	21.8790000	87.0210000
5	C	22.8670000	20.8520000	87.0010000
6	C	21.6320000	21.0090000	87.4850000
7	C	21.0390000	23.4760000	85.5320000
8	C	20.4210000	20.1280000	87.2650000
9	C	19.4910000	20.8880000	86.2520000
10	C	19.0980000	22.2980000	86.6320000
11	C	19.7570000	23.4410000	86.3480000
12	C	19.1990000	24.7780000	86.7720000
13	C	24.9660000	23.5880000	88.6350000
14	C	19.6890000	19.9330000	88.6090000
15	C	20.7590000	18.7600000	86.6600000
16	H	23.2000000	25.2060000	87.7480000
17	H	22.9370000	24.4090000	85.1890000
18	H	21.7930000	25.4350000	86.0220000
19	H	24.8950000	21.3940000	87.4010000
20	H	24.2140000	22.1090000	85.9610000
21	H	23.1350000	19.9350000	86.4630000
22	H	21.4150000	21.9260000	88.0340000
23	H	20.7600000	23.8610000	84.5320000
24	H	21.4160000	22.4620000	85.3660000
25	H	18.1650000	22.3920000	87.2020000
26	H	18.2090000	24.6680000	87.2410000
27	H	19.8570000	25.2750000	87.5030000
28	H	19.1150000	25.4690000	85.9150000
29	H	25.2190000	22.7720000	89.3280000
30	H	25.8670000	23.8050000	88.0280000
31	H	24.7510000	24.4920000	89.2250000
32	H	20.3260000	19.3900000	89.3260000
33	H	19.4250000	20.9010000	89.0640000
34	H	18.7590000	19.3540000	88.4730000
35	H	19.8380000	18.1780000	86.4930000

36	H	21.2750000	18.8520000	85.6920000
37	H	21.4120000	18.1800000	87.3310000
38	H	18.5760000	20.2830000	86.1220000
39	H	19.9990000	20.8840000	85.2740000
40	O	21.3750000	24.4180000	89.1570000
41	O	22.1930000	23.9660000	90.0280000
42	O	22.5730000	22.7660000	89.8250000

2a

	Symbol	X	Y	Z
1	C	23.9510000	24.1030000	86.9740000
2	C	22.9490000	24.6770000	86.2800000
3	C	22.4640000	24.3240000	84.8880000
4	C	24.7030000	22.8800000	86.4890000
5	C	24.0080000	21.5580000	86.7650000
6	C	22.7530000	21.4450000	87.2140000
7	C	21.6400000	23.0330000	84.6600000
8	C	21.8650000	20.2180000	87.2600000
9	C	20.8290000	20.3250000	86.0950000
10	C	19.8760000	21.5270000	86.0560000
11	C	20.2330000	22.8950000	85.2990000
12	C	19.7970000	24.0750000	86.1710000
13	C	24.3580000	24.6130000	88.3330000
14	C	21.1420000	20.1590000	88.6240000
15	C	22.6500000	18.9110000	87.0680000
16	H	22.4470000	25.5280000	86.7550000
17	H	23.3400000	24.2350000	84.2230000
18	H	21.8840000	25.1750000	84.5040000
19	H	25.7180000	22.8630000	86.9270000
20	H	24.8660000	22.9410000	85.3970000
21	H	24.5750000	20.6630000	86.4800000
22	H	22.2380000	22.3730000	87.4900000
23	H	21.4750000	22.9630000	83.5740000
24	H	22.2500000	22.1670000	84.9340000
25	H	19.5560000	21.7940000	87.0780000
26	H	18.7320000	23.9630000	86.4260000
27	H	20.3750000	24.1110000	87.1060000
28	H	19.9320000	25.0290000	85.6440000
29	H	24.2990000	23.8110000	89.0900000
30	H	25.4080000	24.9570000	88.3200000
31	H	23.7280000	25.4510000	88.6700000
32	H	21.8690000	19.9920000	89.4350000
33	H	20.6060000	21.0930000	88.8560000
34	H	20.4090000	19.3360000	88.6490000
35	H	21.9700000	18.0450000	87.1170000

36	H	23.1700000	18.8710000	86.1000000
37	H	23.4100000	18.7980000	87.8550000
38	H	20.1740000	19.4390000	86.1570000
39	H	21.3420000	20.2330000	85.1250000
40	O	19.3460000	22.8080000	84.1570000
41	O	18.1790000	22.2000000	84.6940000
42	O	18.7370000	21.0380000	85.3300000

2b

	Symbol	X	Y	Z
1	C	23.9620000	22.5960000	87.4630000
2	C	23.1080000	23.7850000	86.9040000
3	C	22.8290000	23.8670000	85.3950000
4	C	23.8880000	21.2340000	86.7680000
5	C	22.5800000	20.4860000	86.7350000
6	C	21.3900000	20.9320000	87.1500000
7	C	21.5590000	23.2080000	84.8090000
8	C	20.0210000	20.3330000	86.8950000
9	C	19.3840000	21.1490000	85.7120000
10	C	19.3260000	22.6510000	85.8640000
11	C	20.2410000	23.5640000	85.4760000
12	C	19.9610000	25.0390000	85.6250000
13	C	23.8340000	22.4890000	88.9860000
14	C	19.1580000	20.4770000	88.1650000
15	C	20.0790000	18.8560000	86.4790000
16	H	22.1790000	23.8870000	87.4870000
17	H	23.7130000	23.5020000	84.8500000
18	H	22.7890000	24.9450000	85.1820000
19	H	24.6580000	20.5950000	87.2300000
20	H	24.2350000	21.3740000	85.7310000
21	H	22.6570000	19.5100000	86.2430000
22	H	21.3360000	21.9110000	87.6330000
23	H	21.5060000	23.5540000	83.7610000
24	H	21.6770000	22.1190000	84.7720000
25	H	18.4080000	23.0430000	86.3210000
26	H	18.9610000	25.2260000	86.0460000
27	H	20.6910000	25.5500000	86.2750000
28	H	20.0230000	25.5530000	84.6490000
29	H	22.8650000	22.0530000	89.2670000
30	H	24.6310000	21.8360000	89.3740000
31	H	23.9290000	23.4770000	89.4560000
32	H	19.5890000	19.9010000	89.0010000
33	H	19.0870000	21.5300000	88.4850000
34	H	18.1340000	20.1080000	87.9910000
35	H	19.0620000	18.4630000	86.3150000

36	H	20.6370000	18.7230000	85.5390000
37	H	20.5630000	18.2440000	87.2580000
38	H	18.3590000	20.7700000	85.5580000
39	H	19.9380000	20.8830000	84.7990000
40	O	23.9170000	24.9220000	87.2500000
41	O	25.2690000	24.4130000	87.5810000
42	O	25.2710000	23.0870000	87.1050000

2c

	Symbol	X	Y	Z
1	C	23.6550000	23.6030000	87.4780000
2	C	22.9960000	24.6510000	86.9450000
3	C	22.5840000	24.8900000	85.5060000
4	C	24.0410000	22.3890000	86.6620000
5	C	23.4370000	21.0410000	87.1070000
6	C	22.0160000	21.0360000	87.7720000
7	C	21.5720000	23.9170000	84.8480000
8	C	20.8690000	20.2960000	87.0290000
9	C	20.4860000	21.1060000	85.7500000
10	C	19.8540000	22.4540000	85.9820000
11	C	20.2930000	23.6750000	85.6150000
12	C	19.4750000	24.9070000	85.9200000
13	C	24.0660000	23.5890000	88.9310000
14	C	19.6670000	20.2110000	87.9930000
15	C	21.2540000	18.8640000	86.6160000
16	H	22.7620000	25.4710000	87.6370000
17	H	23.4780000	24.9160000	84.8600000
18	H	22.1620000	25.9020000	85.4490000
19	H	25.1370000	22.2470000	86.7000000
20	H	23.7940000	22.5420000	85.6040000
21	H	23.4510000	20.3380000	86.2610000
22	H	21.6870000	22.0680000	87.9670000
23	H	21.3030000	24.3490000	83.8670000
24	H	22.0660000	22.9630000	84.6190000
25	H	18.8870000	22.4170000	86.4980000
26	H	18.5220000	24.6500000	86.4090000
27	H	20.0150000	25.6050000	86.5820000
28	H	19.2600000	25.4830000	85.0020000
29	H	23.6280000	22.7380000	89.4750000
30	H	25.1620000	23.4760000	89.0230000
31	H	23.7720000	24.5190000	89.4410000
32	H	19.8950000	19.5370000	88.8320000
33	H	19.4070000	21.1920000	88.4210000
34	H	18.7780000	19.8230000	87.4690000
35	H	20.3670000	18.3380000	86.2270000

36	H	22.0170000	18.8430000	85.8240000
37	H	21.6450000	18.2960000	87.4740000
38	H	19.7690000	20.4810000	85.1850000
39	H	21.3770000	21.1920000	85.1060000
40	O	22.2750000	20.4860000	89.0740000
41	O	23.4290000	19.6490000	88.8640000
42	O	24.2870000	20.5230000	88.1400000

2a'

	Symbol	X	Y	Z
1	C	23.8080000	23.1900000	87.5840000
2	C	23.1180000	24.2140000	87.0460000
3	C	22.6120000	24.3750000	85.6260000
4	C	24.1440000	21.9180000	86.8350000
5	C	23.0290000	20.8870000	86.7780000
6	C	21.7710000	21.1220000	87.1720000
7	C	21.4080000	23.5100000	85.1700000
8	C	20.5360000	20.2830000	86.9270000
9	C	19.5570000	21.0590000	85.9750000
10	C	19.1270000	22.5210000	86.2180000
11	C	20.0560000	23.7780000	85.8680000
12	C	19.2400000	24.8160000	85.0880000
13	C	24.2300000	23.2110000	89.0330000
14	C	19.8550000	19.9640000	88.2800000
15	C	20.8660000	18.9510000	86.2330000
16	H	22.8780000	25.0410000	87.7210000
17	H	23.4290000	24.1520000	84.9180000
18	H	22.3680000	25.4370000	85.4650000
19	H	25.0480000	21.4550000	87.2710000
20	H	24.4210000	22.1550000	85.7890000
21	H	23.3030000	19.9370000	86.3050000
22	H	21.5600000	22.0790000	87.6610000
23	H	21.2530000	23.7020000	84.0980000
24	H	21.6790000	22.4560000	85.2630000
25	H	18.1990000	22.6640000	85.6340000
26	H	18.3440000	25.1040000	85.6570000
27	H	19.8420000	25.7190000	84.9180000
28	H	18.9370000	24.4120000	84.1110000
29	H	23.8140000	22.3430000	89.5760000
30	H	25.3290000	23.1430000	89.1290000
31	H	23.8990000	24.1260000	89.5470000
32	H	20.5140000	19.3300000	88.8940000
33	H	19.6250000	20.8770000	88.8430000
34	H	18.9100000	19.4170000	88.1230000
35	H	19.9470000	18.3650000	86.0620000

36	H	21.3500000	19.1050000	85.2550000
37	H	21.5490000	18.3490000	86.8520000
38	H	18.6260000	20.4700000	85.9400000
39	H	19.9490000	21.0240000	84.9450000
40	O	18.8380000	22.6950000	87.6070000
41	O	19.0890000	24.0920000	87.8590000
42	O	20.3260000	24.2900000	87.1870000

2b'

	Symbol	X	Y	Z
1	C	23.7980000	23.0890000	88.0540000
2	C	22.7730000	24.2280000	87.6160000
3	C	22.2040000	24.3920000	86.1990000
4	C	23.9230000	21.8040000	87.2140000
5	C	22.7840000	20.8210000	87.0950000
6	C	21.5440000	20.9360000	87.5820000
7	C	21.1050000	23.4760000	85.6140000
8	C	20.3410000	20.0740000	87.2470000
9	C	19.5030000	20.8710000	86.1830000
10	C	19.0940000	22.2770000	86.5600000
11	C	19.7660000	23.4240000	86.3320000
12	C	19.1750000	24.7550000	86.7320000
13	C	25.1850000	23.7220000	88.2270000
14	C	19.5060000	19.8540000	88.5240000
15	C	20.7070000	18.7140000	86.6360000
16	H	23.3090000	25.1720000	87.8180000
17	H	23.0740000	24.3710000	85.5210000
18	H	21.8380000	25.4300000	86.1560000
19	H	24.8090000	21.2590000	87.5880000
20	H	24.2210000	22.1230000	86.1980000
21	H	23.0410000	19.9450000	86.4890000
22	H	21.3020000	21.8030000	88.1990000
23	H	20.9040000	23.8850000	84.6050000
24	H	21.4920000	22.4650000	85.4550000
25	H	18.1290000	22.3640000	87.0770000
26	H	18.1560000	24.6370000	87.1340000
27	H	19.7820000	25.2450000	87.5110000
28	H	19.1430000	25.4560000	85.8790000
29	H	25.9080000	22.9770000	88.5940000
30	H	25.5540000	24.1360000	87.2760000
31	H	25.1360000	24.5430000	88.9570000
32	H	20.0800000	19.2870000	89.2750000
33	H	19.2160000	20.8120000	88.9830000
34	H	18.5830000	19.2900000	88.3020000
35	H	19.7920000	18.1480000	86.3930000

36	H	21.2880000	18.8180000	85.7060000
37	H	21.3070000	18.1130000	87.3380000
38	H	18.5930000	20.2840000	85.9640000
39	H	20.0880000	20.8830000	85.2510000
40	O	21.7330000	24.1130000	88.5820000
41	O	22.4740000	23.8150000	89.7660000
42	O	23.2820000	22.6980000	89.3420000

TS2a-1

	Symbol	X	Y	Z
1	C	23.7470000	24.0170000	88.4480000
2	C	22.6830000	24.7810000	88.1300000
3	C	21.9860000	24.8870000	86.7890000
4	C	24.3490000	23.0020000	87.4960000
5	C	23.6080000	21.6760000	87.4610000
6	C	22.4700000	21.4390000	88.1200000
7	C	20.9750000	23.8020000	86.3430000
8	C	21.4790000	20.3060000	87.9740000
9	C	20.1780000	20.9130000	87.3480000
10	C	19.5670000	22.1600000	88.0350000
11	C	19.6920000	23.5840000	87.1630000
12	C	19.2740000	24.7480000	88.0540000
13	C	24.3730000	24.0750000	89.8180000
14	C	21.1680000	19.7050000	89.3620000
15	C	21.9850000	19.1890000	87.0500000
16	H	22.3060000	25.4480000	88.9170000
17	H	22.7540000	24.9140000	85.9960000
18	H	21.4830000	25.8650000	86.7450000
19	H	25.4100000	22.8270000	87.7500000
20	H	24.3630000	23.4070000	86.4660000
21	H	24.0200000	20.9160000	86.7900000
22	H	22.1290000	22.2330000	88.7920000
23	H	20.6290000	24.0890000	85.3380000
24	H	21.4920000	22.8460000	86.2080000
25	H	20.0890000	22.4500000	88.9700000
26	H	18.3300000	24.5230000	88.5630000
27	H	20.0480000	24.9350000	88.8090000
28	H	19.1630000	25.6610000	87.4470000
29	H	24.3950000	23.0750000	90.2860000
30	H	25.4220000	24.4150000	89.7510000
31	H	23.8350000	24.7590000	90.4930000
32	H	22.0680000	19.2410000	89.7970000
33	H	20.8070000	20.4670000	90.0720000
34	H	20.3900000	18.9280000	89.2830000
35	H	21.2230000	18.3970000	86.9600000

36	H	22.1950000	19.5650000	86.0360000
37	H	22.9010000	18.7250000	87.4460000
38	H	19.3840000	20.1500000	87.3840000
39	H	20.3560000	21.1190000	86.2810000
40	O	17.5420000	23.0260000	86.8630000
41	O	18.2580000	22.0280000	88.3100000
42	O	18.6810000	23.2490000	86.2180000

TS2a-2

	Symbol	X	Y	Z
1	C	23.3390000	24.3990000	88.1760000
2	C	22.1730000	25.0020000	87.8670000
3	C	21.3320000	24.8610000	86.6100000
4	C	24.0210000	23.3710000	87.2930000
5	C	23.5210000	21.9480000	87.4520000
6	C	22.4110000	21.6040000	88.1140000
7	C	20.5680000	23.5390000	86.3490000
8	C	21.6410000	20.2990000	88.0610000
9	C	20.4050000	20.4990000	87.1200000
10	C	19.2920000	21.4760000	87.5120000
11	C	19.3920000	23.1640000	87.3180000
12	C	19.4420000	23.7570000	88.7390000
13	C	24.0450000	24.6830000	89.4790000
14	C	21.1890000	19.9030000	89.4820000
15	C	22.4740000	19.1520000	87.4660000
16	H	21.7840000	25.7090000	88.6110000
17	H	21.9890000	24.9880000	85.7300000
18	H	20.6220000	25.7020000	86.5700000
19	H	25.1120000	23.4060000	87.4590000
20	H	23.8910000	23.6410000	86.2270000
21	H	24.0790000	21.1930000	86.8880000
22	H	21.9080000	22.3970000	88.6750000
23	H	20.1070000	23.6100000	85.3550000
24	H	21.2930000	22.7240000	86.2890000
25	H	19.0120000	21.3830000	88.5720000
26	H	18.5250000	23.4580000	89.2700000
27	H	20.3160000	23.4390000	89.3250000
28	H	19.4480000	24.8540000	88.6830000
29	H	24.1880000	23.7540000	90.0610000
30	H	25.0550000	25.0910000	89.2950000
31	H	23.4910000	25.3970000	90.1080000
32	H	22.0630000	19.6730000	90.1110000
33	H	20.6320000	20.7120000	89.9810000
34	H	20.5460000	19.0080000	89.4580000
35	H	21.9000000	18.2130000	87.4730000

36	H	22.7700000	19.3540000	86.4240000
37	H	23.3850000	18.9790000	88.0580000
38	H	19.9020000	19.5190000	87.0420000
39	H	20.7590000	20.7360000	86.1060000
40	O	17.2010000	21.9790000	87.0180000
41	O	18.1870000	21.1480000	86.7190000
42	O	18.2300000	23.5470000	86.7210000

