

Homopyrrole and Homofuran as Masked 1, 5-Dipoles in Metal-Free (5+2) Cycloadditions with Dienophiles: A DFT Study

Pei-Jun Cai, Fu-Qiang Shi, Yi Wang, Xin Li, and Zhi-Xiang Yu*

College of Chemistry, Peking University, Beijing 100871, China.

yuzx@pku.edu.cn

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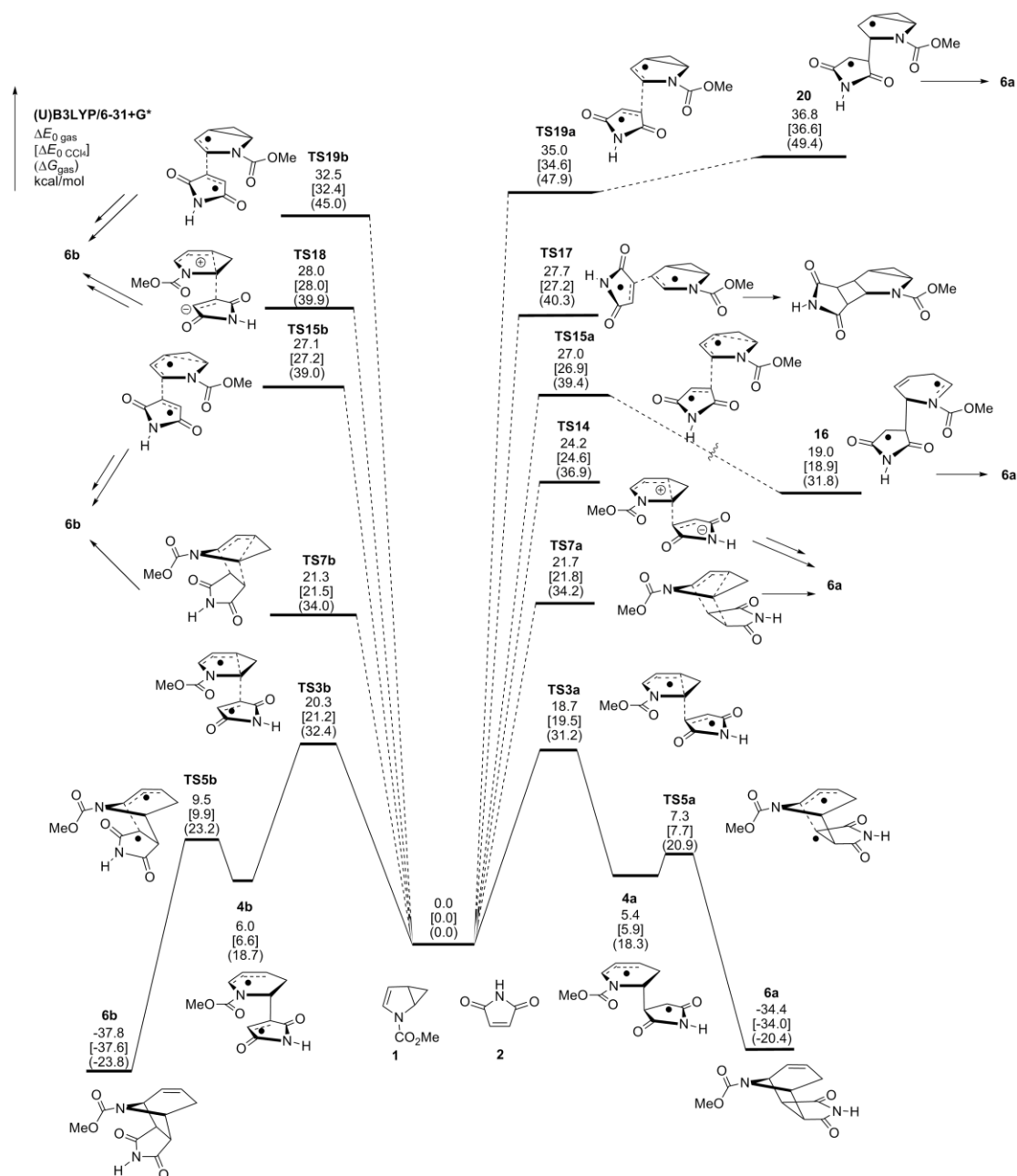


Figure S1. The computed energy surfaces for pathways *a-d* between **1** and **2** at the (U)B3LYP/6-31+G* level

Note: Every species in this Figure could have two conformers because the amide group can have two different conformations. Every species listed here is the one with the lower energy compared to another conformer. It is interesting to note that the energy difference between each pair of conformers is very small (for example, **TS3a** here is lower than its another conformer by about 0.5 kcal/mol).

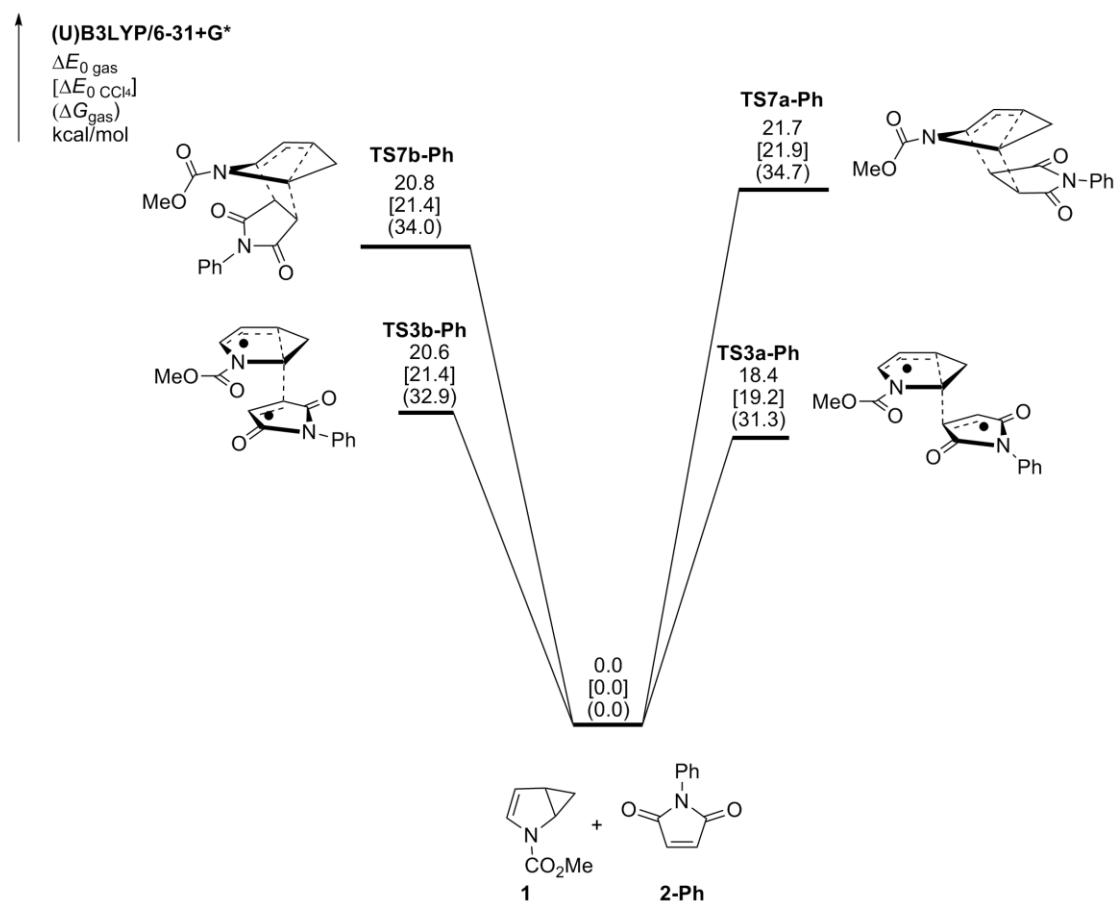


Figure S2. The computed energy surfaces for pathways *a* and *c* between **1** and **2-ph** at the (U)B3LYP/6-31+G* level

Note: Every species in this Figure could have two conformers because the amide group can have two different conformations. Every species listed here is the one with the lower energy compared to another conformer. It is interesting to note that the energy difference between each pair of conformers is very small (for example, **TS3a-Ph** here is lower than its another conformer by about 0.3 kcal/mol).

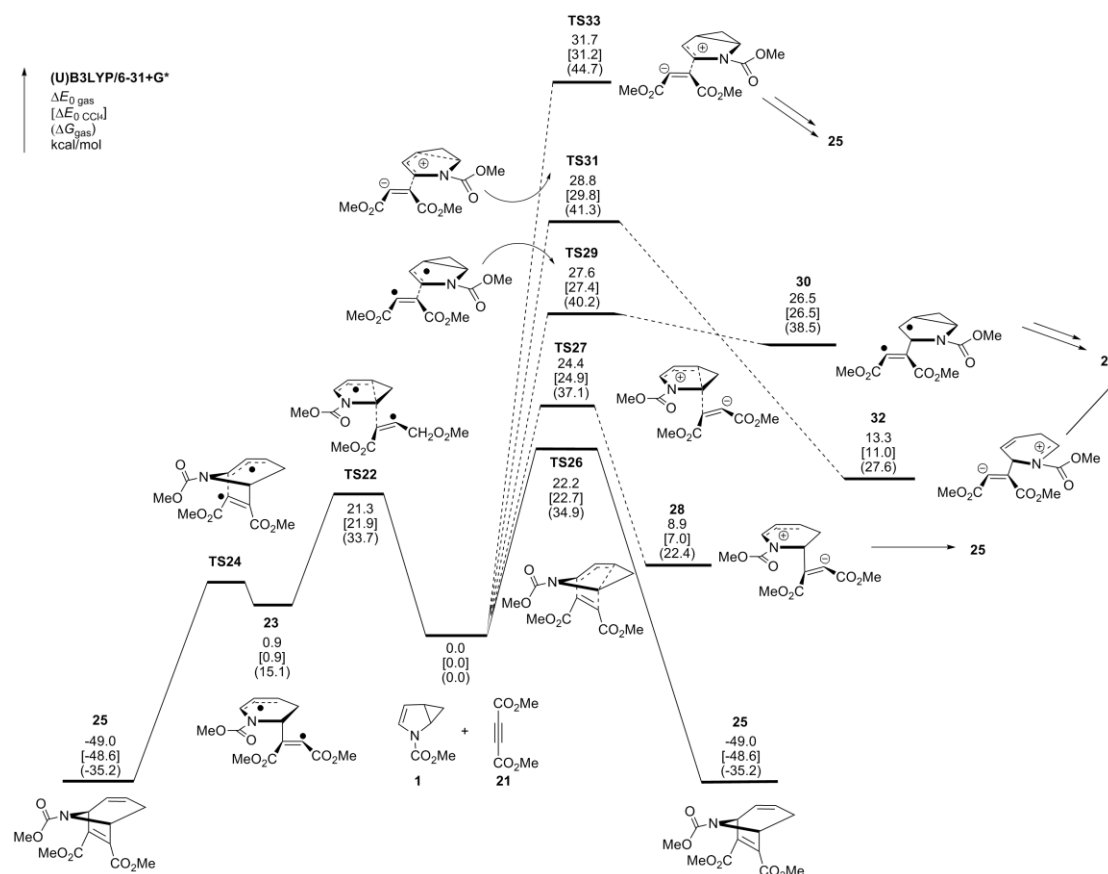


Figure S3. The computed energy surfaces for pathways *a-d* between **1** and **21** at the (U)B3LYP/6-31+G* level

Note: Here we only consider the conformation changes through the amide bond rotations in **TS22** and **TS26** because these are rate-determining transition states in two competing pathways.

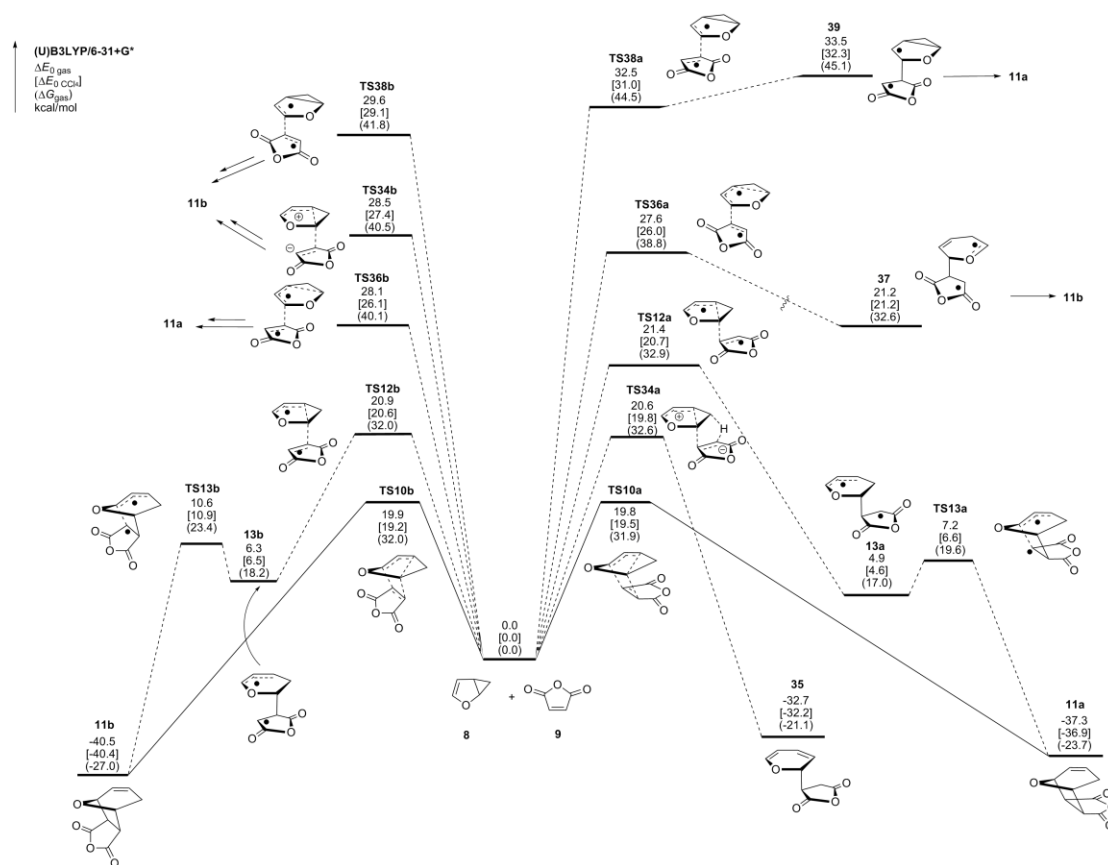


Figure S4. The computed energy surfaces for pathways *a-d* between **8** and **9** at the (U)B3LYP/6-31+G* level

Note: The zwitterionic pathway *c* via **TS34b** is not favored than the diradical pathway *c*. It was found that **TS34a** led to an ene-type reaction to give **35** (this pathway is not favored by about 0.3 kcal/mol in solution than pathway *a*). Experimentally no such product was reported. The reason for this is not known. All efforts to locate a zwitterionic transition state in pathway *c* to get endo **11a** always led to location of **TS34a** corresponding to the ene-like reaction.

