Supporting Information

Mechanism and Regioselectivity of Intramolecular [2+2] Cycloaddition of Ene–Ketenes: A DFT Study

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Contents:

S1. Benchmark Calculations

To assess the performance of different density functionals (B3LYP,[1] B3LYP-D3(BJ),[1,2] M06-2X,[3] PBE0-D3(BJ),[2,4] and ωB97XD[5]) on [2+2] cycloadditions, we performed benchmark calculations by performing single-point energy calculations with the cc-pVTZ basis set[6] on the optimized geometries computed at the B3LYP[1]/def2-SVP[7] level (**Figure S1** and **Table S1**). Results from CCSD(T)[8]/cc-pVTZ[6] calculations (the frozen core approximation was applied) were utilized as the reference.

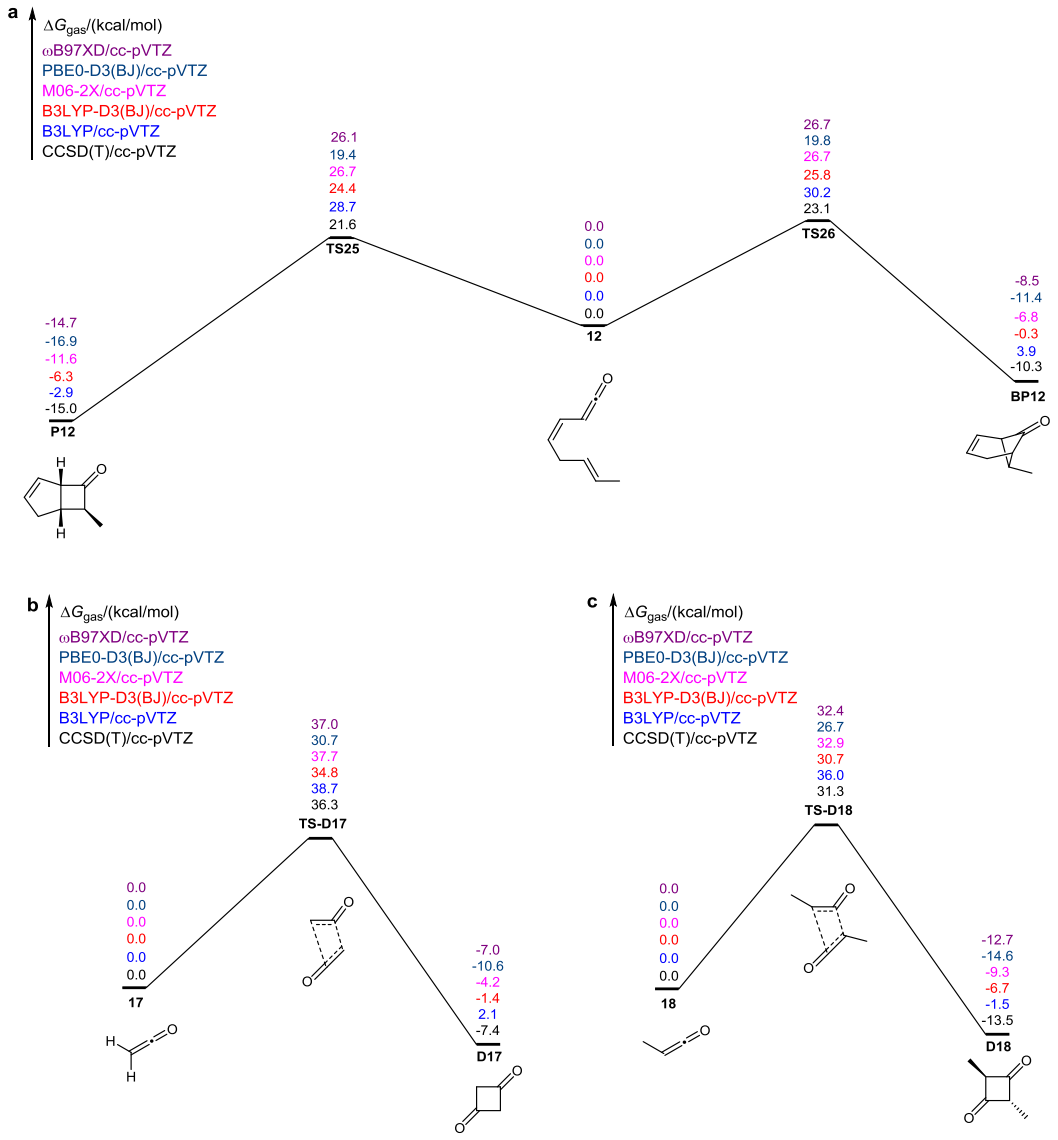


Figure S1. Benchmark calculations.

B3LYP performs badly with a mean absolute deviation (MAD) of 8.6 kcal/mol. B3LYP-D3(BJ) and M06-2X perform much better, with MADs of 4.9 and 3.2 kcal/mol, respectively. Though PBE0-D3(BJ) performs well on intramolecular [2+2] cycloadditions, it performs badly on dimerizations. Among all the tested functionals, ωB97XD performs best (MAD = 1.6 kcal/mol). Consequently, ωB97XD was chosen for single-point energy refinements.

Table S1. Absolute deviation from CCSD(T) calculations.[a]

Functional	B3LYP	B3LYP-D3(BJ)	M06-2X	PBE0-D3(BJ)	ωB97XD
TS25	7.1	2.9	5.2	2.2	4.6
TS26	7.1	2.7	3.6	3.3	3.6
P12	12.0	8.7	3.4	2.0	0.2
BP12	14.1	10.0	3.5	1.1	1.7
TS-D17	2.4	1.5	1.3	5.6	0.7
D17	9.5	6.0	3.2	3.3	0.4
TS-D18	4.7	0.6	1.6	4.5	1.1
D18	12.0	6.9	4.2	2.1	0.8
MAD	**8.6**	**4.9**	**3.2**	**3.0**	**1.6**

[a] Reported in kcal/mol. MAD, mean absolute deviation.

S2. Natural Population Analysis

To investigate the charge distribution, we carried out natural population analysis on **1**, **TS1**, and **TS2** (**Figure S2**).[9] In **TS1**, the internal carbon becomes less negatively charged (**1**: −0.20 e vs. **TS1**: −0.06 e). Similarly, in **TS2**, the external carbon becomes less negatively charged (**1**: −0.38 e vs. **TS2**: −0.26 e).

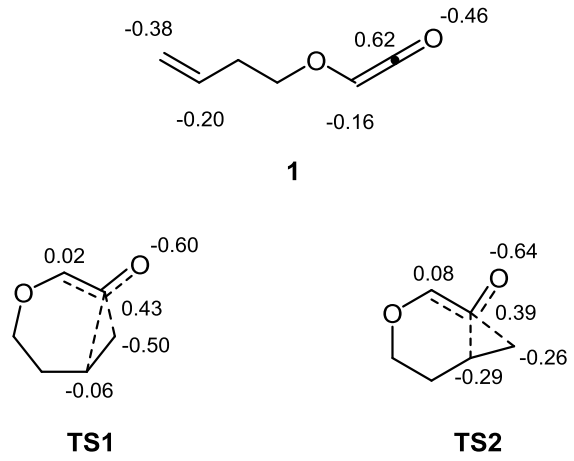


Figure S2. Natural atomic charges (in e). Computed at the B3LYP/def2-SVP level.

S3. Discussion on Diradical Stepwise Mechanism

Besides the concerted mechanism, we have also considered the diradical stepwise mechanism. For oxygen-tethered substrate **1**, the activation free energy of the normal [2+2] cycloaddition via diradical mechanism is 33.3 kcal/mol (**Figure S3a**), which is higher than that of the concerted mechanism (**Figure 2**) by 11.8 kcal/mol. For the cross-[2+2] cycloaddition, the diradical mechanism is also disfavored (by 14.5 kcal/mol). Similarly, the activation free energies of both normal and cross-[2+2] cycloadditions of carbon-tethered substrate **7** are much lower than those of the diradical mechanism (**Figure S3b**). We envision that the same conclusion may hold for the other substrates.

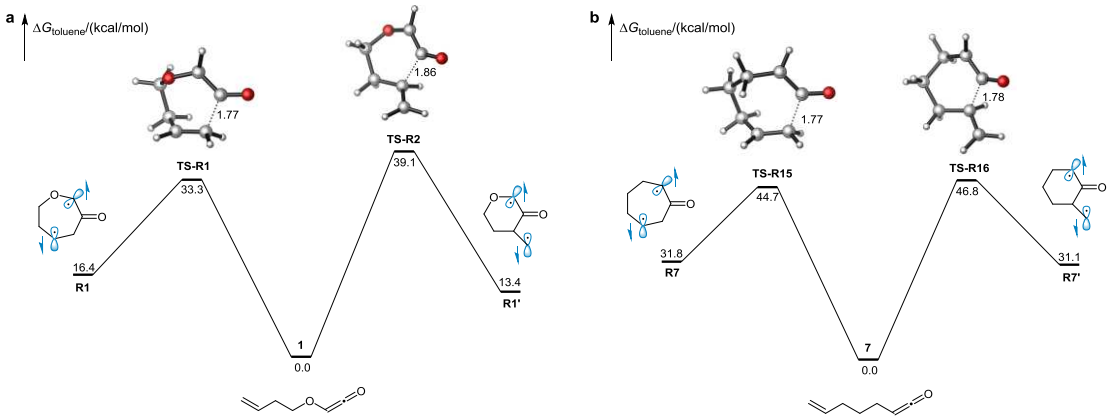
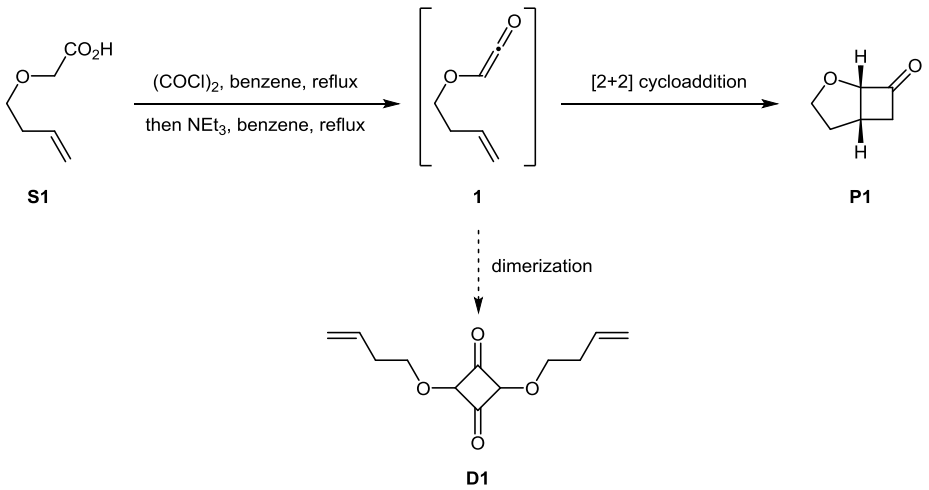


Figure S3. DFT-computed free energy surfaces of intramolecular [2+2] cycloadditions via singlet diradical mechanism.

S4. ^{13}C NMR Analysis on the Crude Product

General Information. The reactions were carried out in oven-dried glassware under N_2 atmosphere. All chemicals were used as received without further purification. The $^{13}C\{^1H\}$ nuclear magnetic resonance (NMR) spectrum was measured on a Bruker AVANCE III 400 NMR spectrometer.

Following Snider's procedure,[10] acid **S1** (181 mg, 1.39 mmol, 1.0 equiv) was dissolved in benzene (2 mL). Oxalyl chloride (1.4 mL) was added, and the solution was heated at reflux for 1.5 h. The solution was cooled and concentrated by rotary evaporation. The residue was taken up in benzene (5 mL) and concentrated by rotary evaporation. This process was repeated twice to remove all of the excess oxalyl chloride. The resulting acyl chloride was taken up in benzene (3 mL) and added to a solution of NEt_3 (0.27 mL, 1.9 mmol, 1.4 equiv) in benzene (20 mL) at reflux. The solution was refluxed for an additional 24 h, cooled, quenched with semi-saturated aqueous NH_4Cl solution (30 mL), and extracted with Et_2O (20 mL × 2). The combined organic phases were washed with brine (20 mL), dried over Na_2SO_4, filtered, and concentrated by rotary evaporation at 0 °C. ^{13}C NMR analysis on the crude product indicated that there are two carbonyl peaks. The peak at 211.1 ppm is assigned to the carbonyl carbon of the normal [2+2] cycloadduct **P1**, whereas the peak at 172.9 ppm cannot be assigned to the carbonyl carbons of the dimerized product **D1**.



Scheme S1. Reaction of substrate **1**.

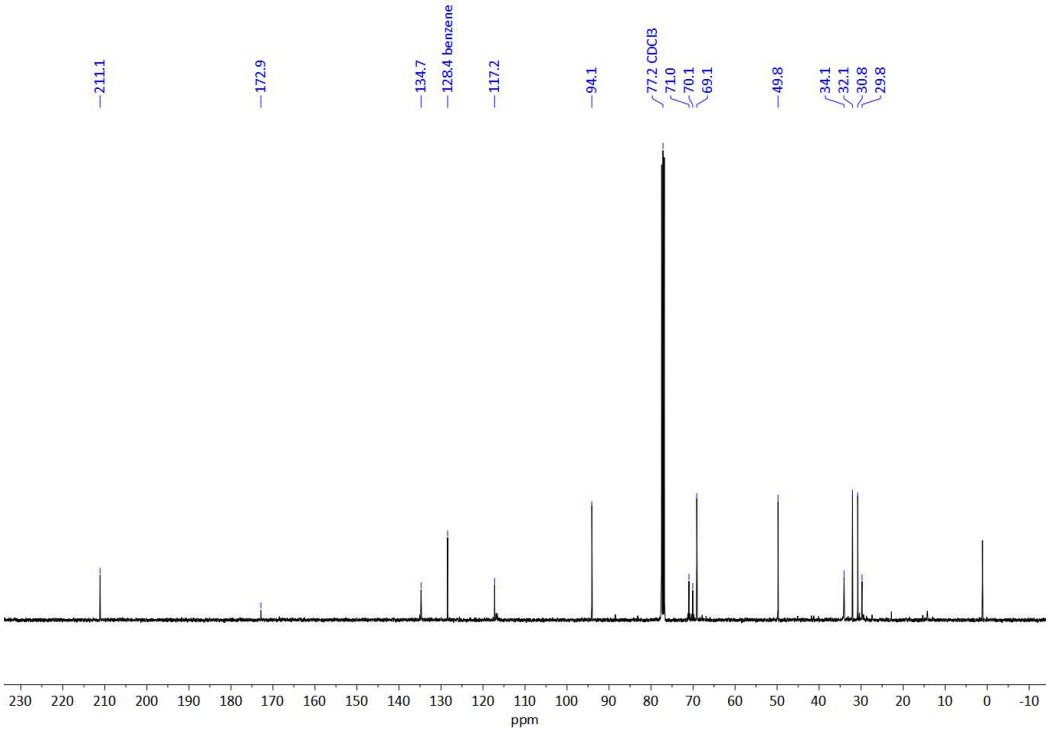


Figure S4. $^{13}C\{^{1}H\}$ NMR spectrum of the crude product.