TS2b-1

	Symbol	X	Y	Z
1	C	23.3940000	23.7400000	88.8150000
2	C	22.0840000	24.6940000	88.2970000
3	C	22.0050000	24.9670000	86.7780000
4	C	23.8390000	22.5790000	87.9270000
5	C	22.8890000	21.4480000	87.6210000
6	C	21.5810000	21.3750000	87.8860000
7	C	21.1230000	24.0370000	85.9140000
8	C	20.5610000	20.4160000	87.3050000
9	C	19.8070000	21.2140000	86.1770000
10	C	19.1840000	22.5400000	86.5560000
11	C	19.7190000	23.7750000	86.4330000
12	C	18.9030000	25.0020000	86.7650000
13	C	23.1750000	23.3700000	90.2760000
14	C	19.5720000	19.9860000	88.4070000
15	C	21.1940000	19.1670000	86.6740000
16	H	21.2510000	24.0550000	88.6630000
17	H	23.0160000	25.0170000	86.3430000
18	H	21.6130000	25.9920000	86.7130000
19	H	24.7590000	22.1660000	88.3810000
20	H	24.1750000	23.0070000	86.9650000
21	H	23.3550000	20.6460000	87.0370000
22	H	21.1190000	22.1660000	88.4830000
23	H	21.0330000	24.5190000	84.9240000
24	H	21.6370000	23.0860000	85.7400000
25	H	18.1570000	22.4850000	86.9400000
26	H	17.8740000	24.7380000	87.0540000
27	H	19.3440000	25.5860000	87.5910000
28	H	18.8650000	25.6940000	85.9050000
29	H	22.5260000	22.4870000	90.3460000
30	H	24.1470000	23.1170000	90.7290000
31	H	22.7330000	24.2040000	90.8320000
32	H	20.0880000	19.4140000	89.1960000
33	H	19.0930000	20.8580000	88.8820000
34	H	18.7750000	19.3470000	87.9920000
35	H	20.4070000	18.5200000	86.2530000

36	H	21.8810000	19.4210000	85.8500000
37	H	21.7590000	18.5830000	87.4180000
38	H	19.0140000	20.5560000	85.7790000
39	H	20.5200000	21.3630000	85.3530000
40	O	24.3710000	24.7400000	88.6420000
41	O	24.1120000	25.7550000	89.4360000
42	O	22.1530000	25.7930000	89.0380000

TS2b-2

	Symbol	X	Y	Z
1	C	23.4470000	23.6880000	88.8830000
2	C	22.2770000	24.6920000	88.2390000
3	C	22.0300000	24.8800000	86.7320000
4	C	23.8850000	22.5820000	87.8530000
5	C	22.9480000	21.4350000	87.5660000
6	C	21.6250000	21.4150000	87.7540000
7	C	21.0850000	23.9550000	85.9370000
8	C	20.5920000	20.4250000	87.2640000
9	C	19.7360000	21.1800000	86.1820000
10	C	19.1280000	22.5070000	86.5830000
11	C	19.6860000	23.7330000	86.4830000
12	C	18.9010000	24.9780000	86.8230000
13	C	22.9520000	23.0820000	90.2120000
14	C	19.6940000	20.0100000	88.4470000
15	C	21.2050000	19.1750000	86.6190000
16	H	21.3610000	24.4400000	88.7990000
17	H	23.0060000	24.9140000	86.2230000
18	H	21.6400000	25.9070000	86.6540000
19	H	24.8340000	22.1780000	88.2420000
20	H	24.1540000	23.0860000	86.9100000
21	H	23.4400000	20.5740000	87.0970000
22	H	21.1610000	22.2710000	88.2460000
23	H	20.9800000	24.4290000	84.9440000
24	H	21.5670000	22.9910000	85.7570000
25	H	18.1020000	22.4590000	86.9710000
26	H	17.8720000	24.7400000	87.1340000
27	H	19.3670000	25.5660000	87.6330000
28	H	18.8600000	25.6610000	85.9550000
29	H	21.9930000	22.5520000	90.1440000
30	H	23.7120000	22.3720000	90.5750000
31	H	22.8660000	23.8910000	90.9500000
32	H	20.2790000	19.4730000	89.2110000
33	H	19.2360000	20.8890000	88.9300000
34	H	18.8800000	19.3470000	88.1100000
35	H	20.4040000	18.5040000	86.2660000

36	H	21.8300000	19.4270000	85.7470000
37	H	21.8290000	18.6140000	87.3330000
38	H	18.9240000	20.5030000	85.8670000
39	H	20.3760000	21.3150000	85.2960000
40	O	24.5580000	24.4180000	89.0920000
41	O	23.3670000	26.0190000	89.7410000
42	O	22.7170000	26.0020000	88.6100000

TS2c-1

	Symbol	X	Y	Z
1	C	24.2520000	21.8600000	71.4980000
2	C	23.7260000	23.0760000	71.7520000
3	C	22.5030000	23.7140000	71.1310000
4	C	23.6210000	20.8660000	70.5460000
5	C	22.6210000	19.7940000	71.1120000
6	C	22.4630000	19.8000000	72.7700000
7	C	21.1180000	23.1730000	71.5700000
8	C	21.0560000	19.4070000	73.2930000
9	C	20.0950000	20.6160000	73.0390000
10	C	20.4550000	21.9360000	73.6700000
11	C	20.8950000	23.0570000	73.0630000
12	C	21.1710000	24.3030000	73.8700000
13	C	25.5460000	21.4180000	72.1400000
14	C	21.2040000	19.1540000	74.8090000
15	C	20.4340000	18.1660000	72.6290000
16	H	24.2630000	23.6960000	72.4820000
17	H	22.5420000	23.6230000	70.0310000
18	H	22.5380000	24.7960000	71.3390000
19	H	24.4090000	20.2810000	70.0490000
20	H	23.0790000	21.4020000	69.7500000
21	H	21.5750000	20.0690000	70.8560000
22	H	22.7310000	20.7950000	73.1480000
23	H	20.3610000	23.8580000	71.1470000
24	H	20.9380000	22.2090000	71.0760000
25	H	20.3030000	21.9890000	74.7540000
26	H	20.8650000	24.1850000	74.9200000
27	H	22.2440000	24.5610000	73.8580000
28	H	20.6440000	25.1790000	73.4540000
29	H	25.4330000	20.4550000	72.6640000
30	H	26.3220000	21.2610000	71.3700000
31	H	25.9230000	22.1610000	72.8600000
32	H	21.8350000	18.2730000	75.0000000
33	H	21.6550000	20.0120000	75.3300000
34	H	20.2150000	18.9670000	75.2590000
35	H	19.4230000	18.0070000	73.0370000

36	H	20.3330000	18.2850000	71.5410000
37	H	21.0340000	17.2690000	72.8220000
38	H	19.1100000	20.3030000	73.4260000
39	H	19.9580000	20.7220000	71.9530000
40	O	22.8810000	18.5480000	70.7470000
41	O	23.3930000	17.7970000	72.5280000
42	O	23.5380000	18.9790000	73.0920000

TS2c-2

	Symbol	X	Y	Z
1	C	24.0080000	21.6110000	71.4360000
2	C	23.6830000	22.9030000	71.6300000
3	C	22.4990000	23.6790000	71.0870000
4	C	23.1230000	20.6690000	70.6400000
5	C	22.6300000	19.4210000	71.3850000
6	C	22.3500000	19.4980000	73.0360000
7	C	21.0740000	23.2440000	71.5180000
8	C	20.8390000	19.3800000	73.4280000
9	C	20.0430000	20.6200000	72.9230000
10	C	20.3950000	21.9350000	73.5690000
11	C	20.8530000	23.0680000	73.0010000
12	C	21.1650000	24.2760000	73.8520000
13	C	25.2940000	21.0300000	71.9740000
14	C	20.7920000	19.2940000	74.9690000
15	C	20.1990000	18.0990000	72.8600000
16	H	24.3900000	23.4900000	72.2310000
17	H	22.5180000	23.6650000	69.9830000
18	H	22.6360000	24.7360000	71.3650000
19	H	23.6830000	20.2900000	69.7640000
20	H	22.2560000	21.2050000	70.2390000
21	H	21.6790000	19.0370000	70.9880000
22	H	22.7220000	20.5250000	73.2580000
23	H	20.3920000	24.0310000	71.1510000
24	H	20.7770000	22.3400000	70.9730000
25	H	20.2260000	21.9680000	74.6510000
26	H	20.8330000	24.1390000	74.8920000
27	H	22.2500000	24.4820000	73.8690000
28	H	20.6890000	25.1880000	73.4500000
29	H	25.1170000	20.1600000	72.6270000
30	H	25.9440000	20.6830000	71.1510000
31	H	25.8590000	21.7810000	72.5470000
32	H	21.2600000	18.3600000	75.3110000
33	H	21.3310000	20.1270000	75.4450000
34	H	19.7490000	19.3160000	75.3280000
35	H	19.2310000	17.9110000	73.3520000

36	H	19.9900000	18.1700000	71.7810000
37	H	20.8490000	17.2280000	73.0370000
38	H	18.9760000	20.4060000	73.1210000
39	H	20.1300000	20.6770000	71.8260000
40	O	23.6210000	18.4460000	71.2660000
41	O	23.3510000	17.4170000	72.0400000
42	O	23.1440000	18.6080000	73.6320000

TS2a-1'

	Symbol	X	Y	Z
1	C	23.8140000	23.2310000	87.5870000
2	C	23.1040000	24.2700000	87.1080000
3	C	22.5750000	24.4870000	85.7030000
4	C	24.1470000	21.9910000	86.7810000
5	C	23.0650000	20.9210000	86.7860000
6	C	21.8260000	21.1350000	87.2450000
7	C	21.4420000	23.5610000	85.1890000
8	C	20.5740000	20.3110000	87.0240000
9	C	19.7840000	20.9240000	85.8160000
10	C	19.1180000	22.3220000	85.8100000
11	C	20.0700000	23.6960000	85.8580000
12	C	19.2370000	24.8590000	85.3230000
13	C	24.2670000	23.1900000	89.0250000
14	C	19.7130000	20.3040000	88.3050000
15	C	20.9110000	18.8600000	86.6320000
16	H	22.8770000	25.0700000	87.8210000
17	H	23.4060000	24.3760000	84.9830000
18	H	22.2510000	25.5350000	85.6080000
19	H	25.1010000	21.5610000	87.1330000
20	H	24.3310000	22.2700000	85.7250000
21	H	23.3350000	19.9780000	86.2950000
22	H	21.6340000	22.0920000	87.7350000
23	H	21.2880000	23.7840000	84.1240000
24	H	21.7850000	22.5230000	85.2490000
25	H	18.6750000	22.4540000	84.7980000
26	H	18.2230000	24.8280000	85.7380000
27	H	19.7040000	25.8140000	85.6040000
28	H	19.1920000	24.8070000	84.2260000
29	H	23.8830000	22.2870000	89.5330000
30	H	25.3700000	23.1390000	89.0900000
31	H	23.9320000	24.0720000	89.5920000
32	H	20.2380000	19.7700000	89.1150000
33	H	19.4860000	21.3220000	88.6490000
34	H	18.7510000	19.7960000	88.1260000
35	H	19.9890000	18.2640000	86.5280000

36	H	21.4480000	18.8190000	85.6710000
37	H	21.5520000	18.3850000	87.3920000
38	H	18.9460000	20.2370000	85.6040000
39	H	20.4360000	20.8690000	84.9290000
40	O	18.1720000	22.5150000	86.7410000
41	O	19.0210000	23.8290000	87.8180000
42	O	20.2230000	23.7580000	87.2640000

TS2a-2'

	Symbol	X	Y	Z
1	C	23.9760000	22.8450000	87.6200000
2	C	23.3720000	23.9400000	87.1170000
3	C	22.9110000	24.1730000	85.6940000
4	C	24.1680000	21.5650000	86.8260000
5	C	22.9130000	20.7130000	86.6950000
6	C	21.7480000	21.0730000	87.2450000
7	C	21.5380000	23.6310000	85.2270000
8	C	20.3540000	20.5050000	87.0830000
9	C	19.4310000	21.5800000	86.3990000
10	C	19.4380000	23.0440000	86.8650000
11	C	20.2660000	24.2100000	85.9300000
12	C	19.2010000	24.6600000	84.9000000
13	C	24.4170000	22.7870000	89.0620000
14	C	19.7920000	20.1510000	88.4810000
15	C	20.3230000	19.2460000	86.2010000
16	H	23.2030000	24.7740000	87.8050000
17	H	23.6510000	23.7360000	85.0010000
18	H	22.9290000	25.2580000	85.5060000
19	H	24.9720000	20.9540000	87.2760000
20	H	24.5220000	21.8030000	85.8060000
21	H	23.0140000	19.8110000	86.0820000
22	H	21.7640000	21.9730000	87.8590000
23	H	21.4430000	23.8970000	84.1610000
24	H	21.5450000	22.5360000	85.2630000
25	H	18.4230000	23.4660000	86.8590000
26	H	18.3790000	25.1660000	85.4270000
27	H	19.6440000	25.3750000	84.1930000
28	H	18.8110000	23.8020000	84.3280000
29	H	23.9240000	21.9510000	89.5910000
30	H	25.5050000	22.6060000	89.1390000
31	H	24.1880000	23.7190000	89.6020000
32	H	20.4220000	19.3860000	88.9620000
33	H	19.7650000	21.0270000	89.1440000
34	H	18.7670000	19.7470000	88.4050000
35	H	19.2890000	18.8900000	86.0580000

36	H	20.7520000	19.4330000	85.2040000
37	H	20.9030000	18.4370000	86.6710000
38	H	18.3930000	21.2170000	86.4830000
39	H	19.6340000	21.5880000	85.3170000
40	O	19.9890000	23.2430000	88.1210000
41	O	19.8620000	24.5260000	88.4210000
42	O	20.5570000	25.2030000	86.7880000

TS2b-1'

	Symbol	X	Y	Z
1	C	23.7860000	23.0760000	88.0610000
2	C	22.7360000	24.2470000	87.6540000
3	C	22.2070000	24.3680000	86.1930000
4	C	23.9200000	21.8060000	87.2100000
5	C	22.7820000	20.8190000	87.0940000
6	C	21.5410000	20.9440000	87.5740000
7	C	21.0980000	23.4670000	85.6110000
8	C	20.3380000	20.0780000	87.2450000
9	C	19.4980000	20.8700000	86.1810000
10	C	19.0860000	22.2760000	86.5550000
11	C	19.7590000	23.4230000	86.3270000
12	C	19.1700000	24.7570000	86.7160000
13	C	25.1540000	23.7440000	88.2350000
14	C	19.5050000	19.8580000	88.5240000
15	C	20.7080000	18.7160000	86.6390000
16	H	23.3170000	25.1790000	87.7940000
17	H	23.0930000	24.3020000	85.5390000
18	H	21.8710000	25.4150000	86.1200000
19	H	24.8160000	21.2640000	87.5640000
20	H	24.2010000	22.1430000	86.1950000
21	H	23.0410000	19.9390000	86.4940000
22	H	21.2980000	21.8220000	88.1760000
23	H	20.9010000	23.8820000	84.6030000
24	H	21.4750000	22.4540000	85.4450000
25	H	18.1180000	22.3640000	87.0670000
26	H	18.1520000	24.6430000	87.1200000
27	H	19.7800000	25.2530000	87.4890000
28	H	19.1380000	25.4480000	85.8540000
29	H	25.9070000	23.0140000	88.5670000
30	H	25.4840000	24.1870000	87.2830000
31	H	25.0890000	24.5500000	88.9810000
32	H	20.0800000	19.2900000	89.2740000
33	H	19.2140000	20.8160000	88.9830000
34	H	18.5840000	19.2940000	88.3020000
35	H	19.7940000	18.1490000	86.3960000

36	H	21.2900000	18.8180000	85.7100000
37	H	21.3060000	18.1180000	87.3440000
38	H	18.5900000	20.2800000	85.9630000
39	H	20.0820000	20.8810000	85.2480000
40	O	21.6910000	24.2130000	88.5510000
41	O	22.7090000	23.6960000	89.9400000
42	O	23.2740000	22.6390000	89.3380000

TS2b-2'

	Symbol	X	Y	Z
1	C	23.8330000	22.9900000	88.1410000
2	C	22.7060000	24.1650000	87.6930000
3	C	22.2580000	24.3700000	86.2470000
4	C	23.8720000	21.7490000	87.2080000
5	C	22.7150000	20.7910000	87.1040000
6	C	21.5220000	20.8460000	87.7060000
7	C	21.1740000	23.4660000	85.6110000
8	C	20.2940000	20.0360000	87.3150000
9	C	19.5540000	20.8520000	86.1950000
10	C	19.1470000	22.2660000	86.5320000
11	C	19.8110000	23.4140000	86.2840000
12	C	19.1800000	24.7470000	86.6100000
13	C	25.1930000	23.7250000	88.0760000
14	C	19.3870000	19.8620000	88.5460000
15	C	20.6310000	18.6520000	86.7360000
16	H	23.2170000	25.0730000	88.0480000
17	H	23.1650000	24.3270000	85.6220000
18	H	21.9260000	25.4200000	86.1860000
19	H	24.7740000	21.1810000	87.5030000
20	H	24.1080000	22.1130000	86.1900000
21	H	22.8930000	19.9930000	86.3740000
22	H	21.3390000	21.6200000	88.4510000
23	H	21.0170000	23.8730000	84.5950000
24	H	21.5640000	22.4530000	85.4750000
25	H	18.1680000	22.3640000	87.0210000
26	H	18.1660000	24.6180000	87.0200000
27	H	19.7660000	25.3140000	87.3500000
28	H	19.1220000	25.3890000	85.7130000
29	H	26.0110000	23.0180000	88.2840000
30	H	25.3670000	24.1850000	87.0920000
31	H	25.2170000	24.5120000	88.8430000
32	H	19.8990000	19.2720000	89.3250000
33	H	19.1210000	20.8350000	88.9910000
34	H	18.4510000	19.3390000	88.2840000
35	H	19.7050000	18.1220000	86.4570000

36	H	21.2570000	18.7180000	85.8330000
37	H	21.1720000	18.0380000	87.4740000
38	H	18.6470000	20.2890000	85.9090000
39	H	20.2040000	20.8470000	85.3060000
40	O	21.6370000	23.9010000	88.5410000
41	O	22.1110000	23.8550000	89.7770000
42	O	23.5230000	22.6400000	89.4090000

TS2c-2

	Symbol	X	Y	Z
1	C	23.2040000	23.2030000	88.3910000
2	C	22.7770000	24.4370000	88.0610000
3	C	22.7980000	25.0890000	86.6950000
4	C	23.7740000	22.2260000	87.3860000
5	C	22.8810000	21.0620000	87.0020000
6	C	21.5790000	20.9190000	87.2810000
7	C	21.6710000	24.6560000	85.7300000
8	C	20.6810000	19.7590000	86.8780000
9	C	19.4110000	20.3080000	86.1460000
10	C	18.3110000	20.8590000	87.0280000
11	C	20.2840000	24.7750000	86.2710000
12	C	19.7280000	25.9210000	87.0170000
13	C	23.1610000	22.7170000	89.8200000
14	C	20.2650000	18.9750000	88.1450000
15	C	21.3890000	18.7960000	85.9150000
16	H	22.3770000	25.0570000	88.8730000
17	H	23.7510000	24.8950000	86.1780000
18	H	22.7620000	26.1820000	86.8230000
19	H	24.7170000	21.8050000	87.7880000
20	H	24.0650000	22.7510000	86.4590000
21	H	23.3940000	20.2780000	86.4330000
22	H	21.0830000	21.7060000	87.8620000
23	H	21.7220000	25.2940000	84.8300000
24	H	21.8060000	23.6190000	85.3920000
25	H	18.5900000	21.6830000	87.7260000
26	H	19.2490000	25.5360000	87.9340000
27	H	20.4790000	26.6890000	87.2290000
28	H	18.8990000	26.3500000	86.4280000
29	H	22.6210000	21.7590000	89.9030000
30	H	24.1820000	22.5310000	90.1990000
31	H	22.6770000	23.4450000	90.4860000
32	H	21.1390000	18.4920000	88.6080000
33	H	19.8010000	19.6330000	88.8970000
34	H	19.5300000	18.1920000	87.8910000
35	H	20.7040000	17.9790000	85.6370000

