

Supporting Information for:

**Controlling the Repair Mechanism of Oxetanes
Through Functional Group Substitution**

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Table S1. Properties of the main excited state geometries of HH-oxetanes involved in the photophysical processes, in which λ is the excitation wavelength (unit in nm) and f is the oscillator strength.

Oxetane	S_n			S_1			$S_{1,\min}$			$T_{1,\min}$	
	Nature	λ	f	Nature	λ	f	Nature	λ	f	Nature	λ
1	$^1(\pi_{A-T}\pi_{B-A}^*)$	224	0.0718	$^1(n_T\pi_T^*/\pi_{CO}\pi_T^*)$	257	0.0011	$^1(n_T\pi_T^*/\pi_{CO}\pi_T^*)$	343	0.0039	$^3(\pi_A\pi_A^*)$	585
2	$^1(\pi_{A-B}\pi_T^*/n_T\pi_T^*)$	221	0.0654	$^1(\pi_A\pi_T^*/n_T\pi_T^*)$	286	0.0012	$^1(n_T\pi_T^*/\pi_{CO}\pi_T^*)$	344	0.0034	$^3(\pi_A\pi_A^*)$	852
3	$^1(\pi_A\pi_{A-B}^*)$	243	0.0504	$^1(\pi_A\pi_T^*)$	319	0.0113	$^1(\pi_A\pi_T^*)$	378	0.0042	$^3(\pi_A\pi_A^*)$	679
4	$^1(\pi_B\pi_{A-B-T}^*)$	237	0.0309	$^1(\pi_{B-A}\pi_{NO2}^*)$	390	0.0039	$^1(\pi_A\pi_{NO2}^*/n_{NO2}\pi_{NO2}^*)$	733	0.0002	$^3(\pi_{NO2}\pi_{NO2}^*)$	1148
5	$^1(\pi_{A-T}\pi_T^*)$	247	0.0361	$^1(\pi_B\pi_T^*)$	288	0.0016	$^1(\pi_B\pi_T^*/n_T\pi_T^*)$	343	0.0097	$^3(\pi_A\pi_A^*)$	579
6	$^1(\pi_{A-B-T}\pi_T^*)$	246	0.0338	$^1(\pi_B\pi_T^*)$	321	0.0022	$^1(\pi_B\pi_T^*)$	377	0.0302	$^3(\pi_A\pi_A^*)$	580
7	$^1(\pi_{B-T}\pi_B^*)$	275	0.1535	$^1(\pi_A\pi_B^*)$	475	0.0029	$^1(\pi_{A-T}\pi_B^*)$	525	0.0058	$^3(\pi_{NO2}\pi_B^*)$	859

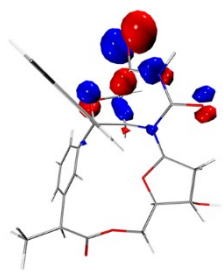
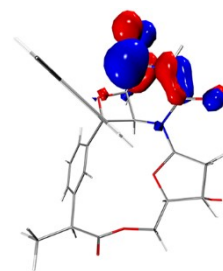
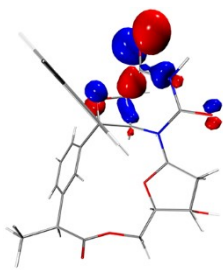
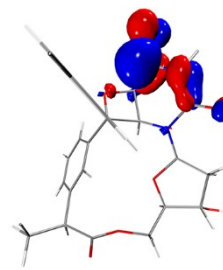
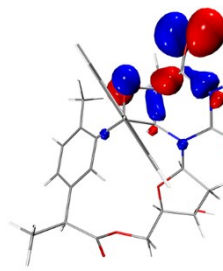
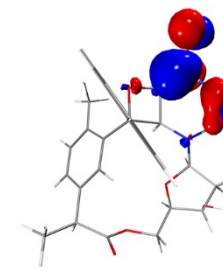
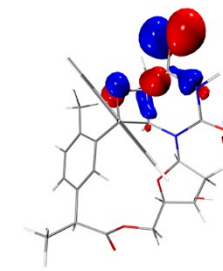
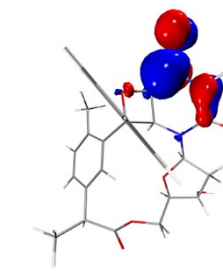
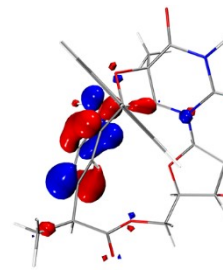
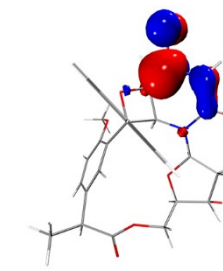
Table S2. Properties of the main excited state geometries of HT-oxetanes involved in the photophysical processes, in which λ is the excitation wavelength (unit in nm) and f is the oscillator strength.

Oxetane	S_n			S_1			$S_{1,min}$			$T_{1,min}$	
	Nature	λ	f	Nature	λ	f	Nature	λ	f	Nature	λ
1	$^1(\pi_{B-A}\pi_{A-B-T}^*)$	224	0.0332	$^1(\pi_{B-A}\pi_T^*)$	275	0.0040	$^1(\pi_{B-A}\pi_T^*)$	336	0.0150	$^3(\pi_A\pi_A^*)$	657
2	$^1(\pi_A\pi_{COO}^*)$	214	0.0267	$^1(\pi_{A-B}\pi_T^*)$	282	0.0177	$^1(\pi_{A-B}\pi_T^*)$	342	0.0370	$^3(\pi_A\pi_A^*)$	797
3	$^1(\pi_A\pi_{B-A}^*)$	251	0.0408	$^1(\pi_A\pi_T^*)$	311	0.0130	$^1(\pi_A\pi_T^*)$	374	0.0403	$^3(\pi_A\pi_A^*)$	722
4	$^1(\pi_A\pi_A^*/n_{NO_2}\pi_A^*)$	261	0.1189	$^1(\pi_B\pi_A^*)$	437	0.0038	$^1(\pi_{A-B}\pi_{NO_2}^*/n_{NO_2}\pi_{NO_2}^*)$	718	0.0009	$^3(\pi_{B-NO_2}\pi_A^*)$	1036
5	$^1(\pi_B\pi_{A-B}^*)$	236	0.0481	$^1(\pi_B\pi_T^*)$	291	0.0026	$^1(\pi_{B-A}\pi_T^*)$	351	0.0101	$^3(\pi_A\pi_A^*)$	657
6	$^1(\pi_B\pi_A^*)$	257	0.0434	$^1(\pi_B\pi_T^*)$	323	0.0013	$^1(\pi_B\pi_T^*)$	391	0.0056	$^3(\pi_A\pi_A^*)$	650
7	$^1(\pi_B\pi_B^*/n_T\pi_B^*)$	274	0.2514	$^1(\pi_A\pi_B^*)$	463	0.0222	$^1(\pi_A\pi_B^*)$	468	0.0455	$^3(\pi_{NO_2}\pi_B^*)$	865

Table S3. Properties of the main excited state geometries of products involved in the photophysical processes, in which λ is the excitation wavelength (unit in nm) and f is the oscillator strength.

Product	S_n			S_1			$S_{1,\min}$			$T_{1,\min}$	
	Nature	λ	f	Nature	λ	f	Nature	λ	f	Nature	λ
1	$^1(\pi_{A-B}\pi_{A-B}^*)$	269	0.2435	$^1(n_{CO}\pi_{A-B}^*)$	338	0.0011	$^1(\pi_B\pi_A^*)$	480	0.0002	$^3(n_{CO}\pi_{A-B}^*/\pi_{A-B}\pi_{A-E}^*)$	512
2	$^1(\pi_T\pi_T^*)$	251	0.1850	$^1(n_{CO}\pi_{B-A}^*)$	338	0.0016	$^1(\pi_B\pi_A^*)$	485	0.0001	$^3(n_{CO}\pi_{A-B}^*/\pi_B\pi_{A-B}^*)$	528
3	$^1(\pi_T\pi_T^*)$	237	0.1771	$^1(\pi_A\pi_B^*)$	385	0.0257	$^1(n_{CO-OCH_3}\pi_{A-B}^*)$	545	0.0038	$^3(n_{CO}\pi_{A-B}^*/\pi_B\pi_{A-B}^*)$	557
4	$^1(\pi_B\pi_A^*)$	254	0.0110	$^1(\pi_T\pi_A^*)$	662	1.2E-06	$^1(n_{CO-NO_2}\pi_A^*)$	998	0.0003	$^3(\pi_{NO_2}\pi_A^*)$	1152
5	$^1(\pi_{B-A}\pi_{A-B}^*)$	278	0.2034	$^1(n_{CO}\pi_{A-B}^*)$	336	0.0016	$^1(\pi_B\pi_A^*)$	505	0.0002	$^3(\pi_B\pi_{A-B}^*)$	527
6	$^1(\pi_B\pi_{A-B}^*)$	300	0.3230	$^1(n_{CO}\pi_{A-B}^*)$	334	0.0074	$^1(\pi_B\pi_A^*)$	544	0.0002	$^3(\pi_B\pi_{A-B}^*)$	550
7	$^1(n_{CO}\pi_B^*/\pi_A\pi_B^*)$	271	0.0186	$^1(\pi_T\pi_B^*)$	776	5.7E-07	$^1(n_{NO_2}\pi_B^*)$	619	9.5E-06	$^3(n_{NO_2}\pi_B^*)$	814

Table S4. The NTO analyses for S_1 and T_1 states at the $S_{1,\min}$ geometries of HH-oxetanes

Oxetane	State	Nature	Hole	Electron
1	S_1	$^1(n_T\pi_T^*/\pi_{CO}\pi_T^*)$ 99.60%		
	T_1	$^3(n_T\pi_T^*/\pi_{CO}\pi_T^*)$ 99.20%		
2	S_1	$^1(n_T\pi_T^*/\pi_{CO}\pi_T^*)$ 99.60%		
	T_1	$^3(n_T\pi_T^*/\pi_{CO}\pi_T^*)$ 99.20%		
3	S_1	$^1(\pi_A\pi_T^*)$ 99.90%		

Oxetane	State	Nature	Hole	Electron
4	T ₁	${}^3(\text{n}_T\pi_T^*/\pi_{\text{CO}}\pi_T^*)$ 99.30%		
	S ₁	${}^1(\pi_A\pi_{\text{NO}_2}^*/\text{n}_{\text{NO}_2}\pi_{\text{NO}_2}^*)$ 99.90%		
	T ₁	${}^3(\pi_{\text{NO}_2}\pi_{\text{NO}_2}^*)$ 99.30%		
	S ₁	${}^1(\pi_B\pi_T^*/\text{n}_T\pi_T^*)$ 99.50%		
5	T ₁	${}^3(\text{n}_T\pi_T^*/\pi_{\text{CO}}\pi_T^*)$ 99.20%		
	S ₁	${}^1(\pi_B\pi_T^*)$ 99.60%		

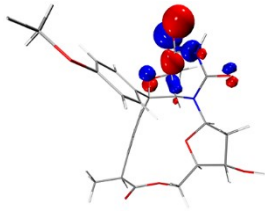
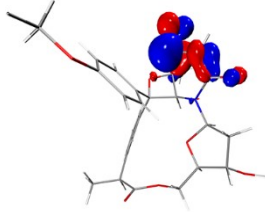
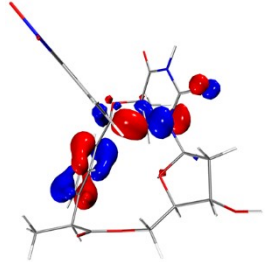


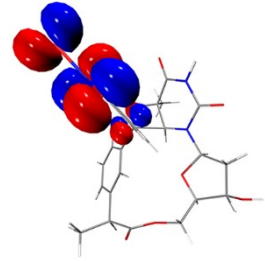

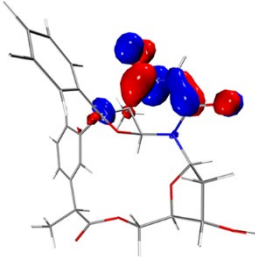
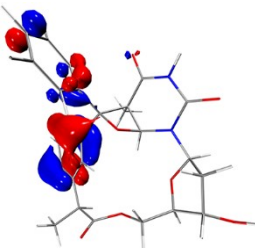
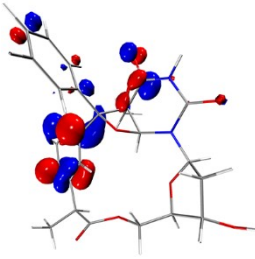
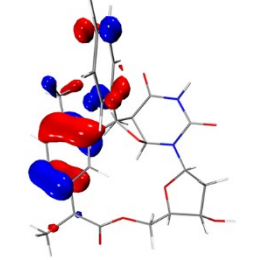
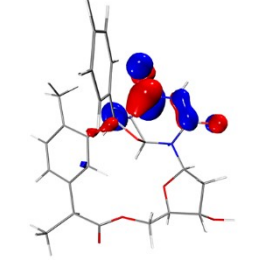
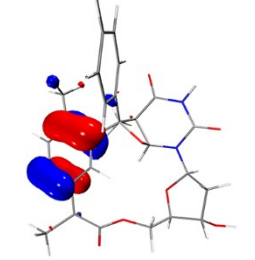
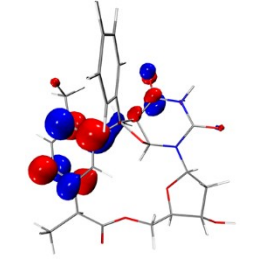
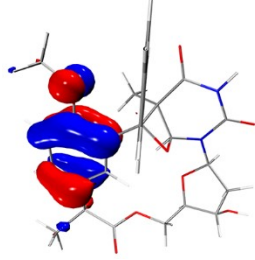
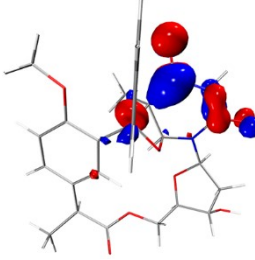
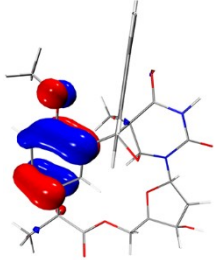
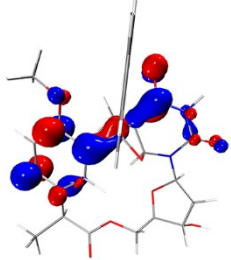
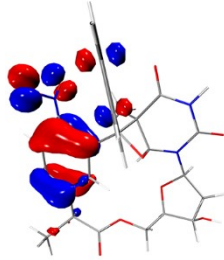
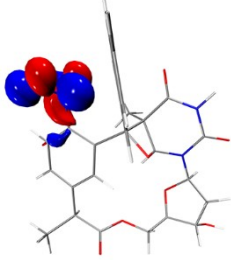
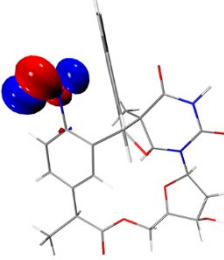
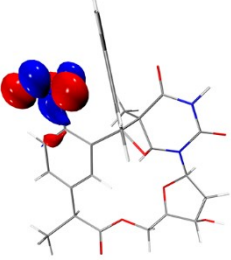
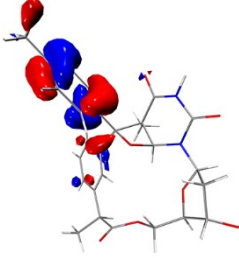
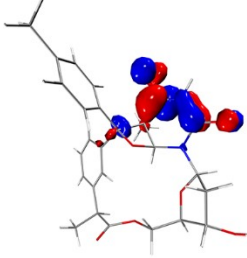
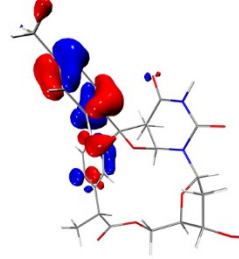
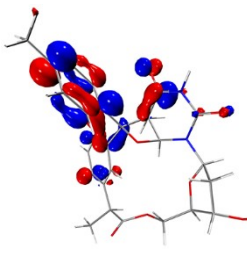
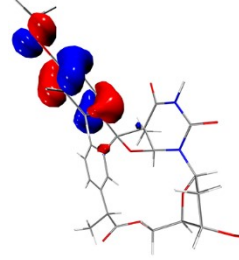
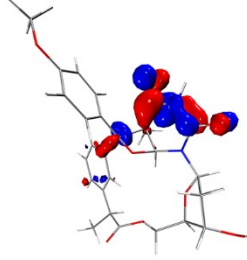
Oxetane	State	Nature	Hole	Electron
	T_1	${}^3(n_T\pi_T^*/\pi_{CO}\pi_T^*)$ 99.20%		
7	S_1	${}^1(\pi_A - \pi_B^*)$ 99.90%		
	T_1	${}^3(\pi_{NO_2}\pi_B^*)$ 98.10%		

Table S5. The NTO analyses for S_1 and T_1 states at the $S_{1,\min}$ geometries of HT-oxetanes

Oxetane	State	Nature	Hole	Electron
1	S_1	${}^1(\pi_{B-A}\pi_T^*)$ 99.60%		
	T_1	${}^3(\pi_{A-B}\pi_{A-T-B}^*)$ 74.20%		
2	S_1	${}^1(\pi_{A-B}\pi_T^*)$ 99.20%		
	T_1	${}^3(\pi_A\pi_{A-T}^*)$ 86.00%		
3	S_1	${}^1(\pi_A\pi_T^*)$ 99.20%		

Oxetane	State	Nature	Hole	Electron
	T ₁	$^3(\pi_A \pi_A^*)$ 95.30%		
4	S ₁	$^1(\pi_{A-B} \pi_{NO2}^* / n_{NO2} \pi_{NO2}^*)$ 99.90%		
	T ₁	$^3(\pi_{NO2} \pi_{NO2}^*)$ 99.30%		
5	S ₁	$^1(\pi_{B-A} \pi_T^*)$ 99.80%		
	T ₁	$^3(\pi_{B-A} \pi_{B-A}^*)$ 70.90%		
6	S ₁	$^1(\pi_B \pi_{T-A}^*)$ 99.90%		

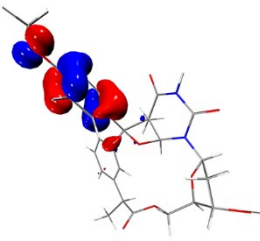
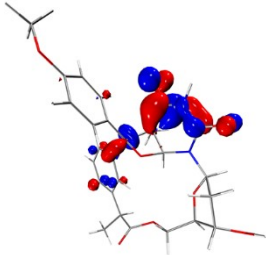
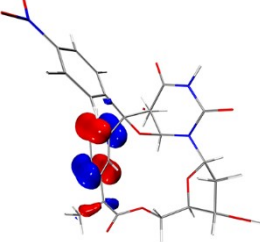
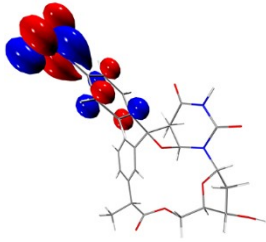
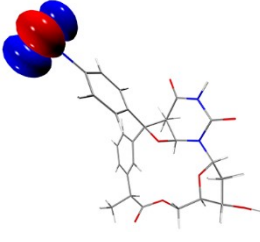
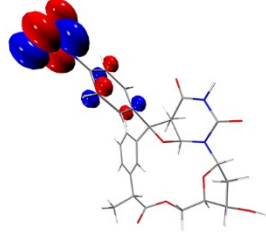
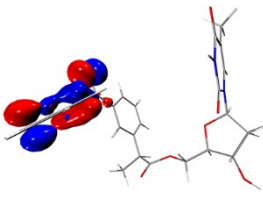
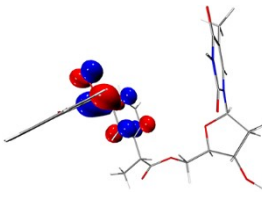
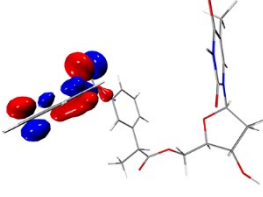
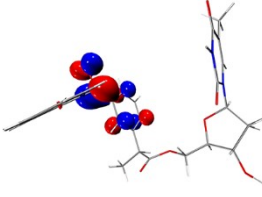
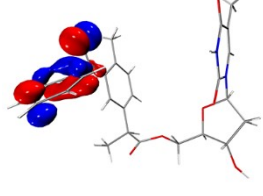
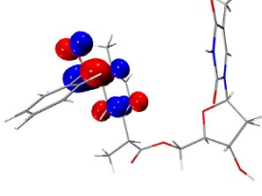
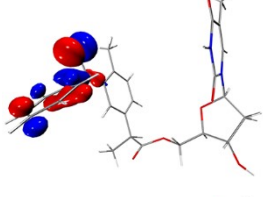
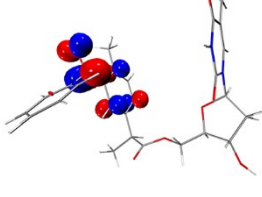
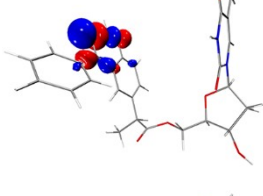
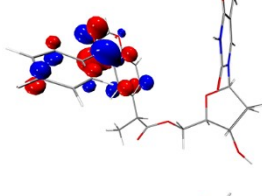
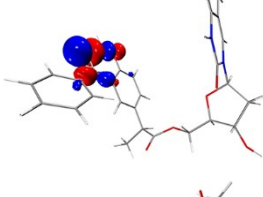
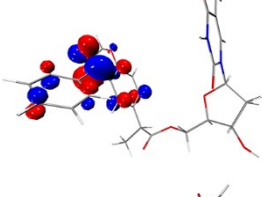
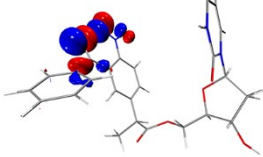
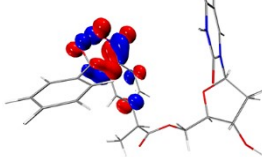
Oxetane	State	Nature	Hole	Electron
	T ₁	${}^3(\pi_B\pi_{T-A}^*)$ 95.30%		
7	S ₁	${}^1(\pi_A\pi_B^*)$ 99.60%		
	T ₁	${}^3(\pi_{NO_2}\pi_B^*)$ 99.00%		

Table S6. The NTO analyses for S_1 and T_1 states at the $S_{1,\min}$ geometries of products

Product	State	Nature	Hole	Electron
1	S_1	$^1(\pi_B\pi_A^*)$ 99.90%		
	T_1	$^3(\pi_B\pi_A^*)$ 99.40%		
2	S_1	$^1(\pi_B\pi_A^*)$ 99.90%		
	T_1	$^3(\pi_B\pi_A^*)$ 99.40%		
3	S_1	$^1(n_{CO-OCH_3}\pi_{A-B}^*)$ 99.70%		
	T_1	$^3(n_{CO-OCH_3}\pi_{A-B}^*)$ 99.00%		
4	S_1	$^1(n_{CO-NO_2}\pi_A^*)$ 99.50%		

Product	State	Nature	Hole	Electron
	T ₁	³ (n _{CO} - NO ₂ π _A [*]) 97.20%		
5	S ₁	¹ (π _B π _A [*]) 99.90%		
	T ₁	³ (π _B π _A [*]) 99.40%		
6	S ₁	¹ (π _B π _A [*]) 99.90%		
	T ₁	³ (π _B π _A [*]) 99.30%		
7	S ₁	¹ (n _{NO2} π _B [*]) 100.00%		
	T ₁	³ (n _{NO2} π _B [*]) 99.50%		

Table S7. The dihedral angles among the A, B rings of BPs and the T ring at the $S_{1,\min}$ geometries of HH-oxetanes (unit in degree).

