

Supplementary Information

Theoretical study on the mechanism of the gas phase
reaction of methoxybenzene with ozone

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Detailed parameters in the kinetic calculations

The rate constants of unimolecular reactions in this paper are obtained by solving the energy-grained master-equation with the MultiWell program.

The energy-dependent specific unimolecular rate constant is given as follows:

$$k(E) = \left[\frac{m^\ddagger \sigma_{ext}}{m \sigma_{ext}^\ddagger} \right] \frac{g^\ddagger \rho(E - E_0)}{g h \rho(E)}$$

where m^\ddagger and m are the number of optical isomers, σ_{ext}^\ddagger and σ_{ext} are the external rotation symmetry numbers, g^\ddagger and g represent the electronic state degeneracies of the transition state and corresponding reactant, respectively. h is the Plank's constant. $\rho(E)$ is the density of states of the reactant and $\rho(E - E_0)$ is the sum of states of the transition state. In this work, the transition states of the entrance channels are treated as tight transition states rather than variational transition states.

The collision rate constants were calculated by Klaus Luther's empirical function with kinetically controlled selective ionization parameters[2]. As the Lennard-Jones parameters for IM1 are not available from the literature, we try to estimate these parameters theoretically. The intermolecular interaction energy between the primary ozonide and argon bath gas has been estimated at the M06-2X/6-31+g(d,p) level as shown in Fig. S3 in Supplementary Information. So the Lennard-Jones parameter of IM1 was set as $\sigma_{IM1} = 5.14 \text{ \AA}$ and $\varepsilon_{IM1}/k_b = 5840.80 \text{ K}$ to confirm that the Lennard-Jones parameters for IM1 + Ar collisions are in confidence with Fig. S3. The Lennard-Jones parameters for other intermediates are also set as $\sigma = 5.14 \text{ \AA}$ and $\varepsilon/k_b = 5840.80 \text{ K}$ in the input files, for convenience.

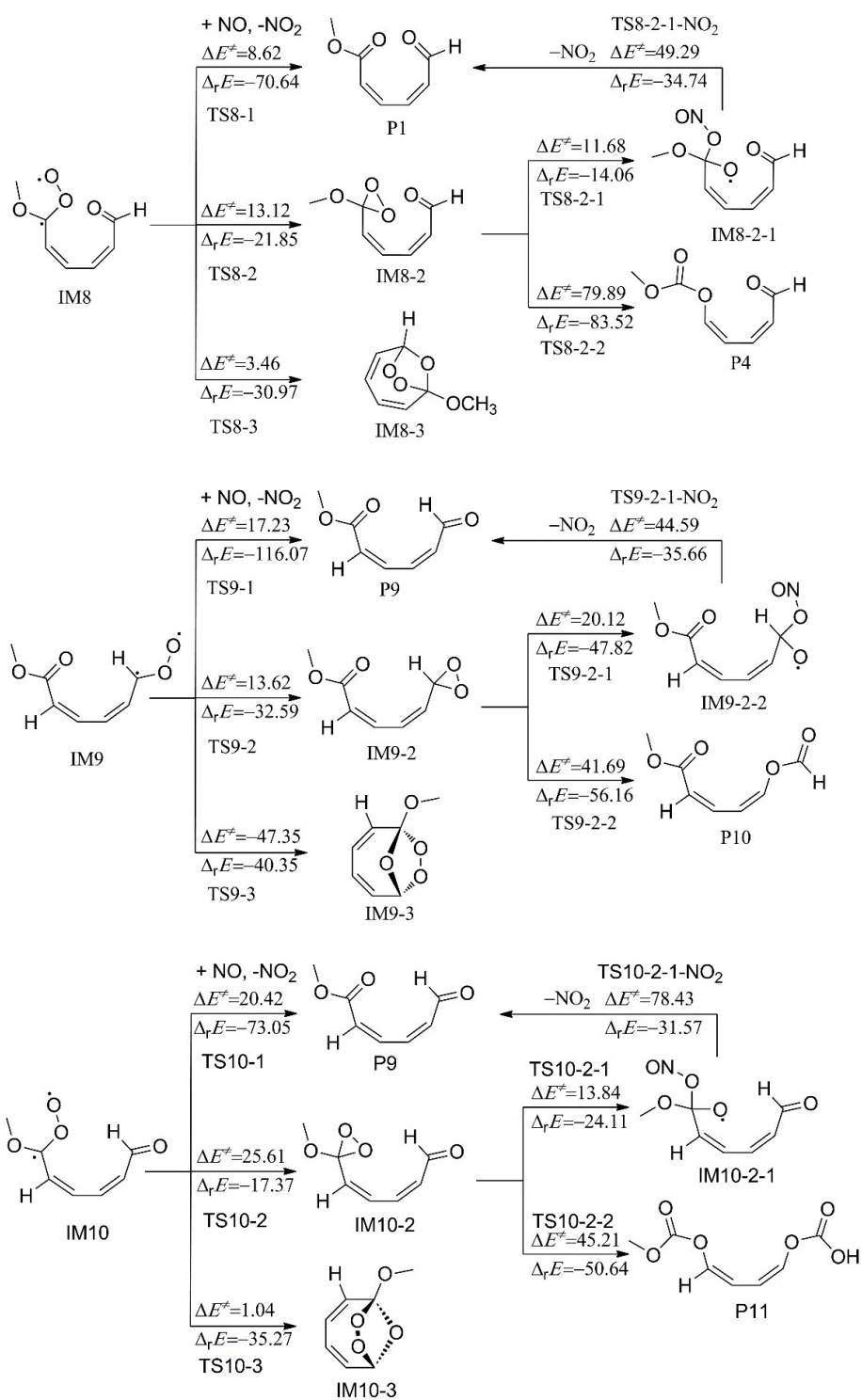


Fig. S1. The detailed mechanisms of the further reaction for the Criegee intermediates IM7, IM8, IM9, IM10, IM11, IM12, IM13, IM14, IM15, IM16, IM17 and IM18 respectively.

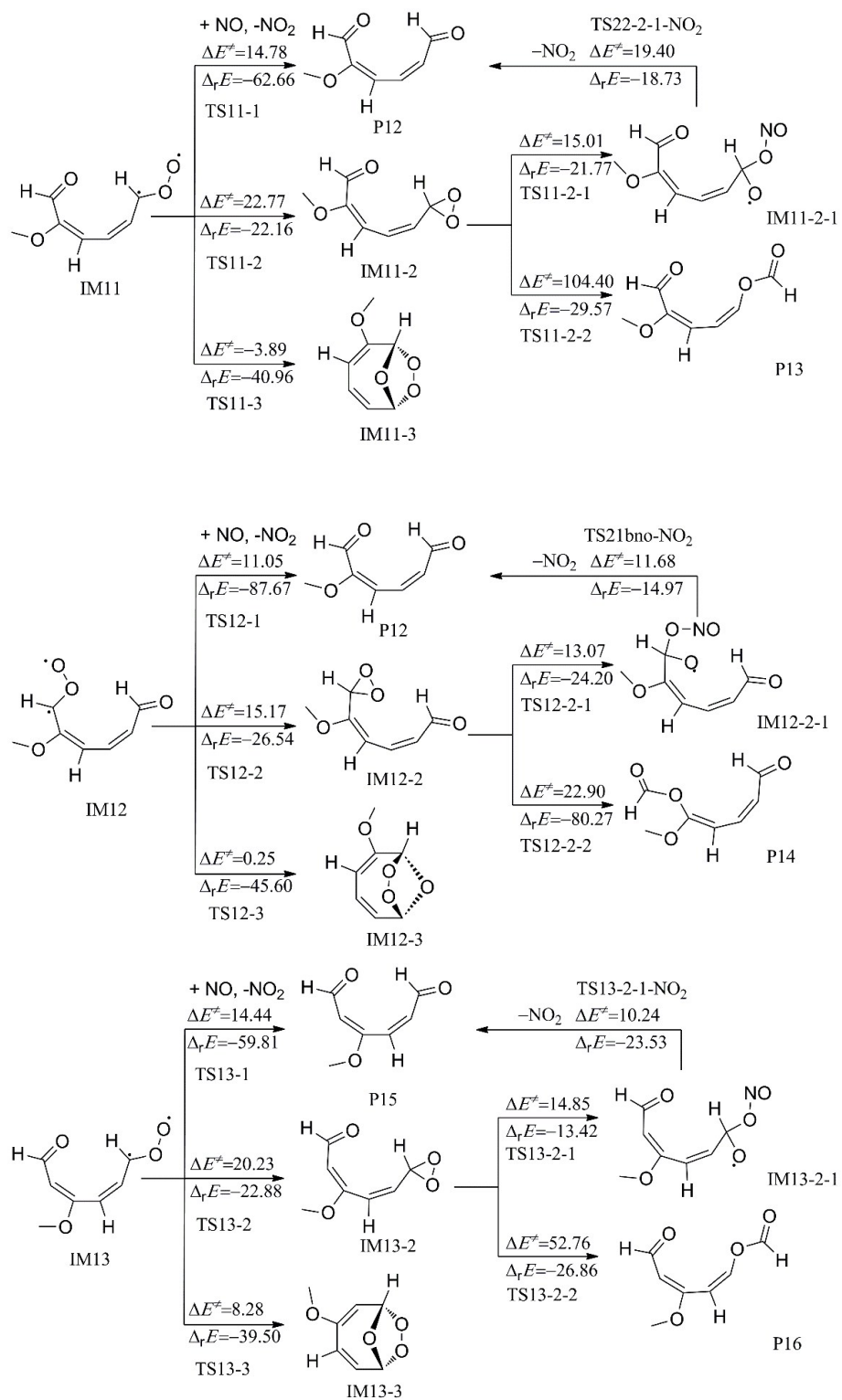


Fig. S1. Continued.

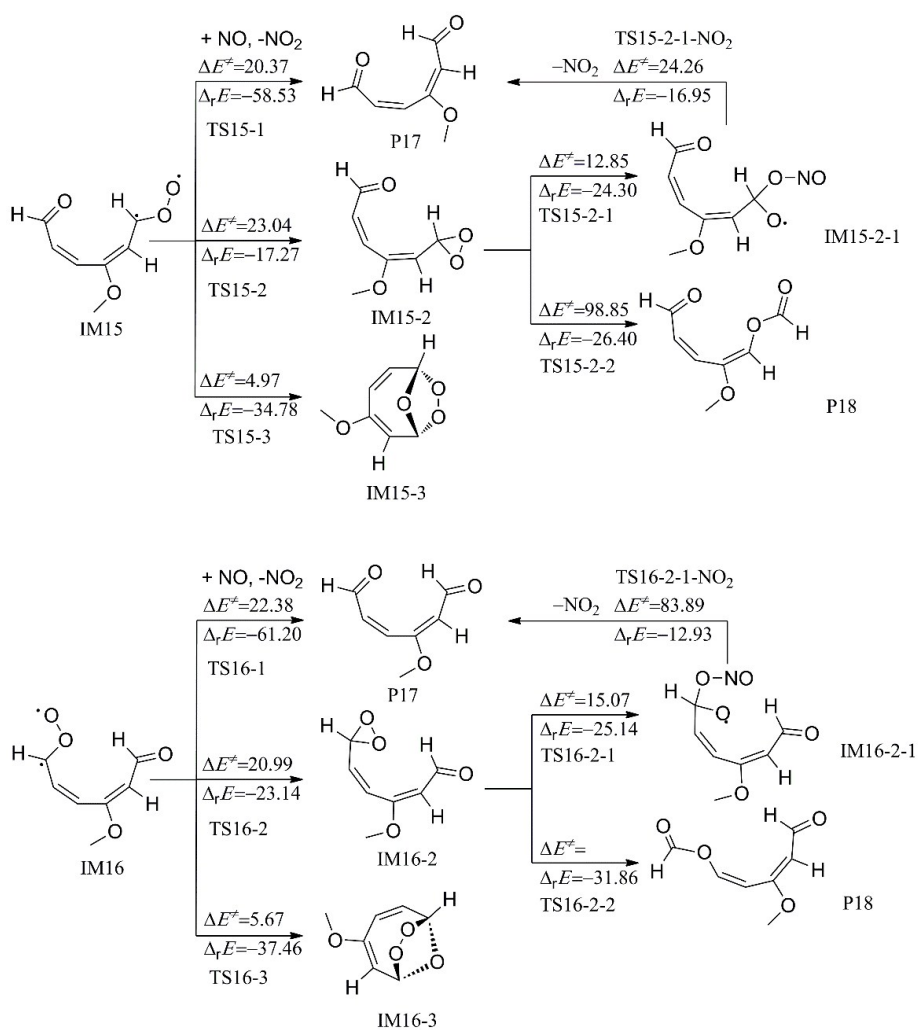


Fig. S1. Continued.

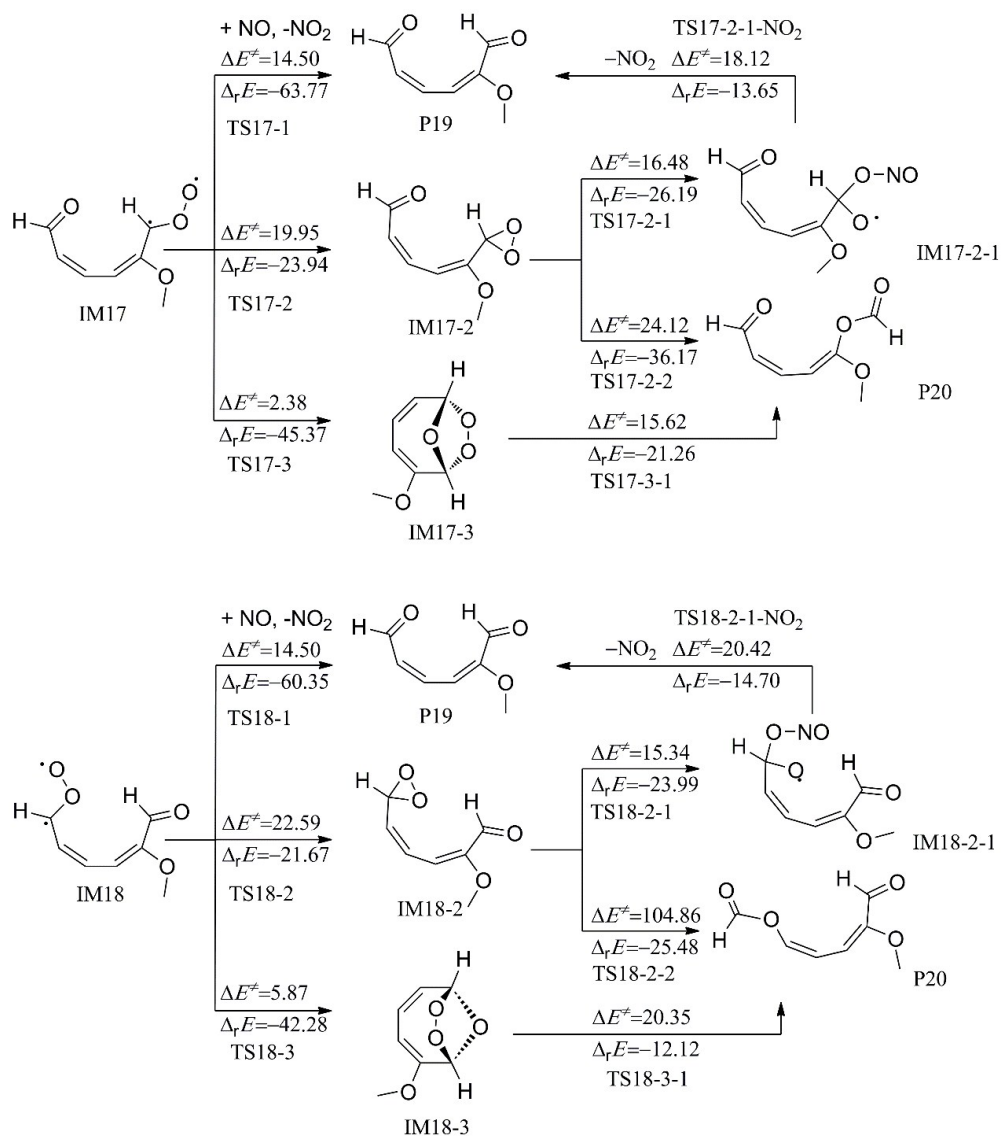


Fig. S1. Continued.

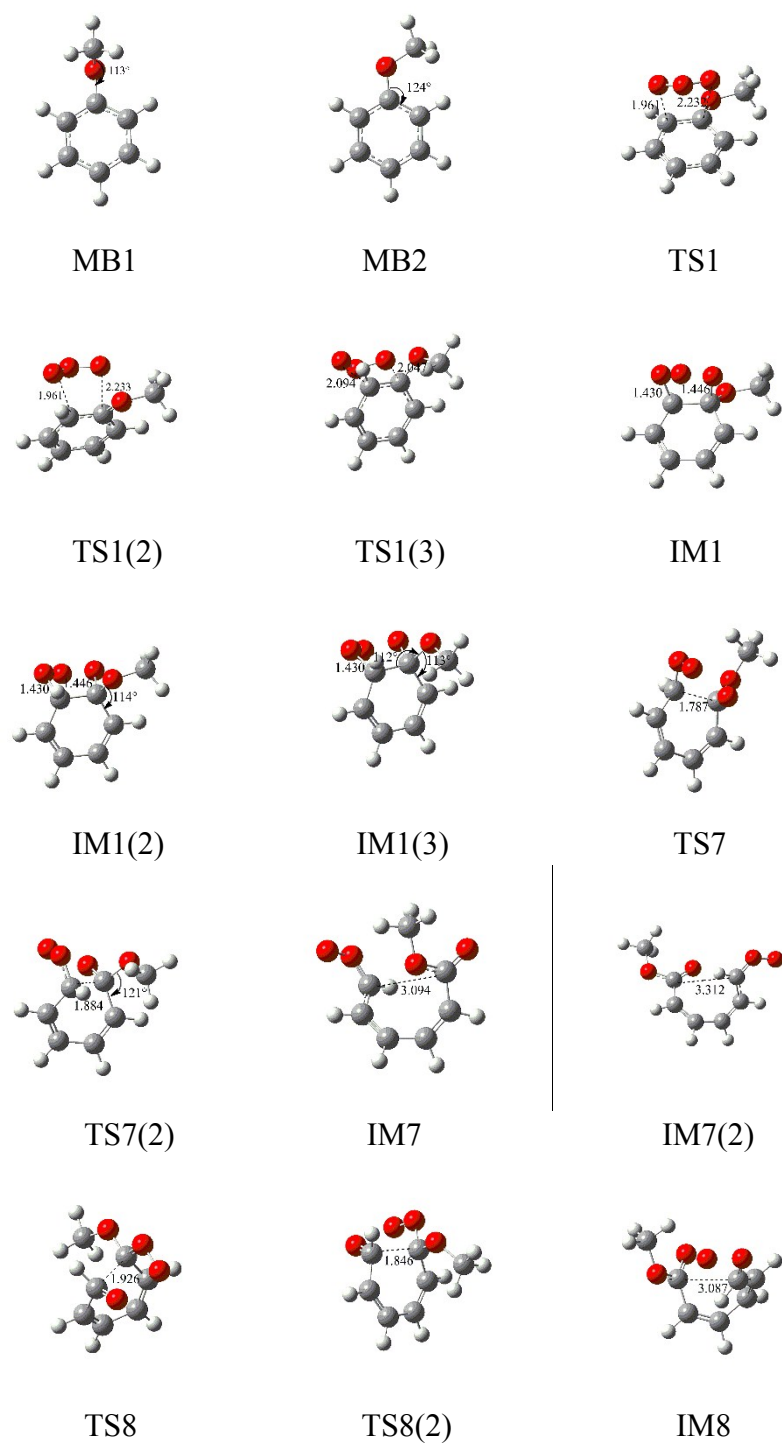
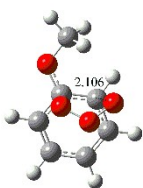


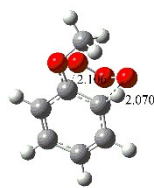
Fig. S2. M06-2X/6-31+g(d,p) optimized geometries for the reactants, transition states, intermediates involved in the initial reaction of MB + O₃ (bond length in Å and angle in degree).



IM8(2)



TS2



TS2(2)



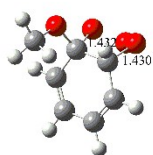
TS3(2)



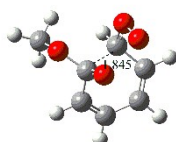
IM2



IM2(2)



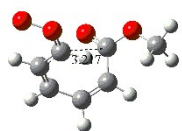
IM2(3)



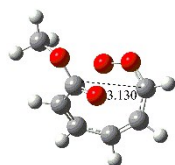
TS9



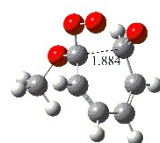
TS9(2)



IM9



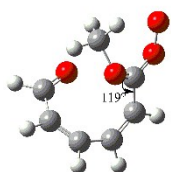
IM9(2)



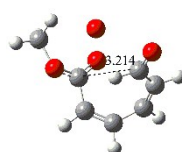
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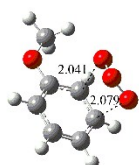
TS10(2)



IM10



IM10(2)



TS3



TS3(2)



IM3

Fig. S2. Continued.

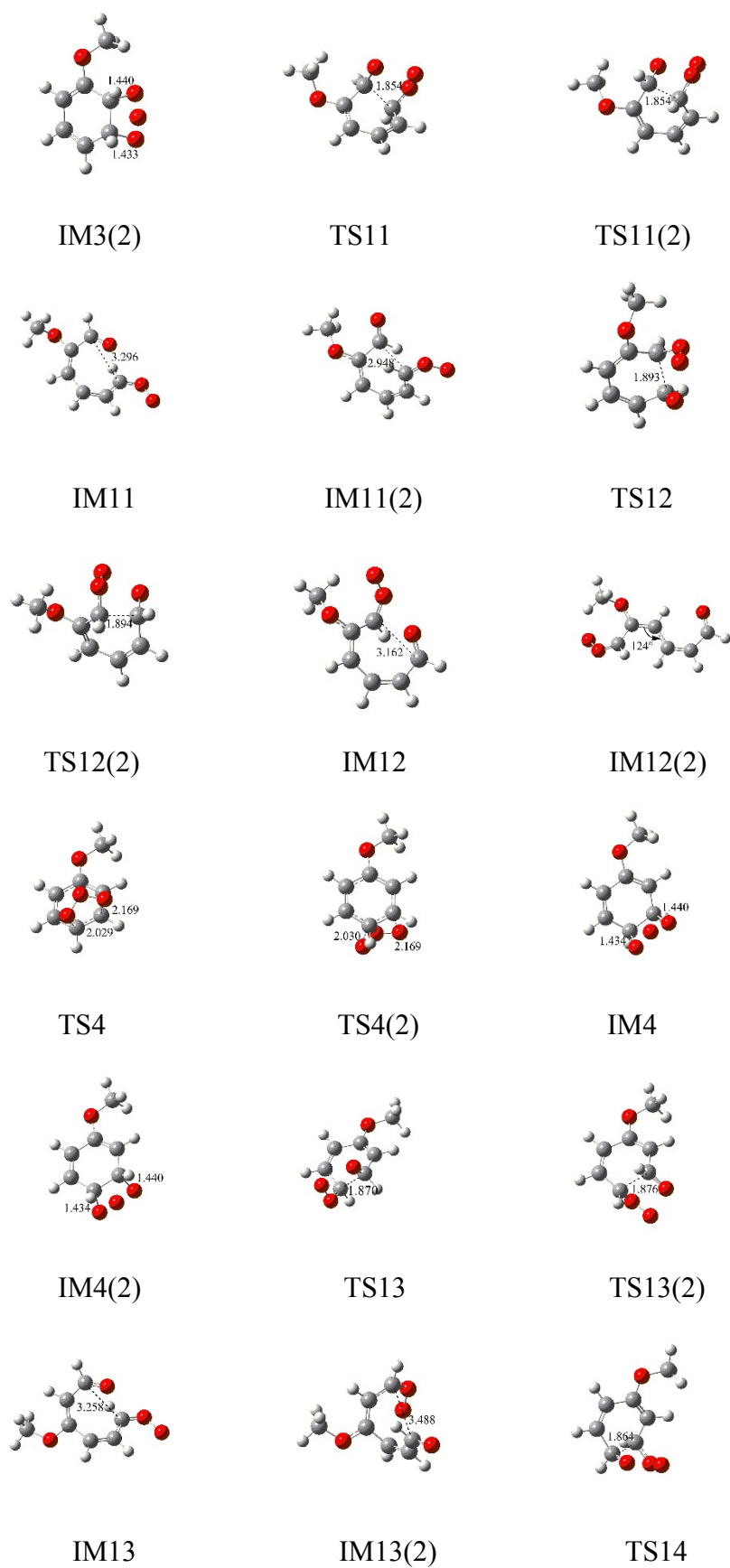
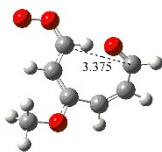


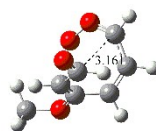
Fig. S2. Continued.



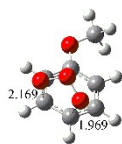
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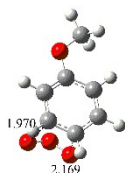
IM14



IM14(2)



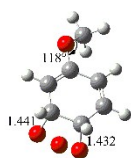
TS5



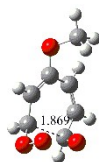
TS5(2)



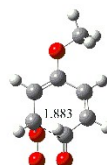
IM5



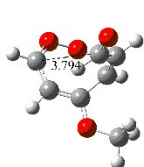
IM5(2)



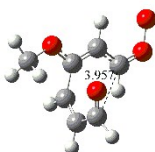
TS15



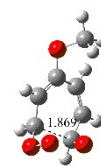
TS15(2)



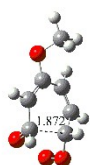
IM15



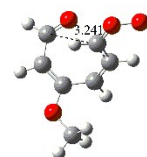
IM1(2)



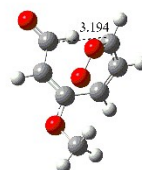
TS16



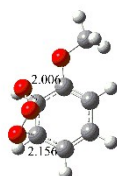
TS16(2)



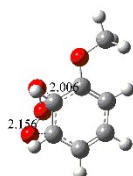
IM16



IM16(2)



TS6

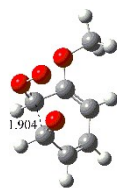


TS6(2)



IM6

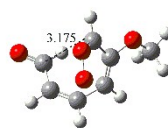
Fig. S2. Continued.



