

CHEMPHYSICHEM

Supporting Information

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Computational Reference Data for the Photochemistry of Cyclobutane Pyrimidine Dimers

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Supporting Information

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I. Thymine monomer

The ground-state geometry of thymine in the singlet, triplet, cation doublet, and anion doublet was optimized with DFT (B3LYP and ω B97XD) and CC2. The ω B97XD geometries are shown in the first row of Fig. S1. Cartesian coordinates for all levels and states are provided later in this Supporting Information. All three methods produce similar geometries. The singlet and the cation doublet ground states are planar. The triplet and the anion doublet ground states show out-of-plane ring distortions. The singlet ground state, with a closed shell electronic configuration, is the most stable state among the four (Table S1). It is energetically closely followed by the anion species (singly occupied π^*), then by the triplet ($\pi\pi^*$) and finally by the cation (singly occupied π).

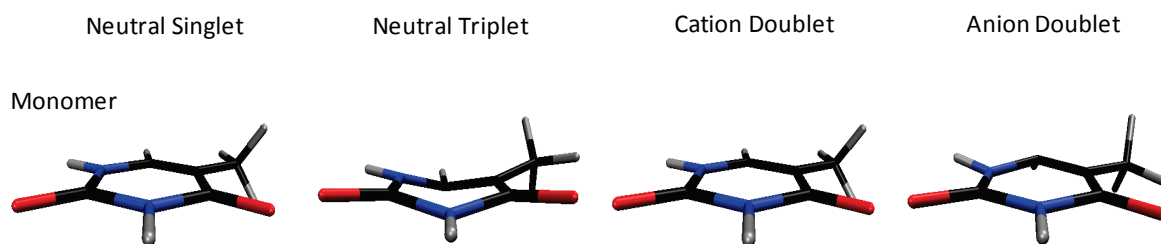


Fig. S1 – Thymine monomer geometries.

Table S1 – Characterization of the ground state of thymine monomer. M – Multiplicity; Q – total charge; S – adiabatic state label; C – diabatic-state character based on the singly-occupied orbitals in the main configuration. E_0 – absolute energy of the state; ΔE_0 – energy relative to the singlet ground state; E_{ZP} – zero-point energy based on un-scaled harmonic frequencies; ΔE_{ZP} – zero-point corrected relative energy. cs – Closed shell.

M	Q	S	Method	E_0 (au)	C	ΔE_0 (eV) [kcal/mol]	E_{ZP} (au)	ΔE_{ZP} (eV) [kcal/mol]
1	0	S_0	B3LYP	-454.084787	cs	0	0.114658	0
			ω B97XD	-454.163746	cs	0	0.116256	0
			CC2	-453.361536	cs	0	-	-
3	0	T_1	B3LYP	-453.977617	$\pi\pi^*$	2.92 [67.2]	0.110604	2.81 [64.7]
			ω B97XD	-454.054286	$\pi\pi^*$	2.98 [68.7]	0.112133	2.87 [66.1]
			CC2	-453.236155	$\pi\pi^*$	3.41 [78.7]	-	-
2	+1	D_1^+	B3LYP	-453.766998	π	8.65 [199.4]	0.113076	8.60 [198.4]
			ω B97XD	-453.841846	π	8.76 [202.0]	0.114808	8.72 [201.1]
			CC2	-452.972622	π	9.45 [217.9]	-	-
2	-1	D_1^-	B3LYP	-454.077002	π^*	0.21 [4.9]	0.109732	0.08 [1.79]
			ω B97XD	-454.158723	π^*	0.14 [3.2]	0.111471	0.01 [0.2]
			CC2	-453.378570	π^*	0.44 [10.1]	-	-

The lowest vertical excitation energies of thymine are given in Table S2. In the singlet state, the lowest excited state is an excitation from the oxygen lone pairs (n_o) into the π^* . The first $\pi\pi^*$ bright state is the next state with values ranging from 5.04 eV to 5.28 depending of the method. As for comparison with experiments, the first dipole-allowed transition of thymine vapor is peaked at 4.95 eV.^[1] The excited-state relaxation of thymine after excitation into this is state is discussed in Ref.^[2]. Excitations with the triplet manifold start at about 2 eV above

the T₁ triplet ground state, also with an n₀π* excitation. The cation manifold is reached right above 1 eV, while the anion states are just below this level. There is a good agreement among the three computational levels provided in Table S2. The first excited state of the singlet, cation and anion are systematically higher in energy with ωB97XD than with the other methods. For the singlet, DFT-MRCI excitations are given later in Table S3. The good agreement between methods can be better visualized in Fig. S2, where energy levels for all multiplicities are given in the same scale relative to the minimum of the singlet state.

Table S2 – Characterization of the excited states of thymine monomer. All single-point calculations for the anion with the aug-cc-pVTZ basis set. ΔE – excitation energy relative to the ground state of the same multiplicity and charge; *f* – oscillator strength for excitation from the ground state. See caption of Table S1 for abbreviations.

M	Q	S	TD-ωB97XD			TD-B3LYP			CC2		
			ΔE (eV)	<i>f</i>	C	ΔE (eV)	<i>f</i>	C	ΔE (eV)	<i>f</i>	C
1	0	S ₁	5.14	0.000	n ₀ π*	4.77	0.000	n ₀ π*	4.87	0.000	n ₀ π*
		S ₂	5.27	0.175	ππ*	5.04	0.132	ππ*	5.28	0.187	ππ*
		S ₃	6.03	0.000	π-Ryd	5.87	0.000	n ₀ π*	6.24	0.000	n ₀ π*
		S ₄	6.46	0.000	n ₀ π ₀ *	6.05	0.064	π ₀ π*	6.37	0.067	π ₀ π*
		S ₅	6.64	0.051	π ₀ π*	6.18	0.000	π-Ryd	6.63	0.000	n ₀ π*
		S ₆	6.69	0.194	ππ ₀ *	6.29	0.000	n ₀ π ₀ *			
3	0	T ₂	2.15	0.000	n ₀ π*	1.72	0.000	n ₀ π*	2.18	0.000	n ₀ π*
		T ₃	2.87	0.013	π ₀ π*	2.34	0.012	π ₀ π*	3.05	0.021	π ₀ π*
		T ₄	3.54	0.020	ππ ₀ *	2.90	0.000	n ₀ π*	3.68	0.001	n ₀ π*
		T ₅	3.57	0.006	π-Ryd	3.10	0.014	ππ ₀ *	4.03	0.027	ππ ₀ *
		T ₆	3.81	0.000	n ₀ π*	3.81	0.008	π-Ryd	4.36	0.075	ππ*
		T ₇	4.28	0.066	ππ*	3.88	0.055	ππ*			
		2	+1	D ₂ ⁺	1.60	0.000	n ₀	1.08	0.000	n ₀	1.13
D ₃ ⁺	2.26			0.012	π ₀ *	1.74	0.010	π ₀	2.12	-	π ₀
D ₄ ⁺	2.73			0.000	n ₀	1.97	0.000	n ₀	2.54	-	n ₀
D ₅ ⁺	4.14			0.056	π	3.08	0.068	π	4.43	-	π
2	-1			D ₂ ⁻	0.91	0.009	Ryd	0.55	0.009	Ryd	0.63
		D ₃ ⁻	1.35	0.004	Ryd	0.90	0.004	Ryd	1.07	0.006	Ryd
		D ₄ ⁻	1.54	0.020	Ryd	1.24	0.007	Ryd	1.33	0.012	Ryd
		D ₅ ⁻	1.76	0.004	Ryd	1.31	0.029	Ryd	1.40	0.022	Ryd
		D ₆ ⁻	1.99	0.003	Ryd	1.57	0.005	Ryd	1.67	0.005	Ryd
		D ₇ ⁻	2.24	0.004	Ryd	1.84	0.004	Ryd	1.96	0.005	Ryd

II. DFT-MRCI results

Table S3 - DFT-MRCI excited states of neutral singlet states of thymine monomer, dimer and complex. Thymine complex based on ω B97XD/cc-pVTZ geometry. s – Contribution of single excitations for the state. ΔE – excitation energy relative to the ground state of the same multiplicity and charge; f – oscillator strength for excitation from the ground state. C – diabatic-state character based on the singly-occupied orbitals in the main configuration; cs – closed shell. For S_0 , the absolute energy is given in atomic units.

DFT-MRCI				
S	ΔE (eV)	f	C	s (%)
Thymine monomer				
S_0	-454.071099	-	cs	0
S_1	4.66	0.000	$n_O\pi^*$	91
S_2	5.26	0.265	$\pi\pi^*$	95
S_3	6.09	0.000	$n_O\pi_O^*$	91
S_4	6.17	0.108	$\pi_O\pi^*$	82
S_5	6.54	0.001	π -Ryd	97
S_6	6.60	0.271	$\pi\pi_O^*$	94
Thymine dimer				
S_0	-908.111909	-	cs	0
S_1	4.69	0.001	$n_O\pi_O^*$	97
S_2	4.77	0.001	$n_O\pi_O^*$	97
S_3	5.79	0.001	$n_O\pi_O^*$	97
S_4	5.85	0.000	$n_O\pi_O^*$	97
S_5	6.23	0.026	$\pi_{66}\pi_O^*$	96
S_6	6.56	0.148	$\pi_{66}\pi_O^*$	96
S_7	6.76	0.216	$\pi_O\pi_O^*$	95
S_8	6.87	0.573	$\pi_O\pi_O^*$	96
Thymine complex				
S_0	-908.144941	-	cs	0
S_2	4.52	0.000	$n_O\pi^*$	91
S_3	4.61	0.000	$n_O\pi^*$	91
S_4	5.11	0.259	$\pi\pi^*$	94
S_5	5.14	0.158	$\pi\pi^*$	95
S_7	5.56	0.006	$\pi\pi^*$	63
S_8	5.88	0.028	$\pi\pi^*$	93
S_9	5.99	0.001	$n_O\pi_O^*$	92

III. Energy levels

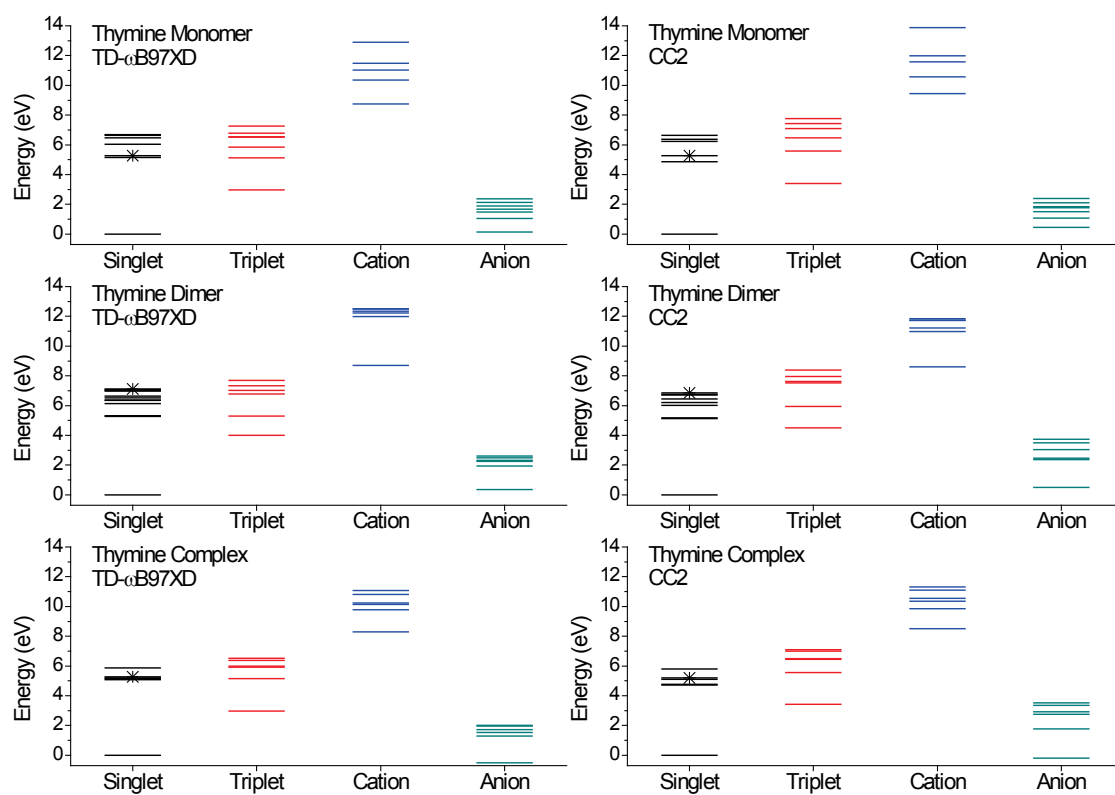


Fig. S2 – Energy levels of thymine monomer, dimer and complex relative to the ground-state singlet of each species. Crosses indicate bright states ($f > 0.1$).

IV. Grid definition

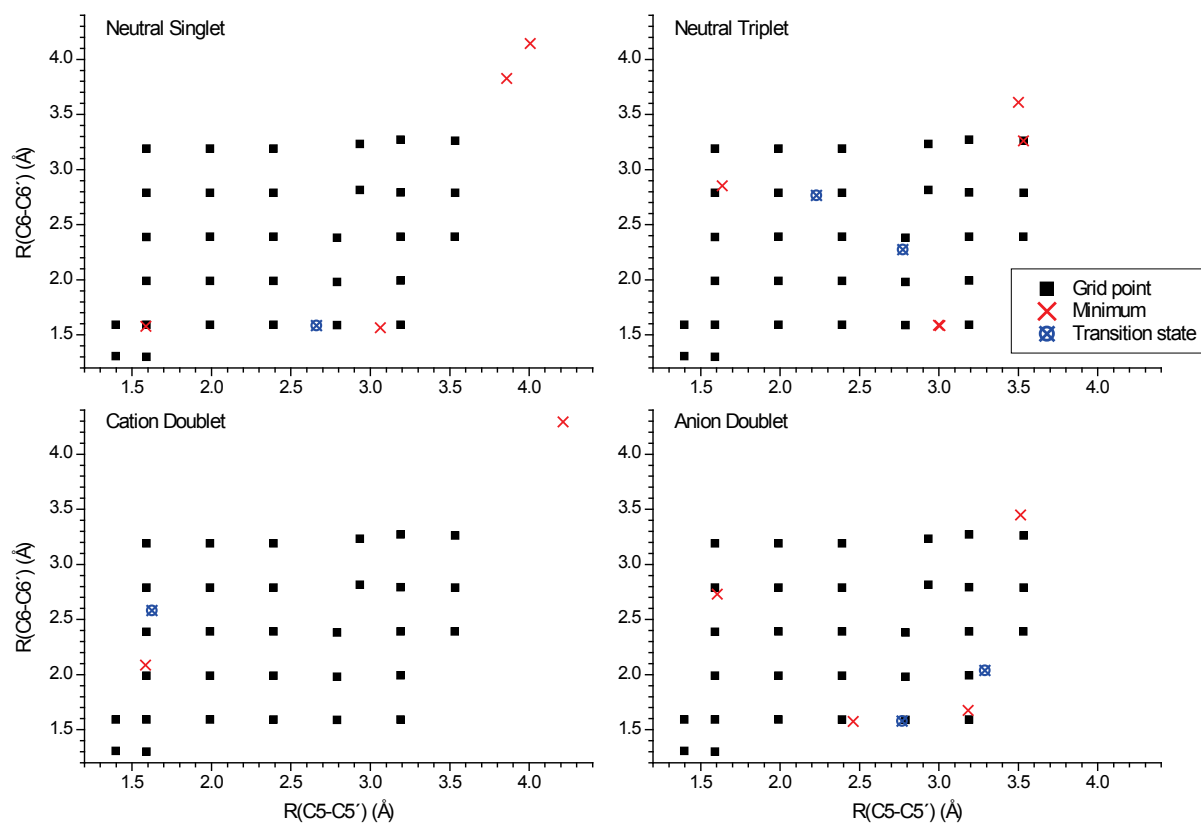


Fig. S3 – Definition of the grid used to compute the potential energy surface. In addition to the points with fixed values of $R(C5-C5')$ and $R(C6-C6')$, fully optimized geometries and transition states (still keeping the sugar restrictions) were included as well.