36	H	21.6920000	19.3090000	84.9890000
37	H	22.2830000	18.3490000	86.3750000
38	H	18.9520000	19.5010000	85.5560000
39	H	19.7190000	21.1090000	85.4530000
40	O	18.2270000	23.8360000	86.4580000
41	O	17.1730000	20.4490000	86.9820000
42	O	19.5260000	23.7840000	86.0290000

3a2

	Symbol	X	Y	Z
1	C	23.1860000	24.1140000	88.3660000
2	C	22.3710000	25.0960000	87.9380000
3	C	22.0400000	25.4720000	86.5120000
4	C	23.9260000	23.1670000	87.4440000
5	C	23.4130000	21.7360000	87.4480000
6	C	22.1460000	21.3500000	87.6520000
7	C	20.8630000	24.6990000	85.8800000
8	C	21.6170000	19.9230000	87.6610000
9	C	20.6520000	19.7120000	86.4390000
10	C	19.3550000	20.4370000	86.4880000
11	C	19.5420000	24.7180000	86.6330000
12	C	19.0590000	26.0310000	87.2130000
13	C	23.4430000	23.8980000	89.8380000
14	C	20.8420000	19.6880000	88.9760000
15	C	22.7380000	18.8800000	87.5430000
16	H	21.8950000	25.7090000	88.7130000
17	H	22.9150000	25.3210000	85.8600000
18	H	21.8190000	26.5510000	86.4790000
19	H	24.9880000	23.1470000	87.7470000
20	H	23.9290000	23.5510000	86.4090000
21	H	24.1780000	20.9750000	87.2560000
22	H	21.3910000	22.1220000	87.8510000
23	H	20.6440000	25.1340000	84.8860000
24	H	21.1270000	23.6460000	85.7100000
25	H	19.2240000	21.5310000	86.4550000
26	H	18.0560000	25.8960000	87.6400000
27	H	19.7420000	26.3750000	88.0060000
28	H	19.0490000	26.8190000	86.4440000
29	H	23.2110000	22.8610000	90.1360000
30	H	24.5100000	24.0610000	90.0730000
31	H	22.8480000	24.5790000	90.4650000
32	H	21.5230000	19.7440000	89.8390000
33	H	20.0510000	20.4420000	89.1230000
34	H	20.3640000	18.6950000	88.9820000
35	H	22.3320000	17.8600000	87.6250000

36	H	23.2700000	18.9570000	86.5830000
37	H	23.4710000	19.0000000	88.3550000
38	H	20.4200000	18.6380000	86.3460000
39	H	21.1870000	20.0200000	85.5240000
40	O	17.0940000	20.3160000	86.5920000
41	O	18.3070000	19.7320000	86.5710000
42	O	18.8680000	23.7090000	86.7340000

3b1

	Symbol	X	Y	Z
1	C	24.0350000	21.9530000	88.9350000
2	C	22.3730000	24.8940000	87.1660000
3	C	21.8710000	25.4050000	85.8400000
4	C	23.9510000	20.5090000	88.5490000
5	C	22.7360000	20.0650000	87.7560000
6	C	21.6620000	20.7890000	87.4120000
7	C	21.0510000	24.3430000	85.0610000
8	C	20.4690000	20.2930000	86.6060000
9	C	20.1320000	21.3420000	85.4900000
10	C	19.4260000	22.5990000	85.9200000
11	C	19.7780000	23.8880000	85.7440000
12	C	18.8610000	24.9940000	86.2130000
13	C	23.2600000	22.6140000	90.0000000
14	C	19.2710000	20.1050000	87.5670000
15	C	20.7520000	18.9500000	85.9110000
16	H	23.4590000	24.6450000	87.2660000
17	H	22.7180000	25.7360000	85.2220000
18	H	21.2270000	26.2760000	86.0380000
19	H	24.0040000	19.8990000	89.4720000
20	H	24.8620000	20.2770000	87.9720000
21	H	22.8020000	19.0140000	87.4590000
22	H	21.5840000	21.8370000	87.7320000
23	H	20.7780000	24.7970000	84.0930000
24	H	21.6980000	23.4880000	84.8130000
25	H	18.4520000	22.4270000	86.3930000
26	H	17.8710000	24.6040000	86.4980000
27	H	19.2900000	25.4950000	87.0960000
28	H	18.7290000	25.7690000	85.4380000
29	H	22.6360000	21.9030000	90.5550000
30	H	23.9700000	23.1480000	90.6580000
31	H	22.6380000	23.4190000	89.5570000
32	H	19.4740000	19.2800000	88.2690000
33	H	19.0760000	21.0080000	88.1650000
34	H	18.3520000	19.8610000	87.0070000
35	H	19.8660000	18.6260000	85.3430000

36	H	21.5940000	19.0320000	85.2050000
37	H	20.9970000	18.1600000	86.6370000
38	H	19.4740000	20.8290000	84.7660000
39	H	21.0580000	21.5740000	84.9420000
40	O	24.8980000	22.6210000	88.2790000
41	O	25.0570000	23.9460000	88.5690000
42	O	21.6380000	24.7360000	88.1240000

3b2

	Symbol	X	Y	Z
1	C	23.8450000	22.0390000	88.5670000
2	C	22.1920000	25.1690000	87.6090000
3	C	21.7610000	25.4070000	86.2100000
4	C	23.3200000	20.6260000	88.8590000
5	C	22.4080000	20.0470000	87.8130000
6	C	21.1900000	20.5350000	87.5470000
7	C	21.0910000	24.2120000	85.5020000
8	C	20.2250000	20.0950000	86.4640000
9	C	19.9920000	21.2930000	85.4840000
10	C	19.2980000	22.5130000	86.0270000
11	C	19.7300000	23.7900000	86.0320000
12	C	18.8050000	24.8990000	86.4830000
13	C	24.9500000	22.5550000	89.4600000
14	C	18.8920000	19.6710000	87.1210000
15	C	20.7660000	18.9130000	85.6460000
16	H	21.6130000	24.5960000	88.3440000
17	H	22.6270000	25.7600000	85.6330000
18	H	21.0530000	26.2540000	86.2370000
19	H	22.8080000	20.7160000	89.8380000
20	H	24.1860000	19.9710000	89.0540000
21	H	22.8060000	19.2080000	87.2330000
22	H	20.8290000	21.3790000	88.1500000
23	H	20.9680000	24.5120000	84.4460000
24	H	21.7890000	23.3660000	85.5060000
25	H	18.2760000	22.3390000	86.3890000
26	H	17.8020000	24.5110000	86.7170000
27	H	19.1760000	25.4180000	87.3840000
28	H	18.7070000	25.6790000	85.7060000
29	H	24.9350000	22.0890000	90.4570000
30	H	25.9150000	22.2960000	88.9890000
31	H	24.8560000	23.6500000	89.5360000
32	H	19.0360000	18.7640000	87.7310000
33	H	18.4940000	20.4550000	87.7830000
34	H	18.1290000	19.4520000	86.3550000
35	H	20.0320000	18.6090000	84.8830000

36	H	21.7020000	19.1720000	85.1250000
37	H	20.9730000	18.0470000	86.2950000
38	H	19.3750000	20.9070000	84.6520000
39	H	20.9610000	21.5680000	85.0430000
40	O	23.3880000	22.7180000	87.6700000
41	O	23.5970000	25.5740000	89.3410000
42	O	23.2450000	25.7140000	88.0260000

3c1

	Symbol	X	Y	Z
1	C	24.9800000	21.9210000	70.6070000
2	C	24.1380000	22.7000000	71.3140000
3	C	22.9620000	23.5050000	70.8290000
4	C	24.8680000	21.6820000	69.1150000
5	C	24.3970000	20.2760000	68.7680000
6	C	22.2130000	19.4940000	73.2740000
7	C	21.5900000	23.0320000	71.3640000
8	C	20.7800000	19.5920000	73.7030000
9	C	20.1420000	20.9030000	73.1200000
10	C	20.7410000	22.2000000	73.5960000
11	C	21.3760000	23.1380000	72.8640000
12	C	21.8400000	24.4170000	73.5220000
13	C	26.1220000	21.1890000	71.2670000
14	C	20.7460000	19.5870000	75.2430000
15	C	19.9970000	18.3700000	73.1600000
16	H	24.3260000	22.7640000	72.3950000
17	H	22.9040000	23.5090000	69.7310000
18	H	23.1080000	24.5610000	71.1200000
19	H	25.8310000	21.8420000	68.6000000
20	H	24.1280000	22.3690000	68.6710000
21	H	23.5600000	19.8880000	69.4030000
22	H	23.0340000	19.4480000	74.0020000
23	H	20.8220000	23.6550000	70.8680000
24	H	21.4280000	22.0000000	71.0280000
25	H	20.5880000	22.4220000	74.6600000
26	H	21.4980000	24.4810000	74.5660000
27	H	22.9400000	24.4990000	73.5240000
28	H	21.4690000	25.3050000	72.9810000
29	H	26.0490000	20.0970000	71.1100000
30	H	27.0900000	21.4890000	70.8300000
31	H	26.1610000	21.3760000	72.3510000
32	H	21.1420000	18.6410000	75.6470000
33	H	21.3330000	20.4120000	75.6740000
34	H	19.7090000	19.6930000	75.5970000
35	H	18.9440000	18.4650000	73.4700000

36	H	20.0320000	18.3350000	72.0650000
37	H	20.3890000	17.4250000	73.5700000
38	H	19.0830000	20.8680000	73.4280000
39	H	20.1690000	20.8210000	72.0290000
40	O	24.8580000	19.6160000	67.8660000
41	O	21.8220000	19.4970000	71.0210000
42	O	22.6590000	19.4470000	72.0940000

3c2

	Symbol	X	Y	Z
1	C	24.8230000	22.2820000	71.5550000
2	C	24.0260000	23.2320000	72.0810000
3	C	22.9800000	24.0650000	71.3910000
4	C	24.7720000	21.8870000	70.0710000
5	C	23.6350000	20.9490000	69.8720000
6	C	22.4110000	19.9130000	73.8570000
7	C	21.5270000	23.5800000	71.6320000
8	C	20.9040000	19.7440000	73.6920000
9	C	20.3370000	21.0170000	72.9790000
10	C	20.5850000	22.3510000	73.6330000
11	C	21.0970000	23.4700000	73.0800000
12	C	21.2280000	24.7370000	73.8950000
13	C	25.7580000	21.4550000	72.3980000
14	C	20.2930000	19.5850000	75.1000000
15	C	20.6050000	18.5190000	72.8200000
16	H	24.1210000	23.4030000	73.1600000
17	H	23.1400000	24.0910000	70.3020000
18	H	23.0670000	25.1090000	71.7400000
19	H	25.7120000	21.3970000	69.7710000
20	H	24.6170000	22.7660000	69.4300000
21	H	22.5980000	21.2760000	69.7070000
22	H	22.7090000	20.7760000	74.5090000
23	H	20.8550000	24.2940000	71.1240000
24	H	21.3860000	22.6230000	71.1120000
25	H	20.2490000	22.4280000	74.6740000
26	H	20.7570000	24.6390000	74.8840000
27	H	22.2860000	25.0130000	74.0550000
28	H	20.7690000	25.5980000	73.3770000
29	H	25.4290000	20.4010000	72.4160000
30	H	26.7850000	21.4730000	71.9970000
31	H	25.7800000	21.8090000	73.4390000
32	H	20.6280000	18.6460000	75.5690000
33	H	20.5650000	20.4120000	75.7750000
34	H	19.1930000	19.5570000	75.0350000
35	H	19.5240000	18.4370000	72.6200000

36	H	21.1380000	18.5950000	71.8610000
37	H	20.9340000	17.5910000	73.3140000
38	H	19.2450000	20.8550000	72.9250000
39	H	20.7020000	21.0080000	71.9410000
40	O	23.8170000	19.7090000	70.0030000
41	O	22.7630000	18.8650000	69.9420000
42	O	23.2530000	19.2090000	73.3520000

3) QM/MM Computed Transition States Structures in Stage II

a) Addition reactions of Waters or Acids on Criegee Intermediate 3a1

TS3a1_1w

Symbol		X	Y	Z
1	C	23.3520000	23.0570000	86.9440000
2	O	17.5700000	24.6850000	87.2680000
3	C	22.8160000	24.2900000	86.8810000
4	O	16.9380000	20.3680000	86.5900000
5	C	22.1610000	24.9460000	85.6870000
6	O	18.4790000	24.6540000	86.1520000
7	C	23.3980000	22.0870000	85.7820000
8	C	22.5180000	20.8530000	85.8960000
9	C	21.3680000	20.7490000	86.5770000
10	C	20.6870000	24.5770000	85.4470000
11	C	20.4940000	19.5040000	86.6850000
12	C	19.1440000	19.7180000	85.9300000
13	C	18.1200000	20.6300000	86.5640000
14	C	19.6700000	25.0200000	86.4620000
15	C	19.9010000	26.1570000	87.4030000
16	C	24.0080000	22.5600000	88.2090000
17	C	20.2210000	19.2210000	88.1800000
18	C	21.1610000	18.2700000	86.0600000
19	H	22.8720000	24.8970000	87.7940000
20	H	22.7040000	24.6760000	84.7680000
21	H	22.2580000	26.0400000	85.7720000
22	H	24.4410000	21.7320000	85.6880000
23	H	23.1720000	22.6010000	84.8300000
24	H	22.8920000	19.9810000	85.3480000
25	H	20.9980000	21.6270000	87.1220000
26	H	20.3470000	25.0060000	84.4870000
27	H	20.5820000	23.4880000	85.3390000
28	H	18.4950000	21.5940000	86.9870000
29	H	20.8240000	26.0320000	87.9820000
30	H	20.0210000	27.0590000	86.7790000
31	H	19.0280000	26.2810000	88.0510000
32	H	23.5480000	21.6190000	88.5560000

33	H	25.0760000	22.3370000	88.0320000
34	H	23.9470000	23.2970000	89.0240000
35	H	21.1520000	18.9420000	88.6990000
36	H	19.8020000	20.1040000	88.6910000
37	H	19.5060000	18.3900000	88.3000000
38	H	20.5200000	17.3880000	86.2120000
39	H	21.3020000	18.3940000	84.9740000
40	H	22.1400000	18.0600000	86.5170000
41	H	18.6420000	18.7520000	85.7650000
42	H	19.3650000	20.1300000	84.9270000
43	O	19.6650000	23.5430000	87.9560000
44	H	18.6740000	23.8660000	87.9660000
45	H	20.0420000	23.7720000	88.8160000

TS3a1_2w

Symbol		X	Y	Z
1	C	23.2210000	22.7130000	86.4110000
2	O	17.2330000	24.6660000	86.9560000
3	C	22.7510000	23.9710000	86.5220000
4	O	17.6560000	20.6780000	88.1200000
5	C	21.9730000	24.7590000	85.4910000
6	O	18.3400000	24.2360000	86.1490000
7	C	23.0180000	21.8400000	85.1880000
8	C	22.1090000	20.6360000	85.3720000
9	C	21.1000000	20.5310000	86.2480000
10	C	20.4800000	24.4270000	85.3020000
11	C	20.2120000	19.3130000	86.4750000
12	C	18.7060000	19.6760000	86.2100000
13	C	18.1950000	20.8210000	87.0400000
14	C	19.4820000	24.7820000	86.3820000
15	C	19.5310000	26.0620000	87.1510000
16	C	24.0330000	22.0830000	87.5180000
17	C	20.3900000	18.8580000	87.9430000
18	C	20.5660000	18.1450000	85.5450000
19	H	22.9910000	24.5080000	87.4500000
20	H	22.4420000	24.6130000	84.5040000
21	H	22.0900000	25.8340000	85.6990000
22	H	24.0060000	21.4580000	84.8750000
23	H	22.6550000	22.4380000	84.3340000
24	H	22.3330000	19.7910000	84.7110000
25	H	20.9010000	21.3830000	86.9120000
26	H	20.1220000	24.9770000	84.4120000
27	H	20.3500000	23.3600000	85.0730000
28	H	18.3490000	21.8450000	86.6300000
29	H	18.9130000	25.9870000	88.0510000

30	H	20.5610000	26.3550000	87.3880000
31	H	19.0840000	26.8410000	86.5110000
32	H	23.5650000	21.1520000	87.8790000
33	H	25.0380000	21.8000000	87.1550000
34	H	24.1590000	22.7630000	88.3740000
35	H	21.4250000	18.5240000	88.1120000
36	H	20.1680000	19.6680000	88.6540000
37	H	19.7150000	18.0180000	88.1780000
38	H	19.9080000	17.2860000	85.7500000
39	H	20.4380000	18.4130000	84.4850000
40	H	21.6080000	17.8300000	85.7090000
41	H	18.0910000	18.7900000	86.4360000
42	H	18.5940000	19.9230000	85.1420000
43	O	20.1060000	23.5480000	87.8280000
44	H	19.2650000	23.4440000	88.4440000
45	H	20.8570000	23.8150000	88.3750000
46	O	17.9160000	23.3490000	89.0520000
47	H	17.6250000	22.4220000	88.9500000
48	H	17.4870000	23.8550000	88.2720000

TS3a1_3w

Symbol		X	Y	Z
1	C	23.4900000	23.0020000	86.8850000
2	O	17.4810000	24.8430000	87.1540000
3	C	23.0210000	24.2670000	86.9280000
4	O	17.0920000	20.5550000	86.5670000
5	C	22.2600000	25.0060000	85.8470000
6	O	18.6550000	24.3340000	86.4980000
7	C	23.3540000	22.0890000	85.6830000
8	C	22.4960000	20.8490000	85.8600000
9	C	21.4110000	20.7260000	86.6360000
10	C	20.7790000	24.6250000	85.6520000
11	C	20.5350000	19.4860000	86.7770000
12	C	19.2260000	19.6650000	85.9420000
13	C	18.2830000	20.7360000	86.4090000
14	C	19.7430000	25.0110000	86.6920000
15	C	19.6230000	26.4130000	87.2020000
16	C	24.2700000	22.4200000	88.0390000
17	C	20.1860000	19.2820000	88.2680000
18	C	21.2320000	18.2260000	86.2430000
19	H	23.2310000	24.8410000	87.8390000
20	H	22.7510000	24.8380000	84.8740000
21	H	22.3460000	26.0880000	86.0290000
22	H	24.3700000	21.7440000	85.4210000
23	H	22.9960000	22.6490000	84.8030000