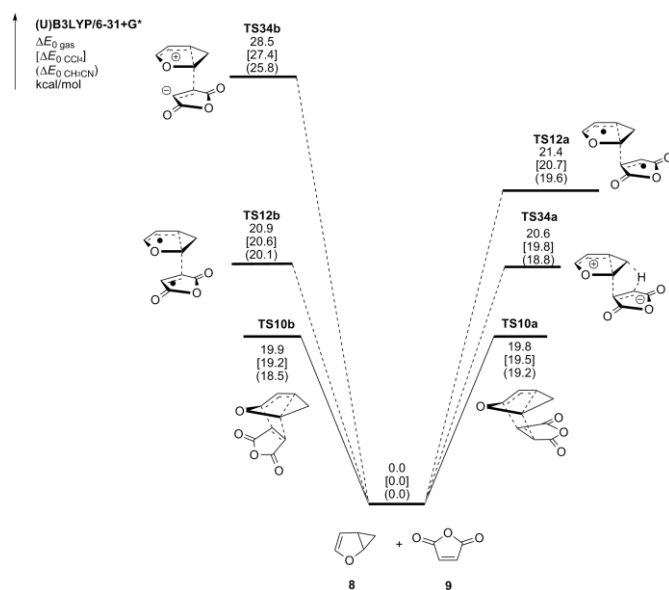


Figure S5. Comparison of ΔE_0 in different solvents for pathways *a* and *c* between **8** and **9** at the (U)B3LYP/6-31+G* level

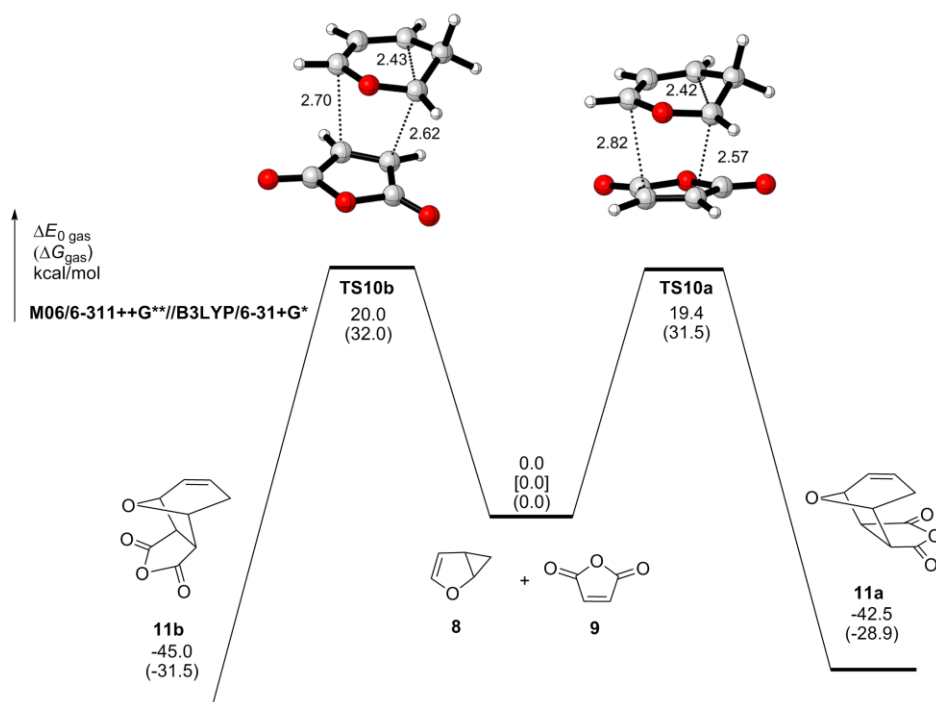


Figure S6. The computed energy surfaces for pathway *a* between **8** and **9** at the M06/6-311++G**//B3LYP/6-31+G* level

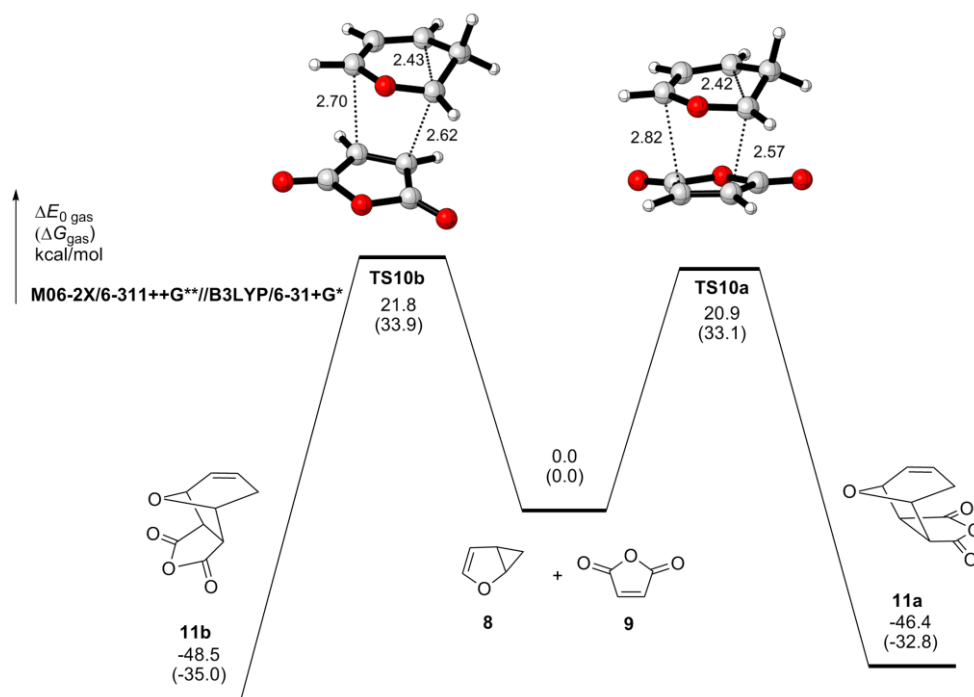


Figure S7. The computed energy surfaces for pathway *a* between **8** and **9** at the M06-2X/6-311++G**//B3LYP/6-31+G* level

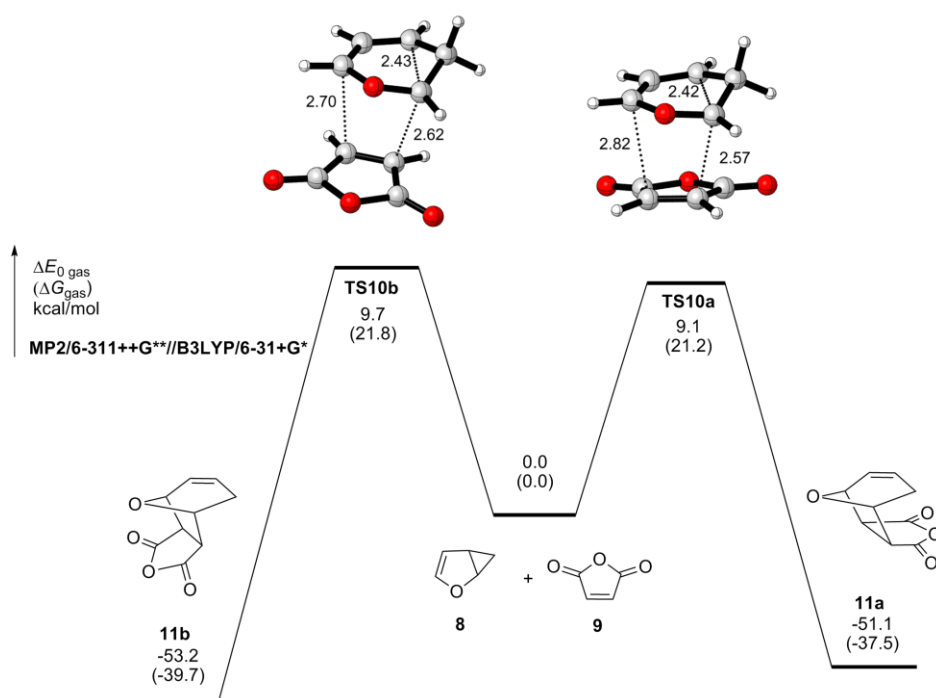


Figure S8. The computed energy surfaces for pathway *a* between **8** and **9** at the MP2/6-311++G**//B3LYP/6-31+G* level

Table S1. Sum of electronic and zero-point energies (E_0 , in Hartree), sum of electronic and thermal enthalpies (H , in Hartree), sum of electronic and thermal free energies (G , in Hartree), total free energy in CCl_4 (SP_{ccl4} , in Hartree), zero-point energy (ZPE , in Hartree) and thermo corrected zero-point energies in CCl_4 ($E_{0-\text{ccl4}}$). Relative energies ($\Delta E_{0-\text{ccl4}}$, $\Delta E_{0-\text{gas}}$, ΔG_{gas}) are reported in kcal/mol. $\Delta E_{0-\text{ccl4}}$, $\Delta E_{0-\text{gas}}$, ΔG_{gas} for all diradical species have been corrected by the YJH spin-projection energy correction.

	E_0	H	G	ZPE	SP_{ccl4}	$E_{0-\text{ccl4}}$	$\Delta E_{0-\text{ccl4}}$	$\Delta E_{0-\text{gas}}$	ΔG_{gas}
1	-477.185493	-477.175431	-477.220177	0.154035	-477.342675	-477.18864	0.0	0.0	0.0
21	-532.984944	-532.972988	-533.023582	0.115105	-533.103798	-532.988693	0.0	0.0	0.0
TS22	-1010.132923	-1010.110583	-1010.18645	0.268338	-1010.40723	-1010.13889	21.9	21.3	33.7
23	-1010.164683	-1010.14308	-1010.2153	0.271426	-1010.44287	-1010.17145	0.9	0.9	15.1
25	-1010.248601	-1010.227782	-1010.29992	0.275226	-1010.53008	-1010.25486	-48.6	-49.0	-35.2
TS26	-1010.135097	-1010.112783	-1010.188182	0.269338	-1010.410503	-1010.141165	22.7	22.2	34.9
TS27	-1010.131491	-1010.109302	-1010.18468	0.269277	-1010.40692	-1010.13764	24.9	24.4	37.1
28	-1010.156264	-1010.134606	-1010.208	0.272015	-1010.43812	-1010.1661	7.0	8.9	22.4
TS29	-1010.121577	-1010.099607	-1010.17476	0.268435	-1010.397276	-1010.128841	27.4	27.6	40.2
30	-1010.121862	-1010.099611	-1010.176072	0.269246	-1010.397972	-1010.128726	26.5	26.5	38.5
TS31	-1010.124495	-1010.10227	-1010.17791	0.269307	-1010.399162	-1010.129855	29.8	28.8	41.3
32	-1010.149302	-1010.127676	-1010.19972	0.271831	-1010.431653	-1010.159822	11.0	13.3	27.6
TS33	-1010.119865	-1010.098088	-1010.17253	0.269034	-1010.396582	-1010.127548	31.2	31.7	44.7
1	-477.185493	-477.175431	-477.220177	0.154035	-477.342675	-477.18864	0.0	0.0	0.0
2	-359.379122	-359.372732	-359.408408	0.06824	-359.453511	-359.385271	0.0	0.0	0.0
TS3a	-836.530156	-836.513618	-836.574233	0.221817	-836.760075	-836.538258	19.5	18.7	31.2
TS3b	-836.52846	-836.511735	-836.573145	0.221272	-836.757622	-836.53635	21.2	20.3	32.4
4a	-836.553556	-836.537201	-836.596972	0.22406	-836.786198	-836.562138	5.9	5.4	18.3
4b	-836.553825	-836.537382	-836.597625	0.223954	-836.786084	-836.56213	6.6	6.0	18.7
TS5a	-836.551424	-836.535759	-836.593689	0.223891	-836.784018	-836.560127	7.7	7.3	20.9
TS5b	-836.549415	-836.533721	-836.59153	0.223719	-836.781774	-836.558055	9.9	9.5	23.2
6a	-836.619448	-836.604385	-836.661109	0.229791	-836.857838	-836.628047	-34.0	-34.4	-20.4
6b	-836.624884	-836.609819	-836.666591	0.229729	-836.762191	-836.633826	-37.6	-37.8	-23.8
TS7a	-836.530057	-836.513564	-836.574116	0.223007	-836.762192	-836.539185	21.8	21.7	34.2
TS7b	-836.530689	-836.514145	-836.574446	0.222823	-836.762487	-836.539664	21.5	21.3	34.0
TS14	-836.526095	-836.509725	-836.569807	0.223029	-836.757799	-836.53477	24.6	24.2	36.9
TS15a	-836.517736	-836.501177	-836.561865	0.221905	-836.749077	-836.527172	26.9	27.0	39.4
TS15b	-836.517012	-836.500223	-836.562027	0.221505	-836.747613	-836.526108	27.2	27.1	39.0
16	-836.529487	-836.512903	-836.573061	0.22321	-836.762147	-836.538937	18.9	19.0	31.8
TS17	-836.51557	-836.499407	-836.559385	0.222489	-836.748123	-836.525634	27.2	27.7	40.3
TS18	-836.520017	-836.503515	-836.564947	0.223102	-836.752366	-836.529264	28.0	28.0	39.9
TS19a	-836.502507	-836.48621	-836.545983	0.221461	-836.733870	-836.512409	34.6	35.0	47.9
TS19b	-836.506045	-836.489693	-836.550082	0.221532	-836.737051	-836.515519	32.4	32.5	45.0
20	-836.503444	-836.486841	-836.547262	0.222309	-836.735372	-836.513063	36.6	36.8	49.4