V. Basis set effects

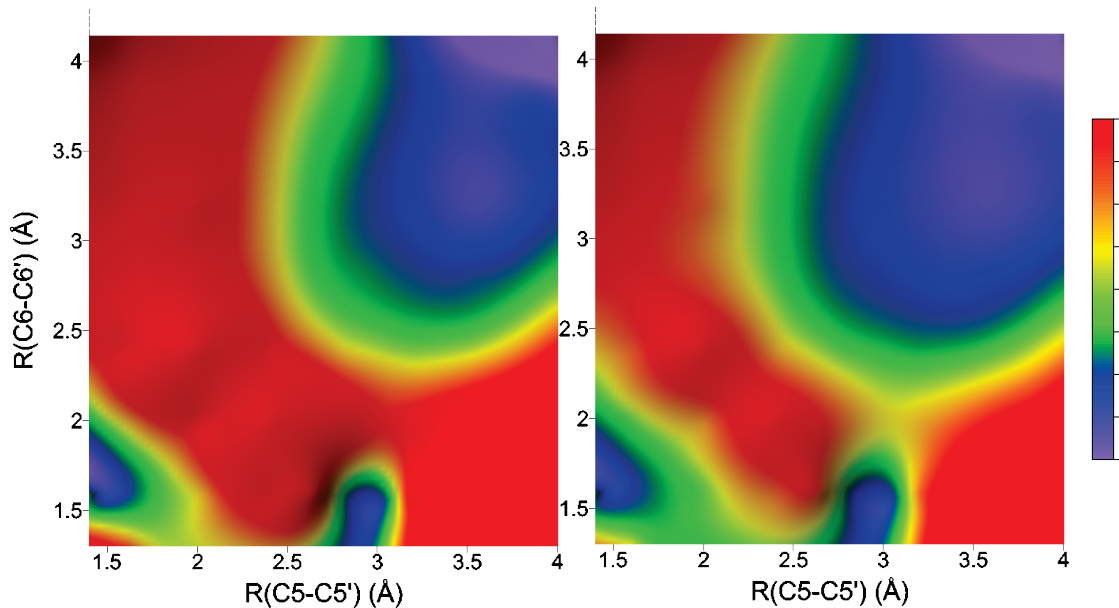


Fig. S4 – 2D cuts of the potential energy and charge difference surfaces of thymidine dimer (ground state neutral singlet). Comparison of calculations with aug-cc-pVDZ and cc-pVTZ for thymines. Sugars were computed with the cc-pVDZ basis set in both cases. Both maps are based on the same geometries, optimized with cc-pVTZ (thymines) and cc-pVDZ (sugars).

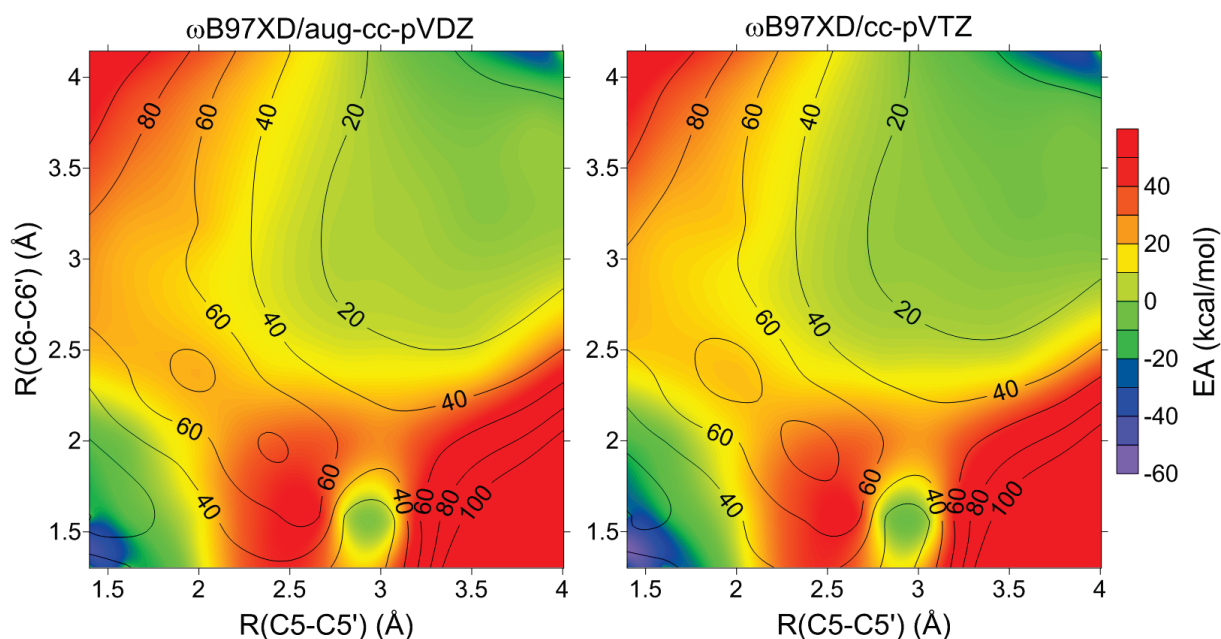


Fig. S5 - Energy difference between the singlet ground state and the anion ground state (EA) computed on singlet geometries. The contours indicate the singlet energies. Comparison of calculations with aug-cc-pVDZ and cc-pVTZ for thymines. Sugars were computed with the cc-pVDZ basis set in both cases. Both maps are based on the same geometries, optimized with cc-pVTZ (thymines) and cc-pVDZ (sugars).

VI. References

- [1] R. Abouaf, J. Pommier, H. Dunet *Chem. Phys. Lett.* **2003**, 381, 486-494.
- [2] J. J. Szymczak, M. Barbatti, J. T. Soo Hoo, J. A. Adkins, T. L. Windus, D. Nachtigallová, H. Lischka *J. Phys. Chem. A* **2009**, 113, 12686-12693.

VII. Cartesian coordinates

A Thymine monomer

1 Neutral Singlet

B3LYP/TZVPP

N	0.253559	1.722643	-0.449987
C	1.019856	1.168012	-1.459893
N	1.046922	-0.211429	-1.411859
C	0.407026	-1.056077	-0.492829
C	-0.376049	-0.363264	0.532839
C	-0.410084	0.981966	0.500437
O	1.601000	1.830359	-2.292274
O	0.526225	-2.262139	-0.584272
C	-1.089731	-1.190373	1.555612
H	0.208251	2.727966	-0.447480
H	1.595299	-0.664748	-2.129177
H	-1.621879	-0.559889	2.267469
H	-1.806832	-1.862775	1.081627
H	-0.388074	-1.821119	2.104023
H	-0.965489	1.560867	1.225763

ω B97XD/cc-pVTZ

N	0.416874	1.627112	-1.664035
C	1.176691	1.073768	-2.671894
N	1.200106	-0.302418	-2.628883
C	0.565921	-1.143620	-1.712966
C	-0.212659	-0.451362	-0.684360
C	-0.244382	0.887265	-0.715143
O	1.756874	1.731849	-3.500977
O	0.681146	-2.344385	-1.804027
C	-0.922350	-1.282422	0.333537
H	0.376093	2.630412	-1.658922
H	1.743959	-0.753377	-3.348170
H	-1.463978	-0.656596	1.041301
H	-1.627920	-1.960064	-0.147404
H	-0.215314	-1.903703	0.883390
H	-0.798282	1.465198	0.011628

CC2/TZVPP

N	0.254346	1.725562	-0.447047
C	1.019715	1.171370	-1.459328
N	1.039691	-0.211020	-1.406509
C	0.401906	-1.059511	-0.487216
C	-0.374725	-0.367667	0.532697
C	-0.410607	0.986348	0.503343
O	1.608182	1.837475	-2.300902
O	0.520196	-2.280959	-0.578008
C	-1.087697	-1.192240	1.553251
H	0.210910	2.732389	-0.445834
H	1.586757	-0.666224	-2.126739
H	-1.626362	-0.558199	2.255565
H	-1.793780	-1.867883	1.072114
H	-0.381049	-1.811371	2.104457
H	-0.967482	1.561927	1.230154

2 Neutral Triplet

B3LYP/TZVPP

N	1.107628	-1.240663	0.049277
C	1.648206	0.038840	0.023875
N	0.724693	1.042379	-0.180850
C	-0.678639	0.908387	-0.055464
C	-1.165588	-0.435895	-0.058009
C	-0.197676	-1.551366	-0.284119
O	2.836764	0.233663	0.169328
O	-1.375635	1.917005	0.031952
C	-2.590414	-0.738176	0.171614
H	1.796669	-1.967155	0.170509
H	1.086901	1.983313	-0.143540
H	-2.709904	-1.399522	1.038950
H	-3.163679	0.171522	0.329679
H	-3.008525	-1.287879	-0.681364
H	-0.498982	-2.576135	-0.129555

ω B97XD/cc-pVTZ

N	1.101474	-1.238603	0.058892
C	1.640958	0.037340	0.025046
N	0.719416	1.038165	-0.185496
C	-0.676576	0.907256	-0.059230
C	-1.164513	-0.435877	-0.065344
C	-0.194142	-1.550122	-0.296909
O	2.822817	0.234657	0.169480
O	-1.371503	1.907897	0.033894
C	-2.585001	-0.737313	0.173181
H	1.789259	-1.962202	0.184993
H	1.082477	1.976603	-0.146225
H	-2.695177	-1.402222	1.036993
H	-3.152827	0.173647	0.340562
H	-3.006435	-1.277844	-0.681679
H	-0.498408	-2.573063	-0.135877

CC2/TZVPP

N	1.072407	-1.245427	0.100338
C	1.624974	0.030995	0.077399
N	0.715768	1.031462	-0.236161
C	-0.683088	0.923092	-0.118324
C	-1.161902	-0.440379	-0.112379
C	-0.187576	-1.530199	-0.403695
O	2.808394	0.235859	0.306039
O	-1.382586	1.928665	-0.037893
C	-2.564377	-0.746056	0.222203
H	1.752185	-1.976270	0.255883
H	1.084983	1.971874	-0.180748
H	-2.615103	-1.396315	1.101464
H	-3.116999	0.170140	0.411707
H	-3.038977	-1.297190	-0.595633
H	-0.496281	-2.561931	-0.337917

3 Cation Doublet

B3LYP/TZVPP

N	0.230883	1.711541	-0.417375
C	1.029291	1.129916	-1.470094
N	1.059199	-0.237365	-1.428376
C	0.418649	-1.070175	-0.506108
C	-0.378583	-0.368558	0.539387
C	-0.419341	1.034151	0.510131
O	1.574215	1.844006	-2.255818
O	0.506858	-2.268207	-0.556029
C	-1.083582	-1.166533	1.547915
H	0.205250	2.728124	-0.443570
H	1.608666	-0.694721	-2.149568
H	-1.623166	-0.558047	2.268405
H	-1.773589	-1.862754	1.053972

H	-0.373814	-1.823995	2.065556
H	-0.980936	1.602617	1.241570

ω B97XD/cc-pVTZ

N	0.393523	1.615330	-1.628707
C	1.186538	1.035162	-2.683911
N	1.214366	-0.329652	-2.646198
C	0.577618	-1.159171	-1.727652
C	-0.215877	-0.458512	-0.679781
C	-0.253556	0.942427	-0.705268
O	1.728582	1.746599	-3.464209
O	0.660348	-2.352110	-1.775541
C	-0.917300	-1.259903	0.325098
H	0.371063	2.629896	-1.653508
H	1.760338	-0.783905	-3.368647
H	-1.464694	-0.655109	1.041882
H	-1.596293	-1.959580	-0.174308
H	-0.199675	-1.903765	0.845121
H	-0.812202	1.509950	0.028704

CC2/TZVPP

N	0.015518	1.682638	-0.587017
C	1.036974	1.138374	-1.455196
N	1.266357	-0.198439	-1.238351
C	0.646200	-1.038680	-0.314670
C	-0.396320	-0.364914	0.531710
C	-0.650712	1.002810	0.330195
O	1.581716	1.851311	-2.258408
O	0.916332	-2.205048	-0.198085
C	-1.094352	-1.177266	1.527751
H	-0.162981	2.673623	-0.739084
H	1.978588	-0.624575	-1.828021
H	-0.355367	-1.628394	2.199576
H	-1.832430	-0.616076	2.091443
H	-1.558191	-2.034103	1.026499
H	-1.391332	1.538738	0.911655

4 Anion Doublet

B3LYP/TZVPP

n	1.150325	-1.227823	0.091869
c	1.669351	0.027956	-0.010250
n	0.727904	1.010335	-0.159360
c	-0.711963	0.859061	-0.146442
c	-1.158419	-0.459807	0.015686
c	-0.241906	-1.523007	0.214762
o	2.885676	0.256781	0.028501
o	-1.370892	1.918501	-0.277143
c	-2.632841	-0.736398	0.021770
h	1.829752	-1.923518	0.344496
h	1.066779	1.952291	-0.250690
h	-2.905954	-1.525598	-0.693200
h	-2.996778	-1.067845	1.004806
h	-3.174729	0.170771	-0.246269
h	-0.501713	-2.540883	-0.066332

ω B97XD/cc-pVTZ

N	1.147003	-1.226645	0.090432
C	1.661190	0.026652	-0.010451
N	0.721625	1.004950	-0.158906
C	-0.710525	0.854896	-0.145082
C	-1.154894	-0.459373	0.017941
C	-0.241247	-1.521530	0.217358
O	2.870837	0.256964	0.026594
O	-1.367093	1.908409	-0.279016
C	-2.626503	-0.734261	0.022184

H	1.826936	-1.917452	0.346742
H	1.060030	1.945430	-0.249082
H	-2.897688	-1.521242	-0.693879
H	-2.988508	-1.064946	-1.004238
H	-3.163373	0.175486	-0.245628
H	-0.503200	-2.536521	-0.071242

CC2/TZVPP

N	1.143459	-1.233993	0.059947
C	1.665570	0.024832	-0.010602
N	0.717645	1.012396	-0.109280
C	-0.714307	0.859661	-0.136515
C	-1.156554	-0.462886	0.014491
C	-0.242580	-1.525346	0.242310
O	2.891839	0.255548	0.010592
O	-1.381824	1.921004	-0.284098
C	-2.626427	-0.737189	0.016424
H	1.830675	-1.925750	0.308976
H	1.059214	1.952867	-0.227520
H	-2.884830	-1.558090	-0.662935
H	-2.998299	-1.017116	1.009388
H	-3.156087	0.160826	-0.301760
H	-0.512902	-2.535947	-0.057216

B Thymine dimer

5 Neutral Singlet

B3LYP/TZVPP

N	1.065681	1.346426	-1.138149
C	1.933093	0.550753	-1.833940
N	1.474931	-0.740873	-2.101638
C	0.300934	-1.337580	-1.691816
C	-0.641506	-0.451471	-0.886690
C	-0.325262	1.069353	-0.874595
O	3.034680	0.911909	-2.188147
O	0.031889	-2.475444	-1.997409
C	-2.071221	-0.728090	-1.350905
H	1.410723	2.282174	-0.993956
H	2.131438	-1.327568	-2.597049
H	-2.323711	-1.775568	-1.206417
H	-2.159777	-0.508939	-2.415847
H	-2.796316	-0.110795	-0.821845
H	-0.976042	1.679963	-1.505493
N	0.091048	1.857426	1.576566
C	1.242658	1.440901	2.179302
N	1.594266	0.111191	1.921223
C	0.928218	-0.833307	1.166544
C	-0.478509	-0.454105	0.699503
C	-0.681030	1.078921	0.651453
O	1.922945	2.141713	2.896439
O	1.410588	-1.923586	0.963734
C	-1.454784	-1.283800	1.530941
H	-0.179785	2.799468	1.804756
H	2.485831	-0.169901	2.305202
H	-1.279328	-2.346285	1.367191
H	-2.487683	-1.053006	1.276745
H	-1.316649	-1.078229	2.594280
H	-1.733862	1.328350	0.775849