24	H	22.8150000	19.9910000	85.2570000
25	H	21.0950000	21.5850000	87.2390000
26	H	20.4200000	25.1110000	84.7280000
27	H	20.6820000	23.5440000	85.4710000
28	H	18.7160000	21.7470000	86.5940000
29	H	19.0400000	26.4140000	88.1280000
30	H	20.6090000	26.8700000	87.3510000
31	H	19.0580000	26.9880000	86.4530000
32	H	23.8260000	21.4710000	88.3830000
33	H	25.3030000	22.1820000	87.7260000
34	H	24.3260000	23.1120000	88.8930000
35	H	21.0940000	19.0460000	88.8450000
36	H	19.7280000	20.1840000	88.7070000
37	H	19.4820000	18.4420000	88.3900000
38	H	20.5930000	17.3460000	86.4200000
39	H	21.4140000	18.2930000	85.1580000
40	H	22.1960000	18.0530000	86.7460000
41	H	18.6590000	18.7210000	85.9110000
42	H	19.5110000	19.9200000	84.9060000
43	O	20.4740000	24.2670000	88.2810000
44	H	19.8360000	23.5850000	88.7080000
45	H	21.3020000	23.7920000	88.0880000
46	O	18.9820000	22.4600000	89.3290000
47	H	18.0020000	22.5380000	88.9810000
48	H	18.9170000	22.4800000	90.2930000
49	O	16.6730000	22.7510000	88.3640000
50	H	16.5120000	22.0440000	87.7140000
51	H	16.9160000	23.5970000	87.8270000

TS3a1_3w'

Symbol		X	Y	Z
1	C	23.2460000	22.6500000	86.4550000
2	O	17.3030000	24.6410000	87.1890000
3	C	22.7900000	23.9070000	86.6030000
4	O	17.6770000	20.5800000	88.2220000
5	C	22.0090000	24.7260000	85.6000000
6	O	18.4010000	24.1900000	86.3630000
7	C	23.0240000	21.8090000	85.2140000
8	C	22.0970000	20.6180000	85.3670000
9	C	21.1310000	20.4680000	86.2830000
10	C	20.5060000	24.4190000	85.4490000
11	C	20.2420000	19.2460000	86.4870000
12	C	18.7260000	19.6110000	86.2890000
13	C	18.2460000	20.7370000	87.1590000
14	C	19.5320000	24.8160000	86.5390000

15	C	19.4960000	26.2150000	87.0760000
16	C	24.0480000	21.9790000	87.5450000
17	C	20.4670000	18.7290000	87.9260000
18	C	20.5640000	18.1160000	85.4990000
19	H	23.0160000	24.4050000	87.5530000
20	H	22.4450000	24.5830000	84.5980000
21	H	22.1500000	25.7960000	85.8200000
22	H	24.0030000	21.4170000	84.8850000
23	H	22.6680000	22.4310000	84.3740000
24	H	22.2730000	19.8130000	84.6460000
25	H	20.9920000	21.2770000	87.0140000
26	H	20.1360000	24.9570000	84.5580000
27	H	20.3550000	23.3490000	85.2440000
28	H	18.4510000	21.7690000	86.7880000
29	H	18.9580000	26.2360000	88.0280000
30	H	20.5070000	26.6270000	87.1820000
31	H	18.9370000	26.8300000	86.3550000
32	H	23.5510000	21.0620000	87.9050000
33	H	25.0390000	21.6650000	87.1680000
34	H	24.2020000	22.6440000	88.4080000
35	H	21.5100000	18.3960000	88.0480000
36	H	20.2610000	19.5040000	88.6800000
37	H	19.8060000	17.8750000	88.1430000
38	H	19.9260000	17.2420000	85.7070000
39	H	20.3820000	18.4150000	84.4550000
40	H	21.6150000	17.8110000	85.6050000
41	H	18.1190000	18.7190000	86.5150000
42	H	18.5760000	19.8890000	85.2330000
43	O	20.2450000	23.9190000	88.0550000
44	H	19.4100000	23.4520000	88.4130000
45	H	20.3790000	24.5450000	88.8090000
46	O	19.5850000	25.0470000	90.4060000
47	H	19.1400000	25.8890000	90.5710000
48	H	18.8580000	24.4050000	90.2320000
49	O	18.0000000	23.2490000	89.1250000
50	H	17.6810000	22.3280000	89.0730000
51	H	17.5520000	23.8040000	88.3360000

TS3a1_R1

Symbol	X	Y	Z
1 C	23.4590000	23.1800000	87.5730000
2 O	17.6150000	24.7220000	86.9320000
3 C	22.8410000	24.3650000	87.4180000
4 O	17.2730000	20.4520000	86.6570000
5 C	22.4090000	25.0120000	86.1250000

6	O	18.8110000	24.3290000	86.3050000
7	C	23.8090000	22.2470000	86.4340000
8	C	22.9280000	21.0220000	86.2880000
9	C	21.6950000	20.8490000	86.7820000
10	C	20.9930000	24.6540000	85.6240000
11	C	20.8250000	19.6120000	86.6000000
12	C	19.4900000	19.9870000	85.8850000
13	C	18.4480000	20.7340000	86.6850000
14	C	19.7990000	25.1210000	86.3990000
15	C	19.6230000	26.4860000	86.9450000
16	C	23.8560000	22.6800000	88.9410000
17	C	20.5240000	18.9980000	87.9870000
18	C	21.5120000	18.5470000	85.7340000
19	H	22.5950000	24.9190000	88.3280000
20	H	23.0950000	24.7380000	85.3090000
21	H	22.4970000	26.1070000	86.2200000
22	H	24.8480000	21.8900000	86.5680000
23	H	23.8050000	22.7830000	85.4680000
24	H	23.3780000	20.2140000	85.7030000
25	H	21.2570000	21.6540000	87.3860000
26	H	20.8590000	25.1220000	84.6290000
27	H	20.8950000	23.5710000	85.4640000
28	H	18.8010000	21.6000000	87.2990000
29	H	19.1270000	26.4400000	87.9190000
30	H	20.5730000	27.0280000	86.9980000
31	H	18.9340000	27.0150000	86.2630000
32	H	23.4600000	21.6660000	89.1240000
33	H	24.9560000	22.6050000	89.0270000
34	H	23.4950000	23.3430000	89.7410000
35	H	21.4480000	18.6180000	88.4490000
36	H	20.0790000	19.7390000	88.6730000
37	H	19.8150000	18.1570000	87.8980000
38	H	20.8510000	17.6720000	85.6370000
39	H	21.7220000	18.9180000	84.7180000
40	H	22.4590000	18.2100000	86.1800000
41	H	18.9940000	19.0780000	85.5120000
42	H	19.7240000	20.6070000	84.9990000
43	C	19.2890000	23.7160000	89.4390000
44	O	20.1150000	24.2980000	88.7390000
45	C	19.6570000	23.1000000	90.7730000
46	O	18.0340000	23.5370000	89.1130000
47	H	17.8060000	24.0140000	88.2010000
48	H	18.8630000	23.2830000	91.5120000
49	H	19.7450000	22.0080000	90.6490000

50	H	20.6180000	23.4970000	91.1230000

TS3a1_R2

Symbol		X	Y	Z
1	C	23.4860000	23.1300000	87.7160000
2	O	17.6370000	24.6830000	86.8410000
3	C	22.8720000	24.3190000	87.5710000
4	O	17.3160000	20.4550000	86.6810000
5	C	22.4650000	24.9840000	86.2790000
6	O	18.8680000	24.2710000	86.3030000
7	C	23.8490000	22.2140000	86.5660000
8	C	22.9660000	20.9950000	86.3780000
9	C	21.7240000	20.8110000	86.8450000
10	C	21.0790000	24.5950000	85.7230000
11	C	20.8480000	19.5880000	86.6090000
12	C	19.5280000	20.0010000	85.8860000
13	C	18.4900000	20.7420000	86.6960000
14	C	19.8440000	25.0740000	86.4240000
15	C	19.6260000	26.4600000	86.9000000
16	C	23.8610000	22.6100000	89.0820000
17	C	20.5180000	18.9310000	87.9690000
18	C	21.5390000	18.5490000	85.7160000
19	H	22.6180000	24.8660000	88.4840000
20	H	23.1870000	24.7490000	85.4830000
21	H	22.5190000	26.0780000	86.3990000
22	H	24.8850000	21.8530000	86.7090000
23	H	23.8610000	22.7680000	85.6100000
24	H	23.4240000	20.2030000	85.7780000
25	H	21.2800000	21.6000000	87.4660000
26	H	20.9830000	25.0350000	84.7100000
27	H	20.9990000	23.5070000	85.5870000
28	H	18.8460000	21.6100000	87.3060000
29	H	19.2660000	26.4500000	87.9350000
30	H	20.5330000	27.0650000	86.8080000
31	H	18.8150000	26.8850000	86.2850000
32	H	23.3920000	21.6310000	89.2790000
33	H	24.9530000	22.4540000	89.1570000
34	H	23.5610000	23.3040000	89.8810000
35	H	21.4320000	18.5340000	88.4370000
36	H	20.0600000	19.6490000	88.6690000
37	H	19.8100000	18.0950000	87.8380000
38	H	20.8710000	17.6850000	85.5760000
39	H	21.7670000	18.9550000	84.7180000
40	H	22.4750000	18.1880000	86.1640000
41	H	19.0240000	19.1080000	85.4850000

42	H	19.7830000	20.6410000	85.0210000
43	C	19.1320000	23.8490000	89.5060000
44	O	20.0130000	24.3580000	88.8140000
45	C	19.3800000	23.3840000	90.9330000
46	O	17.9070000	23.6310000	89.1030000
47	C	20.6310000	23.9670000	91.5780000
48	H	17.7450000	24.0380000	88.1440000
49	H	18.4730000	23.6080000	91.5170000
50	H	19.4330000	22.2800000	90.8940000
51	H	21.5290000	23.7370000	90.9870000
52	H	20.5610000	25.0640000	91.6580000
53	H	20.7700000	23.5600000	92.5920000

TS3a1_R3

Symbol		X	Y	Z
1	C	23.2230000	23.2390000	86.9090000
2	O	17.0950000	24.6480000	86.7130000
3	C	22.5520000	24.4020000	86.8340000
4	O	17.0960000	20.4140000	86.5870000
5	C	21.8830000	24.9980000	85.6210000
6	O	18.2590000	24.2920000	85.9970000
7	C	23.3970000	22.2730000	85.7550000
8	C	22.5650000	21.0030000	85.8310000
9	C	21.4470000	20.8250000	86.5490000
10	C	20.4490000	24.5210000	85.3260000
11	C	20.6380000	19.5380000	86.6690000
12	C	19.2770000	19.6750000	85.9220000
13	C	18.2750000	20.6570000	86.4790000
14	C	19.3190000	24.9640000	86.2100000
15	C	19.2810000	26.2410000	86.9640000
16	C	23.8730000	22.8040000	88.2010000
17	C	20.3880000	19.2530000	88.1670000
18	C	21.3650000	18.3340000	86.0540000
19	H	22.4780000	24.9870000	87.7570000
20	H	22.4720000	24.7710000	84.7190000
21	H	21.8930000	26.0960000	85.7010000
22	H	24.4560000	21.9560000	85.7220000
23	H	23.2080000	22.7700000	84.7860000
24	H	22.9580000	20.1680000	85.2390000
25	H	21.0770000	21.6710000	87.1420000
26	H	20.1620000	24.8940000	84.3240000
27	H	20.4080000	23.4250000	85.2530000
28	H	18.6720000	21.6650000	86.7610000
29	H	18.5150000	26.2100000	87.7430000
30	H	20.2670000	26.4950000	87.3680000

31	H	18.9880000	27.0220000	86.2410000
32	H	23.5030000	21.8160000	88.5220000
33	H	24.9660000	22.7030000	88.0750000
34	H	23.6860000	23.5220000	89.0130000
35	H	21.3420000	19.0920000	88.6940000
36	H	19.8690000	20.0910000	88.6610000
37	H	19.7700000	18.3500000	88.2990000
38	H	20.7690000	17.4220000	86.2140000
39	H	21.5010000	18.4540000	84.9670000
40	H	22.3540000	18.1760000	86.5120000
41	H	18.7690000	18.6990000	85.8630000
42	H	19.4830000	19.9910000	84.8820000
43	C	18.9260000	23.6540000	89.1500000
44	O	19.7740000	23.8080000	88.2640000
45	C	19.3020000	23.2510000	90.5670000
46	O	17.6470000	23.8340000	88.9920000
47	C	20.7800000	22.9360000	90.7870000
48	C	21.1190000	22.6670000	92.2540000
49	H	17.3860000	24.1430000	87.9940000
50	H	18.9720000	24.0770000	91.2240000
51	H	18.6610000	22.3960000	90.8470000
52	H	21.0590000	22.0640000	90.1710000
53	H	21.3860000	23.7730000	90.4020000
54	H	20.9130000	23.5510000	92.8810000
55	H	20.5290000	21.8290000	92.6610000
56	H	22.1840000	22.4150000	92.3780000

TS3a1_R4

Symbol	X	Y	Z
1 C	23.1840000	23.2970000	86.7390000
2 O	16.9460000	24.7830000	86.8400000
3 C	22.4560000	24.4270000	86.6930000
4 O	17.0990000	20.3880000	86.5150000
5 C	21.6960000	24.9760000	85.5120000
6 O	18.0570000	24.3760000	86.0470000
7 C	23.3230000	22.3260000	85.5840000
8 C	22.5250000	21.0400000	85.7120000
9 C	21.4540000	20.8410000	86.4940000
10 C	20.2410000	24.5030000	85.3360000
11 C	20.6640000	19.5430000	86.6370000
12 C	19.2970000	19.6570000	85.8990000
13 C	18.2840000	20.6250000	86.4600000
14 C	19.1750000	24.9760000	86.2810000
15 C	19.2150000	26.2660000	87.0170000
16 C	23.9290000	22.9040000	87.9920000

17	C	20.4220000	19.2710000	88.1380000
18	C	21.4000000	18.3400000	86.0320000
19	H	22.4060000	25.0200000	87.6130000
20	H	22.2060000	24.7010000	84.5770000
21	H	21.7200000	26.0770000	85.5430000
22	H	24.3860000	22.0370000	85.4940000
23	H	23.0680000	22.8110000	84.6250000
24	H	22.8960000	20.2140000	85.0930000
25	H	21.1020000	21.6780000	87.1110000
26	H	19.8880000	24.8520000	84.3460000
27	H	20.1940000	23.4060000	85.3020000
28	H	18.6770000	21.6170000	86.8000000
29	H	18.5530000	26.2530000	87.8870000
30	H	20.2410000	26.5220000	87.3040000
31	H	18.8390000	27.0370000	86.3210000
32	H	23.6170000	21.9070000	88.3460000
33	H	25.0160000	22.8420000	87.8010000
34	H	23.7690000	23.6270000	88.8050000
35	H	21.3770000	19.1070000	88.6630000
36	H	19.9110000	20.1170000	88.6270000
37	H	19.7990000	18.3730000	88.2780000
38	H	20.8250000	17.4210000	86.2280000
39	H	21.5090000	18.4350000	84.9400000
40	H	22.4010000	18.2100000	86.4710000
41	H	18.8020000	18.6740000	85.8440000
42	H	19.4900000	19.9740000	84.8570000
43	C	18.9420000	23.6530000	89.0710000
44	O	19.7780000	23.7570000	88.1350000
45	C	19.4200000	23.0690000	90.3980000
46	O	17.7180000	23.9870000	89.0090000
47	C	20.7270000	23.6800000	90.9140000
48	C	21.1900000	23.0820000	92.2470000
49	C	22.4900000	23.6980000	92.7670000
50	H	17.2610000	24.3880000	87.8430000
51	H	18.6040000	23.1820000	91.1280000
52	H	19.5620000	21.9840000	90.2410000
53	H	21.5080000	23.5450000	90.1480000
54	H	20.5980000	24.7720000	91.0310000
55	H	20.3920000	23.2110000	93.0020000
56	H	21.3200000	21.9910000	92.1270000
57	H	22.3780000	24.7820000	92.9380000
58	H	23.3120000	23.5640000	92.0440000
59	H	22.8070000	23.2410000	93.7190000

TS3a1_R5

	Symbol	X	Y	Z
1	C	23.3370000	23.1760000	87.1550000
2	O	17.3200000	24.3690000	86.5230000
3	C	22.7230000	24.3690000	87.0500000
4	O	17.1140000	20.4240000	86.6480000
5	C	22.1430000	24.9930000	85.8030000
6	O	18.5710000	24.0570000	85.9470000
7	C	23.5140000	22.2030000	86.0060000
8	C	22.6560000	20.9500000	86.0670000
9	C	21.5120000	20.7980000	86.7500000
10	C	20.7530000	24.4900000	85.3680000
11	C	20.6570000	19.5370000	86.8210000
12	C	19.3250000	19.7390000	86.0350000
13	C	18.2960000	20.6720000	86.6300000
14	C	19.5280000	24.8730000	86.1440000
15	C	19.2860000	26.2180000	86.7180000
16	C	23.9200000	22.7160000	88.4700000
17	C	20.3480000	19.2290000	88.3040000
18	C	21.3630000	18.3220000	86.2020000
19	H	22.6280000	24.9610000	87.9660000
20	H	22.8120000	24.8130000	84.9460000
21	H	22.1210000	26.0880000	85.9180000
22	H	24.5690000	21.8700000	85.9830000
23	H	23.3410000	22.7040000	85.0360000
24	H	23.0440000	20.1070000	85.4830000
25	H	21.1430000	21.6500000	87.3340000
26	H	20.5410000	24.8980000	84.3600000
27	H	20.7480000	23.3970000	85.2540000
28	H	18.6740000	21.6430000	87.0350000
29	H	18.5440000	26.1720000	87.5190000
30	H	20.2210000	26.6840000	87.0490000
31	H	18.8520000	26.8310000	85.9100000
32	H	23.5310000	21.7250000	88.7600000
33	H	25.0190000	22.6100000	88.3940000
34	H	23.7010000	23.4250000	89.2820000
35	H	21.2720000	18.9790000	88.8490000
36	H	19.8790000	20.0880000	88.8110000
37	H	19.6580000	18.3720000	88.3920000
38	H	20.7350000	17.4250000	86.3330000
39	H	21.5290000	18.4570000	85.1220000
40	H	22.3340000	18.1270000	86.6820000
41	H	18.8180000	18.7720000	85.8840000
42	H	19.5670000	20.1300000	85.0290000
43	C	19.0140000	23.7960000	89.1720000