8	-269.204619	-269.199132	-269.232161	0.098349	-269.304754	-269.206405	0.0	0.0	0.0
9	-379.250646	-379.244507	-379.27973	0.055666	-379.311488	-379.255822	0.0	0.0	0.0
TS10a	-648.423667	-648.411937	-648.46099	0.154533	-648.585657	-648.431124	19.5	19.8	31.9
TS10b	-648.423571	-648.411857	-648.46094	0.15457	-648.586166	-648.431596	19.2	19.9	32.0
11a	-648.514698	-648.504532	-648.549654	0.161316	-648.682424	-648.521108	-36.9	-37.3	-23.7
11b	-648.519879	-648.509651	-648.554989	0.161211	-648.687872	-648.526661	-40.4	-40.5	-27.0
TS12a	-648.417419	-648.405558	-648.455693	0.15351	-648.57901	-648.4255	20.7	21.4	32.9
TS12b	-648.417308	-648.405256	-648.456258	0.152797	-648.577629	-648.424832	20.6	20.9	32.0
13a	-648.445269	-648.433487	-648.482591	0.155089	-648.607737	-648.452648	4.6	4.9	17.0
13b	-648.444008	-648.432239	-648.481534	0.15501	-648.605542	-648.450532	6.5	6.3	18.2
TS13a	-648.439979	-648.428828	-648.476883	0.155153	-648.603062	-648.447909	6.6	7.2	19.6
TS13b	-648.438223	-648.427152	-648.474492	0.154756	-648.599505	-648.444749	10.9	10.6	23.4
TS34a	-648.422459	-648.410871	-648.459995	0.154492	-648.585209	-648.430717	19.8	20.6	32.6
TS34b	-648.409858	-648.398216	-648.447416	0.154673	-648.573199	-648.418526	27.4	28.5	40.5
35	-648.507433	-648.495796	-648.54555	0.158293	-648.671773	-648.513480	-32.2	-32.7	-21.1
TS36a	-648.406088	-648.394022	-648.444939	0.152976	-648.568514	-648.415538	26.0	27.6	38.8
TS36b	-648.408184	-648.396504	-648.445609	0.153763	-648.572076	-648.418313	26.1	28.1	40.1
37	-648.419197	-648.407085	-648.457598	0.154203	-648.580328	-648.426125	21.2	21.2	32.6
TS38a	-648.397309	-648.385779	-648.434724	0.15287	-648.559547	-648.406678	31.0	32.5	44.5
TS38b	-648.401966	-648.390521	-648.439162	0.153043	-648.562872	-648.409830	29.1	29.6	41.8
39	-648.397011	-648.385039	-648.435118	0.153421	-648.559399	-648.405978	32.3	33.5	45.1
2-Ph	-590.353138	-590.342213	-590.389602	0.148892	-590.507243	-590.358352	0	0	0
TS3a-Ph	-1067.504772	-1067.483662	-1067.555350	0.302503	-1067.814339	-1067.511836	19.2	18.4	31.3
TS3b-Ph	-1067.502146	-1067.480834	-1067.553572	0.301923	-1067.811085	-1067.509162	21.4	20.6	32.9
TS7a-Ph	-1067.504077	-1067.483053	-1067.55449	0.303739	-1067.815861	-1067.512122	21.9	21.7	34.7
TS7b-Ph	-1067.505531	-1067.484404	-1067.555526	0.303399	-1067.816218	-1067.512819	21.4	20.8	34.0

Table S2. Relative energies ΔE_0 (before YJH Spin-projection Energy Corrections, kcal/mol) for main diradical species. $^1E_{\text{mix}}$ is the uncorrected energy (in Hartree) of the singlet diradical, $^3E_{\text{pure}}$ is the energy (in Hartree) of the triplet diradical, $^1\langle S^2 \rangle_{\text{mix}}$ is the total spin-squared operator of singlet diradical, $^3\langle S^2 \rangle_{\text{pure}}$ is the total spin-squared operator of triplet diradical.

	ΔE_0	$^1E_{\text{mix}}$	$^1\langle S^2 \rangle_{\text{mix}}$	$^3E_{\text{pure}}$	$^3\langle S^2 \rangle_{\text{pure}}$
TS3a	21.6	-836.7519726	0.4904	-836.7372514	2.0425
TS3b	22.7	-836.7497317	0.8054	-836.7438946	2.0407
4a	6.9	-836.7776152	0.9038	-836.7746129	2.0292
4b	6.8	-836.7777792	0.9606	-836.77645	2.0288
TS5a	8.3	-836.775315	0.9454	-836.7735513	2.0278
TS5b	9.5	-836.7731344	1.022	-836.7730678	2.0293
TS12a	23.7	-648.5709258	0.2842	-648.5480177	2.0434
TS12b	23.8	-648.5701047	0.7791	-648.5626482	2.0448
TS13a	9.6	-648.5951305	0.7615	-648.5888629	2.031
TS13b	10.7	-648.5929789	1.017	-648.592842	2.0319
13a	6.3	-648.6003583	0.8859	-648.5974964	2.0327
13b	7.1	-648.5990177	0.9391	-648.5975284	2.0319
TS15a	29.4	-836.7396407	0.3116	-836.7182188	2.0196
TS15b	29.9	-836.738517	0.4608	-836.7233747	2.0205
16	22.0	-836.7526973	0.6764	-836.7432504	2.0119

TS17	30.8	-836.7380592	0.4609	-836.7215197	2.0115
TS19a	39.0	-836.7239675	0.7124	-836.7124953	2.0114
TS19b	36.8	-836.7275766	0.6883	-836.7146599	2.0115
20	38.4	-836.7257537	0.9337	-836.7227837	2.0117
TS22	23.5	-1010.401261	0.3222	-1010.382172	2.0395
23	3.6	-1010.436109	0.4578	-1010.420988	2.0358
TS29	30.7	-1010.390012	0.3103	-1010.363316	2.0161
30	30.5	-1010.391108	0.6886	-1010.378847	2.0176
TS36a	30.9	-648.5590639	0.4593	-648.5413774	2.0217
TS36b	29.5	-648.5619477	0.1326	-648.5290657	2.0169
37	22.6	-648.5734001	0.8879	-648.5704173	2.0125
TS38a	36.4	-648.5501788	0.6622	-648.5375487	2.0125
TS38b	33.4	-648.5550092	0.7112	-648.5438636	2.0129
39	36.6	-648.5504321	0.7974	-648.5430531	2.0131
TS3a-Ph	21.2	-1067.807276	0.4811	-1067.792427	2.0421
TS3b-Ph	22.9	-1067.804069	0.8092	-1067.798387	2.0422

Computed Coordinates of All Species

1

C	1.09872700	1.38388700	0.05479400
C	2.36486500	0.98424100	-0.16004600
C	2.40141500	-0.48916600	-0.39673900
C	0.93737800	-0.91699500	-0.31690000
N	0.19814800	0.30639200	-0.05943700
C	1.90544600	-1.37284100	0.74255200
C	-1.16128400	0.44373300	0.03206600
O	-1.74157600	1.49967000	0.23090600
O	-1.78071500	-0.75376000	-0.13058000
C	-3.21657300	-0.70974700	-0.07122000
H	0.70402100	2.35887600	0.30487900
H	3.23286600	1.63135200	-0.15324300
H	3.08500600	-0.91229700	-1.12861200
H	0.46705300	-1.62343700	-0.98999400
H	2.18494000	-2.42284700	0.71324800
H	1.83843500	-0.93858100	1.73672200
H	-3.53924100	-1.74101000	-0.21949400
H	-3.54798600	-0.33855100	0.90205800
H	-3.61365000	-0.06419900	-0.85915200

2

C	-0.66950900	1.26662300	0.00002900
C	0.66950900	1.26662200	0.00003100
C	1.15577600	-0.15638000	-0.00039200
N	0.00000000	-0.94217000	-0.00014000
C	-1.15577700	-0.15638000	-0.00038900
O	-2.29996400	-0.56125500	0.00026100
O	2.29996500	-0.56125500	0.00026200
H	-1.35716600	2.10323700	0.00029700
H	1.35716700	2.10323600	0.00030100
H	-0.00000100	-1.95411400	0.00052200

TS3a

C	0.08243300	2.11231600	1.25116400
C	-0.30944700	0.73073500	0.78654400
C	-0.44084900	3.15826600	0.30148600
C	-1.46593500	2.87716500	-0.55995700
C	-2.05933500	1.59928800	-0.61582500
N	-1.51060500	0.57986000	0.12132100
C	2.48728600	0.82175100	-0.46081100
C	1.24470900	0.38486900	-0.87384500
C	3.24770100	-0.31745700	0.06751900

C	1.23111600	-1.11315500	-0.76342300
N	2.40733000	-1.44587800	-0.10852700
O	0.37523100	-1.89791200	-1.14860100
O	4.36694400	-0.36556300	0.55525800
C	-2.16386100	-0.70511500	0.02657300
O	-3.05003600	-0.92312200	-0.76367600
O	-1.69606300	-1.54384100	0.94503200
C	-2.14948200	-2.91242100	0.82070300
H	-0.26448700	2.30781900	2.28514100
H	1.18388900	2.14199300	1.31045000
H	-0.03385500	-0.11421500	1.40054700
H	-0.01700300	4.15815100	0.34166200
H	-1.86799900	3.64650300	-1.21297200
H	-2.92028000	1.34178500	-1.21372200
H	2.90017200	1.82089000	-0.50382100
H	0.57230100	0.88694200	-1.55986800
H	2.70707000	-2.39579600	0.06869100
H	-3.23950200	-2.95153900	0.87176500
H	-1.79273100	-3.32027900	-0.12685700
H	-1.69927800	-3.43406800	1.66456000

TS3b

C	-1.97950300	-1.47517000	-0.98927400
C	-0.93971000	-0.41303800	-0.72115200
C	-3.05081800	-1.47336400	0.07179400
C	-3.27076300	-0.34943200	0.83031100
C	-2.47994200	0.80161500	0.69378800
N	-1.36875900	0.77179800	-0.13977100
C	1.20912100	-0.42232800	1.44514200
C	0.38918900	-1.35976800	0.83498700
C	2.48289000	-0.35885100	0.72247100
C	1.21705400	-2.08119300	-0.18986900
N	2.41176100	-1.37641400	-0.25739800
O	0.91979100	-3.05908400	-0.86063300
O	3.44475800	0.38218700	0.87841500
C	-0.56957000	1.95189700	-0.18033100
O	-0.85389700	2.96045800	0.42816900
O	0.49319200	1.79125400	-0.97213100
C	1.41183500	2.90915000	-1.02456900
H	-2.43045800	-1.31267100	-1.98902000
H	-1.47028800	-2.44486700	-1.05971900
H	-0.16071000	-0.27789200	-1.45774600
H	-3.68115700	-2.35081800	0.18298100
H	-4.07993200	-0.31767600	1.55456400

H	-2.64819600	1.73294700	1.21283100
H	0.99234600	0.20572200	2.29956100
H	-0.46990100	-1.83732500	1.28804900
H	3.18180400	-1.62605500	-0.86449300
H	1.85218900	3.06986200	-0.03873300
H	0.88779400	3.80700600	-1.35871700
H	2.17604200	2.60843900	-1.73972300
4a			
C	0.17455400	2.29362300	1.06402200
C	0.09799200	0.80443900	0.67616800
C	-0.34052000	3.17190100	-0.04231500
C	-1.27153100	2.66526800	-0.92845100
C	-1.76438400	1.35959400	-0.80861000
N	-1.24365600	0.51143400	0.15643700
C	2.57877000	0.61844200	0.07832000
C	1.18598000	0.42673900	-0.40546300
C	3.28367800	-0.64648300	0.10849600
C	1.15659200	-1.07046700	-0.78237700
N	2.36926900	-1.60456400	-0.39200000
O	0.25793500	-1.67529200	-1.33746400
O	4.42993200	-0.90185800	0.45755700
C	-1.83880400	-0.69446900	0.52851800
O	-1.37186000	-1.44457700	1.36578300
O	-2.99843300	-0.89474500	-0.12227500
C	-3.65550300	-2.14459400	0.16734500
H	-0.41669100	2.44618200	1.98192300
H	1.20766500	2.54487900	1.33380900
H	0.24561200	0.17391300	1.55222400
H	-0.01115500	4.20456100	-0.10843600
H	-1.67329700	3.28295900	-1.72665900
H	-2.56185300	0.96546400	-1.42179100
H	3.05348600	1.55098000	0.35260100
H	0.95371000	1.01087500	-1.30690000
H	2.61390800	-2.57849300	-0.52921500
H	-3.01008500	-2.98019500	-0.11295400
H	-3.90052300	-2.20708000	1.23036100
H	-4.56161100	-2.13431000	-0.43875300
4b			
C	0.70429600	-2.18942400	1.03484000
C	0.33625200	-0.75570800	0.61202300
C	1.27646300	-2.96066400	-0.11881800
C	2.00452400	-2.28131200	-1.08294800

C	2.16747800	-0.89769500	-1.03474100
N	1.48844300	-0.13436100	-0.08465900
C	-1.14784800	0.49424400	-1.10313700
C	-0.91983100	-0.75349600	-0.31931500
C	-2.46578800	1.03104000	-0.82903100
C	-2.22731900	-0.90082300	0.48515600
N	-3.04532400	0.14957300	0.11608800
O	-2.50238300	-1.76242800	1.30101100
O	-3.02158600	2.02504800	-1.27812100
C	1.83750200	1.20141000	0.06426600
O	2.72152500	1.74764000	-0.57282100
O	1.08644500	1.81564000	1.00722700
C	1.38318900	3.21068100	1.21484400
H	1.44195800	-2.12720100	1.85210700
H	-0.18618500	-2.67138600	1.45020000
H	0.12778000	-0.14862400	1.49110800
H	1.17704800	-4.04130400	-0.15022900
H	2.49249500	-2.81654300	-1.89271700
H	2.82301700	-0.34258700	-1.69207200
H	-0.46486800	0.94628900	-1.81000800
H	-0.83187300	-1.62833400	-0.98703200
H	-3.97603100	0.28428600	0.49503600
H	1.20426000	3.77656100	0.29741800
H	2.42328100	3.33563000	1.52542000
H	0.70177000	3.53001200	2.00355100

TS5a

C	-1.07599500	-0.00673500	1.31261900
C	1.14024400	1.63230900	-0.00564500
C	0.12827800	2.43085700	-0.55741700
C	-0.70620800	1.96128500	-1.54757000
C	-0.52627600	0.55537800	-2.04512600
C	0.13352600	-0.37205600	-1.00337600
N	1.28987300	0.30302200	-0.39443700
H	1.87421900	2.01129200	0.69089900
H	0.03872700	3.44736800	-0.18498000
H	-1.45875200	2.60073200	-1.99866600
H	-1.47209900	0.11153300	-2.37162900
H	0.11770000	0.55721900	-2.94066100
H	0.50985000	-1.25644400	-1.51473200
C	2.36252100	-0.48962100	-0.00879700
O	2.41508500	-1.69418200	-0.19667300
O	3.33152200	0.23292600	0.59146800
C	4.48524300	-0.51880100	1.01793800

H	4.96586300	-0.99372100	0.15929600
H	5.14831400	0.21638200	1.47420800
H	4.19487600	-1.28265400	1.74331200
H	-0.35730200	0.35641400	2.03395900
H	-0.31627200	-1.83701200	0.49266300
C	-0.80231800	-0.90839000	0.15672400
C	-2.21272900	-1.26589700	-0.34774600
O	-2.49539700	-2.01234300	-1.26765900
O	-3.12162700	0.86896900	2.27960200
C	-2.49985200	0.20297300	1.46108800
N	-3.10806300	-0.56061900	0.43088600
H	-4.11306300	-0.61869600	0.31113500