S5. Discussion on Ketene Dimerization

As shown in **Figure S5a**, the intermolecular [2+2] cycloaddition of oxygen-tethered substrate **1** possesses an activation free energy of 20.5 kcal/mol, which is 1.0 kcal/mol lower than the intramolecular normal [2+2] cycloaddition (**Figure 2**). However, considering that the reaction solution is dilute (0.03 M), the ketene dimerization should be disfavored over the intramolecular [2+2] cycloaddition. For carbon-tethered substrate **7**, the ketene dimerization requires an activation free energy of 27.5 kcal/mol (**Figure S5b**), which is favored over the intramolecular normal [2+2] cycloaddition (**Scheme 2**) by 2.6 kcal/mol. As a result, the yield of the normal [2+2] cycloadduct was only 3%.[11]

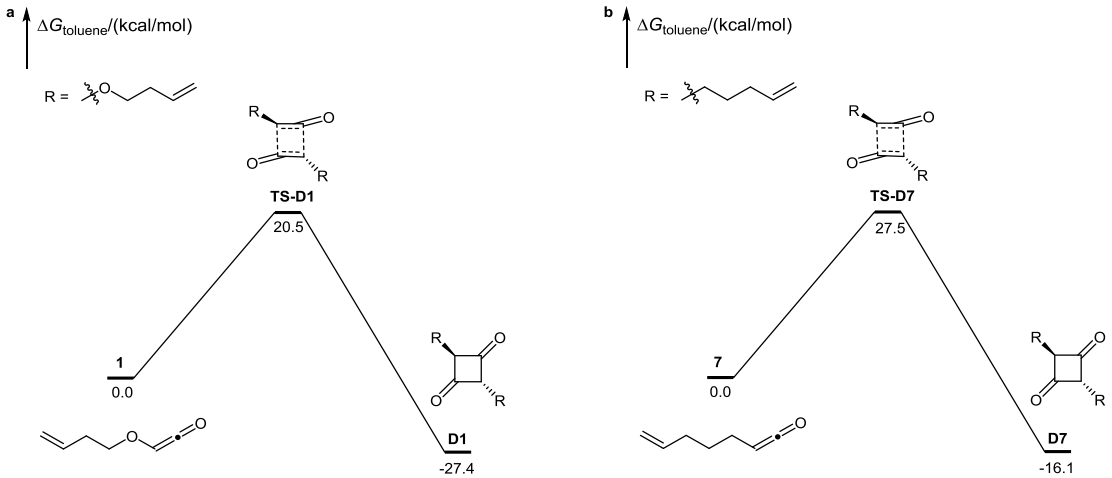


Figure S5. DFT-computed free energy surfaces of the dimerization of substrates **1** and **7**.

S6. Discussion on Interconversion between Normal and Cross-[2+2] Cycloadducts

Besides **TS1** and **TS2**, we have also located an unexpected [1,2]-acyl shift transition state **TS-int**, which connects normal [2+2] cycloadduct **P1** with cross-[2+2] cycloadduct **BP1** (**Figure S6**). However, due to the high activation Gibbs energy, such an interconversion may not occur at normal reaction temperatures. Therefore, the presence of **TS-int** would not influence our regiochemistry prediction model. We suggest that the same conclusions may hold for the other substrates.

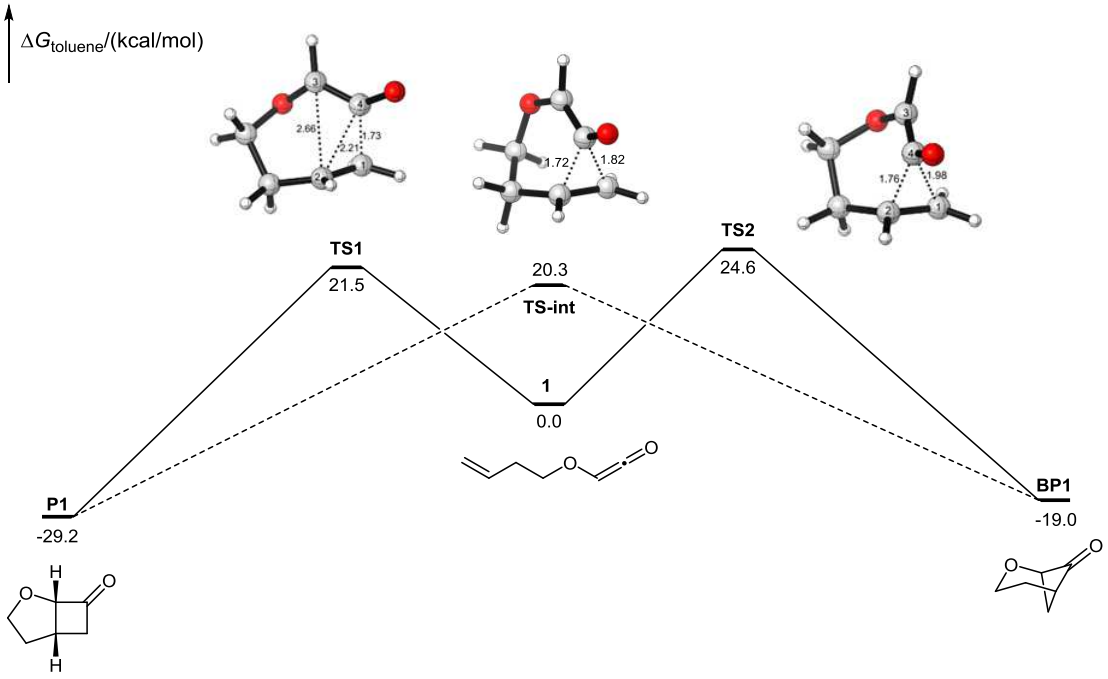


Figure S6. Free energy surface of the interconversion between **P1** and **BP1**. Bond lengths are reported in Å.

S7. Geometries of TS21 and TS22

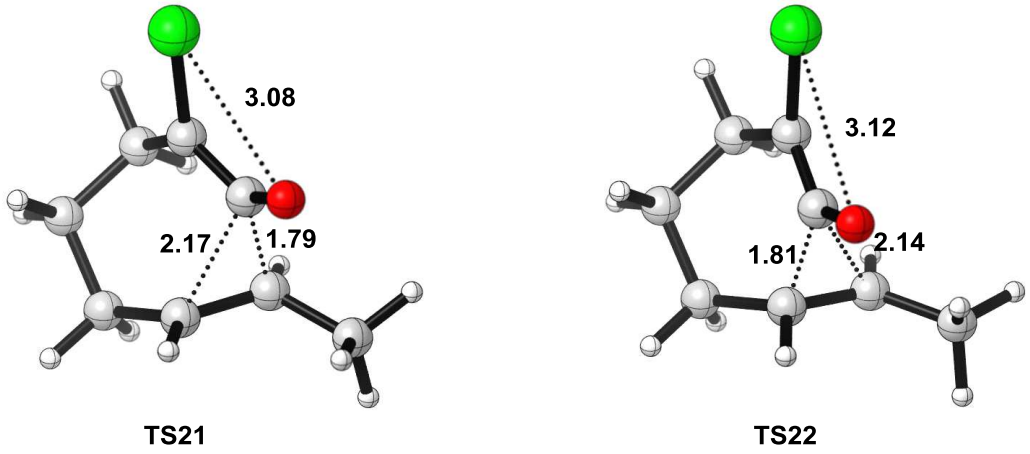


Figure S7. Geometries of **TS21** and **TS22**. Color scheme: H, white; C, gray; O, red; Cl, green. Bond lengths are reported in Å.

S8. Computed Energies of the Stationary Points

Table S2. Single-point energies (SPEs), thermal corrections to enthalpies (TCHs), and thermal corrections to Gibbs energies (TCGs).[a]

	SPE(DZ)[b]	SPE(TZ)[c]	TCH[b]	TCG[b]
1	−383.528277	−383.840823	0.136981	0.091468
TS1	−383.496446	−383.812260	0.135937	0.097217
TS2	−383.488577	−383.807311	0.135994	0.097118
TS-int	−383.492606	−383.814793	0.136286	0.097806
P1	−383.569787	−383.896321	0.139150	0.100449
BP1	−383.556216	−383.881607	0.139708	0.101927
TS-R1	−383.479585	−383.790870	0.134588	0.094617
TS-R2	−383.469887	−383.779338	0.133530	0.092351
R1	−383.503230	−383.819033	0.136478	0.095823
R1'	−383.506811	−383.823652	0.136019	0.095693
TS-D1	−767.039360	−767.667196	0.275188	0.204157
D1	−767.109325	−767.747702	0.277894	0.208306
2	−422.817587	−423.162914	0.166281	0.116944
TS3	−422.791692	−423.138966	0.165089	0.122511
TS4	−422.784440	−423.136652	0.165378	0.123927
P2	−422.857362	−423.216773	0.167959	0.126068
BP2	−422.847470	−423.204780	0.168711	0.127581
3	−462.107152	−462.484197	0.195694	0.142778
TS5	−462.067218	−462.448659	0.194975	0.150146
TS6	−462.079652	−462.459054	0.194376	0.149762
P3	−462.143438	−462.536072	0.197925	0.152980
BP3	−462.131716	−462.522471	0.197948	0.154366
4	−422.819276	−423.163665	0.166390	0.117112
TS7	−422.787307	−423.135098	0.165698	0.122353
TS8	−422.790782	−423.135688	0.165277	0.123093
P4	−422.857114	−423.215490	0.168578	0.125894
BP4	−422.846371	−423.203632	0.168914	0.127991
5	−460.878051	−461.246975	0.172520	0.121029
TS9	−460.839123	−461.213060	0.171588	0.126534
TS10	−460.847119	−461.215132	0.171438	0.126370
TS11	−460.848269	−461.216043	0.171802	0.127652
TS12	−460.855665	−461.222226	0.172793	0.130914
P5	−460.907229	−461.291649	0.174385	0.129052
BP5	−460.897030	−461.280182	0.174746	0.131309
CP	−460.917164	−461.292904	0.176340	0.134750
6	−539.476067	−539.916106	0.234016	0.180267
TS13	−539.446449	−539.888651	0.232973	0.186947
TS14	−539.443398	−539.886360	0.232978	0.186722
P6	−539.503575	−539.957174	0.236001	0.188922
BP6	−539.504796	−539.957669	0.236346	0.191129
7	−347.681797	−347.962084	0.161234	0.115417
TS15	−347.635954	−347.919742	0.160241	0.121046
TS16	−347.626965	−347.912264	0.160302	0.121494

P7	−347.711084	−348.002808	0.163029	0.123881
BP7	−347.703438	−347.994630	0.126182	0.126182
TS-R15	−347.614463	−347.893697	0.158270	0.118219
TS-R16	−347.611264	−347.888588	0.157593	0.116462
R7	−347.631104	−347.915002	0.159725	0.119042
R7'	−347.631555	−347.915133	0.159113	0.117968
TS-D7	−695.331821	−695.899783	0.323739	0.253318
D7	−695.402136	−695.973423	0.326723	0.257493
8	−386.971151	−387.284284	0.190547	0.141152
TS17	−386.933013	−387.248829	0.189624	0.148195
TS18	−386.916462	−387.233273	0.189360	0.147468
P8	−386.995533	−387.319971	0.191918	0.149648
BP8	−386.994169	−387.317418	0.193152	0.151827
9	−807.136760	−807.562556	0.153737	0.104254
TS19	−807.103853	−807.533729	0.152507	0.109774
TS20	−807.097468	−807.528758	0.152451	0.110161
P9	−807.173552	−807.612105	0.154943	0.112366
BP9	−807.171543	−807.609984	0.155791	0.114503
10	−846.427627	−846.885125	0.183095	0.129644
TS21	−846.393619	−846.855012	0.182015	0.136221
TS22	−846.395272	−846.856742	0.181735	0.135725
P10	−846.462169	−846.932605	0.184519	0.138641
BP10	−846.459885	−846.930264	0.184999	0.140505
11	−346.458252	−346.730338	0.137517	0.093058
TS23	−346.425656	−346.701554	0.136311	0.098726
TS24	−346.414738	−346.691127	0.136221	0.098725
P11	−346.481773	−346.766634	0.138917	0.100583
BP11	−346.474366	−346.758511	0.139840	0.102675
12	−385.749054	−386.052859	0.166946	0.118716
TS25	−385.714723	−386.021512	0.165644	0.124703
TS26	−385.712984	−386.020382	0.165764	0.125353
P12	−385.770132	−386.086684	0.168523	0.126821
BP12	−385.762238	−386.078777	0.168990	0.128559
13	−535.854389	−536.267717	0.163279	0.114227
TS27	−535.837559	−536.250513	0.161838	0.117265
TS28	−535.826183	−536.247609	0.161969	0.118649
P13	−535.895498	−536.324711	0.164779	0.120773
BP13	−535.887232	−536.315044	0.165446	0.122626
14	−575.145483	−575.590694	0.192569	0.139385
TS29	−575.129043	−575.573900	0.191306	0.143149
TS30	−575.122692	−575.572369	0.191198	0.143937
P14	−575.182815	−575.643867	0.194372	0.146192
BP14	−575.174985	−575.635014	0.194739	0.148600
15	−441.053069	−441.406247	0.184321	0.132771
TS31	−441.028417	−441.384221	0.182639	0.137768
TS32	−441.022823	−441.378465	0.182824	0.138980
P15	−441.093848	−441.459011	0.185724	0.140620

BP15	−441.083690	−441.448101	0.186390	0.142770
16	−480.343800	−480.728789	0.213785	0.158734
TS33	−480.318291	−480.704982	0.212060	0.164588
TS34	−480.321756	−480.708582	0.212453	0.165957
P16	−480.382085	−480.779356	0.215322	0.166844
BP16	−480.370758	−480.768512	0.215754	0.169136
17	−152.488394		0.035937	0.007837
TS-D17	−304.940560		0.074242	0.037911
D17	−305.009847		0.076913	0.041362
18	−191.773906		0.066350	0.033882
TS-D18	−383.516228		0.133817	0.089668
D18	−383.586522		0.136771	0.093338

[a] Reported in atomic units. $G_{toluene}$ = SPE(TZ) + TCG + 1.89 kcal/mol.

[b] Computed at the (U)B3LYP/def2-SVP level.

[c] Computed at the SMD(toluene)/(U)ωB97XD/def2-TZVPP//(U)B3LYP/def2-SVP level.

Table S3. Single-point energies (SPEs) in benchmark calculations.[a]

	CCSD(T)[b]	B3LYP[c]	B3LYP-D3(BJ)[d]	M06-2X[e]	PBE0-D3(BJ)[f]	ωB97XD[g]
12	−385.342455	−386.173765	−386.200907	−385.990538	−385.710378	−386.028981
TS25	−385.314094	−386.134048	−386.167998	−385.953948	−385.685497	−385.993340
TS26	−385.312292	−386.132272	−386.166421	−385.954629	−385.685417	−385.993136
P12	−385.374441	−386.186560	−386.219056	−386.017060	−385.745482	−386.060569
BP12	−385.368660	−386.177450	−386.211234	−386.011164	−385.738353	−386.052441
17	−152.358114	−152.663527	−152.667166	−152.595947	−152.483743	−152.604562
TS-D17	−304.680543	−305.287615	−305.301040	−305.154113	−304.940731	−305.172352
D17	−304.753671	−305.349326	−305.362208	−305.224306	−305.010122	−305.245987
18	−191.595888	−191.990908	−191.998529	−191.901196	−191.762729	−191.918270
TS-D18	−383.163875	−383.946404	−383.970091	−383.771895	−383.504761	−383.806811
D18	−383.238931	−384.009855	−384.033284	−383.842862	−383.575910	−383.882360

[a] Reported in atomic units.

[b] Computed at the CCSD(T)/cc-pVTZ//B3LYP/def2-SVP level.

[c] Computed at the B3LYP/cc-pVTZ//B3LYP/def2-SVP level.