44	O	19.9150000	24.0830000	88.3770000
45	C	19.2950000	23.4760000	90.6320000
46	O	17.7510000	23.7110000	88.8680000
47	C	20.5810000	24.0730000	91.2040000
48	C	20.7250000	23.8280000	92.7090000
49	C	22.0120000	24.3990000	93.3130000
50	C	22.0900000	24.2410000	94.8320000
51	H	17.5410000	23.9560000	87.8370000
52	H	18.4120000	23.7910000	91.2110000
53	H	19.3190000	22.3720000	90.7100000
54	H	21.4500000	23.6560000	90.6680000
55	H	20.6020000	25.1600000	91.0090000
56	H	19.8540000	24.2640000	93.2330000
57	H	20.6770000	22.7420000	92.9120000
58	H	22.0930000	25.4710000	93.0540000
59	H	22.8830000	23.9100000	92.8380000
60	H	21.2660000	24.7800000	95.3280000
61	H	22.0180000	23.1820000	95.1340000
62	H	23.0350000	24.6400000	95.2360000

TS3a1_R6

Symbol		X	Y	Z
1	C	23.3350000	23.1660000	87.0540000
2	O	17.2270000	24.3720000	86.5610000
3	C	22.7160000	24.3600000	87.0170000
4	O	17.0800000	20.4640000	86.6130000
5	C	22.0630000	25.0100000	85.8200000
6	O	18.4770000	24.0660000	85.9530000
7	C	23.4430000	22.2290000	85.8680000
8	C	22.5820000	20.9790000	85.9380000
9	C	21.4770000	20.8090000	86.6780000
10	C	20.6680000	24.4890000	85.4270000
11	C	20.6390000	19.5380000	86.7760000
12	C	19.2790000	19.7170000	86.0380000
13	C	18.2710000	20.6700000	86.6360000
14	C	19.4560000	24.8550000	86.2310000
15	C	19.2200000	26.1930000	86.8280000
16	C	23.9860000	22.6620000	88.3200000
17	C	20.3870000	19.2270000	88.2690000
18	C	21.3410000	18.3310000	86.1350000
19	H	22.6740000	24.9280000	87.9520000
20	H	22.6950000	24.8680000	84.9290000
21	H	22.0230000	26.1010000	85.9680000
22	H	24.4920000	21.8890000	85.7850000
23	H	23.2320000	22.7600000	84.9220000

24	H	22.9400000	20.1490000	85.3160000
25	H	21.1370000	21.6480000	87.3010000
26	H	20.4220000	24.8930000	84.4250000
27	H	20.6730000	23.3970000	85.3120000
28	H	18.6730000	21.6130000	87.0820000
29	H	18.4720000	26.1480000	87.6230000
30	H	20.1580000	26.6260000	87.1890000
31	H	18.8200000	26.8320000	86.0210000
32	H	23.6090000	21.6620000	88.5940000
33	H	25.0780000	22.5580000	88.1870000
34	H	23.8110000	23.3390000	89.1690000
35	H	21.3350000	19.0060000	88.7850000
36	H	19.9130000	20.0760000	88.7890000
37	H	19.7270000	18.3510000	88.3830000
38	H	20.7340000	17.4250000	86.2910000
39	H	21.4640000	18.4650000	85.0480000
40	H	22.3330000	18.1550000	86.5780000
41	H	18.7690000	18.7460000	85.9290000
42	H	19.4830000	20.0770000	85.0120000
43	C	19.0510000	23.7880000	89.1160000
44	O	19.9810000	23.9960000	88.2990000
45	C	19.3970000	23.4300000	90.5590000
46	O	17.8050000	23.8300000	88.8500000
47	C	20.6080000	24.1640000	91.1380000
48	C	20.8160000	23.8760000	92.6280000
49	C	22.0210000	24.5940000	93.2440000
50	C	22.1460000	24.3990000	94.7590000
51	C	23.3820000	25.0730000	95.3570000
52	H	17.4650000	24.0860000	87.6480000
53	H	18.4960000	23.6080000	91.1650000
54	H	19.5740000	22.3380000	90.5810000
55	H	21.5070000	23.8900000	90.5610000
56	H	20.4790000	25.2530000	90.9930000
57	H	19.9020000	24.1630000	93.1800000
58	H	20.9240000	22.7850000	92.7800000
59	H	21.9570000	25.6780000	93.0300000
60	H	22.9480000	24.2450000	92.7500000
61	H	21.2350000	24.7950000	95.2460000
62	H	22.1650000	23.3180000	94.9910000
63	H	23.3910000	26.1570000	95.1460000
64	H	24.3110000	24.6510000	94.9370000
65	H	23.4280000	24.9470000	96.4500000

TS3a1_R7

Symbol	X	Y	Z

1	C	23.2490000	23.2140000	86.9820000
2	O	17.2440000	24.2410000	86.6360000
3	C	22.6340000	24.4110000	86.9650000
4	O	17.0150000	20.3030000	86.6000000
5	C	21.9980000	25.0920000	85.7760000
6	O	18.4920000	24.0100000	86.0150000
7	C	23.3610000	22.2970000	85.7810000
8	C	22.5280000	21.0260000	85.8500000
9	C	21.4080000	20.8430000	86.5640000
10	C	20.6150000	24.5720000	85.3400000
11	C	20.6060000	19.5510000	86.6840000
12	C	19.2350000	19.6820000	85.9560000
13	C	18.1910000	20.5810000	86.5760000
14	C	19.3970000	24.8950000	86.1520000
15	C	19.0910000	26.2380000	86.6990000
16	C	23.8940000	22.6920000	88.2440000
17	C	20.3780000	19.2520000	88.1840000
18	C	21.3330000	18.3560000	86.0510000
19	H	22.5850000	24.9600000	87.9110000
20	H	22.6540000	24.9880000	84.8960000
21	H	21.9410000	26.1750000	85.9620000
22	H	24.4150000	21.9800000	85.6800000
23	H	23.1250000	22.8340000	84.8440000
24	H	22.9220000	20.1920000	85.2570000
25	H	21.0340000	21.6850000	87.1600000
26	H	20.3820000	25.0160000	84.3520000
27	H	20.6310000	23.4850000	85.1820000
28	H	18.5450000	21.5550000	86.9930000
29	H	18.3210000	26.1730000	87.4710000
30	H	19.9970000	26.7320000	87.0650000
31	H	18.6880000	26.8340000	85.8620000
32	H	23.4640000	21.7210000	88.5440000
33	H	24.9750000	22.5190000	88.0910000
34	H	23.7780000	23.3940000	89.0830000
35	H	21.3380000	19.0800000	88.6950000
36	H	19.8700000	20.0870000	88.6940000
37	H	19.7560000	18.3500000	88.3130000
38	H	20.7440000	17.4400000	86.2180000
39	H	21.4470000	18.4800000	84.9620000
40	H	22.3290000	18.2010000	86.4910000
41	H	18.7660000	18.6910000	85.8450000
42	H	19.4160000	20.0580000	84.9320000
43	C	19.0680000	23.7640000	89.2050000
44	O	19.8890000	24.2190000	88.4020000

45	C	19.4410000	23.4470000	90.6440000
46	O	17.8250000	23.4890000	88.9260000
47	C	20.6460000	24.2130000	91.1870000
48	C	20.8900000	23.9450000	92.6740000
49	C	22.0940000	24.6950000	93.2520000
50	C	22.2560000	24.5250000	94.7650000
51	C	23.4650000	25.2600000	95.3530000
52	C	23.5710000	25.1400000	96.8740000
53	H	17.5470000	23.7750000	87.9280000
54	H	18.5450000	23.6190000	91.2620000
55	H	19.6240000	22.3570000	90.6890000
56	H	21.5430000	23.9510000	90.6000000
57	H	20.4920000	25.2950000	91.0290000
58	H	19.9830000	24.2190000	93.2450000
59	H	21.0240000	22.8580000	92.8360000
60	H	21.9970000	25.7720000	93.0170000
61	H	23.0160000	24.3600000	92.7410000
62	H	21.3360000	24.8790000	95.2680000
63	H	22.3320000	23.4470000	95.0060000
64	H	23.4100000	26.3290000	95.0730000
65	H	24.3890000	24.8770000	94.8820000
66	H	24.4550000	25.6710000	97.2630000
67	H	22.6830000	25.5690000	97.3700000
68	H	23.6460000	24.0850000	97.1910000

b) Addition reactions of Waters or Acids on Criegee Intermediate 3b1

TS3b1_1w

	Symbol	X	Y	Z
1	C	25.2540000	22.5650000	91.0060000
2	O	25.4230000	22.7990000	89.7470000
3	C	22.5860000	24.9350000	88.9630000
4	O	25.7090000	24.1880000	89.5190000
5	C	21.7390000	24.8030000	87.7180000
6	O	22.1770000	25.3760000	90.0170000
7	C	25.3780000	21.1030000	91.3440000
8	C	24.2060000	20.2410000	90.9160000
9	C	23.1480000	20.6090000	90.1830000
10	C	21.2040000	23.3600000	87.5400000
11	C	21.9890000	19.7010000	89.7710000
12	C	21.1310000	20.4170000	88.6760000
13	C	20.3080000	21.5970000	89.1220000
14	C	20.3000000	22.8630000	88.6570000
15	C	19.3240000	23.8750000	89.2190000
16	C	24.4300000	23.4700000	91.8720000

17	C	21.1280000	19.3620000	91.0090000
18	C	22.5180000	18.3840000	89.1660000
19	H	23.6430000	24.5760000	88.8910000
20	H	22.3620000	25.0560000	86.8440000
21	H	20.9180000	25.5330000	87.7620000
22	H	25.5260000	21.0090000	92.4330000
23	H	26.3030000	20.7310000	90.8710000
24	H	24.2940000	19.2030000	91.2590000
25	H	23.0680000	21.6490000	89.8490000
26	H	20.6430000	23.3370000	86.5860000
27	H	22.0500000	22.6690000	87.3980000
28	H	19.5740000	21.3680000	89.9050000
29	H	18.5950000	23.4010000	89.8930000
30	H	19.8530000	24.6640000	89.7780000
31	H	18.7680000	24.3950000	88.4170000
32	H	23.3800000	23.1440000	91.7710000
33	H	24.7080000	23.3690000	92.9300000
34	H	24.4920000	24.5090000	91.5330000
35	H	21.7050000	18.7500000	91.7200000
36	H	20.8010000	20.2670000	91.5420000
37	H	20.2300000	18.7900000	90.7190000
38	H	21.6790000	17.7050000	88.9420000
39	H	23.0700000	18.5710000	88.2300000
40	H	23.1910000	17.8560000	89.8590000
41	H	20.4330000	19.6600000	88.2690000
42	H	21.7920000	20.6850000	87.8370000
43	O	27.0340000	23.3620000	91.4520000
44	H	27.0010000	23.9560000	92.2160000
45	H	26.7620000	23.9590000	90.6410000

TS3b1_2w

	Symbol	X	Y	Z
1	C	24.9290000	22.4760000	90.2540000
2	O	24.5800000	23.3910000	89.4200000
3	C	22.0560000	25.1870000	90.4820000
4	O	24.5790000	24.7280000	89.9380000
5	C	21.6630000	25.3750000	89.0370000
6	O	21.8020000	24.2130000	91.1570000
7	C	24.7440000	21.0800000	89.7180000
8	C	23.3510000	20.4880000	89.7410000
9	C	22.1840000	21.0850000	90.0120000
10	C	20.9250000	24.2030000	88.3700000
11	C	20.8110000	20.4350000	89.9170000
12	C	19.9730000	21.2180000	88.8350000
13	C	19.2820000	22.4910000	89.2610000

14	C	19.6390000	23.7730000	89.0540000
15	C	18.7210000	24.8930000	89.4870000
16	C	24.9050000	22.7500000	91.7230000
17	C	20.1280000	20.5160000	91.3000000
18	C	20.8890000	18.9630000	89.4780000
19	H	22.5680000	26.0720000	90.9340000
20	H	22.5990000	25.5950000	88.4980000
21	H	21.0800000	26.3130000	88.9740000
22	H	25.4350000	20.4320000	90.2770000
23	H	25.0940000	21.0920000	88.6720000
24	H	23.3560000	19.4320000	89.4490000
25	H	22.1570000	22.1380000	90.3120000
26	H	20.6840000	24.5270000	87.3390000
27	H	21.6140000	23.3520000	88.2760000
28	H	18.3270000	22.3340000	89.7790000
29	H	17.7460000	24.5080000	89.8230000
30	H	19.1510000	25.4710000	90.3240000
31	H	18.5500000	25.6140000	88.6680000
32	H	25.2300000	21.8660000	92.2870000
33	H	25.5330000	23.6150000	91.9580000
34	H	23.8720000	23.0240000	91.9920000
35	H	20.6760000	19.9080000	92.0380000
36	H	20.0960000	21.5520000	91.6680000
37	H	19.0940000	20.1360000	91.2490000
38	H	19.8830000	18.5150000	89.4620000
39	H	21.3130000	18.8660000	88.4640000
40	H	21.5060000	18.3660000	90.1680000
41	H	19.1820000	20.5250000	88.4960000
42	H	20.6180000	21.3840000	87.9580000
43	O	27.1150000	25.0060000	90.3430000
44	H	27.2360000	25.5420000	91.1400000
45	H	26.1140000	25.0380000	90.1540000
46	O	26.9200000	22.4430000	90.0690000
47	H	27.1170000	22.3080000	89.1250000
48	H	27.1560000	23.4110000	90.2510000

TS3b1_3w

	Symbol	X	Y	Z
1	C	25.1580000	22.4990000	90.1580000
2	O	24.6050000	23.3460000	89.3390000
3	C	21.9870000	25.8080000	90.3280000
4	O	24.3680000	24.6670000	89.8690000
5	C	21.6110000	25.7710000	88.8600000
6	O	22.2660000	26.8330000	90.9090000
7	C	24.9080000	21.0670000	89.7240000

8	C	23.4940000	20.5380000	89.7260000
9	C	22.3340000	21.1730000	89.9350000
10	C	20.9700000	24.4670000	88.3600000
11	C	20.9490000	20.5570000	89.7810000
12	C	20.1210000	21.4600000	88.7950000
13	C	19.4510000	22.6950000	89.3460000
14	C	19.7520000	23.9950000	89.1400000
15	C	18.8240000	25.0740000	89.6490000
16	C	25.1940000	22.8230000	91.6260000
17	C	20.2670000	20.4820000	91.1650000
18	C	21.0020000	19.1410000	89.1790000
19	H	21.9610000	24.8320000	90.8720000
20	H	22.5420000	25.9460000	88.3010000
21	H	20.9770000	26.6480000	88.6590000
22	H	25.5550000	20.4170000	90.3310000
23	H	25.2770000	20.9910000	88.6880000
24	H	23.4650000	19.4770000	89.4550000
25	H	22.3370000	22.2350000	90.2050000
26	H	20.6750000	24.6330000	87.3060000
27	H	21.7350000	23.6770000	88.3400000
28	H	18.5470000	22.4930000	89.9350000
29	H	17.9210000	24.6460000	90.1120000
30	H	19.3080000	25.7220000	90.3990000
31	H	18.5130000	25.7460000	88.8290000
32	H	25.7750000	22.0670000	92.1710000
33	H	25.5950000	23.8300000	91.7830000
34	H	24.1580000	22.8170000	91.9980000
35	H	20.8130000	19.7880000	91.8240000
36	H	20.2370000	21.4660000	91.6570000
37	H	19.2300000	20.1170000	91.0720000
38	H	19.9830000	18.7300000	89.0940000
39	H	21.4440000	19.1470000	88.1690000
40	H	21.5830000	18.4470000	89.8060000
41	H	19.3130000	20.8180000	88.3970000
42	H	20.7620000	21.7020000	87.9320000
43	O	26.4720000	25.8640000	90.7250000
44	H	26.2170000	26.7290000	91.0990000
45	H	25.6380000	25.4160000	90.3390000
46	O	28.4410000	24.3130000	90.6270000
47	H	28.7200000	24.1710000	91.5430000
48	H	27.7510000	25.0640000	90.6880000
49	O	26.9240000	22.4720000	89.8110000
50	H	27.0660000	22.4030000	88.8460000
51	H	27.5440000	23.2330000	90.1690000

TS3b1_3w

	Symbol	X	Y	Z
1	C	25.0890000	22.6700000	90.8100000
2	O	24.8590000	23.4400000	89.7680000
3	C	22.0020000	25.2180000	90.3460000
4	O	24.6130000	24.8290000	90.0950000
5	C	21.7130000	25.3230000	88.8690000
6	O	21.7000000	24.2780000	91.0480000
7	C	25.1550000	21.2160000	90.3790000
8	C	23.8540000	20.5150000	90.0510000
9	C	22.6050000	20.9970000	90.0080000
10	C	21.1660000	24.0570000	88.1930000
11	C	21.3570000	20.2010000	89.6490000
12	C	20.5680000	20.9800000	88.5330000
13	C	19.7070000	22.1400000	88.9660000
14	C	19.9140000	23.4630000	88.8160000
15	C	18.8510000	24.4510000	89.2420000
16	C	24.4890000	23.0240000	92.1430000
17	C	20.4930000	20.0500000	90.9200000
18	C	21.6870000	18.8020000	89.0990000
19	H	22.4640000	26.1350000	90.7900000
20	H	22.6510000	25.6380000	88.3870000
21	H	21.0320000	26.1850000	88.7360000
22	H	25.6800000	20.6550000	91.1690000
23	H	25.8100000	21.1760000	89.4880000
24	H	24.0100000	19.4570000	89.8180000
25	H	22.4070000	22.0470000	90.2530000
26	H	20.9450000	24.3250000	87.1420000
27	H	21.9650000	23.3020000	88.1580000
28	H	18.7580000	21.8480000	89.4340000
29	H	17.9210000	23.9410000	89.5360000
30	H	19.1820000	25.0520000	90.1050000
31	H	18.6170000	25.1690000	88.4340000
32	H	24.8120000	22.3010000	92.9020000
33	H	24.7870000	24.0390000	92.4280000
34	H	23.3940000	23.0290000	92.0550000
35	H	21.0160000	19.4360000	91.6710000
36	H	20.2750000	21.0270000	91.3760000
37	H	19.5320000	19.5590000	90.6890000
38	H	20.7550000	18.2590000	88.8720000
39	H	22.2770000	18.8620000	88.1690000
40	H	22.2510000	18.1950000	89.8250000
41	H	19.8950000	20.2460000	88.0520000
42	H	21.2830000	21.2790000	87.7510000