Oxetane	φ_{A-B}	φ_{A-T}	φ_{B-T}
1	66.07	36.05	60.23
2	69.30	34.98	57.75
3	67.94	60.84	68.21
4	64.17	52.21	55.17
5	63.04	34.92	56.52
6	64.74	42.76	65.56
7	62.21	27.60	52.70

Table S8. Fluorescence and phosphorescence radiation rate constants (unit in s⁻¹) on the photophysical processes of oxetanes formed by BP derivatives.

Regioisomer	Oxetane	k_{FL}	k_{PH}
HH	2	6.23×10^6	1.33×10^2
	3	3.71×10^6	2.92×10^2
	4	1.95×10^5	4.61×10^7
	5	1.05×10^7	1.79×10^2
	6	2.09×10^7	8.47×10^1
	7	1.32×10^6	2.41×10^3
	HT	2	2.77×10^7
3		4.04×10^7	1.63×10^2
4		7.68×10^5	7.98×10^3
5		2.08×10^7	2.97×10^2
6		9.35×10^6	1.98×10^2
7		9.64×10^6	3.15×10^3

Table S9. Fluorescence and phosphorescence radiation rate constants rate constants (unit in s^{-1}) on the photophysical processes of products formed by BP derivatives.

Product	k_{FL}	k_{PH}
2	7.38×10^4	1.66×10^3
3	3.88×10^6	2.43×10^3
4	4.20×10^5	9.54×10^3
5	1.32×10^5	7.60×10^2
6	4.00×10^5	7.40×10^2
7	9.36×10^3	6.80×10^3

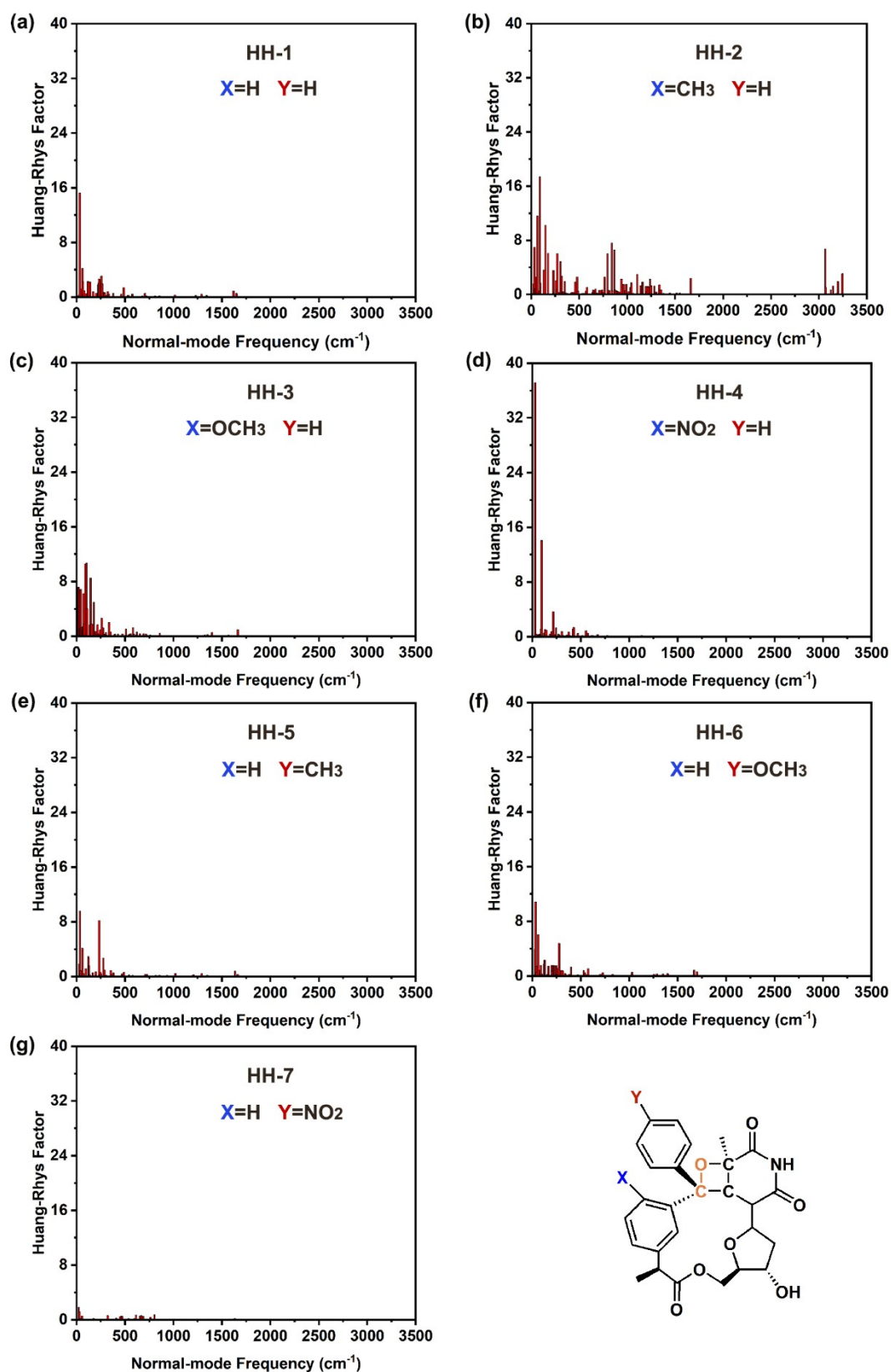


Figure S1. Huang-Rhys factors in ISC processes of HH-oxetanes formed by BPs and Thy.

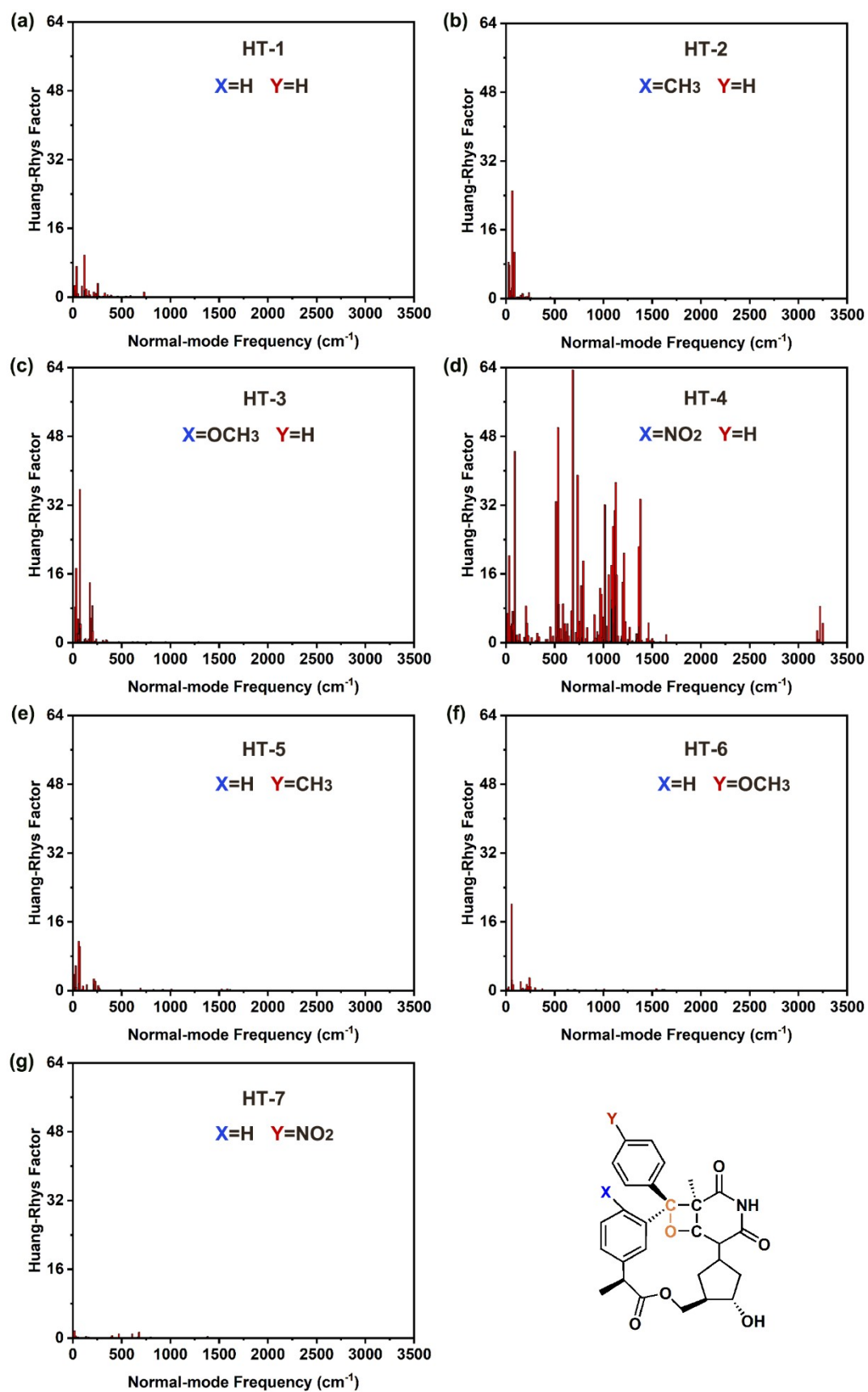


Figure S2. Huang-Rhys factors in ISC processes of HT-oxetanes formed by BPs and Thy.

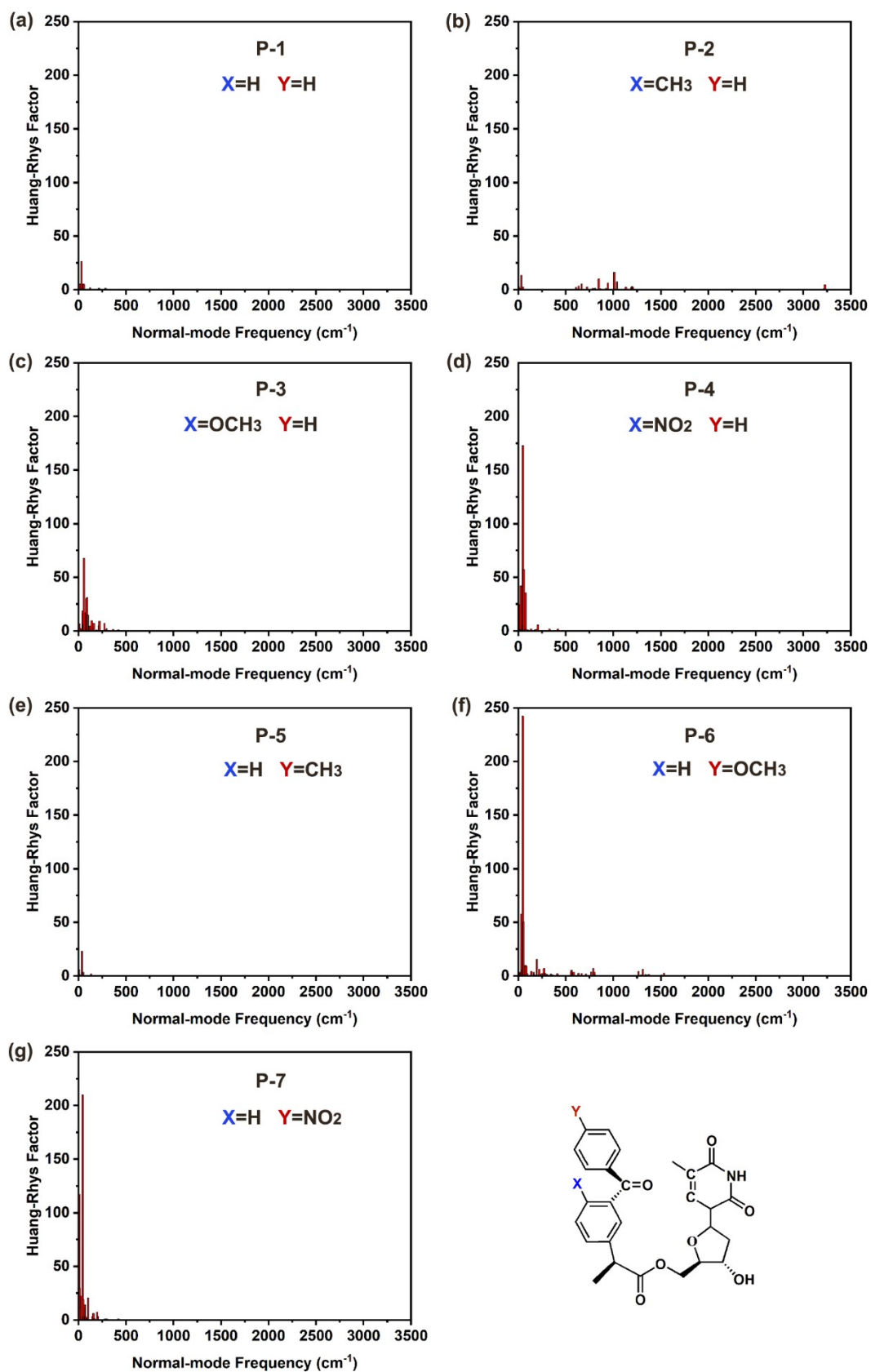


Figure S3. Huang-Rhys factors in ISC processes of products formed by BPs and Thy.

Cartesian Coordinates

HH-1-S₀

C	4.557840	-2.564527	0.775404
H	4.740168	-3.455738	0.166610
H	5.494459	-2.284016	1.268013
H	3.824884	-2.818799	1.547789
O	3.503128	0.889431	-0.126785
C	3.012646	2.110464	0.474338
H	2.695338	1.908234	1.499397
H	3.826299	2.842370	0.483506
O	0.800637	1.649625	-0.364982
C	1.240466	3.944072	0.137835
C	-0.234694	3.576188	0.405516
H	1.728899	4.299831	1.052562
H	-0.909710	4.407486	0.196284
H	-0.363893	3.272333	1.446151
O	1.406238	4.915307	-0.901330
H	1.128664	5.782019	-0.562058
N	-1.510849	1.416724	-0.284090
C	-2.651006	1.748605	0.398889
O	-2.814920	2.761483	1.071923
N	-3.715785	0.828270	0.309450
H	-4.503972	1.064300	0.906821
C	1.862380	2.619585	-0.375313
H	2.199520	2.773758	-1.409016
C	-1.425061	0.197818	-1.070876
H	-0.796434	0.404922	-1.937095
O	-2.138429	-1.796092	-1.219460
C	4.043535	-1.424668	-0.119080
H	4.806083	-1.200763	-0.876886
C	2.757585	-1.795917	-0.858712
C	1.507055	-1.493679	-0.309981
C	2.809963	-2.441412	-2.101423
C	0.316898	-1.749299	-1.001339
H	1.460338	-1.005678	0.656255
C	1.628076	-2.758221	-2.775644
H	3.771488	-2.688495	-2.546025
C	0.386408	-2.398140	-2.242469

HH-1-S_{1,min}

C	4.470577	-2.652568	0.713533
H	4.641841	-3.521818	0.070694
H	5.402277	-2.422539	1.240507
H	3.711058	-2.917181	1.456092
O	3.563246	0.869073	-0.070120
C	3.082484	2.083542	0.552128
H	2.786978	1.872954	1.581871
H	3.897650	2.813483	0.548112
O	0.845811	1.641307	-0.230306
C	1.319212	3.934810	0.242269
C	-0.163485	3.594589	0.505288
H	1.811552	4.278359	1.159660
H	-0.823637	4.433749	0.279818
H	-0.304719	3.307161	1.548554
O	1.509973	4.905157	-0.793580
H	1.252678	5.777186	-0.452030
N	-1.474652	1.451235	-0.172814
C	-2.615631	1.811375	0.521767
O	-2.709126	2.806627	1.253314
N	-3.712325	0.996695	0.355698
H	-4.508595	1.259589	0.926264
C	1.916612	2.598889	-0.271509
H	2.232381	2.743552	-1.313715
C	-1.438511	0.275037	-1.013074
H	-0.839288	0.507744	-1.896079
O	-2.143201	-1.690285	-1.348942
C	4.014302	-1.459449	-0.141774
H	4.800943	-1.227061	-0.871493
C	2.735450	-1.755516	-0.925651
C	1.481560	-1.475970	-0.372945
C	2.798086	-2.309922	-2.211592
C	0.299253	-1.676586	-1.094891
H	1.425727	-1.055818	0.624516
C	1.623171	-2.563959	-2.922858
H	3.763313	-2.536347	-2.658896
C	0.377545	-2.234437	-2.379671

H	1.673389	-3.266396	-3.735512	H	1.676448	-3.001828	-3.916243
H	-0.524556	-2.613297	-2.790045	H	-0.527233	-2.407756	-2.951728
C	-1.011729	-1.218892	-0.471783	C	-1.031830	-1.185856	-0.529992
C	-1.202897	-1.431746	1.026340	C	-1.239737	-1.543780	0.935432
C	-1.916110	-2.557243	1.468472	C	-1.897150	-2.741386	1.260583
C	-0.653370	-0.563025	1.982424	C	-0.736390	-0.743809	1.972543
C	-2.076089	-2.809505	2.833205	C	-2.053176	-3.127812	2.592731
H	-2.352866	-3.231947	0.739225	H	-2.295867	-3.365404	0.466914
C	-0.817972	-0.814237	3.348675	C	-0.899095	-1.130054	3.307737
H	-0.097431	0.313045	1.666979	H	-0.219641	0.182211	1.745539
C	-1.528868	-1.937233	3.779889	C	-1.556529	-2.321218	3.623531
H	-2.631433	-3.686651	3.155544	H	-2.567131	-4.056836	2.825891
H	-0.388856	-0.127166	4.073609	H	-0.508657	-0.494544	4.098516
H	-1.656517	-2.130515	4.841797	H	-1.682239	-2.619267	4.661112
C	-0.423696	2.374656	-0.521106	C	-0.368636	2.382817	-0.404676
H	-0.503273	2.708006	-1.568242	H	-0.427791	2.706475	-1.457322
C	-3.884146	-0.240460	-0.538335	C	-3.817963	-0.212623	-0.359607
O	-4.901903	-0.920124	-0.524205	O	-5.026094	-0.632523	-0.615553
C	-2.723871	-0.498056	-1.503297	C	-2.760581	-0.393892	-1.474996
C	-3.185430	-0.360376	-2.943947	C	-3.292559	-0.137743	-2.874190
H	-2.357197	-0.584546	-3.622362	H	-2.481674	-0.208280	-3.606027
H	-4.010740	-1.050640	-3.143554	H	-4.064017	-0.869927	-3.128437
H	-3.532967	0.660988	-3.138707	H	-3.735151	0.862575	-2.931013
C	3.845440	-0.136263	0.679579	C	3.830561	-0.200958	0.706080
O	3.953581	-0.034448	1.888325	O	3.887688	-0.156491	1.921630

HH-1-T_{1,min}

C	4.073082	-3.129536	0.514506
H	4.150042	-3.947205	-0.209208
H	5.019474	-3.061465	1.061619
H	3.285274	-3.375067	1.232073
O	3.682410	0.532228	0.057412
C	3.257073	1.744212	0.721152
H	2.909656	1.507891	1.728740
H	4.121446	2.412246	0.777227
O	1.026911	1.494416	-0.161523
C	1.642707	3.729367	0.434842
C	0.146435	3.463478	0.692863
H	2.155833	4.019358	1.359311

HT-1-S₀

O	-3.033824	1.575473	0.004313
C	-3.479208	0.498552	0.862985
H	-2.693216	0.293316	1.595648
H	-4.378507	0.815386	1.399801
O	-2.694670	-1.133715	-0.818231
C	-4.090536	-1.943771	0.928062
C	-2.719659	-2.630746	1.005043
H	-4.459860	-1.642080	1.915216
H	-2.792882	-3.694756	1.239805
H	-2.094226	-2.152138	1.766746
O	-5.070272	-2.744722	0.260089
H	-5.267264	-3.519196	0.812489

H	-0.466278	4.351926	0.528626	N	-0.661933	-2.277489	-0.471365
H	-0.000322	3.119892	1.717565	C	0.057587	-3.434756	-0.382352
O	1.882603	4.716649	-0.575091	O	-0.438726	-4.537519	-0.161939
H	1.668691	5.591085	-0.210253	N	1.441821	-3.310744	-0.577936
N	-1.310511	1.468959	-0.127546	H	1.947898	-4.190096	-0.513472
C	-2.371586	1.802366	0.675446	C	-3.800416	-0.734075	0.023917
O	-2.387116	2.695436	1.517028	H	-4.647530	-0.529961	-0.637135
N	-3.544264	1.043515	0.491983	C	-0.006636	-1.020387	-0.600484
H	-4.283286	1.280056	1.148973	H	-0.715014	-0.320206	-1.037066
C	2.162475	2.377891	-0.118917	O	0.525282	-0.484146	0.647089
H	2.528439	2.542676	-1.141083	C	2.925138	0.044980	0.756526
C	-1.384443	0.353336	-1.051572	C	4.197774	0.153768	0.175798
H	-0.743265	0.580686	-1.903585	C	2.825089	-0.067931	2.151192
O	-2.353343	-1.519755	-1.368565	C	5.344246	0.155384	0.974449
C	3.780848	-1.815756	-0.220156	H	4.307403	0.210414	-0.902020
H	4.608204	-1.597853	-0.905450	C	3.972757	-0.064642	2.949880
C	2.486073	-1.817876	-1.032418	H	1.846833	-0.160891	2.611690
C	1.286550	-2.103872	-0.464026	C	5.236968	0.049456	2.364894
C	2.543265	-1.435974	-2.451424	H	6.322120	0.232875	0.506222
C	0.043290	-1.876026	-1.217917	H	3.875438	-0.152490	4.028979
H	1.225647	-2.396255	0.579737	H	6.129977	0.049992	2.984398
C	1.381412	-1.560232	-3.271174	C	-2.144568	-2.376273	-0.393799
H	3.503323	-1.193195	-2.895619	H	-2.439057	-3.163806	-1.093376
C	0.172717	-1.863951	-2.714460	C	2.153405	-2.237839	-1.085293
H	1.486135	-1.482679	-4.351675	O	3.326375	-2.370549	-1.408772
H	-0.695527	-2.085976	-3.326343	C	1.377877	-0.938243	-1.261706
C	-1.131409	-1.178174	-0.603810	C	1.440801	-0.508851	-2.726901
C	-1.311791	-1.476788	0.879053	H	2.474010	-0.340117	-3.042568
C	-2.244596	-2.441631	1.286673	H	1.017635	-1.294186	-3.364279
C	-0.530617	-0.832974	1.851056	H	0.868057	0.406738	-2.889256
C	-2.399306	-2.752947	2.640881	C	1.653445	0.111037	-0.069805
H	-2.854468	-2.941674	0.541221	C	1.284945	1.550413	-0.483687
C	-0.689807	-1.141910	3.205455	C	0.016012	2.029121	-0.137337
H	0.204095	-0.093169	1.550477	C	2.117921	2.370112	-1.255479
C	-1.624790	-2.101587	3.605878	C	-0.483723	3.250577	-0.599835
H	-3.126756	-3.503312	2.940095	H	-0.593825	1.395833	0.490698
H	-0.080216	-0.630885	3.946482	C	1.650656	3.612054	-1.696960
H	-1.747362	-2.340187	4.659117	H	3.116554	2.051072	-1.535511
C	-0.132825	2.326452	-0.290648	C	0.355855	4.044725	-1.394564
H	-0.165445	2.717720	-1.319693	H	2.296636	4.240334	-2.304602
C	-3.874277	0.165323	-0.512455	H	0.008300	4.995838	-1.788097