ω B97XD/cc-pVTZ

N	0.038452	1.426937	-1.099953
C	0.802200	2.170999	-0.251144
N	1.843085	1.485426	0.369101

C	2.118974	0.138946	0.328991
C	1.207776	-0.688087	-0.559901
C	0.312959	0.091894	-1.551344
O	0.601649	3.340125	-0.027678
O	3.046369	-0.333578	0.933791
C	2.047744	-1.744080	-1.264335
H	-0.698031	1.948629	-1.543050
H	2.392862	2.040280	1.006245
H	2.531266	-2.390544	-0.536413
H	2.827286	-1.259745	-1.851853
H	1.447517	-2.354305	-1.938357
H	0.651217	0.081837	-2.589203
N	-2.179105	-0.424247	-1.067712
C	-2.696295	0.124833	0.065583
N	-1.853505	0.085455	1.176267
C	-0.590399	-0.447890	1.284132
C	-0.104726	-1.270668	0.097479
C	-0.838830	-0.899667	-1.203906
O	-3.800644	0.605937	0.136514
O	0.053753	-0.326707	2.295189
C	-0.110931	-2.726302	0.538685
H	-2.805972	-0.425595	-1.852223
H	-2.209814	0.561592	1.990690
H	0.572787	-2.862774	1.374820
H	0.188045	-3.385260	-0.274082
H	-1.111388	-3.018451	0.860791
H	-0.828119	-1.736733	-1.899249

C	0.299482	-1.318378	-1.664139
C	-0.678583	-0.515122	-0.865314
C	-0.412191	1.032361	-0.898898
O	3.096048	0.919540	-1.850443
O	0.023567	-1.669556	-2.919908
C	-2.104488	-0.840464	-1.307229
H	1.227426	2.337662	-1.196607
H	2.354288	-1.408573	-2.066833
H	-2.350065	-1.882206	-1.103928
H	-2.200941	-0.674133	-2.379656
H	-2.837169	-0.212809	-0.801532
H	-1.125872	1.606925	-1.491189
N	0.159362	1.844541	1.511455
C	1.356342	1.434242	2.021744
N	1.671317	0.092717	1.773470
C	0.895232	-0.893778	1.195323
C	-0.496667	-0.475543	0.722369
C	-0.676481	1.059815	0.649803
O	2.100683	2.145911	2.660756
O	1.289297	-2.036091	1.130710
C	-1.496027	-1.253162	1.579011
H	-0.073084	2.802002	1.716750
H	2.565758	-0.200840	2.141266
H	-1.353829	-2.324566	1.446262
H	-2.522787	-0.996694	1.325008
H	-1.345809	-1.024761	2.636144
H	-1.716036	1.330325	0.830702

CC2/TZVPP

N	1.102561	1.259734	-1.017712
C	1.961485	0.456301	-1.722951
N	1.418810	-0.767868	-2.126260
C	0.234113	-1.344263	-1.708381
C	-0.664474	-0.437396	-0.898428
C	-0.316574	1.067006	-0.885890
O	3.121686	0.756655	-1.970880
O	-0.075392	-2.487562	-2.020169
C	-2.105424	-0.682797	-1.315618
H	1.500736	2.157367	-0.779074
H	2.076166	-1.382556	-2.590832
H	-2.367184	-1.726050	-1.154334
H	-2.216044	-0.467167	-2.378725
H	-2.798984	-0.048093	-0.764832
H	-0.892786	1.703178	-1.562815
N	0.012822	1.871968	1.557299
C	1.182956	1.487945	2.154545
N	1.563916	0.164494	1.895486
C	0.960430	-0.753656	1.056323
C	-0.469497	-0.438512	0.662976
C	-0.723625	1.079439	0.620696
O	1.855696	2.215195	2.873134
O	1.515390	-1.802367	0.744823
C	-1.372749	-1.313408	1.513217
H	-0.275975	2.811122	1.784549
H	2.488499	-0.076907	2.232124
H	-1.154217	-2.363760	1.320840
H	-2.421273	-1.120247	1.292925
H	-1.200453	-1.111443	2.571922
H	-1.787158	1.293650	0.721873

6 Neutral Triplet

B3LYP/TZVPP

N	0.933959	1.378097	-1.293584
C	1.956278	0.546178	-1.655543
N	1.614449	-0.803637	-1.740139

ωB97XD/cc-pVTZ

N	0.161149	1.604356	1.097056
C	-0.165796	2.334753	-0.001852
N	-1.185747	1.809139	-0.793722
C	-1.827360	0.602492	-0.667501
C	-1.410858	-0.254567	0.507509
C	-0.422923	0.365531	1.520701
O	0.368056	3.377927	-0.293249
O	-2.673921	0.253326	-1.452775
C	-2.658287	-0.802187	1.185878
H	0.911404	2.002933	1.634413
H	-1.421840	2.367265	-1.599254
H	-3.244296	-1.398988	0.491397
H	-3.280482	0.023006	1.533485
H	-2.401427	-1.413010	2.051017
H	-0.840535	0.476585	2.522237
N	1.898840	-0.717827	1.155235
C	2.427493	-0.158933	0.025787
N	1.531417	-0.142352	-1.048438
C	0.422434	-1.017408	-1.151497
C	-0.326933	-1.346083	0.117815
C	0.493936	-0.896265	1.363371
O	3.544058	0.289333	-0.059245
O	0.864114	-1.990830	-1.939068
C	-0.781802	-2.794090	0.093865
H	2.521423	-0.709933	1.943978
H	1.928101	0.208969	-1.906416
H	-1.473093	-2.967919	-0.730419
H	-1.282805	-3.063696	-1.020903
H	0.075486	-3.452397	-0.037042
H	0.350574	-1.583517	2.195021

CC2/TZVPP

N	0.915066	1.369012	-1.213969
C	1.966118	0.528804	-1.465481
N	1.619217	-0.828476	-1.541757
C	0.286690	-1.302773	-1.626085
C	-0.703139	-0.509336	-0.844202
C	-0.441339	1.028365	-0.870606
O	3.128356	0.897538	-1.583486
O	0.123429	-1.462253	-2.938817

C	-2.117177	-0.826837	-1.298099
H	1.212788	2.328240	-1.098687
H	2.360984	-1.427863	-1.882385
H	-2.365933	-1.866567	-1.089244
H	-2.193424	-0.659550	-2.372384
H	-2.846146	-0.187737	-0.800001
H	-1.136196	1.608357	-1.480493
N	0.116264	1.809756	1.533203
C	1.409465	1.457500	1.821204
N	1.710086	0.111908	1.565868
C	0.866189	-0.904891	1.156442
C	-0.528990	-0.490635	0.724985
C	-0.724405	1.037401	0.670075
O	2.237859	2.213802	2.309608
O	1.225782	-2.077507	1.172311
C	-1.514477	-1.292087	1.557383
H	-0.071402	2.791581	1.674307
H	2.641728	-0.167750	1.850680
H	-1.349570	-2.357286	1.402428
H	-2.541407	-1.042366	1.297196
H	-1.366742	-1.075126	2.616716
H	-1.766214	1.296777	0.859120

7 Cation Doublet

B3LYP/TZVPP

N	2.195856	-0.916285	-1.015703
C	2.775541	-0.351432	0.147058
N	1.885536	-0.205387	1.191300
C	0.551108	-0.591513	1.253997
C	-0.046983	-1.266973	0.003373
C	0.901186	-1.211200	-1.170283
O	3.930826	-0.044273	0.175800
O	-0.083457	-0.440721	2.261828
C	-0.373101	-2.714644	0.424295
H	2.854482	-1.035712	-1.776196
H	2.275552	0.181786	2.043862
H	-1.120352	-2.699339	1.215888
H	0.522133	-3.203127	0.810661
H	-0.745363	-3.299536	-0.413049
H	0.658751	-1.778803	-2.059075
N	-0.219812	1.652831	-1.365793
C	-0.596989	2.372513	-0.192192
N	-1.481255	1.698079	0.615009
C	-2.000134	0.415972	0.432247
C	-1.277015	-0.449522	-0.618152
C	-0.542297	0.386109	-1.646924
O	-0.188871	3.482227	-0.007881
O	-2.938822	0.021140	1.059955
C	-2.308719	-1.343841	-1.313646
H	0.250123	2.236127	-2.048209
H	-1.855406	2.227974	1.394117
H	-2.836576	-1.953778	-0.586419
H	-1.844807	-1.993300	-2.055917
H	-3.046539	-0.724201	-1.822837
H	-0.577473	0.124164	-2.696722

ωB97XD/cc-pVTZ

N	2.122452	-0.790674	-1.015949
C	2.632038	-0.126081	0.120745
N	1.739546	-0.055709	1.167721
C	0.488481	-0.644641	1.272328
C	-0.080875	-1.307125	0.011758
C	0.852848	-1.181926	-1.168889
O	3.738122	0.314486	0.132921
O	-0.111857	-0.636796	2.306388

C	-0.394299	-2.760524	0.374954
H	2.789155	-0.868887	-1.771522
H	2.101780	0.366286	2.013468
H	-1.152260	-2.777610	1.155140
H	0.501067	-3.250174	0.757214
H	-0.750517	-3.319071	-0.486791
H	0.667749	-1.818727	-2.025430
N	-0.088609	1.532686	-1.355528
C	-0.400377	2.261434	-0.175492
N	-1.333925	1.655430	0.626970
C	-1.959179	0.428609	0.425884
C	-1.291710	-0.480515	-0.609210
C	-0.492260	0.287947	-1.640441
O	0.097654	3.325303	0.024174
O	-2.922674	0.101793	1.046414
C	-2.347190	-1.349029	-1.281427
H	0.426090	2.080644	-2.031177
H	-1.664291	2.207395	1.407532
H	-2.875243	-1.942675	-0.540955
H	-1.907082	-2.014097	-2.023999
H	-3.077161	-0.714969	-1.782538
H	-0.590351	0.052553	-2.693873

CC2/TZVPP

N	2.107481	-0.810122	-1.026361
C	2.586016	-0.044766	0.066138
N	1.678304	0.043852	1.108371
C	0.456958	-0.614606	1.248892
C	-0.094365	-1.315660	0.010643
C	0.829855	-1.214089	-1.174072
O	3.686060	0.458113	0.051990
O	-0.142839	-0.615283	2.309080
C	-0.431304	-2.751267	0.408920
H	2.772866	-0.888203	-1.789735
H	2.027194	0.514168	1.940653
H	-1.183391	-2.732872	1.196616
H	0.462867	-3.241900	0.795461
H	-0.802233	-3.320142	-0.440152
H	0.649807	-1.871470	-2.019014
N	-0.024165	1.496823	-1.313491
C	-0.313278	2.199636	-0.105895
N	-1.297698	1.606987	0.654800
C	-1.963923	0.403097	0.408968
C	-1.296466	-0.490048	-0.630581
C	-0.477050	0.269246	-1.642846
O	0.244021	3.244458	0.147103
O	-2.959502	0.077220	1.022092
C	-2.332999	-1.366683	-1.313944
H	0.526621	2.045054	-1.968000
H	-1.619021	2.148793	1.452659
H	-2.862083	-1.966606	-0.578400
H	-1.871601	-2.023118	-2.051978
H	-3.060464	-0.733903	-1.821868
H	-0.578546	0.068630	-2.705654

8 Anion Doublet

B3LYP/TZVPP

N	-0.964483	1.367427	-1.117243
C	-0.895230	2.314649	-0.122842
N	0.198843	2.214534	0.685354
C	1.179271	1.178245	0.721630
C	1.293959	0.350340	-0.557078
C	0.093635	0.485652	-1.539311
O	-1.763975	3.175922	0.014161
O	2.112381	1.284213	1.531878

C	2.648818	0.577126	-1.227506
H	-1.771444	1.476602	-1.707071
H	0.230309	2.860143	1.458515
H	3.447227	0.374522	-0.514992
H	2.738942	1.618985	-1.545337
H	2.785471	-0.057279	-2.107271
H	0.412763	0.746488	-2.554378
N	-1.505199	-1.520561	-1.068458
C	-2.073595	-1.421600	0.188335
N	-1.189916	-1.200348	1.200503
C	0.242870	-1.134781	1.162977
C	0.866785	-1.135863	-0.243767
C	-0.182159	-1.053038	-1.381737
O	-3.283326	-1.566499	0.358034
O	0.864002	-1.487612	2.177775
C	1.892173	-2.254206	-0.365916
H	-2.198339	-1.536356	-1.798214
H	-1.581438	-1.243714	2.127836
H	2.603297	-2.192643	0.456832
H	2.431381	-2.209337	-1.315171
H	1.396498	-3.226195	-0.302830
H	0.168778	-1.584736	-2.268989

H	2.793349	-0.064740	-2.162815
H	0.434447	0.726260	-2.604210
N	-1.460491	-1.528630	-1.074572
C	-2.043989	-1.125895	0.125920
N	-1.144252	-0.803124	1.104085
C	0.279778	-1.011011	1.107854
C	0.899733	-1.135546	-0.287950
C	-0.139832	-1.074214	-1.420498
O	-3.272515	-1.111305	0.276838
O	0.819147	-1.462744	2.146272
C	1.921081	-2.244881	-0.332640
H	-2.153176	-1.549556	-1.810560
H	-1.553271	-0.663545	2.018368
H	2.614343	-2.129492	0.499909
H	2.472016	-2.234624	-1.275994
H	1.425230	-3.212375	-0.226898
H	0.201289	-1.620118	-2.303493

C Thymine complex

ωB97XD/cc-pVTZ

N	-0.917363	1.373944	-1.188543
C	-0.973350	2.127440	-0.043727
N	0.121460	2.046275	0.759459
C	1.176983	1.088350	0.718327
C	1.318624	0.338579	-0.605951
C	0.124874	0.472251	-1.584116
O	-1.928941	2.852752	0.196341
O	2.132770	1.243251	1.487849
C	2.673683	0.574734	-1.244758
H	-1.788704	1.355781	-1.686576
H	0.069045	2.580614	1.609476
H	3.458251	0.345162	-0.525584
H	2.775884	1.623466	-1.531422
H	2.811500	-0.039359	-2.138263
H	0.446301	0.713847	-2.601112
N	-1.482180	-1.494291	-1.056492
C	-2.046065	-1.228024	0.175796
N	-1.157196	-0.900896	1.148976
C	0.281218	-1.022953	1.126678
C	0.889084	-1.128544	-0.282794
C	-0.163287	-1.058019	-1.404922
O	-3.252516	-1.315955	0.353519
O	0.833896	-1.484534	2.134898
C	1.901620	-2.247591	-0.361408
H	-2.175162	-1.562382	-1.780638
H	-1.550354	-0.842239	2.072638
H	2.627324	-2.141493	0.443295
H	2.421835	-2.247966	-1.322173
H	1.405027	-3.211554	-0.236062
H	0.164039	-1.610564	-2.286990

CC2/TZVPP

N	-0.938794	1.339454	-1.169635
C	-1.010451	2.042572	0.018070
N	0.142300	2.037717	0.758652
C	1.200327	1.074708	0.706379
C	1.324618	0.337499	-0.617363
C	0.123500	0.465121	-1.587468
O	-2.025674	2.681273	0.331485
O	2.179293	1.211125	1.485024
C	2.670119	0.564023	-1.276649
H	-1.851336	1.213124	-1.583217
H	0.067798	2.523730	1.642358
H	3.462611	0.345630	-0.561427
H	2.761098	1.609646	-1.580104

9 Neutral Singlet

ωB97XD/cc-pVTZ

N	2.301967	-0.560570	0.387059
C	2.106265	-0.324759	-0.956128
N	1.447188	0.857382	-1.209609
C	0.861307	1.715481	-0.281608
C	1.059404	1.334132	1.116010
C	1.756756	0.218960	1.373521
O	2.467999	-1.090150	-1.818166
O	0.229881	2.682561	-0.648882
C	0.445865	2.196114	2.169131
H	2.677137	-1.466249	0.611456
H	1.227466	1.031202	-2.179427
H	-0.626700	2.300128	1.998903
H	0.864189	3.202406	2.140729
H	0.609161	1.777916	3.161572
H	1.922509	-0.139283	2.379691
N	-1.442949	-1.187988	1.566836
C	-0.566493	-1.945333	0.826267
N	-0.609560	-1.659968	-0.517201
C	-1.340324	-0.650115	-1.150878
C	-2.184935	0.148136	-0.261952
C	-2.199579	-0.168291	1.039074
O	0.172485	-2.770668	1.316540
O	-1.232361	-0.479544	-2.343187
C	-2.944109	1.286547	-0.857577
H	-1.445810	-1.374398	2.553323
H	0.019739	-2.188553	-1.105393
H	-2.248095	2.035750	-1.236939
H	-3.591280	1.754588	-0.117248
H	-3.551674	0.948161	-1.696222
H	-2.802131	0.373524	1.754365

CC2/TZVPP

N	2.283110	-0.600325	0.392377
C	2.103205	-0.387189	-0.964261
N	1.469988	0.810765	-1.240215
C	0.818474	1.661106	-0.335042
C	0.970501	1.286245	1.062129
C	1.688336	0.173267	1.358013
O	2.465179	-1.186490	-1.820923
O	0.169871	2.630325	-0.737476
C	0.319614	2.144245	2.094817