[d] Computed at the B3LYP-D3(BJ)/cc-pVTZ//B3LYP/def2-SVP level.

[e] Computed at the M06-2X/cc-pVTZ//B3LYP/def2-SVP level.

[f] Computed at the PBE0-D3(BJ)/cc-pVTZ//B3LYP/def2-SVP level.

[g] Computed at the ωB97XD/cc-pVTZ//B3LYP/def2-SVP level.

S9. Cartesian Coordinates of the Stationary Points

1

C	1.612785	−0.267912	0.576887
H	1.489805	0.593599	1.253077
H	1.627972	−1.173591	1.209934
C	2.898178	−0.157602	−0.194621
C	−1.938573	−0.700877	−0.199631
C	3.741962	0.877054	−0.148411
C	−2.887109	0.226051	−0.108565
O	−3.746303	1.010203	−0.008482
H	3.546974	1.748348	0.486160
H	3.141012	−1.007531	−0.846939
H	−2.129568	−1.589902	−0.813244
H	4.663445	0.890588	−0.737151
C	0.390756	−0.365884	−0.331259
O	−0.756052	−0.569155	0.490565
H	0.272186	0.554911	−0.932633
H	0.499021	−1.209782	−1.042261

TS1

C	−1.617232	0.958718	−0.257783
H	−2.158194	1.410156	−1.104406
H	−2.040065	1.370331	0.676975
C	−0.162355	1.315311	−0.304717
C	0.382766	−1.273810	−0.050780
C	0.708201	1.118947	0.790610
C	1.354218	−0.271129	−0.007573
O	2.478488	−0.165307	−0.451008
H	0.251487	0.836808	1.745028
H	1.601536	1.743416	0.869177
H	0.247574	1.766358	−1.213782
H	0.694453	−2.289542	−0.328569
C	−1.845233	−0.564931	−0.243540
O	−0.839904	−1.178302	0.558941
H	−1.806700	−0.975176	−1.269061
H	−2.820944	−0.812111	0.203869

TS2

C	−1.279120	1.111756	−0.426195
H	−1.509089	1.572984	−1.399190
H	−1.813880	1.693988	0.344204
C	0.221259	1.196440	−0.143965
C	0.257125	−1.318868	0.252793
C	0.690324	0.994332	1.172994
C	1.104062	−0.323162	−0.242868
O	2.227323	−0.303495	−0.714424
H	0.021100	0.635355	1.957415
H	1.708036	1.276062	1.449822
H	0.821175	1.832869	−0.799471
H	0.566116	−2.371076	0.193781
C	−1.771231	−0.334097	−0.419892
O	−1.060061	−1.121556	0.546756
H	−1.631100	−0.796715	−1.414120
H	−2.834964	−0.401468	−0.148296

TS-int

C	1.178514	−1.012958	−0.678915
H	1.247096	−0.755102	−1.748131
H	1.731305	−1.959139	−0.539830
C	−0.269495	−1.174251	−0.286843
C	−0.178357	1.343140	0.032790
C	−0.690904	−1.028564	1.063852
C	−1.126359	0.306385	−0.086629
O	−2.319220	0.360967	−0.407273
H	0.007187	−0.809452	1.872511
H	−1.691256	−1.348367	1.353824
H	−0.918229	−1.716475	−0.978733
H	−0.527741	2.363026	−0.159312
C	1.856688	0.057437	0.170896
O	1.158344	1.298491	0.142389
H	2.871387	0.278327	−0.190268
H	1.946737	−0.275616	1.218107

P1

C	1.640578	0.758987	−0.287704
H	2.535180	0.882295	0.342252
H	1.750018	1.418790	−1.162278
C	0.378535	1.053814	0.541644
C	−0.132694	−0.390415	0.891732
C	−0.932702	1.359317	−0.238554
C	−1.366303	−0.100046	−0.022594
O	−2.259777	−0.773827	−0.446610
H	−0.837277	1.660252	−1.295450
H	0.573263	1.722604	1.390168
H	−0.389923	−0.627929	1.936571
H	−1.604896	2.075793	0.262087
C	1.476293	−0.722166	−0.679794

O	0.794516	−1.327538	0.413436
H	0.885209	−0.824271	−1.612259
H	2.428276	−1.253557	−0.824071

BP1

C	−0.962242	1.264421	−0.321761
H	−0.662786	1.687146	−1.294767
H	−1.626016	2.002514	0.159552
C	0.303677	1.030173	0.541611
C	0.286461	−1.106745	0.301127
C	0.053327	−0.163556	1.519704
C	1.186665	0.034992	−0.231823
O	2.200813	0.109704	−0.863961
H	−0.918853	−0.222170	2.029160
H	0.860418	−0.268521	2.259504
H	0.756510	1.965224	0.903141
H	0.690529	−2.119758	0.439111
C	−1.719315	−0.067758	−0.497527
O	−0.856971	−1.200163	−0.543201
H	−2.296673	−0.079689	−1.434225
H	−2.445295	−0.190240	0.327837

TS-R1

C	−1.637950	0.757247	0.588448
H	−2.634108	1.229699	0.560565
H	−1.190312	0.966008	1.573579
C	−0.738792	1.257615	−0.502491
C	0.571123	−1.266968	−0.151318
C	0.652619	1.376827	−0.289816
C	1.431275	−0.176765	0.063457
O	2.570340	−0.075554	0.451239
H	0.911403	1.805486	0.688363
H	1.253945	1.806862	−1.099454
H	−1.157697	1.351507	−1.509341
H	1.051317	−2.209030	−0.439830
C	−1.742982	−0.761949	0.337708
O	−0.708784	−1.134590	−0.594137
H	−2.684605	−1.024526	−0.167648
H	−1.654146	−1.360901	1.261026

TS-R2

C	−0.751099	1.459552	0.196347
H	−0.700213	2.355202	−0.445749
H	−1.114673	1.791650	1.183255
C	0.644596	0.854252	0.367622
C	−0.555232	−1.494252	−0.006967
C	0.729933	−0.970259	0.013907
O	1.846370	−1.417119	−0.084388
H	−0.695836	−2.479464	−0.471746
C	−1.757826	0.484362	−0.398407
O	−1.690067	−0.786374	0.244075
H	−1.573727	0.348575	−1.481536
H	−2.788147	0.845839	−0.262954
C	1.754322	1.478651	−0.211620
H	2.762929	1.108450	−0.016223
H	0.831956	0.505867	1.401812
H	1.639126	2.277997	−0.949640

R1

C	−1.809221	0.762883	0.084403
H	−2.703995	1.185302	−0.403976
H	−1.977019	0.817467	1.177450
C	−0.579603	1.524177	−0.289034
C	0.612919	−1.277192	0.028482
C	0.690922	1.272914	0.440290
C	1.372342	−0.047907	0.010218
O	2.561764	−0.074613	−0.305372
H	0.503561	1.203119	1.529709
H	1.438382	2.060886	0.272696
H	−0.552731	2.079275	−1.231680
H	1.185499	−2.209652	−0.038687
C	−1.735842	−0.715994	−0.305017
O	−0.678797	−1.448519	0.340509
H	−1.610927	−0.823883	−1.396852
H	−2.655610	−1.240741	−0.005807

R1'

C	−0.986576	0.912697	0.810688
H	−1.407106	1.930902	0.856499
H	−1.093318	0.472612	1.816285
C	0.493333	0.946868	0.398241
C	0.010881	−1.463146	−0.222171
C	0.997715	−0.488723	0.139460
O	2.192792	−0.784241	0.224999
H	0.300606	−2.508092	−0.359869
C	−1.787829	0.090760	−0.188325
O	−1.305487	−1.256314	−0.285256
H	−1.727889	0.543077	−1.195220

H	−2.846751	0.002490	0.091029
C	0.745048	1.740970	−0.838388
H	1.721842	1.682255	−1.323552
H	1.115556	1.324382	1.234497
H	0.003187	2.440258	−1.234655

TS-D1

C	4.396392	−1.149701	−0.527144
H	4.279341	−2.003758	0.159674
H	4.286244	−1.545885	−1.553307
C	5.752501	−0.522958	−0.364005
C	0.881011	−0.102487	−0.417347
C	6.673020	−0.889604	0.532188
C	0.626073	0.644779	0.701315
O	1.128552	1.189666	1.654616
H	6.492204	−1.709798	1.235420
H	5.982739	0.307299	−1.045725
H	0.081892	−0.389371	−1.099250
H	7.642889	−0.388038	0.595502
C	3.257963	−0.160561	−0.289064
O	2.033905	−0.828264	−0.565603
H	3.275299	0.210343	0.751235
H	3.357071	0.722758	−0.950944
C	−4.058480	−1.210073	−0.071475
H	−3.968135	−1.241584	−1.169201
H	−3.490099	−2.070233	0.324898
C	−5.500824	−1.305436	0.344604
C	−1.245451	1.075570	0.532226
C	−6.543303	−1.318254	−0.490409
C	−1.116933	2.111669	−0.389764
O	−0.895233	2.903232	−1.196565
H	−6.409448	−1.263924	−1.576200
H	−5.686923	−1.366126	1.425288
H	−1.380608	1.413092	1.569827
H	−7.570004	−1.393431	−0.121757
C	−3.391379	0.058993	0.446979
O	−2.007723	0.014800	0.088160
H	−3.869096	0.958301	0.012962
H	−3.482921	0.133267	1.548082

D1

C	4.587865	−0.417829	−0.487781
H	4.675675	−1.508307	−0.355176
H	4.425544	−0.236358	−1.565783
C	5.841556	0.276837	−0.033590
C	1.007582	−0.220643	0.274539
C	6.894598	−0.320837	0.530575
C	0.273939	1.110416	−0.047083
O	0.597893	2.262194	−0.030546
H	6.916506	−1.402605	0.701463
H	5.868795	1.364512	−0.184365
H	1.024886	−0.263804	1.393480
H	7.778107	0.246389	0.836488
C	3.348666	0.075676	0.251366
O	2.207704	−0.577373	−0.299883
H	3.425372	−0.154733	1.333026
H	3.242696	1.171805	0.153530
C	−4.600316	0.554823	0.392595
H	−4.495341	0.253323	1.447341
H	−4.601246	1.659712	0.371330
C	−5.884685	0.026858	−0.183865
C	−1.031500	0.365024	−0.424219
C	−6.742729	−0.777466	0.449458
C	−0.294857	−0.967374	−0.109333
O	−0.614925	−2.119749	−0.136211
H	−6.561301	−1.115319	1.475479
H	−6.112921	0.337644	−1.212456
H	−1.060636	0.411043	−1.542487
H	−7.662231	−1.124215	−0.030260
C	−3.375125	0.082826	−0.383409
O	−2.224973	0.722468	0.164131
H	−3.271248	−1.015010	−0.319541
H	−3.468218	0.345740	−1.457504

2

C	1.184059	0.139895	0.749943
H	0.921623	1.104430	1.211603
H	1.258244	−0.598536	1.568312
C	2.510323	0.248011	0.026033
C	−2.279138	−0.759081	−0.016363
C	3.080716	1.438238	−0.208327
C	−3.292495	0.081529	−0.199886
O	−4.207495	0.794134	−0.334586
H	2.611873	2.371359	0.117952
H	−2.375537	−1.787322	−0.386273
C	0.025465	−0.281043	−0.151386
O	−1.147121	−0.361625	0.656395
H	−0.121302	0.453264	−0.965474

H	0.218354	−1.263472	−0.624579
H	4.039014	1.521083	−0.729699
C	3.157087	−1.045922	−0.404540
H	2.518521	−1.610004	−1.106351
H	4.125334	−0.873200	−0.896552
H	3.324698	−1.707433	0.463752

TS3

C	−0.788328	1.398251	−0.427797
H	−0.666283	1.341236	−1.521800
H	−0.993953	2.464827	−0.208739
C	0.509291	0.996573	0.219906
C	−0.662841	−1.428279	−0.426112
C	0.555054	0.140607	1.314052
C	0.637031	−1.232225	−0.019371
O	1.760986	−1.599684	−0.268741
H	−0.342275	−0.102162	1.885859
H	−0.869160	−2.338321	−0.999259
C	−1.989182	0.590514	0.039895
O	−1.789325	−0.825545	0.056985
H	−2.255527	0.882237	1.070217
H	−2.866019	0.813162	−0.594184
H	1.506120	−0.016713	1.827913
C	1.790278	1.472494	−0.391393
H	2.363375	2.093394	0.316896
H	2.415428	0.587883	−0.624588
H	1.627192	2.048684	−1.313340

TS4

C	0.622877	−1.407131	−0.386276
H	0.586544	−1.436848	−1.487890
H	0.643489	−2.456423	−0.041065
C	−0.624789	−0.706000	0.128887
C	0.805891	1.380572	−0.209852
C	−0.572026	−0.103927	1.431593
C	−0.539457	0.966633	−0.067038
O	−1.563771	1.620780	−0.310058
H	0.309327	−0.146260	2.071620
H	0.980522	2.400360	−0.570284
C	1.906709	−0.735332	0.079435
O	1.934100	0.664036	−0.205916
H	2.055424	−0.869274	1.163071
H	2.788356	−1.156566	−0.424862
H	−1.493538	0.250814	1.894019
C	−1.937813	−1.206344	−0.432967
H	−2.188991	−2.188349	0.001225
H	−2.739493	−0.489558	−0.214167
H	−1.872632	−1.317257	−1.526558

P2

C	1.366809	0.687620	0.758889
H	2.345525	0.911775	0.305577
H	1.521321	0.543339	1.839473
C	0.752308	−0.550068	0.065380
C	−0.300324	0.126653	−0.896269
C	−0.403166	−1.238868	0.863395
C	−1.420653	−0.481105	0.001121
O	−2.610618	−0.351556	0.041441
H	−0.469962	−1.029465	1.944227
H	−0.331943	−0.198833	−1.949133
C	0.378819	1.824991	0.445929
O	−0.147445	1.519604	−0.841067
H	−0.434302	1.869184	1.198293
H	0.845802	2.819440	0.396087
H	−0.461193	−2.331487	0.722571
C	1.777634	−1.489520	−0.556060
H	2.426774	−1.938404	0.214402
H	1.289395	−2.315233	−1.099618
H	2.424521	−0.952918	−1.269185

BP2

C	0.271337	−1.304597	−0.723157
H	0.028142	−1.163883	−1.789546
H	0.146139	−2.379624	−0.504124
C	−0.728152	−0.474365	0.132720
C	0.748997	1.030375	0.622194
C	−0.001385	−0.048896	1.457729
C	−0.504045	0.993673	−0.281140
O	−1.142917	1.793552	−0.904863
H	0.606330	−0.801639	1.979974
H	1.071324	1.974417	1.083696
C	1.722957	−0.886768	−0.419071
O	1.850230	0.495541	−0.103740
H	2.114247	−1.493946	0.418539
H	2.381105	−1.071008	−1.281601
H	−0.696974	0.418198	2.171399
C	−2.140285	−1.025391	0.140639
H	−2.173628	−2.035373	0.581393

H	−2.817083	−0.374479	0.715977
H	−2.534654	−1.089583	−0.886367

3

C	0.577237	−0.533322	0.806550
H	0.514597	0.445217	1.305210
H	0.448132	−1.295614	1.596011
C	1.897327	−0.733504	0.114235
C	−2.962157	−0.688999	−0.124884
C	2.886053	0.160291	−0.074970
C	−3.786563	0.341319	−0.285437
O	−4.541807	1.224442	−0.401878
H	2.055123	−1.742495	−0.289641
H	−3.236026	−1.654485	−0.568121
C	−0.604590	−0.663889	−0.150314
O	−1.807077	−0.560079	0.610006
H	−0.573394	0.126127	−0.924106
H	−0.575436	−1.638813	−0.677202
C	4.150293	−0.228331	−0.802103
H	5.036608	−0.089342	−0.157159
H	4.131250	−1.276507	−1.135390
H	4.309600	0.411709	−1.688466
C	2.855095	1.590718	0.402109
H	2.973713	2.285039	−0.448635
H	1.929223	1.857594	0.928348
H	3.701506	1.790956	1.083014