43	O	26.9920000	25.3540000	90.5040000
44	H	27.0900000	26.1940000	90.9790000
45	H	25.9450000	25.2570000	90.2850000
46	O	28.2740000	23.2400000	89.1070000
47	H	27.8750000	22.9010000	88.2820000
48	H	27.9370000	24.1500000	89.2440000
49	O	26.8150000	22.9170000	91.2560000
50	H	26.9130000	23.9310000	91.2520000
51	H	27.3880000	22.7240000	90.4550000

TS3b1_R1

	Symbol	X	Y	Z
1	C	24.8560000	22.3900000	90.5240000
2	O	25.0580000	23.1930000	89.5560000
3	C	22.3760000	25.2100000	89.6680000
4	O	25.3650000	24.5300000	89.9030000
5	C	21.7460000	25.1950000	88.3020000
6	O	22.1500000	24.3940000	90.5340000
7	C	24.6850000	20.9680000	90.0850000
8	C	23.2860000	20.3940000	90.0090000
9	C	22.1080000	21.0220000	90.1120000
10	C	20.8740000	23.9760000	87.9700000
11	C	20.7360000	20.3710000	89.9940000
12	C	19.8980000	21.1440000	88.9120000
13	C	19.3280000	22.4850000	89.3020000
14	C	19.7030000	23.7180000	88.9060000
15	C	18.9200000	24.9330000	89.3470000
16	C	24.5670000	22.8690000	91.8960000
17	C	20.0400000	20.4570000	91.3710000
18	C	20.8200000	18.8980000	89.5590000
19	H	23.0780000	26.0560000	89.8630000
20	H	22.5590000	25.3020000	87.5610000
21	H	21.1900000	26.1450000	88.2040000
22	H	25.2930000	20.3630000	90.7780000
23	H	25.1740000	20.8890000	89.1010000
24	H	23.3020000	19.3140000	89.8250000
25	H	22.0730000	22.1000000	90.3040000
26	H	20.4790000	24.1350000	86.9480000
27	H	21.5130000	23.0830000	87.9150000
28	H	18.4620000	22.4330000	89.9730000
29	H	18.0090000	24.6470000	89.8950000
30	H	19.5160000	25.5790000	90.0150000
31	H	18.6270000	25.5630000	88.4880000
32	H	24.6410000	22.0480000	92.6190000
33	H	25.2290000	23.7020000	92.1540000

34	H	23.5440000	23.2830000	91.8790000
35	H	20.5770000	19.8450000	92.1130000
36	H	20.0130000	21.4920000	91.7460000
37	H	19.0010000	20.0880000	91.3110000
38	H	19.8120000	18.4570000	89.5120000
39	H	21.2790000	18.7990000	88.5610000
40	H	21.4100000	18.2970000	90.2690000
41	H	19.0410000	20.4910000	88.6600000
42	H	20.5000000	21.2110000	87.9930000
43	C	27.9590000	22.9020000	90.9190000
44	O	27.0700000	22.0610000	91.0560000
45	C	29.3840000	22.5950000	91.3260000
46	O	27.7920000	24.1050000	90.4440000
47	H	26.7830000	24.3220000	90.2010000
48	H	30.0460000	22.6860000	90.4510000
49	H	29.7250000	23.3330000	92.0690000
50	H	29.4530000	21.5810000	91.7390000

TS3b1_R2

	Symbol	X	Y	Z
1	C	24.8290000	22.3690000	90.5130000
2	O	25.0340000	23.1590000	89.5360000
3	C	22.3710000	25.2080000	89.6400000
4	O	25.3540000	24.4950000	89.8690000
5	C	21.7170000	25.1950000	88.2860000
6	O	22.1420000	24.4080000	90.5200000
7	C	24.6430000	20.9420000	90.0930000
8	C	23.2400000	20.3760000	90.0240000
9	C	22.0690000	21.0160000	90.1370000
10	C	20.8280000	23.9840000	87.9650000
11	C	20.6890000	20.3810000	90.0360000
12	C	19.8520000	21.1590000	88.9580000
13	C	19.2990000	22.5090000	89.3400000
14	C	19.6760000	23.7350000	88.9260000
15	C	18.9090000	24.9560000	89.3770000
16	C	24.5620000	22.8710000	91.8830000
17	C	20.0080000	20.4680000	91.4220000
18	C	20.7450000	18.9070000	89.6020000
19	H	23.0970000	26.0400000	89.8120000
20	H	22.5140000	25.3050000	87.5290000
21	H	21.1610000	26.1470000	88.2040000
22	H	25.2470000	20.3420000	90.7940000
23	H	25.1360000	20.8460000	89.1120000
24	H	23.2480000	19.2950000	89.8400000
25	H	22.0520000	22.0960000	90.3240000

26	H	20.4110000	24.1580000	86.9540000
27	H	21.4570000	23.0860000	87.8850000
28	H	18.4410000	22.4710000	90.0230000
29	H	18.0090000	24.6770000	89.9450000
30	H	19.5230000	25.5990000	90.0310000
31	H	18.6020000	25.5860000	88.5230000
32	H	24.5690000	22.0500000	92.6090000
33	H	25.2820000	23.6520000	92.1470000
34	H	23.5720000	23.3620000	91.8580000
35	H	20.5470000	19.8450000	92.1530000
36	H	19.9920000	21.5000000	91.8060000
37	H	18.9670000	20.1070000	91.3700000
38	H	19.7280000	18.4870000	89.5600000
39	H	21.1940000	18.7990000	88.6010000
40	H	21.3250000	18.2930000	90.3090000
41	H	18.9870000	20.5140000	88.7140000
42	H	20.4520000	21.2140000	88.0350000
43	C	27.9420000	22.8620000	90.8840000
44	O	27.0470000	22.0250000	91.0160000
45	C	29.3710000	22.5450000	91.2910000
46	O	27.7800000	24.0650000	90.4110000
47	C	29.5510000	21.1640000	91.9130000
48	H	26.7730000	24.2820000	90.1650000
49	H	29.9920000	22.6670000	90.3880000
50	H	29.6990000	23.3490000	91.9730000
51	H	28.9460000	21.0640000	92.8280000
52	H	29.2320000	20.3700000	91.2210000
53	H	30.6060000	20.9900000	92.1800000

TS3b1_R3

	Symbol	X	Y	Z
1	C	24.5450000	22.2090000	90.5730000
2	O	24.4790000	22.9270000	89.5150000
3	C	22.1200000	25.1590000	90.0760000
4	O	24.7180000	24.3140000	89.6960000
5	C	21.6980000	25.1500000	88.6310000
6	O	21.8160000	24.3200000	90.8950000
7	C	24.3800000	20.7450000	90.2830000
8	C	22.9700000	20.2100000	90.1580000
9	C	21.8120000	20.8760000	90.2380000
10	C	20.8520000	23.9490000	88.1790000
11	C	20.4270000	20.2810000	90.0340000
12	C	19.6930000	21.1170000	88.9250000
13	C	19.1400000	22.4670000	89.3100000
14	C	19.5870000	23.6960000	88.9820000

15	C	18.7920000	24.9200000	89.3720000
16	C	24.4110000	22.7870000	91.9350000
17	C	19.6560000	20.3500000	91.3710000
18	C	20.4750000	18.8190000	89.5580000
19	H	22.7320000	26.0470000	90.3750000
20	H	22.6310000	25.2040000	88.0430000
21	H	21.1970000	26.1150000	88.4290000
22	H	24.9330000	20.1900000	91.0570000
23	H	24.9150000	20.5690000	89.3380000
24	H	22.9620000	19.1350000	89.9500000
25	H	21.8060000	21.9520000	90.4530000
26	H	20.5730000	24.1360000	87.1240000
27	H	21.4830000	23.0490000	88.1730000
28	H	18.2110000	22.4280000	89.8920000
29	H	17.8250000	24.6460000	89.8210000
30	H	19.3330000	25.5390000	90.1090000
31	H	18.5990000	25.5730000	88.5020000
32	H	24.6960000	22.0490000	92.6930000
33	H	24.9980000	23.7060000	92.0310000
34	H	23.3530000	23.0790000	92.0620000
35	H	20.1320000	19.6970000	92.1210000
36	H	19.6400000	21.3730000	91.7780000
37	H	18.6130000	20.0160000	91.2430000
38	H	19.4530000	18.4280000	89.4330000
39	H	20.9880000	18.7300000	88.5860000
40	H	20.9910000	18.1690000	90.2810000
41	H	18.8370000	20.5030000	88.5880000
42	H	20.3660000	21.1920000	88.0560000
43	C	27.5030000	22.9590000	90.4930000
44	O	26.7300000	22.0250000	90.7500000
45	C	28.9920000	22.8190000	90.7490000
46	O	27.1560000	24.1180000	90.0310000
47	C	29.4640000	21.4110000	91.1040000
48	C	30.9620000	21.3410000	91.4100000
49	H	26.0850000	24.2410000	89.8720000
50	H	29.5040000	23.2170000	89.8570000
51	H	29.2330000	23.5320000	91.5590000
52	H	28.8870000	21.0530000	91.9720000
53	H	29.2060000	20.7220000	90.2810000
54	H	31.5770000	21.6670000	90.5530000
55	H	31.2310000	21.9840000	92.2640000
56	H	31.2690000	20.3130000	91.6600000

TS3b1_R4

Symbol	X	Y	Z

1	C	24.5930000	22.2640000	90.6170000
2	O	24.5230000	22.9920000	89.5670000
3	C	22.1080000	25.1780000	90.1030000
4	O	24.7420000	24.3810000	89.7680000
5	C	21.6900000	25.1710000	88.6560000
6	O	21.8180000	24.3270000	90.9150000
7	C	24.4530000	20.8010000	90.3130000
8	C	23.0520000	20.2460000	90.1720000
9	C	21.8820000	20.8930000	90.2470000
10	C	20.8700000	23.9560000	88.1920000
11	C	20.5070000	20.2760000	90.0370000
12	C	19.7640000	21.0980000	88.9220000
13	C	19.1800000	22.4350000	89.3050000
14	C	19.6050000	23.6740000	88.9860000
15	C	18.7830000	24.8810000	89.3770000
16	C	24.4390000	22.8310000	91.9830000
17	C	19.7320000	20.3360000	91.3730000
18	C	20.5790000	18.8140000	89.5650000
19	H	22.7040000	26.0730000	90.4100000
20	H	22.6210000	25.2510000	88.0700000
21	H	21.1680000	26.1260000	88.4620000
22	H	25.0040000	20.2490000	91.0910000
23	H	25.0030000	20.6380000	89.3730000
24	H	23.0610000	19.1710000	89.9610000
25	H	21.8590000	21.9680000	90.4650000
26	H	20.5930000	24.1440000	87.1370000
27	H	21.5190000	23.0690000	88.1850000
28	H	18.2490000	22.3750000	89.8810000
29	H	17.8180000	24.5850000	89.8140000
30	H	19.3060000	25.5030000	90.1230000
31	H	18.5870000	25.5360000	88.5090000
32	H	24.7150000	22.0870000	92.7390000
33	H	25.0230000	23.7500000	92.0940000
34	H	23.3790000	23.1200000	92.0970000
35	H	20.2200000	19.6950000	92.1250000
36	H	19.6960000	21.3600000	91.7750000
37	H	18.6950000	19.9810000	91.2440000
38	H	19.5620000	18.4070000	89.4400000
39	H	21.0950000	18.7300000	88.5950000
40	H	21.1030000	18.1730000	90.2910000
41	H	18.9230000	20.4670000	88.5790000
42	H	20.4420000	21.1870000	88.0580000
43	C	27.5430000	23.0340000	90.5270000
44	O	26.7790000	22.0990000	90.8060000

45	C	29.0400000	22.8980000	90.7350000
46	O	27.1820000	24.1920000	90.0760000
47	C	29.5410000	21.4950000	91.0730000
48	C	31.0530000	21.4430000	91.3150000
49	C	31.5870000	20.0320000	91.5670000
50	H	26.1070000	24.3170000	89.9360000
51	H	29.5150000	23.2930000	89.8210000
52	H	29.3060000	23.6160000	91.5330000
53	H	29.0070000	21.1250000	91.9640000
54	H	29.2630000	20.8020000	90.2580000
55	H	31.5860000	21.8820000	90.4510000
56	H	31.3070000	22.0930000	92.1730000
57	H	31.3680000	19.3630000	90.7170000
58	H	31.1270000	19.5830000	92.4630000
59	H	32.6780000	20.0370000	91.7170000

TS3b1_R5

	Symbol	X	Y	Z
1	C	24.6180000	22.2720000	90.6230000
2	O	24.5470000	22.9940000	89.5680000
3	C	22.1400000	25.1870000	90.0910000
4	O	24.7630000	24.3850000	89.7620000
5	C	21.7260000	25.1740000	88.6430000
6	O	21.8460000	24.3400000	90.9050000
7	C	24.4670000	20.8080000	90.3240000
8	C	23.0580000	20.2620000	90.2200000
9	C	21.8980000	20.9290000	90.2810000
10	C	20.8970000	23.9630000	88.1890000
11	C	20.5090000	20.3310000	90.1100000
12	C	19.7680000	21.1260000	88.9720000
13	C	19.1880000	22.4760000	89.3170000
14	C	19.6220000	23.7060000	88.9760000
15	C	18.8060000	24.9250000	89.3390000
16	C	24.4630000	22.8490000	91.9840000
17	C	19.7490000	20.4660000	91.4480000
18	C	20.5500000	18.8490000	89.7010000
19	H	22.7360000	26.0830000	90.3970000
20	H	22.6600000	25.2390000	88.0580000
21	H	21.2160000	26.1330000	88.4390000
22	H	25.0350000	20.2550000	91.0890000
23	H	24.9900000	20.6410000	89.3690000
24	H	23.0530000	19.1800000	90.0470000
25	H	21.8950000	22.0110000	90.4590000
26	H	20.6310000	24.1380000	87.1290000
27	H	21.5350000	23.0680000	88.2010000

28	H	18.2510000	22.4350000	89.8870000
29	H	17.8360000	24.6420000	89.7760000
30	H	19.3260000	25.5580000	90.0770000
31	H	18.6170000	25.5660000	88.4590000
32	H	24.7430000	22.1150000	92.7490000
33	H	25.0410000	23.7730000	92.0860000
34	H	23.4010000	23.1320000	92.0950000
35	H	20.2270000	19.8480000	92.2260000
36	H	19.7420000	21.5080000	91.8030000
37	H	18.7030000	20.1330000	91.3430000
38	H	19.5270000	18.4490000	89.6110000
39	H	21.0500000	18.7120000	88.7280000
40	H	21.0780000	18.2340000	90.4480000
41	H	18.9230000	20.4900000	88.6480000
42	H	20.4430000	21.1890000	88.1040000
43	C	27.5620000	23.0440000	90.5370000
44	O	26.8040000	22.1040000	90.8150000
45	C	29.0600000	22.9250000	90.7420000
46	O	27.1970000	24.1980000	90.0780000
47	C	29.5900000	21.5290000	91.0640000
48	C	31.1120000	21.5130000	91.2440000
49	C	31.7190000	20.1170000	91.4150000
50	C	33.2490000	20.1280000	91.4440000
51	H	26.1220000	24.3200000	89.9330000
52	H	29.5190000	23.3330000	89.8260000
53	H	29.3230000	23.6420000	91.5420000
54	H	29.0960000	21.1500000	91.9740000
55	H	29.2960000	20.8330000	90.2590000
56	H	31.5920000	21.9960000	90.3710000
57	H	31.3880000	22.1430000	92.1110000
58	H	31.3700000	19.4660000	90.5910000
59	H	31.3290000	19.6590000	92.3420000
60	H	33.6640000	20.5230000	90.5010000
61	H	33.6320000	20.7630000	92.2600000
62	H	33.6600000	19.1160000	91.5890000

TS3b1_R6

	Symbol	X	Y	Z
1	C	24.7700000	22.2800000	90.3900000
2	O	25.0680000	23.0810000	89.4510000
3	C	22.4280000	25.1550000	89.5930000
4	O	25.4890000	24.3710000	89.8260000
5	C	21.7350000	25.1610000	88.2580000
6	O	22.1820000	24.3760000	90.4880000
7	C	24.5070000	20.8850000	89.9160000

8	C	23.0940000	20.3500000	89.8990000
9	C	21.9420000	21.0010000	90.0970000
10	C	20.7950000	23.9800000	87.9710000
11	C	20.5520000	20.3890000	90.0140000
12	C	19.7130000	21.2020000	88.9640000
13	C	19.2270000	22.5710000	89.3680000
14	C	19.6490000	23.7820000	88.9520000
15	C	18.9440000	25.0340000	89.4160000
16	C	24.5610000	22.7420000	91.7810000
17	C	19.9020000	20.4690000	91.4130000
18	C	20.5810000	18.9220000	89.5520000
19	H	23.2060000	25.9440000	89.7370000
20	H	22.5150000	25.2350000	87.4790000
21	H	21.2150000	26.1340000	88.1850000
22	H	25.1370000	20.2440000	90.5560000
23	H	24.9350000	20.8260000	88.9030000
24	H	23.0710000	19.2820000	89.6590000
25	H	21.9460000	22.0710000	90.3360000
26	H	20.3700000	24.1550000	86.9640000
27	H	21.3910000	23.0600000	87.8960000
28	H	18.3830000	22.5660000	90.0690000
29	H	18.0400000	24.7940000	89.9970000
30	H	19.5940000	25.6510000	90.0610000
31	H	18.6500000	25.6760000	88.5660000
32	H	24.4790000	21.8930000	92.4690000
33	H	25.3590000	23.4320000	92.0770000
34	H	23.6270000	23.3340000	91.7830000
35	H	20.4470000	19.8270000	92.1240000
36	H	19.9200000	21.4960000	91.8090000
37	H	18.8520000	20.1330000	91.3840000
38	H	19.5600000	18.5090000	89.5250000
39	H	21.0070000	18.8270000	88.5400000
40	H	21.1740000	18.2920000	90.2350000
41	H	18.8170000	20.5920000	88.7410000
42	H	20.2900000	21.2390000	88.0260000
43	C	27.9890000	22.5210000	90.8560000
44	O	27.0520000	21.7280000	90.8890000
45	C	29.3660000	22.1520000	91.3830000
46	O	27.9120000	23.7520000	90.4130000
47	C	29.4470000	20.7640000	92.0190000
48	C	30.8060000	20.4690000	92.6610000
49	C	30.8580000	19.1270000	93.4020000
50	C	32.1930000	18.8530000	94.1040000
51	C	32.2210000	17.5340000	94.8810000