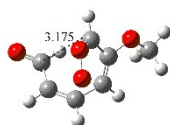
IM6(2)



TS17



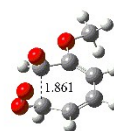
TS17(2)



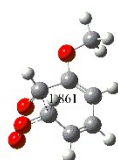
IM17



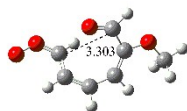
IM17(2)



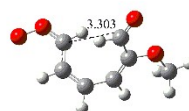
TS18



TS18(2)



IM18



IM18(2)

Fig. S2. Continued.

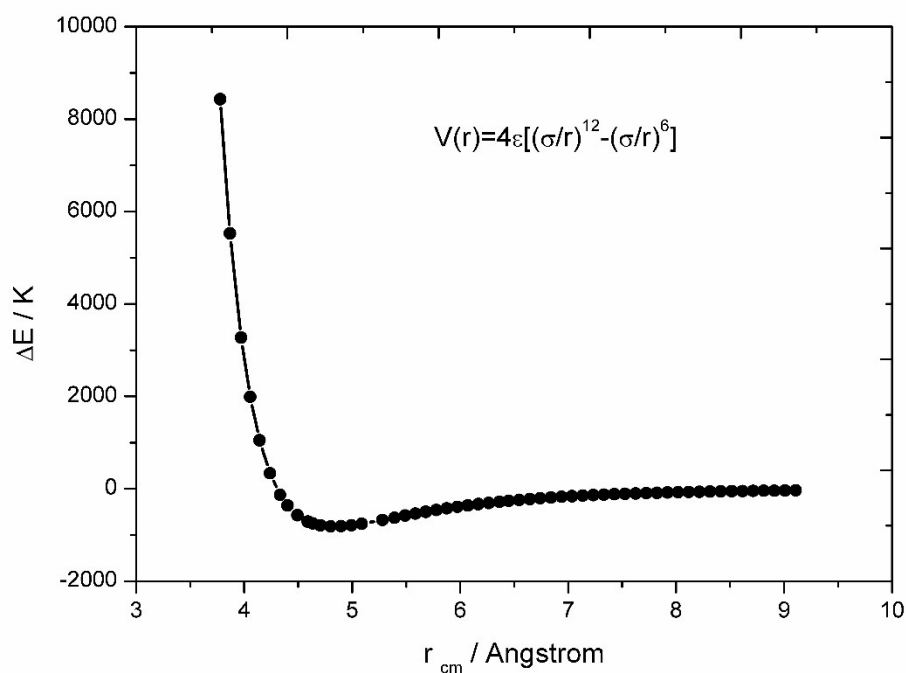


Fig. S3. The intermolecular interaction energy between the primary ozonide and argon bath gas has been estimated at the M06-2X/6-31+g(d,p).

Table S1. The energy barriers (ΔE^\ddagger , kcal mol⁻¹) and reaction heats ($\Delta_r E$, kcal mol⁻¹) of MB + O₃ → IM1 at different levels.

Functionals	with dispersion corrections		without dispersion corrections	
	ΔE^\ddagger	$\Delta_r E$	ΔE^\ddagger	$\Delta_r E$
B2PLYP/aug-cc-pVDZ//B2PLYP/aug-cc-pVDZ	9.80	-32.65	7.23	-34.80
wB97X/aug-cc-pVDZ//wB97X/aug-cc-pVDZ	7.52	-28.13	8.74	-30.16
CCSD(T)/6-31+g(d,p)//M06-2X/6-31+g(d,p)	-	-	7.18	32.04
M06-2X/TZVP//M06-2X/TZVP	-	-	10.13	-41.23
M06-2X/aug-cc-pVDZ//M06-2X/6-31+g(d,p)	-	-	7.28	-31.50
M06-2X/aug-cc-pVQZ//M06-2X/6-31+g(d,p)	-	-	8.12	-33.94
M06-2X/aug-cc-pVTZ//M06-2X/6-31+g(d,p)	-	-	8.43	-38.97
M06-2X/6-311++g(3df, 2p)//M06-2X/6-31+g(d,p)	-	-	5.80	-36.74

Table S2. The overall and individual rate constants ($k_i/\text{cm}^{-3} \text{ molecule}^{-1} \text{ s}^{-1}$) at 1 atm and over the temperature range of 200-400 K.

T/K	k_1	k_2	k_3	k_4	k_5	k_6	k_{tot}
200	1.89E-24	2.79E-24	6.80E-28	3.79E-25	4.73 E-27	3.46E-26	5.10E-24
225	1.51E-23	2.07E-23	1.37 E-26	3.84E-24	7.94 E-26	4.71E-25	4.01E-23
250	8.11E-23	1.05E-22	1.55E-25	2.51E-23	7.77 E-25	3.86E-24	2.16E-22
275	3.20E-22	4.06E-22	1.15E-24	1.19E-22	5.14E-24	2.20E-23	8.82E-22
298	9.85E-22	1.17 E-21	5.48E-24	4.01E-22	2.24 E-23	8.63E-23	2.67E-21
325	2.98 E-21	3.41 E-21	2.63E-23	1.36E-21	9.83E-23	3.37E-22	8.22E-21
350	7.24E-21	8.06 E-21	9.19 E-23	3.63E-21	3.19 E-22	1.00E-21	2.03E-20
375	1.59E-20	1.72E-20	2.74E-22	8.60E-21	8.96E-22	2.63E-21	4.54E-20
400	3.19E-20	3.37E-20	7.25E-22	1.85E-20	2.25E-21	6.15E-21	9.32E-20

Table S3. The calculated TST rate constants ($\text{cm}^{-3} \text{ molecule}^{-1} \text{ s}^{-1}$) for the entrance channels over the temperature range of 200-400 K.

T/K	k_1	k_2	k_3	k_4	k_5	k_6	k_{tot}
200	2.73E-24	4.08E-24	1.07E-27	1.38E-24	7.20E-27	5.11E-26	8.24E-24
225	1.99E-23	2.76E-23	1.93E-26	1.16E-23	1.10E-25	6.30E-25	5.99E-23
250	1.01E-22	1.32E-22	2.03E-25	6.58E-23	1.00E-24	4.87E-24	3.05E-22
275	3.93E-22	4.86E-22	1.43E-24	2.79E-22	6.29E-24	2.66E-23	1.19E-21
298	1.25E-21	1.48E-21	7.41E-24	9.52E-22	2.97E-23	1.12E-22	3.82E-21
325	3.37E-21	3.85E-21	3.04E-23	2.74E-21	1.13E-22	3.84E-22	1.05E-20
350	8.05E-21	8.91E-21	1.04E-22	6.87E-21	3.59E-22	1.12E-21	2.54E-20
375	1.74E-20	1.87E-20	3.05E-22	1.55E-20	9.93E-22	2.89E-21	5.57E-20
400	3.44E-20	3.63E-20	7.93E-22	3.19E-20	2.45E-21	6.67E-21	1.12E-19

Table S4. Relative energies (kcal/mol) with respect to the total energies of MB1 and O₃ for the intermediates, transition states involved in the initial reaction of MB + O₃. (ΔE values are from M06-2X/aug-cc-pVDZ//M06-2X/6-31+g(d,p) level of theory.)

Compound	ΔE	Compound	ΔE
MB1+O3	0	TS12(2)	-1.08
TS1	7.28	IM12(2)	-35.19
IM1	-34.60	TS4	7.76
TS1(2)	7.28	IM4	-36.51
IM1(2)	-34.60	TS4(2)	7.75
TS1(3)	12.93	IM4(2)	-36.51
IM1(3)	-33.37	TS13	-7.49
TS7	-14.67	IM13	-42.49
IM7	-59.80	TS13(2)	-8.41
TS7(2)	-12.16	IM13(2)	-43.47
IM7(2)	-59.47	TS14	-8.41
TS8	-7.47	IM14	-43.80
IM8	-49.10	TS14(2)	-10.70
TS8(2)	-7.47	IM14(2)	-42.35
IM8(2)	-50.30	TS5	9.92
TS2	7.04	IM5	-31.32
IM2	-33.37	TS5(2)	9.92
TS2(2)	7.04	IM5(2)	-31.69
IM2(2)	-36.19	TS15	-4.07
TS2(3)	10.93	IM15	-42.55
IM2(3)	-33.37	TS15(2)	-8.83
TS9	-9.65	IM15(5)	-40.66
IM9	-50.35	TS16	-3.18
TS9(2)	-9.65	IM16	-39.88
IM9(2)	-54.42	TS16(2)	-3.18
TS10	-7.47	IM16(2)	-40.02
IM10	-46.68	TS6	9.13
TS10(2)	-7.47	IM6	-35.96
IM10(2)	-45.35	TS6(2)	9.41
TS3	10.55	IM6(2)	-35.95
IM3	-32.18	TS17	-4.87
TS3(2)	10.56	IM17	-36.28
IM3(2)	-35.13	TS17(2)	-9.52
TS11	-6.23	IM17(2)	-31.13
IM11	-35.11	TS18	-8.55
TS11(2)	-6.23	IM18	-39.70
IM11(2)	-39.26	TS18(2)	-8.55
TS12	-1.06	IM18(2)	-39.69

Table S5. Coordinates for various species involved in the MB + O₃ reaction (the M06-2X/6-31+g(d,p) optimized data, in Å)

MB			
C	-3.157087	-1.690750	-0.079768
C	-1.761927	-1.690750	-0.079768
C	-1.064389	-0.482999	-0.079768
C	-1.762043	0.725510	-0.080967
C	-3.156868	0.725432	-0.081446
C	-3.854469	-0.482774	-0.080450
H	-3.706846	-2.643067	-0.079318
H	-1.212419	-2.643263	-0.078453
H	0.035291	-0.482919	-0.079134
H	-3.706990	1.677713	-0.082399
H	-4.954073	-0.482591	-0.080630
O	-1.046575	1.963656	-0.081043
C	0.359250	1.701821	-0.081027
H	0.617454	1.140179	-0.954405
H	0.894600	2.628266	-0.081561
H	0.617606	1.141100	0.792897
O ₃			
O	-0.284091	0.892857	0.000000
O	1.035909	0.892857	0.000000
O	1.476534	-0.351430	0.000002

TS1

C	1.112021	1.981218	0.134117
C	-0.206244	1.620316	0.009029
C	-0.521918	0.304374	-0.403473
C	0.553623	-0.595081	-0.794248
C	1.891229	-0.105763	-0.825348
C	2.164150	1.123425	-0.297619
H	1.358002	2.959783	0.533035
H	-1.000158	2.299672	0.294811
H	2.658576	-0.770065	-1.205663
H	3.189890	1.469669	-0.232696
O	-1.730567	-0.131237	-0.797445
C	-2.863506	0.564534	-0.291082
H	-2.937086	1.557577	-0.745819
H	-3.731655	-0.030033	-0.569728
H	-2.791823	0.645611	0.797569
O	0.768081	-1.566969	0.954751
O	0.413419	-0.729378	1.868533
O	-0.807942	-0.346882	1.671228
H	0.342302	-1.611104	-1.054902

IM1

C	1.082784	2.080307	0.182151
C	-0.178705	1.652241	0.278868
C	-0.540859	0.207205	0.078736
C	0.621350	-0.719862	-0.466059
C	1.984366	-0.095183	-0.494769
C	2.188770	1.187546	-0.192296
H	1.314055	3.121728	0.385022
H	-0.977200	2.321435	0.582694
H	2.785159	-0.761881	-0.798567
H	3.190511	1.603596	-0.234150
O	-1.624555	0.000531	-0.768470
C	-2.861585	0.583870	-0.372009
H	-2.845949	1.668891	-0.513479
H	-3.618966	0.150828	-1.024560
H	-3.092125	0.337476	0.668321
O	0.581641	-1.795692	0.499226
O	0.298407	-1.118957	1.692320
O	-0.864986	-0.375531	1.351315
H	0.422339	-1.144240	-1.427931

TS2

C	-1.248694	-1.407145	-1.121864
C	0.046156	-0.859194	-1.071987
C	0.224054	0.398267	-0.396836
C	-0.937085	1.131778	0.070685
C	-2.164050	0.532903	0.060165
C	-2.301705	-0.754098	-0.518147
H	-1.399512	-2.358824	-1.617368
H	0.832884	-1.227233	-1.718285
H	-3.013073	1.055833	0.484076
H	-3.285683	-1.213026	-0.525794
O	1.315597	1.177601	-0.543165
C	2.551452	0.528950	-0.847307
H	2.581070	0.254610	-1.906575
H	3.330065	1.261458	-0.640544
H	2.674584	-0.353405	-0.215565
O	0.641354	-0.174874	1.461595
O	0.362621	-1.437799	1.445428
O	1.001453	-2.012853	0.477902
H	-0.785605	2.122694	0.472604

IM2

C	1.338713	0.971970	1.036284
C	0.532576	-0.285523	0.933806
C	-0.492440	-0.347211	-0.244248
C	-0.549520	0.878419	-1.129285
C	0.227616	1.949486	-0.934238
C	1.180892	1.985256	0.176105
H	2.060032	1.021474	1.845341
H	0.009704	-0.512630	1.869185
H	0.158648	2.787693	-1.618815
H	1.783448	2.881913	0.287456
O	-1.774644	-0.741590	0.142550
C	-2.516395	0.270698	0.814165
H	-2.749834	1.104668	0.143303
H	-3.437192	-0.205280	1.148682
H	-1.968016	0.651389	1.685020
O	-0.033072	-1.458980	-1.015468
O	1.348746	-1.493838	-0.728403
O	1.343065	-1.441979	0.682991
H	-1.258199	0.823301	-1.929058

TS3

C	1.411509	0.038612	1.106627
C	0.107712	-0.565160	0.976818
C	-0.897618	0.146679	0.325696
C	-0.630761	1.405300	-0.200792
C	0.608852	2.055729	0.034837
C	1.588231	1.415789	0.732744
H	2.081345	-0.390428	1.842825
H	-0.105491	-1.482689	1.508030
H	0.731831	3.062714	-0.348754
H	2.540790	1.894663	0.926926
O	-2.162384	-0.309579	0.081156
C	-2.449106	-1.662459	0.407418
H	-2.443899	-1.806927	1.493666
H	-3.450590	-1.855406	0.024908
H	-1.729751	-2.334374	-0.069398
O	0.679033	-1.947274	-0.726579
O	1.467213	-1.032336	-1.207069
O	2.374205	-0.723454	-0.335826
H	-1.312255	1.882750	-0.706459

IM3

C	1.596620	0.143711	0.772624
C	0.321123	-0.738529	0.561533
C	-0.895983	0.005591	0.113268
C	-0.902844	1.330733	-0.095139
C	0.292375	2.148585	0.096663
C	1.450122	1.610023	0.484873
H	2.012070	-0.011958	1.772561
H	0.121143	-1.344115	1.450696
H	0.191820	3.209894	-0.108734
H	2.344986	2.212548	0.602258
O	-2.032386	-0.687215	-0.224873
C	-2.299833	-1.885238	0.487678
H	-2.371517	-1.694682	1.565586
H	-3.259066	-2.247447	0.119582
H	-1.531532	-2.640456	0.289481
O	0.752098	-1.689896	-0.425149
O	1.718791	-0.957290	-1.153119
O	2.542030	-0.477935	-0.108915
H	-1.769448	1.856115	-0.438464

TS4

C	0.93611	-0.70422	1.17528
C	-0.405753	-1.006667	0.810152
C	-1.158047	-0.046390	0.192209
C	-0.665883	1.297109	0.045037
C	0.566987	1.641508	0.528863
C	1.419349	0.639367	1.046514
H	1.473762	-1.390528	1.817551
H	-0.781405	-2.011031	0.959556
H	0.896917	2.670749	0.451286
H	2.317778	0.923815	1.579456
O	-2.416109	-0.202635	-0.297595
C	-2.991421	-1.496012	-0.221243
H	-3.104387	-1.805922	0.823386
H	-3.970974	-1.420096	-0.690424
H	-2.373465	-2.222175	-0.760015
O	1.888841	-1.599673	-0.437283
O	1.992597	-0.570724	-1.201971
O	2.701493	0.341322	-0.638258
H	-1.298081	2.029188	-0.412440

IM4

C	1.094100	-0.871841	0.776479
C	-0.357088	-1.104550	0.483750
C	-1.171966	-0.103169	0.133859
C	-0.707114	1.301917	0.055597
C	0.559726	1.628012	0.325143
C	1.591593	0.608168	0.682058
H	1.372390	-1.317997	1.735514
H	-0.697232	-2.132007	0.533392
H	0.874387	2.663336	0.254641
H	2.132006	0.896014	1.588182
O	-2.488214	-0.203343	-0.177878
C	-3.062036	-1.499545	-0.170071
H	-2.996096	-1.939033	0.831120
H	-4.105769	-1.372034	-0.452179
H	-2.553087	-2.145573	-0.893109
O	1.925867	-1.544135	-0.181215
O	2.161633	-0.532208	-1.141721
O	2.620558	0.520498	-0.320886
H	-1.433420	2.039534	-0.215143

TS5

C	-0.45344	-1.75213	-0.77232
C	0.77378	-1.43806	-0.25473
C	1.18074	-0.07979	-0.13665
C	0.35405	0.94125	-0.55563
C	-0.96262	0.65682	-0.97054
C	-1.38758	-0.71474	-1.06568
H	-0.7513	-2.78658	-0.89533
H	1.45325	-2.23012	0.03881
H	-1.52448	1.43974	-1.4653
H	-2.26067	-0.9366	-1.66735
O	2.3976	0.32721	0.33105
C	3.34397	-0.66087	0.69522
H	3.59584	-1.29769	-0.15996
H	4.23201	-0.12004	1.01947
H	2.97053	-1.27644	1.52083
O	-2.52553	-0.85286	0.57876
O	-1.94355	0.01107	1.3374
O	-1.98524	1.17953	0.79488
H	0.66636	1.96436	-0.53128

IM5

C	0.534496	-1.841482	0.201186
C	-0.696663	-1.544839	-0.225291
C	-1.213930	-0.177996	-0.184574
C	-0.453863	0.849265	0.219458
C	0.959567	0.679849	0.681316
C	1.470736	-0.797086	0.741832
H	0.927288	-2.851334	0.143016
H	-1.344528	-2.311895	-0.640944
H	1.093618	1.198761	1.635045
H	1.811626	-1.055003	1.748888
O	-2.485830	0.095818	-0.641138
C	-3.518583	-0.453563	0.171463
H	-3.477512	-0.031270	1.182290
H	-4.463813	-0.191508	-0.304318
H	-3.434037	-1.544155	0.233334
O	2.669882	-0.725398	-0.039151
O	2.324327	0.229696	-1.019432
O	1.884577	1.308202	-0.214328
H	-0.787315	1.865912	0.231237

TS6

C	-0.357339	2.246888	-0.115926
C	0.877630	1.556344	-0.287622
C	0.999521	0.283190	0.193442
C	-0.143018	-0.384010	0.770930
C	-1.361702	0.336409	0.967498
C	-1.419931	1.686837	0.545640
H	-0.431257	3.263722	-0.488339
H	1.703649	2.048479	-0.786026
H	-2.065121	-0.071439	1.683439
H	-2.328815	2.252110	0.714892
O	2.095972	-0.510460	0.160824
C	3.225304	-0.025375	-0.545545
H	3.606201	0.890321	-0.080427
H	3.979237	-0.808624	-0.486932
H	2.964840	0.167009	-1.591715
O	-2.462134	-0.679676	-0.479497
O	-1.587302	-0.630403	-1.422086
O	-0.523131	-1.274576	-1.080334
H	-0.077717	-1.414657	1.050932

IM6

C	1.094100	-0.871841	0.776479
C	-0.357088	-1.104550	0.483750
C	-1.171966	-0.103169	0.133859
C	-0.707114	1.301917	0.055597
C	0.559726	1.628012	0.325143
C	1.591593	0.608168	0.682058
H	1.372390	-1.317997	1.735514
H	-0.697232	-2.132007	0.533392
H	0.874387	2.663336	0.254641
H	2.132006	0.896014	1.588182
O	-2.488214	-0.203343	-0.177878
C	-3.062036	-1.499545	-0.170071
H	-2.996096	-1.939033	0.831120
H	-4.105769	-1.372034	-0.452179
H	-2.553087	-2.145573	-0.893109
O	1.925867	-1.544135	-0.181215
O	2.161633	-0.532208	-1.141721
O	2.620558	0.520498	-0.320886
H	-1.433420	2.039534	-0.215143

TS7

C	-2.022363	1.432569	-0.164844
C	-0.722470	1.725427	-0.153665
C	0.372240	0.681077	-0.290006
C	-0.332642	-0.772264	0.573935
C	-1.724859	-0.984487	0.075272
C	-2.511217	0.046749	-0.229164
H	-2.753788	2.234167	-0.130518
H	-0.355263	2.744575	-0.084160
H	-2.049578	-2.018861	0.006031
H	-3.538297	-0.127162	-0.534311
O	1.436613	1.023316	0.569701
C	2.732089	0.647488	0.102059
H	2.956633	1.146035	-0.843972
H	3.428526	0.972669	0.874872
H	2.803103	-0.435011	-0.040814
O	0.607261	-1.639853	0.096097
O	0.546029	-1.667965	-1.212916
O	0.648070	0.243517	-1.451359
H	-0.345424	-0.849214	1.641088

IM7

C	1.159137	2.001643	-0.298398
C	1.989813	1.017494	0.077951
C	1.810247	-0.459221	0.016788
C	-1.366536	0.392616	0.572749
C	-1.270689	1.273706	-0.580186
C	-0.176602	1.969098	-0.916706
H	1.558509	3.011481	-0.206560
H	2.964723	1.286294	0.471971
H	-2.166875	1.278581	-1.190737
H	-0.275485	2.634673	-1.773336
O	0.627922	-0.846906	-0.469901
C	0.392257	-2.262408	-0.558670
H	0.555376	-2.725719	0.416895
H	-0.647506	-2.349873	-0.874138
H	1.079341	-2.701949	-1.284146
O	-2.088726	-0.633745	0.585604
O	-2.645807	-1.001796	-0.664209
O	2.671195	-1.226297	0.384011
H	-0.904274	0.622717	1.398254

TS8

C	-1.459053	-1.080410	-1.272134
C	-0.554350	-0.149489	-1.579198
C	0.211823	0.622062	-0.545182
C	0.441501	-0.531542	0.912717
C	-0.921819	-1.158253	1.118489
C	-1.745572	-1.467401	0.116451
H	-2.020918	-1.560245	-2.067882
H	-0.344536	0.145407	-2.604805
H	-1.146990	-1.398646	2.153786
H	-2.667321	-2.003734	0.319417
O	-0.253568	1.841258	-0.198577
C	-1.538070	1.913000	0.415436
H	-1.481198	1.523783	1.435702
H	-1.791797	2.971708	0.430940
H	-2.282980	1.359643	-0.163757
O	1.363436	-1.307646	0.492024
O	2.050962	-0.416441	-1.054450
O	1.537194	0.756510	-0.767718
H	0.664790	0.128882	1.724432

IM8

C	1.139745	-1.413876	1.055354
C	-0.097244	-1.049151	1.407498
C	-1.037420	-0.473165	0.442589
C	1.267553	1.251362	-0.374451
C	1.728174	-0.045172	-0.935887
C	1.672230	-1.223347	-0.303202
H	1.794527	-1.854009	1.804425
H	-0.445386	-1.095493	2.434028
H	2.016845	-0.001016	-1.980649
H	1.998876	-2.118554	-0.825692
O	-1.661155	0.616495	0.833773
C	-2.537962	1.251454	-0.118658
H	-3.336163	0.563888	-0.403602
H	-2.934589	2.120020	0.401509
H	-1.956556	1.548642	-0.993477
O	0.554492	2.024248	-0.976921
O	-0.701776	-2.128254	-1.106533
O	-1.321607	-0.938384	-0.691755
H	1.627914	1.458984	0.611416

TS9

C	-1.539275	1.243643	-0.634797
C	-1.014399	-0.133080	-0.811853
C	0.287471	-0.370028	0.451972
C	1.173553	0.874042	0.239308
C	0.708827	2.074313	-0.130279
C	-0.714112	2.267624	-0.396527
H	-2.616623	1.356918	-0.718352
H	-0.605878	-0.381248	-1.793678
H	1.390885	2.916786	-0.147778
H	-1.108911	3.277662	-0.348895
O	1.006245	-1.544597	0.155781
C	1.479772	-1.732141	-1.169502
H	1.858333	-0.799291	-1.606825
H	2.296244	-2.452656	-1.107670
H	0.692974	-2.149595	-1.807278
O	-0.375024	-0.440143	1.525495
O	-2.186470	-0.880666	0.838723
O	-1.765441	-1.151294	-0.364525
H	2.206055	0.702814	0.461841

IM9

C	-1.622779	1.240131	0.051709
C	-1.588115	0.016332	-0.694870
C	1.141538	-0.276605	0.871224
C	1.478316	0.728919	-0.214048
C	0.748597	1.821585	-0.492053
C	-0.576821	2.096820	0.053505
H	-2.555067	1.459998	0.559887
H	-0.847620	-0.178237	-1.466874
H	1.210343	2.570070	-1.132789
H	-0.722147	3.084727	0.485989
O	1.466203	-1.560225	0.591638
C	1.146135	-2.111938	-0.692108
H	1.342989	-1.402103	-1.501091
H	1.784427	-2.986240	-0.811602
H	0.097836	-2.421108	-0.697882
O	0.772795	0.051374	1.961457
O	-3.430196	-0.763023	0.339767
O	-2.459580	-0.893160	-0.598385
H	2.414362	0.570764	-0.707712