TS5

C	−1.385268	−0.741815	1.237787
H	−1.756605	−0.106957	2.057722
H	−1.576785	−1.788533	1.548173
C	0.085129	−0.511306	1.084428
C	−0.720281	1.458992	−0.363889
C	0.909394	−0.657056	−0.063354
C	0.600445	1.120436	−0.048402
O	1.562528	1.811099	0.244574
H	0.609877	−0.237878	2.004231
H	−0.898937	2.517431	−0.584596
C	−2.176210	−0.497343	−0.039845
O	−1.781387	0.694043	−0.719465
H	−2.048875	−1.343349	−0.731632
H	−3.255344	−0.409821	0.170939
C	2.402854	−0.796167	0.185294
H	2.671722	−1.866036	0.193149
H	2.970881	−0.296665	−0.612315
H	2.706210	−0.343580	1.137194
C	0.477915	−1.319835	−1.366809
H	1.300359	−1.253339	−2.093937
H	0.264157	−2.391819	−1.209374
H	−0.399661	−0.856027	−1.831690

TS6

C	−1.099841	−0.870015	1.226676
H	−1.369762	−0.738613	2.286393
H	−0.990415	−1.954637	1.063907
C	0.247142	−0.177802	0.963060
C	−0.900663	1.135893	−0.915424
C	1.169141	−0.729011	0.025280
C	0.141505	1.269653	−0.022122
O	0.955462	2.152116	0.225969
H	0.715880	0.257849	1.852066
H	−1.249071	2.008602	−1.481053
C	−2.227013	−0.325515	0.347593
O	−1.733615	0.042953	−0.941339
H	−2.693023	0.561868	0.814378
H	−3.008634	−1.082754	0.181874
C	2.577889	−0.262124	0.091845
H	3.043803	−0.542175	1.052526
H	3.196638	−0.636145	−0.734915
H	2.555190	0.852992	0.087411
C	0.764764	−1.741962	−0.994837
H	1.461349	−1.759552	−1.845039
H	0.787134	−2.748636	−0.531353
H	−0.261408	−1.574052	−1.355671

P3

C	1.322698	−1.456571	−0.009423
H	1.958374	−2.013910	−0.714687
H	0.969469	−2.169035	0.750601
C	0.190964	−0.764291	−0.790209
C	0.701527	0.719255	−0.856692
C	−1.112544	−0.312715	−0.030615
C	−0.462949	1.081282	0.112397
O	−0.695626	2.023243	0.816266
H	−0.010143	−1.256509	−1.751515
H	0.674755	1.244331	−1.824455
C	2.122653	−0.289089	0.601317
O	1.997338	0.783569	−0.325466

H	1.713252	0.002729	1.589165
H	3.193705	−0.503798	0.729944
C	−2.323906	−0.252824	−0.976322
H	−2.673403	−1.271508	−1.213590
H	−3.155066	0.297625	−0.508200
H	−2.080899	0.248109	−1.927299
C	−1.480115	−0.986160	1.289994
H	−2.305768	−0.439474	1.772090
H	−1.807466	−2.026397	1.127288
H	−0.640474	−0.999989	2.001575

BP3

C	−1.163341	−0.739206	1.219838
H	−1.886645	−0.386032	1.972652
H	−0.780675	−1.710148	1.570275
C	0.000732	0.267553	1.089142
C	0.019664	0.229320	−1.065389
C	1.053522	−0.243543	0.023535
C	−0.402766	1.278197	0.002322
O	−0.723176	2.432398	−0.018621
H	0.364364	0.642215	2.058269
H	0.377894	0.555739	−2.053380
C	−1.880057	−0.859809	−0.140869
O	−0.990791	−0.746824	−1.250181
H	−2.643946	−0.061050	−0.213562
H	−2.397660	−1.824301	−0.250287
C	2.310142	0.633412	0.027887
H	2.919548	0.430579	0.923803
H	2.932751	0.425916	−0.857572
H	2.074284	1.709838	0.026360
C	1.421938	−1.724176	0.007692
H	2.151614	−1.922585	−0.794217
H	1.886600	−2.024573	0.961435
H	0.554603	−2.370683	−0.178315

4

C	0.926324	−0.631352	0.632411
H	0.814110	0.059966	1.483517
H	0.836523	−1.655234	1.038732
C	2.264842	−0.447192	−0.026846
C	−2.588679	−0.566455	−0.394409
C	3.160499	0.495173	0.293127
C	−3.469853	0.392870	−0.129301
O	−4.273481	1.203899	0.115663
H	2.914192	1.193576	1.104980
H	2.507149	−1.148964	−0.837566
H	−2.802736	−1.265095	−1.212708
C	−0.236771	−0.418979	−0.331884
O	−1.448944	−0.704812	0.362576
H	−0.248862	0.620597	−0.709825
H	−0.141096	−1.086327	−1.212166
C	4.497537	0.685018	−0.359421
H	5.317833	0.586654	0.373560
H	4.668741	−0.048491	−1.162641
H	4.590154	1.696124	−0.793846

TS7

C	−1.326027	−1.149689	0.790378
H	−1.718948	−0.735601	1.732755
H	−1.567781	−2.230251	0.797354
C	0.155526	−0.950400	0.720881
C	−0.641891	1.455396	−0.081465
C	0.877706	−0.789285	−0.463532
C	0.653344	1.010089	0.115370
O	1.680909	1.489119	0.547678
H	0.340544	−0.884003	−1.411113
H	0.713506	−0.966798	1.662299
H	−0.783661	2.537869	−0.004676
C	−2.032907	−0.528820	−0.408942
O	−1.765251	0.855192	−0.553481
H	−1.740201	−1.058322	−1.332615
H	−3.126288	−0.625949	−0.317040
C	2.366156	−0.990027	−0.558360
H	2.580049	−2.030207	−0.857279
H	2.806374	−0.319046	−1.310007
H	2.859690	−0.785763	0.400771

TS8

C	−1.063995	−1.234153	0.807624
H	−1.528322	−0.844661	1.727053
H	−1.089251	−2.335345	0.874571
C	0.363913	−0.743413	0.702668
C	−0.923783	1.391232	−0.273679
C	1.131685	−0.994642	−0.431721
C	0.332613	1.100844	0.196161
O	1.353651	1.709929	0.449264
H	0.631023	−1.363104	−1.332329
H	0.893817	−0.581137	1.647408

H	−1.189821	2.452330	−0.275361
C	−1.893055	−0.789496	−0.396212
O	−2.024682	0.609023	−0.451572
H	−1.442982	−1.163956	−1.336177
H	−2.916883	−1.187397	−0.338793
C	2.578146	−0.694561	−0.510058
H	3.143611	−1.167673	0.310137
H	3.022004	−0.980824	−1.473013
H	2.691908	0.405289	−0.353727

P4

C	−1.474145	−1.339157	−0.102313
H	−2.166999	−1.747601	0.650356
H	−1.317770	−2.108478	−0.874729
C	−0.174129	−0.884222	0.572926
C	−0.422316	0.645755	0.817197
C	1.043936	−0.572718	−0.358028
C	0.834095	0.924321	−0.059771
O	1.453437	1.911947	−0.336459
H	0.814579	−0.779187	−1.420844
H	0.089856	−1.474377	1.461838
H	−0.360483	1.054746	1.838952
C	−2.033735	−0.026691	−0.675877
O	−1.673737	0.980478	0.262395
H	−1.597174	0.188803	−1.672369
H	−3.128868	−0.016269	−0.780882
C	2.413294	−1.145288	−0.005050
H	2.449751	−2.232056	−0.182307
H	3.196704	−0.670642	−0.616135
H	2.660803	−0.966343	1.054142

BP4

C	−1.297458	−0.477310	1.209900
H	−1.827215	0.090627	1.992007
H	−1.318314	−1.540108	1.502090
C	0.172831	−0.012835	1.094873
C	0.167103	−0.035163	−1.064014
C	0.888109	−0.903382	0.018594
C	0.239539	1.084642	0.017281
O	0.491993	2.255524	0.006969
H	0.540578	−1.948252	0.001219
H	0.659721	0.164195	2.065730
H	0.634912	0.119848	−2.047529
C	−2.003964	−0.248166	−0.139935
O	−1.157597	−0.498953	−1.256228
H	−2.355285	0.802054	−0.182824
H	−2.884163	−0.897131	−0.258184
C	2.408942	−0.816778	0.011610
H	2.828365	−1.326225	−0.870820
H	2.760621	0.228253	−0.007210
H	2.835000	−1.291882	0.909737

5

C	0.408376	−0.771753	0.661821
H	0.353429	−0.028558	1.473524
H	0.237102	−1.762052	1.122423
C	1.753511	−0.735302	−0.001342
C	−3.094139	−0.493112	−0.368064
C	2.735176	0.142313	0.279143
C	−3.897265	0.544608	−0.154979
O	−4.634052	1.427772	0.045351
H	2.565776	0.901156	1.054299
H	1.935293	−1.490096	−0.778768
H	−3.366770	−1.218740	−1.144198
C	−0.737789	−0.522065	−0.315621
O	−1.963838	−0.676718	0.394259
H	−0.671178	0.493491	−0.748799
H	−0.695863	−1.241639	−1.158022
C	4.036633	0.159780	−0.376105
C	5.020301	1.031279	−0.097195
H	4.201262	−0.601976	−1.148457
H	5.978628	0.999491	−0.621280
H	4.896620	1.806006	0.666450

TS9

C	−1.471152	−1.192887	0.919368
H	−2.146270	−0.765105	1.677487
H	−1.425395	−2.282457	1.111929
C	−0.110964	−0.585033	1.034818
C	−1.207783	1.280017	−0.398046
C	0.796022	−0.506328	−0.047058
C	0.112788	1.201700	0.043904
O	0.884291	2.029018	0.491118
H	0.501295	−0.968505	−0.992594
H	0.228685	−0.256432	2.020661
H	−1.594501	2.293919	−0.544203
C	−2.043177	−1.003722	−0.483849
O	−2.080035	0.360892	−0.868187

H	−1.450943	−1.578529	−1.215827	H	−1.688505	−1.188273	−1.292900
H	−3.079323	−1.370039	−0.547011	H	−3.149263	−1.294183	−0.276508
C	2.255184	−0.378077	0.128800	C	2.269823	−0.779088	−0.671449
C	3.149137	−0.854318	−0.745105	C	3.070529	−0.057656	0.146513
H	2.586903	0.153761	1.024832	H	2.668064	−1.104212	−1.638230
H	4.222952	−0.742741	−0.575401	H	4.088377	0.200165	−0.157553
H	2.842216	−1.371265	−1.660322	H	2.748215	0.292017	1.127362

TS10

C	−1.265608	−1.207251	0.951227	C	1.402100	−1.339134	−0.489997
H	−1.971185	−0.782812	1.682328	H	1.661321	−1.864920	−1.422853
H	−1.098665	−2.260821	1.235304	H	1.459519	−2.086441	0.317815
C	0.034377	−0.434156	0.971266	C	−0.029633	−0.756587	−0.568850
C	−1.425417	1.172668	−0.601383	C	0.844735	1.247083	0.586296
C	1.047255	−0.754462	0.059447	C	−0.838133	−1.046696	0.654709
C	−0.268007	1.263188	0.142650	C	−0.101139	0.776906	−0.343610
O	0.533776	2.112823	0.449227	O	−1.066430	1.467076	−0.751431
H	0.827740	−1.444142	−0.762036	H	−0.313013	−1.454411	1.523435
H	0.332401	0.002979	1.929488	H	−0.539474	−1.014945	−1.509904
H	−1.910720	2.130890	−0.812643	H	0.744889	2.240074	1.039367
C	−1.901049	−1.166336	−0.439570	C	2.439054	−0.247003	−0.260610
O	−2.286113	0.136597	−0.799667	O	2.054455	0.689877	0.755252
H	−1.201159	−1.575373	−1.193845	H	2.591627	0.329212	−1.191687
H	−2.818523	−1.772036	−0.475110	H	3.406641	−0.656895	0.060373
C	2.375915	−0.202354	0.096161	C	−2.171763	−0.659254	0.781766
C	3.358696	−0.570807	−0.752332	C	−2.861023	−0.036214	−0.242094
H	2.572425	0.562546	0.853716	H	−2.622518	−0.699308	1.778950
H	4.356912	−0.130535	−0.694007	H	−3.819572	0.451581	−0.045317
H	3.192488	−1.328992	−1.524475	H	−2.578816	−0.134183	−1.286396

TS11

C	−1.278726	−1.245844	0.844056	C	−1.353597	−1.618099	−0.055066
H	−1.729542	−0.848848	1.766687	H	−1.975934	−2.167319	0.669014
H	−1.286482	−2.346720	0.929145	H	−0.915057	−2.350367	−0.750569
C	0.134860	−0.734184	0.687905	C	−0.302197	−0.783033	0.687382
C	−1.301239	1.397535	−0.296326	C	−0.974972	0.629492	0.775064
C	0.888577	−1.092370	−0.425347	C	0.885306	−0.216394	−0.165711
C	−0.011771	1.204205	0.106117	C	0.227948	1.189833	−0.038571
O	1.015740	1.803215	0.296364	O	0.551984	2.282434	−0.399016
H	0.375461	−1.621754	−1.234550	H	0.851507	−0.548196	−1.219667
H	0.654055	−0.441015	1.604195	H	0.015447	−1.226279	1.641054
H	−1.629217	2.441487	−0.300388	H	−1.111615	1.108477	1.758538
C	−2.149943	−0.839792	−0.347549	C	−2.197018	−0.547583	−0.768324
O	−2.363720	0.546097	−0.395212	O	−2.216149	0.568958	0.114821

P5

H	−1.746936	−0.269655	−1.743074	H	1.681774	0.558117	−1.592695
H	−3.238196	−0.850127	−0.953958	H	3.236632	0.712050	−0.716353
C	2.276241	−0.358178	0.367955	C	−2.134202	0.845991	−0.537880
C	3.342871	−0.732099	−0.345429	C	−2.339090	−0.626355	−0.298883
H	2.406565	−0.112150	1.429997	H	−2.918545	1.359751	−1.103936
H	4.336297	−0.795975	0.106589	H	−2.366196	−1.158103	−1.274212
H	3.263746	−0.983186	−1.408169	H	−3.314208	−0.804194	0.186482

BP5

C	−1.383290	−0.812079	1.210152
H	−2.075571	−0.457029	1.990797
H	−1.038065	−1.816045	1.506736
C	−0.162549	0.129933	1.095511
C	−0.158439	0.103053	−1.065852
C	0.821218	−0.477800	0.023283
C	−0.467572	1.179416	0.014219
O	−0.617855	2.367736	0.000581
H	0.846660	−1.577716	0.003505
H	0.235043	0.462912	2.065081
H	0.233829	0.403310	−2.047741
C	−2.123652	−0.841810	−0.140016
O	−1.239309	−0.788342	−1.254956
H	−2.813166	0.024313	−0.186881
H	−2.726845	−1.753673	−0.258951
C	2.196910	0.106324	0.022770
C	3.328740	−0.604785	−0.002342
H	2.261114	1.202717	0.041979
H	4.307515	−0.117786	−0.006841
H	3.318597	−1.699667	−0.019035