TS5b

C	0.74323200	-1.13701800	1.15436100
C	-2.24181400	0.21484500	1.04415200
C	-2.92185500	-0.99969000	0.97652900
C	-2.81355300	-1.83469400	-0.12258900
C	-2.01387000	-1.35813900	-1.30127300
C	-0.83149700	-0.46589800	-0.87272400
N	-1.31093100	0.56922200	0.06437700
H	-2.37989600	0.94440200	1.83039000
H	-3.56521300	-1.26042400	1.81253600
H	-3.36874900	-2.76574800	-0.18050100
H	-1.62367600	-2.18954500	-1.89998000
H	-2.65682000	-0.77289000	-1.97951500
H	-0.44827000	0.04347800	-1.75577600
C	0.36584600	-1.30551000	-0.28001300
C	1.69198300	-1.02287900	-1.01775800
O	1.86129600	-0.98633600	-2.22117300
N	2.66117800	-0.83145000	-0.05117500
H	3.63299900	-0.64312200	-0.26951100
C	2.16638400	-0.86850800	1.27286200
O	2.85015100	-0.70416300	2.27420600
H	0.13486100	-2.36662400	-0.46923300
H	0.08955600	-1.23600000	2.01066000
C	-0.72759300	1.82697100	0.14148200
O	-1.07683800	2.69874100	0.91688600
O	0.28230200	1.95505700	-0.75006100
H	1.39864700	3.43917000	0.20435400
C	0.93318700	3.24059800	-0.76411100
H	1.68577100	3.16729300	-1.54933900
H	0.21107600	4.02874500	-0.99088100

6a

C	0.05037900	-1.63132000	1.13836200
C	-0.12480200	-1.25920100	-0.34972200
C	0.17912600	-0.39294400	1.99898800
C	0.02141900	0.84354100	1.50762600
C	-0.30835900	1.04245000	0.03508100
N	-1.06097100	-0.12584000	-0.45098600
C	0.95875600	0.91585400	-0.86677400
C	1.13088100	-0.62016000	-1.02770400
C	2.26620600	1.40700900	-0.25580700
C	2.50087800	-0.92913600	-0.42947000
N	3.07601900	0.28837800	-0.07088800
O	3.03343600	-2.01281800	-0.29753900
O	2.57917500	2.54658900	0.02233300
C	-2.41295800	-0.31059000	-0.34463700
O	-2.97312800	-1.39246600	-0.43963400
O	-3.06226800	0.86950400	-0.17101700
C	-4.49668800	0.77783900	-0.11634900
H	-0.82029600	-2.22001400	1.46038300
H	0.92242100	-2.28464000	1.26562000
H	-0.50443300	-2.10858100	-0.91716400
H	0.39729500	-0.53770700	3.05588200
H	0.14281600	1.72612100	2.13075600
H	-0.85885400	1.96512200	-0.14152300
H	0.79248800	1.43260000	-1.81685200
H	1.15839000	-0.92027400	-2.08026900
H	3.99844700	0.34914500	0.34870700
H	-4.89112500	0.37786200	-1.05420700
H	-4.80795000	0.13531600	0.71124500
H	-4.84128300	1.80075500	0.03984600

6b

C	0.53518100	2.47362700	-0.11864300
C	-0.10618400	1.18863000	-0.68794300
C	0.90503000	2.30872800	1.34001900
C	0.78602100	1.13838200	1.98096700
C	0.25412700	-0.08069800	1.24231400
N	0.62252500	0.01449400	-0.18109000
C	-1.29133000	0.01077900	1.13522300
C	-1.52458400	0.92232600	-0.10328900
C	-1.94974500	-1.32294300	0.77841100
C	-2.38328800	0.08218100	-1.05023200
N	-2.56399400	-1.16440900	-0.45905900
O	-2.83242600	0.41398800	-2.12777400

O	-1.95684100	-2.34186400	1.43824500
C	1.83304800	-0.34700200	-0.71369100
O	2.26151600	0.04863500	-1.78685500
O	2.47619300	-1.23843800	0.08131800
C	3.72204300	-1.73631500	-0.43734900
H	1.43217400	2.71905800	-0.70460800
H	-0.15262400	3.32142800	-0.24724200
H	-0.10232000	1.19944200	-1.77865500
H	1.29663200	3.18204900	1.85915500
H	1.04044900	1.03410300	3.03357000
H	0.59524600	-1.01996200	1.67691900
H	-1.73768400	0.38395600	2.06091700
H	-2.05094500	1.85602800	0.11126800
H	-3.07994900	-1.91181800	-0.91241700
H	4.09468100	-2.42035200	0.32591000
H	4.42563900	-0.91524000	-0.59716400
H	3.55955000	-2.26402200	-1.38079700

TS7a

C	0.63813100	-2.31656800	0.74377500
C	-0.36339300	-1.60183100	-0.12421900
C	1.19195800	-1.33359700	1.75466800
C	0.52969800	-0.19441800	2.07066000
C	-0.68061600	0.18324500	1.41667200
N	-1.15641100	-0.63890200	0.43241000
C	0.63542400	1.35122300	-0.75160600
C	0.85134500	0.15828100	-1.40450800
C	1.87302500	1.74272900	-0.04226200
C	2.25878900	-0.26414300	-1.14592000
N	2.80315600	0.73283700	-0.33295500
O	2.84968100	-1.25703800	-1.54382500
O	2.10304800	2.72194900	0.65271100
C	-2.35708900	-0.29380200	-0.28840500
O	-2.68500700	-0.84257900	-1.31273100
O	-3.03543800	0.66989500	0.33143500
C	-4.26456400	1.08100500	-0.31219400
H	0.19379100	-3.20468800	1.23975800
H	1.43823700	-2.70802800	0.10120900
H	-0.79252000	-2.09740700	-0.98367400
H	2.13501800	-1.56787600	2.24198700
H	0.93009300	0.49884000	2.80454100
H	-1.32672500	0.97189500	1.76429200
H	-0.19491100	2.03723300	-0.85463300
H	0.29283600	-0.25540200	-2.23311700

H	3.73314200	0.69445100	0.06270200
H	-4.05144400	1.46710900	-1.31126900
H	-4.95058100	0.23384400	-0.37924900
H	-4.66867700	1.86192400	0.33059400
TS7b			
C	2.78045100	-0.77723400	-0.90572100
C	1.30124600	-0.55229500	-1.09376800
C	3.08534100	-0.92324900	0.57120500
C	2.10959200	-1.19245500	1.46864200
C	0.73125800	-1.29452300	1.09322500
N	0.42220200	-1.11567000	-0.22628400
C	0.49934600	1.40611600	1.33156300
C	1.07182400	1.71889700	0.12382600
C	-0.97366200	1.50510500	1.20197500
C	-0.00750500	2.08764700	-0.83219800
N	-1.20652000	1.80894500	-0.15343900
O	0.07139500	2.55685600	-1.95535500
O	-1.84884500	1.36963900	2.04399000
C	-0.93757900	-1.31412700	-0.70673900
O	-1.23073200	-1.20964500	-1.87093800
O	-1.74657300	-1.65709600	0.28718900
C	-3.13340200	-1.85739800	-0.07122500
H	3.12720300	-1.66422500	-1.47653700
H	3.32607100	0.06975200	-1.34459000
H	0.89834700	-0.33157400	-2.07307100
H	4.11842000	-0.83177900	0.89810500
H	2.34349800	-1.31663600	2.52257900
H	-0.03387400	-1.70289500	1.73224000
H	0.97863700	1.27546000	2.29080400
H	2.10675300	1.94848000	-0.08707800
H	-2.11043600	2.09865300	-0.50569000
H	-3.62683400	-2.12451800	0.86194700
H	-3.21585400	-2.65957200	-0.80799000
H	-3.54512500	-0.93102600	-0.47645800
8			
C	-1.41955000	-0.02757000	0.19768100
C	-0.76914100	1.12528800	-0.02460200
C	0.63494100	0.80658000	-0.41607700
C	0.63499400	-0.71683300	-0.40015300
O	-0.67104500	-1.15767900	-0.03981000
C	1.43941200	0.02792900	0.62306100
H	-2.43063100	-0.22116000	0.53182600

H	-1.18986600	2.11840400	0.06771000
H	1.15250900	1.39544700	-1.16934000
H	1.09771400	-1.36193200	-1.13900300
H	2.51839100	-0.00822700	0.49336800
H	1.09631700	0.04653600	1.65445500

9

C	-0.66857200	1.25898100	0.00000200
C	0.66857200	1.25898100	0.00000200
C	1.13235400	-0.15829300	-0.00005600
O	0.00000000	-0.97268800	-0.00000300
C	-1.13235400	-0.15829300	-0.00005800
O	-2.24685200	-0.60044000	0.00003700
O	2.24685200	-0.60044000	0.00003600
H	-1.36242000	2.09013900	0.00004600
H	1.36242000	2.09013900	0.00004600

TS10a

C	-2.12924200	0.94132200	-0.64592400
C	-1.87625200	0.52028800	0.77067000
C	-1.32567300	0.00406000	-1.52839400
C	-1.02902600	-1.25477800	-1.11493600
C	-1.30629600	-1.66098500	0.21670300
O	-1.79823600	-0.77264200	1.07538400
C	1.09880200	-0.60987800	1.23584200
C	0.62658300	0.67020100	1.32152300
C	1.84719100	-0.73889100	-0.02219300
C	1.07303300	1.39708400	0.11267400
O	1.79059000	0.50112800	-0.67996800
O	0.90868400	2.54751000	-0.21232600
O	2.43887600	-1.67381200	-0.50234100
H	-3.20922700	0.93121000	-0.90232900
H	-1.79905100	1.98067700	-0.76983600
H	-2.19177200	1.11522300	1.61935900
H	-1.00266100	0.34957000	-2.50621100
H	-0.48918100	-1.94810800	-1.75279200
H	-1.24335600	-2.66110600	0.62001200
H	1.09343500	-1.39087300	1.98361000
H	0.24778100	1.19540100	2.18640900

TS10b

C	2.55812900	1.11893600	-0.10599500
C	1.21569200	0.99427400	-0.76401000
C	2.76960800	-0.14098700	0.71432400

C	2.17277100	-1.30324000	0.34841700
C	1.19861700	-1.32613000	-0.68812100
O	0.83399300	-0.17593000	-1.25326600
C	-0.76532500	-0.74823900	1.07744000
C	-0.56018400	0.60098700	1.12749200
C	-1.83521300	-1.01378900	0.10022300
C	-1.53584300	1.24027800	0.21623000
O	-2.24248900	0.22225600	-0.42608400
O	-1.76555000	2.40469300	0.00315300
O	-2.34514300	-2.04710100	-0.25365200
H	3.36825600	1.26618800	-0.85076400
H	2.56638900	2.01991000	0.51991300
H	0.71205700	1.82564900	-1.24226500
H	3.43257900	-0.10670000	1.57493400
H	2.35718900	-2.22929400	0.88590100
H	0.76618900	-2.19420700	-1.16359800
H	-0.36626300	-1.52351600	1.71518000
H	0.00761100	1.17807400	1.84349900

11a

C	1.91961000	0.87457900	0.66937900
C	1.49839200	0.57224200	-0.77655400
C	1.43525300	-0.21700500	1.59565400
C	0.86691600	-1.33127300	1.11932100
C	0.72128200	-1.51170100	-0.37822000
O	1.76699800	-0.81077100	-1.06127900
C	-0.54608900	-0.78395700	-0.94251400
C	-0.04382100	0.66582300	-1.07025300
C	-1.73614400	-0.69720200	-0.00739300
C	-0.91052400	1.44995400	-0.10063400
O	-1.87693500	0.61247800	0.44686000
O	-0.85593900	2.61236400	0.19014800
O	-2.48878400	-1.56246700	0.34043700
H	3.01595200	0.94285300	0.71465200
H	1.53747900	1.85367500	0.98375800
H	2.07369500	1.16588900	-1.48891100
H	1.57068100	-0.07592500	2.66612100
H	0.49149500	-2.11321200	1.77466800
H	0.77242300	-2.55995600	-0.67705500
H	-0.85433600	-1.24073700	-1.88660400
H	-0.19936300	1.08580500	-2.06868000

11b

C	-2.30564500	1.21983300	-0.00996500
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C	-0.87582800	1.04078400	0.52962700
C	-2.86843100	-0.09825500	-0.48931300
C	-2.19829800	-1.24272500	-0.31305800
C	-0.85308600	-1.21312400	0.38159500
O	-0.81557500	-0.14313400	1.33723400
C	0.25646600	-0.79340200	-0.62511200
C	0.17105600	0.74578600	-0.59557300
C	1.65851900	-1.10463600	-0.12389400
C	1.56722100	1.18858800	-0.18913400
O	2.35691800	0.07902700	0.08495800
O	1.99435500	2.30372600	-0.08399000
O	2.15830600	-2.17414700	0.08083600
H	-2.94502700	1.62888800	0.78548600
H	-2.31139100	1.96400800	-0.81904000
H	-0.57888700	1.88405200	1.15706500
H	-3.84855400	-0.09193200	-0.96276000
H	-2.58248500	-2.19855200	-0.66239400
H	-0.62747900	-2.14092000	0.91118900
H	0.12147400	-1.24881800	-1.60971200
H	-0.09152900	1.22241300	-1.54318400

TS12a

C	-2.03964200	-1.07910200	-0.48924200
C	-0.96152900	-0.14170600	-0.99302700
C	-3.25188700	-0.22391000	-0.26789900
C	-3.05819300	0.95111400	0.42315300
C	-1.76434300	1.47153800	0.51831500
O	-0.81664000	1.04831200	-0.33102400
C	1.99287900	-0.38426800	-1.22344400
C	0.96059400	-1.12590700	-0.68267500
C	2.55326500	0.45733000	-0.18285100
C	0.99657700	-0.89040000	0.79395100
O	1.89342000	0.11644900	1.04079600
O	0.35517200	-1.42633600	1.66694400
O	3.41797500	1.29728100	-0.19247500
H	-2.20766700	-1.87018400	-1.22590000
H	-1.71135900	-1.54926400	0.45057400
H	-0.78777200	-0.00329600	-2.05650900
H	-4.23153000	-0.52670400	-0.62701100
H	-3.87962400	1.53393400	0.83086700
H	-1.45075200	2.32988500	1.09733000
H	2.34928400	-0.35762700	-2.24444000
H	0.55367400	-2.05052400	-1.07651600

TS12b

C	-1.86794100	1.17918800	0.65005700
C	-0.93226000	0.02487800	0.90369400
C	-2.87120100	0.80241100	-0.41471100
C	-3.15308800	-0.52266500	-0.65114500
C	-2.46411100	-1.53307500	0.02953100
O	-1.41765200	-1.23482200	0.83622200
C	1.37631200	-1.04479600	-0.80275400
C	0.55769500	0.06505400	-0.82640900
C	2.58048700	-0.71489800	-0.05293100
C	1.33971700	1.18763600	-0.23852000
O	2.50276600	0.66454500	0.28894100
O	1.06395800	2.36155700	-0.16402200
O	3.53666100	-1.37528900	0.26786000
H	-2.38483700	1.46424100	1.58834200
H	-1.27314800	2.05630300	0.36564400
H	-0.18951200	0.09574300	1.69161100
H	-3.40366200	1.58873500	-0.94113300
H	-3.91892800	-0.81976400	-1.36210400
H	-2.65194600	-2.59607600	-0.02554000
H	1.20324400	-2.02761200	-1.21960000
H	-0.26074100	0.24811200	-1.51008100