H	2.633266	-1.516916	0.633291
H	1.260435	0.968697	-2.220322
H	-0.751749	2.216997	1.903916
H	0.715251	3.159096	2.059087
H	0.479578	1.738695	3.093400
H	1.831218	-0.169539	2.374119
N	-1.379433	-1.164294	1.595895
C	-0.483178	-1.898204	0.841642
N	-0.533471	-1.579224	-0.499819
C	-1.267550	-0.549543	-1.119658
C	-2.122228	0.210273	-0.220385
C	-2.151598	-0.145134	1.088067
O	0.277033	-2.734676	1.325089
O	-1.147222	-0.345359	-2.327627
C	-2.906681	1.344945	-0.788898
H	-1.387449	-1.379020	2.581042
H	0.099556	-2.096055	-1.103740
H	-2.224331	2.105767	-1.169106
H	-3.547662	1.790071	-0.029081
H	-3.521523	1.004305	-1.620951
H	-2.777221	0.364283	1.808679

H	2.921381	-1.317696	0.616800
H	1.081936	0.887016	-2.200412
H	-0.763226	1.997180	2.056021
H	0.530634	3.180783	2.003544
H	0.638297	1.811758	3.126594
H	2.093491	-0.003136	2.371178
N	-1.429099	-1.039932	1.627162
C	-0.455690	-1.733152	0.926464
N	-0.552388	-1.632566	-0.453747
C	-1.300553	-0.679671	-1.169153
C	-2.245521	0.061170	-0.357531
C	-2.469910	-0.330967	1.052659
O	0.410991	-2.394487	1.490977
O	-1.075020	-0.487284	-2.360947
C	-2.906569	1.259848	-0.901240
H	-1.424829	-1.238102	2.617756
H	0.178695	-2.101043	-0.979025
H	-2.563161	2.146439	-0.358485
H	-3.989322	1.193284	-0.760104
H	-2.669945	1.378464	-1.954879
H	-3.467185	-0.497561	1.443726

10 Neutral Triplet

11 Cation Doublet

ω B97XD/cc-pVTZ

N	2.462829	-0.429662	0.382457
C	2.199106	-0.258135	-0.958492
N	1.415833	0.844441	-1.219758
C	0.768080	1.657750	-0.293765
C	1.041030	1.336673	1.105009
C	1.863995	0.311650	1.366778
O	2.609547	-1.007709	-1.812368
O	0.023781	2.540608	-0.665511
C	0.342133	2.135389	2.155581
H	2.943242	-1.280878	0.616731
H	1.147686	0.966276	-2.185443
H	-0.738921	2.004913	2.073156
H	0.542457	3.199408	2.032814
H	0.655185	1.830515	3.153198
H	2.089696	-0.001804	2.375882
N	-1.454199	-1.094865	1.606096
C	-0.510565	-1.812170	0.897922
N	-0.605325	-1.702718	-0.470319
C	-1.359735	-0.745350	-1.175964
C	-2.263722	0.030008	-0.380830
C	-2.432921	-0.292853	1.060500
O	0.323627	-2.491859	1.453767
O	-1.157089	-0.584336	-2.368564
C	-2.934890	1.216191	-0.934618
H	-1.423518	-1.260063	2.598167
H	0.103018	-2.186272	-1.001874
H	-2.533168	2.116424	-0.455403
H	-4.007209	1.188901	-0.718406
H	-2.771228	1.293565	-2.005583
H	-3.415209	-0.319915	1.516105

CC2/TZVPP

N	2.454163	-0.456130	0.375154
C	2.155137	-0.319728	-0.969605
N	1.392215	0.802302	-1.237500
C	0.724006	1.615812	-0.312032
C	1.006296	1.312521	1.081602
C	1.853790	0.290451	1.358445
O	2.528354	-1.117800	-1.822591
O	-0.051814	2.496380	-0.695510
C	0.318393	2.119966	2.131943

ω B97XD/cc-pVTZ

N	4.041751	0.316772	-0.311451
C	3.677513	-0.880497	0.269868
N	2.300749	-0.998624	0.416944
C	1.336582	-0.088513	0.056535
C	1.817014	1.136353	-0.544045
C	3.149348	1.269564	-0.698195
O	4.451717	-1.728632	0.614331
O	0.148436	-0.360251	0.253046
C	0.834144	2.176115	-0.976482
H	5.030863	0.450222	-0.442514
H	1.991432	-1.866242	0.827698
H	0.245259	2.545151	-0.136967
H	0.134008	1.774558	-1.709453
H	1.340157	3.027014	-1.427485
H	3.583534	2.153015	-1.144920
N	-2.428363	-1.753166	0.400363
C	-2.600200	-1.362026	-0.966684
N	-2.660883	-0.009007	-1.139233
C	-2.452513	0.965153	-0.172218
C	-2.194957	0.453942	1.196608
C	-2.218782	-0.930059	1.398930
O	-2.700912	-2.194072	-1.811121
O	-2.492887	2.136554	-0.427476
C	-1.932548	1.415983	2.273263
H	-2.416239	-2.756775	0.534919
H	-2.811818	0.312634	-2.086030
H	-0.985624	1.923837	2.066142
H	-1.876563	0.942998	3.249527
H	-2.693093	2.199269	2.269605
H	-2.059130	-1.362376	2.377403

CC2/TZVPP

N	3.519326	1.300595	0.310609
C	3.226208	0.306402	1.238595
N	2.011532	-0.319800	0.947945
C	1.148238	-0.048205	-0.092875
C	1.540006	0.984103	-1.001978
C	2.732931	1.610273	-0.753880
O	3.931130	0.015153	2.183698
O	0.078899	-0.721380	-0.200559
C	0.679810	1.323809	-2.178074

H	4.394272	1.785729	0.464563
H	1.777231	-1.095408	1.557867
H	-0.194308	1.889568	-1.860453
H	0.344693	0.417386	-2.679463
H	1.233826	1.930605	-2.891236
H	3.105870	2.396538	-1.396591
N	-2.858277	-1.534420	-0.091730
C	-3.093760	-0.525699	-1.071502
N	-2.573710	0.699027	-0.718044
C	-1.738789	0.986062	0.357262
C	-1.546478	-0.137480	1.307028
C	-2.172152	-1.355967	1.036272
O	-3.714624	-0.771848	-2.080058
O	-1.212697	2.076921	0.503587
C	-0.861698	0.144447	2.581818
H	-3.271504	-2.434193	-0.316397
H	-2.733466	1.447827	-1.385208
H	0.024344	0.753762	2.405634
H	-0.608706	-0.765690	3.120512
H	-1.520415	0.754302	3.209498
H	-2.089737	-2.203530	1.704067

H	2.751236	-2.393609	-0.319272
H	2.535150	1.287091	-1.868696
H	1.538911	2.075445	2.544799
H	2.123378	0.630355	3.398360
H	0.468208	0.692929	2.801456
H	2.400707	-1.574230	1.949179
N	-0.759935	-0.704469	0.421180
C	-1.677935	-1.722907	0.333010
N	-2.928150	-1.288110	-0.095869
C	-3.336111	0.009721	-0.430225
C	-2.292258	1.000271	-0.303040
C	-1.059998	0.595556	0.115098
O	-1.447785	-2.901842	0.601767
O	-4.502350	0.221510	-0.793862
C	-2.597062	2.424617	-0.637934
H	0.208224	-0.942373	0.741903
H	-3.631288	-2.010491	-0.176238
H	-2.952519	2.511515	-1.665115
H	-1.703163	3.035550	-0.518492
H	-3.386551	2.815687	0.004953
H	-0.238673	1.295120	0.229712

12 Anion Doublet

ωB97XD/cc-pVTZ

N	2.788361	-1.399976	-0.144007
C	2.942286	-0.613744	-1.243995
N	2.599682	0.697487	-1.044316
C	2.117198	1.296457	0.159967
C	1.983356	0.420852	1.243013
C	2.176522	-0.970501	1.065940
O	3.347903	-1.039148	-2.319245
O	1.820623	2.507798	0.095315
C	1.479725	0.944200	2.552827
H	2.884843	-2.380974	-0.328428
H	2.705931	1.313760	-1.829901
H	1.344232	2.022471	2.482469
H	2.176923	0.735272	3.371523
H	0.517866	0.497745	2.835009
H	2.384180	-1.610952	1.916213
N	-0.824316	-0.707582	0.379625
C	-1.760624	-1.703748	0.356051
N	-3.014199	-1.265058	-0.032202
C	-3.404930	0.027656	-0.374388
C	-2.336803	1.007173	-0.312205
C	-1.111504	0.588922	0.059156
O	-1.542278	-2.862011	0.643232
O	-4.561480	0.249609	-0.688196
C	-2.640886	2.430024	-0.656646
H	0.137251	-0.952644	0.670279
H	-3.730171	-1.972178	-0.064296
H	-3.063992	2.507066	-1.659398
H	-1.735356	3.033198	-0.608334
H	-3.380373	2.848143	0.028881
H	-0.272212	1.271270	0.125129

CC2/TZVPP

N	2.701284	-1.404918	-0.132829
C	2.790099	-0.640899	-1.264135
N	2.478845	0.686398	-1.060569
C	2.057731	1.308958	0.154442
C	1.970058	0.443798	1.260152
C	2.136221	-0.956274	1.095956
O	3.122989	-1.094793	-2.370256
O	1.757700	2.534056	0.091198
C	1.500795	0.986923	2.572436

D Thymidine dimer

13 Neutral Singlet

Min A

N	0.263147	1.161688	-1.810982
C	0.255973	1.263789	-0.440070
N	0.655756	0.112725	0.244805
C	1.386354	-0.945608	-0.245052
C	1.353410	-1.131917	-1.752893
C	0.404205	-0.128355	-2.435166
O	-0.018630	2.265862	0.169862
O	2.000166	-1.676539	0.490672
C	2.782259	-1.217480	-2.255973
H	0.675980	0.230721	1.246703
H	3.303408	-2.038343	-1.767125
H	3.314566	-0.292553	-2.028024
H	2.813134	-1.368290	-3.333361
H	0.726514	0.025153	-3.459921
N	-1.803996	-1.090593	-1.492777
C	-1.894658	-1.841356	-0.346231
N	-0.922086	-2.824591	-0.164297
C	0.035507	-3.257792	-1.048306
C	0.341304	-2.284538	-2.160805
C	-0.737731	-1.215578	-2.450130
O	-2.765963	-1.706601	0.477848
O	0.603000	-4.310734	-0.908310
C	0.727413	-3.047202	-3.416664
H	-1.076664	-3.400736	0.648458
H	1.573307	-3.702696	-3.224328
H	0.978546	-2.368131	-4.231468
H	-0.118312	-3.656094	-3.735724
H	-1.168237	-1.362152	-3.434343
C	-3.054240	-0.446848	-1.895376
C	-2.909343	0.497398	-3.066901
C	-3.307058	-0.294839	-4.305802
C	-4.358760	-1.261075	-3.691132
O	-3.992490	-1.419640	-2.327108
C	-4.557349	-2.663186	-4.244876
O	-3.327849	-3.432760	-4.288692
H	-3.454893	0.036926	-0.999078
H	-3.652756	1.300362	-2.962620

H	-1.941821	0.991777	-3.129336	C	0.067144	2.530720	-2.303223
H	-2.478490	-0.890471	-4.726161	C	0.254253	3.734931	-4.336451
H	-5.343046	-0.754515	-3.760374	C	-1.170541	3.827338	-3.760250
H	-4.998290	-2.581520	-5.257426	O	-1.245689	2.865877	-2.713949
H	-3.541439	-4.337708	-4.633855	C	0.841276	2.512253	-3.618961
C	0.202666	2.422515	-2.525293	C	-2.267461	3.572174	-4.774073
C	0.234086	3.784525	-4.444269	O	-1.984324	2.464177	-5.655138
C	-1.152449	3.813360	-3.783201	H	0.445801	3.328385	-1.642476
O	-1.142869	2.804944	-2.773719	H	0.589149	1.613114	-4.201673
C	0.842792	2.486234	-3.906562	H	1.931989	2.572511	-3.498345
C	-2.267462	3.571988	-4.774072	O	0.884659	4.942103	-3.984253
O	-1.984278	2.464230	-5.655190	H	0.233694	3.582526	-5.426918
H	0.665649	3.169570	-1.863659	H	-1.291217	4.838264	-3.333756
H	0.494747	1.661093	-4.544613	H	-2.356153	4.454105	-5.425290
H	1.941788	2.494062	-3.883992	H	-3.230109	3.427178	-4.254654
O	0.884752	4.942188	-3.984125	O	-3.704454	0.702131	-5.259426
H	0.156821	3.764940	-5.542736	H	-5.288497	-3.156929	-3.584543
H	-1.280541	4.800483	-3.307979	H	-2.111666	1.617509	-5.159398
H	-2.361571	4.457142	-5.420301	H	-3.829651	0.308706	-6.145861
H	-3.227432	3.424221	-4.250106	H	1.806711	4.935930	-4.309806
O	-3.704278	0.702246	-5.259375				
H	-5.293945	-3.159441	-3.591166	Min D1			
H	-2.111744	1.617507	-5.159420	N	0.193754	1.593509	-1.298963
H	-3.829785	0.308649	-6.145817	C	-0.249080	1.887201	-0.008602
H	1.806669	4.935981	-4.309926	N	0.073936	0.931346	0.924787
				C	0.843705	-0.211022	0.759097
Min B				C	1.324069	-0.414568	-0.605649
N	0.043931	1.296385	-1.533697	C	0.963844	0.474710	-1.540337
C	-0.498328	1.402576	-0.276124	O	-0.847212	2.896638	0.265568
N	-0.371375	0.270139	0.534036	O	1.065252	-0.949138	1.694105
C	0.612153	-0.690222	0.438099	C	2.226696	-1.574655	-0.877389
C	1.346917	-0.638093	-0.855283	H	-0.315637	1.079273	1.842873
C	0.657166	0.053786	-1.999686	H	1.841368	-2.490825	-0.434969
O	-1.056133	2.389067	0.136475	H	3.206481	-1.405487	-0.427761
O	0.843401	-1.464719	1.332353	H	2.358121	-1.727599	-1.947820
C	2.551640	-1.182103	-0.936323	H	1.291607	0.355951	-2.561099
H	-0.840284	0.343684	1.423586	N	-1.979036	-1.598839	-1.513404
H	2.971118	-1.694917	-0.082131	C	-1.859522	-1.738673	-0.137309
H	3.133532	-1.148823	-1.847493	N	-1.059584	-2.786831	0.249789
H	1.461222	-1.731953	-3.665772	C	-0.391801	-3.703809	-0.554528
H	1.431432	0.329312	-2.711634	C	-0.568665	-3.482116	-1.981905
N	-1.489739	-1.337320	-2.086771	C	-1.343985	-2.463421	-2.371058
C	-1.418579	-2.421689	-1.250198	O	-2.390459	-1.001113	0.661713
N	-0.315698	-3.257059	-1.446322	O	0.280739	-4.583839	-0.061866
C	0.624958	-3.191819	-2.438520	C	0.124323	-4.401179	-2.932562
C	0.448663	-2.052183	-3.419971	H	-0.884283	-2.847845	1.241973
C	-0.313260	-0.872172	-2.808082	H	1.207169	-4.330699	-2.818521
O	-2.226443	-2.675121	-0.392593	H	-0.137317	-4.165246	-3.963166
O	1.514935	-4.003497	-2.529633	H	-0.142371	-5.438541	-2.729882
C	-0.210394	-2.576575	-4.696321	H	-1.530178	-2.289461	-3.417939
H	-0.229011	-4.002152	-0.773005	C	-2.930443	-0.607706	-2.013396
H	0.336893	-3.441247	-5.067959	C	-2.467603	0.159633	-3.250355
H	-0.188387	-1.804587	-5.467279	C	-3.249686	-0.400322	-4.438155
H	-1.246281	-2.863036	-4.519193	C	-4.372110	-1.229855	-3.766202
H	-0.659742	-0.262436	-3.637701	O	-4.149940	-1.216537	-2.364083
C	-2.772741	-0.606629	-2.028798	C	-4.557153	-2.662954	-4.244688
C	-2.870040	0.470652	-3.073709	O	-3.328014	-3.433017	-4.288806
C	-3.283786	-0.294610	-4.320758	H	-3.113076	0.054719	-1.161628
C	-4.308611	-1.273625	-3.678354	H	-2.735368	1.212435	-3.112985
O	-3.856034	-1.459664	-2.337635	H	-1.378964	0.123917	-3.382600
C	-4.557260	-2.663118	-4.244653	H	-2.622292	-1.068364	-5.052374
O	-3.327855	-3.432755	-4.288963	H	-5.330308	-0.715444	-3.958729
H	-2.926334	-0.256985	-1.000416	H	-5.010279	-2.624783	-5.254027
H	-3.698434	1.140619	-2.802061	H	-3.541442	-4.337716	-4.633830
H	-1.995526	1.106619	-3.179853	C	0.088937	2.681130	-2.253776
H	-2.445630	-0.876963	-4.742971	C	0.257408	3.728866	-4.324845
H	-5.287197	-0.753833	-3.666170	C	-1.176674	3.814129	-3.751019
H	-5.000538	-2.572202	-5.254570	O	-1.241625	2.844608	-2.703095
H	-3.541454	-4.337736	-4.633769	C	0.860347	2.548060	-3.559934