CP

C	1.477121	1.262708	0.451242
H	2.042964	1.173319	1.392393
H	1.498097	2.327225	0.163132
C	0.026453	0.780733	0.680217
C	0.926780	−1.452836	−0.036067
C	−1.054635	1.503683	−0.099354
C	−0.097607	−0.691290	0.379912
O	−1.357082	−1.217988	0.545468
H	−0.944558	2.580202	−0.273333
H	−0.202159	0.919427	1.755862
H	0.829670	−2.527704	−0.207652
C	2.180366	0.424472	−0.612684
O	2.175259	−0.959854	−0.281557

6

C	4.400663	0.345334	−0.253390
O	5.234958	1.135453	−0.044666
C	3.485554	−0.591405	−0.481693
H	3.613992	−1.251785	−1.348222
O	2.417227	−0.753873	0.368850
C	1.150842	−0.425592	−0.200426
H	0.970340	−1.040008	−1.103838
H	1.147399	0.633797	−0.518959
C	0.074358	−0.697873	0.847876
H	0.348319	−0.140888	1.761667
H	0.107365	−1.768468	1.104385
C	−1.312992	−0.301531	0.393059
C	−2.199747	−1.211198	−0.047146
C	−1.664757	1.172355	0.467318
C	−3.601605	−0.888790	−0.499912
H	−1.899668	−2.265778	−0.082860
C	−2.917881	1.535202	−0.338031
H	−1.805322	1.444469	1.532084
H	−0.807567	1.781024	0.129265
C	−4.040140	0.522986	−0.090840
H	−4.303027	−1.640564	−0.096506
H	−3.662840	−1.001050	−1.600668
H	−3.248865	2.555852	−0.084782
H	−2.669647	1.544782	−1.414954
H	−4.954725	0.811531	−0.634413
H	−4.299002	0.527515	0.983438

TS13

C	−0.310025	1.358576	0.231105
O	0.505977	2.059998	0.815956
C	−1.687564	1.218412	0.430081
H	−2.205991	1.925348	1.091533
O	−2.492547	0.488591	−0.408195
C	−2.647166	−0.858495	0.006094
H	−2.907695	−0.895699	1.080790

H	−3.477794	−1.291749	−0.573059
C	−1.337755	−1.625206	−0.250851
H	−1.313562	−2.531779	0.374530
H	−1.334414	−1.948029	−1.308993
C	−0.089167	−0.807227	−0.037514
C	0.239289	0.279579	−0.928244
C	0.918963	−1.293347	0.966085
C	1.706841	0.574568	−1.264204
H	−0.443665	0.354770	−1.782392
C	2.275343	−0.576026	0.917434
H	1.056806	−2.373858	0.755884
H	0.477095	−1.262141	1.979018
C	2.697852	−0.346850	−0.536580
H	1.842730	0.493257	−2.354222
H	1.907405	1.619117	−0.979220
H	3.023125	−1.181478	1.454746
H	2.201547	0.392359	1.433054
H	3.708459	0.089963	−0.579593
H	2.758845	−1.322698	−1.054596

TS14

C	0.504622	−0.962897	0.641000
O	−0.280612	−1.535307	1.387579
C	1.760903	−1.289946	0.149566
H	2.269243	−2.187404	0.524888
O	2.541411	−0.441907	−0.583091
C	2.606928	0.878789	−0.037792
H	2.942656	0.805753	1.013167
H	3.377123	1.415170	−0.611980
C	1.255936	1.583121	−0.121198
H	1.206377	2.353254	0.664797
H	1.161001	2.107682	−1.087646
C	0.047024	0.637015	0.020351
C	−0.269072	−0.193452	−1.088905
C	−1.094358	1.207267	0.863720
C	−1.617358	−0.816147	−1.253650
H	0.482457	−0.325072	−1.870728
C	−2.444867	0.488994	0.729119
H	−1.204822	2.262194	0.549953
H	−0.780079	1.229306	1.919902
C	−2.739895	0.089269	−0.718423
H	−1.771607	−1.094738	−2.307850
H	−1.625413	−1.755217	−0.664844
H	−3.242026	1.143666	1.118654
H	−2.426725	−0.415931	1.352697
H	−3.704408	−0.439912	−0.782346
H	−2.829354	0.986887	−1.357304

P6

C	−0.044998	1.498235	0.140435
O	0.401077	2.562551	0.468514
C	−1.069039	0.539213	0.758117
H	−1.136083	0.485677	1.862952
O	−2.332186	0.685048	0.142969
C	−2.778891	−0.614492	−0.223533
H	−3.237407	−1.122616	0.648990
H	−3.554813	−0.496554	−0.994540
C	−1.526907	−1.379829	−0.698821
H	−1.561590	−2.436406	−0.391382
H	−1.432882	−1.359428	−1.795859
C	−0.357218	−0.623997	−0.023208
C	0.387771	0.465220	−0.907719
C	0.596233	−1.502027	0.798928
C	1.895393	0.394597	−1.199120
H	−0.182609	0.646927	−1.833441
C	1.960369	−0.847767	1.052582
H	0.770515	−2.447162	0.254345
H	0.105306	−1.780384	1.748026
C	2.672048	−0.573663	−0.277426
H	2.071081	0.124571	−2.251921
H	2.281225	1.421417	−1.078377
H	2.577803	−1.514611	1.676618
H	1.846006	0.087976	1.629516
H	3.685490	−0.180847	−0.097459
H	2.808262	−1.542281	−0.790739

BP6

C	−0.547364	−0.038997	−1.123048
O	−0.355661	0.121895	−2.296006
C	−1.098274	−1.206338	−0.248818
H	−1.163994	−2.219070	−0.672863
O	−2.332944	−0.884523	0.361369
C	−2.542577	0.518194	0.470055
H	−2.911455	0.904466	−0.501121
H	−3.343857	0.663211	1.209772
C	−1.262760	1.280378	0.854562
H	−1.367811	2.334696	0.547072
H	−1.097258	1.269724	1.945044

C	−0.031815	0.642359	0.161637
C	0.091846	−0.836047	0.691554
C	1.210576	1.521664	0.136997
C	1.432637	−1.492725	0.339091
H	−0.156982	−0.950398	1.758480
C	2.480831	0.741101	−0.231151
H	1.337165	1.975382	1.137354
H	1.051931	2.356583	−0.567064
C	2.619110	−0.550494	0.587501
H	1.544732	−2.428878	0.910202
H	1.439412	−1.783643	−0.727452
H	3.363962	1.384101	−0.083494
H	2.456917	0.486187	−1.305078
H	3.562000	−1.061812	0.331844
H	2.680818	−0.304087	1.664128

7

C	1.760833	−0.377989	0.508990
H	1.700258	0.323514	1.359437
H	1.836762	−1.392004	0.947014
C	3.000822	−0.095782	−0.292890
C	−2.063930	−0.615365	−0.329747
C	3.865643	0.896680	−0.064416
C	−3.055224	0.232115	−0.130457
O	−3.935899	0.976779	0.052992
H	3.726340	1.598224	0.765454
H	3.184024	−0.771410	−1.139789
H	−2.194757	−1.312540	−1.163897
H	4.747492	1.044977	−0.694021
C	0.469035	−0.301247	−0.321996
H	0.364201	0.709814	−0.750852
H	0.543354	−0.989930	−1.183269
C	−0.789095	−0.643343	0.490385
H	−0.878854	0.052979	1.340988
H	−0.670129	−1.648265	0.935777

TS15

C	1.491522	−0.964508	−0.551965
H	1.712453	−0.711643	−1.602502
H	2.093710	−1.867432	−0.321308
C	0.048129	−1.312064	−0.402756
C	−0.401664	1.274381	−0.250807
C	−0.680478	−1.132965	0.790113
C	−1.358665	0.307041	0.049693
O	−2.546445	0.208230	−0.183501
H	−0.143759	−0.894636	1.711569
H	−0.473478	−1.755830	−1.256608
H	−0.860986	2.187531	−0.652480
H	−1.583322	−1.726116	0.940269
C	1.888158	0.179474	0.385613
H	1.767371	−0.144744	1.431071
H	2.958549	0.412603	0.270523
C	1.051116	1.435913	0.103426
H	1.166995	2.134722	0.956663
H	1.505316	1.976081	−0.749085

TS16

C	1.157612	−1.233975	−0.397573
H	1.300284	−1.811931	−1.323290
H	1.672360	−1.795353	0.402745
C	−0.335056	−1.181687	−0.059837
C	−0.265630	1.340430	0.248217
C	−0.727907	−0.882525	1.269960
C	−1.105186	0.350781	−0.289468
O	−2.223015	0.351038	−0.764561
H	−0.009872	−0.587896	2.037660
H	−1.760902	−1.041719	1.586707
H	−0.991740	−1.847940	−0.626363
H	−0.647048	2.365302	0.151307
C	1.804088	0.151340	−0.544509
H	1.624973	0.533374	−1.563279
H	2.896907	0.069350	−0.419588
C	1.222600	1.171291	0.451835
H	1.712712	2.148052	0.312840
H	1.483318	0.866528	1.485997

P7

C	1.672702	0.809393	−0.163443
H	2.511583	0.835421	0.553052
H	1.869845	1.589292	−0.916986
C	0.352234	1.031228	0.596344
C	−0.207674	−0.411846	0.887180
C	−0.904285	1.357720	−0.268938
C	−1.395532	−0.075460	−0.031331
O	−2.330163	−0.711963	−0.431574
H	−0.734806	1.618467	−1.327651
H	0.469173	1.691493	1.466875
H	−0.516259	−0.647983	1.918247

H	−1.580667	2.113344	0.164211
C	1.558735	−0.603616	−0.769390
H	0.969240	−0.575553	−1.702824
H	2.536748	−1.038213	−1.028610
C	0.806662	−1.413687	0.303289
H	0.317498	−2.317469	−0.092994
H	1.501903	−1.735488	1.097006

BP7

C	1.051611	−1.290863	−0.127163
H	1.047248	−2.119192	−0.853763
H	1.728255	−1.593436	0.690589
C	−0.364387	−1.085735	0.460289
C	−0.364713	1.086223	0.459342
C	−0.301612	0.000816	1.577595
C	−1.102770	−0.000196	−0.346768
O	−2.006039	−0.000738	−1.135861
H	0.601070	0.001148	2.208307
H	−1.198328	0.001161	2.214227
H	−0.890653	−2.031573	0.656563
H	−0.890357	2.032568	0.654656
C	1.544605	−0.000330	−0.820172
H	1.148856	−0.000894	−1.849760
H	2.642056	−0.000289	−0.915280
C	1.051474	1.290746	−0.128462
H	1.047035	2.118404	−0.855807
H	1.727880	1.594036	0.689197

TS-R15

C	−1.566074	−0.874733	−0.583031
H	−2.500997	−1.459503	−0.618643
H	−1.061653	−0.985333	−1.556929
C	−0.659463	−1.367000	0.492184
C	0.589070	1.316237	0.031882
C	0.746570	−1.359224	0.313293
C	1.453498	0.222437	−0.065214
O	2.617065	0.120548	−0.392381
H	1.040261	−1.767412	−0.664398
H	1.361311	−1.767347	1.124427
H	−1.087047	−1.552918	1.484809
H	1.118741	2.274564	0.003999
C	−1.901262	0.630704	−0.341680
H	−2.869967	0.717937	0.179854
H	−2.009606	1.143850	−1.311871
C	−0.821199	1.312322	0.527424
H	−1.124299	2.350936	0.732694
H	−0.850098	0.796390	1.515958

TS-R16

C	−0.645096	1.501227	0.040741
H	−0.454954	2.270641	−0.725358
H	−0.940339	2.047468	0.954116
C	0.671784	0.769362	0.348375
C	−0.554523	−1.496640	−0.063217
C	0.738507	−0.972454	−0.017080
O	1.849303	−1.434253	−0.136863
H	−0.645916	−2.400623	−0.676296
C	−1.817142	0.614826	−0.402788
H	−1.761167	0.430739	−1.489178
H	−2.769876	1.139010	−0.217081
C	1.877706	1.374631	−0.070700
H	2.839895	0.939793	0.206030
H	0.725795	0.450663	1.411844
H	1.879265	2.215915	−0.769681
C	−1.793367	−0.742879	0.320204
H	−1.852335	−0.573152	1.413082
H	−2.682005	−1.334880	0.054212

R7

C	1.357190	0.843698	−0.739111
H	2.188385	1.478998	−1.084600
H	0.738278	0.621907	−1.631460
C	0.517439	1.572087	0.259474
C	−0.472869	−1.331387	0.040494
C	−0.876218	1.137474	0.596304
C	−1.346599	−0.180500	−0.030525
O	−2.455018	−0.260231	−0.565812
H	−1.626236	1.901083	0.314375
H	−0.981867	1.033130	1.697587
H	0.925901	2.436463	0.791898
H	−0.880008	−2.249608	−0.394740
C	1.930069	−0.504061	−0.226273
H	2.822582	−0.326695	0.397081
H	2.257896	−1.107091	−1.090105
C	0.902222	−1.299118	0.620755
H	1.273019	−2.322583	0.785206
H	0.854791	−0.812917	1.614553

R7'

C	−0.893533	1.030687	0.809614
H	−1.174955	2.094530	0.883300
H	−1.011956	0.606135	1.822468
C	0.579230	0.915694	0.377098
C	−0.015021	−1.484880	−0.254988
C	1.008724	−0.550810	0.139714
O	2.187665	−0.887050	0.259160
H	0.326134	−2.512694	−0.420684
C	−1.819949	0.297537	−0.167319
H	−1.718741	0.746221	−1.170484
H	−2.874281	0.424429	0.126244
C	0.878880	1.649848	−0.885706
H	0.170159	2.359953	−1.320622
H	1.245224	1.276423	1.186794
H	1.853984	1.525952	−1.362765
C	−1.478133	−1.196007	−0.242198
H	−1.913648	−1.720393	0.636410
H	−1.964435	−1.676566	−1.111221

TS-D7

C	4.792209	−0.609560	0.760828
H	5.195273	0.412272	0.869298
H	4.716317	−1.023656	1.784857
C	5.747603	−1.450444	−0.038406
C	1.010177	0.329044	0.424841
C	6.878531	−1.020542	−0.605956
C	0.279535	1.506944	0.372747
O	0.502425	2.680550	0.628200
H	7.204143	0.021544	−0.514837
H	5.464234	−2.505058	−0.163012
H	0.501003	−0.620751	0.232613
H	7.523841	−1.691432	−1.180350
C	3.379146	−0.546320	0.156803
H	3.433811	−0.120220	−0.859781
H	2.988719	−1.574154	0.034019
C	−4.494583	−0.691087	0.814381
H	−4.061451	−1.698822	0.936763
H	−4.524097	−0.238945	1.823962
C	−5.896300	−0.801244	0.280785
C	−1.231122	1.204949	−0.336430
C	−6.503741	−1.937315	−0.072483
C	−0.752467	0.709351	−1.554204
O	−0.460926	0.406060	−2.624024
H	−6.002067	−2.907337	0.014135
H	−6.442090	0.146248	0.174982
H	−1.663975	2.202258	−0.524034
H	−7.527626	−1.943645	−0.456406
C	−3.576241	0.164024	−0.075567
H	−3.525659	−0.289940	−1.081630
H	−4.025144	1.163915	−0.214273
C	2.395114	0.277076	1.003968
H	2.766645	1.310147	1.110469
H	2.381135	−0.148999	2.028380
C	−2.165968	0.315284	0.503169
H	−1.699609	−0.671156	0.644859
H	−2.206754	0.783890	1.499720