13a

C	-1.95488800	1.00168300	0.60913600
C	-0.84962200	-0.04909200	0.77180600
C	-3.24363100	0.31042600	0.26930300
C	-3.19027400	-0.85197600	-0.48210300
C	-1.96528300	-1.40074700	-0.84860300
O	-0.78660700	-0.94564000	-0.36301600
C	1.59793800	-0.55128600	1.17045600
C	0.58750800	0.50764600	0.92563900
C	2.55506800	-0.57278200	0.10315900
C	1.10842300	1.15235800	-0.37102300
O	2.21574500	0.47596200	-0.80391500
O	0.65984200	2.10606100	-0.95080600
O	3.51646000	-1.27614600	-0.10608400
H	-2.03972800	1.57290500	1.54203500
H	-1.67000500	1.71737600	-0.17608300
H	-1.06801300	-0.66605100	1.65414900
H	-4.19190200	0.74523100	0.56942800
H	-4.09333500	-1.34024800	-0.83715400
H	-1.83039800	-2.21081000	-1.55530300
H	1.62115100	-1.25304700	1.99417100

H	0.55727800	1.27535300	1.71270700
13b			
C	-1.86909900	1.18902900	0.56159600
C	-0.82813600	0.09683500	0.83502100
C	-2.71634900	0.81336300	-0.61786000
C	-2.97249600	-0.53439800	-0.83764000
C	-2.38016200	-1.50356400	-0.03916300
O	-1.44810500	-1.21640800	0.90869500
C	1.15541100	-1.14566300	-0.20651100
C	0.28146800	0.05276400	-0.25030600
C	2.53293600	-0.74356500	-0.13205600
C	1.29581400	1.19655400	-0.11205600
O	2.56661100	0.68115400	-0.08516800
O	1.07742500	2.37700600	-0.03281700
O	3.55841100	-1.38333600	-0.10630200
H	-2.49536400	1.29544000	1.46233500
H	-1.35632600	2.14534000	0.41741600
H	-0.37095400	0.22129300	1.81954200
H	-3.17190100	1.58330400	-1.23220700
H	-3.65093000	-0.86425800	-1.61943600
H	-2.61461700	-2.56120500	-0.07297600
H	0.84287700	-2.18010300	-0.22423300
H	-0.21384800	0.16473600	-1.23185900
TS13a			
C	0.67452700	0.88379800	-0.92875500
C	-2.54964500	0.46083500	-0.87049300
C	-2.71251000	0.97911800	0.41937500
C	-2.08415500	0.38297800	1.48261800
C	-1.04648100	-0.67533100	1.26458000
C	-0.84563900	-1.09456800	-0.21986900
O	-1.89349900	-0.68460600	-1.11334000
H	-3.07923700	0.82501600	-1.74382000
H	-3.38091100	1.82518900	0.54850300
H	-2.27713100	0.70343100	2.50219700
H	-0.09024400	-0.30042000	1.66181100
H	-1.27685500	-1.56188000	1.87034600
H	-0.83142900	-2.18222100	-0.30290200
C	0.49439000	-0.58095000	-0.87319100
H	0.54187900	-1.07359000	-1.85380800
H	0.15728300	1.58148300	-1.57264700
C	1.77894400	1.27134200	-0.10791400
O	2.26663400	2.34551600	0.16011700

O	2.36282500	0.06830700	0.43672300
C	1.68844200	-1.02685100	-0.01777400
O	1.99521500	-2.15662100	0.26635700

TS13b

C	-2.09234900	1.31404000	-0.12186600
C	-0.89424700	0.67013100	0.59091400
C	-2.83373100	0.28607600	-0.93136400
C	-2.82851300	-1.02622600	-0.47988400
C	-2.09870800	-1.38867100	0.64627300
O	-1.27834000	-0.51797900	1.30031600
C	0.85352600	-1.00405000	-0.47053900
C	0.30037500	0.37059600	-0.40612400
C	2.26723200	-0.97736500	-0.18885600
C	1.54151900	1.19414200	-0.04026500
O	2.63775600	0.36972500	0.05807700
O	1.60142600	2.37761200	0.15708500
O	3.08657400	-1.86467900	-0.15051400
H	-2.75525500	1.75447900	0.64022300
H	-1.73442200	2.15082600	-0.73421900
H	-0.51851000	1.33550700	1.36978000
H	-3.41881400	0.58554300	-1.79499500
H	-3.41141100	-1.79720400	-0.97661000
H	-2.13291100	-2.35864700	1.12747700
H	0.32632700	-1.91067900	-0.73300200
H	-0.02496300	0.69069800	-1.40810300

TS14

C	0.46751700	2.27116900	1.01116400
C	-0.04717000	0.86319800	0.81305700
C	-0.12227100	3.18445200	-0.03058900
C	-1.21440300	2.82902000	-0.76086500
C	-1.86456600	1.57924400	-0.57280700
N	-1.30239700	0.68629000	0.27528900
C	2.57984200	0.50805200	-0.58169200
C	1.26266800	0.17600400	-0.84363100
C	3.25790500	-0.64921600	0.00459600
C	1.10590500	-1.29718300	-0.57586300
N	2.29091300	-1.69379800	0.01152900
O	0.13599900	-2.00694300	-0.81282500
O	4.40326400	-0.78413400	0.40960400
C	-1.95323600	-0.58851400	0.55681100
O	-1.68741300	-1.23096400	1.53929300
O	-2.85732700	-0.87561200	-0.36868300

C	-3.48901200	-2.17156000	-0.22997200
H	0.28140800	2.65579800	2.03241400
H	1.57067900	2.22256100	0.92284500
H	0.20574200	0.11573600	1.55365200
H	0.32532300	4.16539600	-0.17152700
H	-1.64109400	3.51201900	-1.48971800
H	-2.78750800	1.29723400	-1.05349900
H	3.09475800	1.43789500	-0.78246300
H	0.60374200	0.65567700	-1.56077800
H	2.49641300	-2.64283200	0.29543300
H	-2.72513200	-2.94824700	-0.29956800
H	-4.01047800	-2.23344000	0.72768600
H	-4.18872800	-2.23201000	-1.06257800

TS15a

C	2.33877700	-2.45549700	0.58559700
C	2.42794500	-0.96131700	0.56224600
C	1.45512800	-2.95568400	-0.53728300
C	0.54329200	-2.15272200	-1.10746200
C	0.39230700	-0.74817100	-0.72252900
N	1.53257000	-0.20951300	-0.10140300
C	-1.11744700	-0.80801100	0.69921600
C	-2.31115500	-1.35736700	0.21377800
C	-1.37419600	0.67244000	0.89504800
C	-3.24082700	-0.29172900	-0.10132900
N	-2.58546500	0.92108200	0.29282300
O	-4.36969200	-0.31174000	-0.57612000
O	-0.64884200	1.49229600	1.44653500
C	1.77738900	1.22513700	-0.09709800
O	2.64406000	1.72583200	0.57463200
O	0.98169400	1.84219300	-0.95953600
C	1.03363600	3.28874600	-0.92216700
H	3.35558800	-2.86986500	0.51386700
H	1.96409500	-2.81266700	1.56357700
H	3.22821800	-0.41805000	1.04534600
H	1.56455600	-3.98981200	-0.85290200
H	-0.13445000	-2.52351100	-1.87122400
H	-0.05189400	-0.07614800	-1.44308200
H	-0.45925100	-1.30463100	1.40776000
H	-2.54661900	-2.40108500	0.05501800
H	-3.05648000	1.81633900	0.31792600
H	0.70729600	3.63043400	0.06194000
H	2.04922000	3.63130900	-1.13065800
H	0.34313700	3.61311900	-1.69970000

TS15b

C	3.37756500	-0.58544000	0.79896200
C	2.57978000	0.66178500	0.58989500
C	2.98686500	-1.64674700	-0.20601500
C	1.79674800	-1.61474700	-0.82614400
C	0.83147400	-0.53352500	-0.60178500
N	1.41339900	0.64861800	-0.09523000
C	-1.30182900	-0.27123900	1.38459200
C	-0.48251200	-1.23838800	0.77150600
C	-2.57187100	-0.20272100	0.69172800
C	-1.37771800	-1.99391800	-0.19738500
N	-2.54155300	-1.25591500	-0.27085400
O	-1.12039600	-3.00905800	-0.82670100
O	-3.53109800	0.54954800	0.83274700
C	0.72240000	1.90693200	-0.20993500
O	1.16124700	2.93545100	0.25196800
O	-0.42399400	1.76016400	-0.86238400
C	-1.25761100	2.94256300	-0.95560200
H	4.44721200	-0.33922600	0.72814600
H	3.24774000	-0.96346000	1.83191200
H	2.90109000	1.63095700	0.94533700
H	3.69192500	-2.45102600	-0.39855700
H	1.48375100	-2.40882000	-1.49613700
H	0.14194300	-0.32697200	-1.40932700
H	-1.05753800	0.37338600	2.21923000
H	0.26963000	-1.80455300	1.31347000
H	-3.34259800	-1.52093300	-0.82969100
H	-1.50517400	3.29575300	0.04670100
H	-0.73321700	3.71967300	-1.51576500
H	-2.15350800	2.61012600	-1.47666700

16

C	-2.13338800	2.55612600	0.63874800
C	-2.16311900	1.07040000	0.80755300
C	-1.27026400	2.99867700	-0.51298400
C	-0.41032000	2.17005300	-1.10918100
C	-0.22843000	0.74271200	-0.65033000
N	-1.47137100	0.25556400	-0.03928100
C	0.96381400	0.68290700	0.40891500
C	2.25001300	1.17884600	-0.12421800
C	1.30234600	-0.75570200	0.86768900
C	3.24567700	0.14567500	-0.08573000
N	2.60237700	-0.99128000	0.49712200

O	4.42367600	0.14315400	-0.43130400
O	0.56521600	-1.53364200	1.45306300
C	-1.85458500	-1.10416200	-0.10750300
O	-2.79461800	-1.55676200	0.51036700
O	-1.09056100	-1.78335000	-0.97516500
C	-1.32878700	-3.20593400	-1.01626600
H	-3.16776400	2.91679200	0.49956200
H	-1.79988500	3.04865700	1.56827000
H	-2.89581600	0.58210200	1.43621000
H	-1.36963400	4.02872600	-0.84817700
H	0.22027600	2.50077400	-1.92998400
H	0.01283800	0.09608400	-1.49181900
H	0.57815400	1.24722600	1.27626400
H	2.45865300	2.17912600	-0.47860100
H	3.09675700	-1.84888800	0.71266000
H	-1.09751300	-3.64172700	-0.04177500
H	-2.36904400	-3.40788800	-1.28124500
H	-0.65151400	-3.58375700	-1.78209400

TS17

C	0.75309300	-0.33477000	0.68095500
C	-0.43965600	0.46055500	0.65399300
C	0.02150200	1.84941400	0.23805700
C	1.47322600	1.70815500	-0.16897500
N	1.80579700	0.31128000	0.08590200
C	1.11532800	2.50558600	1.05792800
C	3.06688500	-0.19841200	-0.20072300
O	3.96057200	0.46669700	-0.68920400
O	3.14755800	-1.50307500	0.12935700
C	4.41967800	-2.12884300	-0.14042100
H	0.87021200	-1.35414100	1.01902400
H	-1.08283800	0.39798200	1.53189800
H	-0.66760700	2.47342400	-0.32005400
H	1.93515000	2.14521600	-1.04473300
H	1.20116800	3.58537300	0.97540200
H	1.37271600	2.09735000	2.03238800
H	4.30090400	-3.16200400	0.18543200
H	4.64410300	-2.08189100	-1.20866300
H	5.21234200	-1.63189600	0.42385700
C	-1.56217900	-0.18190400	-0.61307200
C	-2.07691200	-1.49580800	-0.34535900
C	-2.79574700	0.73179400	-0.52082100
C	-3.43855300	-1.41474200	0.11924400
N	-3.78698500	-0.02738500	0.05169400

O	-4.21975000	-2.28217700	0.49360400
O	-2.87693100	1.90207100	-0.86046000
H	-0.95493000	-0.00627000	-1.50164500
H	-1.54758900	-2.43667500	-0.42237800
H	-4.72689800	0.31197700	0.21509600

TS18

C	-2.15555400	-1.32466000	-0.94900200
C	-0.97511700	-0.40204500	-0.68841100
C	-3.20131100	-1.14755000	0.12673300
C	-3.26813500	-0.00842900	0.86299500
C	-2.33553000	1.04858100	0.66305900
N	-1.29005600	0.85555200	-0.16635300
C	1.06734300	-0.50266500	1.47610300
C	0.18876700	-1.33876700	0.77292500
C	2.35214000	-0.49743200	0.81213700
C	1.02874000	-2.10653800	-0.22632600
N	2.25162500	-1.47120600	-0.23256400
O	0.69355100	-3.06003100	-0.91692700
O	3.37654300	0.14925100	1.01941500
C	-0.33882900	1.95107900	-0.25017300
O	-0.52880700	3.01198500	0.29336300
O	0.70446500	1.60827200	-0.98564700
C	1.78907000	2.57276500	-1.05030900
H	-2.60639400	-1.15668000	-1.94671300
H	-1.77508600	-2.35434400	-0.97416600
H	-0.24476000	-0.34229000	-1.48324700
H	-3.93862100	-1.93351500	0.27176100
H	-4.04531600	0.13858400	1.60689100
H	-2.40226400	2.01744700	1.13644000
H	0.86459600	0.07515900	2.36844400
H	-0.65119200	-1.84312400	1.23459500
H	3.04426500	-1.77729900	-0.78210200
H	2.28909400	2.60956300	-0.08079100
H	1.39714300	3.55278900	-1.32757400
H	2.46203800	2.18144600	-1.81113200

TS19a

C	0.03494700	0.96285400	-0.46044700
C	-0.26332300	2.37899400	-0.41567100
C	-1.52655400	2.61955100	0.29197400
C	-2.09200600	1.23542100	0.60218200
N	-1.15286800	0.30159500	0.01520600
C	-2.83023200	2.11487400	-0.35794500