52	H	26.9450000	24.0250000	90.1380000
53	H	30.0900000	22.2600000	90.5570000
54	H	29.6470000	22.9380000	92.1060000
55	H	28.6520000	20.6780000	92.7790000
56	H	29.2050000	19.9990000	91.2620000
57	H	31.5990000	20.4940000	91.8890000
58	H	31.0570000	21.2800000	93.3690000
59	H	30.6390000	18.3060000	92.6930000
60	H	30.0430000	19.1000000	94.1510000
61	H	33.0080000	18.8570000	93.3580000
62	H	32.4180000	19.6870000	94.7940000
63	H	32.0400000	16.6700000	94.2190000
64	H	31.4450000	17.5130000	95.6660000
65	H	33.1930000	17.3770000	95.3760000

TS3b1_R7

	Symbol	X	Y	Z
1	C	24.8810000	22.2670000	90.4450000
2	O	25.0900000	23.0630000	89.4650000
3	C	22.4540000	25.1680000	89.6160000
4	O	25.5110000	24.3750000	89.8130000
5	C	21.7670000	25.1860000	88.2780000
6	O	22.2130000	24.3790000	90.5020000
7	C	24.5900000	20.8640000	89.9970000
8	C	23.1660000	20.3580000	89.9340000
9	C	22.0120000	21.0170000	90.1020000
10	C	20.8360000	24.0040000	87.9670000
11	C	20.6200000	20.4060000	90.0110000
12	C	19.7800000	21.2110000	88.9560000
13	C	19.2760000	22.5750000	89.3540000
14	C	19.6870000	23.7900000	88.9390000
15	C	18.9640000	25.0340000	89.4020000
16	C	24.6200000	22.7610000	91.8210000
17	C	19.9620000	20.4860000	91.4080000
18	C	20.6430000	18.9370000	89.5560000
19	H	23.2220000	25.9660000	89.7710000
20	H	22.5500000	25.2790000	87.5030000
21	H	21.2380000	26.1550000	88.2170000
22	H	25.1710000	20.2110000	90.6680000
23	H	25.0570000	20.7730000	89.0040000
24	H	23.1370000	19.2880000	89.7020000
25	H	22.0180000	22.0880000	90.3320000
26	H	20.4150000	24.1930000	86.9600000
27	H	21.4370000	23.0870000	87.8810000
28	H	18.4260000	22.5620000	90.0480000

29	H	18.0670000	24.7800000	89.9860000
30	H	19.6070000	25.6600000	90.0440000
31	H	18.6580000	25.6690000	88.5510000
32	H	24.6500000	21.9350000	92.5410000
33	H	25.3240000	23.5540000	92.0890000
34	H	23.6170000	23.2240000	91.8060000
35	H	20.5080000	19.8510000	92.1240000
36	H	19.9640000	21.5140000	91.8020000
37	H	18.9170000	20.1360000	91.3710000
38	H	19.6180000	18.5350000	89.5280000
39	H	21.0700000	18.8340000	88.5450000
40	H	21.2260000	18.3040000	90.2440000
41	H	18.8910000	20.5920000	88.7320000
42	H	20.3600000	21.2510000	88.0200000
43	C	27.9060000	22.5490000	90.8760000
44	O	26.9630000	21.7480000	90.9320000
45	C	29.2830000	22.1440000	91.3780000
46	O	27.8280000	23.7650000	90.4370000
47	C	29.3610000	20.7390000	91.9750000
48	C	30.7160000	20.4200000	92.6160000
49	C	30.7600000	19.0620000	93.3270000
50	C	32.0850000	18.7880000	94.0440000
51	C	32.1200000	17.4640000	94.8160000
52	C	33.4400000	17.2200000	95.5500000
53	H	26.8190000	24.0700000	90.1380000
54	H	29.9910000	22.2730000	90.5410000
55	H	29.5820000	22.9090000	92.1170000
56	H	28.5640000	20.6340000	92.7300000
57	H	29.1210000	19.9960000	91.1960000
58	H	31.5160000	20.4590000	91.8530000
59	H	30.9680000	21.2100000	93.3480000
60	H	30.5570000	18.2550000	92.5990000
61	H	29.9330000	19.0130000	94.0600000
62	H	32.9130000	18.8040000	93.3090000
63	H	32.2950000	19.6180000	94.7440000
64	H	31.9230000	16.6290000	94.1180000
65	H	31.2860000	17.4490000	95.5440000
66	H	33.4300000	16.2660000	96.1010000
67	H	34.2920000	17.1890000	94.8500000
68	H	33.6490000	18.0210000	96.2800000

c) Addition reactions of Waters or Acids on Criegee Intermediate 3c1

TS3c1_1w

Symbol	X	Y	Z

1	C	22.2010000	22.6980000	75.2500000
2	O	22.4850000	21.4080000	72.4280000
3	C	21.1370000	22.6560000	76.0780000
4	O	22.9070000	17.1630000	75.8440000
5	C	19.7710000	23.2400000	75.8320000
6	O	22.7810000	18.5740000	75.6610000
7	C	22.1460000	23.3230000	73.8600000
8	C	21.7350000	22.2460000	72.8700000
9	C	21.5730000	18.9400000	75.5390000
10	C	18.7380000	22.2700000	75.1940000
11	C	20.5020000	18.2390000	74.7100000
12	C	19.3560000	19.2660000	74.4490000
13	C	18.6340000	19.7780000	75.6660000
14	C	18.3610000	21.0520000	76.0150000
15	C	17.5690000	21.3520000	77.2660000
16	C	23.5210000	22.0600000	75.5950000
17	C	19.9300000	16.9140000	75.2510000
18	C	21.2280000	17.9430000	73.3700000
19	H	21.2760000	22.1480000	77.0400000
20	H	19.8540000	24.1190000	75.1710000
21	H	19.3690000	23.6170000	76.7880000
22	H	23.1450000	23.6940000	73.5780000
23	H	21.4310000	24.1570000	73.8150000
24	H	20.6470000	22.2300000	72.6030000
25	H	21.4670000	20.0260000	75.6640000
26	H	17.8120000	22.8510000	75.0200000
27	H	19.1020000	21.9750000	74.2000000
28	H	18.2470000	19.0010000	76.3360000
29	H	17.3230000	20.4370000	77.8240000
30	H	18.1190000	22.0260000	77.9460000
31	H	16.6190000	21.8550000	77.0120000
32	H	23.8170000	21.3340000	74.8190000
33	H	24.3190000	22.8230000	75.6340000
34	H	23.4920000	21.5390000	76.5630000
35	H	20.7390000	16.2040000	75.4560000
36	H	19.3410000	17.0580000	76.1690000
37	H	19.2540000	16.4860000	74.4950000
38	H	20.5290000	17.4300000	72.6930000
39	H	21.5860000	18.8670000	72.8880000
40	H	22.0960000	17.2980000	73.5690000
41	H	18.6320000	18.7540000	73.7890000
42	H	19.7640000	20.0990000	73.8580000
43	O	21.2370000	18.2900000	77.5080000
44	H	21.8940000	17.5900000	77.1970000

45	H	20.4400000	17.7960000	77.7400000

TS3c1_2w

	Symbol	X	Y	Z
1	C	21.8140000	22.5470000	75.4100000
2	O	22.2990000	21.5680000	72.4540000
3	C	20.7950000	22.3670000	76.2740000
4	O	22.9660000	16.6680000	75.6430000
5	C	19.3710000	22.8400000	76.1400000
6	O	22.7250000	18.0650000	75.9320000
7	C	21.6640000	23.2500000	74.0660000
8	C	21.4230000	22.1950000	72.9990000
9	C	21.4930000	18.4400000	75.8970000
10	C	18.3620000	21.7880000	75.6040000
11	C	20.4410000	17.8900000	74.9320000
12	C	19.2560000	18.9000000	74.8220000
13	C	18.5560000	19.3070000	76.0900000
14	C	18.1670000	20.5450000	76.4530000
15	C	17.4120000	20.7640000	77.7440000
16	C	23.1980000	22.0110000	75.6740000
17	C	19.9240000	16.4810000	75.2790000
18	C	21.1520000	17.8560000	73.5530000
19	H	21.0240000	21.8240000	77.1990000
20	H	19.3260000	23.7150000	75.4710000
21	H	19.0260000	23.1940000	77.1270000
22	H	22.5920000	23.7880000	73.8160000
23	H	20.8260000	23.9630000	74.0680000
24	H	20.3460000	21.9810000	72.7770000
25	H	21.4340000	19.5230000	76.0740000
26	H	17.3780000	22.2880000	75.5240000
27	H	18.6540000	21.5170000	74.5790000
28	H	18.3130000	18.4900000	76.7770000
29	H	17.3120000	19.8320000	78.3190000
30	H	17.9070000	21.5090000	78.3930000
31	H	16.3950000	21.1460000	77.5390000
32	H	23.5370000	21.3690000	74.8430000
33	H	23.9280000	22.8370000	75.7460000
34	H	23.2510000	21.4290000	76.6060000
35	H	20.7670000	15.7820000	75.3460000
36	H	19.3750000	16.4690000	76.2310000
37	H	19.2340000	16.1500000	74.4870000
38	H	20.4540000	17.4420000	72.8100000
39	H	21.4510000	18.8640000	73.2220000
40	H	22.0530000	17.2320000	73.6170000
41	H	18.5240000	18.4180000	74.1490000

42	H	19.6190000	19.7880000	74.2840000
43	O	20.7920000	17.9630000	77.5970000
44	H	21.3070000	17.0480000	77.8020000
45	H	21.1780000	18.6030000	78.2160000
46	O	22.1750000	15.9200000	77.8840000
47	H	22.6340000	16.1280000	76.9470000
48	H	21.7190000	15.0740000	77.7760000

TS3c1_3w

	Symbol	X	Y	Z
1	C	22.2560000	22.4860000	75.3420000
2	O	22.6140000	21.2740000	72.4970000
3	C	21.1410000	22.5250000	76.1010000
4	O	22.2580000	16.5840000	75.8200000
5	C	19.8600000	23.2550000	75.7900000
6	O	22.3170000	18.0110000	76.0420000
7	C	22.3600000	23.1650000	73.9800000
8	C	21.9220000	22.1740000	72.9100000
9	C	21.2560000	18.6920000	75.7560000
10	C	18.8020000	22.4240000	75.0140000
11	C	20.2010000	18.2230000	74.7450000
12	C	19.2570000	19.4040000	74.3540000
13	C	18.3490000	19.9650000	75.4160000
14	C	18.1550000	21.2620000	75.7440000
15	C	17.1840000	21.6460000	76.8360000
16	C	23.4790000	21.7030000	75.7440000
17	C	19.3900000	17.0120000	75.2350000
18	C	21.0170000	17.8530000	73.4820000
19	H	21.1640000	21.9650000	77.0440000
20	H	20.0760000	24.1540000	75.1890000
21	H	19.4160000	23.6180000	76.7330000
22	H	23.4090000	23.4440000	73.7860000
23	H	21.7340000	24.0660000	73.9180000
24	H	20.8710000	22.2940000	72.5460000
25	H	21.5130000	19.7550000	75.6820000
26	H	17.9870000	23.1130000	74.7260000
27	H	19.2490000	22.0870000	74.0700000
28	H	17.7280000	19.2290000	75.9430000
29	H	16.7220000	20.7630000	77.3020000
30	H	17.6760000	22.2370000	77.6290000
31	H	16.3660000	22.2690000	76.4340000
32	H	23.7560000	20.9820000	74.9560000
33	H	24.3460000	22.3770000	75.8700000
34	H	23.3310000	21.1530000	76.6850000
35	H	20.0770000	16.2020000	75.5000000

36	H	18.7970000	17.2510000	76.1300000
37	H	18.7020000	16.6780000	74.4450000
38	H	20.3440000	17.4000000	72.7380000
39	H	21.4950000	18.7410000	73.0370000
40	H	21.7940000	17.1330000	73.7670000
41	H	18.6300000	19.0140000	73.5300000
42	H	19.8720000	20.1990000	73.9100000
43	O	20.3860000	18.9470000	77.3120000
44	H	20.1260000	18.0830000	77.8510000
45	H	19.5640000	19.4370000	77.1220000
46	O	21.3530000	15.2060000	77.7300000
47	H	21.8170000	15.7950000	77.0080000
48	H	21.0410000	14.4220000	77.2520000
49	O	19.7040000	16.9000000	78.6080000
50	H	20.3170000	16.1350000	78.2670000
51	H	19.9240000	16.9880000	79.5460000

TS3c1_3w'

	Symbol	X	Y	Z
1	C	22.1060000	22.6290000	75.3110000
2	O	22.4540000	21.4930000	72.4210000
3	C	21.0710000	22.5070000	76.1640000
4	O	22.7900000	16.1200000	75.8260000
5	C	19.6680000	23.0280000	75.9870000
6	O	22.7010000	17.4340000	76.4100000
7	C	21.9930000	23.3060000	73.9500000
8	C	21.6480000	22.2450000	72.9160000
9	C	21.6170000	18.0860000	76.2050000
10	C	18.6520000	22.0020000	75.4130000
11	C	20.7410000	17.9580000	74.9620000
12	C	19.8160000	19.2030000	74.8190000
13	C	18.9160000	19.5530000	75.9820000
14	C	18.4070000	20.7680000	76.2620000
15	C	17.4960000	20.9740000	77.4480000
16	C	23.4610000	22.0350000	75.5980000
17	C	19.9110000	16.6630000	74.9340000
18	C	21.7270000	17.9730000	73.7620000
19	H	21.2600000	21.9640000	77.0980000
20	H	19.6730000	23.9080000	75.3230000
21	H	19.3000000	23.3830000	76.9660000
22	H	22.9590000	23.7580000	73.6730000
23	H	21.2200000	24.0880000	73.9430000
24	H	20.5600000	22.1550000	72.6680000
25	H	21.6760000	19.0790000	76.6680000
26	H	17.6860000	22.5280000	75.2950000

27	H	18.9740000	21.7200000	74.3990000
28	H	18.6520000	18.7330000	76.6550000
29	H	17.3960000	20.0580000	78.0490000
30	H	17.8670000	21.7750000	78.1150000
31	H	16.4870000	21.2770000	77.1170000
32	H	23.7740000	21.3630000	74.7810000
33	H	24.2290000	22.8280000	75.6600000
34	H	23.4750000	21.4730000	76.5440000
35	H	20.5390000	15.7990000	75.1750000
36	H	19.0750000	16.7170000	75.6430000
37	H	19.4910000	16.5320000	73.9310000
38	H	21.1500000	17.8680000	72.8310000
39	H	22.2830000	18.9210000	73.7000000
40	H	22.4400000	17.1430000	73.8540000
41	H	19.1990000	19.0080000	73.9200000
42	H	20.4460000	20.0670000	74.5610000
43	O	22.2260000	16.7230000	79.5050000
44	H	22.0360000	15.8420000	79.1160000
45	H	23.1070000	16.9310000	79.1580000
46	O	21.3850000	14.9300000	77.5880000
47	H	22.0310000	15.2920000	76.8650000
48	H	21.0400000	14.0870000	77.2540000
49	O	20.4210000	17.4040000	77.6560000
50	H	20.4910000	16.4190000	77.5120000
51	H	21.0210000	17.4650000	78.4500000

TS3c1_R1

	Symbol	X	Y	Z
1	C	22.2750000	22.5440000	75.2950000
2	O	22.6320000	21.1940000	72.5130000
3	C	21.1400000	22.6240000	76.0190000
4	O	22.4230000	16.9600000	76.2180000
5	C	19.8650000	23.3260000	75.6320000
6	O	22.2750000	18.3690000	76.2880000
7	C	22.4190000	23.1560000	73.9050000
8	C	21.9610000	22.1300000	72.8810000
9	C	21.1750000	18.8420000	75.8780000
10	C	18.8040000	22.4230000	74.9430000
11	C	20.2550000	18.2550000	74.8320000
12	C	19.2460000	19.3670000	74.4020000
13	C	18.4340000	19.9810000	75.5090000
14	C	18.2420000	21.2880000	75.7760000
15	C	17.3720000	21.7130000	76.9360000
16	C	23.4810000	21.7730000	75.7650000
17	C	19.5140000	16.9730000	75.2550000

18	C	21.1770000	17.9320000	73.6210000
19	H	21.1380000	22.1290000	76.9970000
20	H	20.0890000	24.1590000	74.9470000
21	H	19.4210000	23.7790000	76.5350000
22	H	23.4790000	23.3920000	73.7150000
23	H	21.8230000	24.0730000	73.7970000
24	H	20.9130000	22.2580000	72.5100000
25	H	21.1110000	19.9170000	76.0850000
26	H	17.9610000	23.0760000	74.6500000
27	H	19.2260000	22.0460000	74.0020000
28	H	17.9440000	19.2670000	76.1780000
29	H	17.0190000	20.8500000	77.5170000
30	H	17.9090000	22.3880000	77.6260000
31	H	16.4810000	22.2610000	76.5770000
32	H	23.7630000	21.0060000	75.0230000
33	H	24.3550000	22.4410000	75.8700000
34	H	23.3100000	21.2770000	76.7320000
35	H	20.2260000	16.2120000	75.5930000
36	H	18.8090000	17.1850000	76.0690000
37	H	18.9540000	16.5850000	74.3910000
38	H	20.5490000	17.5110000	72.8210000
39	H	21.6810000	18.8310000	73.2330000
40	H	21.9370000	17.1970000	73.9180000
41	H	18.5700000	18.8920000	73.6670000
42	H	19.7970000	20.1390000	73.8440000
43	C	20.2760000	17.4550000	78.5460000
44	O	19.9950000	18.4070000	77.8040000
45	C	19.5310000	17.2580000	79.8490000
46	O	21.1850000	16.5600000	78.3220000
47	H	21.7520000	16.6920000	77.4040000
48	H	19.2220000	16.2060000	79.9490000
49	H	20.2110000	17.4710000	80.6900000
50	H	18.6620000	17.9250000	79.9040000

TS3c1_R2

	Symbol	X	Y	Z
1	C	22.2890000	22.5410000	75.2970000
2	O	22.6580000	21.1650000	72.5320000
3	C	21.1440000	22.6390000	76.0030000
4	O	22.3670000	16.9870000	76.2730000
5	C	19.8820000	23.3490000	75.5900000
6	O	22.2270000	18.3980000	76.3180000
7	C	22.4590000	23.1420000	73.9040000
8	C	22.0000000	22.1190000	72.8770000
9	C	21.1380000	18.8730000	75.8840000