D7

C	−4.697420	−0.179181	0.223740
H	−4.603571	−0.301488	1.316804
H	−5.191282	0.798282	0.060906
C	−5.569228	−1.269698	−0.334648
C	−1.020736	1.018556	−0.474071
C	−6.093610	−2.279973	0.364596
C	0.000036	2.075913	−0.000013
O	0.000095	3.274575	−0.000219
H	−5.920818	−2.382048	1.441557
H	−5.769583	−1.214080	−1.413538
H	−1.069569	1.021631	−1.581389
H	−6.717135	−3.042827	−0.110052
C	−3.299568	−0.133741	−0.415002
H	−2.781065	−1.090865	−0.238920
H	−3.398894	−0.038875	−1.511899
C	4.697422	−0.179146	−0.223519
H	4.603620	−0.301291	−1.316604
H	5.191241	0.798309	−0.060509
C	5.569220	−1.269727	0.334748
C	1.020697	1.018465	0.474138
C	6.093455	−2.280016	−0.364589
C	0.000020	−0.038761	−0.000172
O	0.000120	−1.239334	−0.000498
H	5.920555	−2.382027	−1.441539
H	5.769688	−1.214173	1.413620
H	1.069189	1.021372	1.581482
H	6.716967	−3.042941	0.109962
C	3.299533	−0.133821	0.415159
H	2.781032	−1.090911	0.238858

H	3.398792	−0.039178	1.512082
C	−2.436646	1.018133	0.111278
H	−2.374010	0.963841	1.212984
H	−2.905446	1.990183	−0.121609
C	2.436655	1.018153	−0.110964
H	2.374152	0.964059	−1.212689
H	2.905431	1.990168	0.122127

8

C	3.454831	−0.048017	−0.264912
C	2.417029	0.722601	−0.000863
O	4.377087	−0.728180	−0.489899
C	1.198516	0.272687	0.781253
H	1.058432	0.946621	1.646348
H	1.378804	−0.728423	1.207588
C	−0.091623	0.250363	−0.053025
H	−0.247145	1.249223	−0.496750
H	0.033770	−0.444757	−0.900497
C	−1.324066	−0.162277	0.771473
H	−1.444920	0.553580	1.607208
H	−1.133621	−1.146671	1.231093
C	−2.615711	−0.222844	−0.017729
C	−3.235231	−1.387471	−0.257180
H	−2.832660	−2.335774	0.111610
H	−4.167170	−1.434607	−0.828558
H	2.462653	1.737563	−0.409191
C	−3.169589	1.090200	−0.513824
H	−2.470681	1.591145	−1.205671
H	−4.125799	0.956391	−1.040360
H	−3.333293	1.789703	0.325221

TS17

C	−1.035624	−0.972978	−0.063875
C	0.158854	−1.536350	0.386636
O	−2.193961	−1.107426	0.317362
C	1.546558	−1.254568	−0.116483
H	2.219359	−2.060767	0.215560
H	1.600544	−1.253879	−1.223526
C	2.082908	0.094493	0.402576
H	3.152926	0.225586	0.159652
H	1.990405	0.115339	1.501230
C	1.279543	1.266977	−0.202471
H	1.510320	2.192789	0.348381
H	1.627879	1.405071	−1.243263
C	−0.210693	1.070228	−0.245947
C	−0.795094	0.195943	−1.221690
H	−0.132709	−0.136422	−2.028944
H	−1.808193	0.428346	−1.563887
H	0.032682	−2.358614	1.100043
C	−1.115119	1.835000	0.657303
H	−1.522026	2.717161	0.126753
H	−0.605587	2.189242	1.565291
H	−1.981901	1.203087	0.927526

TS18

C	0.451441	1.031842	0.257089
C	−0.866215	1.413764	−0.036878
O	1.425029	1.626571	0.678813
C	−2.018912	0.452668	−0.193828
H	−2.938349	0.937225	0.172030
H	−2.230382	0.206061	−1.255036
C	−1.763867	−0.841851	0.595863
H	−2.627477	−1.522982	0.511108
H	−1.671024	−0.573364	1.661423
C	−0.488794	−1.564643	0.141820
H	−0.158178	−2.254634	0.933484
H	−0.716107	−2.192646	−0.738975
C	0.682565	−0.639194	−0.233172
C	0.575253	0.048357	−1.474679
H	−0.310439	−0.019713	−2.108079
H	1.446787	0.556791	−1.894822
H	−1.106571	2.455434	0.213001
C	2.049719	−1.074125	0.260451
H	2.295084	−2.071466	−0.141330
H	2.060474	−1.130831	1.359418
H	2.828804	−0.363351	−0.042724

P8

C	−1.587619	0.053077	0.043103
C	−0.310610	−0.320365	0.813845
O	−2.638488	−0.502059	−0.120437
C	0.319071	−1.704151	0.545599
H	0.564615	−2.246164	1.470960
H	−0.389031	−2.337238	−0.014716
C	1.571774	−1.386055	−0.302731
H	1.862951	−2.215406	−0.966872
H	2.432719	−1.191388	0.359889
C	1.206350	−0.103691	−1.070613

H	2.082583	0.416528	−1.490028
H	0.551517	−0.360756	−1.921613
C	0.434248	0.767097	−0.046244
C	−0.941496	1.306112	−0.558802
H	−1.081355	1.467207	−1.639671
H	−1.271804	2.213184	−0.023596
H	−0.403488	−0.066691	1.883487
C	1.323073	1.764234	0.687272
H	1.694996	2.544198	0.001735
H	2.200667	1.268371	1.134214
H	0.774788	2.267075	1.501130

BP8

C	0.321920	0.979292	0.366686
C	−0.798239	0.997861	−0.687696
O	0.779571	1.784489	1.130563
C	−1.994900	0.151642	−0.199892
H	−2.738983	0.791143	0.301468
H	−2.497074	−0.284829	−1.080462
C	−1.512412	−0.942999	0.775938
H	−2.248024	−1.760099	0.847285
H	−1.455607	−0.494978	1.782164
C	−0.112722	−1.493804	0.426426
H	0.349077	−1.919964	1.332361
H	−0.173296	−2.313970	−0.310421
C	0.807388	−0.388252	−0.159936
C	0.171289	0.093772	−1.507366
H	−0.295208	−0.682645	−2.133766
H	0.880938	0.679656	−2.110559
H	−1.097442	1.972680	−1.099787
C	2.287573	−0.710903	−0.081523
H	2.516495	−1.664738	−0.585768
H	2.609184	−0.797074	0.968799
H	2.893987	0.079251	−0.551637

9

C	1.680358	1.276955	−0.021113
C	1.556979	−0.041481	−0.007743
O	1.791714	2.439264	−0.031939
C	0.264205	−0.811468	0.069777
H	0.310229	−1.480047	0.948955
H	0.199270	−1.472001	−0.814339
C	−0.986003	0.070854	0.153415
H	−0.920156	0.721700	1.043731
H	−1.029762	0.743785	−0.720597
C	−2.285169	−0.749804	0.219208
H	−2.222526	−1.435361	1.085745
H	−2.368828	−1.387207	−0.677801
C	−3.516476	0.102575	0.353750
H	−3.556705	0.744853	1.244181
C	−4.532450	0.140342	−0.512807
H	−4.539440	−0.479304	−1.416242
Cl	3.064956	−0.952142	−0.094904
H	−5.398713	0.788056	−0.351665

TS19

C	−0.388105	1.143159	−0.062798
C	−0.692936	−0.207089	−0.171159
O	−0.906462	2.140831	0.376246
C	0.162619	−1.346372	−0.661182
H	−0.494826	−2.215608	−0.797678
H	0.594709	−1.133743	−1.658215
C	1.293718	−1.702161	0.319971
H	1.778440	−2.652781	0.036302
H	0.861609	−1.839083	1.324399
C	2.355360	−0.582283	0.350399
H	3.023549	−0.724959	1.214324
H	2.970005	−0.677510	−0.563820
C	1.784277	0.803182	0.381695
H	1.795058	1.358028	1.325380
C	1.253225	1.442539	−0.745653
H	1.383108	0.965545	−1.722627
Cl	-2.380446	−0.590870	0.125607
H	1.198675	2.532412	−0.770997

TS20

C	−0.125271	0.992010	0.259874
C	−0.693738	−0.193105	−0.231878
O	−0.537276	2.032897	0.721837
C	0.047987	−1.485318	−0.487770
H	−0.670040	−2.311537	−0.389920
H	0.436291	−1.548735	−1.522406
C	1.196740	−1.661930	0.519724
H	1.685374	−2.640000	0.374388
H	0.763056	−1.666005	1.533254
C	2.235476	−0.538297	0.402424
H	2.827090	−0.477210	1.328273
H	2.945031	−0.783362	−0.407600

C	1.630611	0.832597	0.101703
H	1.935003	1.659603	0.749119
C	1.247978	1.162051	−1.214967
H	1.246373	0.422162	−2.017832
Cl	-2.419403	−0.338887	−0.001840
H	1.021188	2.194936	−1.485356

P9

C	1.252298	−0.885010	−0.281327
C	0.208306	0.236099	−0.108498
O	2.351051	−0.929740	−0.749267
C	−0.786880	0.438604	−1.270025
H	−0.561298	1.346169	−1.846424
H	−0.720526	−0.417518	−1.964868
C	−2.153588	0.440182	−0.567965
H	−2.995690	0.307348	−1.265107
H	−2.295668	1.406922	−0.056980
C	−2.038068	−0.693813	0.472986
H	−2.721371	−0.552446	1.323599
H	−2.297043	−1.662532	0.012944
C	−0.553005	−0.684927	0.903367
H	−0.402400	−0.378186	1.946495
C	0.376581	−1.874645	0.504303
H	−0.098834	−2.640450	−0.130635
Cl	0.855117	1.797312	0.514056
H	0.913575	−2.384626	1.319107

BP9

C	0.149433	1.079245	0.364350
C	−0.547649	−0.208382	−0.136562
O	−0.136013	1.952970	1.127639
C	0.145907	−1.445952	0.468737
H	−0.374566	−1.737312	1.392988
H	0.035904	−2.281385	−0.242539
C	1.629187	−1.134285	0.777029
H	2.210116	−2.066517	0.854690
H	1.671320	−0.662263	1.772622
C	2.271799	−0.162082	−0.235695
H	3.127461	0.348656	0.233539
H	2.667152	−0.697246	−1.115718
C	1.227688	0.868880	−0.719801
H	1.674652	1.770718	−1.162017
C	0.097028	0.138477	−1.505441
H	0.392926	−0.717907	−2.129469
Cl	-2.331043	−0.307525	−0.036368
H	−0.529497	0.832009	−2.082653

10

C	2.157762	1.322219	0.001626
C	2.125182	−0.001436	−0.017371
O	2.189716	2.489467	0.019015
C	0.890618	−0.860621	0.068996
H	1.003835	−1.545669	0.929247
H	0.849853	−1.502559	−0.830173
C	−0.415047	−0.069346	0.202881
H	−0.372519	0.563794	1.107251
H	−0.526063	0.619284	−0.652862
C	−1.653931	−0.978271	0.277061
H	−1.522088	−1.679011	1.123697
H	−1.711193	−1.599528	−0.633358
C	−2.938483	−0.217138	0.454346
H	−3.014815	0.392999	1.365737
C	−3.966376	−0.220912	−0.403451
H	−3.883314	−0.831236	−1.313733
Cl	3.690524	−0.802130	−0.162269
C	−5.248192	0.539464	−0.233548
H	−5.416405	1.233530	−1.075933
H	−6.117812	−0.141204	−0.214764
H	−5.255306	1.126316	0.698093

TS21

C	−0.117248	−0.961829	0.099544
C	0.935040	−0.099033	−0.192658
O	−0.222777	−2.041202	0.640141
C	0.902676	1.277367	−0.799683
H	1.929415	1.541283	−1.087262
H	0.307523	1.299089	−1.732791
C	0.345974	2.321530	0.183722
H	0.481183	3.346364	−0.204043
H	0.905778	2.250028	1.130265
C	−1.151461	2.059158	0.433462
H	−1.485945	2.618990	1.321252
H	−1.711286	2.453435	−0.435023
C	−1.521091	0.612393	0.596871
H	−1.776557	0.244838	1.596796
C	−1.668225	−0.286718	−0.480101
Cl	2.529599	−0.787290	0.048713
H	−1.519262	0.153017	−1.474337

C	−2.660581	−1.429253	−0.457065
H	−2.350531	−2.229744	−1.143506
H	−3.650676	−1.061279	−0.772578
H	−2.741104	−1.864161	0.547434

TS22

C	−0.065831	−0.682125	0.514902
C	0.928469	−0.081474	−0.244029
O	−0.205361	−1.700289	1.159344
C	0.907309	1.324975	−0.788287
H	1.944262	1.625673	−0.991883
H	0.377746	1.393916	−1.757954
C	0.263950	2.281777	0.228005
H	0.336687	3.325421	−0.121851
H	0.833277	2.215590	1.169537
C	−1.206812	1.922871	0.471128
H	−1.550590	2.368986	1.416867
H	−1.820353	2.375539	−0.327032
C	−1.506368	0.420347	0.501309
H	−1.990146	0.044028	1.408759
C	−1.789495	−0.274424	−0.687962
H	−1.509500	0.194960	−1.636019
Cl	2.511504	−0.828317	−0.114167
C	−2.479230	−1.589567	−0.723712
H	−2.416946	−2.068731	−1.710342
H	−3.544454	−1.476002	−0.453264
H	−2.024610	−2.249955	0.041147

P10

C	−1.019368	−0.678582	−0.625646
C	0.412460	−0.391463	−0.145301
O	−1.580489	−1.651461	−1.038501
C	1.379211	0.248617	−1.162940
H	2.114770	−0.476247	−1.537577
H	0.806102	0.615809	−2.032562
C	1.978521	1.432369	−0.387235
H	2.480391	2.162687	−1.041059
H	2.731551	1.051942	0.322407
C	0.780780	2.027910	0.387345
H	1.095849	2.523263	1.317786
H	0.266058	2.790686	−0.221129
C	−0.158471	0.828739	0.650177
H	−0.305262	0.602758	1.715257
C	−1.503465	0.701796	−0.145618
Cl	1.195457	−1.713542	0.793348
H	−1.518521	1.409508	−0.994455
C	−2.836612	0.736622	0.589828
H	−3.653458	0.435527	−0.084293
H	−3.057418	1.747513	0.967935
H	−2.837243	0.042394	1.445125

BP10

C	−0.227658	0.249453	−1.113712
C	0.409864	−0.375575	0.145020
O	0.005203	0.218286	−2.285718
C	−0.507748	−1.488920	0.694387
H	−0.190726	−2.456256	0.277650
H	−0.361845	−1.542895	1.785999
C	−1.981685	−1.213218	0.318071
H	−2.659072	−1.767568	0.986277
H	−2.150331	−1.617293	−0.693864
C	−2.331350	0.289809	0.293520
H	−3.195539	0.458596	−0.368308
H	−2.623222	0.653829	1.293300
C	−1.114386	1.107498	−0.188564
H	−1.374959	2.115393	−0.544555
C	0.060685	0.982594	0.839486
H	−0.267661	0.853755	1.883496
Cl	2.121923	−0.898629	0.069196
C	1.115913	2.074625	0.736848
H	2.007075	1.813636	1.327033
H	0.716776	3.029076	1.115413
H	1.443382	2.232535	−0.303356