C	-1.46898200	-0.97152400	-0.40170400
O	-0.76174700	-1.65380800	-1.12344000
O	-2.66704000	-1.35382800	0.09266300
C	-3.05957700	-2.70072800	-0.23152200
H	0.42919600	0.51215200	-1.36799900
H	0.46207400	3.14779100	-0.65402000
H	-1.61527300	3.44478300	0.99395800
H	-2.50880600	0.97171200	1.56842900
H	-3.74244000	2.58782600	-0.00349300
H	-2.81541000	1.86004200	-1.41373700
H	-4.03300500	-2.83422700	0.24145000
H	-3.13544600	-2.82690900	-1.31453500
H	-2.33339500	-3.41156900	0.17024200
C	1.40579500	0.70038700	0.69504900
C	2.65838300	1.09881800	0.10961400
C	1.54560200	-0.81405300	0.88187400
C	3.39733300	-0.07877800	-0.32418500
N	2.64673300	-1.18826300	0.13348500
O	4.45881500	-0.16339900	-0.92790000
O	0.84651900	-1.53909300	1.56293300
H	1.03080900	1.20589400	1.58295000
H	3.03244800	2.10340200	-0.04118400
H	2.95149600	-2.14809100	0.02773800

TS19b

C	0.01577600	0.76251500	-0.43998400
C	-0.16692000	2.19663100	-0.48714200
C	-1.37356400	2.58724300	0.25450400
C	-2.05972000	1.28526000	0.64047300
N	-1.21822200	0.23114300	0.10246600
C	-2.73086700	2.18020800	-0.35496400
C	-1.65495300	-1.02836900	-0.22184400
O	-1.00566300	-1.84346200	-0.85738600
O	-2.89620900	-1.25232800	0.27388100
C	-3.43895400	-2.55729800	-0.00269900
H	0.35102500	0.23829500	-1.33332100
H	0.60791600	2.87953000	-0.81017700
H	-1.36527100	3.45056200	0.91501300
H	-2.49055400	1.11251800	1.62094700
H	-3.59238900	2.74822200	-0.01318900
H	-2.75463600	1.87655200	-1.39754000
H	-4.42739100	-2.55672300	0.45772100
H	-3.51508700	-2.71832400	-1.08099600
H	-2.80836700	-3.33445800	0.43652600

C	1.55296700	-1.02217200	0.87290400
C	1.34164300	0.39292900	0.72234600
C	2.74086400	-1.42589800	0.13971800
C	2.61138900	0.90416900	0.03889800
N	3.30499300	-0.21894400	-0.36183200
O	2.93338600	2.06335600	-0.16449800
O	3.24596200	-2.52818200	-0.01390500
H	0.93404700	-1.72862800	1.40779700
H	1.01843300	0.96617300	1.58972700
H	4.18909900	-0.18549000	-0.85494100

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C	0.07652400	0.92403400	-0.38119800
C	-0.26262400	2.37473000	-0.38094200
C	-1.54053500	2.61095800	0.29986500
C	-2.09408400	1.23883300	0.64768400
N	-1.14820600	0.28475300	0.10357000
C	-2.83472700	2.07683400	-0.35005700
C	-1.49867800	-0.95631000	-0.36923200
O	-0.79551800	-1.64358700	-1.09300300
O	-2.72377300	-1.31716700	0.07796200
C	-3.15181900	-2.63509400	-0.30980100
H	0.34744600	0.50587900	-1.35402000
H	0.44708400	3.15153900	-0.64071600
H	-1.64952000	3.45552900	0.97597600
H	-2.52051300	1.00864300	1.61874000
H	-3.75770400	2.55081600	-0.02469300
H	-2.80335000	1.78495900	-1.39597000
H	-4.14075300	-2.75472600	0.13420600
H	-3.20534300	-2.71635400	-1.39858400
H	-2.46046400	-3.38708100	0.07869300
C	1.33991600	0.65265700	0.60395600
C	2.61171200	1.09415200	-0.00781300
C	1.58270200	-0.85131500	0.84928500
C	3.44152000	-0.05635300	-0.32991500
N	2.74729200	-1.17735500	0.17195900
O	4.52795400	-0.10106600	-0.89265600
O	0.91727500	-1.60285400	1.53139300
H	1.08610400	1.13644000	1.55269300
H	2.91124000	2.10846500	-0.23967100
H	3.12522000	-2.11726600	0.14408800

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C	0.60266700	0.18746000	0.06108300
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C	-0.60262900	0.18794200	-0.06072900
C	-2.03445500	0.24882800	-0.27843700
O	-2.55725300	0.98526600	-1.08955500
O	-2.68659100	-0.60718600	0.52608200
C	-4.12463800	-0.62191000	0.38776000
C	2.03440100	0.24722900	0.27950100
O	2.55665700	0.97896000	1.09519600
O	2.68693600	-0.60403700	-0.52959000
C	4.12487600	-0.61951800	-0.39062500
H	-4.46956500	-1.36418300	1.10693600
H	-4.53452400	0.36463000	0.61787800
H	-4.40162400	-0.90596800	-0.63043100
H	4.46994900	-1.35937100	-1.11221900
H	4.53501900	0.36774400	-0.61722600
H	4.40141500	-0.90706700	0.62668700

TS22

C	-1.20175000	0.90102700	2.70610500
C	0.07275500	0.40915500	2.78044400
C	0.42320000	-0.88032100	2.07784700
C	-0.42425300	-0.98881300	0.84181400
C	0.79895900	0.49206500	-0.56324900
C	1.96983300	0.10514900	-0.65006000
C	-2.16400000	0.31979000	1.85593000
N	-1.73993100	-0.60282900	0.93523400
C	3.22338000	-0.57761800	-0.68027800
O	-1.34521600	1.07960700	-1.41534500
O	0.13395000	2.69343900	-0.84459000
C	-0.83127200	3.68532000	-1.24864700
C	-2.71415200	-1.01323100	-0.05074000
C	-0.25370100	1.41064600	-0.98668300
O	3.47620000	-1.53274900	-1.40156900
O	4.11873500	-0.02796800	0.18332100
C	5.41871200	-0.64393800	0.19665000
O	-3.84774800	-0.59782400	-0.05628800
O	-2.20442300	-1.91777800	-0.88017900
C	-3.06026800	-2.30291100	-1.97779700
H	-1.49908200	1.76912900	3.28816400
H	0.82204000	0.90413000	3.39209700
H	0.29790600	-1.75316900	2.75231700
H	1.47727700	-0.89435900	1.76842700
H	-0.22526200	-1.75263000	0.10793500
H	-3.19580100	0.62608100	1.78089100
H	-1.05529500	3.58508300	-2.31396500

H	-1.75319500	3.57630600	-0.67155000
H	-0.35503800	4.64409000	-1.04262200
H	5.88464200	-0.57459400	-0.79029300
H	5.34293800	-1.69613300	0.48542100
H	5.99318400	-0.08208600	0.93392500
H	-3.98143100	-2.74971200	-1.59683900
H	-2.47888700	-3.02853400	-2.54556500
H	-3.29111800	-1.42554900	-2.58579400

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C	-0.36361000	2.54128600	-1.64970200
C	0.88430800	2.84071200	-1.18211100
C	1.28340400	2.40819400	0.19092700
C	0.59017300	1.10886300	0.64676800
C	1.16834400	-0.16978200	0.03037900
C	0.43556700	-1.01248400	-0.68340500
C	-1.25997300	1.78888000	-0.86375100
N	-0.87009400	1.18479000	0.29002200
C	-0.82034700	-1.16348600	-1.30157200
O	3.25520000	0.24668400	1.12446300
O	3.09221300	-1.53234400	-0.25806500
C	4.45706900	-1.86245700	0.04869800
C	-1.85623800	0.54161700	1.06558300
C	2.59726500	-0.44237000	0.35546200
O	-1.18809300	-0.48045700	-2.27234100
O	-1.58521700	-2.16638300	-0.77561200
C	-2.84585400	-2.39415700	-1.42799700
O	-3.03403500	0.51899700	0.76734200
O	-1.32267600	-0.00209100	2.16766900
C	-2.23590700	-0.75736700	2.99016900
H	-0.71459900	2.88579800	-2.61650200
H	1.56776000	3.44747100	-1.76983200
H	1.01366000	3.20665900	0.90341700
H	2.36339600	2.27532200	0.28766600
H	0.65128400	1.05631300	1.73434800
H	-2.30691500	1.68097900	-1.11119100
H	5.12510600	-1.04788800	-0.24525900
H	4.57343300	-2.05538500	1.11885200
H	4.66965700	-2.76187300	-0.53002800
H	-2.69543200	-2.62102700	-2.48745000
H	-3.49730000	-1.52157700	-1.32900700
H	-3.28114100	-3.25266900	-0.91375200
H	-3.06021000	-0.12220900	3.32277600
H	-1.63815000	-1.09557900	3.83625300

H	-2.62424600	-1.60780600	2.42522800
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O	-1.52194900	-2.82933100	-0.81628100
O	-2.87119800	-1.05644700	-0.42134300
C	-3.99107900	-1.80924000	-0.92476000
O	-2.02085300	1.55814200	-1.44997300
O	-1.30708500	2.65822400	0.39757400
C	-2.13225800	3.78006300	0.02709600
O	3.09901000	-1.48123800	-1.00934200
O	3.21768300	0.78271500	-0.78454400
C	4.33957800	0.77955700	-1.68419600
C	0.65269700	0.81652900	2.24124400
C	0.91123300	0.84240400	0.73695500
C	0.47937400	-0.36577200	2.84779700
C	0.54104700	-1.67872400	2.09205300
C	0.70948400	-1.44909300	0.56753800
N	1.68461600	-0.36192100	0.40902200
C	-0.55370700	-0.81246600	-0.02419700
C	-0.43136200	0.52907800	0.03307300
C	2.68935700	-0.44169400	-0.51796200
C	-1.35526700	1.59060700	-0.43636500
C	-1.67833000	-1.67115500	-0.47026700
H	-4.84873700	-1.14359700	-0.82826000
H	-4.13424800	-2.71872600	-0.33505200
H	-3.82447100	-2.07605700	-1.97153000
H	-1.97097200	4.52551700	0.80604100
H	-1.82955400	4.16667500	-0.94965500
H	-3.18284500	3.48090800	-0.01140000
H	4.62680300	1.82700100	-1.78522900
H	5.16250100	0.19344500	-1.26648600
H	4.05351400	0.36274400	-2.65319500
H	0.57086300	1.76065400	2.77179500
H	1.40446300	1.75099300	0.39909300
H	0.27636700	-0.41254100	3.91636100
H	-0.36186200	-2.27425700	2.29030300
H	1.38927000	-2.27659100	2.45363300
H	1.02711000	-2.34981500	0.04363100
TS26			
C	0.78961700	-0.45262200	2.48605700
C	-0.48428600	-0.50447100	2.94017400
C	-1.52425600	0.49394300	2.47920500
C	-1.07217300	1.10052500	1.17733000

C	-0.94776600	-0.81265000	-0.36912600
C	0.23315400	-1.13666400	-0.51764500
C	1.19882600	0.48564200	1.48948000
N	0.25427600	1.32219600	0.96927100
C	1.56763400	-1.51330600	-0.86672600
O	-3.14426100	-1.36711200	0.31287300
O	-2.79433700	-0.37403700	-1.69753300
C	-4.21423900	-0.40454500	-1.93601300
C	0.59669500	2.23127100	-0.10867200
C	-2.38542700	-0.89921300	-0.52082400
O	2.24564900	-0.95987400	-1.72315700
O	2.00205200	-2.58346900	-0.14837700
C	3.32860900	-3.03949300	-0.46247400
O	-0.23607900	2.86566800	-0.70711900
O	1.90870000	2.27065100	-0.30358400
C	2.35079000	3.06164000	-1.43131100
H	1.53412900	-1.16400300	2.83085100
H	-0.78007400	-1.26969800	3.65324900
H	-1.71242100	1.26902200	3.25127800
H	-2.48914100	-0.00216100	2.31304900
H	-1.73014900	1.73717000	0.60161400
H	2.22710500	0.68043700	1.23377600
H	-4.57877800	-1.43526700	-1.93724400
H	-4.74395200	0.16551500	-1.16760400
H	-4.34762100	0.05365500	-2.91631500
H	4.06453800	-2.25562400	-0.25953100
H	3.39646000	-3.33079300	-1.51426200
H	3.49571500	-3.90045100	0.18604100
H	1.94525100	2.63892600	-2.35257200
H	3.43707100	2.98565200	-1.41661700
H	2.02507300	4.09729900	-1.31216100

TS27

C	-1.14642800	0.55423300	2.79069600
C	0.12310400	0.05347700	2.76184500
C	0.42905100	-1.16908900	1.92874500
C	-0.42923400	-1.08715500	0.70048900
C	0.77970300	0.54041200	-0.46969000
C	1.95240600	0.17217800	-0.61995400
C	-2.14054400	0.07153200	1.90907600
N	-1.73805200	-0.71112800	0.87309600
C	3.19680800	-0.51234400	-0.74079900
O	-1.37643200	1.27597100	-1.17606100
O	0.20094400	2.78266800	-0.58260800

C	-0.73311900	3.83816800	-0.88483700
C	-2.73652900	-0.97739100	-0.15091800
C	-0.25077700	1.52885800	-0.78251000
O	3.43750200	-1.37799300	-1.57226700
O	4.10562200	-0.07544700	0.17413200
C	5.39924300	-0.69932500	0.10223800
O	-3.86322400	-0.55464300	-0.08080500
O	-2.24771000	-1.76665000	-1.09803100
C	-3.12288600	-1.99866200	-2.22426700
H	-1.41471200	1.36263400	3.46538500
H	0.90312300	0.49107400	3.37924600
H	0.27998800	-2.10614100	2.50491700
H	1.47921200	-1.17891100	1.60585000
H	-0.25020500	-1.73846000	-0.13878500
H	-3.17229200	0.38708400	1.90017400
H	-1.00710600	3.81142100	-1.94288600
H	-1.63386500	3.73636700	-0.27386900
H	-0.20426500	4.76115800	-0.64621400
H	5.85320700	-0.52815800	-0.87788000
H	5.31820600	-1.77604300	0.27741000
H	5.98904900	-0.22501600	0.88754400
H	-4.03954600	-2.49027000	-1.89071600
H	-2.55366300	-2.64284800	-2.89329900
H	-3.35916500	-1.04659600	-2.70411800

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C	0.57541000	-1.94209700	-2.29861300
C	-0.61355300	-2.23726000	-1.70006700
C	-0.81265400	-2.00330000	-0.23973300
C	0.12370500	-0.90776000	0.30187300
C	-0.46819100	0.52154300	-0.02605100
C	-1.73463300	0.77900000	0.22555400
C	1.65723300	-1.47338500	-1.51304600
N	1.48153400	-1.12605800	-0.23609600
C	-2.91402200	0.29000700	0.82551000
O	1.69082300	1.53553900	-0.37367500
O	-0.15518100	2.65464900	-1.00552600
C	0.68717000	3.75450400	-1.38698600
C	2.65658200	-0.73590400	0.50091300
C	0.46851700	1.58893500	-0.47663200
O	-3.15093900	0.30393300	2.03722500
O	-3.85089100	-0.13189400	-0.09810400
C	-5.13478600	-0.46803300	0.44478300
O	3.76544500	-0.78717700	0.02510700