C	-2.267411	3.572118	-4.774225	O	0.884546	4.941830	-3.984165
O	-1.984381	2.464190	-5.655175	H	-0.108616	4.484810	-5.751996
H	0.403156	3.598403	-1.727210	H	-1.156221	4.504633	-3.150480
H	0.596394	1.608907	-4.068937	H	-2.416737	4.466785	-5.393143
H	1.951943	2.620740	-3.456136	H	-3.183793	3.387392	-4.188810
O	0.884479	4.942032	-3.983963	O	-3.705017	0.702286	-5.259637
H	0.243639	3.554190	-5.411494	H	-5.293037	-3.169348	-3.598536
H	-1.296925	4.822518	-3.316808	H	-2.111719	1.617496	-5.159223
H	-2.339127	4.458166	-5.421574	H	-3.829361	0.308692	-6.145896
H	-3.238280	3.437671	-4.266025	H	1.806667	4.935942	-4.309930
O	-3.704635	0.702159	-5.259310				
H	-5.280687	-3.141018	-3.563680	TS A-B			
H	-2.111656	1.617509	-5.159395	N	0.202969	1.245429	-1.657256
H	-3.829440	0.308727	-6.145901	C	0.044857	1.396631	-0.293173
H	1.806642	4.935970	-4.310002	N	0.464230	0.307052	0.467871
				C	1.434723	-0.610045	0.077242
Min D2				C	1.570769	-0.737233	-1.361552
N	0.724921	0.643729	-3.568539	C	0.513578	-0.068479	-2.196966
C	1.571187	0.035023	-2.650212	O	-0.380554	2.397006	0.227035
N	1.730381	-1.317276	-2.855195	O	2.082575	-1.233642	0.893211
C	1.148747	-2.118781	-3.832804	C	2.807492	-1.321913	-1.929113
C	0.243484	-1.405780	-4.727698	H	0.343735	0.430015	1.461087
C	0.100927	-0.088239	-4.552022	H	3.208743	-2.070614	-1.248328
O	2.133493	0.625141	-1.758229	H	3.574008	-0.547398	-2.053269
O	1.409859	-3.298810	-3.905289	H	2.637742	-1.773771	-2.905407
C	-0.474838	-2.176082	-5.787009	H	0.926994	0.071687	-3.192534
H	2.305575	-1.789179	-2.170016	N	-1.798647	-0.902961	-1.435873
H	0.213272	-2.840339	-6.307854	C	-1.823141	-1.615572	-0.250601
H	-0.926497	-1.500524	-6.514218	N	-0.854649	-2.602960	-0.132942
H	-1.263615	-2.792597	-5.351870	C	-0.188790	-3.215110	-1.187086
H	-0.530757	0.492795	-5.205093	C	-0.177715	-2.444916	-2.410555
N	-2.060101	-1.058183	-1.388350	C	-0.716758	-1.049704	-2.387247
C	-1.246384	-0.286773	-0.583160	O	-2.620933	-1.419751	0.632953
N	-0.119488	-0.937275	-0.140237	O	0.345356	-4.299385	-1.054402
C	0.257048	-2.254136	-0.386109	C	0.218201	-3.069389	-3.689105
C	-0.696084	-3.012738	-1.180380	H	-0.868863	-3.106682	0.739474
C	-1.779280	-2.376325	-1.653415	H	0.761857	-3.995292	-3.518338
O	-1.501133	0.863628	-0.301268	H	0.821282	-2.395816	-4.303333
O	1.321118	-2.671367	0.026276	H	-0.693695	-3.293123	-4.256756
C	-0.401990	-4.449984	-1.464086	H	-1.122028	-0.838660	-3.368861
H	0.543048	-0.363944	0.360531	C	-3.093526	-0.391765	-1.869356
H	-0.363346	-5.023769	-0.537251	C	-3.019237	0.561548	-3.037692
H	0.563454	-4.554320	-1.956993	C	-3.327334	-0.268969	-4.278106
H	-1.167879	-4.875024	-2.111106	C	-4.350416	-1.270714	-3.668160
H	-2.492066	-2.875916	-2.291287	O	-3.915289	-1.462122	-2.329336
C	-3.309495	-0.400297	-1.838604	C	-4.557283	-2.663148	-4.244799
C	-3.093203	0.565654	-2.984420	O	-3.327859	-3.432773	-4.288760
C	-3.352049	-0.258028	-4.245002	H	-3.559307	0.045090	-0.980053
C	-4.428143	-1.246814	-3.715787	H	-3.830453	1.298728	-2.953185
O	-4.208218	-1.362920	-2.307651	H	-2.092992	1.134004	-3.079806
C	-4.556892	-2.663018	-4.244732	H	-2.461640	-0.848246	-4.647373
O	-3.328115	-3.433185	-4.288686	H	-5.342698	-0.773676	-3.687673
H	-3.724739	0.096300	-0.953346	H	-4.994021	-2.566519	-5.257391
H	-3.870524	1.344477	-2.945771	H	-3.541442	-4.337713	-4.633837
H	-2.120095	1.062518	-2.942178	C	0.156117	2.472617	-2.425491
H	-2.461579	-0.832124	-4.548330	C	0.243754	3.760568	-4.399148
H	-5.417484	-0.776536	-3.881469	C	-1.159826	3.815330	-3.771105
H	-4.987754	-2.604544	-5.262454	O	-1.182770	2.824642	-2.745698
H	-3.541434	-4.337701	-4.633874	C	0.843852	2.489777	-3.785379
C	0.609441	2.092760	-3.565007	C	-2.267541	3.572030	-4.774054
C	0.169303	4.049106	-4.776784	O	-1.984301	2.464253	-5.655226
C	-1.042488	3.719225	-3.912600	H	0.578079	3.258946	-1.780487
O	-0.724132	2.479814	-3.266220	H	0.523262	1.632753	-4.397067
C	0.916046	2.735450	-4.913726	H	1.941486	2.509927	-3.729019
C	-2.267573	3.572414	-4.773984	O	0.884678	4.942183	-3.984245
O	-1.984121	2.464124	-5.655126	H	0.189495	3.685036	-5.496524
H	1.287579	2.442631	-2.777420	H	-1.284513	4.811863	-3.314194
H	0.505355	2.154094	-5.745998	H	-2.354289	4.456796	-5.421689
H	1.995971	2.872823	-5.072950	H	-3.230496	3.428417	-4.254724

O	-3.704237	0.702262	-5.259411
H	-5.295167	-3.167820	-3.599498
H	-2.111666	1.617509	-5.159397
H	-3.829823	0.308647	-6.145811
H	1.806711	4.935888	-4.309806

O	-3.704320	0.702222	-5.259433
H	-5.295428	-3.170179	-3.601334
H	-2.111744	1.617507	-5.159420
H	-3.829777	0.308648	-6.145818
H	1.806669	4.935913	-4.309923

14 Neutral Triplet

Min B

N	0.180885	1.268262	-1.602443
C	-0.150077	1.425274	-0.270743
N	0.154312	0.348237	0.549305
C	1.085171	-0.643470	0.273867
C	1.410004	-0.778014	-1.127149
C	0.598239	-0.025694	-2.126495
O	-0.640271	2.432732	0.178155
O	1.559841	-1.331965	1.156117
C	2.501167	-1.697820	-1.525131
H	-0.095249	0.475085	1.517153
H	2.349755	-2.688035	-1.092060
H	3.457577	-1.339923	-1.132474
H	2.582668	-1.796027	-2.606125
H	1.235094	0.153886	-2.992223
N	-1.699029	-1.049957	-1.740033
C	-1.652454	-2.086237	-0.830385
N	-0.685736	-3.052418	-1.098927
C	-0.133901	-3.303209	-2.349251
C	-0.176388	-2.175635	-3.252108
C	-0.621826	-0.867281	-2.695031
O	-2.383406	-2.179949	0.122829
O	0.374325	-4.377577	-2.613033
C	0.141455	-2.352575	-4.683789
H	-0.657644	-3.810568	-0.435561
H	0.844758	-3.171076	-4.826629
H	0.539309	-1.438724	-5.128385
H	-0.778905	-2.615588	-5.220226
H	-0.989108	-0.252318	-3.507122
C	-3.033135	-0.456068	-1.909014
C	-3.086480	0.567583	-3.008421
C	-3.347946	-0.258351	-4.263877
C	-4.370628	-1.269455	-3.672904
O	-3.975999	-1.438477	-2.313633
C	-4.557312	-2.663183	-4.244853
O	-3.327852	-3.432766	-4.288685
H	-3.348041	-0.083106	-0.928832
H	-3.973896	1.198877	-2.855908
H	-2.230827	1.241228	-3.046772
H	-2.464118	-0.828732	-4.600609
H	-5.367270	-0.784296	-3.715343
H	-4.993579	-2.571626	-5.258541
H	-3.541436	-4.337702	-4.633871
C	0.140288	2.485044	-2.387824
C	0.252514	3.747862	-4.379161
C	-1.159453	3.806882	-3.766619
O	-1.195374	2.808750	-2.749993
C	0.858613	2.494058	-3.732269
C	-2.267434	3.572075	-4.774039
O	-1.984276	2.464207	-5.655161
H	0.529686	3.291302	-1.746309
H	0.568934	1.619131	-4.334990
H	1.954179	2.536839	-3.653466
O	0.884723	4.942195	-3.984138
H	0.209438	3.647815	-5.475042
H	-1.281408	4.801097	-3.303484
H	-2.348837	4.458018	-5.420389
H	-3.231217	3.430252	-4.255913

Min C

N	0.332117	1.216952	-1.768701
C	-0.226074	1.229526	-0.506075
N	-0.011116	0.077359	0.235887
C	0.758878	-1.021368	-0.065576
C	1.311914	-1.104196	-1.482169
C	1.193767	0.207957	-2.177301
O	-0.845750	2.158751	-0.051356
O	0.973826	-1.860667	0.773198
C	2.794001	-1.491750	-1.350370
H	-0.394004	0.104848	1.168849
H	2.892279	-2.506026	-0.970592
H	3.293249	-0.812551	-0.660542
H	3.292901	-1.418069	-2.314444
H	1.688768	0.354670	-3.119107
N	-1.851491	-1.649769	-1.881693
C	-1.936106	-2.529658	-0.823627
N	-0.940993	-3.503389	-0.808654
C	0.274601	-3.483195	-1.457965
C	0.506607	-2.247846	-2.329077
C	-0.808756	-1.738039	-2.774430
O	-2.795224	-2.487124	0.023457
O	1.067430	-4.382941	-1.339523
C	1.315534	-2.655452	-3.559722
H	-1.040090	-4.188945	-0.076709
H	2.214603	-3.195809	-3.281670
H	1.586815	-1.779128	-4.149669
H	0.708803	-3.308177	-4.185516
H	-0.908297	-1.256471	-3.727576
C	-2.948611	-0.673311	-2.009109
C	-2.720245	0.325792	-3.122235
C	-3.296448	-0.346281	-4.362573
C	-4.399380	-1.243306	-3.738763
O	-4.165941	-1.286211	-2.334079
C	-4.557072	-2.662888	-4.244346
O	-3.328032	-3.433037	-4.288976
H	-3.071379	-0.214162	-1.021171
H	-3.331071	1.212543	-2.906302
H	-1.691395	0.668715	-3.222105
H	-2.558203	-0.992827	-4.867519
H	-5.372882	-0.746219	-3.901672
H	-5.003722	-2.612571	-5.257554
H	-3.541434	-4.337699	-4.633880
C	0.229053	2.478333	-2.500346
C	0.246241	3.776929	-4.441271
C	-1.144299	3.790039	-3.783629
O	-1.123773	2.750601	-2.803981
C	0.893204	2.515742	-3.868697
C	-2.267465	3.572180	-4.774312
O	-1.984248	2.464151	-5.655084
H	0.625720	3.276314	-1.849318
H	0.585013	1.641390	-4.460936
H	1.990072	2.578521	-3.841996
O	0.884401	4.941870	-3.983866
H	0.177800	3.739209	-5.539544
H	-1.268709	4.763788	-3.279331
H	-2.350926	4.462470	-5.414389
H	-3.227783	3.428255	-4.250037
O	-3.704270	0.702098	-5.259567
H	-5.288498	-3.153332	-3.580012
H	-2.111785	1.617506	-5.159432
H	-3.829789	0.308752	-6.145863
H	1.806667	4.935943	-4.309930