TS10

C	-0.885778	1.944222	-0.369845
C	-1.335429	0.559856	-0.801928
C	0.188330	-0.446880	-0.454280
C	0.560424	-0.128221	0.982366
C	0.485821	1.106645	1.474744
C	-0.080761	2.190523	0.667501
H	-1.285461	2.757298	-0.970351
H	-1.350644	0.430216	-1.896362
H	0.825305	1.288745	2.488909
H	0.150096	3.215022	0.944594
O	1.065341	-0.231025	-1.445495
C	2.404417	0.154386	-1.104338
H	2.831803	-0.539495	-0.376458
H	2.957451	0.105236	-2.040616
H	2.418221	1.174045	-0.712698
O	-0.420080	-1.640397	-0.602119
O	-1.354247	-1.748295	0.329150
O	-2.242954	-0.047648	-0.131291
H	0.965575	-0.957028	1.524428

IM10

C	2.429957	0.084369	-0.652597
C	1.878054	1.452889	-0.517720
C	-0.885235	-0.159417	0.349125
C	-0.040197	-0.688974	1.404991
C	1.246653	-1.057805	1.282914
C	2.164603	-0.963550	0.145852
H	3.187069	-0.044146	-1.422974
H	2.393512	2.222214	-1.123294
H	1.693640	-1.545910	2.149273
H	2.769738	-1.857861	-0.011444
O	-0.580379	-0.204274	-0.930099
C	-0.733633	-1.476478	-1.579197
H	-0.172401	-2.253162	-1.042653
H	-1.794168	-1.732124	-1.651474
H	-0.309456	-1.333627	-2.568315
O	-2.182419	0.404905	0.784158
O	-3.061035	0.793856	-0.172855
O	0.971090	1.770544	0.219443
H	-0.549893	-0.814178	2.357450

TS11

C	1.532406	0.344674	0.818603
C	0.278513	-0.932681	0.304734
C	-0.986253	-0.091890	0.238218
C	-1.053215	1.213948	-0.062709
C	0.143602	1.982412	-0.389360
C	1.353201	1.525374	-0.063572
H	1.402681	0.487329	1.893074
H	0.291960	-1.559156	1.214295
H	0.009000	2.892145	-0.965634
H	2.271848	1.983792	-0.420957
O	-2.150928	-0.748529	0.545751
C	-2.397000	-1.907897	-0.255396
H	-1.604714	-2.651436	-0.123486
H	-3.347527	-2.316504	0.086087
H	-2.455574	-1.632316	-1.313199
O	0.776782	-1.441235	-0.755660
O	2.658363	-0.677585	-0.711635
O	2.587667	-0.430420	0.569906
H	-1.979589	1.745316	-0.128883

IM11

C	-1.957757	-0.007575	-0.569912
C	0.756365	-1.573046	0.228916
C	1.338296	-0.274776	-0.134709
C	0.843137	0.978145	0.070040
C	-0.410245	1.389574	0.714309
C	-1.652583	0.938508	0.473101
H	-1.235748	-0.338473	-1.310324
H	1.447646	-2.417478	0.035606
H	-0.274388	2.199834	1.427194
H	-2.505749	1.313489	1.027287
O	2.590191	-0.330675	-0.728820
C	3.652403	-0.609234	0.188740
H	3.514552	-1.586018	0.662907
H	4.572521	-0.616568	-0.395413
H	3.704138	0.163787	0.964504
O	-0.352023	-1.769853	0.682360
O	-4.098502	-0.151112	0.119500
O	-3.113616	-0.477177	-0.745695
H	1.440734	1.824501	-0.197279

TS12

C	1.934174	-0.428305	0.310210
C	0.145151	-0.746781	0.819821
C	-0.689673	0.283922	0.141664
C	-0.268404	1.540608	-0.061645
C	1.084496	1.962354	0.295696
C	2.063257	1.076705	0.488711
H	2.422269	-0.997921	1.119334
H	0.135976	-0.803865	1.910129
H	1.259717	3.031037	0.375643
H	3.059495	1.413084	0.765047
O	-1.904289	-0.090391	-0.371112
C	-2.775098	-0.769754	0.528492
H	-2.901497	-0.193215	1.452421
H	-3.731912	-0.862868	0.015595
H	-2.395232	-1.770341	0.760189
O	0.099002	-1.972161	0.296629
O	0.236915	-1.912850	-0.999650
O	1.995799	-0.930507	-0.861894
H	-0.883024	2.286243	-0.521179

IM12

C	2.613888	-1.134913	-0.408348
C	-0.428991	-0.852397	0.696301
C	-0.519243	0.419423	0.028330
C	0.550130	1.274017	0.032702
C	1.879948	1.074028	0.605729
C	2.737869	0.041848	0.486598
H	3.583261	-1.590475	-0.687139
H	0.374175	-1.009478	1.410860
H	2.224195	1.954640	1.147114
H	3.704371	0.141316	0.974693
O	-1.639829	0.912232	-0.564434
C	-2.826965	0.885405	0.242400
H	-2.664880	1.467755	1.156980
H	-3.604506	1.351308	-0.362140
H	-3.098143	-0.151137	0.456550
O	-1.175953	-1.858100	0.572977
O	-2.169288	-1.856982	-0.360918
O	1.579821	-1.582724	-0.850911
H	0.430438	2.258747	-0.368397

TS13

C	0.919146	-1.366064	0.142837
C	-0.592636	-1.237521	0.198290
C	-1.251931	-0.078281	0.109703
C	-0.555544	1.224868	0.009795
C	0.736839	1.338925	0.322033
C	1.504402	0.233446	0.934327
H	1.307818	-2.067481	0.899515
H	-1.121282	-2.183330	0.251156
H	1.278607	2.260349	0.127957
H	1.441580	0.084086	2.014227
O	-2.599456	0.086676	0.045847
C	-3.397508	-1.084791	0.014697
H	-3.272351	-1.655918	0.940997
H	-4.428815	-0.747574	-0.074250
H	-3.127630	-1.707020	-0.845125
O	1.509636	-1.361759	-0.989702
O	2.832529	0.145832	-0.770021
O	2.768209	0.090343	0.531623
H	-1.122269	2.054034	-0.359266

IM13

C	-0.520827	2.153136	0.108993
C	-1.428770	1.032813	-0.209670
C	-1.326516	-0.253916	0.199680
C	-0.210182	-0.911965	0.936211
C	1.099525	-0.880960	0.611700
C	1.598076	-0.214880	-0.546900
H	-0.986226	3.143567	-0.058930
H	-2.340874	1.336603	-0.711015
H	1.819757	-1.427122	1.209924
H	0.968165	0.288454	-1.273589
O	-2.323776	-1.159139	0.073649
C	-3.541339	-0.771867	-0.550097
H	-3.360222	-0.468347	-1.585557
H	-4.175571	-1.655938	-0.530143
H	-4.014139	0.045003	0.004669
O	0.612881	2.080406	0.527952
O	3.712291	-0.802846	-0.014387
O	2.822003	-0.202154	-0.852938
H	-0.517877	-1.506515	1.770917

TS14

C	0.916550	-0.450889	0.972430
C	-0.459395	-0.688215	0.475999
C	-1.265616	0.330406	0.161781
C	-0.777179	1.727030	0.152217
C	0.527898	2.001558	0.095762
C	1.627680	0.961634	-0.009805
H	1.055926	-0.194541	2.024303
H	-0.739087	-1.730281	0.359355
H	0.850092	3.038185	0.070798
H	2.490449	1.197528	0.635040
O	-2.563332	0.251876	-0.209403
C	-3.136761	-1.044193	-0.288093
H	-3.092469	-1.539514	0.687941
H	-4.173086	-0.900524	-0.588361
H	-2.610329	-1.645355	-1.036288
O	1.835562	-1.337346	0.585105
O	1.726435	-1.548414	-0.700721
O	1.893465	0.415313	-1.136378
H	-1.517598	2.499094	0.176655

IM14

C	1.491703	-0.411321	-0.623133
C	0.732937	0.654794	-0.047183
C	-0.616450	0.646019	0.010511
C	-1.529778	-0.434629	-0.458023
C	-1.480221	-1.755676	-0.175971
C	-0.605917	-2.441152	0.786173
H	1.057406	-1.295243	-1.078223
H	1.327275	1.493486	0.293080
H	-2.284713	-2.351272	-0.597866
H	-0.978881	-3.441321	1.078137
O	-1.363198	1.699645	0.400062
C	-0.689808	2.883311	0.822455
H	-0.072475	3.280224	0.010719
H	-1.474965	3.590055	1.083258
H	-0.067952	2.671427	1.696567
O	2.749815	-0.368749	-0.691719
O	3.398112	0.706199	-0.156283
O	0.423667	-2.016244	1.271133
H	-2.338826	-0.083457	-1.063845

TS15

C	-0.337854	2.101623	0.225127
C	0.897007	1.629736	0.036875
C	1.174780	0.201756	-0.094643
C	0.282321	-0.735082	0.250738
C	-1.007222	-0.427288	0.932335
C	-1.603948	1.264028	0.224838
H	-0.507207	3.169876	0.334629
H	1.738099	2.313435	-0.041127
H	-1.004606	-0.350867	2.019659
H	-2.298094	1.510092	1.046333
O	2.347892	-0.223705	-0.678978
C	3.499219	-0.037898	0.139649
H	3.398512	-0.596774	1.077205
H	4.349871	-0.413610	-0.429206
H	3.656867	1.022567	0.364698
O	-2.122967	0.927493	-0.887317
O	-2.128682	-1.104115	-0.787262
O	-2.070958	-1.095946	0.510606
H	0.434007	-1.784922	0.110287

IM15

C	1.471682	-1.204603	0.543316
C	0.462237	-0.476449	1.047244
C	-0.138554	0.658094	0.301760
C	-1.258502	0.653727	-0.479782
C	-2.165770	-0.423707	-0.712111
C	1.988787	-1.020799	-0.824678
H	1.948119	-1.977956	1.138955
H	0.105788	-0.649871	2.056453
H	-2.749519	-0.425315	-1.629095
H	1.443289	-0.295268	-1.463620
O	0.555210	1.821856	0.209599
C	1.723756	2.026059	1.005025
H	2.550663	1.403943	0.653995
H	1.970149	3.079531	0.883807
H	1.516984	1.807641	2.055712
O	2.956283	-1.609575	-1.255708
O	-1.838322	-1.381666	1.288874
O	-2.436199	-1.379645	0.068579
H	-1.482437	1.491617	-1.106435

TS16

C	0.67938	-1.59725	-0.05134
C	-0.56854	-1.40564	-0.48759
C	-1.25478	-0.14428	-0.24218
C	-0.58	0.97486	0.0704
C	0.92629	1.0861	0.22491
C	1.34785	-0.62436	0.84937
H	1.28765	-2.44404	-0.35774
H	-1.06541	-2.14667	-1.10765
H	1.19163	1.68521	1.11104
H	1.09098	-0.63947	1.91051
O	-2.61017	-0.02655	-0.47175
C	-3.40932	-0.87113	0.34966
H	-3.23913	-0.65011	1.40978
H	-4.44812	-0.66877	0.08856
H	-3.18703	-1.92721	0.1608
O	2.6625	-0.47241	0.68371
O	2.92642	-0.3452	-0.59128
O	1.66398	1.20609	-0.80956
H	-1.06059	1.92082	0.20855

IM16

C	-1.232805	-0.868229	0.637103
C	0.073912	-0.913993	0.962468
C	1.195921	-0.258926	0.292999
C	1.345775	1.046229	-0.050766
C	0.408643	2.167196	0.213125
C	-1.710722	-0.236869	-0.564109
H	-1.987385	-1.356359	1.243459
H	0.373223	-1.529536	1.810554
H	0.911053	3.151495	0.180289
H	-1.051246	0.148354	-1.336537
O	2.346237	-1.004776	0.165131
C	2.190790	-2.289929	-0.439295
H	1.756827	-2.189530	-1.439578
H	3.191369	-2.714815	-0.507693
H	1.557389	-2.938896	0.171717
O	-2.934231	-0.142800	-0.849515
O	-3.855422	-0.568481	0.047346
O	-0.774228	2.063530	0.443112
H	2.276572	1.405351	-0.437482

TS17

C	-0.697051	2.206072	-0.133288
C	0.643496	1.616367	-0.179749
C	0.845031	0.335077	0.157557
C	-0.247270	-0.540940	0.719654
C	-1.869787	-0.033521	-0.181941
C	-1.814753	1.476378	-0.101277
H	-0.762054	3.290329	-0.130093
H	1.473333	2.234902	-0.500886
H	-2.544325	-0.492732	0.560878
H	-2.785813	1.961461	-0.039136
O	2.000156	-0.355716	0.146686
C	3.107272	0.261680	-0.488814
H	3.424942	1.153226	0.064199
H	3.905510	-0.478466	-0.484495
H	2.847668	0.532622	-1.517658
O	-1.762759	-0.603301	-1.314287
O	-0.178633	-1.799815	-1.042319
O	-0.272087	-1.791528	0.266903
H	-0.419949	-0.502396	1.774925

IM17

C	1.063977	-0.275794	-1.516499
C	-0.307218	-0.692655	-1.172802
C	-1.025618	-0.120133	-0.197775
C	-0.591506	1.057704	0.581890
C	2.088855	-1.083707	0.611079
C	2.130849	-0.447380	-0.715405
H	1.203221	0.141847	-2.509792
H	-0.730436	-1.527454	-1.726184
H	1.115232	-1.503493	0.935014
H	3.112893	-0.119190	-1.043159
O	-2.218707	-0.548627	0.310467
C	-2.767225	-1.734873	-0.243718
H	-2.067352	-2.570244	-0.128029
H	-3.682295	-1.931542	0.311792
H	-3.002005	-1.587402	-1.302712
O	3.061194	-1.183140	1.329405
O	0.325744	2.105687	-1.217388
O	0.031610	2.050652	0.142087
H	-0.833321	1.062465	1.624196

TS18

C	0.057042	2.212917	0.072556
C	-1.176456	1.430435	0.051773
C	-1.145383	0.085388	0.023644
C	0.152768	-0.737383	0.066052
C	1.321165	0.319014	-0.824258
C	1.238384	1.690920	-0.267844
H	-0.002107	3.241851	0.413709
H	-2.120605	1.954209	0.133026
H	1.102403	0.177202	-1.885313
H	2.176502	2.228541	-0.161387
O	-2.198515	-0.739911	0.043146
C	-3.486510	-0.149997	0.040610
H	-3.619216	0.477550	-0.847897
H	-4.194044	-0.977037	0.022241
H	-3.637813	0.450888	0.944507
O	2.397777	-0.414962	-0.483965
O	2.555690	-0.361351	0.811859
O	0.706093	-0.881301	1.207349
H	0.065096	-1.604467	-0.554737

IM18

C	-0.587695	-1.401338	1.027269
C	0.735318	-1.242346	0.409809
C	1.410832	-0.128155	0.070690
C	0.947085	1.291802	0.306567
C	-1.950713	-0.174075	-0.589402
C	-1.782809	-0.934660	0.619241
H	-0.587458	-2.062944	1.892262
H	1.268667	-2.183962	0.300412
H	-1.140949	0.035824	-1.281099
H	-2.691180	-1.157343	1.166226
O	2.670015	-0.121442	-0.448362
C	3.323451	-1.357533	-0.687699
H	2.742938	-1.968866	-1.386551
H	4.286810	-1.106113	-1.127622
H	3.473372	-1.901238	0.251223
O	-3.065421	0.269565	-0.975345
O	-4.158759	0.079840	-0.197874
O	-0.258050	1.521838	0.586394
H	1.643674	2.100886	0.235527

TS7-1

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.343092
C	1.144425	0.000000	2.298018
C	2.426043	-1.855415	-0.112943
C	2.177020	-0.770572	-1.061825
C	1.098743	0.021593	-0.979844
H	-0.982573	0.076433	-0.466014
H	-0.953770	0.042747	1.859449
H	2.931115	-0.627783	-1.826299
H	0.980045	0.774101	-1.758325
O	2.337297	-0.117394	1.709883
C	3.490793	-0.152875	2.567205
H	3.370817	-0.942773	3.311301
H	4.326636	-0.357405	1.898035
H	3.599446	0.808565	3.072614
O	3.541554	-2.283516	0.189617
O	4.746224	-1.257029	-0.276853
O	0.984550	0.089798	3.492921
N	5.521993	-0.085103	-1.592251
O	5.188722	0.378476	-2.598092
H	1.600608	-2.329218	0.296402

P1

C	-0.146304	2.180331	-0.099677
C	1.051186	1.675065	0.224468
C	1.535192	0.277573	0.081492
C	-1.517357	-0.697287	0.399795
C	-1.921713	0.383948	-0.530511
C	-1.323048	1.564533	-0.734385
H	-0.277367	3.244601	0.093655
H	1.781429	2.319144	0.703842
H	-2.782110	0.114075	-1.133967
H	-1.797600	2.213389	-1.470010
O	0.903415	-0.428629	-0.865235
C	1.304386	-1.797045	-0.986342
H	1.175381	-2.314101	-0.032544
H	0.648731	-2.226557	-1.741153
H	2.351294	-1.857017	-1.290546
O	-1.802827	-1.858750	0.217774
O	2.431329	-0.170595	0.760002
H	-0.968978	-0.369513	1.258133

TS7-2

C	-0.573297	2.122981	-0.043863
C	-1.622882	1.444928	-0.523154
C	-1.960304	0.019026	-0.276661
C	1.502253	-0.311818	-0.216485
C	1.396570	0.712293	0.809471
C	0.494088	1.705187	0.879763
H	-0.507880	3.174716	-0.323551
H	-2.308376	1.933759	-1.207824
H	2.176468	0.623015	1.554398
H	0.618525	2.383773	1.723417
O	-1.484172	-0.455096	0.881857
C	-1.716796	-1.846069	1.113611
H	-1.237642	-2.442146	0.332197
H	-1.276149	-2.059600	2.085642
H	-2.787594	-2.058597	1.115866
O	2.412898	-1.210117	-0.211450
O	3.530910	-0.229445	-0.228584
O	-2.610812	-0.642650	-1.052684
H	0.812307	-0.379982	-0.900166

IM7-2

C	0.804742	2.169285	-0.077447
C	1.743088	1.307007	0.332511
C	1.776962	-0.169077	0.174082
C	-1.532566	-0.029622	0.297956
C	-1.421924	1.067844	-0.696152
C	-0.437374	1.958925	-0.839791
H	0.998438	3.219224	0.140333
H	2.591439	1.680142	0.897302
H	-2.268893	1.090483	-1.374201
H	-0.589573	2.702061	-1.621658
O	1.016671	-0.635999	-0.826008
C	1.023106	-2.057901	-0.983130
H	0.681701	-2.540067	-0.064209
H	0.334919	-2.264498	-1.800883
H	2.030859	-2.405718	-1.219896
O	-1.752212	-1.303801	-0.212725
O	-2.806969	-0.542286	0.503305
O	2.456694	-0.880317	0.879402
H	-0.903561	0.054956	1.159408

TS7-2-1

C	-1.110995	2.219308	0.177990
C	-2.052706	1.565791	-0.512789
C	-2.361063	0.113388	-0.496628
C	0.888394	-0.358549	0.156296
C	0.691706	0.704626	1.190816
C	-0.146400	1.745040	1.185476
H	-1.065811	3.296300	0.016624
H	-2.661694	2.112938	-1.225350
H	1.325917	0.544253	2.058158
H	-0.084077	2.401095	2.053681
O	-1.997908	-0.512962	0.629476
C	-2.261339	-1.918336	0.660629
H	-1.744978	-2.416723	-0.162700
H	-1.872116	-2.266828	1.615494
H	-3.335187	-2.101196	0.580528
O	0.694673	-1.646187	0.569245
O	2.179338	-0.890272	0.125968
O	-2.917064	-0.442372	-1.418168
N	3.496409	0.475209	-0.468315
O	4.488016	-0.047793	-0.612584
H	0.491337	-0.097293	-0.802344

IM7-2-1

C	-0.827673	2.172155	0.297453
C	-1.807978	1.690315	-0.473645
C	-2.278828	0.282921	-0.550802
C	1.003594	-0.546222	0.116909
C	0.795341	0.420383	1.262809
C	0.020401	1.513152	1.303229
H	-0.632917	3.241637	0.220834
H	-2.306501	2.350679	-1.175926
H	1.383268	0.151393	2.133985
H	0.108508	2.090272	2.224535
O	-2.149700	-0.401990	0.628658
C	-2.564851	-1.769692	0.591572
H	-2.033072	-2.303036	-0.197638
H	-2.307595	-2.180217	1.566205
H	-3.640914	-1.827497	0.412663
O	0.460186	-1.689885	0.597204
O	2.405002	-0.834370	-0.070807
O	-2.751965	-0.192137	-1.558716
N	3.098712	0.332516	-0.419664
O	4.219432	0.082183	-0.645112
H	0.579671	-0.191148	-0.799121

TS 7-2-1-NO₂

C	-1.512574	2.111903	-0.231226
C	-2.277688	1.177278	-0.809124
C	-2.347222	-0.277349	-0.517854
C	0.849545	0.008313	0.309976
C	0.453259	1.187418	1.122815
C	-0.553981	2.031794	0.884064
H	-1.642673	3.127088	-0.605215
H	-2.923662	1.462530	-1.632985
H	1.053255	1.296779	2.020034
H	-0.669280	2.838270	1.607520
O	-1.849023	-0.627232	0.676182
C	-1.889661	-2.027554	0.972537
H	-1.336671	-2.589740	0.216634
H	-1.416748	-2.133264	1.947039
H	-2.924252	-2.375479	0.995764
O	1.025481	-1.107633	0.864306
O	2.646835	0.207270	0.389619
O	-2.823803	-1.071528	-1.297128
N	3.164994	-0.506679	-0.643904
O	4.309429	-0.249518	-0.794692
H	0.985307	0.108137	-0.746671

TS7-2-2

C	-0.015836	1.972336	0.375711
C	-1.004379	1.611865	-0.453785
C	-1.741168	0.315022	-0.482479
C	1.840804	-0.464825	-0.188121
C	1.406713	0.051674	1.194850
C	0.640842	1.153910	1.392336
H	0.327994	3.006327	0.331849
H	-1.357542	2.317406	-1.199200
H	1.718570	-0.592599	2.010850
H	0.569252	1.524079	2.416804
O	-1.796485	-0.293636	0.707997
C	-2.391852	-1.595062	0.688821
H	-1.801318	-2.256788	0.051182
H	-2.378423	-1.938967	1.721262
H	-3.414006	-1.537372	0.310072
O	0.668173	-1.079606	-0.329318
O	2.672484	-1.499062	-0.252681
O	-2.279053	-0.097187	-1.481831
H	2.081554	0.354694	-0.832580

P2

C	-1.894624	1.636573	-0.352607
C	-2.112290	0.377961	-0.763898
C	-1.328264	-0.814398	-0.346089
C	2.032099	0.121633	-0.240473
C	0.439867	1.700464	0.520344
C	-0.816991	2.153454	0.500248
H	-2.576194	2.395811	-0.731963
H	-2.888383	0.173719	-1.494976
H	1.258231	2.122717	1.092956
H	-1.025916	3.037512	1.092989
O	-1.248501	-0.938557	0.977674
C	-0.463015	-2.035509	1.454802
H	0.579799	-1.916944	1.147974
H	-0.546148	-2.004631	2.539051
H	-0.847744	-2.976922	1.058704
O	0.762215	0.620194	-0.256610
O	2.957370	0.626222	0.324152
O	-0.822325	-1.605755	-1.120786
H	2.058434	-0.706477	-0.751973

CO₂

O	0.000000	0.000000	1.162895
C	0.000000	0.000000	0.000000
O	0.000000	0.000000	-1.162895

TS7-3

C	0.835266	2.238803	-0.036859
C	-0.465104	1.930273	-0.131473
C	-0.973279	0.547260	-0.324086
C	1.160212	-1.077267	0.040697
C	2.131424	0.009550	-0.106794
C	1.990969	1.347477	-0.088850
H	1.089400	3.289450	0.072422
H	-1.218358	2.709547	-0.063228
H	3.126858	-0.393831	-0.274461
H	2.935831	1.881348	-0.174703
O	-2.293770	0.484675	-0.071516
C	-2.860997	-0.819418	-0.133464
H	-2.743359	-1.245029	-1.132302
H	-2.374907	-1.460234	0.608282
H	-3.915508	-0.696497	0.108833
O	0.337057	-1.249654	1.018447
O	-0.202243	-0.043923	1.452871
O	-0.411190	-0.294015	-1.059794
H	1.405376	-1.894596	-0.428301

IM7-3

C	0.689995	2.243545	-0.098131
C	-0.540676	1.768067	-0.326567
C	-0.819938	0.288389	-0.245731
C	1.077916	-0.899629	-0.115844
C	2.093512	0.145872	0.262006
C	1.891691	1.471865	0.264151
H	0.840789	3.317083	-0.175224
H	-1.365950	2.414592	-0.604532
H	3.053402	-0.257180	0.569823
H	2.738105	2.081359	0.571216
O	-2.085974	-0.035588	-0.682547
C	-3.033238	-0.426940	0.306237
H	-2.730049	-1.353616	0.799937
H	-3.169854	0.355305	1.060156
H	-3.965598	-0.580320	-0.235991
O	0.267979	-1.271015	1.008216
O	-0.553510	-0.113502	1.113579
O	0.103565	-0.434983	-1.014788
H	1.566106	-1.773773	-0.493261