11

C	2.894780	−0.316428	−0.002062
C	1.583344	−0.260171	0.197552
O	4.044816	−0.378912	−0.172551
C	0.749700	0.879604	−0.180135
H	1.272679	1.713033	−0.659933
C	−0.579810	0.998182	0.007631
H	−1.055615	1.919599	−0.344779
C	−1.510010	−0.010471	0.632319
H	−2.018498	0.443271	1.502387
H	−0.937594	−0.870473	1.021670
C	−2.553672	−0.509492	−0.338823
H	−2.164399	−1.021924	−1.227983
C	−3.873171	−0.353283	−0.201099

H	−4.302419	0.159222	0.666918
H	−4.575892	−0.733393	−0.947944
H	1.156241	−1.145684	0.677779

TS23

C	1.349108	0.163723	−0.081775
C	0.422607	1.194576	0.318804
O	2.540136	0.127084	0.177789
C	−0.912306	1.426343	−0.169617
H	−1.166246	2.458271	−0.446331
C	−1.904232	0.500899	−0.230376
H	−2.873914	0.743009	−0.674936
C	−1.698487	−0.862748	0.354015
H	−2.189506	−0.944307	1.339964
H	−2.214378	−1.602418	−0.296811
C	−0.273666	−1.249634	0.402959
H	0.123662	−1.752105	1.289278
C	0.619064	−1.062079	−0.736398
H	0.096011	−0.794567	−1.666408
H	0.923845	2.057628	0.776841
H	1.366912	−1.848668	−0.889581

TS24

C	1.088229	0.263017	0.269835
C	0.241718	1.345328	−0.115838
O	2.256067	0.241645	0.611250
C	−1.201640	1.267461	−0.150093
H	−1.742744	2.177552	−0.425373
C	−1.893162	0.148133	0.179056
H	−2.986091	0.151380	0.191282
C	−1.163719	−1.102380	0.585812
H	−1.144590	−1.178348	1.690931
H	−1.710996	−1.996942	0.240000
C	0.253244	−1.145359	0.039637
H	0.892190	−1.933081	0.449840
C	0.476911	−0.792175	−1.337231
H	−0.313428	−0.390935	−1.971899
H	1.446277	−1.007290	−1.791238
H	0.701349	2.340356	−0.100612

P11

C	1.429144	−0.059213	0.053623
C	0.200281	−0.520476	−0.763079
O	2.504041	−0.537683	0.274768
C	−0.752208	−1.404497	0.003101
H	−0.567436	−2.470221	0.157950
C	−1.811819	−0.725980	0.467214
H	−2.620076	−1.171303	1.054036
C	−1.795264	0.733633	0.075368
H	−2.616249	0.962653	−0.628645
H	−1.941924	1.404898	0.941286
C	−0.404201	0.919309	−0.566585
H	−0.422605	1.540924	−1.472092
C	0.770823	1.287421	0.389832
H	0.492337	1.382634	1.453071
H	1.383248	2.161010	0.114640
H	0.439840	−0.890313	−1.775230

BP11

C	1.105820	−0.037520	0.303923
C	0.354345	1.111638	−0.399933
O	2.058328	−0.116976	1.025185
C	−0.961473	1.258189	0.354625
H	−1.299138	2.254037	0.653969
C	−1.666515	0.152685	0.636546
H	−2.627467	0.209963	1.157057
C	−1.122890	−1.206886	0.258963
H	−0.987560	−1.826231	1.164763
H	−1.839503	−1.758489	−0.378335
C	0.236081	−1.049210	−0.463586
H	0.688637	−2.017863	−0.722659
C	0.143963	0.074175	−1.547291
H	−0.803667	0.152217	−2.100380
H	0.993339	0.043227	−2.245162
H	0.872751	2.060518	−0.590216

12

C	3.502983	−0.422279	0.027071
C	2.214891	−0.201915	0.260499
O	4.632798	−0.625983	−0.168645
C	1.414461	0.791546	−0.453706
H	1.941754	1.360947	−1.225792
C	0.111044	1.067821	−0.250110
H	−0.341664	1.839511	−0.882069
C	−0.821237	0.419097	0.741247
H	−1.219521	1.188081	1.428213
H	−0.269225	−0.300270	1.371380
C	−1.978219	−0.285427	0.073230

H	−1.709309	−1.108840	−0.602163
C	−3.268973	0.033505	0.229048
H	−3.523038	0.865319	0.901135
H	1.779347	−0.827843	1.045199
C	−4.424221	−0.654297	−0.436568
H	−5.013968	0.052749	−1.046652
H	−4.089531	−1.472856	−1.092567
H	−5.121616	−1.077247	0.308213

TS25

C	−0.814765	0.901992	−0.035487
C	0.501750	1.471249	−0.161174
O	−1.862384	1.434804	−0.367877
C	1.730899	1.013056	0.430226
H	2.362959	1.771542	0.910708
C	2.214477	−0.254252	0.361612
H	3.130034	−0.538137	0.888396
C	1.523845	−1.275866	−0.487243
H	2.057069	−1.412916	−1.444897
H	1.583320	−2.259162	0.029018
C	0.088479	−0.983824	−0.680507
H	−0.368469	−1.130656	−1.664344
C	−0.791137	−0.610051	0.425247
H	−0.267742	−0.691630	1.392446
C	−2.190706	−1.209549	0.461728
H	−2.820048	−0.654174	1.172026
H	−2.158704	−2.267460	0.765986
H	−2.674588	−1.137033	−0.522822
H	0.478186	2.524663	−0.469904

TS26

C	−0.449529	0.879894	−0.452364
C	0.438045	1.293905	0.588310
O	−1.399349	1.476364	−0.941961
C	1.711539	0.653663	0.843796
H	2.351055	1.094136	1.614487
C	2.138622	−0.430459	0.151088
H	3.131137	−0.852469	0.329889
C	1.271936	−1.032810	−0.922630
H	1.617945	−0.685214	−1.916691
H	1.385064	−2.130758	−0.939632
C	−0.198416	−0.678545	−0.731815
H	−0.845467	−0.978196	−1.564753
C	−0.778083	−0.867862	0.598034
H	−0.114689	−1.067679	1.441111
C	−2.248008	−0.925703	0.784270
H	−2.547216	−0.812797	1.835722
H	−2.645017	−1.889518	0.410320
H	−2.723726	−0.135583	0.171504
H	0.269065	2.294671	1.001606

P12

C	−0.925209	0.906118	0.047362
C	0.416750	0.814027	−0.707175
O	−1.733293	1.778280	0.200777
C	1.649414	1.096727	0.116027
H	1.971869	2.111785	0.360432
C	2.276994	−0.026964	0.493313
H	3.190410	−0.050654	1.094185
C	1.602994	−1.279409	−0.019614
H	2.234286	−1.787417	−0.771725
H	1.424819	−2.021461	0.780316
C	0.283897	−0.751363	−0.618024
H	−0.006354	−1.242603	−1.557805
C	−0.926958	−0.599221	0.361916
H	−0.598948	−0.752767	1.406675
C	−2.223815	−1.354182	0.102767
H	−3.023263	−0.982230	0.762515
H	−2.103043	−2.433994	0.286061
H	−2.562140	−1.221100	−0.937779
H	0.414300	1.319804	−1.688524

BP12

C	0.274399	1.095767	0.035290
C	0.192874	0.062610	−1.105872
O	0.503042	2.269439	0.108307
C	−1.289886	−0.244656	−1.263972
H	−1.733147	−0.248882	−2.263345
C	−2.014574	−0.494060	−0.163270
H	−3.079263	−0.738550	−0.228544
C	−1.368454	−0.411835	1.201645
H	−1.876024	0.354701	1.815845
H	−1.482615	−1.363913	1.753467
C	0.127040	−0.048087	1.052647
H	0.632808	0.063715	2.024223
C	0.799448	−0.933120	−0.056257
H	0.383838	−1.950488	−0.130704
C	2.321021	−0.961798	−0.003533

H	2.739888	−1.439522	−0.903904	C	−2.479608	0.221484	−0.318198
H	2.673451	−1.529182	0.873375	O	−3.462149	−0.248547	−0.797306
H	2.747216	0.053082	0.064564	H	−2.073589	2.252226	−0.600614
H	0.718299	0.254605	−2.051498	H	−2.527496	−1.634557	1.306979

13

C	−0.335475	−1.583354	0.175373
C	−0.229761	−0.189891	0.156179
C	−1.368523	0.630703	−0.054966
C	−2.598964	−0.032335	−0.234903
C	−2.716620	−1.421831	−0.212250
C	−1.576392	−2.199606	−0.007142
H	0.562243	−2.185277	0.320812
H	−3.490195	0.579961	−0.397332
H	−3.691812	−1.892311	−0.356115
H	−1.643142	−3.290318	0.008311
C	−1.370775	2.101624	−0.099499
C	−0.362893	2.981912	0.025208
H	−2.373385	2.514731	−0.263895
H	0.669993	2.679579	0.188366
O	0.972869	0.454059	0.338798
C	2.082082	−0.276015	0.715066
C	3.136292	−0.354633	−0.089739
O	4.084447	−0.412286	−0.764973
H	2.127454	−0.732990	1.708557
H	−0.573514	4.052989	−0.039269

TS28

C	1.964423	1.266865	0.066494
C	0.666947	0.741003	0.107197
C	0.424745	−0.642007	0.033501
C	1.524655	−1.492293	−0.188334
C	2.817456	−0.980500	−0.250457
C	3.038883	0.399723	−0.103040
H	2.099184	2.347927	0.136903
H	1.352528	−2.568291	−0.274575
H	3.662996	−1.655957	−0.399115
H	4.055051	0.798831	−0.142955
C	−0.948352	−1.129713	0.243073
C	−1.720138	−0.627507	1.342062
H	−1.205201	−2.110508	−0.166008
H	−1.289246	0.074018	2.059575
O	−0.372519	1.634376	0.132707
C	−1.628789	1.278384	−0.195655
C	−2.112794	−0.035440	−0.374962
O	−3.119672	−0.457905	−0.928830
H	−2.230861	2.132449	−0.517351
H	−2.669161	−1.101329	1.593227

TS27

C	1.903772	1.323295	0.175020
C	0.657292	0.679270	0.194558
C	0.563931	−0.720149	0.015990
C	1.743656	−1.427537	−0.319220
C	2.974045	−0.787517	−0.364743
C	3.054562	0.590855	−0.094175
H	1.933549	2.402809	0.334625
H	1.675689	−2.504001	−0.498689
H	3.877764	−1.353485	−0.601263
H	4.021826	1.098311	−0.126883
C	−0.682783	−1.416538	0.248822
C	−1.664373	−0.994311	1.118469
H	−0.837867	−2.352682	−0.300163
H	−1.453474	−0.220758	1.859908
O	−0.440214	1.462916	0.356152
C	−1.636742	1.297345	−0.297303

P13

C	1.843462	−1.394739	−0.137375
C	0.663744	−0.771722	0.262960
C	0.543621	0.625410	0.339350
C	1.636291	1.428685	0.017542
C	2.834885	0.822688	−0.385576
C	2.930311	−0.572807	−0.461536
H	1.905722	−2.482954	−0.190135
H	1.561280	2.517894	0.077735
H	3.697665	1.441397	−0.642603
H	3.869651	−1.032967	−0.778880
C	−0.851315	0.966024	0.806054
C	−1.872608	1.403158	−0.290879
H	−0.871126	1.563416	1.729890
H	−1.468900	1.845132	−1.215082
O	−0.466976	−1.440662	0.642561
C	−1.483892	−0.468751	0.851783

C	−2.313998	−0.066190	−0.404371
O	−2.970588	−0.681727	−1.189998
H	−2.093188	−0.752339	1.724269
H	−2.683602	2.049006	0.086581

BP13

C	1.825783	1.294737	−0.261750
C	0.556544	0.765137	−0.023539
C	0.379886	−0.614682	0.210993
C	1.493025	−1.456167	0.182360
C	2.769375	−0.935034	−0.063006
C	2.929619	0.436652	−0.281943
H	1.928274	2.367616	−0.436117
H	1.358975	−2.526936	0.357840
H	3.635485	−1.600203	−0.081715
H	3.924015	0.847273	−0.473988
C	−1.048724	−1.055697	0.488885
C	−1.679455	0.004830	1.453422
H	−1.160675	−2.132660	0.669514
H	−1.050350	0.355284	2.283918
O	−0.527873	1.601247	−0.023190
C	−1.779309	0.956089	0.226558
C	−1.901360	−0.362910	−0.586905
O	−2.556164	−0.718480	−1.522464
H	−2.561675	1.722036	0.160150
H	−2.674057	−0.292279	1.815173

14

C	0.487407	−1.950270	0.171222
C	0.058238	−0.620599	0.157840
C	−1.306173	−0.287449	−0.050082
C	−2.193356	−1.367909	−0.233023
C	−1.777015	−2.698910	−0.215581
C	−0.427622	−2.990393	−0.013517
H	1.546473	−2.167611	0.314625
H	−3.250238	−1.138438	−0.393905
H	−2.503092	−3.501878	−0.361598
H	−0.077140	−4.025417	−0.002419
C	−1.868459	1.070955	−0.089673
C	−1.273658	2.271837	0.047831
H	−2.952769	1.074271	−0.260789
H	−0.197170	2.323346	0.218729
C	−2.006873	3.577127	−0.019697
H	−3.085107	3.439838	−0.196765
H	−1.883785	4.151737	0.916129
H	−1.606157	4.217868	−0.825827
O	0.932105	0.429193	0.343343
C	2.234982	0.169227	0.715405
C	3.239222	0.495456	−0.090954
O	4.137453	0.802699	−0.767412
H	2.452365	−0.243278	1.705752

TS29

C	2.355575	1.090477	0.469488
C	1.026937	0.681962	0.275501
C	0.727190	−0.622593	−0.177668
C	1.807138	−1.451245	−0.570930
C	3.121554	−1.039151	−0.407497
C	3.395116	0.229579	0.137805
H	2.540666	2.100757	0.839463
H	1.587074	−2.447714	−0.963581
H	3.942240	−1.701470	−0.691866
H	4.429587	0.555540	0.270966
C	−0.626565	−1.126693	−0.156977
C	−1.616456	−0.730858	0.731806
H	−0.870614	−1.920327	−0.874087
H	−1.307494	−0.129983	1.593173
C	−2.909020	−1.487012	0.876419
H	−2.828969	−2.215710	1.701030
H	−3.744711	−0.809795	1.105276
H	−3.163116	−2.030676	−0.044933
O	0.056807	1.604619	0.493372
C	−1.095905	1.722228	−0.239802
C	−2.054465	0.781435	−0.509750
O	−3.055854	0.588360	−1.132852
H	−1.378876	2.766764	−0.389972

TS30

C	2.385661	1.032123	0.460897
C	1.035593	0.717322	0.255572
C	0.638618	−0.554874	−0.189045
C	1.641303	−1.480945	−0.534084
C	2.986771	−1.171070	−0.356299
C	3.356752	0.081297	0.162418
H	2.645429	2.030679	0.817632
H	1.347659	−2.465228	−0.908563
H	3.753244	−1.908053	−0.606414
H	4.412156	0.322487	0.310085

C	−0.796128	−0.888038	−0.209500
C	−1.625620	−0.656939	0.915682
H	−1.116322	−1.653931	−0.923941
H	−1.200340	−0.106941	1.759368
C	−2.983847	−1.252034	1.048036
H	−2.924643	−2.350772	1.140580
H	−3.522368	−0.854233	1.919113
H	−3.560315	−1.028913	0.129169
O	0.119670	1.714888	0.426634
C	−1.101508	1.682917	−0.172193
C	−1.763611	0.566883	−0.664622
O	−2.746352	0.394213	−1.365996
H	−1.464954	2.682250	−0.423300