O	-4.986905	-0.342040	-0.580631	C	-2.604602	2.689760	0.640510
C	-2.762977	-0.132595	-1.519974	O	-2.717973	2.844301	1.842833
C	-3.212378	0.193975	-2.933683	C	-1.930548	3.681745	-0.304602
H	-2.417769	-0.050843	-3.644211	H	-2.481517	3.638191	-1.253682
H	-4.108306	-0.381263	-3.186473	C	-2.032708	5.108063	0.263451
H	-3.449321	1.260413	-3.024183	H	-1.485927	5.193727	1.207143
C	3.676650	-0.631437	0.741918	H	-1.619110	5.831867	-0.443951
O	3.556043	-0.710565	1.950485	H	-3.078916	5.375582	0.444797

HT-1-S_{1,min}

O	-2.874342	1.750949	-0.054359
C	-3.404524	0.722160	0.818041
H	-2.633498	0.466786	1.550997
H	-4.272167	1.120453	1.352373
O	-2.784237	-0.996840	-0.853293
C	-4.176950	-1.658377	0.955001
C	-2.852209	-2.429031	1.020048
H	-4.502578	-1.302279	1.939940
H	-2.984562	-3.476765	1.296022
H	-2.175013	-1.966457	1.746940
O	-5.225579	-2.412922	0.337017
H	-5.435852	-3.172702	0.904685
N	-0.829629	-2.283671	-0.551355
C	-0.169219	-3.490620	-0.308874
O	-0.788324	-4.521817	0.038387
N	1.174227	-3.446041	-0.501932
H	1.651530	-4.330367	-0.369228
C	-3.830233	-0.498909	0.006193
H	-4.681851	-0.247475	-0.633037
C	-0.099451	-1.085559	-0.682641
H	-0.750391	-0.330491	-1.117617
O	0.450821	-0.542094	0.595339
C	2.849684	-0.080355	0.752990
C	4.150120	-0.192336	0.179772
C	2.718190	0.053705	2.165713
C	5.264383	-0.242358	0.997805
H	4.253365	-0.303632	-0.891734
C	3.836539	-0.001461	2.974310
H	1.728086	0.163328	2.593467

HT-1-T_{1,min}

O	-3.182410	1.279742	-0.001579
C	-3.615005	0.203786	0.859969
H	-2.860720	0.068463	1.641175
H	-4.562522	0.471876	1.337056
O	-2.679476	-1.321902	-0.838541
C	-3.910079	-2.293303	0.948487
C	-2.453719	-2.777629	1.004685
H	-4.302906	-2.035488	1.939289
H	-2.369251	-3.837724	1.255463
H	-1.886326	-2.203165	1.745283
O	-4.776849	-3.230874	0.303335
H	-4.854378	-4.020250	0.864295
N	-0.505485	-2.172618	-0.541160
C	0.345987	-3.236602	-0.658994
O	0.000550	-4.410570	-0.536498
N	1.676008	-2.919931	-0.963283
H	2.273545	-3.732043	-1.093042
C	-3.803021	-1.064192	0.031282
H	-4.685835	-0.971767	-0.607517
C	-0.005625	-0.835007	-0.497703
H	-0.825729	-0.165484	-0.751193
O	0.577748	-0.453672	0.781229
C	2.987398	0.068328	0.800227
C	4.198366	0.365125	0.156509
C	3.017968	-0.406434	2.120358
C	5.415077	0.187216	0.819558
H	4.200534	0.710665	-0.872185
C	4.236072	-0.581746	2.783467
H	2.086943	-0.644923	2.624111

C	5.116380	-0.145175	2.394695	C	5.439094	-0.283941	2.136533
H	6.252367	-0.362065	0.565612	H	6.344417	0.412678	0.302876
H	3.737245	0.068767	4.052567	H	4.242163	-0.952109	3.805424
H	5.994699	-0.170390	3.031926	H	6.386538	-0.420935	2.651043
C	-2.300531	-2.267596	-0.403316	C	-1.951623	-2.469002	-0.411419
H	-2.692365	-3.051705	-1.058079	H	-2.151299	-3.302358	-1.089598
C	1.947444	-2.443326	-1.177857	C	2.174578	-1.718434	-1.441956
O	3.202723	-2.674226	-1.363460	O	3.273847	-1.678330	-1.983431
C	1.309911	-1.096636	-1.310178	C	1.290098	-0.501706	-1.255574
C	1.427010	-0.550082	-2.734392	C	1.157828	0.256774	-2.572529
H	2.476592	-0.475864	-3.037110	H	2.139040	0.539793	-2.961712
H	0.932509	-1.240535	-3.427064	H	0.667081	-0.378928	-3.319152
H	0.959571	0.433817	-2.845987	H	0.554735	1.158318	-2.446358
C	1.611842	-0.057197	-0.093374	C	1.642194	0.301175	0.124863
C	1.431601	1.438254	-0.422611	C	1.296527	1.776568	0.133817
C	0.213232	2.038353	-0.047299	C	-0.106088	2.173464	0.401658
C	2.357623	2.190815	-1.189594	C	2.141701	2.802678	-0.539053
C	-0.194668	3.257824	-0.573866	C	-0.719890	3.067357	-0.415404
H	-0.442566	1.454772	0.581614	H	-0.632975	1.675013	1.208030
C	1.995434	3.453964	-1.648233	C	1.523834	3.710422	-1.342797
H	3.322916	1.780255	-1.462399	H	3.217650	2.818010	-0.393736
C	0.725498	3.976537	-1.374492	C	0.086272	3.764867	-1.415511
H	2.691884	4.026830	-2.252803	H	2.105179	4.440976	-1.901736
H	0.449591	4.939520	-1.792306	H	-0.392688	4.443429	-2.114267
C	-2.393689	2.848916	0.568604	C	-2.922231	2.455154	0.610245
O	-2.521262	3.043120	1.763355	O	-3.198302	2.668988	1.777011
C	-1.627695	3.770177	-0.379950	C	-2.202615	3.430881	-0.312325
H	-2.120660	3.704058	-1.359031	H	-2.632568	3.303579	-1.315254
C	-1.690962	5.227063	0.113413	C	-2.420930	4.886134	0.141230
H	-1.183257	5.338219	1.075766	H	-2.021888	5.043202	1.147574
H	-1.221754	5.900043	-0.609288	H	-1.918157	5.576375	-0.542657
H	-2.732980	5.539997	0.233455	H	-3.488102	5.131987	0.147943

HH-2-S₀

C	5.548997	-1.293107	-0.847257
H	5.616358	-2.155476	-1.517960
H	6.300399	-0.562287	-1.163978
H	5.800302	-1.618594	0.166736
O	3.231020	1.483760	-0.560534

HH-2-S_{1,min}

C	4.123414	-2.743168	1.227650
H	4.246155	-3.707546	0.725479
H	5.036090	-2.526963	1.792106
H	3.294128	-2.825391	1.936399
O	3.706661	0.705045	-0.070380

C	2.658276	2.472734	0.320194	C	3.322997	2.032582	0.347812
H	2.363474	1.983226	1.252803	H	3.039351	2.013726	1.401428
H	3.396969	3.248580	0.544565	H	4.188202	2.688188	0.212500
O	0.589352	2.034857	-0.873157	O	1.047216	1.629163	-0.324140
C	0.613549	3.968282	0.550844	C	1.681883	3.934009	-0.226288
C	-0.686535	3.164351	0.710275	C	0.205654	3.728408	0.171437
H	1.113806	4.134498	1.512172	H	2.247323	4.394863	0.593908
H	-1.550476	3.803522	0.894701	H	-0.423011	4.571505	-0.119938
H	-0.597106	2.440035	1.526704	H	0.117105	3.581065	1.248014
O	0.415416	5.222804	-0.112002	O	1.846299	4.689091	-1.424921
H	-0.073145	5.813755	0.484582	H	1.619707	5.611315	-1.222986
N	-1.615510	1.213944	-0.686989	N	-1.280402	1.625725	-0.189700
C	-2.952308	1.489479	-0.647214	C	-2.316732	2.131782	0.579341
O	-3.413165	2.590909	-0.347282	O	-2.261327	3.167520	1.247685
N	-3.841358	0.455848	-0.983351	N	-3.494049	1.415959	0.552182
H	-4.821439	0.702434	-0.872446	H	-4.203754	1.784307	1.174112
C	1.461915	3.083633	-0.391909	C	2.174739	2.494285	-0.530300
H	1.792453	3.677785	-1.251359	H	2.475728	2.456720	-1.585959
C	-1.090279	-0.075525	-1.127653	C	-1.416093	0.393298	-0.936427
H	-0.232513	0.115252	-1.764441	H	-0.873684	0.508037	-1.877795
O	-1.747840	-2.103291	-0.859667	O	-2.318987	-1.508298	-1.084347
C	4.151561	-0.670346	-0.914263	C	3.847031	-1.645493	0.188543
H	3.962661	-0.329802	-1.939184	H	4.697783	-1.581477	-0.500983
C	2.995652	-1.604042	-0.506480	C	2.598456	-1.933479	-0.643545
C	1.677653	-1.114873	-0.520234	C	1.338913	-1.516674	-0.210634
C	3.195828	-2.921332	-0.094019	C	2.676499	-2.638465	-1.845191
C	0.581622	-1.881708	-0.118145	C	0.163433	-1.730723	-0.944828
H	1.516593	-0.090056	-0.827513	H	1.272168	-0.981928	0.727771
C	2.103300	-3.707394	0.289067	C	1.514853	-2.902308	-2.564776
H	4.190864	-3.353248	-0.062760	H	3.636936	-2.985518	-2.218791
C	0.790597	-3.221752	0.299799	C	0.244179	-2.458505	-2.159544
H	2.281559	-4.733640	0.602568	H	1.589391	-3.467805	-3.490184
C	-0.816996	-1.257391	-0.094447	C	-1.106496	-1.068869	-0.385292
C	-1.309942	-1.001780	1.326540	C	-1.280621	-1.298055	1.115957
C	-2.603257	-1.361311	1.728438	C	-1.990980	-2.430596	1.544040
C	-0.464953	-0.376432	2.257346	C	-0.708205	-0.455922	2.080810
C	-3.044598	-1.098504	3.029837	C	-2.133301	-2.710338	2.901906
H	-3.260709	-1.868653	1.030670	H	-2.443715	-3.084396	0.805824
C	-0.906523	-0.107284	3.554755	C	-0.856495	-0.736678	3.442601
H	0.547305	-0.105240	1.971754	H	-0.145765	0.419076	1.775089
C	-2.200351	-0.467384	3.946895	C	-1.568237	-1.861527	3.858747

H	-4.048733	-1.392846	3.324350	H	-2.689427	-3.590410	3.213581
H	-0.236609	0.377618	4.260192	H	-0.411098	-0.069778	4.175853
H	-2.542939	-0.263529	4.957971	H	-1.682547	-2.076913	4.917536
C	-0.754840	2.425122	-0.628808	C	-0.119980	2.427020	-0.561275
H	-1.097163	3.104476	-1.421105	H	-0.188018	2.624863	-1.644198
C	-3.564793	-0.729499	-1.612458	C	-3.755616	0.170548	-0.049188
O	-4.452717	-1.495316	-1.966670	O	-5.013540	-0.166355	-0.158317
C	-2.083115	-1.049659	-1.801761	C	-2.826686	-0.167891	-1.233743
C	-1.789423	-1.437010	-3.241948	C	-3.478458	0.068462	-2.585828
H	-0.740677	-1.731970	-3.340918	H	-2.766906	-0.114166	-3.396382
H	-2.426828	-2.273072	-3.543979	H	-4.337616	-0.595623	-2.712262
H	-1.982403	-0.591308	-3.912527	H	-3.830552	1.102819	-2.653294
C	4.045501	0.556554	-0.013221	C	3.715815	-0.278946	0.854858
O	4.548899	0.675515	1.088943	O	3.596792	-0.091951	2.049396
C	-0.323016	-4.141389	0.749473	C	-0.918911	-2.817718	-3.064311
H	-0.919815	-3.696829	1.553087	H	-1.710554	-3.349163	-2.531831
H	-1.013303	-4.366505	-0.069941	H	-1.380112	-1.936217	-3.520413
H	0.090343	-5.085191	1.118714	H	-0.563402	-3.458930	-3.876975

HH-2-T_{1,min}

C	3.592835	-3.343443	1.098594
H	3.527131	-4.273075	0.524444
H	4.555609	-3.326817	1.620672
H	2.802711	-3.345461	1.854184
O	3.844196	0.192857	0.051130
C	3.605115	1.557686	0.465368
H	3.314592	1.577732	1.517317
H	4.541493	2.104833	0.327829
O	1.306636	1.396753	-0.229838
C	2.184352	3.622311	-0.164472
C	0.676683	3.595699	0.160150
H	2.758819	4.030684	0.675178
H	0.159247	4.487328	-0.201851
H	0.528152	3.515389	1.236319
O	2.504608	4.346381	-1.358233
H	2.418194	5.296316	-1.175619
N	-1.023408	1.649699	-0.200820
C	-1.959986	2.201228	0.638122
O	-1.780584	3.144482	1.401886

HT-2-S₀

O	-2.920797	1.859580	0.007108
C	-3.489492	0.832284	0.852324
H	-2.733171	0.524445	1.580254
H	-4.345676	1.245616	1.394261
O	-2.892005	-0.850161	-0.850451
C	-4.389871	-1.521022	0.871435
C	-3.112913	-2.369930	0.941221
H	-4.725686	-1.195281	1.863021
H	-3.316445	-3.421824	1.150703
H	-2.441685	-1.987872	1.718317
O	-5.455423	-2.185775	0.185362
H	-5.746429	-2.941741	0.721837
N	-1.011798	-2.231952	-0.508110
C	-0.438639	-3.462811	-0.373493
O	-1.066631	-4.493568	-0.140764
N	0.953835	-3.511055	-0.544396
H	1.341532	-4.448857	-0.482397
C	-3.950936	-0.338889	-0.007944
H	-4.762408	-0.023714	-0.670201

N	-3.244540	1.626078	0.587906	C	-0.209071	-1.060161	-0.634341
H	-3.893266	2.029549	1.258789	H	-0.814935	-0.292625	-1.111891
C	2.524702	2.132980	-0.432420	O	0.328181	-0.571921	0.621318
H	2.831746	2.038586	-1.483008	C	2.723211	-0.331113	0.926834
C	-1.313359	0.450701	-0.967380	C	3.977388	-0.846992	0.579725
H	-0.694820	0.470799	-1.865009	C	2.506257	0.069221	2.258315
O	-2.575004	-1.263626	-1.024820	C	4.988515	-0.967416	1.540850
C	3.477629	-2.142182	0.153865	H	4.174531	-1.171644	-0.433921
H	4.313039	-2.162674	-0.555669	C	3.513622	-0.050843	3.216203
C	2.180488	-2.085576	-0.654534	H	1.539953	0.472704	2.546103
C	0.960624	-2.281742	-0.085616	C	4.763232	-0.571307	2.860362
C	2.260793	-1.763831	-2.086475	H	5.953363	-1.374681	1.249394
C	-0.245591	-2.002287	-0.875568	H	3.322170	0.262205	4.239407
H	0.870673	-2.513671	0.970972	H	5.549734	-0.666928	3.604431
C	1.137779	-1.937361	-2.908506	C	-2.497225	-2.156270	-0.447579
H	3.233187	-1.559856	-2.524451	H	-2.875215	-2.889392	-1.166348
C	-0.104859	-2.235625	-2.361679	C	1.789474	-2.550008	-1.081903
H	1.276602	-1.984555	-3.988582	O	2.919386	-2.851605	-1.445689
C	-1.280429	-1.038173	-0.345756	C	1.200069	-1.152822	-1.247199
C	-1.443651	-1.124850	1.168232	C	1.324231	-0.740867	-2.715302
C	-2.486583	-1.888902	1.711875	H	2.354757	-0.818683	-3.067946
C	-0.543443	-0.488464	2.036827	H	0.710161	-1.408174	-3.331807
C	-2.633075	-2.009332	3.097077	H	0.968850	0.280747	-2.866258
H	-3.188881	-2.381238	1.046988	C	1.562782	-0.129970	-0.042484
C	-0.694129	-0.605439	3.422049	C	1.399043	1.350029	-0.476480
H	0.277996	0.094374	1.633353	C	0.181075	1.962400	-0.148618
C	-1.739004	-1.364833	3.957713	C	2.352746	2.086758	-1.215088
H	-3.447455	-2.605096	3.501598	C	-0.182640	3.241343	-0.576750
H	0.008870	-0.102278	4.081193	H	-0.507033	1.382195	0.448391
H	-1.854297	-1.454274	5.034838	C	1.994479	3.382928	-1.623455
C	0.241049	2.304294	-0.535469	C	0.753713	3.952883	-1.335948
H	0.226027	2.461624	-1.625413	H	2.710857	3.957518	-2.206278
C	-3.765671	0.718571	-0.302389	H	0.527660	4.945518	-1.715325
O	-4.945225	0.390915	-0.267914	C	-2.353160	2.903378	0.653168
C	-2.775607	0.145277	-1.318495	O	-2.432429	3.051807	1.859223
C	-3.256873	0.397822	-2.736998	C	-1.578547	3.819751	-0.289545
H	-2.547783	-0.020894	-3.456255	H	-2.128721	3.832403	-1.239962
H	-4.238056	-0.061832	-2.890469	C	-1.537621	5.250031	0.276425
H	-3.347673	1.474612	-2.922275	H	-0.986298	5.282621	1.220817
C	3.566680	-0.814132	0.906788	H	-1.053191	5.927994	-0.431493
O	3.372177	-0.663961	2.098445	H	-2.552109	5.621701	0.455424

C	-1.169371	-2.941085	-3.148548	C	3.728592	1.579385	-1.584957
H	-1.388812	-3.918187	-2.688905	H	4.397603	1.574583	-0.716607
H	-2.118178	-2.395502	-3.154289	H	3.713981	0.561087	-1.981213
H	-0.846232	-3.113136	-4.180867	H	4.177451	2.224454	-2.346680

HT-2-S_{1,min}

O	-2.846002	1.853440	-0.042115
C	-3.460673	0.861142	0.819581
H	-2.716992	0.551670	1.559833
H	-4.304098	1.318339	1.344777
O	-2.950709	-0.871357	-0.874241
C	-4.368875	-1.470607	0.933775
C	-3.083767	-2.306566	0.994875
H	-4.678919	-1.107210	1.921116
H	-3.268326	-3.348866	1.261141
H	-2.386664	-1.885368	1.727880
O	-5.451703	-2.166409	0.306371
H	-5.701948	-2.919332	0.867000
N	-1.049686	-2.233665	-0.568603
C	-0.442459	-3.469220	-0.349893
O	-1.093402	-4.469994	0.019334
N	0.896746	-3.488120	-0.592637
H	1.331188	-4.400103	-0.506377
C	-3.960654	-0.323015	-0.004312
H	-4.797868	-0.013922	-0.637065
C	-0.266764	-1.058166	-0.670338
H	-0.889951	-0.274130	-1.095554
O	0.289119	-0.583206	0.614146
C	2.687084	-0.389960	0.932439
C	3.809695	-1.177051	0.622329
C	2.621596	0.245348	2.196437
C	4.832687	-1.329322	1.557680
H	3.861455	-1.689838	-0.333745
C	3.648472	0.092893	3.125729
H	1.753606	0.846797	2.451084
C	4.762190	-0.691998	2.807083
H	5.689776	-1.952706	1.317232
H	3.582152	0.584095	4.092431
H	5.568802	-0.811985	3.525112

HT-2-T_{1,min}

O	-3.096497	1.598753	0.049847
C	-3.633641	0.569980	0.908098
H	-2.876491	0.320672	1.657825
H	-4.522265	0.945812	1.424305
O	-2.947826	-1.018305	-0.846893
C	-4.255938	-1.868520	0.946407
C	-2.872867	-2.535365	0.960275
H	-4.594857	-1.588844	1.951116
H	-2.919909	-3.604126	1.181389
H	-2.224839	-2.058776	1.704080
O	-5.247047	-2.670459	0.297182
H	-5.410217	-3.460817	0.837890
N	-0.887724	-2.134389	-0.605005
C	-0.178395	-3.300035	-0.679046
O	-0.671374	-4.416571	-0.526250
N	1.182319	-3.166383	-0.984410
H	1.659162	-4.053805	-1.121209
C	-4.008517	-0.640056	0.057707
H	-4.884972	-0.414166	-0.556156
C	-0.223123	-0.867251	-0.577961
H	-0.945506	-0.106934	-0.869782
O	0.363375	-0.539271	0.708196
C	2.794896	-0.417687	0.862998
C	4.031418	-0.704565	0.269869
C	2.681679	-0.501132	2.262467
C	5.127876	-1.074982	1.056508
H	4.144699	-0.660877	-0.806801
C	3.775619	-0.869845	3.046714
H	1.728987	-0.284477	2.735954
C	5.006194	-1.158412	2.445421
H	6.076799	-1.300265	0.576432
H	3.666235	-0.932406	4.126392
H	5.859061	-1.447554	3.053988