TS7-3-1

C	-1.339763	2.023854	-0.182359
C	-2.036079	0.946464	-0.610206
C	-1.827035	-0.478558	-0.279519
C	1.335847	0.246535	0.009989
C	0.973196	1.372108	0.755003
C	-0.157652	2.155523	0.640814
H	-1.760318	2.984949	-0.479042
H	-2.874915	1.100844	-1.281176
H	1.705593	1.642599	1.508734
H	-0.137574	3.066856	1.234114
O	-1.192570	-0.670342	0.889183
C	-0.893220	-2.028465	1.203939
H	-0.235552	-2.456042	0.441245
H	-0.389960	-2.003922	2.169412
H	-1.808683	-2.621355	1.255762
O	2.342069	-0.502732	0.415076
O	3.368330	-0.599687	-0.751569
O	-2.229013	-1.389318	-0.971248
H	4.072572	-0.055934	-0.365541
H	0.871622	-0.019672	-0.803473

P3

C	3.525333	0.166626	-5.001053
C	2.241974	0.599822	-5.196135
C	1.350986	1.294025	-4.250266
C	2.660103	-0.484580	-2.080922
C	3.923138	-0.181063	-2.482656
C	4.316563	0.022932	-3.828759
H	4.038185	-0.140499	-5.912793
H	1.793770	0.472050	-6.176028
H	4.698471	-0.167868	-1.725291
H	5.387595	-0.029386	-4.004140
O	2.006944	2.035678	-3.342771
C	1.189102	2.655643	-2.350931
H	0.650414	1.897160	-1.775777
H	1.874400	3.206164	-1.708577
H	0.466536	3.328625	-2.817272
O	2.247716	-0.715661	-0.812052
O	3.310672	-0.530660	0.095692
O	0.138403	1.227930	-4.293892
H	3.138804	0.382103	0.371176
H	1.807457	-0.615158	-2.740329

TS7-H₂O

C	-1.939310	-1.672954	-0.565173
C	-2.401642	-0.429740	-0.165970
C	-1.839648	0.890089	0.001808
C	0.881225	-1.076211	0.569991
C	0.598660	-1.685375	-0.641093
C	-0.672955	-2.147186	-0.966654
H	-2.747881	-2.368036	-0.781689
H	-3.485104	-0.344086	-0.144029
H	1.438675	-1.872669	-1.297269
H	-0.708762	-2.949411	-1.702583
O	-0.562029	0.944644	0.511174
C	-0.017853	2.165332	0.699916
H	0.700153	2.178216	1.512435
H	1.223300	2.075375	-0.757330
H	-0.649963	3.014869	0.472936
O	1.978809	-0.375991	0.848468
O	2.877990	-0.337509	-0.244557
O	-2.445045	1.926042	-0.221217
H	2.596211	0.516226	-0.708017
O	1.940440	1.775363	-1.382691
H	2.475974	2.551282	-1.580524
H	0.317202	-1.204701	1.353228

IM7-H₂O

C	-2.451532	0.961031	-1.299275
C	-2.589412	1.182434	0.142897
C	-1.697243	1.361120	1.101779
C	0.140983	-1.109704	-1.197215
C	-0.071571	0.100264	-1.720708
C	-1.432686	0.557446	-2.075861
H	-3.375170	1.197595	-1.822599
H	-3.595545	1.311994	0.534199
H	0.779066	0.685828	-2.057595
H	-1.641967	0.569824	-3.145608
O	1.335572	-1.715634	-0.946263
O	2.419244	-0.927946	-1.411718
O	-1.015085	1.595012	2.018422
H	2.729408	-0.527255	-0.575798
H	-0.654890	-1.781430	-0.890532

IM8-2

C	0.592675	-1.997377	0.594901
C	-0.560070	-1.441079	0.966132
C	-1.250892	-0.373989	0.182473
C	1.692997	0.816851	-0.120481
C	1.819502	-0.419581	-0.938274
C	1.358764	-1.633038	-0.611726
H	0.991231	-2.814932	1.192665
H	-1.068543	-1.750401	1.874184
H	2.286746	-0.257418	-1.904293
H	1.542512	-2.445094	-1.314158
O	-1.118740	0.840133	0.762781
C	-1.667325	1.952000	0.039320
H	-2.686694	1.730818	-0.282374
H	-1.664039	2.782538	0.743412
H	-1.030829	2.183719	-0.816561
O	1.479967	1.923073	-0.681250
O	-2.475890	-0.701539	-0.384697
O	-1.252971	-0.457204	-1.196768
H	1.783153	0.765465	0.944475

IM8-2-1

C	0.746144	-2.038839	0.483851
C	-0.358315	-1.316415	0.651638
C	-0.749791	-0.131065	-0.212825
C	2.393588	0.540826	0.143228
C	2.468235	-0.670146	-0.722485
C	1.760653	-1.797711	-0.558778
H	0.914972	-2.886799	1.145013
H	-1.047615	-1.517442	1.465622
H	3.115995	-0.552796	-1.585460
H	1.924264	-2.606927	-1.268968
O	-0.532251	1.012581	0.529960
C	-0.707221	2.240407	-0.184991
H	-1.713377	2.302010	-0.610863
H	-0.569510	3.030180	0.552062
H	0.048517	2.329912	-0.968690
O	2.466635	1.687165	-0.370720
O	-2.137643	-0.215305	-0.616487
O	-0.127201	-0.139912	-1.438934
N	-2.984633	-0.201778	0.497927
O	-4.102486	-0.182823	0.152213
H	2.277889	0.435463	1.201723

P4

C	2.368406	-1.102293	-0.706958
C	2.523100	0.229833	-0.673398
C	1.848655	1.214975	0.204847
C	-1.765416	-0.400198	-0.013536
C	0.125832	-1.727922	0.206020
C	1.425793	-1.958568	0.017975
H	3.024836	-1.641726	-1.389365
H	3.221995	0.699171	-1.358048
H	-0.554086	-2.416720	0.693419
H	1.789069	-2.926440	0.349056
O	-2.115982	0.774796	-0.515802
O	-0.450309	-0.570929	-0.253300
O	-2.485006	-1.178848	0.557881
O	1.770407	2.391525	-0.066500
C	-3.499622	1.105352	-0.352745
H	-3.615756	2.086853	-0.806970
H	-4.124016	0.366709	-0.858838
H	-3.757263	1.134489	0.707466
H	1.482582	0.819184	1.129098

TS8-2

C	0.878541	-1.688271	0.891865
C	-0.298198	-1.142509	1.217169
C	-1.067817	-0.272771	0.304988
C	1.560721	0.978127	-0.316472
C	1.854815	-0.334772	-0.957461
C	1.555898	-1.513163	-0.403453
H	1.361320	-2.334690	1.621269
H	-0.727689	-1.274190	2.204464
H	2.253206	-0.273681	-1.964964
H	1.792764	-2.423316	-0.950498
O	-1.506524	0.820700	0.855538
C	-2.229323	1.744724	0.006113
H	-3.020294	1.206661	-0.515964
H	-2.631439	2.491513	0.685976
H	-1.527393	2.185792	-0.702504
O	0.900671	1.850509	-0.836309
O	-1.852011	-1.837464	-0.746208
O	-1.255736	-0.474433	-0.935265
H	1.955926	1.078730	0.567713

TS8-2-1-NO₂

C	1.117000	-1.887644	0.788948
C	0.038579	-1.117006	0.922351
C	-0.345124	0.066785	0.049992
C	2.873497	0.586663	0.418039
C	2.967407	-0.656900	-0.382540
C	2.201387	-1.747184	-0.197525
H	1.202863	-2.738145	1.464382
H	-0.679280	-1.288418	1.719325
H	3.736478	-0.651122	-1.150869
H	2.413996	-2.634905	-0.791582
O	-0.409071	1.165823	0.884416
C	-0.550168	2.420383	0.211837
H	-1.419854	2.408534	-0.452514
H	-0.694307	3.161787	0.995896
H	0.355033	2.649741	-0.356793
O	3.545461	1.562430	0.163120
O	-2.135575	-0.237553	-0.435874
O	-0.285140	0.081768	-1.314197
N	-3.378937	-0.445507	-0.374398
O	-4.092106	-0.494468	-1.301413
H	2.173301	0.585679	1.272753

TS8-3

C	0.113548	2.098070	0.056293
C	-0.960023	1.322959	0.308721
C	-1.127307	-0.122712	0.508470
C	1.348180	-0.647190	-0.463516
C	2.097807	0.636727	-0.470830
C	1.512243	1.823057	-0.255813
H	-0.119015	3.161964	0.049946
H	-1.913249	1.835574	0.422130
H	3.163145	0.577417	-0.673439
H	2.135330	2.710163	-0.325111
O	-2.263985	-0.690154	0.178334
C	-2.933329	-0.192147	-0.989053
H	-2.197532	0.002502	-1.771990
H	-3.609878	-0.989495	-1.290403
H	-3.504975	0.707888	-0.751494
O	0.217760	-0.718910	-1.011766
O	0.844835	-0.368679	1.435914
O	-0.461614	-0.832229	1.349417
H	1.769862	-1.510228	0.007917

TS8-1

C	-0.159986	-1.247582	1.481675
C	0.092561	0.043374	1.707158
C	0.240136	1.022771	0.609196
C	1.930813	-1.099393	-0.709544
C	0.605623	-1.761416	-0.834483
C	-0.311637	-1.827272	0.136364
H	-0.258625	-1.917963	2.333109
H	0.278419	0.425899	2.705380
H	0.370467	-2.104623	-1.836286
H	-1.266969	-2.301582	-0.074207
O	1.345940	1.739709	0.701788
C	1.602347	2.667020	-0.371267
H	0.774984	3.372919	-0.457344
H	2.523741	3.173519	-0.093215
H	1.725539	2.108613	-1.301341
O	2.328487	-0.312988	-1.607872
O	-0.544530	1.218299	-0.324327
O	-1.955056	0.360670	-0.257041
N	-3.690205	-0.442750	-0.245054
O	-4.554806	0.257783	-0.495907
H	2.546492	-1.291566	0.144217

TS8-2-2

C	0.813318	0.743026	1.569078
C	1.590525	-0.274240	1.171575
C	2.128158	-0.525538	-0.195028
C	-1.488254	0.255848	-0.419471
C	-0.751649	1.593564	-0.210811
C	0.208470	1.774882	0.728910
H	0.628267	0.851544	2.638217
H	1.926602	-1.007098	1.898219
H	-1.031002	2.363444	-0.923380
H	0.510790	2.802399	0.938940
O	-1.760806	-0.307559	0.812804
O	-0.560614	-0.228866	-1.131237
O	-2.463284	0.211199	-1.318875
O	2.489383	-1.684729	-0.525729
C	-2.198265	-1.664360	0.721527
H	-2.289260	-2.016972	1.748476
H	-3.162096	-1.728738	0.213359
H	-1.452933	-2.262845	0.186401
H	2.311077	0.298730	-0.886428

P4

C	-0.456754	2.046891	-0.048852
C	-1.465171	1.275437	-0.485307
C	-1.741767	-0.164022	-0.231441
C	1.618793	0.765341	0.605510
C	0.719405	1.738292	0.782570
H	-0.527704	3.100940	-0.319067
H	2.450905	0.678118	1.272504
H	0.895977	2.450500	1.586986
O	-0.884396	-0.753095	0.610585
C	-1.104835	-2.149690	0.842829
H	-1.060474	-2.696779	-0.100927
H	-0.299770	-2.462777	1.505092
H	-2.080820	-2.302591	1.307468
O	-2.672756	-0.739203	-0.748253
H	-2.239150	1.727624	-1.097437
O	1.468850	-0.158918	-0.475306
C	2.533401	-1.021136	-0.489870
O	2.345487	-2.206163	-0.509888
H	3.532394	-0.637899	-0.483397

IM9-2

C	0.806416	-1.840897	0.311653
C	1.578107	-0.835190	-0.140059
C	1.382547	0.646178	0.005342
C	-1.741706	-0.341512	-0.546555
C	-1.613838	-1.193358	0.651582
C	-0.489827	-1.832407	0.999726
H	1.251022	-2.826135	0.176856
H	-2.517349	-1.289088	1.247248
H	-0.538712	-2.492395	1.864496
O	0.297444	1.011267	0.666246
C	0.074109	2.425906	0.776240
H	-0.005212	2.864550	-0.219954
H	-0.866209	2.523864	1.314411
H	0.897148	2.890096	1.322122
O	-2.265173	0.937631	-0.376740
O	-3.026361	-0.133139	-1.037659
O	2.200470	1.416198	-0.456913
H	-0.964323	-0.425361	-1.307477
H	2.499245	-1.063464	-0.634322

IM9-2-1

C	-0.387146	2.133587	-0.074669
C	-1.395563	1.362133	-0.511124
C	-1.672159	-0.077326	-0.257258
C	1.637114	-0.143038	-0.511840
C	1.688401	0.852037	0.579693
C	0.789013	1.824988	0.756753
H	-0.458096	3.187636	-0.344884
H	2.538351	0.751353	1.249139
H	0.965585	2.537196	1.561169
O	-0.814788	-0.666399	0.584768
C	-1.035227	-2.062994	0.817012
H	-0.990866	-2.610083	-0.126744
H	-0.230162	-2.376081	1.479275
H	-2.011212	-2.215895	1.281651
O	1.798920	-1.476601	-0.154719
O	2.844777	-0.731345	-0.872590
O	-2.603148	-0.652507	-0.774070
H	0.945954	0.038550	-1.335298
H	-2.169542	1.814320	-1.123254
N	3.889690	0.037104	-0.401376
O	4.905530	-0.457757	-0.704826

IM9-3

C	1.507058	1.542254	0.022983
C	0.164395	1.492932	0.030462
C	-0.562463	0.157970	-0.024707
C	0.824650	-1.530684	-0.456039
C	2.166356	-0.914288	-0.186708
C	2.411752	0.396231	-0.001823
H	1.957644	2.528183	0.069870
H	2.993307	-1.615031	-0.123719
H	3.452695	0.659527	0.173281
O	-1.904116	0.398008	-0.164623
C	-2.735466	-0.766012	-0.147812
H	-2.484852	-1.415544	-0.988985
H	-2.607720	-1.300852	0.796085
H	-3.756718	-0.401081	-0.242555
O	0.128514	-1.877381	0.732022
O	-0.248358	-0.563222	1.174027
O	-0.078816	-0.639724	-1.066894
H	0.880008	-2.438128	-1.061422
H	-0.438249	2.376611	0.059298

TS9-2

C	0.677114	-1.848952	0.296442
C	1.562656	-0.942425	-0.164271
C	1.563825	0.555283	-0.014667
C	-1.675435	-0.126104	-0.494723
C	-1.658976	-0.925923	0.704027
C	-0.585859	-1.686211	1.014130
H	1.014392	-2.878672	0.183392
H	-2.535484	-0.902723	1.336664
H	-0.671595	-2.317776	1.897625
O	0.490150	1.075119	0.558562
C	0.480781	2.506315	0.697083
H	0.583527	2.972604	-0.284000
H	-0.483428	2.742569	1.141687
H	1.302650	2.820101	1.342378
O	-2.497347	0.822280	-0.754187
O	-3.663577	-0.063375	-0.583546
O	2.516758	1.199258	-0.400820
H	-0.860373	-0.263889	-1.214116
H	2.450234	-1.287823	-0.651924

TS9-2-1-NO₂

C	-0.768495	2.015734	-0.146936
C	-1.776912	1.244280	-0.583391
C	-2.053508	-0.195179	-0.329525
C	1.255765	-0.260891	-0.584107
C	1.307052	0.734184	0.507426
C	0.407664	1.707135	0.684486
H	-0.839445	3.069783	-0.417151
H	2.157002	0.633500	1.176872
H	0.584236	2.419343	1.488902
O	-1.196137	-0.784252	0.512501
C	-1.416576	-2.180847	0.744745
H	-1.372215	-2.727936	-0.199011
H	-0.611511	-2.493934	1.407008
H	-2.392561	-2.333748	1.209384
O	1.417571	-1.594454	-0.226986
O	3.048188	-0.744350	-0.880565
O	-2.984497	-0.770360	-0.846337
H	0.564605	-0.079303	-1.407565
H	-2.550891	1.696467	-1.195521
N	4.009811	-0.037154	-0.446912
O	5.025651	-0.532016	-0.750361

TS9-3

C	-1.382972	-1.615386	0.179950
C	0.645612	0.068154	0.192276
C	0.083076	1.469304	-0.020601
C	-1.255877	1.726257	-0.069838
C	-2.302119	0.777306	0.073764
C	-2.358155	-0.586363	0.254990
H	-1.588307	-2.547474	0.704599
H	-3.283132	1.246818	0.137537
H	-3.311554	-0.971206	0.607054
O	0.241515	-0.592566	1.197235
O	0.029491	-0.603438	-1.171114
O	-0.460845	-1.820321	-0.714644
O	2.012962	0.149786	-0.058737
C	2.725759	-1.054351	0.205142
H	2.619457	-1.336158	1.254359
H	2.346491	-1.856610	-0.435409
H	3.767939	-0.848067	-0.036151
H	-1.543258	2.768210	-0.159782
H	0.766507	2.284460	-0.136107

TS9-1

C	2.205965	1.896208	-0.226324
C	2.926847	0.800685	0.101554
C	2.609676	-0.650858	0.003620
C	-0.375248	0.752289	0.961441
C	-0.312568	1.534360	-0.248378
C	0.839020	2.061099	-0.725324
H	2.757544	2.836858	-0.183059
H	-1.262321	1.698321	-0.746117
H	0.756941	2.744175	-1.570904
O	1.334330	-0.928010	-0.320024
C	0.982608	-2.325177	-0.454451
H	1.226566	-2.863094	0.463666
H	-0.090882	-2.328144	-0.637317
H	1.527805	-2.766108	-1.291816
O	-1.357680	0.061214	1.308549
O	-2.488471	-0.104176	0.175271
O	3.459896	-1.500589	0.198745
N	-4.174761	-0.683646	-0.557684
O	-5.117406	-0.113526	-0.200185
H	0.449923	0.781532	1.679798
H	3.954586	0.951052	0.417863

IM10-2

C	2.507417	-0.078196	0.238366
C	2.210970	-0.439705	-1.157422
C	-0.971693	-0.329386	-0.138411
C	-0.576097	1.098139	0.166702
C	0.581396	1.523378	0.704978
C	1.814535	0.803570	0.990956
H	3.454238	-0.447530	0.623812
H	3.069741	-0.867338	-1.711523
H	0.574021	2.569576	1.005103
H	2.288219	1.105631	1.925923
O	-0.251566	-1.330839	0.402937
C	-0.470939	-1.520880	1.800350
H	-0.154893	-0.641365	2.370888
H	-1.526805	-1.737376	1.990456
H	0.136840	-2.379231	2.080995
O	-1.490952	-0.565498	-1.381130
O	-2.361267	-0.516757	-0.180827
O	1.154874	-0.263979	-1.730106
H	-1.355400	1.808942	-0.013148

IM10-2-1

C	-2.732759	0.775869	0.669458
C	-3.072809	0.025466	-0.561394
C	0.516713	-0.189899	-0.693627
C	0.155588	-0.941127	0.605406
C	-0.775599	-0.617487	1.512574
C	-1.768060	0.458415	1.551280
H	-3.407431	1.591203	0.919618
H	-4.026471	0.332232	-1.035912
H	-0.721024	-1.221141	2.418729
H	-1.763090	1.021976	2.485616
O	-0.144601	0.990810	-0.919287
C	0.291074	2.138874	-0.202348
H	0.384175	1.937842	0.870382
H	1.244437	2.502686	-0.597600
H	-0.479804	2.892707	-0.360330
O	0.235910	-1.094411	-1.660841
O	1.948647	-0.002030	-0.760533
O	-2.427768	-0.884046	-1.030474
N	2.515531	0.384518	0.474222
O	3.663206	0.554585	0.346812
H	0.808076	-1.765753	0.803271

P13

C	-2.518085	-0.916078	0.633394
C	-2.645726	0.415668	0.512682
C	-1.955178	1.225003	-0.511103
C	1.654860	-0.349798	-0.039582
C	-0.292933	-1.590367	-0.306445
C	-1.596466	-1.794192	-0.099973
H	-3.159325	-1.426323	1.351083
H	-3.331500	0.964431	1.152684
H	0.364863	-2.297914	-0.797913
H	-1.979614	-2.754967	-0.430898
O	2.044347	0.813248	0.454733
O	0.317494	-0.442537	0.136877
O	2.352126	-1.183143	-0.557868
O	-2.013995	2.435743	-0.536101
C	3.447315	1.077002	0.330764
H	3.595001	2.056092	0.780576
H	4.020252	0.313915	0.860500
H	3.734951	1.085575	-0.721946
H	-1.407131	0.669277	-1.293634

TS10-2

C	2.538202	-0.380496	0.145820
C	2.144578	-0.665878	-1.243999
C	-0.845346	-0.147829	-0.194214
C	-0.308044	1.202456	0.138485
C	0.887182	1.469712	0.706296
C	2.011346	0.578275	0.940383
H	3.446190	-0.875594	0.479807
H	2.950969	-1.096037	-1.867350
H	1.016365	2.496618	1.041981
H	2.561265	0.795714	1.855976
O	-0.441104	-1.224152	0.408706
C	-0.536481	-1.352558	1.837235
H	-0.251681	-0.421748	2.332319
H	-1.571654	-1.617451	2.059382
H	0.147795	-2.154189	2.107309
O	-1.769927	-0.171938	-1.060389
O	-2.866931	-0.762705	-0.222366
O	1.062631	-0.432040	-1.746188
H	-0.930083	2.041045	-0.095474

TS10-2-1-NO₂

C	3.340073	-0.833627	0.059973
C	4.295109	0.281099	0.261743
C	-0.981432	-0.521510	-0.580223
C	-0.011088	0.655124	-0.622038
C	1.322828	0.531233	-0.458543
C	2.028833	-0.725984	-0.242810
H	3.768488	-1.828092	0.155973
H	5.351024	-0.030587	0.377096
H	1.922486	1.435425	-0.489489
H	1.452843	-1.638477	-0.366951
O	-0.740333	-1.484703	0.383685
C	-0.905189	-1.084325	1.737890
H	-0.348910	-0.164333	1.951222
H	-1.963056	-0.942142	1.979682
H	-0.505809	-1.901151	2.338489
O	-0.742460	-1.004638	-1.802478
O	-2.724168	0.029114	-0.487553
O	4.005547	1.458789	0.307367
N	-2.910573	1.092618	0.386498
O	-4.046142	1.379383	0.449211
H	-0.445410	1.611643	-0.889773

TS10-1

C	-2.857179	0.821634	0.373990
C	-3.030931	-0.263341	-0.609167
C	0.362462	-0.327688	-0.574822
C	0.034592	-0.661954	0.876921
C	-0.885230	-0.101904	1.680854
C	-1.954197	0.840747	1.377110
H	-3.630048	1.586414	0.362902
H	-4.021942	-0.271468	-1.105975
H	-0.803325	-0.390142	2.727825
H	-2.095119	1.613077	2.134476
O	-0.247175	0.777643	-1.093976
C	0.279038	2.027413	-0.677583
H	0.349753	2.093186	0.414689
H	1.264009	2.197701	-1.126695
H	-0.418162	2.782559	-1.039642
O	0.421505	-1.386577	-1.414433
O	1.741048	-0.424074	-0.811144
O	-2.226583	-1.135762	-0.862305
N	2.870373	0.705292	0.402140
O	3.944282	0.414526	0.206067
H	0.707996	-1.380516	1.295366

TS10-3

C	-2.490426	0.084531	-0.549511
C	-1.672754	-1.153481	-0.497161
C	0.807248	-0.333556	0.480804
C	0.509351	1.091267	0.212217
C	-0.629758	1.737983	-0.109326
C	-1.988631	1.322682	-0.415284
H	-3.559358	-0.038164	-0.709768
H	-2.195423	-2.075868	-0.206007
H	-0.465251	2.812226	-0.172607
H	-2.679136	2.154871	-0.523236
O	2.004453	-0.800790	0.194266
C	2.460033	-0.597817	-1.166469
H	2.622341	0.463718	-1.356631
H	3.395116	-1.149799	-1.229299
H	1.710631	-1.012239	-1.841619
O	0.171118	-1.078375	1.300348
O	-1.140836	-0.711101	1.464201
O	-0.568270	-1.228719	-1.060811
H	1.395506	1.689435	0.254933

TS10-1

C	-2.557237	-0.392496	-0.362206
C	-1.969328	-1.050348	0.823947
C	0.743311	0.834117	-0.079214
C	-0.211177	1.903412	0.205507
C	-1.510189	1.912058	-0.128693
C	-2.344083	0.877263	-0.753165
H	-3.310612	-0.972425	-0.889594
H	-2.550354	-1.911059	1.208406
H	-2.043496	2.844651	0.054147
H	-2.959427	1.243781	-1.574982
O	0.441796	-0.054703	-0.978235
C	0.934415	-1.417607	-0.904598
H	1.859589	-1.496979	-1.467903
H	1.098659	-1.699900	0.132630
H	0.127980	-2.003951	-1.350162
O	1.853788	0.930101	0.511842
O	3.062201	-0.098254	0.059375
O	-0.945867	-0.715593	1.383322
H	0.225905	2.768106	0.693118
N	4.431732	-1.263720	-0.453434
O	4.719940	-1.057974	-1.537041

IM11-1

C	-2.119616	0.008574	-0.394565
C	0.688098	-1.569645	0.227900
C	1.255609	-0.268396	-0.138435
C	0.769528	0.973674	0.131723
C	-0.436979	1.347552	0.885282
C	-1.685273	0.919924	0.688118
H	-1.380092	-0.314191	-1.125708
H	1.360282	-2.415196	-0.022112
H	-0.248242	2.102553	1.645347
H	-2.494766	1.283460	1.315498
O	2.465105	-0.310980	-0.819216
C	3.584758	-0.580786	0.027656
H	3.484176	-1.558984	0.509133
H	4.467434	-0.581078	-0.612089
H	3.679741	0.191344	0.800407
O	-0.394998	-1.769075	0.739438
O	-3.390247	0.262980	-0.903976
O	-3.097692	-0.915548	-0.072458
H	1.339404	1.831499	-0.158584