P14

C	2.395572	−1.179245	−0.196107
C	1.118680	−0.797773	0.209485
C	0.746538	0.549689	0.340975
C	1.679070	1.550499	0.074029
C	2.972436	1.189384	−0.330821
C	3.319263	−0.160996	−0.465154
H	2.654944	−2.234925	−0.291873
H	1.407278	2.604582	0.177206
H	3.712095	1.964481	−0.543909
H	4.329974	−0.429640	−0.783201
C	−0.698401	0.605768	0.766998
C	−1.763350	0.825984	−0.367415
H	−0.874688	1.203241	1.674690
H	−1.307288	1.133981	−1.324468
C	−2.972664	1.704525	−0.052675
H	−2.683130	2.765609	0.008186
H	−3.736087	1.601579	−0.839231
H	−3.437461	1.424833	0.906985
O	0.125539	−1.676389	0.539085
C	−1.047255	−0.920861	0.838044
C	−2.027708	−0.693626	−0.346543
O	−2.735474	−1.417211	−0.983740
H	−1.519237	−1.325022	1.747951

BP14

C	−2.196807	1.247711	−0.135502
C	−0.886727	0.770109	−0.076617
C	−0.622255	−0.614297	−0.016173
C	−1.692698	−1.509560	0.002183
C	−3.010942	−1.039581	−0.051163
C	−3.256349	0.334989	−0.121039
H	−2.366716	2.325075	−0.184177
H	−1.491706	−2.582915	0.054547
H	−3.842880	−1.747188	−0.039089
H	−4.283583	0.705656	−0.162581
C	0.847740	−1.000203	0.015280
C	1.595502	−0.096115	−1.033383
H	1.028583	−2.082851	0.059544
H	1.025063	0.077722	−1.958707
C	3.034606	−0.499241	−1.326535
H	3.068472	−1.439516	−1.899029
H	3.546739	0.275490	−1.919347
H	3.616791	−0.653456	−0.402842
O	0.151667	1.662502	−0.073983
C	1.449574	1.066792	−0.000301
C	1.482255	−0.068565	1.059198
O	1.979770	−0.201472	2.138979
H	2.184359	1.881511	0.036023

15

C	−2.404505	−0.417956	0.515667
C	−1.273540	−0.464084	−0.182269
O	−3.392956	−0.391251	1.131756
C	−0.452292	0.790426	−0.282369
C	1.706737	−0.278382	−0.397327
H	1.801386	−0.710460	−1.414183
H	1.348618	−1.089793	0.262438
C	3.077170	0.163940	0.050971
H	3.464992	1.050663	−0.464517
C	3.806888	−0.439692	0.991333
H	3.434344	−1.315906	1.533586
H	4.805928	−0.083528	1.257789
C	−0.971488	−1.743833	−0.956957
H	−0.229858	−2.387688	−0.460829
H	−1.884335	−2.340751	−1.102671
H	−0.585063	−1.489583	−1.955538
C	−1.224545	2.092047	−0.228465
H	−1.917934	2.176809	−1.081838
H	−1.833444	2.155573	0.690374
H	−0.520800	2.933779	−0.243211
N	0.810467	0.859443	−0.448421

TS31

C	0.950772	0.960439	−0.119355
C	−0.412614	0.753918	0.156198
O	1.701769	1.900355	0.042627
C	−1.145151	−0.491640	−0.075869
C	0.572421	−1.947369	0.655664
H	0.483011	−1.966489	1.759134
H	0.895936	−2.976243	0.386331
C	1.668310	−1.035612	0.245452
H	2.488719	−0.838849	0.943516
C	1.652996	−0.368499	−0.987697
H	0.950578	−0.726393	−1.747459
H	2.582713	0.065865	−1.359089
C	−1.177430	2.014257	0.488535
H	−1.639555	2.477048	−0.403193
H	−0.489334	2.756605	0.918083
H	−1.988023	1.821593	1.208072
C	−2.596111	−0.361703	−0.501580
H	−2.712810	0.315622	−1.362746
H	−3.209163	0.051081	0.316583
H	−2.983667	−1.356400	−0.755030
N	−0.724532	−1.709862	0.083814

TS32

C	1.064821	0.703403	0.192719
C	−0.347745	0.776377	0.012116
O	1.885713	1.581439	0.393961
C	−1.194411	−0.432247	0.036706
C	0.603212	−1.813347	0.676542
H	0.726326	−1.736560	1.774669
H	0.879442	−2.851589	0.420451
C	1.554036	−0.857856	−0.015659
H	2.595997	−0.878990	0.319093
C	1.314936	−0.546157	−1.389899
H	0.434415	−0.907278	−1.922251
C	−0.957995	2.141258	0.143174
H	−0.194543	2.905278	−0.064916
H	−1.332895	2.327884	1.167337
H	−1.812234	2.275267	−0.537404
C	−2.663972	−0.270189	−0.282605
H	−2.813862	0.181142	−1.277582
H	−3.164759	0.386277	0.447943
H	−3.142068	−1.257387	−0.256576
N	−0.793485	−1.618737	0.355563
H	2.055582	0.028151	−1.949953

P15

C	1.399483	−0.165041	0.430962
C	0.191343	−0.213968	−0.529831
O	2.136250	−1.009147	0.857987
C	−1.112885	−0.465015	0.243390
C	−1.190669	1.763588	−0.079606
H	−1.818914	2.149573	−0.902256
H	−1.162611	2.560573	0.684560
C	0.217625	1.353429	−0.550875
H	0.521214	1.809884	−1.503099
C	1.342936	1.363054	0.529233
H	1.036309	1.731727	1.523190
H	2.289098	1.857192	0.256468
C	0.366457	−1.057436	−1.788255
H	0.497453	−2.119069	−1.526683
H	1.261033	−0.744221	−2.349245
H	−0.505676	−0.969895	−2.456104
C	−1.494878	−1.842983	0.691119
H	−0.674647	−2.302594	1.267532
H	−1.682434	−2.499520	−0.175074
H	−2.402832	−1.800782	1.306927
N	−1.823495	0.569507	0.476152

BP15

C	0.993624	0.704075	0.532642
C	−0.288815	0.646326	−0.321072
O	1.367262	1.417624	1.421838
C	−0.994147	−0.665248	0.129990
C	1.092611	−1.735294	0.055294
H	1.582972	−2.059398	0.990644
H	1.350130	−2.496863	−0.703151
C	1.632219	−0.348056	−0.369476
H	2.723816	−0.340006	−0.505464
C	0.688276	0.222469	−1.471585
H	0.296543	−0.496378	−2.207289
C	−1.144167	1.892743	−0.435097
H	−0.524230	2.748511	−0.744288
H	−1.598045	2.153317	0.533064
H	−1.952368	1.776428	−1.173701
C	−2.473686	−0.641302	0.402017
H	−3.039191	−0.310470	−0.484472
H	−2.714459	0.063746	1.214533

H	−2.804036	−1.647736	0.688801
N	−0.344393	−1.754646	0.266432
H	1.116028	1.096094	−1.984681

16

C	−2.841130	−0.427559	0.702986
C	−1.816270	−0.460840	−0.142858
O	−3.736152	−0.409855	1.449158
C	−1.010988	0.796217	−0.329081
C	1.115807	−0.278029	−0.700302
H	1.094155	−0.694477	−1.727779
H	0.821346	−1.096574	−0.018098
C	2.527013	0.149828	−0.388061
H	2.887231	1.016923	−0.955966
C	3.325357	−0.443067	0.506151
H	2.929957	−1.296338	1.075314
C	−1.621546	−1.723260	−0.977390
H	−0.829401	−2.382383	−0.591189
H	−2.550057	−2.311966	−1.024938
H	−1.356864	−1.446256	−2.009007
C	−1.771539	2.096829	−0.176893
H	−2.561175	2.185624	−0.941677
H	−2.268068	2.154149	0.807684
H	−1.074709	2.939417	−0.269616
N	0.223555	0.864308	−0.640773
C	4.738979	−0.044232	0.812427
H	5.441873	−0.873203	0.615052
H	5.057200	0.821791	0.211619
H	4.858750	0.216655	1.878881

TS33

C	0.693931	0.899644	0.076499
C	−0.712859	0.746078	0.201627
O	1.385982	1.873188	0.339767
C	−1.468652	−0.441202	−0.206021
C	−0.014869	−1.967414	0.836129
H	−0.340503	−2.055397	1.889638
H	0.355665	−2.982428	0.571228
C	1.146764	−1.058452	0.705775
H	1.792508	−0.878846	1.572576
C	1.478610	−0.427450	−0.531081
H	0.904956	−0.817587	−1.383271
C	−1.455529	2.022258	0.499234
H	−1.715557	2.577732	−0.421693
H	−0.806051	2.684431	1.091123
H	−2.393315	1.839789	1.045185
C	−2.790852	−0.210682	−0.913836
H	−2.685080	0.485930	−1.760796
H	−3.531332	0.229541	−0.225907
H	−3.179761	−1.173417	−1.268990
N	−1.161048	−1.681339	0.017245
C	2.920430	−0.085826	−0.855550
H	2.964746	0.697804	−1.625003
H	3.444428	−0.979514	−1.229860
H	3.446928	0.294112	0.030255

TS34

C	0.712996	0.573249	0.712601
C	−0.572829	0.775511	0.120938
O	1.493437	1.413191	1.146871
C	−1.483479	−0.364652	−0.118540
C	0.016656	−1.889670	0.865581
H	−0.134402	−1.887759	1.963343
H	0.296898	−2.925290	0.605885
C	1.150614	−0.944176	0.501768
H	2.084823	−1.105335	1.053716
C	1.299822	−0.600566	−0.904461
H	0.523073	−0.907818	−1.607608
C	−1.080997	2.185778	0.079627
H	−0.229590	2.880176	0.131448
H	−1.735757	2.411996	0.942353
H	−1.671487	2.384929	−0.827599
C	−2.811566	−0.081951	−0.784179
H	−2.674546	0.390255	−1.771406
H	−3.426098	0.606917	−0.181532
H	−3.354592	−1.027286	−0.908154
N	−1.249413	−1.585837	0.229751
C	2.524367	0.062562	−1.410321
H	2.389866	0.498964	−2.409855
H	3.356669	−0.666245	−1.458454
H	2.840036	0.845320	−0.693446

P16

C	0.760460	−0.951702	0.362333
C	−0.346679	−0.340894	−0.518642
O	1.005506	−2.076781	0.701971
C	−1.515441	0.217232	0.309312
C	−0.371248	2.092318	−0.194503

H	−0.731706	2.701121	−1.043103
H	0.131858	2.792742	0.495655
C	0.548948	0.939964	−0.634239
H	1.035209	1.087828	−1.609529
C	1.526328	0.375173	0.451225
H	1.335831	0.849371	1.432291
C	−0.765766	−1.168176	−1.729842
H	−1.240995	−2.108345	−1.409345
H	0.108716	−1.435939	−2.343189
H	−1.477702	−0.618404	−2.366312
C	−2.571565	−0.685422	0.871628
H	−2.115554	−1.491575	1.470545
H	−3.142415	−1.174009	0.064179
H	−3.265849	−0.108297	1.496347
N	−1.521601	1.483586	0.471270
C	3.023857	0.323809	0.177871
H	3.535700	−0.276559	0.946007
H	3.464798	1.333480	0.182035
H	3.235908	−0.136077	−0.801094

BP16

C	0.674101	0.179762	−1.072405
C	−0.054117	−0.660293	−0.008489
O	0.997133	−0.021303	−2.210808
C	−1.419918	0.061195	0.182951
C	−0.272922	2.107363	0.182475
H	−0.387163	2.807889	−0.664246
H	−0.166501	2.735703	1.085495
C	0.987561	1.234416	−0.016919
H	1.907349	1.830654	−0.120260
C	0.937759	0.046491	1.001013
H	0.467362	0.302816	1.964444
C	−0.095885	−2.167478	−0.168848
H	0.915988	−2.567533	−0.329569
H	−0.695252	−2.451555	−1.046835
H	−0.522686	−2.669309	0.713565
C	−2.678193	−0.762500	0.240594
H	−2.636264	−1.503970	1.055195
H	−2.826144	−1.325839	−0.695267
H	−3.536348	−0.097147	0.399117
N	−1.494096	1.329662	0.296750
C	2.270293	−0.655410	1.223831
H	2.146150	−1.588407	1.796325
H	2.954152	−0.004728	1.792783
H	2.768880	−0.907068	0.273256

17

O	1.269244	0.000009	−0.000005
C	0.104785	−0.000032	0.000021
C	−1.212991	0.000005	−0.000036
H	−1.752293	0.948125	0.000065
H	−1.752425	−0.948037	0.000065

TS-D17

O	−1.731847	−0.731735	−0.654130
O	2.131866	0.189058	−0.623261
C	−1.034686	−0.008152	0.016054
C	−0.851955	1.352858	0.222464
C	1.260752	−0.105478	0.067983
C	0.297818	−0.764884	0.828365
H	−1.528792	2.058862	−0.265667
H	−0.276619	1.714711	1.075559
H	0.246974	−0.418118	1.866971
H	0.326716	−1.860103	0.733063

D17

O	−2.258232	0.000009	0.000162
O	2.258256	0.000000	0.000173
C	−1.062188	0.000027	0.000070
C	0.000010	1.119374	−0.000035
C	1.062212	−0.000021	0.000021
C	−0.000028	−1.119373	−0.000220
H	−0.000079	1.765685	−0.895040
H	0.000028	1.768624	0.892758
H	−0.000078	−1.766539	0.894154
H	−0.000091	−1.767872	−0.893572

18

C	0.772697	0.122363	0.000719
O	1.874569	−0.265381	−0.000298
C	−0.471026	0.562525	−0.000242
H	−0.581174	1.651906	−0.000241
C	−1.694159	−0.326562	−0.000018
H	−2.319705	−0.143885	0.889998
H	−2.320201	−0.142963	−0.889464
H	−1.420550	−1.391968	−0.000657

TS-D18

C	1.158831	0.245049	−0.582788
C	0.576508	−0.415911	0.486294
C	−1.108019	−0.552727	0.216443
C	−1.367394	0.818321	0.148852
O	−1.682587	1.922729	0.204268
H	−1.508801	−0.932017	1.170908
C	−1.491895	−1.429622	−0.980759
O	0.950688	−0.822443	1.574670
H	0.571293	0.399594	−1.492086
C	2.635617	0.500338	−0.641738
H	3.076891	0.432861	0.364423
H	−1.117800	−1.010152	−1.923558
H	−1.029336	−2.416280	−0.837480
H	−2.583296	−1.556099	−1.056869
H	3.173641	−0.218593	−1.289564
H	2.850711	1.505700	−1.045102

D18

C	0.033821	−1.124760	0.000000
C	0.000001	0.000004	1.059018
C	−0.033812	1.124746	0.000000
C	0.000001	0.000004	−1.059018
O	0.000001	0.000018	−2.257538
H	0.950736	1.634395	0.000000
C	−1.161597	2.152056	0.000000
O	0.000001	0.000018	2.257538
H	−0.950746	−1.634369	0.000000
C	1.161584	−2.152079	0.000000
H	1.098583	−2.792004	0.893259
H	−2.148672	1.663375	0.000000
H	−1.098584	2.791963	0.893267
H	−1.098584	2.791963	−0.893267
H	1.098583	−2.792004	−0.893259
H	2.148676	−1.663425	0.000000

S10. References

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