O	2.34274400	-0.42409700	1.75310800
C	3.43213000	0.07739800	2.55879700
H	0.75028600	-2.12871000	-3.35296800
H	-1.41926800	-2.68924300	-2.27322900
H	-0.70062300	-2.95266400	0.31059100
H	-1.83851300	-1.66772800	-0.04652900
H	0.19944600	-0.99072000	1.38381700
H	2.66987500	-1.39148100	-1.89004800
H	1.23640400	4.13593700	-0.52156400
H	1.39887600	3.44685400	-2.15853900
H	0.00529600	4.51288400	-1.77326500
H	-5.57640000	0.39254000	0.95652900
H	-5.06005100	-1.29942900	1.15307600
H	-5.74531700	-0.75325300	-0.41424700
H	4.22391300	-0.67185000	2.62873200
H	2.99132200	0.27451800	3.53524000
H	3.82057000	0.99524500	2.11219200

TS29

C	-0.17374900	-0.71671900	-0.69045500
C	-0.22755100	-0.54266500	-2.10814300
C	-1.59850600	-0.39774000	-2.58399500
C	-2.47009500	-0.53923500	-1.34154300
N	-1.54917900	-0.75963800	-0.24916900
C	-2.53458500	-1.61423600	-2.37505500
C	-1.99538200	-1.04385100	1.01712200
O	-3.17392000	-1.08434100	1.33221700
O	-0.95880100	-1.26408500	1.85502600
C	-1.30790000	-1.53871700	3.22275900
H	0.46030700	-1.47822700	-0.24034000
H	0.66025900	-0.43314200	-2.71922500
H	-1.84068500	0.29710900	-3.38146500
H	-3.30926900	0.11555700	-1.13889200
H	-3.40638400	-1.63284200	-3.02347000
H	-2.09189600	-2.58232900	-2.15918000
H	-0.35527300	-1.68363900	3.73242900
H	-1.85261900	-0.69443700	3.65334800
H	-1.92327600	-2.44003900	3.28621700
C	1.91108700	0.62385000	0.22336100
C	0.67293900	0.71880500	-0.11688300
C	-0.19246300	1.92923100	-0.15675900
O	-0.96857000	2.18412700	-1.05901300
O	-0.00592100	2.71613000	0.91597500
C	-0.76622700	3.94083000	0.93240900

C	2.96227200	-0.35243200	0.25492900
O	2.90608200	-1.38380200	0.91609100
O	4.03061400	-0.00177700	-0.50106400
C	5.13197700	-0.92824700	-0.49266800
H	-0.47636000	4.44124200	1.85649100
H	-0.51549800	4.55524300	0.06362100
H	-1.83777000	3.72416200	0.92868800
H	5.89066800	-0.47538500	-1.13170500
H	5.51226400	-1.05993700	0.52400000
H	4.82302100	-1.89911300	-0.89067300

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C	0.29230800	-0.42420600	0.83561500
C	0.55240100	0.03481600	2.21004600
C	1.97474600	0.23721500	2.45656600
C	2.67575600	-0.14358600	1.16666700
N	1.63234000	-0.56541100	0.25855600
C	2.89841600	-1.00600500	2.36722100
C	1.93928800	-1.23011800	-0.89955300
O	3.07636100	-1.41753200	-1.30368500
O	0.81577100	-1.63495200	-1.53644800
C	1.01630000	-2.31589900	-2.78615200
H	-0.27820300	-1.35118600	0.74013000
H	-0.24557900	0.31872700	2.88590700
H	2.31462600	1.06953000	3.06503400
H	3.47098700	0.45617600	0.73885700
H	3.84885900	-0.91246500	2.88638800
H	2.44559300	-1.99290200	2.39609700
H	0.01395600	-2.56662100	-3.13400600
H	1.52173700	-1.66047200	-3.50054700
H	1.61288400	-3.21993700	-2.63792300
C	-1.87163200	0.46471400	-0.18530700
C	-0.60946100	0.67452100	0.06999500
C	0.08705600	1.96363000	-0.23498600
O	0.98432200	2.42688900	0.44389600
O	-0.40084400	2.55972600	-1.33650900
C	0.18761400	3.83146100	-1.67295200
C	-2.89901900	-0.52724800	-0.01408500
O	-2.84818700	-1.64671000	-0.50838100
O	-3.94058000	-0.07407200	0.72271700
C	-5.02625400	-1.00209800	0.90673600
H	-0.33741400	4.15807600	-2.57074800
H	0.04297000	4.54509000	-0.85743600
H	1.25668100	3.71593200	-1.87013100

H	-5.76525300	-0.46250400	1.49954000
H	-5.44491300	-1.29485100	-0.06001100
H	-4.68317000	-1.89468600	1.43738500
TS31			
C	-1.60313300	0.99181900	-0.23112500
C	-0.36144500	1.08227900	-0.21376100
C	0.78784100	1.79032200	-0.77623600
O	1.80297200	1.25993200	-1.19404200
O	0.58438800	3.12325300	-0.79542600
C	1.63732100	3.90904800	-1.38562400
C	-2.90691100	0.45888700	-0.04334500
O	-3.41181500	-0.42979700	-0.72605100
O	-3.56275600	1.06830100	0.98266100
C	-4.90348900	0.61033100	1.22151500
H	1.29195400	4.94114800	-1.32060900
H	2.56919700	3.77720100	-0.82902700
H	1.79225400	3.61741200	-2.42787300
H	-5.26537900	1.21029800	2.05751100
H	-5.52683700	0.76729100	0.33661100
H	-4.90958800	-0.45250200	1.48113900
C	3.58890000	-0.32218700	0.92450900
C	2.75072900	-1.35195100	0.23709200
C	2.82312200	0.23782100	2.10733800
C	1.47444600	0.20300300	2.13249300
C	0.68842600	-0.45453600	1.11148900
N	1.42843300	-1.35569800	0.32685200
C	0.73363000	-2.36115100	-0.48542600
O	1.32930200	-3.17288500	-1.15011300
O	-0.57087300	-2.22015500	-0.37389600
C	-1.39771200	-3.07758600	-1.20266200
H	4.53679100	-0.78665500	1.23277100
H	3.86603900	0.46893500	0.20479700
H	3.17784800	-2.10488900	-0.41244700
H	3.38601100	0.68879600	2.91987200
H	0.92276000	0.65356800	2.95380300
H	-0.29290600	-0.82051300	1.36439500
H	-1.01901600	-3.07250200	-2.22627700
H	-1.37968300	-4.09308400	-0.79949900
H	-2.38856100	-2.63040300	-1.14573700
32			
C	1.32643700	-1.23373900	-0.45291000
C	0.07849200	-0.88307700	-0.09862200

C	-1.12791600	-1.53023600	-0.65701800
O	-2.28208300	-1.16954500	-0.40069800
O	-0.87986500	-2.54548100	-1.50058700
C	-2.02729200	-3.17729300	-2.08428600
C	2.55915400	-0.64242800	-0.07421900
O	3.18296100	0.21330900	-0.71748500
O	3.09038300	-1.20509700	1.06961500
C	4.45511100	-0.87032200	1.35067300
H	-1.62394600	-3.96118900	-2.72671100
H	-2.66883000	-3.60838700	-1.30989500
H	-2.60793100	-2.46041300	-2.67273800
H	4.71053500	-1.42878200	2.25374000
H	5.10649500	-1.16960000	0.52331900
H	4.57335800	0.20434700	1.52272500
C	-3.03682400	0.65912100	1.73681300
C	-2.35412700	1.39200300	0.64580700
C	-2.08638000	-0.11041600	2.60959800
C	-0.81930000	-0.31063600	2.24620400
C	-0.21036300	0.20986100	0.97296100
N	-1.08315700	1.29475200	0.39855000
C	-0.54191900	2.15478400	-0.67075000
O	-1.26557500	2.79093500	-1.39662400
O	0.76286600	2.10156600	-0.63805400
C	1.50983200	2.75423600	-1.70254000
H	-3.63318900	1.39200500	2.30427000
H	-3.77085700	-0.01112600	1.26062200
H	-2.90453900	2.08879400	0.01768100
H	-2.47847200	-0.52561500	3.53416200
H	-0.13911100	-0.89764400	2.85771300
H	0.74354000	0.68485400	1.19535200
H	1.00774100	2.58089500	-2.65556600
H	1.56518000	3.82381300	-1.48704000
H	2.48320800	2.26815000	-1.66707900

TS33

C	-0.17374900	-0.71671900	-0.69045500
C	-0.22755100	-0.54266500	-2.10814300
C	-1.59850600	-0.39774000	-2.58399500
C	-2.47009500	-0.53923500	-1.34154300
N	-1.54917900	-0.75963800	-0.24916900
C	-2.53458500	-1.61423600	-2.37505500
C	-1.99538200	-1.04385100	1.01712200
O	-3.17392000	-1.08434100	1.33221700
O	-0.95880100	-1.26408500	1.85502600

C	-1.30790000	-1.53871700	3.22275900
H	0.46030700	-1.47822700	-0.24034000
H	0.66025900	-0.43314200	-2.71922500
H	-1.84068500	0.29710900	-3.38146500
H	-3.30926900	0.11555700	-1.13889200
H	-3.40638400	-1.63284200	-3.02347000
H	-2.09189600	-2.58232900	-2.15918000
H	-0.35527300	-1.68363900	3.73242900
H	-1.85261900	-0.69443700	3.65334800
H	-1.92327600	-2.44003900	3.28621700
C	1.91108700	0.62385000	0.22336100
C	0.67293900	0.71880500	-0.11688300
C	-0.19246300	1.92923100	-0.15675900
O	-0.96857000	2.18412700	-1.05901300
O	-0.00592100	2.71613000	0.91597500
C	-0.76622700	3.94083000	0.93240900
C	2.96227200	-0.35243200	0.25492900
O	2.90608200	-1.38380200	0.91609100
O	4.03061400	-0.00177700	-0.50106400
C	5.13197700	-0.92824700	-0.49266800
H	-0.47636000	4.44124200	1.85649100
H	-0.51549800	4.55524300	0.06362100
H	-1.83777000	3.72416200	0.92868800
H	5.89066800	-0.47538500	-1.13170500
H	5.51226400	-1.05993700	0.52400000
H	4.82302100	-1.89911300	-0.89067300

TS34a

C	-0.98903900	-0.40687600	-1.02268100
C	-1.01362200	0.86120500	-0.20501200
C	-2.40363500	-0.78633500	-1.26958000
C	-3.25793100	-0.74320900	-0.19046600
C	-2.89510300	0.02425700	0.91966700
O	-1.93172500	0.93935700	0.79815700
C	1.11144500	-0.60007600	1.23885400
C	0.84424800	0.72098700	0.94801300
C	2.06215800	-1.11240300	0.26085800
C	1.75262500	1.10500800	-0.17679100
O	2.39895300	-0.03367000	-0.61004400
O	1.91734900	2.18341800	-0.69104500
O	2.56914900	-2.19584400	0.11361600
H	-0.41684400	-0.24827700	-1.94027300
H	-0.46140600	-1.19291100	-0.43252500
H	-0.82283200	1.84557600	-0.62300900

H	-2.73502300	-1.12266600	-2.24788600
H	-4.24173400	-1.20373700	-0.20000300
H	-3.45202600	0.12356100	1.84219900
H	0.75984400	-1.19885700	2.06840300
H	0.47335200	1.47588000	1.63044500

TS34b

C	-1.60994100	0.69503900	1.28768500
C	-0.91790700	-0.59034500	0.92146900
C	-2.42320800	1.11123300	0.07798300
C	-2.98181000	0.15742700	-0.71759500
C	-2.67662400	-1.20704600	-0.49233800
O	-1.71154900	-1.54182300	0.34075900
C	1.62860400	-1.18846700	-0.53464800
C	0.52779800	-0.35279600	-0.66016000
C	2.73557600	-0.44142600	0.00864400
C	1.03941800	1.03335800	-0.37362300
O	2.31440200	0.93708500	0.10221700
O	0.46289500	2.09021200	-0.49229900
O	3.85438400	-0.74445400	0.34274800
H	-2.25493400	0.59109000	2.18386500
H	-0.86239900	1.45502400	1.53391800
H	-0.25407900	-1.06191600	1.63614600
H	-2.58801700	2.16595300	-0.11823400
H	-3.63578500	0.40941500	-1.54696800
H	-3.12971500	-2.05560200	-0.98859500
H	1.70288800	-2.24270200	-0.76546300
H	-0.27044300	-0.49127000	-1.38657800

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C	1.22662200	0.35312200	1.09473800
C	0.93790000	0.49429900	-0.38149000
C	2.47784300	0.04413000	1.47994700
C	3.48208100	-0.28233600	0.47550800
C	3.06365600	-0.53133900	-0.78046700
O	1.76241800	-0.40606600	-1.16703500
C	-1.06099200	-1.19098300	-0.38044900
C	-0.50577800	0.17551100	-0.79980200
C	-2.43818200	-0.89158800	0.17904700
C	-1.49929800	1.17218300	-0.20928200
O	-2.59838300	0.49265900	0.29118500
O	-1.42049800	2.36763900	-0.15998500
O	-3.30618400	-1.64425800	0.51341600
H	0.44128100	0.57762500	1.81235300

H	-0.46153200	-1.65849700	0.41016800
H	1.16464600	1.52004500	-0.71722600
H	2.74170200	-0.00914900	2.53308300
H	4.52446000	-0.42127100	0.73809400
H	3.68266300	-0.92709200	-1.57909600
H	-1.13972000	-1.91515400	-1.19485200
H	-0.55544200	0.29569700	-1.88966600

TS36a

C	-0.83915100	-0.02434300	-0.81005300
C	1.41462500	-1.08837500	0.69375400
C	0.53357900	-0.00254200	0.70203700
C	1.34830100	1.17725800	0.23892200
O	2.54314000	0.71060800	-0.24149500
C	2.63998500	-0.69726000	0.04183700
O	3.64374400	-1.30001500	-0.25120400
H	1.24826900	-2.09325800	1.05744000
H	-0.22046600	0.16064500	1.46582100
O	1.04580900	2.34568200	0.22382400
C	-1.74760400	1.10410000	-0.63388000
C	-2.90281600	0.95200800	0.03751600
C	-3.22870000	-0.36582700	0.71392800
C	-2.54868200	-1.46284400	-0.03883600
O	-1.44089600	-1.25925800	-0.72744100
H	-0.16561100	-0.02620900	-1.66065100
H	-1.45505300	2.05424100	-1.06809500
H	-3.61675100	1.76664500	0.11861700
H	-2.91943500	-0.35115600	1.77665900
H	-4.30911800	-0.56103700	0.73343900
H	-2.91342700	-2.47906400	-0.12406200