Min D				C	1.297945	-0.815379	-0.027616
N	0.728022	0.697933	-3.207757	C	1.670973	-0.806846	-1.416834
C	1.685241	0.253537	-2.282728	C	0.842200	-0.013014	-2.325398
N	2.059111	-1.057703	-2.411296	O	-0.673286	2.122121	0.051323
C	1.614567	-1.984687	-3.364656	O	1.807890	-1.503439	0.835315
C	0.534417	-1.544332	-4.176635	C	2.929246	-1.476142	-1.829899
C	0.005835	-0.161364	-4.010527	H	-0.027631	0.089664	1.254144
O	2.170904	0.980140	-1.449496	H	2.926042	-2.523027	-1.516864
O	2.126988	-3.095634	-3.413698	H	3.788964	-1.009708	-1.340321
C	-0.081234	-2.427154	-5.179782	H	3.076728	-1.426014	-2.906488
H	2.688612	-1.404081	-1.703862	H	1.223784	0.112234	-3.326076
H	0.465887	-3.362567	-5.258714	N	-1.704305	-1.461568	-1.819704
H	-0.108799	-1.933780	-6.157871	C	-1.701134	-2.218532	-0.652670
H	-1.123727	-2.645086	-4.912846	N	-0.724021	-3.185458	-0.596485
H	-0.458630	0.303066	-4.868476	C	0.187235	-3.537374	-1.588015
N	-2.148137	-0.962493	-1.327800	C	0.145177	-2.693108	-2.758103
C	-1.400595	-0.177105	-0.474696	C	-0.718088	-1.604421	-2.773899
N	-0.258798	-0.787339	-0.009504	O	-2.486095	-2.041695	0.246512
C	0.179316	-2.086549	-0.255808	O	0.939662	-4.479880	-1.432774
C	-0.675993	-2.842003	-1.159230	C	0.975304	-3.041661	-3.943488
C	-1.772316	-2.240817	-1.652102	H	-0.686249	-3.713861	0.260517
O	-1.720779	0.948993	-0.164838	H	1.890873	-3.544857	-3.640109
O	1.205628	-2.491614	0.249812	H	1.227351	-2.156006	-4.528888
C	-0.304507	-4.251672	-1.487444	H	0.427515	-3.724301	-4.598161
H	0.328789	-0.215164	0.578089	H	-0.918666	-1.131344	-3.718483
H	-0.289205	-4.863550	-0.584648	C	-2.877271	-0.595829	-2.003767
H	0.690873	-4.300972	-1.928321	C	-2.728122	0.378406	-3.143831
H	-1.019767	-4.678674	-2.189484	C	-3.285278	-0.338130	-4.362254
H	-2.433001	-2.754312	-2.334863	C	-4.356674	-1.254067	-3.709511
C	-3.406307	-0.354756	-1.817819	O	-4.021908	-1.352600	-2.326606
C	-3.197293	0.610876	-2.963992	C	-4.557252	-2.663155	-4.244788
C	-3.379028	-0.236586	-4.221933	O	-3.327872	-3.432795	-4.288736
C	-4.447644	-1.245127	-3.717549	H	-3.059780	-0.117568	-1.036444
O	-4.249583	-1.359015	-2.306150	H	-3.380525	1.238761	-2.944253
C	-4.556754	-2.662867	-4.244669	H	-1.725075	0.780004	-3.268759
O	-3.328120	-3.433185	-4.288799	H	-2.535516	-0.975964	-4.862777
H	-3.864026	0.128215	-0.946352	H	-5.332853	-0.740758	-3.798601
H	-4.008126	1.355514	-2.958942	H	-5.002493	-2.588835	-5.256387
H	-2.243610	1.141261	-2.901005	H	-3.541435	-4.337701	-4.633874
H	-2.456288	-0.786321	-4.472576	C	0.186134	2.423688	-2.493030
H	-5.440835	-0.788779	-3.901061	C	0.242484	3.771165	-4.422943
H	-4.985559	-2.608364	-5.263497	C	-1.152450	3.793951	-3.774033
H	-3.541453	-4.337735	-4.633774	O	-1.155524	2.761851	-2.786722
C	0.561852	2.135543	-3.350919	C	0.865011	2.492857	-3.854910
C	0.185866	3.986885	-4.725071	C	-2.267412	3.572262	-4.774041
C	-1.061181	3.720977	-3.883782	O	-1.984269	2.464172	-5.655138
O	-0.797793	2.501162	-3.175680	H	0.605917	3.182939	-1.812225
C	0.923856	2.659575	-4.736206	H	0.549357	1.648382	-4.485376
C	-2.267538	3.572471	-4.774014	H	1.962624	2.527271	-3.808974
O	-1.984329	2.464171	-5.655233	O	0.884641	4.941941	-3.984110
H	1.181012	2.592824	-2.570474	H	0.173278	3.725503	-5.521151
H	0.524045	2.010223	-5.523849	H	-1.278661	4.771934	-3.279050
H	2.009453	2.773249	-4.872712	H	-2.348182	4.461357	-5.416252
O	0.884422	4.941595	-3.984000	H	-3.230888	3.429637	-4.255294
H	-0.058468	4.343760	-5.739950	O	-3.704413	0.702166	-5.259452
H	-1.177684	4.541077	-3.158746	H	-5.291693	-3.154544	-3.584850
H	-2.395101	4.469700	-5.394465	H	-2.111709	1.617512	-5.159382
H	-3.195753	3.399475	-4.203770	H	-3.829694	0.308689	-6.145847
O	-3.705054	0.702330	-5.259696	H	1.806657	4.935963	-4.309958
H	-5.292204	-3.173166	-3.600861	TS C-D			
H	-2.111473	1.617465	-5.159159	N	0.377830	1.165667	-1.846182
H	-3.829361	0.308683	-6.145893	C	-0.032713	1.185582	-0.519138
H	1.806637	4.935959	-4.310015	N	0.228159	0.024511	0.184988
TS B-D				C	1.162766	-0.958467	-0.148930
N	0.265451	1.145740	-1.787821	C	1.494587	-1.037840	-1.570535
C	-0.101239	1.183601	-0.442740	C	0.989887	0.049991	-2.400156
N	0.251811	0.062925	0.285988	O	-0.567916	2.139017	-0.010159
				O	1.618264	-1.675094	0.716057

C	2.875578	-1.558418	-1.850950
H	-0.030236	0.066779	1.158931
H	3.024023	-2.521694	-1.365454
H	3.623573	-0.867423	-1.451505
H	3.055299	-1.659562	-2.919423
H	1.346966	0.154565	-3.408720
N	-1.895528	-1.590269	-1.725642
C	-1.897746	-2.182969	-0.466137
N	-0.927835	-3.146008	-0.282478
C	0.106519	-3.493797	-1.139993
C	0.180447	-2.660865	-2.348678
C	-0.951171	-1.905744	-2.657204
O	-2.686835	-1.891038	0.398526
O	0.855901	-4.404845	-0.879863
C	0.967163	-3.223899	-3.495526
H	-0.931510	-3.592096	0.621196
H	1.880264	-3.694854	-3.145039
H	1.212980	-2.448668	-4.221905
H	0.377452	-3.987440	-4.005680
H	-1.111896	-1.553440	-3.658228
C	-2.973209	-0.625658	-1.993393
C	-2.676561	0.305754	-3.150284
C	-3.290421	-0.356183	-4.376741
C	-4.397575	-1.239883	-3.743652
O	-4.171680	-1.268986	-2.337521
C	-4.557072	-2.662888	-4.244346
O	-3.328032	-3.433037	-4.288976
H	-3.137597	-0.102853	-1.045956
H	-3.216595	1.244216	-2.972750
H	-1.622148	0.561305	-3.254707
H	-2.573730	-1.007690	-4.905923
H	-5.368322	-0.741104	-3.917108
H	-5.004641	-2.614622	-5.256747
H	-3.541434	-4.337699	-4.633880
C	0.248917	2.432952	-2.555407
C	0.240852	3.787648	-4.459287
C	-1.142294	3.781561	-3.784705
O	-1.110699	2.723681	-2.824892
C	0.889182	2.507688	-3.933465
C	-2.267465	3.572180	-4.774312
O	-1.984248	2.464151	-5.655084
H	0.659721	3.213082	-1.893403
H	0.559539	1.663302	-4.555622
H	1.987254	2.553029	-3.920780
O	0.884401	4.941870	-3.983866
H	0.157289	3.779830	-5.557329
H	-1.267890	4.746092	-3.263595
H	-2.348988	4.463531	-5.413121
H	-3.229224	3.429307	-4.251997
O	-3.704270	0.702098	-5.259567
H	-5.287114	-3.152340	-3.577885
H	-2.111785	1.617506	-5.159432
H	-3.829789	0.308752	-6.145863
H	1.806667	4.935943	-4.309930

15 Cation Doublet

Min A

N	0.430356	1.208354	-1.852679
C	0.297088	1.331827	-0.446678
N	0.581401	0.179300	0.262866
C	1.175507	-0.985992	-0.183586
C	1.292203	-1.147720	-1.697595
C	0.651810	0.011645	-2.427695
O	-0.024424	2.352956	0.076873
O	1.578214	-1.811354	0.585574

C	2.777782	-1.317077	-2.021093
H	0.523303	0.285814	1.267251
H	3.149051	-2.218333	-1.536971
H	3.343529	-0.465874	-1.642657
H	2.942983	-1.392336	-3.092951
H	0.837421	0.061144	-3.490867
N	-1.853509	-1.312400	-1.650127
C	-1.908975	-2.075164	-0.442803
N	-0.998870	-3.101462	-0.361959
C	0.060935	-3.374991	-1.210211
C	0.340437	-2.290389	-2.243330
C	-0.859308	-1.423324	-2.527630
O	-2.727053	-1.848116	0.394958
O	0.710645	-4.372791	-1.116874
C	0.833020	-2.937272	-3.533036
H	-1.106805	-3.709694	0.437942
H	1.705854	-3.553394	-3.337694
H	1.084140	-2.191226	-4.286827
H	0.046554	-3.574190	-3.935631
H	-1.104615	-1.209199	-3.556439
C	-3.085259	-0.500417	-1.936561
C	-2.889312	0.462181	-3.078104
C	-3.321342	-0.304136	-4.324191
C	-4.397602	-1.250955	-3.723167
O	-4.115940	-1.345286	-2.315388
C	-4.557227	-2.663066	-4.244691
O	-3.327858	-3.432759	-4.288982
H	-3.332212	-0.026243	-0.981109
H	-3.613107	1.279097	-2.947994
H	-1.909234	0.937827	-3.128579
H	-2.517286	-0.924289	-4.761945
H	-5.378902	-0.757572	-3.840182
H	-5.000310	-2.599855	-5.256248
H	-3.541461	-4.337751	-4.633726
C	0.291679	2.469688	-2.608295
C	0.230960	3.814746	-4.493256
C	-1.139213	3.810765	-3.801042
O	-1.067748	2.773247	-2.794761
C	0.871970	2.506521	-4.010574
C	-2.267550	3.572040	-4.773936
O	-1.984381	2.464310	-5.655324
H	0.770653	3.232399	-1.975953
H	0.482785	1.685706	-4.631486
H	1.969982	2.519924	-4.047528
O	0.884499	4.942186	-3.984570
H	0.136652	3.835549	-5.589404
H	-1.270993	4.777561	-3.291605
H	-2.362481	4.460063	-5.414202
H	-3.225967	3.427404	-4.246841
O	-3.704346	0.702208	-5.259365
H	-5.292365	-3.158612	-3.589504
H	-2.111544	1.617511	-5.159361
H	-3.829700	0.308679	-6.145843
H	1.806801	4.935769	-4.309548

Min D

N	0.715173	0.620175	-3.876585
C	1.491077	-0.082155	-2.970903
N	1.556776	-1.439651	-3.228263
C	0.913168	-2.160318	-4.232162
C	0.101904	-1.347149	-5.122568
C	0.066966	-0.025081	-4.903914
O	2.051462	0.411460	-2.021438
O	1.036533	-3.365611	-4.296695
C	-0.647555	-2.022633	-6.225111
H	2.195114	-1.954845	-2.637765
H	0.020770	-2.634830	-6.828821
H	-1.123746	-1.288811	-6.874471
H	-1.414166	-2.685337	-5.818681

H	-0.497836	0.626341	-5.552651
N	-1.936851	-1.141902	-1.477801
C	-1.041158	-0.362984	-0.659340
N	0.073090	-1.035165	-0.248462
C	0.412042	-2.349081	-0.530698
C	-0.579500	-3.084932	-1.344293
C	-1.710724	-2.394988	-1.798986
O	-1.303738	0.769133	-0.395014
O	1.445882	-2.835835	-0.158386
C	-0.318448	-4.481247	-1.697357
H	0.772232	-0.474763	0.223854
H	0.416647	-4.485360	-2.518414
H	-1.213883	-4.988336	-2.046514
H	0.145576	-5.010352	-0.865828
H	-2.441492	-2.882020	-2.438824
C	-3.221024	-0.435430	-1.877646
C	-3.006841	0.538005	-3.014775
C	-3.332658	-0.269201	-4.275611
C	-4.404839	-1.250006	-3.721941
O	-4.120628	-1.382123	-2.310003
C	-4.557032	-2.663219	-4.244775
O	-3.328050	-3.433051	-4.288767
H	-3.557497	0.038414	-0.947697
H	-3.767073	1.328777	-2.926426
H	-2.026547	1.027361	-3.006964
H	-2.462163	-0.853579	-4.616460
H	-5.394165	-0.770424	-3.826997
H	-4.989194	-2.603511	-5.259574
H	-3.541432	-4.337738	-4.633778
C	0.642342	2.077670	-3.760427
C	0.151673	4.109624	-4.816785
C	-1.029132	3.723565	-3.938560
O	-0.658694	2.461806	-3.342541
C	0.897987	2.810867	-5.071291
C	-2.267393	3.572416	-4.773964
O	-1.984435	2.464174	-5.655386
H	1.373277	2.346618	-2.988856
H	0.468398	2.292482	-5.933800
H	1.971168	2.967980	-5.252449
O	0.884977	4.942113	-3.984064
H	-0.155225	4.609645	-5.751034
H	-1.138430	4.472385	-3.141946
H	-2.436615	4.463245	-5.391308
H	-3.175787	3.381557	-4.178373
O	-3.705525	0.702031	-5.259521
H	-5.293187	-3.165629	-3.596696
H	-2.111433	1.617437	-5.159130
H	-3.829205	0.308781	-6.145958
H	1.806664	4.936011	-4.309942

C	0.213660	-2.368678	-2.458563
C	-1.007361	-1.555992	-2.619620
O	-2.842358	-2.203551	0.227343
O	0.679440	-4.503327	-1.469756
C	0.611610	-2.909333	-3.834217
H	-1.157888	-4.053096	0.119063
H	1.435315	-3.608797	-3.732555
H	0.903180	-2.100369	-4.503020
H	-0.232697	-3.436313	-4.278236
H	-1.072172	-0.929212	-3.493212
C	-3.155339	-0.552631	-1.946160
C	-2.920692	0.441274	-3.051592
C	-3.343870	-0.302058	-4.318911
C	-4.441631	-1.243302	-3.747612
O	-4.245966	-1.297615	-2.317437
C	-4.557227	-2.663066	-4.244691
O	-3.327858	-3.432759	-4.288982
H	-3.305673	-0.126150	-0.949100
H	-3.646745	1.253289	-2.901138
H	-1.940507	0.925335	-3.069907
H	-2.540494	-0.929519	-4.747316
H	-5.422435	-0.768930	-3.919621
H	-4.997924	-2.620052	-5.258262
H	-3.541461	-4.337751	-4.633726
C	0.365688	2.426708	-2.688658
C	0.235880	3.826609	-4.526550
C	-1.121608	3.775983	-3.808937
O	-1.015403	2.686124	-2.867653
C	0.916961	2.522460	-4.099072
C	-2.267550	3.572040	-4.773936
O	-1.984381	2.464310	-5.655324
H	0.805665	3.205835	-2.048330
H	0.542271	1.701106	-4.727118
H	2.013195	2.571865	-4.158575
O	0.884499	4.942186	-3.984570
H	0.124131	3.889908	-5.619744
H	-1.248788	4.715187	-3.248201
H	-2.355837	4.464914	-5.407755
H	-3.224608	3.428851	-4.243648
O	-3.704346	0.702208	-5.259365
H	-5.289798	-3.163403	-3.590334
H	-2.111544	1.617511	-5.159361
H	-3.829700	0.308679	-6.145843
H	1.806801	4.935769	-4.309548

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TS A-D

N	0.542415	1.156347	-1.977992
C	0.270070	1.209919	-0.620398
N	0.514092	0.024023	0.073164
C	1.066203	-1.146907	-0.374510
C	1.272069	-1.277439	-1.887296
C	1.033209	0.025294	-2.597592
O	-0.142343	2.184048	-0.055966
O	1.345372	-2.036865	0.385305
C	2.701969	-1.780857	-2.112966
H	0.390511	0.101105	1.073649
H	2.836556	-2.765713	-1.671145
H	3.400868	-1.090909	-1.642080
H	2.934047	-1.823581	-3.174519
H	1.434628	0.161186	-3.586661
N	-1.961658	-1.493973	-1.773137
C	-2.018232	-2.380967	-0.607708
N	-1.096181	-3.382506	-0.635575
C	-0.005489	-3.527639	-1.496495

Min B

N	0.078705	1.267725	-1.572649
C	-0.371279	1.394157	-0.276357
N	-0.191832	0.286608	0.512576
C	0.791324	-0.711104	0.313304
C	1.269059	-0.790668	-1.014014
C	0.660213	0.016878	-2.061895
O	-0.885772	2.413004	0.149602
O	1.151017	-1.372753	1.282691
C	2.348852	-1.736078	-1.377334
H	-0.492186	0.401149	1.465732
H	2.637401	-2.329843	-0.512615
H	3.232517	-1.209053	-1.758950
H	2.029882	-2.407702	-2.182807
H	1.409513	0.264683	-2.813341
N	-1.560451	-1.297946	-2.143025
C	-1.484667	-2.532764	-1.533574
N	-0.548338	-3.373132	-2.085217
C	0.103074	-3.214226	-3.331535