C	-2.519108	-2.161064	-0.425498	C	-2.359004	-2.253457	-0.457892
H	-2.938067	-2.925716	-1.086355	H	-2.669673	-3.039419	-1.151209
C	1.653932	-2.522132	-1.334464	C	1.819490	-2.054945	-1.511609
O	2.812442	-2.866375	-1.775415	O	2.877826	-2.184256	-2.117914
C	1.130187	-1.128489	-1.318449	C	1.129417	-0.719071	-1.304003
C	1.242105	-0.494229	-2.708871	C	1.123306	0.059193	-2.617128
H	2.275239	-0.510688	-3.066855	H	2.141497	0.238086	-2.971375
H	0.643466	-1.081351	-3.414685	H	0.592980	-0.515988	-3.385377
H	0.872317	0.535599	-2.740182	H	0.617004	1.018914	-2.501001
C	1.522870	-0.160577	-0.012308	C	1.560657	0.030321	0.083427
C	1.440219	1.338668	-0.324667	C	1.443184	1.555124	0.080792
C	0.261614	2.001118	0.035174	C	0.120932	2.125649	0.400790
C	2.446079	2.070938	-1.079508	C	2.383131	2.488912	-0.645902
C	-0.100081	3.227581	-0.514909	C	-0.430564	3.045889	-0.431630
H	-0.433078	1.447537	0.649218	H	-0.430742	1.713572	1.238931
C	2.090134	3.335038	-1.592764	C	1.788231	3.388340	-1.510331
C	0.853330	3.901096	-1.346184	C	0.391626	3.594364	-1.516269
H	2.815358	3.875413	-2.192535	H	2.414434	4.032507	-2.126786
H	0.609288	4.863647	-1.781916	H	-0.050303	4.300278	-2.213142
C	-2.338048	2.930412	0.590156	C	-2.653150	2.713360	0.668159
O	-2.499784	3.148221	1.775738	O	-2.847258	2.937743	1.849570
C	-1.495875	3.809396	-0.336523	C	-1.847447	3.596992	-0.273440
H	-1.972701	3.794762	-1.327021	H	-2.326598	3.537611	-1.259967
C	-1.467703	5.265736	0.175083	C	-1.854420	5.064741	0.193801
H	-0.976753	5.328495	1.149725	H	-1.408238	5.157569	1.188246
H	-0.940477	5.915035	-0.528169	H	-1.282757	5.686084	-0.502118
H	-2.490622	5.640144	0.275788	H	-2.878265	5.451848	0.233818
C	3.821800	1.549949	-1.330291	C	3.853427	2.541070	-0.355125
H	4.439647	1.642175	-0.426779	H	4.035106	2.612051	0.726674
H	3.815024	0.484624	-1.583486	H	4.380205	1.640033	-0.691198
H	4.310125	2.109302	-2.131641	H	4.313598	3.406079	-0.843502

HH-3-S₀

C	4.255445	-2.222817	1.896114
H	4.410246	-3.273875	1.631798
H	5.158627	-1.852906	2.391974
H	3.426483	-2.166758	2.609252
O	3.531809	0.781593	-0.186779
C	3.089622	2.153323	-0.069468

HH-3-S_{1,min}

C	4.486640	-2.043535	1.606801
H	4.689353	-3.070876	1.292322
H	5.386128	-1.640718	2.079507
H	3.688981	-2.065163	2.355089
O	3.384801	0.958404	-0.262218
C	2.852036	2.269167	-0.026298

H	2.764451	2.345154	0.955135	H	2.513328	2.343936	1.008964
H	3.933321	2.807229	-0.311731	H	3.639630	3.007604	-0.201364
O	0.846328	1.532707	-0.711485	O	0.657034	1.560488	-0.717700
C	1.420949	3.821981	-1.096024	C	1.089091	3.892418	-0.898606
C	-0.056426	3.670499	-0.680987	C	-0.354501	3.621773	-0.463283
H	1.959348	4.475996	-0.400214	H	1.613493	4.522824	-0.172436
H	-0.699721	4.408903	-1.163143	H	-1.049274	4.359800	-0.860928
H	-0.151716	3.776552	0.400664	H	-0.428900	3.624989	0.626290
O	1.591360	4.304413	-2.434088	O	1.178531	4.481661	-2.193191
H	1.364070	5.248513	-2.453510	H	0.871642	5.399675	-2.141431
N	-1.474171	1.494023	-0.514583	N	-1.626181	1.385877	-0.387073
C	-2.499699	2.097441	0.162918	C	-2.773288	1.950675	0.111529
O	-2.550677	3.280102	0.488288	O	-2.948338	3.161014	0.259387
N	-3.585844	1.267556	0.509973	N	-3.788312	1.085933	0.445647
H	-4.275905	1.732133	1.094382	H	-4.574924	1.528216	0.905616
C	1.961807	2.369281	-1.065359	C	1.711594	2.487133	-0.997704
H	2.302950	2.106355	-2.075371	H	2.063982	2.333681	-2.024665
C	-1.523502	0.085164	-0.872550	C	-1.575467	-0.010766	-0.765830
H	-1.042788	-0.026191	-1.844657	H	-1.179595	-0.080560	-1.780750
O	-2.254116	-1.816445	-0.282512	O	-2.061565	-1.976580	-0.202598
C	3.951384	-1.414618	0.625899	C	4.081144	-1.207110	0.393349
H	4.805990	-1.499624	-0.058586	H	4.906622	-1.206950	-0.329307
C	2.712845	-1.894399	-0.124521	C	2.841468	-1.718659	-0.319164
C	1.438704	-1.541752	0.335539	C	1.583243	-1.455729	0.221671
C	2.800058	-2.602595	-1.320684	C	2.900987	-2.344386	-1.554108
C	0.263609	-1.762981	-0.388208	C	0.395324	-1.688751	-0.459093
H	1.367372	-1.002313	1.272254	H	1.531852	-0.975117	1.191263
C	1.646616	-2.904626	-2.049137	C	1.732255	-2.650624	-2.247979
H	3.768279	-2.905419	-1.713385	H	3.861314	-2.573268	-2.008839
C	0.387617	-2.456490	-1.624431	C	0.486164	-2.288645	-1.737120
H	1.745175	-3.452010	-2.978624	H	1.808551	-3.128914	-3.215858
C	-1.026497	-1.085208	0.081234	C	-0.905513	-1.134634	0.109071
C	-1.061795	-0.804846	1.586405	C	-0.867510	-0.905602	1.614554
C	-1.712645	-1.723652	2.425242	C	-1.328928	-1.919462	2.458634
C	-0.450478	0.317228	2.168403	C	-0.348945	0.259118	2.184073
C	-1.755962	-1.525857	3.807765	C	-1.283430	-1.769496	3.840745
H	-2.195859	-2.592005	1.989844	H	-1.739029	-2.826244	2.027623
C	-0.501660	0.519906	3.551502	C	-0.310723	0.412784	3.568655
H	0.079825	1.028214	1.545545	H	0.040903	1.042126	1.546090
C	-1.154411	-0.399084	4.377211	C	-0.778790	-0.598131	4.402445
H	-2.264289	-2.251192	4.438093	H	-1.648516	-2.568054	4.480039

H	-0.025016	1.397820	3.980404	H	0.092632	1.327596	3.993285
H	-1.192450	-0.240516	5.451846	H	-0.748036	-0.476729	5.481190
C	-0.346832	2.228444	-1.098177	C	-0.581649	2.210618	-0.991319
H	-0.451202	2.160824	-2.192424	H	-0.739692	2.222949	-2.081060
C	-3.864338	-0.025231	0.134219	C	-3.717886	-0.320203	0.480630
O	-4.857674	-0.613355	0.542028	O	-4.827634	-0.942660	0.716089
C	-2.875996	-0.640907	-0.859878	C	-2.839382	-0.885541	-0.670808
C	-3.579435	-0.918235	-2.178769	C	-3.652037	-1.203288	-1.906083
H	-2.871958	-1.350168	-2.888697	H	-2.985830	-1.473953	-2.726742
H	-4.406772	-1.617402	-2.020904	H	-4.328466	-2.037550	-1.704607
H	-3.987885	0.008835	-2.598013	H	-4.251296	-0.335490	-2.197372
C	3.801309	0.079782	0.933850	C	3.854222	0.252112	0.775190
O	3.885637	0.583223	2.039708	O	4.039529	0.727977	1.875917
O	-0.736049	-2.637651	-2.377776	O	-0.663426	-2.461596	-2.442312
C	-0.631342	-3.323990	-3.626563	C	-0.595911	-3.049574	-3.733917
H	-1.643348	-3.344306	-4.033578	H	-1.623235	-3.087262	-4.095797
H	0.032089	-2.793042	-4.319392	H	0.009523	-2.442813	-4.415356
H	-0.275846	-4.351149	-3.485030	H	-0.192380	-4.066042	-3.683985

HH-3- $T_{1,\min}$

C	3.710344	-2.738713	2.057089
H	3.655281	-3.803382	1.808769
H	4.678501	-2.543821	2.530586
H	2.928670	-2.512025	2.787041
O	3.800102	0.289117	-0.080464
C	3.546480	1.712804	-0.095414
H	3.272115	2.048106	0.906469
H	4.470997	2.204786	-0.409979
O	1.232756	1.344377	-0.657186
C	2.101618	3.480141	-1.299062
C	0.610028	3.564925	-0.917636
H	2.708179	4.126333	-0.653806
H	0.072335	4.311494	-1.506549
H	0.510317	3.812994	0.138595
O	2.364376	3.794518	-2.671821
H	2.280482	4.754780	-2.790934
N	-1.091909	1.617700	-0.586595
C	-1.998035	2.408160	0.074312
O	-1.812419	3.560809	0.452792

HT-3- S_0

O	-2.805532	2.142358	0.022955
C	-3.550417	1.142826	0.757417
H	-2.893437	0.708979	1.517048
H	-4.394357	1.623440	1.261689
O	-3.021060	-0.525271	-0.986008
C	-4.736887	-1.072062	0.565043
C	-3.586032	-2.079005	0.698717
H	-5.123577	-0.751907	1.539747
H	-3.935606	-3.104737	0.831749
H	-2.948471	-1.819734	1.551130
O	-5.805357	-1.563231	-0.250827
H	-6.232404	-2.304548	0.209342
N	-1.355625	-2.138014	-0.549266
C	-0.941208	-3.431711	-0.418535
O	-1.702635	-4.387340	-0.280157
N	0.445958	-3.638088	-0.467971
H	0.720418	-4.612903	-0.379483
C	-4.075293	0.082576	-0.204275
H	-4.778107	0.531919	-0.911693

N	-3.258955	1.828844	0.315171	C	-0.412331	-1.070776	-0.587610
H	-3.880867	2.428674	0.850946	H	-0.886059	-0.223108	-1.078000
C	2.442778	1.979943	-1.104081	O	0.096424	-0.674995	0.715623
H	2.728273	1.565130	-2.080186	C	2.504930	-0.687451	1.121311
C	-1.387553	0.230192	-0.897496	C	3.807366	-1.034977	0.736544
H	-0.838626	-0.031145	-1.803476	C	2.204975	-0.604823	2.491231
O	-2.570560	-1.427165	-0.272928	C	4.785478	-1.295448	1.701101
C	3.562520	-1.902153	0.781617	H	4.058140	-1.111470	-0.312852
H	4.388205	-2.139323	0.100369	C	3.184834	-0.859615	3.454481
C	2.254685	-2.113993	0.021101	H	1.199045	-0.345003	2.805247
C	1.044358	-2.070369	0.651576	C	4.481469	-1.206131	3.062747
C	2.319987	-2.288554	-1.434802	H	5.787986	-1.571067	1.383078
C	-0.185920	-2.007626	-0.129689	H	2.931558	-0.789642	4.509378
H	0.992962	-1.930374	1.726228	H	5.244806	-1.408407	3.809776
C	1.164747	-2.626670	-2.151347	C	-2.821551	-1.885235	-0.617310
H	3.286988	-2.279785	-1.926540	H	-3.214407	-2.536172	-1.404130
C	-0.066784	-2.607584	-1.508443	C	1.439953	-2.764927	-0.874747
H	1.259439	-2.997922	-3.167607	O	2.573342	-3.177211	-1.083529
C	-1.235448	-0.967187	0.169410	C	1.015006	-1.318807	-1.103024
C	-1.277024	-0.559523	1.638032	C	1.302747	-0.941477	-2.556181
C	-2.240244	-1.125526	2.486387	H	2.360436	-1.067319	-2.793622
C	-0.348439	0.345312	2.175653	H	0.718860	-1.586050	-3.224201
C	-2.280299	-0.790085	3.843081	H	1.015355	0.094237	-2.751917
H	-2.964730	-1.822964	2.078790	C	1.400813	-0.349708	0.127639
C	-0.393630	0.685305	3.531198	C	1.385061	1.140457	-0.283706
H	0.414109	0.778794	1.537584	C	0.270136	1.901605	0.077532
C	-1.359343	0.120633	4.370092	C	2.380593	1.761969	-1.067023
H	-3.033705	-1.238878	4.485604	C	0.052745	3.212778	-0.356774
H	0.330434	1.391441	3.930047	H	-0.466811	1.405183	0.693462
H	-1.392537	0.386395	5.423586	C	2.205183	3.090915	-1.481907
C	0.148732	2.128601	-1.171776	C	1.047346	3.798163	-1.147413
H	0.077228	1.947766	-2.255640	H	2.955857	3.575645	-2.095249
C	-3.797791	0.660919	-0.168837	H	0.930290	4.810182	-1.526506
O	-4.957163	0.344424	0.068690	C	-2.193068	3.085090	0.775451
C	-2.855114	-0.205633	-1.005187	O	-2.363272	3.177184	1.977848
C	-3.441273	-0.464060	-2.382606	C	-1.250177	3.963529	-0.042256
H	-2.775305	-1.117232	-2.951973	H	-1.755575	4.158954	-0.997729
H	-4.420964	-0.943257	-2.291602	C	-1.011841	5.304480	0.673255
H	-3.567262	0.478925	-2.927575	H	-0.509449	5.152259	1.633214
C	3.643425	-0.400282	1.069477	H	-0.387092	5.956276	0.055763
O	3.539448	0.115594	2.166492	H	-1.960316	5.820358	0.856959

O	-1.184124	-3.219584	-1.957928	O	3.462458	1.006369	-1.407506
C	-1.123448	-3.950848	-3.192061	C	4.479124	1.575523	-2.235073
H	-2.113510	-4.387585	-3.322509	H	4.075882	1.863903	-3.212799
H	-0.899790	-3.278759	-4.027271	H	4.941176	2.443940	-1.751840
H	-0.366623	-4.740455	-3.133697	H	5.224883	0.790041	-2.363892

HT-3-S_{1,min}

O	-2.796000	2.109087	-0.061555
C	-3.547529	1.161761	0.741302
H	-2.879430	0.771779	1.514821
H	-4.374546	1.685559	1.229013
O	-3.102460	-0.576770	-0.964030
C	-4.661526	-1.079962	0.757922
C	-3.466520	-2.037741	0.851059
H	-4.977706	-0.707492	1.739930
H	-3.762249	-3.061824	1.086506
H	-2.761843	-1.699487	1.619225
O	-5.778479	-1.655586	0.071348
H	-6.121412	-2.392661	0.603358
N	-1.379383	-2.153613	-0.639619
C	-0.920428	-3.454338	-0.439884
O	-1.692604	-4.392032	-0.140106
N	0.419601	-3.610616	-0.618604
H	0.748675	-4.566843	-0.546509
C	-4.105336	0.042186	-0.134756
H	-4.879372	0.435617	-0.800441
C	-0.468671	-1.068454	-0.657126
H	-0.980256	-0.211420	-1.090073
O	0.058171	-0.693101	0.671221
C	2.458458	-0.765561	1.094179
C	3.551078	-1.567384	0.740306
C	2.368792	-0.279797	2.411371
C	4.533388	-1.875555	1.688190
H	3.621170	-1.969512	-0.265126
C	3.349240	-0.590287	3.357205
H	1.523095	0.338613	2.701722
C	4.439377	-1.388797	2.996273
H	5.373621	-2.503549	1.401502
H	3.262133	-0.207100	4.370854

HT-3-T_{1,min}

O	-2.957523	1.986063	0.044982
C	-3.679794	1.036993	0.858849
H	-2.998622	0.657329	1.626618
H	-4.516858	1.537499	1.354955
O	-3.192842	-0.607443	-0.912409
C	-4.672892	-1.274362	0.824350
C	-3.414368	-2.153426	0.858570
H	-4.990860	-0.962433	1.826407
H	-3.638619	-3.205344	1.049630
H	-2.723030	-1.803880	1.633208
O	-5.760458	-1.896935	0.134112
H	-6.063058	-2.659398	0.654652
N	-1.340273	-2.034748	-0.636596
C	-0.814848	-3.292390	-0.742380
O	-1.476971	-4.324733	-0.646450
N	0.558686	-3.357590	-1.008320
H	0.902810	-4.302591	-1.156621
C	-4.209582	-0.084345	-0.030236
H	-5.020710	0.285713	-0.663585
C	-0.490842	-0.887362	-0.547173
H	-1.081527	-0.014630	-0.819082
O	0.113537	-0.698761	0.760764
C	2.542447	-0.955322	0.925507
C	3.782065	-1.227512	0.330124
C	2.360450	-1.264985	2.283155
C	4.813593	-1.806010	1.074458
H	3.946166	-0.998817	-0.715816
C	3.393894	-1.838585	3.028477
H	1.403694	-1.063656	2.754346
C	4.625901	-2.112094	2.425952
H	5.765452	-2.018029	0.593903
H	3.233414	-2.073403	4.077692

H	5.206255	-1.631240	3.727661	H	5.430321	-2.561812	3.002363
C	-2.834448	-1.920511	-0.542705	C	-2.815997	-1.927097	-0.536378
H	-3.312867	-2.614893	-1.239872	H	-3.220916	-2.641127	-1.258143
C	1.328160	-2.704572	-1.253805	C	1.377037	-2.338645	-1.470329
O	2.441762	-3.171179	-1.695805	O	2.434546	-2.605348	-2.031018
C	0.947969	-1.265206	-1.231151	C	0.881171	-0.923381	-1.246113
C	1.219291	-0.616099	-2.592742	C	1.021965	-0.116259	-2.534381
H	2.284484	-0.659328	-2.836528	H	2.061135	-0.094167	-2.872022
H	0.680577	-1.169759	-3.370037	H	0.418757	-0.575068	-3.326927
H	0.887420	0.426011	-2.639940	H	0.673880	0.909120	-2.394961
C	1.360843	-0.369584	0.120804	C	1.391127	-0.293759	0.174312
C	1.387568	1.133773	-0.167049	C	1.484335	1.229468	0.206561
C	0.269260	1.897703	0.109335	C	0.267187	1.996742	0.492534
C	2.487230	1.804786	-0.826800	C	2.555557	2.021846	-0.486834
C	0.097301	3.214630	-0.360979	C	-0.087462	3.036806	-0.311402
H	-0.530939	1.397925	0.633949	H	-0.387347	1.638850	1.279473
C	2.364845	3.161744	-1.242812	C	2.194991	3.075392	-1.308215
C	1.186386	3.841703	-1.036013	C	0.852976	3.507059	-1.334098
H	3.191400	3.652409	-1.740761	H	2.940078	3.624618	-1.875993
H	1.092885	4.857880	-1.400138	H	0.553518	4.300746	-2.010947
C	-2.215915	3.114625	0.624050	C	-2.378760	3.011128	0.706011
O	-2.415779	3.323784	1.804897	O	-2.587229	3.241339	1.883766
C	-1.242495	3.924661	-0.237073	C	-1.414125	3.784500	-0.182400
H	-1.662394	3.963553	-1.253253	H	-1.858260	3.820888	-1.186550
C	-1.118247	5.365974	0.299619	C	-1.224349	5.226269	0.327153
H	-0.663441	5.375420	1.293557	H	-0.800824	5.228756	1.335730
H	-0.515079	5.981944	-0.371372	H	-0.548799	5.776090	-0.334553
H	-2.111186	5.819116	0.367767	H	-2.183399	5.754641	0.351126
O	3.564024	1.076477	-1.028726	O	3.816578	1.676809	-0.159550
C	4.743444	1.608914	-1.683451	C	4.907633	2.434272	-0.705092
H	4.491814	1.923335	-2.698101	H	5.810498	1.992165	-0.284236
H	5.143132	2.439198	-1.098160	H	4.923641	2.351135	-1.796709
H	5.446348	0.779245	-1.701558	H	4.827609	3.485610	-0.409022

HH-4-S₀

C	3.285171	-4.010466	1.190831
H	2.971701	-4.974921	0.780766
H	4.339514	-4.085897	1.475811
H	2.696861	-3.807852	2.090559

HH-4-S_{1,min}

C	4.146132	-2.147177	2.052315
H	4.222670	-3.229084	1.913548
H	5.066840	-1.784646	2.517027
H	3.310930	-1.937590	2.726996

O	3.842301	-0.703963	-0.340247	O	3.406625	0.655256	-0.251697
C	4.100083	0.685372	-0.023763	C	3.106782	2.072646	-0.214974
H	3.913130	0.855963	1.037723	H	2.810153	2.347900	0.799888
H	5.150400	0.890342	-0.249676	H	4.002947	2.632999	-0.497832
O	1.828259	1.197721	-0.620034	O	0.849845	1.516189	-0.849586
C	3.326115	3.060579	-0.635498	C	1.498052	3.784469	-1.252542
C	1.903105	3.475403	-0.204110	C	0.034829	3.690680	-0.774231
H	4.056624	3.282122	0.151261	H	2.087290	4.431974	-0.592904
H	1.652457	4.484421	-0.534428	H	-0.597829	4.453746	-1.230047
H	1.807782	3.426229	0.882491	H	-0.011567	3.799498	0.311116
O	3.746420	3.662948	-1.864195	O	1.624494	4.234048	-2.605419
H	3.940453	4.600148	-1.699043	H	1.422958	5.183813	-2.636497
N	-0.302131	2.104056	-0.373645	N	-1.446757	1.568610	-0.528530
C	-1.066190	3.087802	0.207619	C	-2.460854	2.222020	0.126428
O	-0.637565	4.121879	0.706902	O	-2.496034	3.424115	0.364296
N	-2.456757	2.866607	0.219203	N	-3.536815	1.420208	0.555615
H	-2.974969	3.578756	0.727633	H	-4.210870	1.921710	1.128367
C	3.198836	1.538035	-0.896438	C	1.989728	2.315469	-1.215740
H	3.408848	1.347407	-1.956987	H	2.320230	2.029649	-2.222137
C	-0.910167	0.898018	-0.911264	C	-1.517468	0.153205	-0.814051
H	-0.295778	0.557903	-1.743693	H	-1.059156	-0.025398	-1.786999
O	-2.613718	-0.359623	-0.706652	O	-2.231727	-1.721472	-0.127968
C	3.087818	-2.899661	0.142477	C	3.956353	-1.453906	0.685962
H	3.688279	-3.137599	-0.744469	H	4.819364	-1.695334	0.052786
C	1.626461	-2.803480	-0.306148	C	2.704388	-1.914530	-0.018069
C	0.806791	-1.722277	0.030222	C	1.443042	-1.460309	0.448274
C	1.076825	-3.847559	-1.064871	C	2.764669	-2.763131	-1.149836
C	-0.546370	-1.644427	-0.331990	C	0.258439	-1.689443	-0.228533
H	1.229421	-0.884133	0.566913	H	1.426986	-0.852361	1.343484
C	-0.264391	-3.818239	-1.426670	C	1.604221	-3.065085	-1.818086
H	1.689444	-4.692429	-1.366290	H	3.719821	-3.146389	-1.494376
C	-1.062963	-2.740737	-1.034984	C	0.357270	-2.508754	-1.401143
H	-0.704874	-4.635146	-1.989012	H	1.605831	-3.701772	-2.695815
C	-1.324183	-0.362883	-0.019971	C	-1.020209	-0.976325	0.205617
C	-1.492099	-0.145716	1.482307	C	-1.030097	-0.612526	1.691320
C	-2.685739	-0.547402	2.100505	C	-1.691602	-1.466613	2.587664
C	-0.471050	0.407781	2.270097	C	-0.379736	0.525028	2.195218
C	-2.855237	-0.398715	3.479335	C	-1.706471	-1.187340	3.956451
H	-3.480996	-0.973428	1.498285	H	-2.204178	-2.344828	2.209622
C	-0.643726	0.557247	3.649595	C	-0.401507	0.806534	3.564755
H	0.457393	0.738537	1.817189	H	0.152097	1.189219	1.523541