IM11-1-1

C	1.678370	0.637299	0.179893
C	-1.495564	1.343809	-0.879746
C	-1.706368	0.025977	-0.271492
C	-1.147813	-0.474647	0.863421
C	-0.204597	0.164458	1.796790
C	1.008928	0.645753	1.534890
H	0.953577	0.450746	-0.628299
H	-2.127275	1.513380	-1.775060
H	-0.538760	0.132508	2.831876
H	1.618474	1.039861	2.342519
O	-2.596058	-0.811879	-0.927537
C	-3.966616	-0.449075	-0.742684
H	-4.165219	0.549125	-1.146217
H	-4.559051	-1.184199	-1.287713
H	-4.229952	-0.466469	0.321397
O	-0.716127	2.191567	-0.496485
O	2.627349	-0.442894	0.208153
O	2.253620	1.829750	-0.058024
N	2.875405	-0.886115	-1.087105
O	3.705136	-1.713199	-1.095251
H	-1.444376	-1.442625	1.209786

IM11-2-2

C	1.696818	-1.555621	-0.495793
C	2.549057	-0.505339	-0.463393
C	2.428244	0.706055	0.356985
C	-0.841424	1.535265	0.005530
C	-0.608859	-0.793869	0.063703
C	0.373094	-1.710475	0.076428
H	2.063947	-2.448216	-1.002921
O	-0.913211	2.558009	-0.599686
O	-0.521785	0.363721	-0.645404
O	1.474424	1.019896	1.046206
H	-1.027270	1.400620	1.078445
H	3.331567	1.345889	0.360467
H	0.096482	-2.685415	0.463427
H	-1.494556	-0.981755	0.633913
O	3.793778	-0.636147	-1.155100
C	4.872391	-0.461689	-0.232572
H	5.748336	-0.944659	-0.612522
H	5.067645	0.582642	-0.105490
H	4.608267	-0.892510	0.710578

P12

C	2.650568	-0.752032	-0.480007
C	-0.481822	-1.236603	0.594596
C	-0.726867	0.095073	0.025800
C	0.155887	1.122957	0.111756
C	1.482270	1.132986	0.737167
C	2.534710	0.319333	0.538062
H	3.691968	-0.969043	-0.787619
H	0.438848	-1.326827	1.194326
H	1.624687	1.993290	1.390616
H	3.454954	0.546922	1.070366
O	-1.895216	0.384486	-0.622761
C	-3.116947	-0.009850	0.014651
H	-3.102545	0.279472	1.071194
H	-3.907147	0.533358	-0.503743
H	-3.265529	-1.085182	-0.075055
O	-1.247641	-2.168482	0.461875
O	1.729134	-1.350611	-0.988997
H	-0.118248	2.093787	-0.244949

TS11-2-2-NO₂

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	3.325461
C	1.449029	0.000000	3.099030
C	2.145069	0.640335	2.122487
C	1.645646	1.548663	1.076584
C	0.716625	1.312688	0.152558
H	0.350874	-0.798738	0.715857
H	-0.291416	-0.520265	4.259467
H	2.180830	2.495700	1.037567
H	0.446660	2.057384	-0.588404
O	2.201098	-0.748963	3.988836
C	2.401381	-0.106829	5.250987
H	1.445123	0.081791	5.749918
H	2.997509	-0.790087	5.855986
H	2.932649	0.843229	5.120041
O	-0.839485	0.484642	2.594199
O	1.123822	-0.705704	-1.301146
O	-1.155340	-0.029613	-0.411625
N	1.755427	-1.528357	-0.579505
O	2.612079	-2.219322	-1.037948
H	3.199658	0.459660	2.112496

TS11-2

C	2.025757	0.284624	-0.328917
C	-0.934752	1.608034	0.217690
C	-1.340455	0.249080	-0.150840
C	-0.720276	-0.929965	0.135235
C	0.495202	-1.155948	0.931597
C	1.717191	-0.627440	0.755392
H	1.227824	0.620238	-0.995290
H	-1.720195	2.361164	0.010010
H	0.351696	-1.892446	1.719298
H	2.539240	-0.890437	1.408678
O	-2.540548	0.148396	-0.839120
C	-3.693982	0.284091	-0.003890
H	-3.716251	1.267549	0.476689
H	-4.562582	0.179098	-0.654116
H	-3.704533	-0.493931	0.768704
O	0.134786	1.946003	0.687113
O	3.829083	-0.508415	-0.526805
O	3.179500	0.804916	-0.509484
H	-1.186333	-1.849538	-0.151254

TS11-1

C	-1.038789	1.111920	0.084227
C	1.062354	-1.083645	1.109413
C	1.856722	-0.519006	0.008542
C	1.938603	0.774605	-0.404887
C	1.274027	1.961207	0.154115
C	-0.029281	2.117020	0.419474
H	-0.786983	0.225378	-0.506129
H	1.298605	-2.147440	1.307670
H	1.955294	2.793763	0.318138
H	-0.397954	3.041574	0.852611
O	2.665150	-1.415884	-0.670509
C	3.841671	-1.793041	0.051272
H	3.582299	-2.307637	0.981960
H	4.397723	-2.472152	-0.594988
H	4.449435	-0.910891	0.284068
O	0.219734	-0.504082	1.762153
O	-2.209938	1.285178	0.401788
O	-3.141995	0.068339	-0.198291
N	-4.347662	-1.269579	-0.788601
O	-5.413501	-1.166290	-0.395959
H	2.620746	1.036374	-1.186589

TS11-2-1

C	1.481190	0.813423	-0.026809
C	-1.734708	1.488417	-0.385549
C	-1.839851	0.034280	-0.230672
C	-1.117930	-0.783092	0.582085
C	-0.058162	-0.429064	1.539076
C	1.047318	0.277946	1.298209
H	0.803792	0.599946	-0.859941
H	-2.516442	1.904053	-1.053944
H	-0.212587	-0.862344	2.525237
H	1.760871	0.460145	2.098687
O	-2.817342	-0.584202	-1.000663
C	-4.141400	-0.404566	-0.494370
H	-4.411701	0.656167	-0.470050
H	-4.810188	-0.933082	-1.174459
H	-4.228294	-0.819787	0.516933
O	-0.904632	2.214105	0.121861
O	2.823597	0.536157	-0.307845
O	2.046258	2.058097	-0.016628
N	3.146137	-1.379713	-0.602461
O	4.253142	-1.510423	-0.798369
H	-1.356108	-1.825659	0.617099

TS11-3

C	2.434986	-0.159655	-0.322064
C	-0.030437	-1.226254	-0.124992
C	-0.963432	-0.078428	0.093258
C	-0.594185	1.221797	0.041807
C	0.711924	1.741938	-0.283880
C	1.923164	1.172565	-0.509651
H	3.302515	-0.466714	-0.901881
H	-0.359015	-2.166848	0.344083
H	0.669544	2.816128	-0.458187
H	2.674506	1.823189	-0.951173
O	-2.256630	-0.339624	0.450972
C	-2.971027	-1.201043	-0.439388
H	-2.470606	-2.167666	-0.542582
H	-3.956016	-1.346038	0.002973
H	-3.063527	-0.731274	-1.423844
O	0.722941	-1.265417	-1.129846
O	1.079549	-0.722857	1.309933
O	2.274914	-0.930676	0.693069
H	-1.311328	1.996752	0.215159

TS11-2-2

C	-0.275776	-1.352399	-0.516047
C	0.902332	-1.995171	-0.335841
C	1.922792	-1.702246	0.675107
C	1.125002	1.395382	-0.436639
C	-0.018471	0.999884	0.444668
C	-0.752358	-0.139680	0.189815
H	-0.413821	1.809409	1.046647
O	1.726144	2.573644	-0.282695
O	0.134273	1.888076	-1.244717
O	1.978460	-0.714420	1.381876
H	1.739343	0.580925	-0.837109
H	2.687364	-2.495276	0.777663
H	-1.764906	-0.149064	0.535587
H	-0.935900	-1.766046	-1.249554
O	1.091199	-3.178932	-1.115545
C	2.490561	-3.424813	-1.277499
H	2.895447	-3.798882	-0.360416
H	2.638406	-4.146679	-2.053353
H	2.984907	-2.512856	-1.539908

IM12-2

C	2.617369	-0.980232	-0.575593
C	-0.551115	-0.993725	0.501543
C	-0.550065	0.401369	0.010058
C	0.497959	1.238165	0.183421
C	1.792240	0.960012	0.811464
C	2.688497	-0.006932	0.536784
H	3.603682	-1.347959	-0.918732
H	0.378583	-1.323034	0.956008
H	2.079283	1.724446	1.533243
H	3.629505	0.004973	1.080790
O	-1.610344	0.935402	-0.662002
C	-2.951111	0.583196	-0.304093
H	-3.117120	0.730232	0.766322
H	-3.582544	1.260624	-0.878868
H	-3.163696	-0.451346	-0.574419
O	-1.704001	-1.484348	1.118048
O	-1.255530	-1.949232	-0.209321
O	1.604471	-1.358014	-1.124924
H	0.414169	2.267261	-0.097366

IM12-2-1

C	-2.568573	-1.453351	0.861001
C	0.704392	-0.257364	0.578573
C	-0.036291	0.954564	0.059966
C	-1.127316	0.898897	-0.728922
C	-1.811300	-0.289319	-1.247499
C	-2.383206	-1.322647	-0.600997
H	-3.430854	-2.081308	1.156346
H	0.008040	-1.110782	0.594886
H	-1.928560	-0.250509	-2.330437
H	-2.890389	-2.074841	-1.199803
O	0.437707	2.199409	0.350117
C	1.856425	2.358999	0.386014
H	2.301147	2.079185	-0.573291
H	2.032459	3.412695	0.597229
H	2.290575	1.747914	1.185868
O	1.774184	-0.558046	-0.345023
O	1.144653	-0.091632	1.831891
O	-1.884329	-0.920159	1.708393
N	1.922458	-1.935575	-0.460751
O	2.832083	-2.204793	-1.148474
H	-1.518336	1.794975	-1.163718

IM15

C	1.461291	-1.488778	-0.617415
C	2.472896	-0.597900	-0.600584
C	2.590335	0.601765	0.244122
C	-0.537884	1.920916	0.166579
C	-0.700876	-0.392872	-0.002969
C	0.142898	-1.439603	-0.005082
H	1.625985	-2.425184	-1.150189
H	3.362048	-0.837644	-1.177318
O	-0.487975	3.003180	-0.326763
O	-0.438230	0.792375	-0.618440
O	1.741690	1.028253	1.002706
H	-0.687751	1.696263	1.230520
O	-1.933241	-0.532364	0.554990
H	3.574952	1.103731	0.189722
C	-3.028389	-0.206421	-0.314789
H	-3.016248	0.854638	-0.575892
H	-2.976470	-0.809533	-1.226578
H	-3.932764	-0.440590	0.244283
H	-0.186940	-2.394867	0.346454

TS12-2-2

C	1.778865	0.846788	0.710810
C	2.659662	-0.116971	0.368856
C	2.518415	-1.049425	-0.767092
C	-0.634872	-0.991798	0.715537
C	-0.540220	0.221228	-0.193372
C	0.474840	1.134370	0.134019
H	2.090618	1.592744	1.439716
H	3.617773	-0.135433	0.880400
O	-1.711926	-1.778855	0.715201
O	-1.043560	-0.243380	1.778246
O	1.474220	-1.314873	-1.326658
H	0.331482	-1.498335	0.824618
O	-1.555134	0.759823	-0.839820
H	3.467202	-1.493939	-1.121561
C	-2.782908	0.029846	-1.033227
H	-2.567968	-0.951778	-1.457821
H	-3.281505	-0.097351	-0.072746
H	-3.361184	0.646700	-1.718606
H	0.264062	2.164469	-0.064395

TS12-1

C	2.986292	-1.157163	-0.442302
C	-0.348907	-0.721609	-0.553609
C	0.014355	0.686408	-0.211918
C	0.976579	1.015415	0.678951
C	1.873147	0.128987	1.422457
C	2.698785	-0.836343	0.972393
H	3.976269	-1.626389	-0.605396
H	0.320571	-1.444275	-0.083842
H	1.926968	0.382877	2.481131
H	3.335915	-1.336739	1.697294
O	-0.625960	1.752425	-0.776326
C	-2.004508	1.664948	-1.142659
H	-2.622815	1.445504	-0.266465
H	-2.255103	2.651322	-1.533139
H	-2.158176	0.901231	-1.904312
O	-1.704847	-1.055477	-0.410378
O	-0.722934	-0.991825	-1.840415
O	2.263160	-0.922979	-1.387093
N	-2.274002	-1.063303	1.473144
O	-3.393475	-1.230765	1.489666
H	1.098857	2.061983	0.865078

TS12-2-1

C	2.717587	-0.254162	-1.158546
C	-0.489406	0.069670	-1.080999
C	-0.115158	0.569595	0.327750
C	0.822847	-0.034310	1.194623
C	1.633064	-1.206300	0.884026
C	2.422514	-1.351593	-0.192387
H	3.230854	-0.553183	-2.089425
H	0.093194	-0.840369	-1.322301
H	1.579937	-1.996915	1.630147
H	2.933278	-2.297171	-0.351773
O	-0.689579	1.618094	0.850644
C	-1.779353	2.310667	0.180562
H	-2.530053	1.589162	-0.139109
H	-2.160078	2.994110	0.936442
H	-1.366886	2.821976	-0.687627
O	-1.924283	-0.579488	-0.765643
O	-0.567655	1.013200	-1.911947
O	2.454190	0.906119	-0.941449
N	-1.757160	-1.712862	-0.083822
O	-2.785816	-2.246475	0.192433
H	0.949569	0.405858	2.161625

TS12-2

C	-3.514737	-0.048709	0.387366
C	1.428589	-1.164715	-0.271115
C	0.785783	0.096388	-0.259572
C	-0.575727	0.188035	-0.500510
C	-1.470486	-0.930267	-0.812873
C	-2.774520	-0.988125	-0.503404
H	-4.585144	0.091651	0.143269
H	0.843750	-2.016475	-0.628190
H	-1.049931	-1.743736	-1.394667
H	-3.360969	-1.817395	-0.893870
O	1.363671	1.284620	0.024832
C	2.745994	1.481043	-0.309262
H	2.916855	1.206833	-1.355298
H	2.920444	2.547629	-0.173672
H	3.370270	0.889753	0.361451
O	2.674858	-1.394109	-0.033567
O	2.586910	-0.888551	1.357031
O	-3.022627	0.489888	1.348518
H	-1.013512	1.163287	-0.454377

TS12-1

C	0.172753	2.591919	0.887784
C	-0.226880	-0.536052	-0.077647
C	1.212801	-0.624732	-0.001971
C	2.021660	0.385209	-0.426402
C	1.624718	1.685765	-0.979830
C	0.799562	2.610504	-0.460736
H	-0.034551	3.597682	1.299987
H	-0.689575	0.309005	-0.593943
H	2.156619	1.929236	-1.898575
H	0.679468	3.542531	-1.007546
O	1.850911	-1.725155	0.493576
C	1.430480	-3.005907	-0.002190
H	1.336397	-2.975911	-1.092672
H	2.217836	-3.703010	0.283156
H	0.481556	-3.298452	0.447171
O	-0.082261	1.602909	1.535932
O	-0.957097	-1.419369	0.374000
O	-2.530982	-1.083999	0.013685
N	-4.281969	-0.467272	-0.337873
O	-4.374460	0.649565	-0.560943
H	3.074150	0.209581	-0.346900

TS12-3

C	2.095105	-0.021328	0.720305
C	0.026582	-1.411292	-0.287668
C	-0.830843	-0.267627	-0.318922
C	-0.593647	1.086003	-0.282850
C	0.598337	1.867874	0.023986
C	1.780928	1.422705	0.469334
H	3.166067	-0.267632	0.748952
H	-0.441799	-2.355861	-0.016726
H	0.439255	2.933677	-0.110894
H	2.573035	2.146966	0.646205
O	-2.176263	-0.634348	-0.380447
C	-2.760709	-0.800506	0.917624
H	-2.683243	0.126738	1.496346
H	-3.806855	-1.062124	0.756584
H	-2.256804	-1.603908	1.465051
O	1.141467	-1.613537	-0.897946
O	1.840502	-0.457253	-1.075823
O	1.292689	-0.749332	1.362709
H	-1.448928	1.680753	-0.527118

IM13-2

C	-0.056576	2.208208	0.512974
C	-1.081106	1.363546	-0.127749
C	-1.194379	0.017268	-0.035188
C	-0.258529	-0.949032	0.601903
C	1.055640	-1.046131	0.378891
C	1.821070	-0.222671	-0.572465
H	-0.357606	3.271516	0.586994
H	-1.883043	1.919397	-0.600575
H	1.612191	-1.827766	0.887041
H	1.280113	0.506323	-1.173637
O	-2.285316	-0.669517	-0.446698
C	-3.377902	0.036147	-1.017825
H	-3.069337	0.542254	-1.937775
H	-4.128735	-0.718102	-1.246025
H	-3.779646	0.763995	-0.305465
O	1.016098	1.853284	0.951302
O	2.854981	-0.879697	-1.238411
O	3.106327	0.144607	-0.209603
H	-0.728591	-1.639367	1.270767

IM13-2-1

C	-1.306807	2.213041	-0.699130
C	-1.800178	0.830762	-0.837490
C	-1.525530	-0.213849	-0.019784
C	-0.581963	-0.261977	1.131830
C	0.695051	0.126573	1.124610
C	1.433328	0.663058	-0.055838
H	-0.644780	2.349578	0.177749
H	-2.554311	0.703522	-1.605721
H	1.274377	0.015331	2.037416
H	0.820610	0.702702	-0.962381
O	-2.177010	-1.396498	-0.072788
C	-3.182951	-1.594642	-1.056619
H	-2.755642	-1.515015	-2.060817
H	-3.559903	-2.602609	-0.894626
H	-3.990347	-0.865689	-0.932547
O	-1.545780	3.155506	-1.424317
O	2.595231	-0.121981	-0.320200
O	2.060686	1.870442	0.205846
N	2.377008	-1.448210	-0.614514
O	3.429633	-1.969375	-0.725459
H	-0.999153	-0.677025	2.025467

P14

C	-0.289688	2.126533	-0.013150
C	-1.286427	1.081702	-0.274122
C	-1.278003	-0.176221	0.241936
C	-0.249430	-0.792442	1.105479
C	1.057059	-0.888664	0.854628
H	-0.656656	3.147465	-0.237644
H	-2.156230	1.418180	-0.826369
H	1.701041	-1.381251	1.552872
O	-2.302658	-1.038632	0.107992
C	-3.452541	-0.640395	-0.621857
H	-3.192666	-0.406052	-1.659254
H	-4.128604	-1.492949	-0.594341
H	-3.926366	0.227752	-0.151384
O	0.839672	1.976857	0.410630
H	-0.656801	-1.261001	1.998287
O	1.597099	-0.333506	-0.347477
C	3.025492	-0.361927	-0.285937
H	3.515964	-0.760638	0.577409
O	3.798392	0.142510	-1.378213

P13

C	1.207067	1.437862	-0.723167
C	-0.121642	1.268305	-0.107274
C	-0.764493	0.092477	-0.010733
C	-0.250764	-1.241725	-0.430679
C	0.931531	-1.816758	-0.118530
C	1.947744	-1.323826	0.819393
H	1.677342	0.542828	-1.163455
H	-0.588846	2.190907	0.219167
H	1.076192	-2.825325	-0.494779
H	2.651395	-2.111519	1.151351
O	-2.052291	-0.062113	0.397031
C	-2.768630	1.101097	0.787333
H	-2.837072	1.807412	-0.046786
H	-3.761414	0.757464	1.072202
H	-2.280630	1.580468	1.641410
O	1.736221	2.525061	-0.799190
O	2.063964	-0.194176	1.251385
H	-0.945171	-1.810023	-1.013548

TS13-2

C	0.188723	2.283525	-0.457297
C	1.098628	1.340563	0.229728
C	1.184367	0.004473	0.045047
C	0.312709	-0.869805	-0.796096
C	-1.035344	-0.953036	-0.735724
C	-1.806190	-0.205601	0.205268
H	0.500788	3.339767	-0.349279
H	1.844400	1.820282	0.853706
H	-1.543889	-1.669323	-1.371697
H	-1.349291	0.482941	0.910622
O	2.178133	-0.768301	0.534162
C	3.175920	-0.175449	1.357222
H	2.721108	0.255713	2.253955
H	3.845815	-0.986511	1.635195
H	3.722934	0.593919	0.802772
O	-0.796566	2.005217	-1.103050
O	-3.074633	-0.568010	1.672850
O	-3.081151	-0.320652	0.221938
H	0.803053	-1.490626	-1.516543

TS2213-2-1-NO₂

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.471416
C	1.076066	0.000000	2.302079
C	2.520986	-0.098593	1.945347
C	3.130762	-1.096706	1.278072
C	2.458208	-2.304141	0.744755
H	-0.996219	0.231764	-0.429644
H	-0.985288	0.107917	1.912084
H	4.202900	-1.042973	1.125603
H	1.348182	-2.324574	0.814406
O	0.998724	0.201474	3.641892
C	-0.279904	0.344034	4.275906
H	-0.881222	-0.557857	4.126846
H	-0.062509	0.472915	5.335386
H	-0.808030	1.222393	3.890001
O	0.947580	-0.209852	-0.739657
O	2.615103	-3.450883	2.166804
O	2.971907	-2.858531	-0.259093
N	1.392841	-3.596892	2.555555
O	1.183591	-4.284882	3.526318
H	3.130851	0.691691	2.330593

TS13-1

C	-1.608562	2.130340	-0.725425
C	-1.936476	0.697862	-0.848857
C	-1.545050	-0.295354	-0.016252
C	-0.593639	-0.223845	1.125346
C	0.645662	0.272959	1.091623
C	1.336814	0.821297	-0.105530
H	-2.290002	2.779986	-1.309903
H	-2.668888	0.475683	-1.616695
H	1.243210	0.232548	1.998568
H	0.750885	0.806183	-1.030151
O	-2.068566	-1.544807	-0.049257
C	-3.057847	-1.856823	-1.018517
H	-2.653868	-1.741603	-2.029102
H	-3.324616	-2.897645	-0.843910
H	-3.937686	-1.217074	-0.892399
O	-0.721743	2.626290	-0.066018
O	2.636240	0.319146	-0.266598
O	2.107383	1.936372	0.083163
N	2.637676	-1.600777	-0.637776
O	3.711614	-1.958644	-0.597687
H	-0.935228	-0.607458	2.063993

TS7-2-2

C	-0.693820	0.482939	-0.050275
C	-2.030539	0.795923	-0.033271
C	-3.195850	-0.062055	-0.026751
C	2.458070	-0.132176	-0.269813
C	1.285996	-1.090264	-0.194040
C	-0.069434	-0.870321	-0.052953
H	-2.285047	1.848235	-0.033523
H	1.605265	-2.120966	-0.068989
O	3.664777	-0.650772	-0.504649
O	2.533401	-0.085572	1.075332
O	-3.231051	-1.291367	0.009689
H	2.262125	0.807378	-0.805580
H	-4.153909	0.478823	-0.053473
O	0.239639	1.427717	-0.063884
C	-0.104918	2.805856	-0.021555
H	-0.665576	3.028836	0.891153
H	0.844877	3.336886	-0.011689
H	-0.684506	3.087391	-0.905953
H	-0.708841	-1.720646	0.061092

TS13-3

C	-1.224332	-1.417351	-0.564488
C	0.273220	-1.408621	-0.560256
C	1.011271	-0.311913	-0.364617
C	0.548007	1.084949	-0.185997
C	-0.703801	1.614115	-0.050135
C	-1.984777	1.037295	0.185110
H	-1.674387	-2.398791	-0.358688
H	0.799954	-2.351073	-0.695314
H	-0.744577	2.687796	-0.210336
H	-2.858784	1.624342	-0.086891
O	2.395218	-0.395958	-0.391331
C	2.958497	-0.770518	0.870454
H	2.618194	-1.771638	1.150792
H	4.040592	-0.766185	0.740121
H	2.668620	-0.056987	1.650616
O	-1.872726	-0.586651	-1.251167
O	-1.305630	-0.791970	1.192929
O	-2.315771	0.108862	1.019561
H	1.335770	1.808536	-0.158589

TS13-1

C	0.670636	-1.170472	1.865506
C	1.526751	-1.289473	0.664635
C	1.983450	-0.285051	-0.117318
C	1.633679	1.163570	-0.050766
C	0.390438	1.679729	-0.026137
C	-0.794407	0.858949	-0.129520
H	0.712679	-2.065770	2.514359
H	1.919606	-2.286686	0.500232
H	0.268360	2.756555	0.018879
H	-0.730605	-0.218836	-0.307744
O	2.946854	-0.433303	-1.054297
C	3.486696	-1.727374	-1.291992
H	2.702133	-2.410434	-1.631071
H	4.229551	-1.596972	-2.076242
H	3.960068	-2.117863	-0.385286
O	-0.012859	-0.223853	2.184658
O	-1.917728	1.359358	-0.085721
O	-3.042588	0.181794	-0.356140
N	-4.457110	-1.034474	-0.641315
O	-5.507089	-0.596891	-0.543582
H	2.473180	1.826932	-0.060216

IM14-2

C	1.584300	-0.506586	0.514759
C	0.320208	-1.028820	-0.040715
C	-0.845208	-0.369592	-0.028203
C	-1.087833	1.002310	0.497644
C	-0.403305	2.135741	0.224462
C	0.653779	2.314049	-0.776700
H	1.574230	0.468083	0.998001
H	0.392300	-2.041621	-0.421377
H	-0.783267	3.040460	0.689737
H	0.828040	3.373865	-1.045256
O	-2.046105	-0.900620	-0.395887
C	-2.056003	-2.235395	-0.878053
H	-1.684407	-2.925255	-0.112531
H	-3.094894	-2.460575	-1.112653
H	-1.443902	-2.318593	-1.781766
O	2.747550	-0.833203	-0.158969
O	2.395242	-1.463114	1.125599
O	1.304073	1.441741	-1.318996
H	-1.942362	1.076160	1.137353