C	0.141460	-1.886043	-3.782309	H	-1.035391	-4.364270	-0.326419
C	-0.461589	-0.838001	-2.967660	H	2.402339	-3.159771	-3.196307
O	-2.199140	-2.870119	-0.610666	H	1.798129	-1.757022	-4.111293
O	0.596223	-4.218590	-3.858953	H	1.009703	-3.322291	-4.260041
C	0.909432	-1.507646	-4.999793	H	-1.071302	-2.605676	-3.797429
H	-0.541171	-4.304287	-1.706676	C	-2.833810	-0.751577	-2.059062
H	1.195922	-2.406749	-5.543932	C	-2.611370	0.265503	-3.158867
H	1.837108	-0.960876	-4.764579	C	-3.262916	-0.365479	-4.378635
H	0.330991	-0.860248	-5.671553	C	-4.373769	-1.240130	-3.738029
H	-0.812513	-0.043278	-3.620107	O	-4.134623	-1.270990	-2.346246
C	-2.835538	-0.597704	-2.001193	C	-4.557164	-2.663005	-4.244433
C	-2.985222	0.504259	-3.017312	O	-3.327999	-3.432987	-4.288910
C	-3.312168	-0.278530	-4.283627	H	-2.921288	-0.309566	-1.057216
C	-4.342093	-1.272081	-3.673875	H	-3.144051	1.191163	-2.902256
O	-3.941352	-1.442916	-2.320334	H	-1.549708	0.453256	-3.318334
C	-4.557339	-2.663123	-4.244883	H	-2.529246	-1.003697	-4.897661
O	-3.327879	-3.432810	-4.288650	H	-5.344003	-0.732692	-3.909391
H	-2.980489	-0.289864	-0.958449	H	-5.007096	-2.613103	-5.258867
H	-3.871079	1.101871	-2.752915	H	-3.541434	-4.337699	-4.633880
H	-2.152260	1.198072	-3.085021	C	0.206184	2.491239	-2.486824
H	-2.443865	-0.852379	-4.651562	C	0.235199	3.777046	-4.436946
H	-5.331860	-0.767967	-3.705874	C	-1.153802	3.811326	-3.780293
H	-4.998204	-2.568712	-5.259087	O	-1.147262	2.811722	-2.773305
H	-3.541432	-4.337696	-4.633889	C	0.852902	2.507621	-3.864626
C	0.089628	2.493757	-2.331124	C	-2.267444	3.572149	-4.774304
C	0.254095	3.731933	-4.348905	O	-1.984199	2.464138	-5.655052
C	-1.165866	3.816856	-3.760000	H	0.630238	3.284559	-1.847320
O	-1.234391	2.849505	-2.730640	H	0.506959	1.647586	-4.453440
C	0.844846	2.498897	-3.658633	H	1.951667	2.523493	-3.845723
C	-2.267334	3.572013	-4.774041	O	0.884403	4.941974	-3.983906
O	-1.984400	2.464220	-5.655217	H	0.164766	3.744301	-5.535827
H	0.465656	3.294925	-1.673121	H	-1.279396	4.806794	-3.315632
H	0.593591	1.606408	-4.250367	H	-2.360772	4.460439	-5.418883
H	1.936770	2.554773	-3.544652	H	-3.225966	3.419824	-4.248005
O	0.884640	4.942292	-3.984153	O	-3.704146	0.702173	-5.259559
H	0.225534	3.603250	-5.442684	H	-5.285618	-3.148616	-3.571819
H	-1.284070	4.827769	-3.328050	H	-2.111846	1.617505	-5.159450
H	-2.354566	4.456485	-5.423892	H	-3.829871	0.308731	-6.145842
H	-3.228948	3.424387	-4.252545	H	1.806667	4.935943	-4.309930
O	-3.704613	0.702083	-5.259302				
H	-5.298755	-3.159951	-3.594869	Min AB			
H	-2.111650	1.617508	-5.159392	N	0.179657	1.131177	-1.784957
H	-3.829515	0.308726	-6.145889	C	0.076573	1.194563	-0.405608
H	1.806667	4.935944	-4.309931	N	0.537234	0.076454	0.246697
				C	1.624322	-0.722808	-0.228131
Min C				C	1.679947	-0.822794	-1.633791
N	0.286546	1.243007	-1.756144	C	0.551926	-0.155743	-2.384457
C	-0.194533	1.284705	-0.477433	O	-0.361599	2.166734	0.181002
N	-0.130039	0.080699	0.203543	O	2.388302	-1.200433	0.608436
C	0.524432	-1.081685	-0.143601	C	2.997365	-1.085686	-2.285726
C	1.151426	-1.138106	-1.525062	H	0.482703	0.142188	1.249502
C	0.937300	0.128227	-2.287618	H	3.698863	-1.455266	-1.538939
O	-0.633025	2.283339	0.059608	H	3.423030	-0.172023	-2.726277
O	0.643470	-1.959533	0.680496	H	2.940258	-1.828222	-3.085788
C	2.656970	-1.364978	-1.242987	H	0.908935	0.046407	-3.391711
H	-0.504868	0.105211	1.137796	N	-1.695974	-1.178304	-1.618504
H	2.815321	-2.357188	-0.822103	C	-1.697613	-1.898360	-0.440525
H	3.025988	-0.620088	-0.535362	N	-0.704068	-2.833065	-0.321935
H	3.227070	-1.266693	-2.164056	C	0.066869	-3.367210	-1.375432
H	0.978062	0.074908	-3.357447	C	0.152095	-2.539551	-2.513276
N	-1.806073	-1.778030	-2.033318	C	-0.586402	-1.232328	-2.558625
C	-1.914397	-2.679266	-1.030019	O	-2.531602	-1.736217	0.432099
N	-0.935094	-3.682756	-1.059619	O	0.586546	-4.471270	-2.216307
C	0.324865	-3.587878	-1.612131	C	0.670954	-3.096630	-3.791920
C	0.539148	-2.314593	-2.429627	H	-0.731863	-3.380632	0.520173
C	-0.761836	-1.868606	-3.050538	H	1.275642	-3.980274	-3.593426
O	-2.743559	-2.671102	-0.132095	H	1.282806	-2.375936	-4.345070
O	1.122410	-4.498186	-1.484871	H	-0.156004	-3.386436	-4.454716
C	1.511659	-2.653285	-3.561119	H	-1.011656	-1.124048	-3.554333

C	-2.933231	-0.502182	-1.928519	C	-4.557124	-2.663064	-4.244922
C	-2.843604	0.461540	-3.088408	O	-3.328007	-3.433021	-4.288554
C	-3.291078	-0.311371	-4.317138	H	-2.804407	-0.235048	-1.167181
C	-4.341932	-1.264084	-3.681149	H	-2.666569	1.092581	-3.057138
O	-3.963675	-1.423642	-2.328834	H	-1.301579	0.060160	-3.472850
C	-4.557502	-2.663279	-4.245824	H	-2.662545	-1.099583	-5.126071
O	-3.327905	-3.432865	-4.288404	H	-5.317843	-0.712485	-3.949753
H	-3.282843	-0.030776	-1.004492	H	-5.012989	-2.622774	-5.255227
H	-3.576993	1.267070	-2.939163	H	-3.541436	-4.337702	-4.633871
H	-1.874058	0.943521	-3.183419	C	0.120376	2.496504	-2.348249
H	-2.482502	-0.917246	-4.759799	C	0.255223	3.733314	-4.355131
H	-5.324550	-0.747915	-3.746437	C	-1.167193	3.778185	-3.751055
H	-4.999124	-2.573736	-5.259771	O	-1.225543	2.749069	-2.784563
H	-3.541453	-4.337736	-4.633770	C	0.876980	2.521716	-3.672132
C	0.153324	2.398723	-2.462527	O	-2.267491	3.572010	-4.773908
C	0.238970	3.761700	-4.406383	C	-1.984234	2.464279	-5.655393
C	-1.159662	3.806771	-3.767627	H	0.420660	3.343962	-1.707643
O	-1.187906	2.808944	-2.765302	H	0.640603	1.612010	-4.241431
C	0.837215	2.481929	-3.824502	H	1.967315	2.607338	-3.561522
C	-2.267412	3.572460	-4.774471	O	0.884605	4.942198	-3.984160
O	-1.984400	2.463962	-5.654892	H	0.217389	3.615550	-5.450496
H	0.579539	3.145369	-1.774104	H	-1.287995	4.766987	-3.267624
H	0.527067	1.642131	-4.462405	H	-2.336424	4.462362	-5.418064
H	1.934850	2.497632	-3.761601	H	-3.236434	3.432107	-4.262985
O	0.884640	4.942619	-3.984455	O	-3.704936	0.702217	-5.259429
H	0.174422	3.709631	-5.505572	H	-5.280705	-3.139600	-3.561323
H	-1.284520	4.804428	-3.307851	H	-2.111633	1.617511	-5.159236
H	-2.354283	4.458206	-5.423039	H	-3.829388	0.308706	-6.145898
H	-3.229897	3.424703	-4.254434	H	1.806661	4.935957	-4.309946
O	-3.703014	0.702137	-5.258801				
H	-5.295837	-3.159343	-3.592559	TS AB-B			
H	-2.111737	1.617507	-5.159417	N	0.128692	1.103321	-1.782511
H	-3.830763	0.308549	-6.145634	C	-0.146026	1.129904	-0.420181
H	1.806756	4.935785	-4.309676	N	0.222591	0.001743	0.251668
				C	1.401334	-0.779714	-0.091237
Min D				C	1.670554	-0.797563	-1.443903
N	0.213414	1.288619	-1.592201	C	0.681449	-0.134553	-2.356684
C	-0.312978	1.330572	-0.318531	O	-0.678724	2.091196	0.112317
N	-0.194601	0.166603	0.383096	O	2.010300	-1.284503	0.863714
C	0.694064	-0.926500	0.105840	C	3.007073	-1.254018	-1.947192
C	1.271520	-0.875319	-1.163419	H	0.062210	0.051469	1.243893
C	0.924315	0.138552	-2.075115	H	3.698501	-1.321163	-1.105422
O	-0.867159	2.323399	0.133639	H	3.430487	-0.543209	-2.672359
O	0.838053	-1.771206	1.009440	H	3.011093	-2.239142	-2.431972
C	2.278357	-1.907707	-1.565136	H	1.221214	0.144415	-3.261955
H	-0.585450	0.176273	1.308834	N	-1.562225	-1.389809	-1.994472
H	3.306814	-1.583253	-1.364714	C	-1.518645	-2.356435	-1.020944
H	2.208322	-2.121083	-2.635509	N	-0.525309	-3.306397	-1.167726
H	2.120483	-2.837302	-1.018113	C	0.307696	-3.471492	-2.257970
H	1.596730	0.347635	-2.899732	C	0.272718	-2.399827	-3.215901
N	-1.925078	-1.953611	-1.843416	C	-0.430610	-1.127005	-2.881329
C	-1.984872	-2.472495	-0.556149	O	-2.317412	-2.430923	-0.111852
N	-1.200860	-3.583189	-0.357040	O	0.993866	-4.479184	-2.372918
C	-0.374105	-4.218803	-1.270742	C	1.014849	-2.523026	-4.490649
C	-0.384740	-3.626080	-2.592915	H	-0.457235	-3.981919	-0.427229
C	-1.131981	-2.532802	-2.796834	H	1.492260	-3.498074	-4.555229
O	-2.682964	-2.007743	0.316308	H	1.789408	-1.754536	-4.576719
O	0.273577	-5.197721	-0.946281	H	0.335373	-2.394046	-5.340469
C	0.463064	-4.244937	-3.654258	H	-0.828427	-0.717338	-3.809024
H	-1.074771	-3.835966	0.610187	C	-2.791432	-0.608793	-2.014774
H	1.513071	-4.248192	-3.358216	C	-2.812042	0.433059	-3.099828
H	0.368127	-3.699377	-4.593412	C	-3.287939	-0.316592	-4.329806
H	0.180288	-5.285940	-3.823912	C	-4.331387	-1.267041	-3.679122
H	-1.140412	-2.050866	-3.758546	O	-3.931336	-1.418565	-2.326505
C	-2.782974	-0.799111	-2.103879	C	-4.557502	-2.663279	-4.245824
C	-2.386323	0.060885	-3.296763	O	-3.327905	-3.432865	-4.288404
C	-3.237479	-0.426634	-4.467325	H	-2.965804	-0.207641	-1.010516
C	-4.359926	-1.231309	-3.766999	H	-3.578943	1.181064	-2.853149
O	-4.117624	-1.194690	-2.374551	H	-1.881454	0.978952	-3.220716

H	-2.489984	-0.929187	-4.784246
H	-5.312890	-0.749786	-3.718660
H	-4.998137	-2.570485	-5.259807
H	-3.541453	-4.337736	-4.633770
C	0.129158	2.385690	-2.434450
C	0.243641	3.751504	-4.387372
C	-1.161399	3.802074	-3.762137
O	-1.205917	2.801008	-2.766543
C	0.839551	2.479749	-3.782963
C	-2.267412	3.572460	-4.774471
O	-1.984400	2.463962	-5.654892
H	0.535832	3.127895	-1.728531
H	0.549863	1.632759	-4.422311
H	1.935578	2.505106	-3.699908
O	0.884640	4.942619	-3.984455
H	0.187499	3.679802	-5.486112
H	-1.285289	4.799677	-3.301196
H	-2.351691	4.458398	-5.423079
H	-3.230423	3.424751	-4.255403
O	-3.703014	0.702137	-5.258801
H	-5.296570	-3.159363	-3.593384
H	-2.111737	1.617507	-5.159417
H	-3.830763	0.308549	-6.145634
H	1.806756	4.935785	-4.309676

C	0.262457	3.712954	-4.301428
C	-1.173826	3.819973	-3.750116
O	-1.277508	2.867523	-2.711685
C	0.842119	2.518190	-3.534882
C	-2.267412	3.572460	-4.774471
O	-1.984400	2.463962	-5.654892
H	0.366194	3.383789	-1.597823
H	0.631631	1.593324	-4.092116
H	1.926993	2.599416	-3.379348
O	0.884640	4.942619	-3.984455
H	0.258122	3.529393	-5.387667
H	-1.288616	4.838342	-3.333852
H	-2.350669	4.455668	-5.426473
H	-3.230692	3.427677	-4.255514
O	-3.703014	0.702137	-5.258801
H	-5.297529	-3.157932	-3.592931
H	-2.111737	1.617507	-5.159417
H	-3.830763	0.308549	-6.145634
H	1.806756	4.935785	-4.309676

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TS B-D

N	-0.006851	1.350682	-1.442977
C	-0.590615	1.505149	-0.199221
N	-0.466832	0.424460	0.628629
C	0.544516	-0.571488	0.550624
C	1.183287	-0.643034	-0.705564
C	0.723916	0.158401	-1.774503
O	-1.174032	2.522360	0.133345
O	0.776517	-1.225341	1.564576
C	2.296102	-1.615113	-0.917035
H	-0.863514	0.549251	1.544590
H	2.520261	-2.114779	0.023703
H	3.204481	-1.115301	-1.271977
H	2.049698	-2.379764	-1.656782
H	1.451333	0.340183	-2.556389
N	-1.579259	-1.394534	-2.160624
C	-1.534038	-2.598887	-1.486336
N	-0.566196	-3.458796	-1.942164
C	0.279811	-3.293721	-3.053952
C	0.295860	-1.980846	-3.577256
C	-0.483667	-0.980496	-2.957715
O	-2.300392	-2.895922	-0.593127
O	0.936464	-4.264669	-3.436872
C	1.286028	-1.610182	-4.629775
H	-0.544495	-4.359264	-1.496550
H	1.600541	-2.501952	-5.170393
H	2.194183	-1.156877	-4.207001
H	0.873251	-0.892173	-5.346380
H	-0.716216	-0.132342	-3.585378
C	-2.819878	-0.630809	-2.015440
C	-2.923698	0.472119	-3.036941
C	-3.301148	-0.291859	-4.298832
C	-4.342850	-1.268704	-3.682450
O	-3.960420	-1.427135	-2.322023
C	-4.557502	-2.663279	-4.245824
O	-3.327905	-3.432865	-4.288404
H	-2.938251	-0.312131	-0.973051
H	-3.772016	1.116674	-2.762313
H	-2.058648	1.123145	-3.118580
H	-2.451367	-0.875202	-4.693621
H	-5.328589	-0.759611	-3.727825
H	-4.998610	-2.574165	-5.260356
H	-3.541453	-4.337736	-4.633770
C	0.029587	2.552651	-2.241828