C	-1.834904	0.154387	4.259471	C	-1.064928	-0.047151	4.450050
H	-3.786341	-0.715112	3.942303	H	-2.223988	-1.860083	4.635242
H	0.154888	0.993864	4.243601	H	0.103798	1.694420	3.935612
H	-1.967687	0.272367	5.331631	H	-1.081267	0.173253	5.514074
C	1.059088	2.379155	-0.855332	C	-0.329358	2.263368	-1.179956
H	0.995153	2.544627	-1.942797	H	-0.493208	2.200050	-2.266556
C	-3.200372	1.972778	-0.513628	C	-3.822011	0.103338	0.274593
O	-4.423320	1.993924	-0.508026	O	-4.792935	-0.463595	0.755231
C	-2.394573	0.943557	-1.311007	C	-2.874363	-0.561235	-0.728263
C	-2.755611	0.978302	-2.783842	C	-3.627583	-0.885285	-2.007170
H	-2.211731	0.194074	-3.317990	H	-2.951887	-1.338547	-2.735173
H	-3.830780	0.821500	-2.911859	H	-4.448608	-1.574646	-1.786022
H	-2.492402	1.949376	-3.218715	H	-4.053803	0.029193	-2.436236
C	3.594430	-1.561354	0.670025	C	3.948828	0.079359	0.834261
O	3.734845	-1.283968	1.846681	O	4.371469	0.688567	1.794697
N	-2.497423	-2.895429	-1.346921	N	-0.752246	-2.778160	-2.248464
O	-3.275720	-3.001523	-0.400374	O	-1.158479	-4.010268	-2.282496
O	-2.820940	-2.998737	-2.531491	O	-0.686270	-2.039739	-3.334924

HH-4-T_{1,min}

C	-3.831181	3.011591	1.750542
H	-3.707944	4.068115	1.493001
H	-4.839360	2.867491	2.151167
H	-3.109394	2.759577	2.533675
O	-3.752925	-0.073340	-0.326639
C	-3.682865	-1.514468	-0.217314
H	-3.468298	-1.790166	0.817009
H	-4.652793	-1.926102	-0.512007
O	-1.337794	-1.432827	-0.757058
C	-2.404954	-3.533541	-1.171561
C	-0.944888	-3.718732	-0.708510
H	-3.100511	-4.038782	-0.491309
H	-0.471292	-4.585377	-1.172884
H	-0.907633	-3.837198	0.375678
O	-2.638298	-3.978261	-2.512416
H	-2.636773	-4.949469	-2.521131
N	0.923371	-1.917013	-0.504557
C	1.806441	-2.765103	0.115678
O	1.576647	-3.924520	0.441082

HT-4-S₀

O	-2.752530	2.267502	-0.028634
C	-3.537426	1.355232	0.777300
H	-2.884210	0.912973	1.535216
H	-4.329673	1.915046	1.283411
O	-3.167174	-0.383677	-0.931212
C	-4.839897	-0.803909	0.706613
C	-3.737928	-1.867623	0.812252
H	-5.159742	-0.439317	1.689787
H	-4.133934	-2.869565	0.988720
H	-3.046696	-1.622337	1.626036
O	-5.972049	-1.256610	-0.042359
H	-6.422534	-1.952306	0.464437
N	-1.579287	-2.081306	-0.541642
C	-1.237061	-3.394918	-0.401830
O	-2.045717	-4.299619	-0.208715
N	0.130867	-3.686715	-0.519770
H	0.343009	-4.679418	-0.461367
C	-4.158140	0.294393	-0.124992
H	-4.869048	0.757554	-0.815075

N	3.080975	-2.233733	0.396367	C	-0.582059	-1.068094	-0.631078
H	3.669477	-2.861200	0.938512	H	-1.023863	-0.214138	-1.141104
C	-2.598626	-1.995385	-1.163931	O	-0.031989	-0.663020	0.649708
H	-2.824120	-1.669283	-2.187747	C	2.325071	-0.833764	1.135613
C	1.294296	-0.557942	-0.852835	C	3.389769	-1.730506	0.982422
H	0.775130	-0.299362	-1.775949	C	2.151601	-0.202221	2.382202
O	2.538718	1.068908	-0.297371	C	4.254086	-1.993594	2.052352
C	-3.615402	2.143157	0.499593	H	3.554084	-2.225686	0.036160
H	-4.358627	2.423329	-0.257772	C	3.012616	-0.466530	3.447323
C	-2.234082	2.354309	-0.113919	H	1.332459	0.497072	2.523371
C	-1.138525	1.597329	0.314157	C	4.071684	-1.366832	3.285992
C	-2.036018	3.320119	-1.108155	H	5.073946	-2.693313	1.911212
C	0.142873	1.717909	-0.236977	H	2.856324	0.031432	4.400720
H	-1.295165	0.849363	1.080546	H	4.745689	-1.574601	4.112955
C	-0.768380	3.515044	-1.641649	C	-3.030140	-1.745572	-0.543307
H	-2.865917	3.926568	-1.460660	H	-3.497719	-2.387893	-1.295502
C	0.308469	2.723287	-1.215187	C	1.146878	-2.886041	-1.007360
H	-0.594422	4.275500	-2.394660	O	2.215662	-3.383437	-1.336004
C	1.202373	0.682249	0.151471	C	0.822174	-1.401959	-1.169992
C	1.220794	0.381207	1.649600	C	1.078189	-1.004403	-2.625161
C	2.117152	1.091897	2.463539	H	2.096611	-1.244847	-2.929249
C	0.359745	-0.552614	2.246485	H	0.383149	-1.552344	-3.273104
C	2.150826	0.875799	3.842959	H	0.901349	0.063572	-2.776639
H	2.795663	1.808737	2.012481	C	1.299184	-0.467926	0.061880
C	0.398128	-0.771257	3.627613	C	1.425409	1.027125	-0.357218
H	-0.342437	-1.114796	1.640782	C	0.315273	1.839733	-0.099534
C	1.292138	-0.058965	4.430676	C	2.528044	1.681391	-0.946152
H	2.851130	1.436161	4.456900	C	0.216945	3.187211	-0.463865
H	-0.273257	-1.501907	4.071160	H	-0.512303	1.364073	0.403051
H	1.320828	-0.230656	5.503424	C	2.482388	3.038536	-1.285715
C	-0.326861	-2.381383	-1.116171	C	1.329011	3.783744	-1.073578
H	-0.185088	-2.345484	-2.207900	H	3.352235	3.493645	-1.743526
C	3.664853	-1.072408	-0.049228	H	1.310218	4.821024	-1.389526
O	4.812375	-0.770742	0.248065	C	-2.043814	3.194822	0.650297
C	2.785757	-0.203919	-0.953518	O	-2.141657	3.355881	1.852302
C	3.417607	-0.054037	-2.326329	C	-1.087742	3.969621	-0.255842
H	2.800882	0.593085	-2.955412	H	-1.571424	4.043274	-1.239137
H	4.416771	0.382103	-2.233898	C	-0.869577	5.389004	0.297692
H	3.510523	-1.032733	-2.811038	H	-0.355122	5.360221	1.262467
C	-3.845743	0.661431	0.798851	H	-0.277474	5.989904	-0.397106
O	-4.062864	0.192375	1.900502	H	-1.832177	5.891517	0.434308

N	1.579969	2.991333	-1.836653
O	2.498604	3.684026	-1.201726
O	1.615395	3.426247	-3.066107

N	3.778823	0.992409	-1.260679
O	4.812180	1.664997	-1.357669
O	3.746622	-0.229240	-1.421639

HT-4-S_{1,min}

O	-2.778484	2.216351	-0.003257
C	-3.606609	1.300199	0.758108
H	-2.990731	0.855199	1.544893
H	-4.420153	1.860875	1.227383
O	-3.167976	-0.422152	-0.954455
C	-4.886690	-0.866809	0.626942
C	-3.776868	-1.919396	0.765374
H	-5.244229	-0.511282	1.600480
H	-4.168092	-2.926663	0.921477
H	-3.117894	-1.672648	1.605034
O	-5.986111	-1.326680	-0.164094
H	-6.446664	-2.030693	0.321730
N	-1.566642	-2.092876	-0.510719
C	-1.203055	-3.406072	-0.401235
O	-2.000339	-4.326765	-0.246791
N	0.172090	-3.670231	-0.497207
H	0.406959	-4.657389	-0.431338
C	-4.187543	0.243312	-0.174982
H	-4.878946	0.706730	-0.884140
C	-0.587377	-1.066241	-0.567586
H	-1.040911	-0.198425	-1.041722
O	-0.027541	-0.691893	0.729331
C	2.379343	-0.843140	1.104766
C	3.619057	-1.365271	0.704610
C	2.130791	-0.634844	2.475866
C	4.577243	-1.703009	1.660069
H	3.832713	-1.519672	-0.345282
C	3.094406	-0.965665	3.427024
H	1.176193	-0.228398	2.794178
C	4.322130	-1.503233	3.022179
H	5.528370	-2.118760	1.339149
H	2.887347	-0.806607	4.481617
H	5.075539	-1.761106	3.761475
C	-3.022876	-1.782056	-0.563257

HT-4-T_{1,min}

O	-2.900895	2.151901	-0.014768
C	-3.609452	1.224373	0.841612
H	-2.911618	0.852282	1.597618
H	-4.423103	1.749978	1.350419
O	-3.191648	-0.524083	-0.849814
C	-4.720436	-1.036674	0.902404
C	-3.533269	-2.009934	0.947530
H	-4.995426	-0.671021	1.898767
H	-3.835617	-3.034461	1.175699
H	-2.802951	-1.689894	1.699057
O	-5.864433	-1.595277	0.250104
H	-6.221202	-2.308608	0.804905
N	-1.482372	-2.120492	-0.576312
C	-1.061302	-3.419384	-0.603076
O	-1.801967	-4.387061	-0.453454
N	0.307347	-3.611397	-0.853089
H	0.574282	-4.589310	-0.934085
C	-4.187344	0.090165	0.000351
H	-4.977010	0.470335	-0.653959
C	-0.554765	-1.043413	-0.596339
H	-1.073452	-0.174655	-0.993308
O	0.031113	-0.727831	0.704867
C	2.442166	-0.756468	1.040118
C	2.993268	-2.061773	1.182527
C	2.759824	0.201434	2.051049
C	3.846981	-2.364014	2.231339
H	2.789828	-2.828570	0.451746
C	3.610103	-0.109677	3.100466
H	2.322617	1.192342	2.000498
C	4.164902	-1.394222	3.196095
H	4.271184	-3.360899	2.304653
H	3.838639	0.641758	3.850129
H	4.834079	-1.640153	4.015461
C	-2.943399	-1.870595	-0.460535

H	-3.450407	-2.430404	-1.333452	H	-3.427739	-2.553172	-1.164146
C	1.185735	-2.837536	-0.933034	C	1.244611	-2.695066	-1.291484
O	2.290258	-3.289625	-1.199118	O	2.315635	-3.078145	-1.745683
C	0.818378	-1.366569	-1.115940	C	0.841064	-1.226717	-1.225277
C	1.095872	-0.955867	-2.560571	C	1.058852	-0.625593	-2.616940
H	2.155713	-1.048519	-2.801604	H	2.119014	-0.643743	-2.880490
H	0.519937	-1.596592	-3.238303	H	0.514356	-1.213583	-3.364335
H	0.789122	0.078399	-2.739162	H	0.692797	0.401631	-2.664937
C	1.278563	-0.454876	0.128438	C	1.310111	-0.388308	0.081184
C	1.370882	1.045907	-0.238861	C	1.340019	1.113240	-0.252465
C	0.286569	1.849421	0.092364	C	0.182310	1.863547	-0.052017
C	2.452920	1.680832	-0.937858	C	2.450461	1.773283	-0.829832
C	0.140107	3.170103	-0.364119	C	0.029844	3.190658	-0.470512
H	-0.501332	1.389831	0.669822	H	-0.633910	1.359649	0.443713
C	2.333471	3.022908	-1.383806	C	2.332881	3.115657	-1.247018
C	1.197356	3.750621	-1.126864	C	1.134668	3.801797	-1.088962
H	3.164152	3.455041	-1.930965	H	3.190311	3.600670	-1.698779
H	1.106610	4.763181	-1.503771	H	1.074728	4.823924	-1.448961
C	-2.141486	3.162257	0.715234	C	-2.236875	3.147013	0.616047
O	-2.323063	3.336116	1.904304	O	-2.341879	3.356962	1.810223
C	-1.139954	3.954838	-0.128727	C	-1.316302	3.919319	-0.327162
H	-1.596609	4.105810	-1.118252	H	-1.796804	3.912060	-1.314920
C	-0.876661	5.339492	0.504100	C	-1.180396	5.377374	0.144963
H	-0.396525	5.237191	1.480582	H	-0.679136	5.431678	1.115789
H	-0.239069	5.947680	-0.141703	H	-0.607364	5.965096	-0.576952
H	-1.825369	5.867228	0.635488	H	-2.168256	5.839851	0.239508
N	3.692011	1.023386	-1.187175	N	3.686637	1.148621	-0.969092
O	4.655681	1.505278	-0.446504	O	4.672905	1.640600	-1.619738
O	3.896305	0.664645	-2.424079	O	3.876085	-0.130372	-0.595241

HH-5-S₀

C	4.344469	-2.986608	0.322373
H	4.517817	-3.723293	-0.468493
H	5.249450	-2.916515	0.934549
H	3.527161	-3.346547	0.955476
O	3.628270	0.664381	0.204275
C	3.174972	1.750483	1.044995
H	2.746322	1.343758	1.963231
H	4.036312	2.378538	1.293556

HH-5-S_{1,min}

C	-4.186815	-3.115406	-0.216713
H	-4.347742	-3.820948	0.603989
H	-5.072139	-3.123828	-0.860443
H	-3.331966	-3.459279	-0.806368
O	-3.744166	0.567224	-0.291469
C	-3.286738	1.636398	-1.148923
H	-2.881740	1.216248	-2.071197
H	-4.147317	2.269933	-1.383932

O	1.027556	1.713491	-0.049876	O	-1.096155	1.620366	-0.136606
C	1.582400	3.767650	1.038441	C	-1.725703	3.691629	-1.151108
C	0.066603	3.483284	1.100133	C	-0.203298	3.450462	-1.236728
H	2.008956	3.846417	2.045309	H	-2.166367	3.775822	-2.152845
H	-0.525475	4.398633	1.056577	H	0.365562	4.380286	-1.187138
H	-0.178877	2.950247	2.020895	H	0.051452	2.932473	-2.161945
O	1.912166	4.940959	0.286570	O	-2.075821	4.825750	-0.360671
H	1.667625	5.722131	0.809386	H	-1.828363	5.619458	-0.861939
N	-1.293177	1.679691	-0.187967	N	1.227311	1.713420	0.063249
C	-2.465839	1.950495	0.466136	C	2.373846	1.981393	-0.664367
O	-2.618276	2.791946	1.346549	O	2.434392	2.731932	-1.641571
N	-3.582160	1.179952	0.081480	N	3.525850	1.367676	-0.216734
H	-4.403474	1.343980	0.657935	H	4.330595	1.545561	-0.805547
C	2.152692	2.553627	0.261029	C	-2.245985	2.440802	-0.392319
H	2.598965	2.919079	-0.673409	H	-2.669536	2.783283	0.561756
C	-1.223816	0.676222	-1.237456	C	1.225695	0.782141	1.167723
H	-0.504507	1.021323	-1.980431	H	0.531118	1.153604	1.924077
O	-2.063895	-1.151870	-1.915402	O	2.067283	-0.965941	2.013972
C	3.997829	-1.626760	-0.305814	C	-3.931047	-1.709194	0.346118
H	4.841320	-1.302710	-0.929873	H	-4.807723	-1.385191	0.920220
C	2.762707	-1.694565	-1.204810	C	-2.721809	-1.660515	1.280820
C	1.491901	-1.412090	-0.693487	C	-1.448593	-1.400697	0.766387
C	2.884038	-2.035652	-2.558596	C	-2.864942	-1.866790	2.657975
C	0.356410	-1.387022	-1.511916	C	-0.333438	-1.268265	1.599080
H	1.389989	-1.158935	0.355172	H	-1.331621	-1.259418	-0.300969
C	1.750797	-2.074178	-3.374670	C	-1.749435	-1.796052	3.493654
H	3.862354	-2.261992	-2.976883	H	-3.846740	-2.074683	3.076501
C	0.494571	-1.732341	-2.863910	C	-0.491648	-1.479360	2.975481
H	1.848556	-2.347002	-4.422373	H	-1.862665	-1.965653	4.561012
H	-0.374031	-1.726435	-3.513124	H	0.364629	-1.394279	3.634815
C	-0.973097	-0.873411	-0.968533	C	0.996346	-0.785017	1.029207
C	-1.320979	-1.409765	0.414921	C	1.369874	-1.431371	-0.296947
C	-2.152613	-2.535917	0.524477	C	2.212782	-2.553299	-0.301715
C	-0.806044	-0.850686	1.592758	C	0.853645	-0.981954	-1.520014
C	-2.457990	-3.081243	1.771399	C	2.529190	-3.201780	-1.492040
H	-2.567298	-2.982730	-0.373634	H	2.626045	-2.910509	0.635701
C	-1.119831	-1.400601	2.840460	C	1.180983	-1.635987	-2.711056
H	-0.156926	0.017096	1.547673	H	0.195282	-0.120574	-1.549876
C	-1.950834	-2.522223	2.956001	C	2.023056	-2.753225	-2.722505
H	-3.103929	-3.955499	1.824669	H	3.183851	-4.070243	-1.467298
H	-0.707419	-0.943330	3.737415	H	0.770803	-1.265378	-3.647608

C	-0.122950	2.563204	-0.106480	C	0.017473	2.520456	-0.044053
H	-0.084833	3.144339	-1.041782	H	-0.083741	3.092826	0.893252
C	-3.746989	0.355174	-1.005431	C	3.685028	0.427213	0.816154
O	-4.807622	-0.214161	-1.227155	O	4.911597	0.257080	1.250050
C	-2.524565	0.224590	-1.917641	C	2.555898	0.389839	1.854142
C	-2.841623	0.740230	-3.311018	C	2.930768	1.015150	3.187935
H	-1.971179	0.614260	-3.961196	H	2.079234	0.981896	3.874143
H	-3.688390	0.190464	-3.733254	H	3.768371	0.475655	3.638133
H	-3.102561	1.804443	-3.275583	H	3.230993	2.058163	3.043841
C	3.819737	-0.548424	0.762850	C	-3.735744	-0.692953	-0.777560
O	3.822804	-0.742135	1.965194	O	-3.550678	-0.969737	-1.945868
C	-2.304693	-3.107079	4.304050	C	2.394094	-3.445655	-4.012620
H	-3.359109	-2.924865	4.549866	H	3.421538	-3.201228	-4.312778
H	-2.154551	-4.193227	4.319238	H	2.341620	-4.535581	-3.910585
H	-1.696518	-2.668380	5.101679	H	1.731933	-3.147264	-4.831330

HH-5- $T_{1,min}$

C	-3.819417	-3.431860	0.408937
H	-3.910992	-3.965710	1.360230
H	-4.703674	-3.652917	-0.198421
H	-2.942016	-3.814682	-0.119679
O	-3.768825	0.194132	-0.378533
C	-3.368880	1.158424	-1.378713
H	-2.899961	0.642520	-2.218690
H	-4.270911	1.673952	-1.720856
O	-1.228678	1.458802	-0.306816
C	-1.957303	3.292558	-1.661181
C	-0.424869	3.130048	-1.700952
H	-2.388352	3.202164	-2.665151
H	0.090757	4.087728	-1.796122
H	-0.138804	2.492511	-2.538227
O	-2.387776	4.522274	-1.065873
H	-2.210126	5.245516	-1.689240
N	1.093080	1.687364	-0.154839
C	2.201667	1.853174	-0.945257
O	2.233642	2.417729	-2.034647
N	3.405903	1.330090	-0.434803
H	4.187637	1.417970	-1.078892
C	-2.421054	2.147884	-0.724334

HT-5- S_0

O	-3.239755	1.574489	0.206881
C	-3.609176	0.496243	1.099182
H	-2.763956	0.291693	1.763019
H	-4.460312	0.811711	1.710447
O	-2.971943	-1.131643	-0.647836
C	-4.208123	-1.947998	1.212244
C	-2.835932	-2.635291	1.165170
H	-4.487954	-1.649466	2.229386
H	-2.889280	-3.700366	1.400512
H	-2.145850	-2.160972	1.871629
O	-5.243422	-2.747381	0.632057
H	-5.387409	-3.525349	1.195806
N	-0.916093	-2.274421	-0.485965
C	-0.189679	-3.430487	-0.462008
O	-0.661542	-4.533583	-0.194191
N	1.169915	-3.304764	-0.786549
H	1.680788	-4.183478	-0.769193
C	-4.000016	-0.735790	0.288990
H	-4.902372	-0.532014	-0.294604
C	-0.276478	-1.016541	-0.675665
H	-1.023598	-0.316676	-1.042445
O	0.371369	-0.481075	0.515697