IM14-2-1

C	1.171746	-0.112154	-0.763723
C	-0.156003	-0.820105	-0.786797
C	-1.191431	-0.495179	-0.006265
C	-1.233009	0.591283	1.014933
C	-1.033541	1.916136	0.840451
C	-0.850957	2.614561	-0.436605
H	1.089465	0.915347	-0.379638
H	-0.201322	-1.682382	-1.441295
H	-1.157166	2.536559	1.723087
H	-1.017777	3.706915	-0.371815
O	-2.339564	-1.219250	0.102721
C	-2.476466	-2.366172	-0.722036
H	-1.692984	-3.098632	-0.497872
H	-3.454963	-2.784106	-0.491742
H	-2.432143	-2.084125	-1.778892
O	1.674664	-0.033060	-2.009983
O	2.018550	-0.869207	0.126555
O	-0.558178	2.109304	-1.502942
N	3.040206	-0.062945	0.610932
O	3.780984	-0.681976	1.276470
H	-1.499684	0.248622	1.992874

P16

C	1.696818	-1.555621	-0.495793
C	2.549057	-0.505339	-0.463393
C	2.428244	0.706055	0.356985
C	-0.841424	1.535265	0.005530
C	-0.608859	-0.793869	0.063703
C	0.373094	-1.710475	0.076428
H	2.063947	-2.448216	-1.002921
H	3.494996	-0.604748	-0.989063
O	-0.913211	2.558009	-0.599686
O	-0.521785	0.363721	-0.645404
O	1.474424	1.019896	1.046206
H	-1.027270	1.400620	1.078445
H	3.331567	1.345889	0.360467
H	-1.494556	-0.981755	0.633913
O	0.008460	-2.995656	0.586576
C	1.190565	-3.743577	0.883461
H	0.922240	-4.652211	1.380740
H	1.705110	-3.973322	-0.026133
H	1.828857	-3.164832	1.517919

TS14-2

C	1.546996	-0.475001	0.145316
C	0.291923	-1.019968	-0.285561
C	-0.885033	-0.399262	-0.036972
C	-1.063793	0.933057	0.608604
C	-0.458060	2.094984	0.282753
C	0.429249	2.367243	-0.860463
H	1.613439	0.442990	0.722512
H	0.329035	-1.993771	-0.758433
H	-0.779796	2.962782	0.851343
H	0.511868	3.444430	-1.098249
O	-2.095283	-0.942749	-0.248448
C	-2.164074	-2.257476	-0.797567
H	-1.658414	-2.969744	-0.138480
H	-3.224338	-2.491416	-0.866414
H	-1.710967	-2.274439	-1.792687
O	2.628167	-1.085605	-0.155946
O	3.082139	-1.065414	1.244402
O	1.027681	1.553920	-1.534536
H	-1.800611	0.948820	1.384330

TS14-2-1-NO₂

C	-0.851164	0.192467	1.039099
C	0.315948	-0.688402	0.771439
C	1.117732	-0.601847	-0.309087
C	1.026572	0.383831	-1.421818
C	1.012247	1.740517	-1.345852
C	1.228162	2.584866	-0.167876
H	-1.038262	1.010002	0.307052
H	0.469297	-1.454442	1.520545
H	0.955379	2.262094	-2.297665
H	1.381192	3.653055	-0.422942
O	2.080385	-1.516685	-0.620912
C	2.303924	-2.622728	0.262588
H	1.398710	-3.232393	0.356545
H	3.102173	-3.204442	-0.196933
H	2.623186	-2.267126	1.247555
O	-1.133973	0.423966	2.240405
O	-2.190016	-0.831835	0.336263
O	1.268551	2.227969	1.001555
N	-2.651066	-0.102214	-0.628084
O	-3.552342	-0.547718	-1.292503
H	0.964413	-0.029041	-2.406995

TS14-2-1

C	-1.002591	-0.922765	-0.362393
C	-0.222698	0.262733	-0.819200
C	0.884705	0.735329	-0.235913
C	1.579118	0.168144	0.952749
C	1.976503	-1.106729	1.161341
C	1.949928	-2.210079	0.194531
H	-0.608448	-1.430360	0.522268
H	-0.667976	0.770175	-1.669066
H	2.503447	-1.293007	2.092435
H	2.600304	-3.059373	0.481473
O	1.507923	1.907063	-0.566928
C	0.969441	2.655020	-1.644025
H	-0.061967	2.956290	-1.428230
H	1.602673	3.535303	-1.743451
H	0.996646	2.070066	-2.568967
O	-1.497188	-1.732972	-1.346190
O	-2.380504	-0.670093	-0.294844
O	1.323789	-2.257047	-0.845910
N	-2.836808	0.607555	1.116355
O	-3.958598	0.760702	1.088697
H	1.813200	0.894234	1.703015

TS14-2-2

C	-0.275776	-1.352399	-0.516047
C	0.902332	-1.995171	-0.335841
C	1.922792	-1.702246	0.675107
C	1.125002	1.395382	-0.436639
C	-0.018471	0.999884	0.444668
C	-0.752358	-0.139680	0.189815
H	1.045737	-2.893988	-0.927862
H	-0.413821	1.809409	1.046647
O	1.726144	2.573644	-0.282695
O	0.134273	1.888076	-1.244717
O	1.978460	-0.714420	1.381876
H	1.739343	0.580925	-0.837109
H	2.687364	-2.495276	0.777663
O	-2.060910	-0.266423	0.472737
C	-2.758467	0.856536	1.008906
H	-3.801684	0.552989	1.066268
H	-2.385145	1.093737	2.008832
H	-2.642481	1.719213	0.344996
H	-0.982333	-1.784747	-1.193360

TS14-3

C	-1.090492	-1.635323	-0.156168
C	0.295085	-1.273797	-0.233264
C	0.970779	-0.100356	-0.069159
C	0.507407	1.305275	0.021023
C	-0.748531	1.748856	-0.144892
C	-1.928121	0.904091	-0.444446
H	-1.404283	-2.533341	-0.682941
H	0.892117	-2.126923	-0.536211
H	-0.909278	2.813898	-0.001356
H	-2.895207	1.342882	-0.161772
O	2.326586	-0.098235	-0.060533
C	3.054844	-1.315967	-0.039121
H	2.962624	-1.837569	-0.996787
H	4.093942	-1.034350	0.123079
H	2.704192	-1.956077	0.776271
O	-1.948468	-1.313798	0.743109
O	-1.709488	-0.084789	1.269125
O	-1.911063	-0.008943	-1.301189
H	1.267542	2.027561	0.234089

TS14-1

C	-0.587808	-0.872535	-0.011440
C	0.821701	-1.164392	0.172315
C	1.787003	-0.264075	-0.101357
C	1.585935	1.147024	-0.537983
C	0.785106	2.079538	0.021244
C	0.022145	1.976464	1.275391
H	-0.926923	0.070262	-0.449665
H	1.060538	-2.171742	0.491960
H	0.831849	3.066558	-0.429703
H	-0.261049	2.959847	1.695138
O	3.109857	-0.534212	-0.114596
C	3.531480	-1.856730	0.202115
H	3.096518	-2.574212	-0.500815
H	4.615834	-1.850403	0.111902
H	3.243929	-2.111057	1.226406
O	-0.285503	0.959581	1.863544
O	-1.431989	-1.724818	0.256098
O	-2.931772	-1.194928	-0.178413
N	-4.588925	-0.385015	-0.565380
O	-4.591634	0.757499	-0.559178
H	2.194369	1.436889	-1.369058

IM15-2

C	1.418639	-1.255591	0.295468
C	0.180578	-0.718622	0.301922
C	-0.233236	0.588411	-0.184436
C	-1.513717	0.951890	-0.425301
C	-2.743202	0.127321	-0.246950
C	2.642314	-0.688765	-0.305308
H	1.563059	-2.235881	0.742193
H	-0.622720	-1.310176	0.730046
H	-3.655100	0.644705	-0.546306
H	2.547189	0.240481	-0.891737
O	0.701985	1.559926	-0.490030
C	1.336744	2.131007	0.660015
H	1.859229	1.364055	1.240029
H	2.053433	2.861435	0.285069
H	0.593364	2.623742	1.296036
O	3.719927	-1.237812	-0.188089
O	-2.857506	-0.704012	0.858229
O	-2.702988	-1.233473	-0.507600
H	-1.758519	1.920707	-0.807880

IM15-2-1

C	2.002395	-1.480540	0.502529
C	0.903505	-0.709808	0.644336
C	0.613242	0.569623	0.019936
C	-0.621847	1.116226	-0.062586
C	-1.901807	0.546576	0.489033
C	3.140163	-1.256235	-0.410203
H	2.074163	-2.397859	1.080971
H	0.124090	-1.064235	1.313100
H	-2.695198	1.300348	0.392095
H	3.073787	-0.413335	-1.118606
O	1.603723	1.292024	-0.618197
C	2.556072	1.881265	0.274310
H	3.072467	1.113395	0.858668
H	3.273928	2.413261	-0.349825
H	2.055670	2.579583	0.953700
O	4.110667	-1.987609	-0.409217
O	-1.806425	0.102071	1.805857
O	-2.257238	-0.617528	-0.238905
N	-3.682248	-0.714014	-0.327947
O	-3.980253	-1.695437	-0.871908
H	-0.794457	2.033219	-0.586255

P18

C	1.696818	-1.555621	-0.495793
C	2.549057	-0.505339	-0.463393
C	2.428244	0.706055	0.356985
C	-0.841424	1.535265	0.005530
C	-0.608859	-0.793869	0.063703
C	0.373094	-1.710475	0.076428
H	2.063947	-2.448216	-1.002921
H	3.494996	-0.604748	-0.989063
O	-0.913211	2.558009	-0.599686
O	-0.521785	0.363721	-0.645404
O	1.474424	1.019896	1.046206
H	-1.027270	1.400620	1.078445
H	3.331567	1.345889	0.360467
H	-1.494556	-0.981755	0.633913
O	0.008460	-2.995656	0.586576
C	1.190565	-3.743577	0.883461
H	0.922240	-4.652211	1.380740
H	1.705110	-3.973322	-0.026133
H	1.828857	-3.164832	1.517919

IM15-3

C	-0.792059	1.958559	-0.274734
C	0.482387	1.574626	-0.443706
C	1.015468	0.217611	-0.379114
C	0.345416	-0.953523	-0.336417
C	-1.153525	-1.135815	-0.330611
C	-1.867687	0.944843	-0.017869
H	-1.071509	3.001901	-0.368229
H	1.233838	2.330818	-0.661392
H	-1.428038	-2.095663	-0.773366
H	-2.878058	1.361494	-0.017275
O	2.400226	0.098999	-0.392357
C	3.014604	0.543946	0.815631
H	2.645389	-0.033852	1.670889
H	4.087600	0.392739	0.694049
H	2.813612	1.606703	0.989428
O	-1.580522	0.304133	1.245592
O	-1.675340	-1.101136	0.977929
O	-1.837952	-0.100934	-0.971004
H	0.857032	-1.892380	-0.295234

P17

C	-0.855654	-1.189529	0.782356
C	0.334989	-0.613782	1.002616
C	1.035487	0.362684	0.161155
C	0.590495	1.551993	-0.309830
C	-0.737730	2.168241	-0.078160
C	-1.639414	-1.032569	-0.463575
H	-1.279169	-1.871324	1.515071
H	0.895915	-0.888544	1.896915
H	-0.731986	3.260880	-0.248156
H	-1.170496	-0.440889	-1.270571
O	2.388200	0.160544	-0.003449
C	2.761635	-1.131267	-0.483267
H	2.301341	-1.322330	-1.458516
H	3.846786	-1.117352	-0.578004
H	2.463829	-1.913734	0.220627
O	-2.710715	-1.572274	-0.622153
O	-1.742093	1.583047	0.258740
H	1.251793	2.228142	-0.810238

TS15-1

C	1.984786	-1.750279	0.216765
C	1.027654	-0.814123	0.373630
C	1.117615	0.596851	0.019297
C	0.054954	1.405578	-0.245189
C	-1.354965	1.024731	-0.230688
C	3.289027	-1.580753	-0.462398
H	1.796078	-2.760272	0.571505
H	0.080353	-1.121177	0.805977
H	-2.097577	1.824135	-0.335451
H	3.482230	-0.621546	-0.972749
O	2.335173	1.216720	-0.109552
C	3.134793	1.266777	1.080877
H	3.403687	0.262754	1.419026
H	4.033979	1.820029	0.813748
H	2.591347	1.788593	1.874574
O	4.110444	-2.473133	-0.482714
O	-1.746193	-0.132298	-0.098161
O	-3.386334	-0.172803	-0.029872
N	-5.290386	-0.373037	0.075019
O	-5.650357	-1.446645	0.203102
H	0.275070	2.424034	-0.488491

TS15-3

C	0.612802	-1.982214	-0.016383
C	-0.579712	-1.435820	-0.300954
C	-0.993734	-0.046698	-0.189021
C	-0.286988	1.103988	0.019145
C	1.129913	1.373012	0.151182
C	1.773415	-1.222309	0.523954
H	0.764857	-3.037739	-0.228404
H	-1.348721	-2.095174	-0.691045
H	1.379436	2.267123	0.717360
H	2.753284	-1.710060	0.422351
O	-2.343215	0.211867	-0.282169
C	-3.272343	-0.775154	0.153829
H	-2.931309	-1.252472	1.077226
H	-4.207016	-0.244579	0.335353
H	-3.437387	-1.529918	-0.620057
O	1.629774	-0.330123	1.390961
O	1.899942	-0.223201	-1.155741
O	2.104108	0.990981	-0.585928
H	-0.813293	2.021945	0.178072

TS15-2-2

C	-0.435423	-1.179379	1.078586
C	-1.746962	-1.324676	0.836532
C	-2.436616	-1.008282	-0.439321
C	-0.227633	1.724257	0.125641
C	0.664419	0.616196	-0.357944
C	0.616278	-0.649094	0.183594
H	-2.360482	-1.790170	1.603539
H	1.512903	0.956770	-0.938972
O	-0.154973	2.936519	-0.423579
O	0.681790	1.941484	1.112137
O	-1.971061	-0.321389	-1.320162
H	-1.233391	1.405521	0.435240
H	-3.438418	-1.464044	-0.553136
H	-0.038800	-1.563822	2.016732
O	1.686560	-1.536202	-0.151719
C	2.937448	-0.888011	0.093287
H	3.721375	-1.616244	0.099256
H	3.123871	-0.169594	-0.677442
H	2.903077	-0.393186	1.041373

TS15-1

C	-1.783198	1.149810	0.832688
C	-0.652627	0.410333	0.838410
C	-0.306874	-0.714334	-0.015761
C	0.949044	-1.194366	-0.165779
C	2.199752	-0.670045	0.489092
C	-2.905013	1.057528	-0.119668
H	-1.896443	1.935458	1.575228
H	0.112170	0.654614	1.570594
H	3.082167	-1.194489	0.103433
H	-2.811502	0.342464	-0.954737
O	-1.266426	-1.343929	-0.791202
C	-2.187878	-2.133888	-0.032332
H	-2.713052	-1.520488	0.706664
H	-2.903464	-2.544062	-0.744934
H	-1.659220	-2.944373	0.480948
O	-3.891994	1.760034	-0.016027
O	2.185662	-0.438688	1.837775
O	2.326453	0.712761	0.563644
N	2.225215	1.582897	-1.227512
O	2.048938	2.684038	-1.050999
H	1.065988	-2.034510	-0.817992

TS15-2

C	1.624849	-1.277702	0.294018
C	0.387505	-0.807975	0.546484
C	-0.141432	0.473306	0.091707
C	-1.430452	0.670419	-0.326169
C	-2.408792	-0.344359	-0.616980
C	2.614349	-0.639748	-0.601393
H	1.934381	-2.231582	0.713376
H	-0.329644	-1.399797	1.115714
H	-3.230221	0.001119	-1.256457
H	2.286289	0.256697	-1.160848
O	0.635829	1.589883	0.002693
C	1.524051	1.875292	1.093060
H	2.418794	1.250244	1.055738
H	1.804110	2.920927	0.973927
H	1.009567	1.727155	2.046088
O	3.733435	-1.083827	-0.744513
O	-2.378541	-1.397672	1.112426
O	-2.364494	-1.598008	-0.353792
H	-1.761845	1.636262	-0.645897

TS15-2-1-NO2

C	-1.951489	1.008508	1.016369
C	-0.905185	0.149022	1.121807
C	-0.468482	-0.763269	0.105765
C	0.907143	-1.127642	-0.023280
C	1.994657	-0.650474	0.927631
C	-2.679696	1.309960	-0.234547
H	-2.232472	1.614844	1.873038
H	-0.270690	0.144626	2.007684
H	2.988791	-0.963190	0.563927
H	-2.206291	0.981418	-1.180025
O	-1.238912	-1.321173	-0.838007
C	-2.610817	-1.682647	-0.576143
H	-2.825968	-1.605311	0.490280
H	-3.270058	-1.028541	-1.147587
H	-2.721631	-2.710888	-0.918794
O	-3.720335	1.929369	-0.243647
O	1.716413	-0.555456	2.132529
O	1.900044	0.862957	0.057244
N	3.012806	1.064336	-0.651913
O	2.973431	2.068507	-1.294545
H	1.187281	-1.770246	-0.831663

TS16-2

C	1.347362	0.495063	0.848609
C	0.041732	0.718951	1.089951
C	-1.111418	0.329779	0.273116
C	-1.470113	-0.914714	-0.130040
C	-0.775405	-2.185621	0.176672
C	1.807568	-0.156976	-0.359735
H	2.112176	0.823872	1.540621
H	-0.226119	1.281871	1.983847
H	-1.445136	-3.062228	0.108994
H	1.074594	-0.542495	-1.072239
O	-2.074162	1.285361	0.063958
C	-1.609473	2.584773	-0.308552
H	-0.975124	2.523578	-1.198249
H	-2.502115	3.169866	-0.525273
H	-1.052475	3.053702	0.506862
O	3.038143	-0.389960	-0.619923
O	3.401154	1.020095	-0.433371
O	0.395202	-2.304081	0.468691
H	-2.410278	-1.087742	-0.610717

TS16-3

C	1.051147	-1.721818	-0.491549
C	-0.283560	-1.429697	-0.516817
C	-1.036935	-0.232731	-0.337294
C	-0.557160	1.034217	-0.197568
C	0.904039	1.383095	-0.164501
C	2.202835	-0.969657	-0.099773
H	1.329653	-2.685085	-0.910816
H	-0.918646	-2.261890	-0.822030
H	1.103952	2.365280	0.287191
H	3.170075	-1.269545	-0.498164
O	-2.422135	-0.336377	-0.413098
C	-3.003990	-0.944606	0.739227
H	-2.751250	-0.379447	1.643788
H	-4.083061	-0.943333	0.582617
H	-2.653630	-1.976341	0.854460
O	2.367588	-0.217654	0.935492
O	1.197791	0.375043	1.324712
O	1.665470	0.935221	-1.060167
H	-1.265164	1.831190	-0.105564

TS16-2-2

C	-1.380464	-0.204404	-0.141357
C	-1.081324	1.092420	0.139038
C	0.090316	1.834953	-0.326482
C	0.745256	-1.405414	-0.590601
C	-0.534605	-1.163115	-0.864570
H	-1.799855	1.693576	0.683232
O	1.045610	1.412931	-0.954446
H	0.048449	2.912413	-0.073803
H	-1.021384	-1.750437	-1.636217
H	1.296246	-2.104920	-1.183897
O	-2.558198	-0.780425	0.163360
C	-3.556043	-0.005884	0.809320
H	-4.409927	-0.669625	0.933903
H	-3.207002	0.336891	1.788634
H	-3.837024	0.854187	0.192322
C	1.432968	-0.678973	0.580269
H	1.009474	0.297227	0.692457
O	2.735128	-0.571453	0.331834
O	1.248407	-1.382951	1.717306

IM16-2-1

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.335115
C	1.120024	0.000000	2.288153
C	2.100770	0.917242	2.455375
C	2.320836	2.128380	1.648826
C	1.214120	-0.030660	-0.899609
H	-0.944616	0.019750	-0.534774
H	-0.971220	-0.050076	1.829642
H	3.044228	2.828560	2.105198
H	1.564270	1.010414	-1.072565
O	1.060061	-0.951860	3.276910
C	0.911984	-2.298393	2.814620
H	1.709335	-2.543445	2.106792
H	0.981857	-2.928360	3.700690
H	-0.060909	-2.441723	2.335954
O	0.924833	-0.532324	-2.112658
O	2.258678	-0.749894	-0.237136
O	1.793823	2.371244	0.581493
N	3.488661	-0.136910	-0.440384
O	4.335255	-0.715509	0.127768
H	2.787608	0.743940	3.257322

IM16-2

C	-1.202805	-0.902914	0.840328
C	0.107567	-0.846404	1.098071
C	1.151828	-0.191646	0.299177
C	1.219010	1.096544	-0.112559
C	0.243919	2.172809	0.173625
C	-1.848777	-0.368450	-0.379003
H	-1.881485	-1.402160	1.526878
H	0.487784	-1.354057	1.984581
H	0.672422	3.182801	0.035046
H	-1.212011	0.078279	-1.141203
O	2.309502	-0.908104	0.096864
C	2.145924	-2.252871	-0.351894
H	1.586179	-2.276160	-1.292762
H	3.151007	-2.643437	-0.506534
H	1.627791	-2.858973	0.396353
O	-3.099280	0.203516	-0.227016
O	-2.923508	-1.114146	-0.859038
O	-0.904472	2.011820	0.522299
H	2.091139	1.474709	-0.603764

TS16-2-1-NO₂

C	0.507351	1.114418	1.371167
C	0.104846	-0.156299	1.554196
C	-0.067200	-1.074803	0.451102
C	0.870914	-1.311671	-0.569734
C	2.338458	-1.054599	-0.510699
C	0.822753	1.684240	0.016728
H	0.598063	1.805146	2.204745
H	-0.235773	-0.487397	2.532082
H	2.865404	-1.430622	-1.405916
H	0.827468	0.891901	-0.782940
O	0.516754	-2.016041	-1.640303
H	-0.444935	-2.157437	-1.646719
O	-1.158596	-1.816656	0.328391
C	-2.325147	-1.505131	1.110515
H	-2.529745	-0.434544	1.054032
H	-3.134403	-2.069247	0.652736
H	-2.174610	-1.830842	2.142355
O	1.555130	2.656910	-0.079422
O	-0.925811	2.111588	-0.467034
O	2.907151	-0.520767	0.408881
N	-1.542749	1.021326	-0.740336
O	-2.705138	1.133319	-1.063972

TS16-1

C	0.520645	-0.708267	-0.325897
C	-0.720291	-0.914425	-0.798926
C	-1.985450	-0.349471	-0.327607
C	-2.307730	0.949464	-0.102803
C	-1.442106	2.138179	-0.305457
C	0.768619	0.036141	0.904458
H	1.399340	-1.137788	-0.792748
H	-0.845168	-1.598341	-1.639143
H	-2.023555	3.060885	-0.484908
H	-0.084108	0.344896	1.521053
O	-3.064165	-1.204199	-0.319999
C	-2.880570	-2.428012	0.394082
H	-2.643705	-2.223801	1.443394
H	-3.825909	-2.964270	0.322107
H	-2.082909	-3.028856	-0.052117
O	1.888539	0.277549	1.349314
O	-0.232548	2.143370	-0.284705
O	3.127522	-0.195120	0.367047
N	4.666072	-0.571049	-0.653825
O	5.600369	0.002782	-0.340043
H	-3.316877	1.235046	0.109247

TS16-2-1

C	0.687721	-0.459952	1.261508
C	-0.418682	0.276201	1.401691
C	-1.422832	0.585974	0.374250
C	-2.154608	-0.268567	-0.376992
C	-2.111341	-1.747923	-0.331671
C	1.187025	-1.042226	-0.019434
H	1.342051	-0.636838	2.112490
H	-0.626207	0.736197	2.368349
H	-3.011289	-2.213927	-0.775412
H	0.548157	-0.859511	-0.889736
O	-1.824381	1.901737	0.287168
C	-0.773872	2.861369	0.194557
H	-0.137311	2.646250	-0.670702
H	-1.257220	3.829895	0.070545
H	-0.163224	2.867866	1.101950
O	1.754961	-2.283443	0.055167
O	2.541575	-0.765902	-0.246435
O	-1.211362	-2.414786	0.127270
N	2.850783	1.140359	-0.559015
O	3.964245	1.290600	-0.700456
H	-2.935764	0.085061	-1.017025

TS17-2

C	1.184483	-0.838448	0.163592
C	0.391227	0.382285	0.168807
C	-0.951726	0.454998	0.058289
C	-1.867445	-0.644749	-0.346059
C	3.396633	0.288351	-0.216361
C	2.526217	-0.874968	0.019418
C	0.641127	-1.762010	0.340428
H	0.911808	1.326056	0.281647
H	2.914243	1.281989	-0.300786
H	3.044834	-1.828716	0.063946
H	-1.676071	1.611011	0.087946
O	-1.010765	2.823753	0.411521
C	-0.284227	3.084125	-0.365293
H	-1.787212	3.584691	0.462561
H	-0.512028	2.732410	1.381301
H	4.600669	0.197455	-0.328526
O	-1.311157	-1.966158	1.144365
O	-1.486524	-1.841550	-0.267722
O	-2.850214	-0.418414	-0.703604

P20

C	1.461291	-1.488778	-0.617415
C	2.472896	-0.597900	-0.600584
C	2.590335	0.601765	0.244122
C	-0.537884	1.920916	0.166579
C	-0.700876	-0.392872	-0.002969
C	0.142898	-1.439603	-0.005082
H	1.625985	-2.425184	-1.150189
H	3.362048	-0.837644	-1.177318
O	-0.487975	3.003180	-0.326763
O	-0.438230	0.792375	-0.618440
O	1.741690	1.028253	1.002706
H	-0.687751	1.696263	1.230520
H	3.574952	1.103731	0.189722
H	-0.188965	-2.325940	0.494091
O	-1.946268	-0.532892	0.685720
C	-1.698813	-0.813505	2.065909
H	-2.610798	-0.720803	2.617806
H	-1.321516	-1.809839	2.165233
H	-0.978965	-0.119840	2.447418