10	C	18.8320000	22.4540000	74.8760000
11	C	20.2260000	18.2740000	74.8360000
12	C	19.2300000	19.3850000	74.3710000
13	C	18.3970000	20.0230000	75.4480000
14	C	18.2230000	21.3360000	75.6990000
15	C	17.3270000	21.7880000	76.8280000
16	C	23.4800000	21.7620000	75.7890000
17	C	19.4680000	17.0060000	75.2700000
18	C	21.1640000	17.9240000	73.6450000
19	H	21.1230000	22.1520000	76.9860000
20	H	20.1270000	24.1810000	74.9120000
21	H	19.4220000	23.8040000	76.4840000
22	H	23.5240000	23.3620000	73.7270000
23	H	21.8790000	24.0680000	73.7820000
24	H	20.9650000	22.2700000	72.4780000
25	H	21.0810000	19.9520000	76.0680000
26	H	18.0080000	23.1150000	74.5480000
27	H	19.2780000	22.0630000	73.9520000
28	H	17.8660000	19.3250000	76.1040000
29	H	16.9220000	20.9360000	77.3920000
30	H	17.8630000	22.4400000	77.5400000
31	H	16.4690000	22.3680000	76.4420000
32	H	23.7640000	20.9870000	75.0560000
33	H	24.3590000	22.4210000	75.9020000
34	H	23.2900000	21.2730000	76.7560000
35	H	20.1680000	16.2430000	75.6300000
36	H	18.7520000	17.2380000	76.0680000
37	H	18.9200000	16.6080000	74.4040000
38	H	20.5480000	17.4850000	72.8440000
39	H	21.6730000	18.8150000	73.2440000
40	H	21.9190000	17.1960000	73.9670000
41	H	18.5670000	18.8990000	73.6320000
42	H	19.7960000	20.1450000	73.8120000
43	C	20.1850000	17.5330000	78.5600000
44	O	19.9370000	18.4860000	77.8070000
45	C	19.4180000	17.3590000	79.8630000
46	O	21.0770000	16.6170000	78.3560000
47	C	18.1810000	18.2400000	79.9930000
48	H	21.6630000	16.7370000	77.4530000
49	H	19.1770000	16.2870000	79.9600000
50	H	20.1400000	17.5610000	80.6750000
51	H	18.4420000	19.3040000	79.8970000
52	H	17.4430000	18.0140000	79.2070000
53	H	17.6950000	18.0870000	80.9700000

TS3c1_R3

	Symbol	X	Y	Z
1	C	21.7830000	22.5580000	75.3880000
2	O	22.3010000	21.5800000	72.4680000
3	C	20.7770000	22.3260000	76.2550000
4	O	23.4060000	16.8590000	75.2640000
5	C	19.3270000	22.7150000	76.1280000
6	O	23.0140000	18.1230000	75.7670000
7	C	21.5950000	23.2620000	74.0500000
8	C	21.4010000	22.2050000	72.9760000
9	C	21.7820000	18.4020000	75.7000000
10	C	18.3940000	21.5890000	75.6030000
11	C	20.7840000	17.8870000	74.6820000
12	C	19.5760000	18.8730000	74.6490000
13	C	18.8970000	19.1350000	75.9670000
14	C	18.3890000	20.3020000	76.4070000
15	C	17.7110000	20.3850000	77.7540000
16	C	23.1890000	22.0790000	75.6430000
17	C	20.2900000	16.4480000	74.9300000
18	C	21.5010000	17.9540000	73.3050000
19	H	21.0360000	21.7860000	77.1750000
20	H	19.2180000	23.5820000	75.4550000
21	H	18.9660000	23.0480000	77.1160000
22	H	22.4980000	23.8430000	73.8010000
23	H	20.7280000	23.9370000	74.0570000
24	H	20.3350000	21.9830000	72.7100000
25	H	21.5610000	19.3380000	76.2270000
26	H	17.3610000	21.9820000	75.5990000
27	H	18.6520000	21.3860000	74.5520000
28	H	18.8040000	18.2710000	76.6340000
29	H	17.7510000	19.4240000	78.2890000
30	H	18.1760000	21.1490000	78.4010000
31	H	16.6500000	20.6700000	77.6380000
32	H	23.5490000	21.4610000	74.8020000
33	H	23.8840000	22.9340000	75.7180000
34	H	23.2670000	21.4910000	76.5690000
35	H	21.1320000	15.7500000	75.0030000
36	H	19.7130000	16.3860000	75.8580000
37	H	19.6370000	16.1540000	74.0940000
38	H	20.8150000	17.5360000	72.5530000
39	H	21.7510000	18.9880000	73.0200000
40	H	22.4250000	17.3620000	73.3230000
41	H	18.8540000	18.4380000	73.9330000
42	H	19.9140000	19.8180000	74.1980000

43	C	21.7180000	16.1460000	77.8920000
44	O	21.1680000	17.2080000	77.5670000
45	C	21.2090000	15.3230000	79.0620000
46	O	22.7210000	15.5960000	77.2810000
47	C	20.1260000	15.9820000	79.9110000
48	C	19.5350000	15.0240000	80.9470000
49	H	23.0590000	16.1200000	76.4060000
50	H	20.8450000	14.3770000	78.6200000
51	H	22.0820000	15.0310000	79.6700000
52	H	20.5420000	16.8730000	80.4110000
53	H	19.3330000	16.3660000	79.2480000
54	H	19.0660000	14.1500000	80.4620000
55	H	20.3120000	14.6390000	81.6280000
56	H	18.7670000	15.5180000	81.5640000

TS3c1_R4

	Symbol	X	Y	Z
1	C	22.3200000	22.4930000	75.3130000
2	O	22.7170000	21.0800000	72.5620000
3	C	21.1580000	22.6430000	75.9790000
4	O	22.1510000	16.9450000	76.4800000
5	C	19.9350000	23.3850000	75.5090000
6	O	21.9970000	18.3510000	76.5950000
7	C	22.5580000	23.0700000	73.9200000
8	C	22.0880000	22.0600000	72.8850000
9	C	20.9300000	18.8410000	76.1210000
10	C	18.8780000	22.5030000	74.7900000
11	C	20.1020000	18.2830000	74.9830000
12	C	19.1810000	19.4190000	74.4390000
13	C	18.3230000	20.1240000	75.4520000
14	C	18.1890000	21.4510000	75.6370000
15	C	17.2620000	21.9850000	76.7030000
16	C	23.4680000	21.6830000	75.8570000
17	C	19.2710000	17.0440000	75.3550000
18	C	21.1070000	17.9040000	73.8590000
19	H	21.0870000	22.1760000	76.9690000
20	H	20.2290000	24.1870000	74.8130000
21	H	19.4650000	23.8840000	76.3740000
22	H	23.6370000	23.2410000	73.7760000
23	H	22.0230000	24.0190000	73.7720000
24	H	21.0730000	22.2520000	72.4540000
25	H	20.8470000	19.9070000	76.3630000
26	H	18.0970000	23.1760000	74.3920000
27	H	19.3480000	22.0500000	73.9060000
28	H	17.7400000	19.4720000	76.1110000

29	H	16.7360000	21.1750000	77.2270000
30	H	17.8050000	22.5830000	77.4570000
31	H	16.4920000	22.6450000	76.2620000
32	H	23.7620000	20.8990000	75.1380000
33	H	24.3590000	22.3200000	76.0040000
34	H	23.2260000	21.2030000	76.8160000
35	H	19.9070000	16.2880000	75.8290000
36	H	18.4650000	17.3170000	76.0480000
37	H	18.8340000	16.6190000	74.4400000
38	H	20.5230000	17.5460000	72.9970000
39	H	21.7050000	18.7690000	73.5330000
40	H	21.7810000	17.1110000	74.2060000
41	H	18.5380000	18.9380000	73.6800000
42	H	19.8060000	20.1380000	73.8890000
43	C	19.8810000	17.4120000	78.6950000
44	O	19.6370000	18.3870000	77.9690000
45	C	19.1790000	17.2110000	80.0300000
46	O	20.7470000	16.4810000	78.4480000
47	C	17.9200000	18.0350000	80.2820000
48	C	17.3410000	17.7920000	81.6810000
49	C	16.0690000	18.5870000	81.9790000
50	H	21.3790000	16.6350000	77.5730000
51	H	18.9850000	16.1300000	80.1330000
52	H	19.9450000	17.4300000	80.7970000
53	H	18.1490000	19.1050000	80.1450000
54	H	17.1620000	17.7920000	79.5150000
55	H	17.1370000	16.7120000	81.8070000
56	H	18.1100000	18.0350000	82.4370000
57	H	15.2610000	18.3400000	81.2680000
58	H	16.2490000	19.6740000	81.9100000
59	H	15.6940000	18.3740000	82.9930000

TS3c1_R5

	Symbol	X	Y	Z
1	C	22.2900000	22.5030000	75.2900000
2	O	22.6690000	21.1140000	72.5160000
3	C	21.1370000	22.6490000	75.9740000
4	O	22.2210000	17.0090000	76.3750000
5	C	19.9070000	23.3950000	75.5290000
6	O	22.0890000	18.4200000	76.4180000
7	C	22.5090000	23.0880000	73.8980000
8	C	22.0280000	22.0760000	72.8700000
9	C	21.0170000	18.9040000	75.9500000
10	C	18.8400000	22.5200000	74.8160000
11	C	20.1340000	18.3160000	74.8720000

12	C	19.1760000	19.4440000	74.3700000
13	C	18.3340000	20.1140000	75.4220000
14	C	18.1880000	21.4340000	75.6490000
15	C	17.2800000	21.9260000	76.7520000
16	C	23.4420000	21.6820000	75.8100000
17	C	19.3380000	17.0690000	75.2950000
18	C	21.0980000	17.9370000	73.7100000
19	H	21.0800000	22.1740000	76.9610000
20	H	20.1910000	24.2060000	74.8390000
21	H	19.4490000	23.8820000	76.4070000
22	H	23.5850000	23.2630000	73.7390000
23	H	21.9660000	24.0340000	73.7600000
24	H	20.9930000	22.2450000	72.4790000
25	H	20.9610000	19.9820000	76.1390000
26	H	18.0400000	23.1950000	74.4620000
27	H	19.2880000	22.1000000	73.9050000
28	H	17.7730000	19.4380000	76.0760000
29	H	16.8700000	21.0940000	77.3400000
30	H	17.8090000	22.6030000	77.4460000
31	H	16.4250000	22.4910000	76.3380000
32	H	23.7090000	20.8920000	75.0870000
33	H	24.3440000	22.3080000	75.9340000
34	H	23.2160000	21.2070000	76.7760000
35	H	20.0130000	16.2930000	75.6740000
36	H	18.6110000	17.3220000	76.0760000
37	H	18.7980000	16.6780000	74.4210000
38	H	20.5000000	17.4940000	72.8990000
39	H	21.6290000	18.8150000	73.3120000
40	H	21.8350000	17.2020000	74.0620000
41	H	18.5180000	18.9710000	73.6180000
42	H	19.7720000	20.1850000	73.8180000
43	C	19.9620000	17.5700000	78.5880000
44	O	19.7560000	18.5350000	77.8370000
45	C	19.1620000	17.3980000	79.8690000
46	O	20.8390000	16.6360000	78.3960000
47	C	17.9140000	18.2710000	79.9810000
48	C	17.2000000	18.1140000	81.3260000
49	C	15.9430000	18.9780000	81.4700000
50	C	15.2570000	18.8260000	82.8290000
51	H	21.4650000	16.7590000	77.5200000
52	H	18.9240000	16.3240000	79.9630000
53	H	19.8570000	17.6050000	80.7040000
54	H	18.1980000	19.3250000	79.8230000
55	H	17.2170000	18.0270000	79.1590000

56	H	16.9310000	17.0510000	81.4800000
57	H	17.9040000	18.3600000	82.1420000
58	H	15.2300000	18.7240000	80.6640000
59	H	16.2130000	20.0380000	81.3070000
60	H	14.9350000	17.7850000	82.9990000
61	H	15.9380000	19.0970000	83.6540000
62	H	14.3660000	19.4690000	82.9110000

TS3c1_R6

	Symbol	X	Y	Z
1	C	22.3250000	22.5360000	75.3270000
2	O	22.7400000	21.0850000	72.6080000
3	C	21.1540000	22.6810000	75.9790000
4	O	22.1310000	16.9880000	76.5520000
5	C	19.9300000	23.4060000	75.4840000
6	O	22.0300000	18.4020000	76.5480000
7	C	22.5720000	23.1000000	73.9300000
8	C	22.1160000	22.0790000	72.8980000
9	C	20.9940000	18.8980000	76.0170000
10	C	18.9060000	22.5110000	74.7340000
11	C	20.1480000	18.3010000	74.9130000
12	C	19.2240000	19.4270000	74.3500000
13	C	18.3450000	20.1210000	75.3550000
14	C	18.2060000	21.4470000	75.5550000
15	C	17.2640000	21.9680000	76.6150000
16	C	23.4730000	21.7420000	75.8930000
17	C	19.3230000	17.0670000	75.3180000
18	C	21.1560000	17.8900000	73.8010000
19	H	21.0760000	22.2230000	76.9720000
20	H	20.2280000	24.2160000	74.8000000
21	H	19.4310000	23.8910000	76.3400000
22	H	23.6520000	23.2740000	73.7940000
23	H	22.0360000	24.0460000	73.7680000
24	H	21.1180000	22.2790000	72.4340000
25	H	20.9600000	19.9830000	76.1690000
26	H	18.1280000	23.1750000	74.3150000
27	H	19.4050000	22.0670000	73.8630000
28	H	17.7510000	19.4610000	75.9950000
29	H	16.7410000	21.1520000	77.1310000
30	H	17.7950000	22.5680000	77.3760000
31	H	16.4930000	22.6240000	76.1710000
32	H	23.7780000	20.9490000	75.1870000
33	H	24.3590000	22.3850000	76.0400000
34	H	23.2240000	21.2730000	76.8560000
35	H	19.9660000	16.3180000	75.7930000

36	H	18.5250000	17.3450000	76.0170000
37	H	18.8710000	16.6310000	74.4150000
38	H	20.5810000	17.4710000	72.9610000
39	H	21.7360000	18.7480000	73.4260000
40	H	21.8490000	17.1290000	74.1870000
41	H	18.5950000	18.9420000	73.5820000
42	H	19.8500000	20.1520000	73.8110000
43	C	19.8030000	17.6760000	78.6520000
44	O	19.6320000	18.6020000	77.8460000
45	C	18.9700000	17.5760000	79.9200000
46	O	20.6750000	16.7230000	78.5380000
47	C	17.7430000	18.4830000	79.9890000
48	C	17.0270000	18.3930000	81.3420000
49	C	15.7860000	19.2820000	81.4590000
50	C	15.0860000	19.1920000	82.8210000
51	C	13.8430000	20.0760000	82.9360000
52	H	21.3310000	16.7940000	77.6770000
53	H	18.7000000	16.5140000	80.0510000
54	H	19.6600000	17.7940000	80.7560000
55	H	18.0490000	19.5230000	79.7870000
56	H	17.0420000	18.2180000	79.1770000
57	H	16.7410000	17.3430000	81.5360000
58	H	17.7400000	18.6590000	82.1450000
59	H	15.0680000	19.0150000	80.6620000
60	H	16.0720000	20.3330000	81.2650000
61	H	14.8090000	18.1400000	83.0180000
62	H	15.8040000	19.4630000	83.6170000
63	H	13.0880000	19.8040000	82.1790000
64	H	14.0910000	21.1410000	82.7860000
65	H	13.3700000	19.9830000	83.9270000

TS3c1_R7

	Symbol	X	Y	Z
1	C	22.3140000	22.5030000	75.3000000
2	O	22.7090000	21.0820000	72.5540000
3	C	21.1490000	22.6530000	75.9630000
4	O	22.0930000	16.9850000	76.4940000
5	C	19.9290000	23.3970000	75.4900000
6	O	22.0200000	18.4010000	76.4810000
7	C	22.5560000	23.0780000	73.9060000
8	C	22.0830000	22.0670000	72.8740000
9	C	20.9860000	18.9090000	75.9600000
10	C	18.8810000	22.5210000	74.7500000
11	C	20.1180000	18.3110000	74.8750000
12	C	19.1900000	19.4380000	74.3240000

13	C	18.3220000	20.1240000	75.3440000
14	C	18.1950000	21.4470000	75.5680000
15	C	17.2740000	21.9530000	76.6530000
16	C	23.4560000	21.6860000	75.8450000
17	C	19.2950000	17.0830000	75.2980000
18	C	21.1100000	17.8940000	73.7510000
19	H	21.0740000	22.1820000	76.9510000
20	H	20.2270000	24.2090000	74.8080000
21	H	19.4500000	23.8830000	76.3570000
22	H	23.6360000	23.2440000	73.7630000
23	H	22.0260000	24.0290000	73.7550000
24	H	21.0710000	22.2610000	72.4400000
25	H	20.9730000	19.9970000	76.0930000
26	H	18.0960000	23.1970000	74.3650000
27	H	19.3540000	22.0920000	73.8570000
28	H	17.7350000	19.4590000	75.9840000
29	H	16.8040000	21.1280000	77.2050000
30	H	17.8120000	22.5850000	77.3820000
31	H	16.4620000	22.5720000	76.2290000
32	H	23.7370000	20.8920000	75.1320000
33	H	24.3560000	22.3130000	75.9820000
34	H	23.2130000	21.2170000	76.8100000
35	H	19.9480000	16.3120000	75.7210000
36	H	18.5400000	17.3610000	76.0430000
37	H	18.7870000	16.6770000	74.4130000
38	H	20.5240000	17.4690000	72.9210000
39	H	21.6850000	18.7500000	73.3650000
40	H	21.8070000	17.1360000	74.1330000
41	H	18.5560000	18.9560000	73.5580000
42	H	19.8110000	20.1670000	73.7830000
43	C	19.7800000	17.7140000	78.6030000
44	O	19.6490000	18.6620000	77.8150000
45	C	18.9370000	17.6260000	79.8660000
46	O	20.6170000	16.7330000	78.4710000
47	C	17.7100000	18.5370000	79.9020000
48	C	16.9540000	18.4550000	81.2320000
49	C	15.7130000	19.3500000	81.3130000
50	C	14.9980000	19.2720000	82.6660000
51	C	13.7460000	20.1480000	82.7760000
52	C	13.0540000	20.0390000	84.1370000
53	H	21.2810000	16.8030000	77.6160000
54	H	18.6640000	16.5660000	80.0090000
55	H	19.6180000	17.8560000	80.7050000
56	H	18.0290000	19.5760000	79.7100000

57	H	17.0330000	18.2740000	79.0700000
58	H	16.6560000	17.4060000	81.4190000
59	H	17.6430000	18.7170000	82.0560000
60	H	15.0080000	19.0720000	80.5070000
61	H	16.0030000	20.3980000	81.1110000
62	H	14.7220000	18.2200000	82.8720000
63	H	15.7060000	19.5530000	83.4680000
64	H	13.0350000	19.8720000	81.9760000
65	H	14.0200000	21.2030000	82.5830000
66	H	12.1550000	20.6750000	84.1900000
67	H	12.7400000	19.0010000	84.3420000
68	H	13.7280000	20.3450000	84.9540000