H	-2.903217	2.596675	0.154359	C	-2.385850	-2.375268	-0.277750
C	1.158403	0.950768	1.093442	H	-2.740805	-3.160587	-0.951387
H	0.418858	1.376091	1.772641	C	1.828247	-2.232209	-1.362853
O	2.229527	-0.599268	2.091723	O	2.964656	-2.365049	-1.797585
C	-3.709602	-1.925147	0.671584	C	1.037997	-0.933905	-1.466014
H	-4.619055	-1.583741	1.179453	C	0.960887	-0.505341	-2.930697
C	-2.511461	-1.517513	1.528616	H	1.959314	-0.337822	-3.344121
C	-1.239663	-1.834525	1.174529	H	0.478090	-1.290728	-3.524113
C	-2.748441	-0.704252	2.731410	H	0.375851	0.410555	-3.038442
C	-0.104619	-1.238033	1.895736	C	1.426649	0.114974	-0.305099
H	-1.045976	-2.439159	0.293828	C	1.017830	1.553663	-0.681592
C	-1.671479	-0.420578	3.624070	C	-0.212441	2.031321	-0.214596
H	-3.766457	-0.440911	3.000212	C	1.770407	2.373588	-1.531853
C	-0.390280	-0.750073	3.287642	C	-0.756495	3.251332	-0.628359
H	-1.893796	-0.005916	4.605473	H	-0.757913	1.398041	0.470306
H	0.425205	-0.658666	3.997631	C	1.260601	3.614115	-1.927962
C	1.070727	-0.660105	1.168932	C	0.000679	4.045544	-1.501943
C	1.429148	-1.407255	-0.107994	H	1.843426	4.242156	-2.596696
C	2.465669	-2.349924	-0.100324	H	-0.385155	4.995402	-1.861496
C	0.712434	-1.213255	-1.298697	C	-2.751742	2.685838	0.804574
C	2.782186	-3.072413	-1.254325	O	-2.752485	2.835622	2.012887
H	3.030777	-2.515316	0.811446	C	-2.168355	3.681632	-0.195198
C	1.037290	-1.935612	-2.449084	H	-2.806717	3.643473	-1.088024
H	-0.106253	-0.501469	-1.327612	C	-2.214157	5.105483	0.386495
C	2.079798	-2.875655	-2.451820	H	-1.579757	5.186460	1.274100
H	3.589829	-3.800740	-1.219764	H	-1.868895	5.831864	-0.354176
H	0.465983	-1.765672	-3.359629	H	-3.237917	5.373310	0.667916
C	-0.161186	2.412568	-0.376465	C	2.771352	0.044302	0.393562
H	-0.271872	3.117796	0.462346	C	2.815902	-0.095110	1.786354
C	3.696903	0.860741	0.823545	C	3.984418	0.171940	-0.301102
O	4.831701	0.520137	1.134140	C	4.038692	-0.098407	2.465741
C	2.515649	0.794224	1.792861	H	1.891763	-0.203792	2.345026
C	2.796374	1.614512	3.040405	C	5.200181	0.166438	0.382432
H	1.955463	1.537833	3.735473	H	3.993651	0.249503	-1.383336
H	3.702762	1.250387	3.533836	C	5.252758	0.034013	1.779855
H	2.943818	2.669550	2.781855	H	4.042965	-0.206778	3.548268
C	-3.596308	-1.122167	-0.624958	H	6.125187	0.260036	-0.183080
O	-3.339161	-1.581999	-1.722221	C	6.577268	0.021267	2.508154
C	2.442245	-3.633378	-3.708460	H	6.434943	-0.004206	3.593336
H	3.068660	-3.021127	-4.371177	H	7.176148	-0.854818	2.227718
H	3.002702	-4.545317	-3.477200	H	7.174274	0.908895	2.265262

H	1.549103	-3.914941	-4.277666	H	2.737174	2.055130	-1.907663
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HT-5-S_{1,min}

O	-3.196349	1.610446	0.154241
C	-3.572884	0.543339	1.058531
H	-2.721233	0.334558	1.713097
H	-4.410976	0.877569	1.677547
O	-2.994024	-1.118880	-0.680137
C	-4.180787	-1.883504	1.233442
C	-2.815796	-2.579305	1.162553
H	-4.429280	-1.553566	2.249710
H	-2.861183	-3.636489	1.431534
H	-2.101954	-2.087823	1.833261
O	-5.243356	-2.688400	0.709549
H	-5.286640	-3.514619	1.218877
N	-0.957534	-2.305590	-0.586104
C	-0.215454	-3.476409	-0.420755
O	-0.744366	-4.544054	-0.034873
N	1.100359	-3.357259	-0.734262
H	1.631882	-4.217590	-0.665213
C	-3.990920	-0.697207	0.272962
H	-4.909626	-0.496398	-0.286657
C	-0.304713	-1.067705	-0.763307
H	-1.032946	-0.344915	-1.122466
O	0.333111	-0.510300	0.464897
C	-2.406745	-2.368780	-0.302028
H	-2.818020	-3.162488	-0.933240
C	1.757242	-2.306316	-1.461005
O	3.005374	-2.466368	-1.744819
C	1.033637	-0.996085	-1.523293
C	0.980708	-0.446717	-2.949444
H	1.988874	-0.358601	-3.367869
H	0.420606	-1.145117	-3.582349
H	0.491364	0.530774	-3.004609
C	1.393283	0.060404	-0.326609
C	1.080464	1.539113	-0.626347
C	-0.152148	2.042255	-0.176877
C	1.895506	2.365638	-1.425303
C	-0.659802	3.266610	-0.609193

HT-5-T_{1,min}

O	3.420744	1.193036	-0.196807
C	3.748169	0.100281	-1.083118
H	2.924524	-0.020664	-1.793624
H	4.656291	0.339917	-1.644368
O	2.925879	-1.389452	0.704148
C	3.973198	-2.404159	-1.172537
C	2.504406	-2.847336	-1.103626
H	4.289794	-2.164625	-2.194708
H	2.369957	-3.906377	-1.336424
H	1.894250	-2.262485	-1.800727
O	4.864359	-3.360987	-0.592049
H	4.872534	-4.157019	-1.148965
N	0.709070	-2.173224	0.592596
C	-0.161146	-3.209367	0.792605
O	0.137048	-4.394500	0.653597
N	-1.450067	-2.849379	1.205364
H	-2.058440	-3.641496	1.394633
C	3.975905	-1.165990	-0.261620
H	4.912545	-1.090597	0.297888
C	0.247266	-0.820973	0.575385
H	1.105811	-0.175212	0.751652
O	-0.428869	-0.433857	-0.654726
C	2.129815	-2.515105	0.346575
H	2.358969	-3.350597	1.012611
C	-1.869328	-1.629039	1.711867
O	-2.915279	-1.551486	2.346914
C	-0.969947	-0.441166	1.434760
C	-0.706051	0.328820	2.725241
H	-1.642578	0.652668	3.186062
H	-0.180075	-0.313891	3.441272
H	-0.083678	1.206158	2.537153
C	-1.414920	0.356620	0.079184
C	-1.031685	1.822164	0.023078
C	0.355826	2.177610	-0.358507
C	-1.792041	2.875883	0.751128
C	1.057132	3.060369	0.398673

H	-0.732975	1.400421	0.468957	H	0.803979	1.657129	-1.197982
C	1.428223	3.622431	-1.812422	C	-1.087925	3.774159	1.492117
C	0.154831	4.064430	-1.436069	C	0.352008	3.790155	1.449612
H	2.049443	4.253922	-2.441497	H	-1.603214	4.524842	2.087997
H	-0.199308	5.025400	-1.796894	H	0.902664	4.461853	2.100538
C	-2.709956	2.725794	0.743409	C	3.150147	2.374032	-0.793258
O	-2.728809	2.896809	1.948834	O	3.338627	2.574529	-1.979611
C	-2.093353	3.698659	-0.259766	C	2.538324	3.375625	0.177904
H	-2.685021	3.623349	-1.181842	H	3.041171	3.236060	1.144711
C	-2.182749	5.139745	0.272319	C	2.770007	4.821274	-0.298641
H	-1.603932	5.253971	1.193464	H	2.298016	4.990275	-1.270921
H	-1.802115	5.848121	-0.468240	H	2.347932	5.530224	0.419754
H	-3.224079	5.404124	0.483364	H	3.841300	5.029110	-0.391414
C	2.708783	0.032039	0.385790	C	-2.815645	0.156411	-0.481154
C	2.721265	0.076971	1.814474	C	-2.972697	-0.314671	-1.791741
C	3.953245	0.013547	-0.317047	C	-3.966289	0.485294	0.252412
C	3.910769	0.047057	2.500899	C	-4.246239	-0.455581	-2.350860
H	1.776142	0.107852	2.343631	H	-2.096301	-0.576955	-2.375684
C	5.138865	-0.007457	0.376746	C	-5.233813	0.339779	-0.311312
H	3.953257	-0.038672	-1.397144	H	-3.881623	0.833991	1.276746
C	5.153462	0.007349	1.801801	C	-5.400081	-0.131926	-1.624163
H	3.917546	0.059110	3.585936	H	-4.339824	-0.823452	-3.370420
H	6.082296	-0.045266	-0.158590	H	-6.109513	0.594544	0.282232
C	6.445227	-0.036157	2.540888	C	-6.779262	-0.300829	-2.218535
H	6.333467	0.261127	3.586005	H	-6.729610	-0.477369	-3.297875
H	6.834908	-1.066474	2.523081	H	-7.303002	-1.153066	-1.765623
H	7.203012	0.587761	2.054516	H	-7.400101	0.586251	-2.045852
H	2.862842	2.027456	-1.781445	H	-2.875682	2.916736	0.695082

HH-6-S₀

C	3.582232	3.873516	0.268263
H	3.687554	4.408506	1.217389
H	4.382592	4.199656	-0.403791
H	2.622369	4.150956	-0.179102
O	3.746469	0.251947	-0.578999
C	3.441076	-0.664891	-1.655236
H	2.806862	-0.163484	-2.389116
H	4.379630	-0.964921	-2.131828
O	1.519485	-1.461076	-0.436903

HH-6-S_{1,min}

C	3.790793	3.604873	0.413885
H	3.923266	4.102589	1.378287
H	4.599949	3.917134	-0.251610
H	2.843038	3.938326	-0.018157
O	3.696923	0.028199	-0.541891
C	3.313886	-0.814939	-1.638376
H	2.698759	-0.245766	-2.337857
H	4.216661	-1.159746	-2.150122
O	1.352377	-1.529486	-0.449921

C	2.364123	-2.956799	-2.098429	C	2.119230	-3.014589	-2.139580
C	0.830983	-3.069019	-1.959204	C	0.591465	-3.052708	-2.006058
H	2.646093	-2.663628	-3.116551	H	2.422184	-2.707603	-3.146445
H	0.476324	-4.086634	-2.129141	H	0.187690	-4.044963	-2.201428
H	0.338619	-2.402665	-2.670347	H	0.130639	-2.345413	-2.698193
O	3.058345	-4.156182	-1.737284	O	2.742825	-4.252992	-1.812199
H	2.926002	-4.813909	-2.439699	H	2.577780	-4.886867	-2.526790
N	-0.701397	-2.067529	-0.112900	N	-0.893834	-2.010436	-0.172798
C	-1.863565	-2.462662	-0.720990	C	-2.063317	-2.457799	-0.736944
O	-1.946079	-3.066030	-1.786509	O	-2.126747	-3.145684	-1.755848
N	-3.057995	-2.133081	-0.048092	N	-3.230553	-2.112570	-0.097443
H	-3.895505	-2.355174	-0.580059	H	-4.069871	-2.383312	-0.595415
C	2.749693	-1.876021	-1.055599	C	2.554577	-1.992258	-1.071272
H	3.395204	-2.340255	-0.298128	H	3.170168	-2.511683	-0.326472
C	-0.709523	-1.379763	1.168121	C	-0.874958	-1.345649	1.111767
H	0.169843	-1.704028	1.724892	H	-0.072343	-1.781097	1.710532
O	-1.836702	-0.062350	2.393566	O	-1.832826	0.047776	2.362604
C	3.656607	2.358269	0.518473	C	3.796829	2.088108	0.611717
H	4.633723	2.122927	0.961182	H	4.761006	1.789514	1.041044
C	2.583427	1.871645	1.492826	C	2.703324	1.617297	1.559767
C	1.349335	1.410602	1.022754	C	1.447322	1.271385	1.066503
C	2.820553	1.873867	2.873925	C	2.941002	1.512975	2.929637
C	0.381625	0.882878	1.885895	C	0.452284	0.758637	1.894494
H	1.156163	1.418039	-0.043462	H	1.254115	1.359924	0.004097
C	1.839916	1.407609	3.752950	C	1.937709	1.053009	3.777602
H	3.772215	2.230566	3.261721	H	3.913538	1.781573	3.334008
C	0.633915	0.894299	3.265314	C	0.704800	0.658782	3.264527
H	2.025004	1.418874	4.824081	H	2.124102	0.978722	4.844914
H	-0.106092	0.497932	3.951778	H	-0.060805	0.271964	3.927033
C	-0.860170	0.197690	1.324333	C	-0.842168	0.220879	1.304916
C	-1.519363	0.951457	0.176321	C	-1.405061	1.065994	0.178369
C	-2.598781	1.802097	0.442331	C	-2.366498	2.033369	0.460194
C	-1.059735	0.865024	-1.150193	C	-0.956164	0.945563	-1.141960
C	-3.212511	2.548753	-0.568762	C	-2.879003	2.865043	-0.533147
H	-2.978683	1.881226	1.455934	H	-2.736748	2.136754	1.474578
C	-1.662283	1.599490	-2.167885	C	-1.459896	1.763211	-2.142509
H	-0.225518	0.217903	-1.398219	H	-0.205062	0.206329	-1.395217
C	-2.743964	2.447551	-1.885458	C	-2.424903	2.728578	-1.845253
H	-4.046926	3.193387	-0.316876	H	-3.628163	3.602284	-0.271465
H	-1.304386	1.523554	-3.190859	H	-1.112904	1.664587	-3.166405
C	0.614707	-2.566196	-0.531380	C	0.393142	-2.574378	-0.573112

H	0.921322	-3.334408	0.196567	H	0.651986	-3.373195	0.139992
C	-3.245691	-1.676737	1.234639	C	-3.373500	-1.275410	1.020680
O	-4.364171	-1.476024	1.689644	O	-4.544818	-1.292262	1.587253
C	-1.965682	-1.466020	2.047551	C	-2.155298	-1.285017	1.964362
C	-1.949596	-2.378675	3.261994	C	-2.324888	-2.225340	3.138414
H	-1.046494	-2.196775	3.851672	H	-1.404914	-2.258885	3.727647
H	-2.829632	-2.193047	3.885408	H	-3.143654	-1.887844	3.778336
H	-1.960653	-3.429996	2.951226	H	-2.556165	-3.234834	2.785283
C	3.583778	1.573919	-0.791757	C	3.680640	1.356338	-0.716267
O	3.382964	2.058151	-1.891042	O	3.559692	1.885053	-1.801461
O	-3.269646	3.124283	-2.949684	O	-2.860948	3.482244	-2.891217
C	-4.373830	4.003928	-2.722537	C	-3.840579	4.481587	-2.643281
H	-4.619326	4.426128	-3.697702	H	-4.035670	4.953462	-3.605720
H	-5.239314	3.457098	-2.330348	H	-4.765815	4.039603	-2.258627
H	-4.100231	4.809821	-2.031543	H	-3.468500	5.231434	-1.937161

HH-6- $T_{1,min}$

C	3.005775	4.032205	1.110239
H	3.085259	4.329639	2.160726
H	3.716910	4.627328	0.527400
H	1.998092	4.270459	0.758446
O	3.749589	0.821562	-0.599074
C	3.473729	0.056886	-1.794467
H	2.782999	0.611219	-2.432615
H	4.421421	-0.090970	-2.320450
O	1.642884	-1.073023	-0.702843
C	2.605668	-2.240959	-2.556606
C	1.089371	-2.497475	-2.448113
H	2.859348	-1.788131	-3.522221
H	0.815573	-3.503805	-2.770691
H	0.544093	-1.773535	-3.054880
O	3.401313	-3.415039	-2.356039
H	3.327403	-3.976734	-3.145054
N	-0.509733	-1.952867	-0.468797
C	-1.639923	-2.230326	-1.194639
O	-1.679333	-2.510814	-2.388999
N	-2.854691	-2.195309	-0.482348
H	-3.670794	-2.340485	-1.071041
C	2.898866	-1.283799	-1.373153

HT-6- S_0

O	3.445930	1.592930	-0.298128
C	3.777659	0.521296	-1.212822
H	2.901488	0.313953	-1.834721
H	4.595759	0.844604	-1.863747
O	3.234344	-1.118084	0.554611
C	4.386842	-1.918356	-1.365365
C	3.022542	-2.614415	-1.257293
H	4.617010	-1.613519	-2.392994
H	3.070844	-3.678010	-1.500515
H	2.297021	-2.140965	-1.927847
O	5.453035	-2.713779	-0.838087
H	5.578450	-3.485939	-1.414170
N	1.180775	-2.273738	0.484309
C	0.461724	-3.434564	0.492415
O	0.928105	-4.534304	0.202189
N	-0.882117	-3.318009	0.879764
H	-1.386341	-4.200692	0.888474
C	4.214711	-0.711547	-0.427850
H	5.142214	-0.504109	0.113497
C	0.541500	-1.019992	0.700549
H	1.299777	-0.314903	1.032677
O	-0.162175	-0.490942	-0.461745

H	3.593210	-1.786463	-0.686708	C	2.639467	-2.363978	0.206530
C	-0.582492	-1.585165	0.933277	H	3.030689	-3.150029	0.858820
H	0.323671	-1.944471	1.422022	C	-1.519378	-2.250350	1.488064
O	-1.856575	-0.672533	2.378981	O	-2.630549	-2.393266	1.981196
C	3.315815	2.536771	0.972690	C	-0.736987	-0.944699	1.549043
H	4.341641	2.352341	1.312408	C	-0.598448	-0.507965	3.006855
C	2.385956	1.620341	1.766993	H	-1.579252	-0.342959	3.461487
C	1.039007	1.649532	1.598376	H	-0.086742	-1.287511	3.583467
C	2.981120	0.634798	2.683942	H	-0.014392	0.411605	3.084246
C	0.199168	0.605997	2.204794	C	-1.185972	0.097657	0.404105
H	0.581720	2.371533	0.928779	C	-0.773630	1.540133	0.760828
C	2.142474	-0.141931	3.537358	C	0.437945	2.025057	0.254732
H	4.059831	0.603649	2.799764	C	-1.507234	2.358382	1.628968
C	0.785352	-0.105718	3.391169	C	0.984248	3.251928	0.645167
H	2.593788	-0.704782	4.352274	H	0.967118	1.393418	-0.444217
H	0.123860	-0.585243	4.105321	C	-0.995657	3.604659	2.003806
C	-0.884067	-0.079351	1.429149	C	0.247368	4.044193	1.537634
C	-1.585016	0.821601	0.423294	H	-1.563249	4.231900	2.686276
C	-2.814603	1.407089	0.741328	H	0.635209	4.999363	1.880322
C	-1.007425	1.124816	-0.822508	C	2.925442	2.705577	-0.865370
C	-3.468888	2.266323	-0.149324	O	2.871734	2.864267	-2.071312
H	-3.280300	1.184802	1.696079	C	2.379750	3.689216	0.167095
C	-1.647404	1.974710	-1.719489	H	3.049756	3.639691	1.035854
H	-0.048105	0.695974	-1.093299	C	2.406456	5.120020	-0.398233
C	-2.884833	2.551330	-1.390134	H	1.739796	5.213231	-1.260615
H	-4.422194	2.696590	0.135645	H	2.091072	5.838089	0.363519
H	-1.199200	2.203040	-2.682524	H	3.419700	5.389443	-0.714121
C	0.841870	-2.232771	-0.962540	H	-2.460772	2.034072	2.033013
H	1.234413	-3.066988	-0.359719	C	-2.557929	0.015266	-0.235708
C	-3.077556	-2.132358	0.872063	C	-3.740106	0.101021	0.507142
O	-4.207963	-2.197003	1.339418	C	-2.660155	-0.085284	-1.633674
C	-1.827798	-1.977808	1.739617	C	-4.994481	0.093379	-0.112794
C	-1.720907	-3.118007	2.737873	H	-3.706775	0.148443	1.590558
H	-0.837010	-2.981328	3.367306	C	-3.900430	-0.093506	-2.264914
H	-2.611483	-3.148267	3.373105	H	-1.758973	-0.161240	-2.233596
H	-1.635593	-4.078037	2.215472	C	-5.078641	-0.000654	-1.508120
C	3.237010	2.065043	-0.480040	H	-5.885390	0.152714	0.501817
O	2.741387	2.688285	-1.400594	H	-3.972317	-0.172349	-3.346060
O	-3.434661	3.369792	-2.336367	O	-6.248707	-0.016445	-2.214630
C	-4.690261	3.993102	-2.054963	C	-7.481945	0.073422	-1.497152
H	-4.926801	4.590110	-2.936517	H	-8.266102	0.047376	-2.254755

H -5.475474 3.244530 -1.896727
H -4.618479 4.646185 -1.177289

H -7.603546 -0.775147 -0.813641
H -7.544379 1.013306 -0.936119

HT-6-S_{1,min}

O 3.612457 1.253859 -0.235229
C 3.818101 0.149624 -1.149442
H 2.923808 0.054191 -1.772834
H 4.669350 0.374253 -1.799092
O 3.109761 -1.420738 0.629634
C 4.069198 -2.337438 -1.343367
C 2.625213 -2.833313 -1.193968
H 4.305821 -2.043398 -2.373343
H 2.506156 -3.884212 -1.465435
H 1.950949 -2.239011 -1.820989
O 5.032778 -3.287495 -0.874033
H 4.959604 -4.094194 -1.410705
N 0.930395 -2.319345 0.664307
C 0.036081 -3.382895 0.594776
O 0.381657 -4.519344 0.205939
N -1.229310 -3.080188 1.000978
H -1.868416 -3.866993 1.019234
C 4.101177 -1.138949 -0.379424
H 5.068456 -1.070019 0.127534
C 0.449941 -0.994739 0.806062
H 1.285570 -0.364097 1.098857
O -0.156955 -0.431496 -0.422978
C 2.336583 -2.578054 0.291727
H 2.671751 -3.423771 0.899573
C -1.660490 -1.936251 1.750033
O -2.806003 -1.998010 2.326782
C -0.809536 -0.726258 1.644752
C -0.612630 -0.040332 2.993548
H -1.579575 0.200589 3.446638
H -0.087042 -0.718075 3.677524
H -0.028284 0.879991 2.906064
C -1.129436 0.319799 0.336455
C -0.665312 1.755933 0.518533
C 0.661317 2.056886 0.162787
C -1.424464 2.764724 1.141301

HT-6-T_{1,min}

O 3.632995 1.211106 -0.279930
C 3.934125 0.121838 -1.179873
H 3.086061 -0.001561 -1.860549
H 4.819929 0.368053 -1.773023
O 3.185976 -1.378104 0.631712
C 4.170581 -2.380951 -1.284836
C 2.708022 -2.833430 -1.163977
H 4.448216 -2.136513 -2.317146
H 2.571438 -3.892563 -1.395172
H 2.069687 -2.250377 -1.836893
O 5.088068 -3.333911 -0.740121
H 5.076763 -4.130406 -1.296361
N 0.971376 -2.175213 0.598416
C 0.114779 -3.217062 0.825463
O 0.414281 -4.399931 0.670612
N -1.160748 -2.866106 1.285170
H -1.757877 -3.662359 1.491944
C 4.198824 -1.145360 -0.370823
H 5.154689 -1.065883 0.154552
C 0.501568 -0.825630 0.603208
H 1.362103 -0.175585 0.751947
O -0.219397 -0.437824 -0.600796
C 2.384243 -2.507610 0.299856
H 2.642530 -3.343509 0.954641
C -1.569097 -1.649957 1.810097
O -2.592947 -1.580801 2.481485
C -0.686939 -0.456161 1.506142
C -0.380711 0.310918 2.789159
H -1.301520 0.629569 3.284057
H 0.173355 -0.331455 3.484059
H 0.230459 1.191721 2.581574
C -1.183690 0.343979 0.171432
C -0.811047 1.812545 0.107702
C 0.558443 2.178593 -0.324844
C -1.549283 2.855432 0.871830