IM17-2-1

C	-1.184853	-0.352414	-1.492429
C	-0.221489	0.738549	-1.262685
C	0.626883	0.843156	-0.220553
C	0.756051	-0.212617	0.905061
C	-2.839269	0.286643	0.271322
C	-2.306938	-0.589233	-0.797171
H	-0.963300	-0.993806	-2.346368
H	-0.126203	1.466551	-2.066033
H	-2.296944	1.229943	0.461214
H	-2.935656	-1.437902	-1.052894
O	1.462077	1.867882	0.024294
C	1.308909	3.053883	-0.744206
H	0.271047	3.400504	-0.701637
H	1.973552	3.789755	-0.295450
H	1.605236	2.877858	-1.783154
O	-3.851923	0.017246	0.877968
O	0.650981	-1.543947	0.429297
O	-0.183089	-0.006347	1.781902
N	1.673536	-1.819146	-0.490549
O	1.601392	-2.930141	-0.849961
H	1.705957	-0.091910	1.382563

IM17-2

C	-1.107958	-0.861304	1.356893
C	0.191058	-1.170966	0.713765
C	1.022475	-0.300516	0.129963
C	0.788123	1.193750	0.029514
C	-2.405861	-0.535976	-0.736911
C	-2.258921	-0.583511	0.732060
H	-1.112503	-0.929673	2.444260
H	0.507180	-2.208639	0.789859
H	-1.498386	-0.756241	-1.329551
H	-3.165487	-0.396365	1.300961
O	2.222585	-0.606824	-0.434955
C	2.633199	-1.963320	-0.439599
H	1.903888	-2.581077	-0.974529
H	3.590772	-1.986608	-0.956737
H	2.753870	-2.331038	0.585051
O	-3.461315	-0.298762	-1.282166
O	0.027237	1.771805	1.017125
O	-0.463812	1.620185	-0.376306
H	1.622059	1.766162	-0.319479

TS17-1

C	-3.040473	1.203877	1.060585
C	-2.562771	-0.177991	1.140052
C	-1.772539	-0.718909	0.190745
C	-1.178380	0.023474	-0.922142
C	-4.205714	0.955457	-1.137583
C	-3.726695	1.724234	0.025284
H	-2.829789	1.837213	1.920036
H	-2.866938	-0.772333	1.997044
H	-4.124950	-0.146964	-1.074139
H	-3.998012	2.776206	0.027483
O	-1.411115	-2.022442	0.081855
C	-1.993140	-2.931741	0.999564
H	-3.087129	-2.870093	0.959726
H	-1.662961	-3.922586	0.692655
H	-1.647851	-2.728277	2.019158
O	-4.707019	1.476855	-2.112023
O	-0.384041	2.397522	0.176004
O	-0.655829	1.171373	-0.860894
H	-1.040241	-0.459710	-1.885828
N	-0.063811	3.842212	1.397712
O	0.587852	4.718608	0.587240

TS17-3

C	0.918349	2.022624	-0.154108
C	-0.415996	1.439250	-0.228502
C	-0.908259	0.185229	-0.148269
C	-0.259429	-1.153575	-0.128707
C	2.179620	0.012053	0.606165
C	2.073815	1.442895	0.202999
H	0.938503	3.080986	-0.400249
H	-1.187412	2.199177	-0.311847
H	3.172099	-0.449316	0.495650
H	2.987950	2.031886	0.190458
O	-2.259085	-0.079747	-0.039326
C	-3.164618	0.996109	0.128304
H	-3.200701	1.618121	-0.771830
H	-4.139443	0.538524	0.290513
H	-2.883674	1.605288	0.994131
O	1.563256	-0.522683	-1.231408
O	0.729582	-1.540267	-0.833260
O	1.336573	-0.515843	1.352317
H	-0.668302	-1.870788	0.551975

P22

C	-0.435423	-1.179379	1.078586
C	-1.746962	-1.324676	0.836532
C	-2.436616	-1.008282	-0.439321
C	-0.227633	1.724257	0.125641
C	0.664419	0.616196	-0.357944
C	0.616278	-0.649094	0.183594
H	1.512903	0.956770	-0.938972
O	-0.154973	2.936519	-0.423579
O	0.681790	1.941484	1.112137
O	-1.971061	-0.321389	-1.320162
H	-1.233391	1.405521	0.435240
H	-3.438418	-1.464044	-0.553136
H	-0.038800	-1.563822	2.016732
H	1.417119	-1.312874	-0.067304
O	-2.554137	-1.937101	1.845642
C	-1.710295	-2.536075	2.832587
H	-1.200605	-1.769902	3.378567
H	-2.305435	-3.117627	3.505272
H	-0.993438	-3.168879	2.352404

TS18-2-1

C	0.124405	0.387892	1.734675
C	-0.971964	0.949937	0.924409
C	-1.838073	0.325665	0.107907
C	-1.890669	-1.162942	-0.143371
C	1.465434	-0.712644	-0.085902
C	1.172949	-0.331056	1.325604
H	0.080645	0.668269	2.786473
H	-1.135489	2.012849	1.087738
H	0.754239	-0.325530	-0.823386
H	1.923035	-0.661721	2.040532
O	-2.861155	0.944755	-0.554983
C	-3.027539	2.341669	-0.395864
H	-2.132896	2.876494	-0.732860
H	-3.878150	2.616402	-1.017359
H	-3.236638	2.589310	0.650653
O	1.897833	-1.993780	-0.295460
O	2.805834	-0.521804	-0.446150
O	-0.932017	-1.895629	0.214018
N	3.308897	1.367243	-0.475547
O	4.417647	1.420451	-0.700844
H	-2.743053	-1.594383	-0.625243

TS18-2-1-NO₂

C	0.262000	-0.418771	1.870609
C	-0.743729	0.441028	1.242464
C	-1.619762	0.187106	0.242952
C	-1.825803	-1.146273	-0.439376
C	1.687295	-1.013428	-0.116688
C	1.316723	-1.052154	1.332656
H	0.196106	-0.450129	2.959250
H	-0.830176	1.412553	1.724387
H	1.008850	-0.415126	-0.768023
H	1.988793	-1.635636	1.952773
O	-2.518975	1.100293	-0.235403
C	-2.494036	2.449147	0.241552
H	-1.507756	2.895766	0.077743
H	-3.245104	2.980765	-0.341807
H	-2.755841	2.489256	1.304706
O	2.221045	-2.028641	-0.612603
O	2.930581	0.339185	-0.074177
O	-1.035387	-2.098546	-0.211365
N	2.356505	1.273383	-0.753263
O	2.932585	2.327018	-0.879879
H	-2.643699	-1.280209	-1.116138

TS18-2

C	-0.700366	-1.070721	1.261024
C	0.575305	-1.159120	0.530163
C	1.367291	-0.173103	0.073154
C	1.096598	1.306693	0.218024
C	-2.030605	0.098125	-0.421483
C	-1.872978	-0.545035	0.862509
H	-0.688617	-1.582590	2.222455
H	0.961800	-2.172971	0.452468
H	-1.154765	0.226180	-1.062727
H	-2.755814	-0.602799	1.486189
O	2.582159	-0.364754	-0.513692
C	3.052121	-1.690819	-0.694442
H	2.358779	-2.261573	-1.320953
H	4.014604	-1.601157	-1.194940
H	3.180678	-2.188649	0.272647
O	-3.118887	0.633110	-0.831790
O	-3.865242	-0.616191	-0.628377
O	-0.062687	1.710080	0.495347
H	1.890673	2.011387	0.084788

P21

C	1.036823	-1.352775	-1.014435
C	-0.302537	-1.236139	-0.412363
C	-1.001666	-0.136194	-0.083001
C	-0.548754	1.290129	-0.294189
C	2.360144	-0.131900	0.708271
C	2.202096	-0.871793	-0.561373
H	1.058581	-1.974065	-1.909280
H	-0.815287	-2.189859	-0.309845
H	1.455435	-0.021200	1.332917
H	3.122051	-1.059558	-1.108253
O	-2.272931	-0.148797	0.413219
C	-2.907737	-1.396345	0.634233
H	-2.329744	-2.001088	1.341171
H	-3.884194	-1.165911	1.056840
H	-3.029419	-1.939436	-0.309407
O	3.430362	0.293211	1.082517
O	0.659494	1.535914	-0.545777
H	-1.255456	2.090956	-0.229785

IM18-2-2

C	1.696818	-1.555621	-0.495793
C	2.549057	-0.505339	-0.463393
C	2.428244	0.706055	0.356985
C	-0.841424	1.535265	0.005530
C	-0.608859	-0.793869	0.063703
C	0.373094	-1.710475	0.076428
H	2.063947	-2.448216	-1.002921
O	-0.913211	2.558009	-0.599686
O	-0.521785	0.363721	-0.645404
O	1.474424	1.019896	1.046206
H	-1.027270	1.400620	1.078445
H	3.331567	1.345889	0.360467
H	0.096482	-2.685415	0.463427
H	-1.494556	-0.981755	0.633913
O	3.793778	-0.636147	-1.155100
C	4.872391	-0.461689	-0.232572
H	5.748336	-0.944659	-0.612522
H	5.067645	0.582642	-0.105490
H	4.608267	-0.892510	0.710578

IM18-2-1

C	0.588355	2.140974	0.132745
C	-0.691824	1.553966	-0.289074
C	-1.356035	0.483085	0.174924
C	-0.921484	-0.388756	1.320833
C	2.228647	0.178440	0.064377
C	1.808990	1.615044	0.267467
H	0.529353	3.218930	0.282251
H	-1.192417	2.136425	-1.058732
H	2.143577	-0.363808	1.030490
H	2.629907	2.260798	0.562631
O	-2.561382	0.054236	-0.302741
C	-3.090734	0.671129	-1.463788
H	-2.369823	0.611340	-2.286094
H	-3.992091	0.114889	-1.715304
H	-3.347200	1.717077	-1.263591
O	3.521781	0.085973	-0.297237
O	1.343017	-0.440159	-0.873264
O	0.182464	-0.179285	1.887395
N	1.181623	-1.783985	-0.578863
O	0.422361	-2.279740	-1.325575
H	-1.551002	-1.187121	1.654329

IM18-2

C	-0.622073	-1.380398	1.166977
C	0.670970	-1.245017	0.473236
C	1.317228	-0.134173	0.078916
C	0.840150	1.282113	0.296819
C	-2.094925	-0.196222	-0.465641
C	-1.821650	-0.932847	0.786663
H	-0.576361	-1.989985	2.068189
H	1.197130	-2.188288	0.346409
H	-1.272134	-0.043190	-1.162102
H	-2.702638	-1.136810	1.389110
O	2.552743	-0.121238	-0.503122
C	3.211072	-1.355001	-0.732104
H	2.611457	-1.993655	-1.389364
H	4.153453	-1.106980	-1.217460
H	3.403898	-1.870924	0.214915
O	-3.024565	0.828245	-0.404003
O	-3.330543	-0.455628	-1.055877
O	-0.361373	1.501754	0.599592
H	1.523789	2.098762	0.193754

TS18-1

C	0.006367	-1.397571	-0.605812
C	-1.404030	-1.275933	-0.206483
C	-2.187130	-0.184876	-0.120623
C	-1.768356	1.230395	-0.452754
C	1.019775	0.104064	1.043835
C	1.094622	-0.794280	-0.100598
H	0.171136	-2.142751	-1.383427
H	-1.891320	-2.237307	-0.061433
H	0.058135	0.241171	1.551451
H	2.089147	-0.988809	-0.483829
O	-3.513540	-0.212327	0.184023
C	-4.125496	-1.457421	0.480387
H	-3.634748	-1.931033	1.336948
H	-5.161073	-1.230150	0.726471
H	-4.086899	-2.122146	-0.389216
O	-0.547032	1.528170	-0.509918
O	1.983678	0.689606	1.533305
O	3.413959	0.444671	0.754347
N	4.914326	0.071008	-0.305157
O	4.753713	-0.710559	-1.125476
H	-2.510640	1.978195	-0.639058

TS18-3

C	-1.119539	1.888854	-0.495135
C	0.273239	1.485353	-0.282890
C	0.847741	0.256659	-0.257718
C	0.154604	-1.045325	-0.586518
C	-2.109182	-0.127577	0.311413
C	-2.259894	1.199978	-0.253701
H	-1.227769	2.892835	-0.901572
H	0.942317	2.328928	-0.144498
H	-2.736814	-0.994777	0.127557
H	-3.229058	1.576119	-0.557399
O	2.159384	0.035635	-0.009700
C	2.959780	1.106034	0.462682
H	2.511014	1.548184	1.358186
H	3.928895	0.671588	0.702780
H	3.082850	1.869399	-0.312921
O	-1.273139	-0.142993	1.293188
O	-0.543946	-1.311829	1.370833
O	-0.978923	-1.034184	-1.132927
H	0.627651	-1.976666	-0.354720

CHOCHO

C	-0.000048565	-0.000004232	-0.000000645
C	0.000049313	-0.000007209	0.000000777
H	0.000004459	0.000021632	0.000000187
O	0.000009157	-0.000019836	0.000000159
O	-0.000004713	-0.000005597	-0.000000225
H	-0.000009651	0.000015242	-0.000000254

IMP1-1

C	-0.109277	-1.184758	-1.217631
C	1.197457	-0.983596	-1.409487
C	2.176063	-0.526379	-0.390419
C	-0.511176	1.494844	-0.246077
C	-1.063516	0.405239	0.656735
C	-0.873375	-1.046345	0.067546
H	-0.724455	-1.473379	-2.067143
H	1.627195	-1.107499	-2.397388
H	-0.582805	0.485623	1.633327
O	1.661724	-0.495396	0.852182
C	2.495960	0.123109	1.838780
H	2.671005	1.164614	1.561374
H	1.941911	0.060314	2.774385
H	3.446326	-0.407534	1.915790
O	0.560201	2.080776	0.057905
O	3.309907	-0.206931	-0.653050
H	-0.461178	-1.678986	0.858415
O	-2.216621	-1.421988	-0.209906
O	-2.469122	0.535683	0.746474
O	-2.916887	-0.814410	0.842899
H	-1.033081	1.764159	-1.140496

IMP1-2

C	0.583359	-1.265433	0.280194
C	0.972729	-0.243120	-0.857332
C	0.385531	1.139428	-0.623191
C	-2.471577	-0.625612	0.018188
C	-1.647380	-0.501196	1.244083
C	-0.342421	-0.768550	1.353369
H	0.634860	-0.608420	-1.828701
H	-2.199913	-0.128078	2.099304
H	0.145771	-0.599193	2.310875
O	0.976510	1.770070	0.386915
C	0.400319	3.035112	0.733299
H	-0.637703	2.896282	1.045392
H	1.006611	3.417258	1.551717
H	0.432027	3.709214	-0.124374
O	-3.668063	-0.235773	0.022180
O	-0.552287	1.566283	-1.250891
H	0.216224	-2.180576	-0.191506
O	2.383170	-0.187036	-0.769920
O	1.840597	-1.503004	0.900991
O	2.726013	-1.440721	-0.187561
H	-2.049117	-1.046889	-0.870042

IMP6

C	-1.485172	0.894325	-0.000051
C	-0.224494	1.348395	-0.000085
C	1.057852	0.588904	0.000001
C	-1.972256	-0.513539	0.000082
H	-2.296336	1.619807	-0.000107
H	-0.047360	2.419696	-0.000149
O	0.920779	-0.744719	-0.000099
C	2.148950	-1.483234	-0.000027
H	2.731908	-1.240189	0.890088
H	1.859375	-2.532090	-0.000120
H	2.732070	-1.240084	-0.890007
O	2.130056	1.146241	0.000139
H	-1.232522	-1.325690	0.000238
O	-3.162886	-0.740341	0.000027

IMP1-1-2

C	-1.043651	-0.116591	-0.000094
C	0.373738	-0.559097	0.000278
H	0.642502	-1.611839	0.000762
O	-1.969037	-0.969369	-0.000153
O	1.275355	0.312961	-0.000026
O	2.542330	-0.070924	-0.000151
H	-1.278189	0.927388	-0.000312

IMP1-1-1

C	0.795646	-1.315013	-0.000179
C	-0.537090	-1.500497	-0.000119
C	-1.618074	-0.480158	0.000052
C	1.503906	-0.056351	0.000055
H	1.439810	-2.190918	-0.000355
H	-0.927799	-2.512408	-0.000199
O	-1.179048	0.787535	-0.000216
C	-2.204234	1.790171	-0.000132
H	-2.826400	1.687956	0.890738
H	-1.679884	2.743564	-0.000466
H	-2.826873	1.687594	-0.890631
O	-2.788006	-0.781653	0.000386
H	1.058285	0.933087	0.000416
O	2.763702	-0.133274	-0.000098
O	3.468594	1.005170	0.000233

P5

C	0.527813	-0.102045	0.000037
C	-0.934234	-0.559940	0.000108
H	-1.039986	-1.659010	0.000417
O	1.453968	-0.953989	-0.000104
O	-1.859149	0.202311	-0.000125
H	0.761410	0.942145	0.000108

P8

C	1.751959	-0.344402	-0.000351
C	-1.448612	-0.005096	0.000014
C	-0.393993	1.044051	0.000211
C	0.938685	0.905266	0.000165
H	-0.825348	2.040318	0.000418
H	1.551675	1.804260	0.000391
O	-2.663282	0.323762	-0.000465
H	1.234015	-1.312699	-0.001068
O	2.961477	-0.273162	-0.000034
H	-1.174365	-1.039353	0.000280

IMP1-2-2

C	0.947633	0.598195	0.000019
C	-0.537905	0.513924	-0.000122
H	1.459657	1.557289	0.000058
O	-0.992589	-0.731297	-0.000208
C	-2.422284	-0.857264	0.000134
H	-2.837696	-0.380668	-0.889606
H	-2.616921	-1.926965	-0.003184
H	-2.836463	-0.386602	0.893632
O	-1.209176	1.517826	0.000035
O	1.619414	-0.459119	-0.000109
O	2.945695	-0.376433	0.000146

IMP1-2-1

C	1.209034	0.004734	-0.000191
C	-1.935995	-0.115126	0.000012
C	-1.053445	1.076729	0.000144
C	0.291538	1.120480	0.000028
H	-1.613364	2.005257	0.000318
H	0.776257	2.094073	0.000143
O	-3.186258	0.027752	-0.000301
H	0.950223	-1.049123	-0.000602
O	2.434560	0.309438	0.000071
O	3.336469	-0.675834	-0.000071
H	-1.509665	-1.096524	0.000183

TS1(2)

C	2.276365	-1.125745	-0.034053
C	1.217251	-1.830531	0.699300
C	-0.054527	-1.420549	0.676241
C	-0.486103	-0.203948	-0.096529
C	0.624080	0.502032	-0.924307
C	2.012441	-0.039909	-0.766553
H	3.292483	-1.500104	0.044032
H	1.494416	-2.695054	1.295169
H	-0.815879	-1.918608	1.267872
H	0.312986	0.511334	-1.973313
H	2.796308	0.492822	-1.296534
O	-1.550794	-0.435399	-0.960705
C	-2.747168	-0.919775	-0.362309
H	-3.023019	-0.316827	0.508473
H	-3.520521	-0.825698	-1.124170
H	-2.652822	-1.973417	-0.079072
O	-1.030238	1.187730	1.171836
O	0.487837	2.361846	-0.320876
O	0.225948	1.692836	0.885595

IM1(2)

C	-2.133539	0.930405	-0.239064
C	-1.095506	1.792212	0.093869
C	0.236643	1.375072	0.025828
C	0.524023	0.071260	-0.383290
C	-0.516029	-0.802776	-0.720249
C	-1.833128	-0.372222	-0.647316
H	-3.163965	1.264560	-0.182809
H	-1.313449	2.807082	0.412619
H	1.027000	2.067090	0.290814
H	-0.344126	-1.126647	-1.725464
H	-2.632314	-1.058304	-0.910963
O	1.781553	-0.438554	-0.485411
C	2.862549	0.407531	-0.155760
H	2.806438	0.733935	0.889777
H	3.765095	-0.185138	-0.302275
H	2.892990	1.286231	-0.811341
O	0.382306	0.054852	1.039576
O	-0.397771	-1.947904	0.128043
O	-0.679556	-0.943106	1.129733

TS1(3)

C	-0.990004	-1.637947	-1.059594
C	-1.736795	-1.602352	0.154063
C	-1.285601	-0.890355	1.229514
C	-0.123853	-0.069020	1.092263
C	0.645070	-0.128182	-0.120250
C	0.203682	-0.972523	-1.170225
H	-1.355783	-2.236728	-1.887637
H	-2.660968	-2.166597	0.226599
H	-1.823777	-0.860650	2.171502
H	0.801847	-1.048340	-2.071729
O	0.109679	1.728985	-0.927321
O	-1.175332	1.651511	0.742135
O	-1.113607	1.729303	-0.536610
H	0.170993	0.584838	1.886263
O	1.987169	0.363357	-0.074842
C	2.832952	-0.613815	0.537273
H	3.852443	-0.296247	0.468794
H	2.562437	-0.725178	1.566505
H	2.716836	-1.551189	0.034535

IM1(3)

C	0.738554	1.755294	1.033024
C	0.817946	0.443507	1.276852
C	0.240509	-0.581146	0.346206
C	-0.506587	-0.028547	-0.912835
C	-0.514337	1.468503	-1.056780
C	0.049551	2.278135	-0.155608
H	1.171677	2.467096	1.729153
H	1.308221	0.061372	2.167512
H	-1.057062	1.847169	-1.918630
H	-0.013428	3.355230	-0.279690
O	-0.766644	-1.373410	0.981716
O	-1.862700	-0.479302	-0.861099
O	-1.936954	-0.635939	0.686963
H	-0.046631	-0.445700	-1.784227
O	1.235488	-1.517557	-0.075755
C	2.180324	-0.860204	-0.924325
H	3.136360	-0.838783	-0.444288
H	2.257904	-1.390972	-1.850158
H	1.853681	0.141009	-1.113474

TS7(2)

C	0.712891	2.095420	0.336088
C	1.289848	0.924558	0.607659
C	0.599103	-0.402296	0.524494
C	-0.698693	-0.219629	-0.887203
C	-1.312239	1.147002	-0.661585
C	-0.667480	2.199148	-0.151574
H	1.283852	3.009760	0.468017
H	2.329154	0.847750	0.920590
H	-2.339296	1.245638	-1.007926
H	-1.157200	3.167151	-0.100790
O	0.059880	-0.924901	1.648162
O	1.280468	-1.362986	-0.101574
C	2.282143	-0.772097	-0.933678
H	3.179073	-0.631865	-0.367329
H	2.481765	-1.416700	-1.764062
H	1.935095	0.174409	-1.292266
O	-1.523717	-1.312315	-0.474563
H	-0.178490	-0.342382	-1.662400
O	-2.412554	-0.885598	0.403094

IM7(2)

C	-0.177331	2.288168	0.128186
C	1.001790	1.653938	0.255030
C	1.397354	0.273069	-0.153584
C	-1.497457	-0.326383	0.761010
C	-2.046962	0.630321	-0.165130
C	-1.459204	1.816095	-0.406283
H	-0.187232	3.332264	0.440500
H	1.831250	2.189140	0.706996
H	-2.961568	0.326067	-0.664349
H	-1.985522	2.526183	-1.040995
O	2.565826	-0.133772	0.344107
C	3.043955	-1.412131	-0.104799
H	2.979944	-1.470901	-1.192981
H	4.082713	-1.455352	0.217850
H	2.442681	-2.207628	0.339837
O	-1.723862	-1.561560	0.672433
O	-2.401649	-1.998649	-0.426433
O	0.698169	-0.396930	-0.878901
H	-0.883013	-0.050956	1.616918

TS8(2)

C	-2.494944	0.068349	-0.423260
C	-1.606690	0.932216	-1.211289
C	-0.275744	0.847449	-1.125099
C	0.406456	0.159035	0.025613
C	-0.506546	-1.243196	0.175858
C	-2.008406	-0.850799	0.415621
H	-3.567318	0.203356	-0.525850
H	-2.058771	1.675654	-1.861053
H	0.366112	1.328981	-1.855787
H	-0.602763	-2.327909	0.069046
H	-2.568211	-1.179207	1.286194
O	1.331524	-0.803508	-0.363742
C	2.397620	-0.348008	-1.188367
H	2.861806	0.550499	-0.769895
H	3.128369	-1.156164	-1.203854
H	2.056508	-0.156836	-2.211296
O	1.102202	1.151718	0.814733
O	0.284329	-1.870299	1.189478
O	0.396169	1.981008	1.741785

IM8(2)

C	1.421569	-0.647107	1.206071
C	0.118903	-0.491745	1.472878
C	-0.884044	-0.382461	0.413063
C	1.140911	1.655431	-0.717341
C	1.844634	0.395156	-1.016204
C	1.983769	-0.625993	-0.152204
H	2.111766	-0.782329	2.037026
H	-0.260203	-0.407263	2.486234
H	2.250156	0.316180	-2.020715
H	2.556975	-1.502160	-0.444605
O	-1.810952	0.532849	0.593139
C	-2.808294	0.679364	-0.435954
H	-3.341471	-0.262479	-0.574641
H	-3.472487	1.459656	-0.073498
H	-2.325247	0.978429	-1.368177
O	0.913717	2.027878	0.416329
O	-0.036738	-2.144155	-0.783931
O	-0.969669	-1.111375	-0.611029
H	0.804962	2.262517	-1.579548

TS2(2)