Min A

N	0.257141	1.168624	-1.794406
C	0.171080	1.266134	-0.414895
N	0.566276	0.106664	0.243956
C	1.544870	-0.735679	-0.326703
C	1.334186	-1.158225	-1.765435
C	0.348957	-0.134143	-2.410077
O	-0.179874	2.258326	0.186619
O	2.028326	-1.637647	0.496785
C	2.678081	-1.372138	-2.450377
H	0.591603	0.220948	1.251836
H	3.219133	-2.213082	-1.993258
H	3.294052	-0.467619	-2.343511
H	2.553733	-1.583728	-3.521203
H	0.611261	0.005783	-3.464383
N	-1.881320	-0.974551	-1.377328
C	-1.971461	-1.619721	-0.159614
N	-0.989997	-2.576684	0.118282
C	-0.049214	-3.113009	-0.732820
C	0.224650	-2.293630	-1.975033
C	-0.813133	-1.201138	-2.317692
O	-2.853425	-1.415444	0.646110
O	0.519222	-4.153005	-0.483092
C	0.469702	-3.236904	-3.147985
H	-1.153611	-3.083924	0.982302
H	1.288806	-3.931400	-2.922665
H	0.705683	-2.681768	-4.067489
H	-0.444760	-3.818898	-3.337748
H	-1.257421	-1.404654	-3.297158
C	-3.132266	-0.404393	-1.861989
C	-2.971450	0.528975	-3.042500
C	-3.318212	-0.281447	-4.286618
C	-4.364433	-1.263655	-3.685173
O	-3.990843	-1.437111	-2.326908
C	-4.557351	-2.663189	-4.244871
O	-3.327849	-3.432761	-4.288688
H	-3.600129	0.072337	-0.994475
H	-3.729940	1.322115	-2.972424
H	-2.008868	1.036476	-3.076643
H	-2.466265	-0.865906	-4.676189
H	-5.352463	-0.762001	-3.752165
H	-4.996379	-2.578850	-5.258151
H	-3.541438	-4.337706	-4.633860
C	0.195360	2.424138	-2.508465

C	0.238877	3.778364	-4.436464	O	-1.984302	2.464253	-5.655226
C	-1.151805	3.809830	-3.782205	H	0.576941	3.259276	-1.790924
O	-1.149332	2.800521	-2.776365	H	0.509867	1.636494	-4.414613
C	0.852559	2.490321	-3.881318	H	1.940481	2.509161	-3.765251
C	-2.267462	3.571990	-4.774071	O	0.884678	4.942181	-3.984257
O	-1.984284	2.464230	-5.655192	H	0.191120	3.707461	-5.509520
H	0.641691	3.174751	-1.838164	H	-1.285204	4.811854	-3.323758
H	0.525658	1.654732	-4.517282	H	-2.361761	4.457590	-5.419502
H	1.950988	2.510981	-3.842278	H	-3.227527	3.423664	-4.250443
O	0.884756	4.942181	-3.984124	O	-3.704264	0.702255	-5.259394
H	0.167250	3.747609	-5.535212	H	-5.290474	-3.164311	-3.591162
H	-1.277930	4.797514	-3.306709	H	-2.111664	1.617509	-5.159396
H	-2.360319	4.457350	-5.420290	H	-3.829800	0.308652	-6.145816
H	-3.227193	3.425038	-4.249499	H	1.806711	4.935893	-4.309807
O	-3.704301	0.702242	-5.259372				
H	-5.295899	-3.162069	-3.595052	Min AD			
H	-2.111738	1.617507	-5.159418	N	0.315345	1.107539	-1.864800
H	-3.829764	0.308654	-6.145822	C	-0.035578	1.120324	-0.512079
H	1.806668	4.935986	-4.309929	N	0.297395	-0.031745	0.178071
				C	1.344127	-0.924796	-0.168197
Min AB				C	1.681878	-0.907144	-1.567039
N	0.254590	1.247724	-1.666585	C	0.967912	-0.007094	-2.414107
C	0.173834	1.411593	-0.283949	O	-0.589627	2.065864	0.009866
N	0.684300	0.346349	0.435974	O	1.845834	-1.625936	0.701317
C	1.642716	-0.569139	-0.039395	C	2.947340	-1.587239	-1.984334
C	1.641030	-0.705839	-1.475880	H	0.070302	0.003190	1.167030
C	0.600968	-0.042222	-2.214083	H	3.012813	-2.587073	-1.527363
O	-0.251805	2.417297	0.241595	H	3.829433	-1.020381	-1.635512
O	2.352380	-1.190466	0.739620	H	3.025085	-1.677590	-3.077328
C	2.804711	-1.319077	-2.159161	H	1.279204	0.104692	-3.449632
H	0.640453	0.464465	1.443279	N	-1.801411	-1.536335	-1.733357
H	3.266028	-2.088052	-1.523840	C	-1.773604	-2.102312	-0.437186
H	3.568224	-0.542747	-2.355063	N	-0.815859	-3.069589	-0.245433
H	2.536253	-1.768429	-3.127583	C	0.148971	-3.512789	-1.155633
H	0.911785	0.097479	-3.253978	C	0.098875	-2.838977	-2.444277
N	-1.765791	-0.924059	-1.455239	C	-0.881294	-1.860546	-2.673088
C	-1.773395	-1.584109	-0.229159	O	-2.550876	-1.761484	0.423236
N	-0.800193	-2.562533	-0.110116	O	0.928947	-4.399722	-0.861591
C	-0.143459	-3.214907	-1.160323	C	0.896488	-3.380706	-3.575158
C	-0.190946	-2.501521	-2.408478	H	-0.743245	-3.431322	0.700194
C	-0.731745	-1.176431	-2.406870	H	1.790728	-3.893759	-3.202393
O	-2.547876	-1.328279	0.665900	H	1.183876	-2.587170	-4.281216
O	0.415136	-4.288405	-0.973831	H	0.295208	-4.120175	-4.133044
C	0.159839	-3.200938	-3.674377	H	-1.057372	-1.503207	-3.681355
H	-0.780577	-3.034856	0.788810	C	-2.916671	-0.608239	-2.004985
H	0.714757	-4.122909	-3.461359	C	-2.654133	0.315737	-3.171269
H	0.751325	-2.568107	-4.359601	C	-3.280153	-0.356789	-4.383382
H	-0.773367	-3.460794	-4.208591	C	-4.372234	-1.246056	-3.729803
H	-1.103636	-0.967013	-3.412141	O	-4.088299	-1.306197	-2.332597
C	-3.055470	-0.389549	-1.885317	C	-4.557363	-2.663234	-4.244876
C	-2.976522	0.556123	-3.056164	O	-3.327847	-3.432759	-4.288660
C	-3.314917	-0.273194	-4.288580	H	-3.084611	-0.084517	-1.059194
C	-4.336531	-1.268804	-3.668433	H	-3.198514	1.250670	-2.989389
O	-3.886841	-1.456091	-2.330665	H	-1.605291	0.584523	-3.291882
C	-4.557285	-2.663150	-4.244820	H	-2.567187	-1.008379	-4.918838
O	-3.327862	-3.432779	-4.288739	H	-5.344086	-0.735524	-3.858892
H	-3.504660	0.059829	-0.993697	H	-5.005203	-2.601842	-5.256106
H	-3.769602	1.311491	-2.960021	H	-3.541435	-4.337701	-4.633877
H	-2.039279	1.109289	-3.114081	C	0.214460	2.394955	-2.541479
H	-2.455225	-0.855739	-4.669285	C	0.241664	3.779234	-4.442056
H	-5.324066	-0.762518	-3.680649	C	-1.147128	3.778983	-3.777452
H	-5.005056	-2.565416	-5.252466	O	-1.136853	2.719601	-2.821853
H	-3.541441	-4.337710	-4.633844	C	0.879338	2.496665	-3.907519
C	0.163688	2.472147	-2.440234	C	-2.267456	3.572018	-4.774081
C	0.242914	3.766240	-4.411058	O	-1.984273	2.464223	-5.655162
C	-1.158577	3.814166	-3.777834	H	0.624000	3.151517	-1.850912
O	-1.176921	2.820486	-2.752376	H	0.567104	1.659776	-4.549111
C	0.842052	2.492294	-3.807052	H	1.976943	2.540474	-3.869711
C	-2.267533	3.572034	-4.774046	O	0.884736	4.942247	-3.984126

H	0.161475	3.758809	-5.540544	H	-5.295080	-3.170989	-3.601427
H	-1.272981	4.744708	-3.258082	H	-2.111738	1.617469	-5.159283
H	-2.345993	4.462992	-5.413979	H	-3.829489	0.308640	-6.145855
H	-3.231570	3.430862	-4.255377	H	1.806697	4.935888	-4.309843
O	-3.704188	0.702277	-5.259405				
H	-5.289250	-3.152192	-3.580120	Min D2			
H	-2.111746	1.617501	-5.159441	N	0.761943	0.681467	-3.396920
H	-3.829865	0.308637	-6.145799	C	1.632937	0.175325	-2.454317
H	1.806672	4.935922	-4.309916	N	1.988336	-1.160383	-2.628061
				C	1.396475	-1.986097	-3.582858
Min D1				C	0.461701	-1.477749	-4.479703
N	0.559342	0.630925	-3.089841	C	0.164666	-0.138586	-4.374900
C	1.505463	0.142643	-2.208267	O	2.102854	0.815027	-1.533611
N	1.788846	-1.198968	-2.372098	O	1.851439	-3.225410	-3.575327
C	1.536391	-1.995259	-3.548912	C	-0.208159	-2.368608	-5.489334
C	0.580228	-1.451332	-4.411778	H	2.370028	-1.597860	-1.788794
C	-0.027248	-0.223901	-4.074172	H	0.490393	-3.121532	-5.882342
O	2.024438	0.806280	-1.319095	H	-0.570057	-1.773436	-6.340305
O	2.118186	-3.108557	-3.592405	H	-1.072474	-2.891677	-5.049471
C	0.113886	-2.240408	-5.600582	H	-0.528101	0.356723	-5.046034
H	2.570375	-1.522271	-1.811027	N	-2.119904	-1.053034	-1.370505
H	0.764701	-3.115172	-5.731714	C	-1.279663	-0.267864	-0.595764
H	0.142033	-1.643433	-6.527891	N	-0.129765	-0.913668	-0.183897
H	-0.922073	-2.606029	-5.474507	C	0.251738	-2.126564	-0.451309
H	-0.597908	0.319628	-4.823058	C	-0.735588	-3.005712	-1.184805
N	-2.003484	-0.945521	-1.395586	C	-1.846746	-2.374848	-1.627782
C	-1.320980	-0.207371	-0.385103	O	-1.533705	0.885903	-0.313415
N	-0.228844	-0.844663	0.145869	O	1.358606	-2.626529	-0.112882
C	0.236700	-2.120325	-0.156315	C	-0.439367	-4.447375	-1.467201
C	-0.455353	-2.765160	-1.299282	H	0.559884	-0.318373	0.268421
C	-1.543880	-2.096155	-1.877977	H	-0.335025	-5.015263	-0.530092
O	-1.726962	0.866909	-0.025254	H	0.507071	-4.545816	-2.016349
O	1.121308	-2.644477	0.477698	H	-1.244525	-4.898747	-2.063842
C	-0.003778	-4.075145	-1.759486	H	-2.586876	-2.887356	-2.240211
H	0.321123	-0.297067	0.802775	C	-3.359220	-0.384471	-1.833488
H	0.369930	-4.675592	-0.919276	C	-3.119572	0.574474	-2.979538
H	0.884826	-3.914488	-2.438144	C	-3.358780	-0.254198	-4.240578
H	-0.772521	-4.599976	-2.339325	C	-4.441387	-1.242168	-3.725123
H	-2.125237	-2.571329	-2.672112	O	-4.258833	-1.342107	-2.309031
C	-3.311381	-0.369049	-1.847705	C	-4.556892	-2.663018	-4.244732
C	-3.163252	0.606704	-2.985245	O	-3.328115	-3.433185	-4.288686
C	-3.364629	-0.242150	-4.239383	H	-3.777984	0.118304	-0.952949
C	-4.416048	-1.253819	-3.706945	H	-3.898623	1.352675	-2.957958
O	-4.116330	-1.404927	-2.307002	H	-2.147786	1.072828	-2.924739
C	-4.556835	-2.662861	-4.244524	H	-2.458802	-0.822340	-4.529112
O	-3.328116	-3.433168	-4.289009	H	-5.428277	-0.777326	-3.917548
H	-3.730985	0.081768	-0.941505	H	-4.988448	-2.610636	-5.262770
H	-3.998534	1.322893	-2.939815	H	-3.541434	-4.337701	-4.633874
H	-2.229108	1.174519	-2.949772	C	0.601334	2.116065	-3.470727
H	-2.444126	-0.788241	-4.498529	C	0.175861	4.022619	-4.756958
H	-5.416336	-0.789847	-3.808673	C	-1.049774	3.717009	-3.899830
H	-4.987912	-2.594069	-5.260701	O	-0.754071	2.485133	-3.232008
H	-3.541460	-4.337761	-4.633701	C	0.920529	2.704666	-4.840263
C	0.482701	2.066243	-3.231843	C	-2.267573	3.572414	-4.773984
C	0.203632	3.928206	-4.669951	O	-1.984121	2.464124	-5.655126
C	-1.074909	3.713521	-3.856623	H	1.242897	2.532689	-2.684427
O	-0.873201	2.511271	-3.109441	H	0.512730	2.084588	-5.645934
C	0.930142	2.596928	-4.590982	H	2.002172	2.833135	-4.997416
C	-2.267814	3.572159	-4.773958	O	0.884546	4.941830	-3.984165
O	-1.983985	2.464291	-5.655203	H	-0.089663	4.428509	-5.748300
H	1.080042	2.484164	-2.411942	H	-1.164410	4.517983	-3.153031
H	0.595976	1.930916	-5.395007	H	-2.405987	4.468386	-5.394010
H	2.023429	2.703534	-4.650719	H	-3.190045	3.394442	-4.195588
O	0.884522	4.941850	-3.984171	O	-3.705017	0.702286	-5.259637
H	-0.016424	4.217771	-5.711964	H	-5.293278	-3.168664	-3.597740
H	-1.191294	4.560417	-3.161216	H	-2.111719	1.617496	-5.159223
H	-2.375835	4.471081	-5.396515	H	-3.829361	0.308692	-6.145896
H	-3.208242	3.411220	-4.218512	H	1.806667	4.935942	-4.309930
O	-3.704800	0.702372	-5.259704				

TS AD-D

N	0.317640	1.043645	-1.944849
C	-0.132688	0.957555	-0.639356
N	-0.042258	-0.303548	-0.075153
C	0.875327	-1.336119	-0.480974
C	1.432275	-1.129373	-1.754798
C	0.977059	-0.066876	-2.574564
O	-0.626764	1.901935	-0.044225
O	1.024616	-2.305078	0.293288
C	2.513654	-2.044226	-2.247597
H	-0.282339	-0.318708	0.909931
H	3.509477	-1.575003	-2.162232
H	2.381705	-2.305902	-3.311977
H	2.536011	-2.961218	-1.640880
H	1.592590	0.213409	-3.428304
N	-2.028130	-1.920520	-1.782806
C	-2.208393	-2.453660	-0.461912
N	-1.572067	-3.644865	-0.229746
C	-0.699512	-4.310459	-1.075589
C	-0.541493	-3.680885	-2.400482
C	-1.246724	-2.507124	-2.675203
O	-2.900949	-1.893065	0.342487
O	-0.166570	-5.352560	-0.772225
C	0.296940	-4.362164	-3.401994
H	-1.605865	-3.970777	0.731770
H	1.341770	-4.363942	-3.051988
H	0.244011	-3.878647	-4.383542
H	0.006414	-5.421443	-3.475029
H	-1.162508	-2.044067	-3.651548
C	-2.871480	-0.723427	-2.102988
C	-2.402440	0.059152	-3.311746
C	-3.256199	-0.424869	-4.479771
C	-4.383517	-1.225209	-3.790518
O	-4.166627	-1.153964	-2.381037
C	-4.557150	-2.663096	-4.244951
O	-3.328003	-3.433016	-4.288533
H	-2.878985	-0.143179	-1.176342
H	-2.608917	1.115672	-3.109010
H	-1.320271	-0.009679	-3.480660
H	-2.682804	-1.102420	-5.135913
H	-5.343342	-0.720977	-3.986570
H	-5.012429	-2.637626	-5.252766
H	-3.541434	-4.337698	-4.633882
C	0.215126	2.342498	-2.558678
C	0.244326	3.774334	-4.438608
C	-1.146487	3.756248	-3.773320
O	-1.146554	2.661948	-2.865270
C	0.894514	2.498307	-3.913138
C	-2.267457	3.572037	-4.773914
O	-1.984241	2.464259	-5.655348
H	0.583718	3.095452	-1.842318
H	0.616906	1.660472	-4.567893
H	1.990089	2.568697	-3.855359
O	0.884585	4.942263	-3.984203
H	0.159928	3.758428	-5.537378
H	-1.270810	4.706676	-3.224375
H	-2.341485	4.464871	-5.411760
H	-3.232770	3.430656	-4.256570
O	-3.704884	0.702213	-5.259408
H	-5.276876	-3.142159	-3.559950
H	-2.111642	1.617503	-5.159268
H	-3.829428	0.308707	-6.145893
H	1.806672	4.935920	-4.309916