C	1.282049	3.264182	0.486170	C	1.282476	3.065340	0.406485
H	1.212545	1.286264	-0.353223	H	0.978457	1.661996	-1.181062
C	-0.832474	3.996391	1.430210	C	-0.823808	3.759954	1.583997
C	0.513915	4.247857	1.133239	C	0.613293	3.790105	1.483042
H	-1.422942	4.769277	1.916183	H	-1.321328	4.503539	2.203420
H	0.947608	5.203754	1.409584	H	1.182945	4.466878	2.111991
C	3.263161	2.427572	-0.812496	C	3.332970	2.391019	-0.864411
O	3.291988	2.600852	-2.017783	O	3.475131	2.593356	-2.056943
C	2.783604	3.464715	0.200851	C	2.752710	3.388832	0.129779
H	3.321729	3.269196	1.138072	H	3.292887	3.251918	1.076639
C	3.141139	4.879096	-0.286243	C	2.958325	4.835778	-0.354755
H	2.608002	5.124498	-1.209564	H	2.449219	5.002198	-1.308590
H	2.885847	5.624324	0.471739	H	2.559541	5.542233	0.379228
H	4.216651	4.956080	-0.477643	H	4.024160	5.049746	-0.487827
H	-2.458210	2.596057	1.428667	H	-2.634903	2.882431	0.865665
C	-2.488369	0.222972	-0.283293	C	-2.598987	0.141601	-0.346537
C	-3.673470	0.327876	0.504624	C	-3.728836	0.440599	0.423595
C	-2.606366	0.045311	-1.692064	C	-2.793478	-0.301629	-1.667089
C	-4.919589	0.270463	-0.070416	C	-5.021084	0.298305	-0.091836
H	-3.587249	0.417714	1.579037	H	-3.619215	0.766906	1.452737
C	-3.837866	-0.019422	-2.286517	C	-4.072319	-0.446007	-2.194163
H	-1.704850	-0.044534	-2.286065	H	-1.933242	-0.542647	-2.283045
C	-5.019379	0.093547	-1.481343	C	-5.197673	-0.145133	-1.409984
H	-5.809074	0.344638	0.541715	H	-5.869497	0.529047	0.542117
H	-3.957498	-0.151422	-3.355892	H	-4.217205	-0.792924	-3.213394
O	-6.152835	0.017430	-2.143732	O	-6.410790	-0.316888	-2.012293
C	-7.436714	0.113327	-1.472280	C	-7.595139	-0.027239	-1.264641
H	-8.171585	0.020221	-2.268415	H	-8.426644	-0.231057	-1.940195
H	-7.538993	-0.705039	-0.757286	H	-7.671639	-0.673118	-0.382259
H	-7.522805	1.084233	-0.981042	H	-7.619911	1.024923	-0.958074

HH-7-S₀

C	3.436282	3.955411	0.807200
H	3.589921	4.318273	1.828352
H	4.165901	4.443338	0.152947
H	2.432558	4.249649	0.484137
O	3.728706	0.563947	-0.698529
C	3.392200	-0.168480	-1.899835
H	2.675799	0.408235	-2.488280

HH-7-S_{1,min}

C	3.707983	3.871397	0.712644
H	3.901211	4.218307	1.732395
H	4.495467	4.263597	0.062264
H	2.748335	4.279640	0.382483
O	3.738630	0.482720	-0.802160
C	3.344281	-0.250763	-1.985095
H	2.595804	0.322513	-2.535723

H	4.306386	-0.314601	-2.483583	H	4.228346	-0.391861	-2.614093
O	1.615947	-1.302071	-0.726136	O	1.660311	-1.396806	-0.682884
C	2.424712	-2.422269	-2.674818	C	2.318080	-2.483806	-2.714016
C	0.921568	-2.694265	-2.445919	C	0.811551	-2.667732	-2.433883
H	2.590971	-1.929801	-3.639941	H	2.477871	-2.000227	-3.684201
H	0.634307	-3.699289	-2.758716	H	0.448375	-3.640495	-2.766621
H	0.319412	-1.969336	-2.997297	H	0.236860	-1.886108	-2.934431
O	3.237247	-3.597749	-2.591542	O	3.059185	-3.704899	-2.653500
H	3.102321	-4.124992	-3.395915	H	2.869012	-4.224642	-3.451780
N	-0.516634	-2.141923	-0.348934	N	-0.503736	-2.127154	-0.239559
C	-1.698212	-2.525468	-0.929950	C	-1.743933	-2.460144	-0.796397
O	-1.829095	-2.950263	-2.072571	O	-1.893386	-2.829840	-1.947139
N	-2.850525	-2.400610	-0.126448	N	-2.844163	-2.368561	0.056640
H	-3.713344	-2.601043	-0.625971	H	-3.733071	-2.564331	-0.398501
C	2.820641	-1.511467	-1.483940	C	2.806578	-1.598672	-1.540339
H	3.546724	-2.052092	-0.862283	H	3.572041	-2.147371	-0.978746
C	-0.461188	-1.685361	1.029036	C	-0.383001	-1.676336	1.089587
H	0.483687	-2.023021	1.454636	H	0.592032	-1.948524	1.483992
O	-1.579393	-0.678271	2.530283	O	-1.505258	-0.575162	2.595147
C	3.601527	2.427093	0.771043	C	3.695949	2.333581	0.669067
H	4.618960	2.175502	1.098685	H	4.674441	1.959183	0.997461
C	2.629165	1.711957	1.710018	C	2.655421	1.738723	1.612618
C	1.401884	1.234459	1.239460	C	1.458117	1.212947	1.164225
C	2.952799	1.520304	3.059893	C	2.916605	1.715425	3.007257
C	0.528763	0.511077	2.060343	C	0.537318	0.601091	2.056555
H	1.144715	1.389528	0.198827	H	1.214089	1.237885	0.111664
C	2.064010	0.852262	3.905482	C	2.003026	1.145849	3.914771
H	3.900974	1.884935	3.448534	H	3.846020	2.132943	3.382992
C	0.864923	0.331132	3.409458	C	0.839159	0.565136	3.450810
H	2.316379	0.713334	4.953500	H	2.228497	1.149695	4.975727
H	0.197553	-0.218344	4.063847	H	0.140190	0.097201	4.131939
C	-0.701529	-0.173679	1.471401	C	-0.687205	-0.044328	1.533767
C	-1.486190	0.717925	0.516252	C	-1.495166	0.746517	0.515182
C	-2.601148	1.419316	1.004746	C	-2.613125	1.467616	0.975428
C	-1.110696	0.884560	-0.827358	C	-1.144547	0.849295	-0.840067
C	-3.327660	2.272137	0.179420	C	-3.362247	2.257398	0.111724
H	-2.904946	1.289335	2.037292	H	-2.904468	1.399551	2.018782
C	-1.830767	1.730300	-1.668449	C	-1.885086	1.635385	-1.718113
H	-0.256517	0.351446	-1.227808	H	-0.284337	0.314686	-1.229630
C	-2.931708	2.414468	-1.152345	C	-3.006006	2.351190	-1.250395
H	-4.185701	2.814993	0.556669	H	-4.226676	2.801232	0.472087

H	-1.545154	1.855516	-2.705738	H	-1.609185	1.703569	-2.762855
C	0.791245	-2.452177	-0.941664	C	0.767380	-2.481202	-0.917643
H	1.214530	-3.299018	-0.378345	H	1.141533	-3.383308	-0.409526
C	-2.956695	-2.205717	1.230440	C	-2.877687	-2.180248	1.421208
O	-4.040390	-2.191182	1.797665	O	-3.921729	-2.202136	2.049450
C	-1.629561	-2.019875	1.969675	C	-1.523438	-1.933386	2.091298
C	-1.439990	-3.102961	3.016340	C	-1.251659	-2.956747	3.179634
H	-0.507736	-2.933945	3.562686	H	-0.304210	-2.734833	3.678426
H	-2.276981	-3.095868	3.721036	H	-2.061065	-2.927939	3.915202
H	-1.395537	-4.089297	2.540514	H	-1.201033	-3.963969	2.752138
C	3.466167	1.886321	-0.652461	C	3.487038	1.805940	-0.749387
O	3.140214	2.541851	-1.625470	O	3.110973	2.466781	-1.697384
N	-3.692262	3.304876	-2.031036	N	-3.759774	3.144532	-2.128825
O	-4.667087	3.900449	-1.559977	O	-4.790095	3.786949	-1.678215
O	-3.326460	3.423061	-3.205431	O	-3.406716	3.223285	-3.372296

HH-7- $T_{1,min}$

C	3.301252	4.032949	0.871413
H	3.445708	4.383695	1.898126
H	4.009941	4.558230	0.223076
H	2.286228	4.295904	0.556834
O	3.707918	0.679876	-0.692939
C	3.391515	-0.043467	-1.905100
H	2.653601	0.518375	-2.481349
H	4.307818	-0.148857	-2.494219
O	1.657853	-1.253909	-0.745910
C	2.499648	-2.316469	-2.713426
C	1.003168	-2.628866	-2.494715
H	2.658173	-1.808195	-3.671689
H	0.740102	-3.633522	-2.829223
H	0.385557	-1.906837	-3.032746
O	3.340688	-3.472657	-2.640600
H	3.217275	-3.996641	-3.448980
N	-0.452510	-2.157062	-0.390152
C	-1.622687	-2.556904	-0.982252
O	-1.741005	-2.958051	-2.135088
N	-2.779077	-2.481591	-0.178722
H	-3.635871	-2.691115	-0.684733
C	2.866987	-1.411516	-1.509157

HT-7- S_0

O	3.549302	1.585941	-0.433915
C	3.818604	0.512807	-1.367317
H	2.903009	0.305336	-1.929180
H	4.592458	0.833813	-2.071206
O	3.387928	-1.118201	0.436184
C	4.409990	-1.929693	-1.552920
C	3.057149	-2.626238	-1.347370
H	4.566926	-1.628717	-2.595401
H	3.089838	-3.690972	-1.587776
H	2.286520	-2.156647	-1.968496
O	5.511187	-2.722225	-1.098514
H	5.599788	-3.494762	-1.680951
N	1.337012	-2.277869	0.511673
C	0.623115	-3.441031	0.575387
O	1.074505	-4.541704	0.269256
N	-0.696699	-3.324365	1.039578
H	-1.202097	-4.205825	1.075012
C	4.303503	-0.719069	-0.610209
H	5.265358	-0.513422	-0.131864
C	0.714911	-1.024188	0.761755
H	1.490246	-0.318556	1.050205
O	-0.051975	-0.489552	-0.362182

H	3.612600	-1.936418	-0.897278	C	-2.422018	0.031713	-0.009048
C	-0.411387	-1.728283	0.997620	C	-3.560878	0.132681	0.806382
H	0.541052	-2.051049	1.417997	C	-2.584101	-0.085589	-1.398679
O	-1.552254	-0.786612	2.522831	C	-4.836425	0.127504	0.250267
C	3.521724	2.512533	0.808666	H	-3.465731	0.187920	1.884199
H	4.548972	2.292484	1.128282	C	-3.853170	-0.090678	-1.971549
C	2.579603	1.745773	1.737610	H	-1.711464	-0.175426	-2.035469
C	1.362622	1.244785	1.264589	C	-4.965880	0.019282	-1.136109
C	2.921563	1.527333	3.078846	H	-5.716048	0.198697	0.878089
C	0.519900	0.471441	2.071598	H	-3.979372	-0.177804	-3.043759
H	1.090383	1.420860	0.230974	C	2.775162	-2.367535	0.137563
C	2.061298	0.809090	3.912895	H	3.210290	-3.148634	0.767430
H	3.861801	1.910200	3.469340	C	-1.311315	-2.246814	1.648817
C	0.874606	0.264457	3.412184	O	-2.412038	-2.370602	2.169793
H	2.327376	0.649448	4.954604	C	-0.518421	-0.944814	1.675143
H	0.230837	-0.324030	4.056382	C	-0.304183	-0.513422	3.124981
C	-0.692748	-0.233419	1.470699	H	-1.259323	-0.357096	3.633940
C	-1.507298	0.651908	0.536138	H	0.242472	-1.293807	3.666987
C	-2.638034	1.318419	1.042728	H	0.278919	0.408528	3.175096
C	-1.146452	0.856117	-0.808117	C	-1.017221	0.102122	0.558698
C	-3.393930	2.166532	0.243676	C	-0.590985	1.547360	0.889344
H	-2.930473	1.163055	2.075318	C	0.586180	2.028817	0.305079
C	-1.888679	1.696073	-1.631664	C	-1.266296	2.364463	1.804199
H	-0.279450	0.354986	-1.222675	C	1.159658	3.253161	0.661960
C	-3.009339	2.352969	-1.096268	H	1.067997	1.396354	-0.426386
H	-4.263877	2.678133	0.641661	C	-0.729462	3.610148	2.144164
H	-1.608115	1.845313	-2.668928	H	-2.190228	2.043056	2.273505
C	0.863838	-2.420542	-0.986206	C	0.481831	4.046569	1.599273
H	1.308090	-3.267342	-0.439114	H	-1.250791	4.237947	2.861823
C	-2.893230	-2.311416	1.180737	H	0.892784	5.000621	1.916877
O	-3.979006	-2.329902	1.744286	C	3.000711	2.701807	-0.967003
C	-1.572166	-2.113260	1.927832	O	2.872951	2.862752	-2.166927
C	-1.360706	-3.219366	2.946289	C	2.524477	3.685800	0.099229
H	-0.432073	-3.046001	3.497509	H	3.246209	3.630544	0.925179
H	-2.197652	-3.247303	3.650603	C	2.523090	5.118309	-0.462157
H	-1.296606	-4.192155	2.445342	H	1.803678	5.218561	-1.280144
C	3.399934	1.991355	-0.623431	H	2.261265	5.835461	0.320482
O	3.048002	2.651546	-1.584217	H	3.515868	5.382906	-0.840652
N	-3.777560	3.164074	-1.917785	N	-6.304212	0.013688	-1.727379
O	-4.736860	3.967835	-1.533592	O	-7.278840	0.117033	-0.974474
O	-3.458263	3.570807	-3.120722	O	-6.402949	-0.093325	-2.954712

HT-7- $S_{1,min}$

O	3.367870	1.782468	-0.343651
C	3.813124	0.783214	-1.299367
H	2.960676	0.512962	-1.929377
H	4.591008	1.218474	-1.932690
O	3.463316	-0.945575	0.432066
C	4.626711	-1.586254	-1.538931
C	3.325481	-2.394879	-1.424350
H	4.807323	-1.233979	-2.561361
H	3.453950	-3.442443	-1.704477
H	2.547071	-1.961701	-2.061823
O	5.764623	-2.304701	-1.055868
H	5.939649	-3.049636	-1.654446
N	1.505571	-2.254430	0.369622
C	0.875327	-3.468906	0.368116
O	1.409520	-4.516261	0.017041
N	-0.454096	-3.467296	0.819921
H	-0.895726	-4.383164	0.806597
C	4.376895	-0.426189	-0.560349
H	5.296005	-0.152621	-0.035018
C	0.791659	-1.068369	0.672848
H	1.512769	-0.316941	0.987374
O	-0.026960	-0.545093	-0.426390
C	-2.434048	-0.144054	-0.025235
C	-3.563537	-0.190792	0.810085
C	-2.629196	-0.055312	-1.414972
C	-4.849916	-0.148892	0.281177
H	-3.451958	-0.291123	1.884965
C	-3.908130	-0.014164	-1.959786
H	-1.770111	-0.020835	-2.077783
C	-5.035924	-0.050923	-1.112832
H	-5.715022	-0.193160	0.930757
H	-4.051107	0.051859	-3.031132
C	2.961298	-2.223215	0.054873
H	3.427278	-2.995433	0.673192
C	-1.140271	-2.475465	1.495525
O	-2.218635	-2.706661	2.022257
C	-0.440205	-1.121452	1.591820

HT-7- $T_{1,min}$

O	3.533049	1.608869	-0.433989
C	3.817047	0.542433	-1.370603
H	2.905645	0.326631	-1.936199
H	4.588984	0.875444	-2.071007
O	3.407467	-1.101357	0.428472
C	4.432797	-1.892608	-1.566073
C	3.084427	-2.598908	-1.365707
H	4.590449	-1.586376	-2.606918
H	3.123640	-3.661830	-1.613131
H	2.310952	-2.130188	-1.983907
O	5.538097	-2.679725	-1.112027
H	5.629721	-3.452269	-1.694004
N	1.362010	-2.272989	0.494879
C	0.656106	-3.441007	0.554684
O	1.114182	-4.537455	0.242520
N	-0.663742	-3.334925	1.021372
H	-1.161663	-4.220621	1.056808
C	4.315734	-0.687096	-0.618335
H	5.276499	-0.473003	-0.141538
C	0.731236	-1.024839	0.753609
H	1.503034	-0.314768	1.040925
O	-0.045443	-0.493164	-0.363831
C	-2.419442	0.001447	0.003956
C	-3.557954	0.093033	0.824293
C	-2.591521	-0.117733	-1.385974
C	-4.836433	0.075013	0.281262
H	-3.457226	0.151315	1.901744
C	-3.859465	-0.134634	-1.955974
H	-1.721407	-0.197174	-2.028004
C	-4.979210	-0.028691	-1.113699
H	-5.711399	0.135281	0.919676
H	-3.985884	-0.222370	-3.029767
C	2.800652	-2.351686	0.120939
H	3.239926	-3.134716	0.745452
C	-1.278693	-2.267485	1.648939
O	-2.371049	-2.405795	2.183827
C	-0.497002	-0.959327	1.674703

C	-0.254111	-0.750885	3.063110	C	-0.277765	-0.530618	3.124608
H	-1.215409	-0.686560	3.579569	H	-1.231333	-0.383747	3.639364
H	0.342808	-1.519689	3.566092	H	0.278419	-1.307824	3.661532
H	0.276611	0.199374	3.172484	H	0.297780	0.396091	3.174279
C	-1.020757	-0.073018	0.522288	C	-1.013079	0.086485	0.563967
C	-0.665348	1.367915	0.911448	C	-0.594535	1.532823	0.899080
C	0.389371	1.994793	0.269629	C	0.574874	2.027585	0.310178
C	-1.353924	2.077309	1.963859	C	-1.270606	2.340176	1.822113
C	0.910255	3.207226	0.736958	C	1.140257	3.254965	0.669550
H	0.858876	1.471777	-0.550045	H	1.058314	1.402555	-0.426584
C	-0.886625	3.317777	2.411041	C	-0.742423	3.588775	2.164992
H	-2.238407	1.646547	2.416125	H	-2.187505	2.007391	2.297315
C	0.235524	3.877610	1.828803	C	0.461597	4.038365	1.614632
H	-1.401698	3.830180	3.214935	H	-1.264403	4.208459	2.889267
H	0.622405	4.821555	2.194514	H	0.865820	4.995011	1.933191
C	2.820027	2.891231	-0.877647	C	2.982861	2.724154	-0.966956
O	2.800865	3.127007	-2.068593	O	2.863500	2.888588	-2.167289
C	2.187280	3.796242	0.185851	C	2.496391	3.703833	0.098826
H	2.892155	3.857125	1.029320	H	3.223272	3.661832	0.921133
C	1.968712	5.226348	-0.366437	C	2.471829	5.134506	-0.466749
H	1.261367	5.216516	-1.198804	H	1.750528	5.220708	-1.284679
H	1.592319	5.893219	0.412619	H	2.198514	5.849449	0.314005
H	2.923516	5.622861	-0.720855	H	3.459987	5.414125	-0.846545
N	-6.333504	0.012747	-1.652102	N	-6.252726	-0.085540	-1.662252
O	-7.351957	-0.012729	-0.854019	O	-7.369519	0.231179	-1.055417
O	-6.482412	0.094832	-2.935088	O	-6.543480	-0.056012	-2.938763

P-1-S₀

C	-3.366208	3.758981	0.424076
H	-4.015881	3.877551	1.297110
H	-3.216265	4.743368	-0.031945
H	-3.876395	3.120552	-0.303192
O	0.210909	2.927317	0.087866
C	1.219453	2.725221	-0.932013
H	0.960110	1.848257	-1.530388
H	1.253702	3.608815	-1.576939
O	2.555089	1.277344	0.455391
C	3.738079	2.487556	-1.219592

P-1-S_{1,min}

C	-3.580903	3.731744	0.602622
H	-4.198490	3.841377	1.499991
H	-3.435718	4.723356	0.159762
H	-4.123951	3.111974	-0.116852
O	-0.027950	2.892954	0.121912
C	0.935886	2.690557	-0.938500
H	0.694740	1.770600	-1.477718
H	0.890614	3.538383	-1.629084
O	2.423423	1.392506	0.445734
C	3.444142	2.566412	-1.354070

C	4.717422	1.518173	-0.534698	C	4.517006	1.704846	-0.665762
H	3.420942	2.092547	-2.188344	H	3.100927	2.088553	-2.275590
H	5.435206	2.099535	0.052782	H	5.225931	2.365081	-0.156301
H	5.272294	0.900275	-1.242551	H	5.072769	1.075952	-1.363214
O	4.238227	3.816655	-1.371776	O	3.850518	3.909489	-1.619428
H	4.789921	3.853296	-2.169258	H	4.356382	3.924821	-2.447365
N	3.707782	-0.752244	0.107881	N	3.695615	-0.576123	0.172755
C	3.275717	-1.147633	-1.153371	C	3.229180	-1.083767	-1.034977
O	3.041359	-0.364780	-2.070544	O	2.889694	-0.382636	-1.984810
N	3.136038	-2.514769	-1.303270	N	3.182879	-2.464406	-1.090272
H	2.827759	-2.819429	-2.222392	H	2.849669	-2.850578	-1.969080
C	2.551896	2.532898	-0.241589	C	2.311361	2.605487	-0.314700
H	2.719936	3.348120	0.476723	H	2.472224	3.467730	0.348470
C	3.921663	-1.686633	1.108526	C	4.038236	-1.424787	1.212974
H	4.232016	-1.263567	2.057913	H	4.368708	-0.918741	2.113534
C	-2.023160	3.150901	0.859174	C	-2.232927	3.096911	0.980415
H	-1.539321	3.826327	1.572774	H	-1.713652	3.755355	1.684989
C	-2.189554	1.797431	1.550585	C	-2.392940	1.734017	1.659978
C	-2.657903	0.681077	0.843498	C	-2.878364	0.641537	0.949749
C	-1.894298	1.656008	2.912486	C	-2.063186	1.590051	3.023201
C	-2.807576	-0.563422	1.475104	C	-3.052657	-0.632275	1.576011
H	-2.879409	0.773713	-0.215754	H	-3.130394	0.749972	-0.102142
C	-2.051316	0.422556	3.555328	C	-2.233750	0.346673	3.657292
H	-1.537438	2.514444	3.476505	H	-1.679417	2.439373	3.581605
C	-2.491435	-0.687743	2.839282	C	-2.715990	-0.751538	2.963383
H	-1.822221	0.332070	4.613581	H	-1.979961	0.244761	4.710007
H	-2.601751	-1.652454	3.324683	H	-2.841248	-1.708434	3.461516
C	3.848405	0.682027	0.426010	C	3.751824	0.882291	0.390699
H	4.267900	0.694552	1.434422	H	4.215266	0.990953	1.374028
C	3.347758	-3.515526	-0.349934	C	3.524801	-3.382405	-0.092514
O	3.170606	-4.699451	-0.650638	O	3.421257	-4.593304	-0.308566
C	3.772183	-3.025487	0.953781	C	3.984789	-2.778280	1.149605
C	4.018735	-4.013336	2.059724	C	4.372005	-3.670461	2.295797
H	4.327632	-3.503240	2.976857	H	4.692713	-3.079672	3.158838
H	3.114801	-4.594830	2.276349	H	3.530887	-4.302738	2.603881
H	4.802079	-4.728422	1.781785	H	5.191856	-4.341391	2.012978
C	-1.067094	3.012312	-0.323989	C	-1.324859	2.959691	-0.236982
O	-1.397839	2.962685	-1.495902	O	-1.698393	2.896944	-1.396204
O	-2.772193	-2.890790	1.054585	O	-3.741731	-2.953199	1.290781
C	-3.220478	-1.790516	0.721290	C	-3.537019	-1.739656	0.859251
C	-4.170434	-1.688915	-0.430024	C	-3.932906	-1.834150	-0.577679