C	-2.184796	-0.724544	-0.801834
C	-1.287452	0.122128	-1.315593
C	-0.057157	0.537889	-0.556054
C	0.067461	-0.020262	0.889372
C	-0.988833	-0.994574	1.315565
C	-2.033972	-1.299325	0.540971
H	-3.043574	-1.025206	-1.394610
H	-1.383715	0.494511	-2.330390
H	-0.865907	-1.430640	2.302429
H	-2.789510	-1.996704	0.889636
O	0.114806	1.915502	-0.474835
C	0.008863	2.482942	0.825525
H	0.894662	2.261900	1.430291
H	-0.057999	3.560180	0.675801
H	-0.894336	2.132422	1.334757
O	1.980766	-0.885827	0.881438
O	2.047017	-1.417213	-0.424759
O	1.715275	-0.293679	-1.216022
H	0.132789	0.827760	1.577804

IM2(2)

C	1.993688	-0.964026	-0.642964
C	0.771089	-0.985776	-1.182231
C	-0.400861	-0.305118	-0.529071
C	-0.116938	0.361115	0.846371
C	1.309705	0.347695	1.305928
C	2.273154	-0.281217	0.626650
H	2.820415	-1.440120	-1.161746
H	0.591810	-1.446183	-2.148478
H	1.516397	0.867531	2.236634
H	3.293090	-0.284716	0.998752
O	-1.507270	-1.130312	-0.359077
C	-1.863844	-1.428432	0.985589
H	-2.336819	-0.569077	1.472461
H	-2.584142	-2.244078	0.928815
H	-0.991679	-1.756241	1.559887
O	-0.606541	1.691230	0.654769
O	-0.247872	1.935467	-0.688592
O	-0.803697	0.815980	-1.349111
H	-0.781991	-0.091478	1.588133

TS2(3)

C	-0.583005	2.214016	0.016061
C	0.069945	1.646760	-1.003470
C	0.358458	0.178766	-1.032510
C	-0.255417	-0.669894	0.127674
C	-0.932733	0.105641	1.218471
C	-1.073291	1.432132	1.156389
H	-0.771108	3.283350	0.010314
H	0.421212	2.232020	-1.847319
H	0.049744	-0.266408	-1.986002
H	-1.302988	-0.483437	2.051191
H	-1.570486	1.959882	1.964271
O	-1.177279	-1.613376	-0.327325
C	-2.497585	-1.152794	-0.589629
H	-2.492968	-0.379287	-1.361842
H	-3.047137	-2.025472	-0.941573
H	-2.982688	-0.756802	0.309737
O	2.407612	-0.075657	-0.782238
O	1.539916	-1.347320	0.791106
O	2.377026	-0.225100	0.623870

IM2(3)

C	0.573303	2.150389	-0.069032
C	0.980549	1.294994	-1.012438
C	0.617613	-0.155980	-0.967248
C	-0.365478	-0.588035	0.168514
C	-0.710172	0.470633	1.173729
C	-0.268605	1.725229	1.054578
H	0.859159	3.196248	-0.126972
H	1.595976	1.620513	-1.845076
H	0.204693	-0.490664	-1.926474
H	-1.343723	0.148949	1.993884
H	-0.539741	2.465270	1.801050
O	-1.573191	-1.081705	-0.326189
C	-2.553960	-0.125060	-0.709683
H	-2.175534	0.521708	-1.505378
H	-3.401341	-0.705141	-1.074226
H	-2.875603	0.496748	0.133463
O	1.805711	-0.897957	-0.676304
O	0.389300	-1.578212	0.865276
O	1.632756	-0.927958	0.727119

TS9(2)

C	-0.529783	1.385636	0.705523
C	-0.594027	-0.126391	0.578743
C	0.433485	-0.445667	-0.968062
C	1.695814	0.338343	-0.799369
C	1.721480	1.543499	-0.230252
C	0.514647	2.140558	0.355470
H	-1.410784	1.839178	1.153974
H	2.658727	2.088151	-0.163996
H	0.502368	3.211301	0.536808
O	0.529303	-1.740745	-0.613341
O	1.116671	-1.825876	0.559152
O	-0.030990	-0.844018	1.473103
H	2.593854	-0.164135	-1.151272
H	-0.162385	-0.347868	-1.851393
O	-1.835082	-0.592194	0.042358
C	-2.384406	0.403872	-0.824242
H	-2.015710	0.254993	-1.817619
H	-3.451640	0.326992	-0.824650
H	-2.096900	1.374940	-0.478892

IM9(2)

C	-1.949883	-0.737618	-0.723694
C	-1.391351	0.493242	-1.212444
C	1.379236	-0.752262	-0.154518
C	0.702750	-0.485545	1.156805
C	-0.582030	-0.778457	1.398511
C	-1.585173	-1.287975	0.450916
H	-2.712274	-1.186001	-1.349604
H	-0.949178	0.605164	-2.198701
H	-0.939390	-0.658888	2.421141
H	-2.122212	-2.174965	0.782344
O	2.328982	0.122504	-0.545722
C	2.575050	1.316160	0.191315
H	3.111664	1.102900	1.120836
H	3.202567	1.932078	-0.450919
H	1.646942	1.852614	0.411761
O	1.131976	-1.706919	-0.841454
O	-1.825583	1.543296	0.734544
O	-1.315645	1.543644	-0.515663
H	1.312445	-0.098376	1.968157

TS10(2)

C	0.176933	0.216437	1.382713
C	-0.370567	0.692750	0.082503
C	-0.425387	-0.766279	-1.046022
C	0.981061	-1.345923	-0.899535
C	1.678064	-1.331603	0.237466
C	1.169273	-0.671618	1.448863
H	-0.261702	0.670292	2.268701
H	2.629684	-1.851863	0.291113
H	1.597729	-0.942704	2.408289
O	-1.413091	-1.383525	-0.569557
O	-2.323381	-0.087604	0.544535
O	-1.688685	0.925574	0.024465
H	1.338209	-1.862958	-1.786521
H	-0.570279	0.164394	-1.553717
O	0.335632	1.758187	-0.558610
C	1.741589	1.505375	-0.493262
H	2.005805	0.768707	-1.222926
H	2.276355	2.410866	-0.690774
H	1.994615	1.147385	0.482813

IM10(2)

C	-2.088987	-0.769467	0.467354
C	-2.115121	0.342436	-0.267859
C	-1.095758	1.437494	-0.188275
C	0.861217	-0.236671	-0.253248
C	0.338056	-0.881827	1.013677
C	-0.924882	-1.268918	1.208573
H	-2.983841	-1.381281	0.533221
H	-2.900891	0.540389	-0.994056
H	1.095996	-1.074695	1.770550
H	-1.155727	-2.021252	1.956998
O	1.148015	-1.003374	-1.233960
O	-0.594994	1.940784	-1.278833
O	0.765105	-2.235597	-0.955741
O	1.715005	0.889143	-0.033041
C	1.476323	1.420135	1.273090
H	2.340328	1.264430	1.884769
H	1.274889	2.468498	1.200571
H	0.635159	0.924793	1.711243
H	-1.276043	2.292380	0.429438

TS3(2)

C	-1.387132	0.314228	0.901109
C	0.103756	-0.144945	0.788714
C	1.010831	0.762260	-0.005171
C	0.570165	1.880662	-0.598309
C	-0.819308	2.310513	-0.457309
C	-1.725679	1.612106	0.235059
H	-1.106095	3.244235	-0.932207
H	-2.748396	1.957020	0.347050
O	2.332016	0.459943	-0.047300
C	2.743742	-0.879814	0.183556
H	2.322106	-1.557505	-0.568633
H	3.828588	-0.872253	0.086534
H	2.474150	-1.216612	1.189197
H	1.273414	2.489730	-1.155486
H	0.501542	-0.231071	1.778284
H	-1.631303	0.399732	1.939362
O	-2.124036	-1.412350	0.005396
O	-0.028464	-2.072173	-0.124244
O	-1.166048	-1.893338	-0.955101

IM3(2)

C	-1.410665	-0.274987	0.744957
C	0.144725	-0.409051	0.650038
C	0.868393	0.768845	0.045949
C	0.224909	1.855395	-0.403674
C	-1.225974	1.976687	-0.279120
C	-1.988788	1.016583	0.254708
H	-1.684310	2.896708	-0.629976
H	-3.062700	1.132241	0.358594
O	2.224070	0.742619	0.033653
C	2.893228	-0.509020	0.091906
H	2.636889	-1.134238	-0.771935
H	3.956044	-0.273312	0.056885
H	2.672496	-1.041037	1.022316
H	0.803639	2.668433	-0.827948
H	0.526794	-0.564397	1.637354
H	-1.693040	-0.397915	1.769677
O	-1.873598	-1.377901	-0.038736
O	0.314853	-1.584606	-0.146220
O	-0.814171	-1.509261	-1.004141

TS11(2)

C	0.203696	-0.745655	-0.112020
C	-1.206814	-0.035031	0.932033
C	-1.565679	1.300684	0.339654
C	-0.638487	2.133974	-0.142259
C	0.760076	1.723075	-0.246336
C	1.143129	0.443385	-0.206026
H	0.546736	-1.508758	0.608139
H	-0.873916	-0.061092	1.971120
H	1.507349	2.501064	-0.374145
O	-2.040856	-1.039047	0.680492
O	-2.346571	-1.062573	-0.587482
O	-0.398956	-1.171340	-1.152142
H	-0.949691	3.114354	-0.486199
H	-2.594512	1.592343	0.303081
O	2.527262	0.094425	-0.291478
C	3.093118	-0.929559	0.530814
H	4.073107	-1.171264	0.175708
H	3.155405	-0.582090	1.540906
H	2.474244	-1.801522	0.491110

IM11(2)

C	-0.734755	1.139471	-0.422857
C	1.932711	-0.188878	0.633493
C	1.710060	-1.313515	-0.281217
C	0.460479	-1.832257	-0.412456
C	-0.790346	-1.330798	0.121405
C	-1.287244	-0.072707	0.208370
H	0.201993	0.969567	-0.987999
H	1.237329	-0.037679	1.455400
H	-1.463164	-2.122970	0.450436
O	2.849436	0.669806	0.599165
O	3.720826	0.694611	-0.428229
O	-1.192320	2.260530	-0.335110
H	0.411001	-2.783290	-0.937188
H	2.525061	-1.722565	-0.840997
O	-2.599763	0.080369	0.754961
C	-3.572779	-0.235257	-0.244297
H	-3.637001	-1.297399	-0.356685
H	-4.525986	0.150367	0.051661
H	-3.283413	0.205091	-1.175565

TS12(2)

C	0.173767	-0.239448	0.806059
C	-1.450655	-0.980194	0.306458
C	-2.356646	0.256358	0.303581
C	-1.969824	1.505184	0.010191
C	-0.584722	1.791072	-0.351839
C	0.402973	0.939794	-0.060852
H	0.118674	-0.082623	1.885458
H	-1.641785	-1.604159	1.198193
H	-0.376373	2.688279	-0.926283
O	-1.192490	-1.584289	-0.786805
O	0.842539	-1.571854	-0.757487
O	0.876615	-1.338828	0.528608
H	-2.718452	2.289516	-0.017451
H	-3.385677	0.109689	0.557518
O	1.731116	1.081806	-0.571508
C	2.661742	0.520861	0.358103
H	2.919855	-0.470775	0.049987
H	3.543803	1.125783	0.388751
H	2.217911	0.487848	1.331151

TS4(2)

C	-0.594042	-0.535394	1.065309
C	0.830616	-0.697646	0.632217
C	1.491269	0.284544	-0.001405
C	0.870437	1.584756	-0.293529
C	-0.383567	1.851336	0.069478
C	-1.247131	0.856369	0.789577
H	1.280437	-1.661710	0.835459
H	-0.846529	2.804491	-0.167594
H	-1.658560	1.289240	1.706070
H	-0.716600	-0.822008	2.113717
O	-2.927203	0.358979	-0.367990
O	-2.006241	-1.588760	-0.008980
O	-2.478106	-0.784847	-1.069523
H	1.482069	2.305934	-0.826628
O	2.767620	0.232072	-0.445727
C	3.470301	-0.979419	-0.247218
H	2.968750	-1.806369	-0.762646
H	4.462768	-0.827456	-0.668820
H	3.551812	-1.208946	0.821633

IM4(2)

C	-0.713095	-0.685345	0.822646
C	0.734565	-0.659914	0.439066
C	1.324885	0.458078	-0.012821
C	0.589668	1.720473	-0.178104
C	-0.708913	1.808706	0.106942
C	-1.507441	0.643435	0.615596
H	1.277184	-1.587161	0.576415
H	-1.243764	2.748217	0.005503
H	-1.942386	0.921222	1.552909
H	-0.776987	-0.951626	1.857011
O	-2.518389	0.254286	-0.317918
O	-1.444682	-1.614245	0.013708
O	-2.021027	-0.858034	-1.027479
H	1.107978	2.586027	-0.534571
O	2.715363	0.419685	-0.344480
C	3.225359	-0.895420	-0.109315
H	2.748696	-1.586689	-0.772519
H	4.281147	-0.904849	-0.282872
H	3.027838	-1.178752	0.903409

TS13(2)

C	-0.888246	-0.551813	1.155344
C	0.515441	-0.674514	0.587135
C	1.232716	0.361375	0.126111
C	0.689151	1.726623	0.082873
C	-0.621740	1.939015	0.156000
C	-1.615464	0.833083	0.130679
H	0.925166	-1.677339	0.636589
H	-1.047167	2.937335	0.233063
O	2.512499	0.318346	-0.313946
C	3.170667	-0.932691	-0.260849
H	2.659782	-1.667644	-0.893903
H	4.178402	-0.761019	-0.636010
H	3.213622	-1.303167	0.769767
H	1.401829	2.543202	0.032666
O	-1.836140	-1.341244	0.432022
H	-1.023153	-0.484685	2.084809
O	-2.064066	0.355841	-1.140500
H	-2.360207	0.915985	0.752433
O	-1.467721	-1.421585	-0.832973

IM13(2)

C	0.240589	1.517546	-1.017005
C	1.004790	0.328975	-0.836240
C	0.708359	-0.576906	0.129774
C	-0.379690	-0.489094	1.130322
C	-1.704912	-0.401446	0.938445
C	-2.425727	-0.445061	-0.361573
H	-0.402482	1.701917	-1.872152
H	1.852888	0.227870	-1.500656
H	-2.344048	-0.417043	1.818329
H	-1.939799	0.134017	-1.170170
O	1.451819	-1.660562	0.393429
C	2.610296	-1.892922	-0.402991
H	3.316683	-1.063811	-0.296840
H	3.048344	-2.813324	-0.022142
H	2.332689	-2.013496	-1.454091
O	0.227861	2.449606	-0.166241
O	1.011537	2.318298	0.948787
O	-3.462073	-1.033404	-0.568419
H	-0.019657	-0.594187	2.152888

TS14(2)

C	-0.541390	-0.960030	1.033039
C	0.840392	-0.867115	0.408299
C	1.449252	0.287825	0.099274
C	0.794897	1.589543	0.295704
C	-0.524265	1.671791	0.443833
C	-1.424735	0.501169	0.270593
H	1.332253	-1.825175	0.281131
H	-1.025651	2.603899	0.695536
O	2.706995	0.427814	-0.382214
C	3.466599	-0.753116	-0.553989
H	2.989072	-1.419830	-1.281571
H	4.438937	-0.436193	-0.927973
H	3.586309	-1.277750	0.400838
H	1.435684	2.463012	0.356332
O	-1.498531	-1.544711	0.145948
H	-0.639660	-1.164058	1.947001
O	-2.238804	0.441958	-0.903581
O	-3.288371	-0.324878	-0.673861
H	-1.931747	0.234236	1.057853

TS5(2)

C	-0.397341	-1.069219	0.723002
C	-1.414490	-0.361980	0.227862
C	-1.288134	1.084541	-0.018537
C	-0.148647	1.745505	0.205839
C	1.074771	1.069280	0.744021
C	0.926587	-0.451290	1.073600
H	-0.470019	-2.144584	0.856837
H	1.466853	1.617316	1.605591
H	1.194425	-0.661060	2.113166
O	2.473510	-1.322245	-0.066824
O	2.534453	-0.463699	-1.189732
O	2.654777	0.798514	-0.566625
H	-0.081093	2.802674	-0.028864
H	-2.135330	1.623098	-0.388829
O	-2.639244	-0.999210	-0.144718
C	-3.554904	-0.019800	-0.641933
H	-3.162519	0.412606	-1.538571
H	-4.495297	-0.484952	-0.852158
H	-3.692040	0.745792	0.092889

IM5(2)

C	0.282963	-1.203538	-0.489014
C	1.283447	-0.373420	-0.189216
C	1.069598	1.081837	-0.114388
C	-0.132575	1.632970	-0.305907
C	-1.344123	0.814623	-0.631684
C	-1.110409	-0.723441	-0.781525
H	0.425262	-2.280260	-0.493830
H	-1.852675	1.218068	-1.512014
H	-1.453676	-1.085095	-1.755081
O	-2.039022	-1.273983	0.160983
O	-2.064320	-0.280678	1.168179
O	-2.336153	0.878093	0.407076
H	-0.259341	2.705312	-0.199744
H	1.902991	1.717738	0.100058
O	2.581783	-0.876078	0.137214
C	3.460882	0.217033	0.415055
H	3.118692	0.737715	1.284938
H	4.449122	-0.155046	0.587799
H	3.472620	0.886350	-0.419676

TS15(2)

C	0.218617	1.653805	-0.367010
C	-0.910799	1.103157	-0.813314
C	-1.386206	-0.188770	-0.289231
C	-0.556976	-1.026461	0.337292
C	0.897382	-0.762235	0.443153
C	1.097710	1.073825	0.732189
H	0.572984	2.597553	-0.774795
H	-1.502899	1.589941	-1.583422
O	-2.691734	-0.526435	-0.481223
C	-3.568926	-0.124095	0.567863
H	-3.578303	0.964359	0.690230
H	-4.562972	-0.464040	0.279636
H	-3.271279	-0.592770	1.511559
H	-0.924209	-1.933301	0.810149
H	0.840839	1.174887	1.632419
O	2.491972	1.203120	0.441988
H	1.318976	-1.013987	1.283969
O	1.745803	-1.106009	-0.655438
O	2.999215	-1.157927	-0.244753

IM15(2)

C	-1.601494	1.459753	0.747082
C	-1.260014	0.220651	1.139907
C	-0.520574	-0.727619	0.268007
C	0.819325	-0.675382	-0.005642
C	1.781399	0.093490	0.687561
C	-1.224743	2.050827	-0.548738
H	-2.196467	2.092033	1.399681
H	-1.615155	-0.171488	2.088305
H	1.482726	0.787808	1.469572
H	-1.789425	2.947563	-0.871471
O	-1.221125	-1.639121	-0.411295
C	-2.645265	-1.676834	-0.297066
H	-3.087344	-0.737769	-0.638417
H	-2.960482	-2.497793	-0.938031
H	-2.945196	-1.875453	0.735153
O	-0.335038	1.604075	-1.241103
O	3.508267	-0.590810	-0.589085
O	3.028369	0.155534	0.449227
H	1.175760	-1.251631	-0.853396

TS16(2)

C	-0.614486	-1.439151	-0.128886
C	0.567080	-1.128325	-0.662994
C	1.281067	0.098332	-0.268933
C	0.639463	1.112647	0.315352
C	-0.831120	1.113048	0.498557
C	-1.324198	-0.632818	0.949796
H	-1.144321	-2.335916	-0.441314
H	1.027262	-1.768118	-1.410995
O	2.613128	0.189157	-0.538461
C	3.462927	-0.276835	0.506823
H	3.294178	-1.337770	0.720680
H	4.483810	-0.137285	0.153144
H	3.298512	0.307601	1.417984
H	1.179099	1.975962	0.695211
H	-1.192562	-0.854122	1.855504
H	-1.327381	1.432286	1.273092
O	-1.128935	1.610784	-0.808526
O	-2.489281	-0.298354	0.611736
O	-2.582787	-0.297090	-0.704947

IM16(2)

C	-0.352145	1.199429	1.352730
C	-0.583651	-0.118777	1.230831
C	-0.165698	-0.991782	0.118816
C	1.089911	-1.141169	-0.376534
C	2.322081	-0.523399	0.121431
C	0.276647	1.983342	0.316039
H	-0.674611	1.754961	2.226206
H	-1.154061	-0.614756	2.013585
H	2.160486	0.141388	0.991428
H	1.256286	2.438657	0.420346
O	-1.103822	-1.817554	-0.395263
C	-2.476102	-1.633561	-0.058987
H	-2.761406	-0.579221	-0.116171
H	-3.036039	-2.207201	-0.795988
H	-2.691471	-2.024259	0.940079
O	-0.245684	2.150260	-0.817369
O	-1.470878	1.635745	-1.069035
O	3.448117	-0.673187	-0.315544
H	1.212697	-1.916183	-1.127744

TS6(2)

C	-1.354241	1.066339	-0.348720
C	-0.377996	2.155058	-0.438740
C	0.841431	2.009851	0.104874
C	1.285236	0.754142	0.807394
C	0.200940	-0.356729	0.965901
C	-1.108522	-0.082095	0.289474
H	-2.317105	1.220782	-0.827049
H	-0.665285	3.066038	-0.949303
H	0.057564	-0.620915	2.018066
O	1.328775	-1.792823	0.063246
O	2.085857	-1.208024	-0.973225
O	2.788306	-0.196660	-0.271104
H	1.744593	1.019496	1.763633
H	1.530549	2.825447	0.035456
O	-2.082433	-1.127430	0.350063
C	-3.261469	-0.721602	-0.349991
H	-3.057185	-0.681835	-1.399556
H	-4.045816	-1.425693	-0.165720
H	-3.563622	0.246384	-0.008515

IM6(2)

C	-1.056331	1.217438	-0.208801
C	0.086121	2.133337	-0.257781
C	1.297308	1.717955	0.147296
C	1.564200	0.323171	0.647945
C	0.316702	-0.605911	0.772075
C	-0.969834	-0.031337	0.259866
H	-2.009267	1.590940	-0.572348
H	-0.073512	3.139647	-0.625139
H	0.205450	-0.982797	1.793341
O	0.724825	-1.751681	0.011783
O	1.495885	-1.164284	-1.012847
O	2.412958	-0.386163	-0.262667
H	2.130465	0.377842	1.581844
H	2.111555	2.411279	0.112612
O	-2.104530	-0.901248	0.284791
C	-3.241761	-0.216673	-0.247151
H	-3.109735	-0.069420	-1.298714
H	-4.121768	-0.800949	-0.076535
H	-3.344715	0.732583	0.235770

TS17(2)

C	-0.059274	2.053901	-0.634748
C	-1.230193	1.201307	-0.429653
C	-1.077669	-0.051359	0.022323
C	0.269902	-0.679581	0.233084
C	1.411534	0.687623	0.905716
C	1.129390	1.809533	-0.075832
H	-0.179846	2.924598	-1.273378
H	-2.213326	1.598014	-0.651465
H	1.981881	2.452033	-0.281006
O	-2.040188	-0.954739	0.284082
C	-3.376378	-0.482374	0.290029
H	-3.682474	-0.170581	-0.715258
H	-3.989378	-1.320385	0.617450
H	-3.477944	0.355862	0.987704
H	1.133879	0.762369	1.802338
O	2.660353	0.032250	0.669418
O	0.916778	-1.258263	-0.903393
O	1.955442	-1.968720	-0.504862
H	0.084263	-0.640433	1.286130

IM17(2)

C	-1.923571	0.763493	-1.051243
C	-0.603555	1.247805	-0.642497
C	0.422821	0.408908	-0.395425
C	0.400846	-1.032746	-0.648063
C	-2.313436	-0.671519	0.958779
C	-2.663321	-0.129555	-0.366586
H	-2.326979	1.181387	-1.971452
H	-0.465840	2.320285	-0.537537
H	-3.019304	-1.400587	1.401597
H	-3.611732	-0.472511	-0.770518
O	1.625939	0.734767	0.141236
C	1.797091	2.072568	0.575707
H	1.012100	2.347726	1.290043
H	2.772028	2.110348	1.058465
H	1.781079	2.761984	-0.275553
O	-1.288090	-0.382483	1.540003
O	2.530022	-1.417839	0.017198
O	1.342603	-1.844768	-0.428527
H	-0.526393	-1.519776	-0.938356

TS18(2)

C	0.171689	1.905134	-0.421414
C	-1.117512	1.221339	-0.319362
C	-1.163644	-0.081325	-0.006863
C	0.070172	-0.924145	0.142754
C	1.386559	0.175242	0.969479
C	1.297421	1.425950	0.115366
H	0.196918	2.847722	-0.961220
H	-2.025238	1.783000	-0.502928
H	2.240568	1.951195	-0.012054
O	-2.255699	-0.852488	0.147351
C	-3.506499	-0.187888	0.196058
H	-3.739306	0.272852	-0.770912
H	-4.244823	-0.954467	0.425119
H	-3.498421	0.576010	0.980979
H	1.102320	0.193898	1.866959
O	0.650020	-1.467751	-1.046014
H	-0.132041	-0.971165	1.192420
O	2.392010	-0.534471	0.706904
O	2.622534	-0.508401	-0.592549

IM18(2)

C	0.246547	-1.430231	-0.845959
C	-1.055657	-1.021990	-0.319302
C	-1.545444	0.224817	-0.130884
C	-0.909052	1.521184	-0.532789
C	1.701969	-0.134641	0.628548
C	1.478604	-1.022945	-0.477713
H	0.192661	-2.218787	-1.595270
H	-1.740419	-1.850514	-0.154074
H	0.905972	0.219297	1.277815
H	2.370712	-1.400677	-0.963868
O	-2.790316	0.503412	0.323569
C	-3.630207	-0.568959	0.706678
H	-3.157040	-1.172668	1.489581
H	-4.542046	-0.114131	1.089770
H	-3.868144	-1.202380	-0.155656
O	2.847445	0.253471	0.982974
O	3.923241	-0.105687	0.238246
O	-1.373366	2.619132	-0.349644
H	0.071367	1.375109	-1.023093