TS36b

C	0.78130900	1.02217700	0.56453600
C	-0.64890800	0.65553600	-0.76951700
C	-1.89862400	1.22088900	-0.45000200
C	-2.74961400	0.22120600	0.10565600
O	-2.01143800	-1.05685400	0.01485700
C	-0.82857200	-0.83097300	-0.58381800
O	-0.03313200	-1.71048300	-0.85810500
H	-0.05553000	0.97454200	-1.62199500
H	-2.21391800	2.24893800	-0.56670900
O	-3.86533400	0.20397100	0.56463100
C	1.97080700	1.56374500	-0.10457800
C	2.97993800	0.75491000	-0.46397000

C	2.85144800	-0.74309600	-0.26212200
C	1.97798700	-0.98514000	0.91906300
O	1.06756600	-0.14274100	1.28882000
H	0.23445800	1.67985400	1.23068200
H	2.00400100	2.63700700	-0.27311600
H	3.89458000	1.14499400	-0.90056400
H	2.39535800	-1.22683700	-1.14360200
H	3.82040700	-1.23204300	-0.10334500
H	2.04471500	-1.85313000	1.56555000

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C	0.77138900	-0.10126100	0.67452400
C	-1.40309700	-1.17813800	-0.20436700
C	-0.43163500	-0.07812100	-0.35263800
C	-1.32872200	1.16434800	-0.22536000
O	-2.62746800	0.77328800	-0.02515900
C	-2.72307800	-0.65021100	-0.01293500
O	-3.79389300	-1.19035100	0.14375200
H	-1.19145500	-2.23842000	-0.22751600
H	0.06287500	-0.06905400	-1.34030000
O	-1.00790600	2.32239100	-0.27770000
C	1.67879000	1.09134500	0.55196800
C	2.92651500	0.99654400	0.08563900
C	3.50457200	-0.30365000	-0.40107400
C	2.47792200	-1.39151900	-0.40171600
O	1.44101500	-1.35053500	0.47667500
H	0.35769600	-0.16394900	1.68593300
H	1.26402200	2.04212400	0.87032800
H	3.56227500	1.87841200	0.04764500
H	3.91491700	-0.18551600	-1.41460600
H	4.37230100	-0.58565300	0.22754700
H	2.72744500	-2.41230300	-0.67382100

TS38a

C	0.72326800	-0.23006400	-0.41349100
C	1.52399400	-1.36433800	0.00828700
C	2.84144600	-0.91485100	0.43027000
C	2.78527600	0.60579500	0.20877800
C	3.71343700	-0.19365200	-0.62842800
H	0.20210700	-0.28313500	-1.37112000
H	1.11910200	-2.35442700	0.17890500
H	3.35097800	-1.38054800	1.26917800
H	3.12485600	1.33612500	0.93611700
H	4.77281200	-0.14616000	-0.39032800

H	3.47252000	-0.33870600	-1.67759300
C	-0.59813600	-0.01337600	0.71553800
C	-1.55169600	-1.09091400	0.66520400
C	-1.40113400	1.17455800	0.19219400
C	-2.69573900	-0.68828500	-0.10976900
O	-3.67751500	-1.29136400	-0.47661800
O	-1.14646600	2.34472900	0.26490600
H	-0.06564700	0.20160300	1.64146900
H	-1.45559900	-2.08733900	1.07603200
O	-2.53362600	0.69241300	-0.42906200
O	1.53692700	0.92214100	-0.36849700

TS38b

C	-0.72461100	-0.09343300	-0.49325200
C	-1.62564900	1.04844400	-0.39609200
C	-2.85597500	0.63900500	0.26987600
C	-2.69224500	-0.87006200	0.44612400
C	-3.73298600	-0.38899900	-0.49720800
H	-0.22233600	-0.24827900	-1.44988800
H	-1.32024400	2.06856000	-0.59112700
H	-3.34983300	1.27884900	0.99624800
H	-2.93484800	-1.40103100	1.36145800
H	-4.77016300	-0.44256900	-0.17587200
H	-3.56295200	-0.50700000	-1.56320000
C	1.43244100	-1.11112600	0.59164900
C	0.55779000	0.03907900	0.64089400
C	2.65992100	-0.75373900	-0.06399100
C	1.45227500	1.18082200	0.17638200
O	1.20652300	2.36079500	0.16707100
O	3.63853300	-1.39243000	-0.37061500
H	1.21713400	-2.11589900	0.92746900
H	0.03168500	0.23781100	1.57526200
O	2.61797300	0.66013000	-0.31697200
O	-1.45230600	-1.25479300	-0.12031300

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C	0.71191000	-0.18354800	-0.34060000
C	1.52247800	-1.35363800	0.04296400
C	2.87124400	-0.93851800	0.38801100
C	2.83230200	0.58654500	0.22884100
C	3.68965500	-0.19243100	-0.70007000
H	0.27770000	-0.21947700	-1.34600200
H	1.11131200	-2.34116000	0.21231600
H	3.42644800	-1.44388800	1.17318300

H	3.23681300	1.27713400	0.96199400
H	4.76355900	-0.17489200	-0.53229900
H	3.37717800	-0.29230300	-1.73568700
C	-0.57631800	0.01314400	0.67278000
C	-1.51701800	-1.10241300	0.61398900
C	-1.42831900	1.18196300	0.16439100
C	-2.69697700	-0.70934400	-0.10926400
O	-3.67621200	-1.33361700	-0.44865700
O	-1.19722100	2.35703900	0.21287800
H	-0.12500400	0.24003300	1.64151500
H	-1.38264800	-2.10477600	0.99874000
O	-2.57748900	0.67439100	-0.40989800
O	1.55853500	0.95828400	-0.24682400

2-Ph

C	-2.99578600	0.65055700	-0.15272700
C	-2.99581700	-0.65060300	0.15232300
C	-1.57654000	1.12246500	-0.26345000
C	-1.57668200	-1.12245300	0.26355100
N	-0.76302500	0.00013600	0.00035900
O	-1.19315400	-2.24294200	0.52815600
O	-1.19316200	2.24304900	-0.52801700
H	-3.82871700	1.32379500	-0.31281500
H	-3.82883300	-1.32381800	0.31208000
C	0.66670300	0.00002500	0.00015200
C	1.36154900	-1.01691700	-0.66400100
C	1.36181200	1.01688300	0.66416400
C	2.75749200	-1.01644600	-0.65368300
H	0.81614600	-1.80468200	-1.17153800
C	2.75775400	1.01632100	0.65347300
H	0.81658300	1.80464900	1.17188300
C	3.45950300	-0.00007400	-0.00022500
H	3.29495600	-1.81140000	-1.16367700
H	3.29541200	1.81122400	1.16334300
H	4.54623300	-0.00012600	-0.00037300

TS3a-Ph

C	2.74269300	-1.60768000	1.28458100
C	1.98051700	-0.39856600	0.80002400
C	3.94561200	-1.85730800	0.41237500
C	4.46206100	-0.86388500	-0.37380400
C	3.87941500	0.41920600	-0.42663400
N	2.69135000	0.63552100	0.22425600
C	0.28845200	-2.52046500	-0.60687400

C	0.83417000	-1.31231100	-0.97774700
C	-1.09879500	-2.31563800	-0.18918300
C	-0.26366400	-0.29525200	-0.96775000
N	-1.38612400	-0.92470300	-0.41410100
O	-0.20243300	0.86364000	-1.35293600
O	-1.90259800	-3.12102700	0.25143600
C	2.14168500	1.97004700	0.13393200
O	2.62207200	2.81929200	-0.57670000
O	1.11562000	2.11570700	0.96438400
C	0.37745300	3.35355200	0.82811400
H	3.03956500	-1.50365800	2.34725900
H	2.04935900	-2.46565800	1.26584200
H	1.11021300	-0.08187500	1.35588500
H	4.42608200	-2.83128300	0.45180900
H	5.35590000	-1.03437100	-0.96707800
H	4.28633400	1.26279900	-0.96317000
H	0.74461000	-3.50145900	-0.61042700
H	1.71323800	-1.14948800	-1.59011800
H	1.04063500	4.20379600	1.00056800
H	-0.05818200	3.39993100	-0.17145200
H	-0.40013700	3.30040900	1.58899800
C	-2.64384800	-0.30246700	-0.16537200
C	-3.19673500	0.57179500	-1.11060500
C	-3.32937800	-0.57045600	1.02704400
C	-4.42565100	1.18264500	-0.85299900
H	-2.66427400	0.77668500	-2.03198700
C	-4.56447900	0.03449700	1.26685200
H	-2.90730200	-1.26024600	1.74885000
C	-5.11554800	0.91609600	0.33277100
H	-4.84695100	1.86257100	-1.58912200
H	-5.09495100	-0.18517200	2.18983200
H	-6.07577900	1.38752100	0.52539900

TS3b-Ph

C	-2.22086800	-2.07884600	-1.19310600
C	-1.79924700	-0.69428800	-0.76223900
C	-3.45951100	-2.52765900	-0.45981800
C	-4.30204500	-1.60220400	0.10671800
C	-4.01967500	-0.22814100	0.07554700
N	-2.80136700	0.20736300	-0.43181000
C	-0.49646400	0.13130100	1.87342300
C	-0.70749000	-1.04870900	1.18516400
C	0.81518900	0.66759100	1.51729200
C	0.58016100	-1.41286000	0.51412500

N	1.44153500	-0.31713200	0.68320500
O	0.83477500	-2.44329000	-0.09140300
O	1.32855000	1.72821600	1.84251000
C	-2.55531600	1.60997300	-0.38411700
O	-3.36403400	2.40654400	0.04017500
O	-1.35041500	1.91002900	-0.87697800
C	-0.97970300	3.30759200	-0.81337600
H	-2.39744100	-2.09156500	-2.28766000
H	-1.37695200	-2.76126300	-1.03108400
H	-0.95874300	-0.24412300	-1.27073000
H	-3.70141200	-3.58625900	-0.43749500
H	-5.22627900	-1.91254900	0.58611100
H	-4.67590200	0.54685900	0.44129000
H	-1.15784500	0.63961400	2.56304200
H	-1.42538000	-1.81556800	1.44551200
H	-0.87465800	3.61239100	0.22984200
H	-1.73417000	3.91804400	-1.31362500
H	-0.02192400	3.36617600	-1.32866800
C	2.75823800	-0.21548300	0.14475100
C	3.20036900	0.99876200	-0.39699900
C	3.61144200	-1.32700600	0.16014600
C	4.49195700	1.09662600	-0.91729900
H	2.54548900	1.86188100	-0.39090700
C	4.89602400	-1.22094000	-0.37599200
H	3.26708000	-2.26652200	0.57561900
C	5.34339900	-0.01133500	-0.91384100
H	4.83048300	2.04432600	-1.32824400
H	5.54985700	-2.08919200	-0.36565800
H	6.34684700	0.06789500	-1.32381400

TS7a-Ph

C	0.85871000	1.89091700	1.63101700
C	1.87760600	1.51768200	0.58737000
C	0.13836800	0.63578400	2.07612200
C	0.67552400	-0.59371200	1.88681700
C	1.90449500	-0.78469300	1.18745800
N	2.53532200	0.32481600	0.69536400
C	0.70379800	-0.72210300	-1.33058200
C	0.64161800	0.64925700	-1.38011800
C	-0.61562700	-1.25150000	-0.94345700
C	-0.74034800	1.06407500	-1.02371100
N	-1.46385200	-0.12279800	-0.75981200
O	-1.18718500	2.19911400	-0.96523800
O	-0.96177500	-2.41505500	-0.81261100

C	3.76466700	0.19521300	-0.04710600
O	4.21541500	1.08624200	-0.72603400
O	4.31889400	-1.00137900	0.13759200
C	5.56230800	-1.22793100	-0.56734900
H	1.32224500	2.42096500	2.48890300
H	0.15394400	2.60763900	1.18830100
H	2.42455200	2.28659500	0.05993600
H	-0.82533700	0.73887500	2.56805000
H	0.15657100	-1.48647000	2.22316200
H	2.44909500	-1.71408100	1.17698000
H	1.47793800	-1.38100800	-1.70067800
H	1.29625100	1.32684700	-1.91083900
H	5.40121400	-1.14302300	-1.64417300
H	6.31042200	-0.50065600	-0.24463900
H	5.85742400	-2.24036400	-0.29494600
C	-2.82589700	-0.17703800	-0.34611300
C	-3.76478800	0.69642100	-0.91284400
C	-3.23393600	-1.10592400	0.62165400
C	-5.09759700	0.64562700	-0.50062400
H	-3.45008700	1.41652400	-1.65840800
C	-4.57235800	-1.15639800	1.01536300
H	-2.51419300	-1.79681500	1.04316300
C	-5.50934000	-0.27988700	0.46183200
H	-5.81650700	1.33111600	-0.94216600
H	-4.88026800	-1.88618200	1.76001800
H	-6.54956000	-0.32020200	0.77443200

TS7b-Ph

C	-3.81290100	0.11251100	-1.34052000
C	-2.38067200	0.51133500	-1.08589000
C	-4.38044900	-0.53556500	-0.09340800
C	-3.81264100	-0.33486600	1.11951300
C	-2.61631600	0.42926300	1.28122900
N	-2.02141300	0.92545300	0.15939600
C	-1.22065200	-1.96360600	0.64716900
C	-1.28334800	-1.77728000	-0.70453600
C	0.11393800	-1.56590600	1.12881300
C	0.03231400	-1.26514100	-1.17598500
N	0.82401600	-1.07942200	-0.01780300
O	0.38654000	-1.04737500	-2.32394500
O	0.57824600	-1.64598700	2.25184500
C	-0.85173300	1.76788000	0.36720200
O	-0.43168700	2.02850800	1.46679500
O	-0.38430300	2.21843400	-0.78842600

C	0.79162300	3.06373700	-0.71027400
H	-4.42652100	0.98251100	-1.65762100
H	-3.83942400	-0.57714000	-2.19599600
H	-1.75605400	0.85156800	-1.89772100
H	-5.27260300	-1.15009100	-0.18635600
H	-4.24105600	-0.77768400	2.01452800
H	-2.22839600	0.77333000	2.22739800
H	-1.92885800	-2.45617800	1.29705100
H	-2.00603500	-2.16676900	-1.40738900
H	1.02236700	3.31092600	-1.74538100
H	1.61236500	2.51392000	-0.24734100
H	0.55932400	3.96100600	-0.13231900
C	2.17809800	-0.63405500	0.00193900
C	2.63373500	0.15167200	1.07157500
C	3.05813500	-0.98263300	-1.03315700
C	3.96253700	0.58004000	1.10036200
H	1.95903400	0.40997800	1.87861300
C	4.38023600	-0.53471900	-0.99855100
H	2.70679100	-1.58606400	-1.86070900
C	4.84056500	0.24485200	0.06592800
H	4.30879200	1.17872700	1.93913400
H	5.05358300	-0.80689100	-1.80740200
H	5.87329300	0.58288100	0.09174600