C	-4.078862	-2.639576	-1.462831
C	-5.189642	-0.721788	-0.476420
C	-4.973750	-2.609954	-2.531103
H	-3.295714	-3.390520	-1.420776
C	-6.100187	-0.708542	-1.535993
H	-5.289679	0.003765	0.324840
C	-5.988886	-1.645394	-2.567904
H	-4.884209	-3.337841	-3.332923
H	-6.894015	0.033097	-1.555302
H	-6.691167	-1.626783	-3.397102

C	-2.972831	-2.200247	-1.554976
C	-5.287132	-1.645208	-0.953744
C	-3.336356	-2.240898	-2.893933
H	-1.952057	-2.405728	-1.248338
C	-5.640816	-1.689296	-2.295354
H	-6.026935	-1.429750	-0.189285
C	-4.668103	-1.986323	-3.265633
H	-2.596276	-2.475626	-3.652729
H	-6.667484	-1.502682	-2.594928
H	-4.952036	-2.036807	-4.312615

P-1- $T_{1,min}$

C	-3.231122	3.911946	0.508846
H	-3.857998	4.045840	1.396263
H	-3.045684	4.895784	0.064633
H	-3.782984	3.307639	-0.216995
O	0.297204	2.937265	0.084896
C	1.271665	2.691428	-0.957810
H	0.979850	1.803789	-1.524811
H	1.302904	3.557011	-1.626862
O	2.619259	1.263259	0.440257
C	3.771986	2.386791	-1.317557
C	4.745116	1.403933	-0.642988
H	3.410784	1.979597	-2.265562
H	5.503924	1.976284	-0.099994
H	5.251890	0.748992	-1.353695
O	4.306269	3.696106	-1.518789
H	4.826508	3.698591	-2.337909
N	3.686626	-0.813493	0.095322
C	3.180755	-1.221097	-1.133970
O	2.923644	-0.450162	-2.055243
N	2.992941	-2.586052	-1.246459
H	2.629146	-2.899979	-2.141821
C	2.620869	2.492521	-0.302504
H	2.830147	3.328060	0.380552
C	3.925116	-1.733374	1.103517
H	4.295945	-1.300672	2.026465
C	-1.909096	3.236568	0.907646
H	-1.378872	3.879657	1.618020

P-2- S_0

C	3.141824	-3.643695	0.980658
H	3.780989	-3.607370	1.868648
H	2.922022	-4.692993	0.755542
H	3.696595	-3.223406	0.136826
O	-0.377930	-2.780802	0.414594
C	-1.367782	-2.753544	-0.642270
H	-1.149200	-1.925651	-1.321864
H	-1.326083	-3.697720	-1.193868
O	-2.843091	-1.270379	0.558255
C	-3.885274	-2.725275	-1.011929
C	-4.952715	-1.771000	-0.448920
H	-3.567320	-2.402073	-2.006615
H	-5.644051	-2.344680	0.176515
H	-5.529460	-1.267795	-1.226816
O	-4.282074	-4.096815	-1.045173
H	-4.795773	-4.253714	-1.853302
N	-4.134735	0.620486	-0.016237
C	-3.682221	0.921667	-1.296181
O	-3.341386	0.073147	-2.116402
N	-3.650767	2.273496	-1.583950
H	-3.325592	2.509057	-2.517413
C	-2.729980	-2.585975	-0.006310
H	-2.863141	-3.335005	0.787526
C	-4.485744	1.628741	0.866694
H	-4.807016	1.279267	1.841925
C	1.845485	-2.860532	1.245841
H	1.313171	-3.322435	2.083623

C	-2.123773	1.883166	1.587343	C	2.103513	-1.400113	1.616854
C	-2.646405	0.804652	0.875360	C	2.704031	-0.515280	0.713588
C	-1.793102	1.718627	2.947037	C	1.766100	-0.913461	2.884273
C	-2.884757	-0.443351	1.505208	C	2.939548	0.829078	1.043377
H	-2.861158	0.913678	-0.183435	H	2.975788	-0.867798	-0.277648
C	-1.994692	0.484894	3.576958	C	2.020034	0.416270	3.229028
H	-1.376303	2.552653	3.505449	H	1.307695	-1.576985	3.613937
C	-2.530176	-0.589908	2.875631	C	2.591000	1.320659	2.324615
H	-1.738774	0.367692	4.626767	H	1.763079	0.761868	4.227643
H	-2.710054	-1.536145	3.375480	C	-4.175449	-0.781817	0.442752
C	3.888359	0.622611	0.372856	H	-4.621028	-0.727278	1.438642
H	4.349228	0.643131	1.362936	C	-4.001874	3.342978	-0.754493
C	3.225488	-3.573426	-0.284016	O	-3.914348	4.500983	-1.172788
O	2.998823	-4.757347	-0.549719	C	-4.451103	2.952377	0.574098
C	3.730718	-3.070214	0.985328	C	-4.848566	4.020589	1.554162
C	4.007470	-4.042248	2.098129	H	-5.164678	3.579752	2.504171
H	4.377098	-3.522580	2.986983	H	-4.014402	4.704255	1.751653
H	3.100822	-4.594004	2.373315	H	-5.674721	4.626046	1.162854
H	4.755966	-4.784278	1.795759	C	0.907816	-2.921080	0.042533
C	-0.986909	3.065105	-0.297099	O	1.257589	-3.054858	-1.117525
O	-1.345866	3.025101	-1.461232	O	2.974099	2.843914	-0.211051
O	-3.081263	-2.775799	1.260973	C	3.487746	1.740100	-0.017049
C	-3.394711	-1.580090	0.770185	C	4.650531	1.294921	-0.847435
C	-4.216674	-1.611007	-0.423512	C	4.842727	1.881865	-2.111558
C	-4.181549	-2.750446	-1.276401	C	5.586305	0.356734	-0.377732
C	-5.129612	-0.567452	-0.730101	C	5.937849	1.525545	-2.896301
C	-4.995448	-2.815196	-2.404309	H	4.121030	2.609827	-2.469277
H	-3.488222	-3.555979	-1.057190	C	6.694282	0.015390	-1.157218
C	-5.921611	-0.639219	-1.869168	H	5.461210	-0.091845	0.602739
H	-5.216102	0.286465	-0.065908	C	6.867926	0.592757	-2.418714
C	-5.864412	-1.761885	-2.714882	H	6.070037	1.972901	-3.877706
H	-4.944155	-3.686867	-3.051508	H	7.418994	-0.700955	-0.780157
H	-6.601835	0.177011	-2.098230	H	7.724966	0.319058	-3.028406
H	-6.494561	-1.811917	-3.598249	C	2.826201	2.751506	2.754226
				H	3.800084	3.126997	2.423688
				H	2.068106	3.422125	2.334618
				H	2.781074	2.830737	3.845028

P-2-S_{1,min}

P-2-T_{1,min}

C	-3.414409	3.757697	0.779445	C	3.263732	-3.711019	0.995136
H	-4.064001	3.785618	1.660378	H	3.883239	-3.708481	1.897821
H	-3.238196	4.786828	0.447082	H	3.074317	-4.751461	0.708827
H	-3.938992	3.225875	-0.019704	H	3.826299	-3.232449	0.188261
O	0.142100	2.913033	0.344702	O	-0.259473	-2.850186	0.398759
C	1.144529	2.804196	-0.693167	C	-1.225506	-2.776227	-0.676770
H	0.907860	1.955327	-1.340054	H	-0.980533	-1.932409	-1.327231
H	1.145561	3.723709	-1.286797	H	-1.187306	-3.704202	-1.255625
O	2.544438	1.322349	0.594127	O	-2.700438	-1.304493	0.537394
C	3.666303	2.668632	-1.017425	C	-3.734733	-2.693819	-1.096482
C	4.686665	1.697972	-0.397627	C	-4.796201	-1.735549	-0.528786
H	3.352186	2.317643	-2.003950	H	-3.390531	-2.349738	-2.075383
H	5.389645	2.270201	0.216097	H	-5.511393	-2.313467	0.065191
H	5.255639	1.141487	-1.144253	H	-5.346575	-1.199541	-1.303863
O	4.117713	4.021232	-1.098939	O	-4.156094	-4.056158	-1.175840
H	4.656742	4.122455	-1.899438	H	-4.662220	-4.178988	-1.994583
N	3.766436	-0.640249	0.119731	N	-3.942837	0.626616	-0.009617
C	3.329138	-0.977085	-1.156568	C	-3.457693	0.955204	-1.270708
O	3.049394	-0.151397	-2.021991	O	-3.119293	0.123777	-2.109219
N	3.238599	-2.337509	-1.385284	N	-3.390238	2.313944	-1.516905
H	2.926499	-2.599393	-2.316173	H	-3.041275	2.569810	-2.436336
C	2.490232	2.615934	-0.027838	C	-2.598066	-2.604617	-0.064290
H	2.638830	3.392806	0.735896	H	-2.760380	-3.374294	0.703943
C	4.039033	-1.623081	1.057376	C	-4.287792	1.615952	0.896718
H	4.352124	-1.245395	2.024717	H	-4.636927	1.245134	1.854317
C	-2.091364	3.062599	1.138188	C	1.945254	-2.971623	1.273410
H	-1.590077	3.634931	1.926203	H	1.405533	-3.491515	2.071923
C	-2.292587	1.639409	1.665188	C	2.161167	-1.528107	1.733501
C	-2.795494	0.639804	0.842644	C	2.736949	-0.585729	0.884759
C	-1.981294	1.331895	3.002187	C	1.776446	-1.129642	3.022802
C	-3.010589	-0.695867	1.315585	C	2.966391	0.758515	1.290830
H	-3.034226	0.868281	-0.192570	H	2.998992	-0.876620	-0.127713
C	-2.189330	0.028866	3.485465	C	1.976179	0.194718	3.432661
H	-1.582235	2.098046	3.661284	H	1.317234	-1.843568	3.701784
C	-2.691630	-0.996910	2.692761	C	2.556435	1.157952	2.606720
H	-1.945759	-0.190041	4.523407	H	1.670515	0.486559	4.435108
C	3.857647	0.777614	0.520540	C	-4.020356	-0.787330	0.407442
H	4.286177	0.746967	1.524928	H	-4.486755	-0.752402	1.394664
C	3.508439	-3.383777	-0.497888	C	-3.731386	3.366057	-0.661529
O	3.370615	-4.553933	-0.865840	O	-3.607349	4.533712	-1.042182
C	3.940882	-2.955387	0.824516	C	-4.216137	2.946620	0.645539

C	4.251698	-3.996057	1.863726	C	-4.607975	3.994069	1.649994
H	4.559711	-3.528511	2.803543	H	-4.950718	3.532486	2.580709
H	3.377387	-4.627119	2.062573	H	-3.762903	4.652890	1.882384
H	5.057354	-4.659681	1.527909	H	-5.413587	4.629071	1.262647
C	-1.139457	3.036225	-0.052887	C	1.034207	-2.985460	0.049598
O	-1.468878	3.097824	-1.225534	O	1.405604	-3.083358	-1.107659
O	-3.793427	-2.921644	0.618195	O	3.607179	2.986932	0.548884
C	-3.519990	-1.659664	0.427012	C	3.553628	1.675351	0.355278
C	-3.882226	-1.482355	-1.015570	C	4.265087	1.370881	-0.898567
C	-2.916898	-1.726335	-2.022133	C	4.056342	2.191792	-2.037843
C	-5.212693	-1.159622	-1.376495	C	5.229303	0.335355	-0.971364
C	-3.247444	-1.522919	-3.356229	C	4.744749	1.940959	-3.223381
H	-1.915247	-2.033550	-1.737804	H	3.331395	2.997373	-1.986339
C	-5.533759	-0.959042	-2.713463	C	5.894083	0.083501	-2.165566
H	-5.961053	-1.035636	-0.599922	H	5.440160	-0.266371	-0.093044
C	-4.553498	-1.139434	-3.703083	C	5.659839	0.885176	-3.297119
H	-2.499519	-1.666940	-4.130033	H	4.561193	2.565569	-4.093305
H	-6.542412	-0.670744	-2.993535	H	6.610188	-0.732238	-2.218365
H	-4.812122	-0.996781	-4.748232	H	6.194091	0.687745	-4.222137
C	-2.889779	-2.376992	3.269976	C	2.752784	2.562411	3.126150
H	-3.936963	-2.700038	3.210241	H	3.812555	2.844790	3.148906
H	-2.295670	-3.132187	2.739638	H	2.234650	3.307310	2.508171
H	-2.592865	-2.397475	4.324273	H	2.360792	2.650926	4.145032

P-3-S₀

C	2.846981	-3.922922	0.823648
H	3.540747	-3.895539	1.670040
H	2.570313	-4.966298	0.636692
H	3.366387	-3.545239	-0.061954
O	-0.661428	-2.902707	0.455713
C	-1.715018	-2.856836	-0.536784
H	-1.473458	-2.101514	-1.288929
H	-1.793578	-3.837103	-1.017187
O	-2.965443	-1.163126	0.638767
C	-4.239708	-2.622310	-0.750627
C	-5.168028	-1.516709	-0.218713
H	-3.960015	-2.423260	-1.788354
H	-5.872102	-1.960473	0.492327
H	-5.739991	-1.022951	-1.006192

P-3-S_{1,min}

C	-2.796864	-4.283998	-0.561497
H	-3.495469	-4.373236	-1.399635
H	-2.453560	-5.288033	-0.289046
H	-3.334069	-3.862979	0.293341
O	0.631614	-2.969312	-0.320028
C	1.680976	-2.756839	0.654770
H	1.387602	-1.951436	1.333264
H	1.828913	-3.678264	1.226386
O	2.807473	-1.105495	-0.693678
C	4.181688	-2.318317	0.826779
C	5.035491	-1.222928	0.164479
H	3.888787	-2.018825	1.836458
H	5.764741	-1.697846	-0.499396
H	5.576159	-0.607634	0.885585

O	-4.772083	-3.942556	-0.631557	O	4.798467	-3.606203	0.856567
H	-5.359115	-4.111781	-1.385516	H	5.389487	-3.652048	1.624815
N	-4.080578	0.800244	-0.053398	N	3.804569	0.988264	-0.255804
C	-3.675612	0.934963	-1.376679	C	3.405394	1.254461	1.049419
O	-3.476489	-0.015594	-2.129003	O	3.276415	0.390333	1.912972
N	-3.518675	2.243953	-1.792504	N	3.167706	2.591320	1.309144
H	-3.227196	2.358290	-2.759211	H	2.880759	2.802064	2.260884
C	-3.010436	-2.519793	0.168514	C	2.948925	-2.400538	-0.089348
H	-3.154695	-3.194625	1.024276	H	3.142378	-3.147745	-0.872373
C	-4.262331	1.915128	0.748687	C	3.902984	2.008198	-1.188263
H	-4.556980	1.691146	1.768262	H	4.199586	1.682703	-2.179364
C	1.604214	-3.078403	1.148811	C	-1.611591	-3.394919	-0.971590
H	1.108312	-3.497126	2.030736	H	-1.093385	-3.859524	-1.816934
C	1.941865	-1.621640	1.463994	C	-2.049307	-1.997404	-1.415873
C	2.524806	-0.783675	0.503312	C	-2.609186	-1.106919	-0.500294
C	1.691969	-1.084971	2.730332	C	-1.921049	-1.619423	-2.763386
C	2.831194	0.554581	0.774227	C	-3.052052	0.184394	-0.893600
H	2.727814	-1.169224	-0.492570	H	-2.745495	-1.422878	0.527357
C	2.013439	0.239750	3.040106	C	-2.379949	-0.366276	-3.192652
H	1.244287	-1.707582	3.501420	H	-1.474742	-2.300553	-3.482197
C	2.576962	1.073687	2.066402	C	-2.940355	0.509244	-2.276278
H	1.818484	0.609089	4.040037	H	-2.286652	-0.073532	-4.234195
C	-4.242552	-0.543302	0.537810	C	4.045647	-0.402767	-0.686890
H	-4.623635	-0.350669	1.543290	H	4.406557	-0.308771	-1.713793
C	-3.698514	3.414889	-1.049713	C	3.262191	3.673872	0.429083
O	-3.513080	4.514373	-1.579158	O	3.011144	4.814840	0.827482
C	-4.101817	3.195518	0.331926	C	3.663107	3.316432	-0.924121
C	-4.316724	4.383648	1.227326	C	3.788713	4.399160	-1.959307
H	-4.617846	4.066555	2.230067	H	4.091784	3.982368	-2.924351
H	-3.401858	4.981661	1.314569	H	2.837179	4.926742	-2.094867
H	-5.095000	5.043435	0.825791	H	4.531276	5.147646	-1.658234
C	0.588112	-3.130304	0.010146	C	-0.589669	-3.277056	0.155626
O	0.853738	-3.327151	-1.163365	O	-0.827809	-3.418424	1.342892
O	2.746788	2.476366	-0.618164	O	-4.187593	2.238674	-0.596942
C	3.335626	1.432388	-0.337167	C	-3.667230	1.161707	-0.042539
C	4.536219	1.000600	-1.116993	C	-3.819417	1.095113	1.414233
C	4.762886	1.570797	-2.383379	C	-4.940842	1.718390	2.016787
C	5.466155	0.080338	-0.602487	C	-2.851108	0.499897	2.257530
C	5.888909	1.218401	-3.124315	C	-5.106678	1.701305	3.400267
H	4.043742	2.282900	-2.776171	H	-5.687705	2.191424	1.387113
C	6.602809	-0.259945	-1.339922	C	-3.028998	0.487047	3.639643

H	5.311510	-0.356958	0.378810	H	-1.942543	0.083188	1.837160
C	6.812904	0.303180	-2.602267	C	-4.157673	1.080202	4.221407
H	6.049806	1.654208	-4.106611	H	-5.982360	2.172276	3.839796
H	7.321558	-0.963880	-0.929616	H	-2.272160	0.024577	4.268147
H	7.693293	0.031731	-3.178805	H	-4.288822	1.067133	5.299880
O	2.939174	2.365112	2.292593	O	-3.371524	1.770646	-2.654390
C	2.736178	2.921742	3.594717	C	-4.482743	1.827610	-3.571383
H	3.098542	3.948273	3.531798	H	-4.768202	2.877729	-3.632230
H	1.673139	2.922833	3.861017	H	-4.161811	1.469693	-4.554885
H	3.309989	2.374210	4.351223	H	-5.312073	1.220312	-3.199081

P-3- $T_{1,\min}$

C	3.038802	-3.983806	0.977293
H	3.700753	-3.960468	1.849033
H	2.797840	-5.028984	0.753849
H	3.579478	-3.568780	0.121639
O	-0.472064	-2.988122	0.499286
C	-1.483908	-2.915872	-0.533181
H	-1.198733	-2.159380	-1.268923
H	-1.562615	-3.890237	-1.025551
O	-2.739133	-1.212712	0.620952
C	-3.991392	-2.609324	-0.846520
C	-4.917619	-1.499439	-0.319458
H	-3.664781	-2.385230	-1.865394
H	-5.656818	-1.947340	0.352246
H	-5.449128	-0.972986	-1.113937
O	-4.555548	-3.920264	-0.789604
H	-5.116639	-4.052834	-1.570226
N	-3.794794	0.791162	-0.042465
C	-3.348224	0.961431	-1.348372
O	-3.152081	0.033321	-2.128806
N	-3.145627	2.279724	-1.712002
H	-2.824228	2.420251	-2.665669
C	-2.799198	-2.559046	0.123983
H	-2.996475	-3.245693	0.959690
C	-3.967835	1.881567	0.794479
H	-4.296887	1.629900	1.796932
C	1.763896	-3.180064	1.277677
H	1.245153	-3.637352	2.126986

P-4- S_0

C	-2.303482	-4.355086	-0.580590
H	-3.032203	-4.384331	-1.396600
H	-1.905646	-5.364707	-0.435356
H	-2.818587	-4.055282	0.336333
O	1.081702	-2.949284	-0.316629
C	2.165352	-2.801943	0.635440
H	1.882041	-2.065973	1.392428
H	2.349250	-3.767453	1.115990
O	3.210543	-1.014929	-0.597939
C	4.664946	-2.331455	0.745769
C	5.482665	-1.183074	0.128877
H	4.412598	-2.107637	1.785820
H	6.183145	-1.601354	-0.600825
H	6.052193	-0.618647	0.868887
O	5.289074	-3.612528	0.655799
H	5.914053	-3.708587	1.391803
N	4.231998	1.047354	-0.081467
C	3.914855	1.228270	1.260684
O	3.842516	0.310881	2.074268
N	3.691278	2.544660	1.618507
H	3.463518	2.693451	2.597545
C	3.395835	-2.356215	-0.122392
H	3.567919	-3.026918	-0.976732
C	4.266381	2.124288	-0.952802
H	4.499917	1.863617	-1.979488
C	-1.168080	-3.378840	-0.933619
H	-0.663909	-3.726141	-1.840590

C	2.051412	-1.724092	1.649897	C	-1.682612	-1.968416	-1.204165
C	2.620888	-0.849528	0.723351	C	-2.277528	-1.214392	-0.181304
C	1.736896	-1.245292	2.929276	C	-1.582957	-1.409902	-2.486175
C	2.904035	0.505579	1.038718	C	-2.777315	0.070431	-0.408153
H	2.827029	-1.201571	-0.282049	H	-2.354827	-1.631962	0.818741
C	1.989762	0.091259	3.275523	C	-2.070309	-0.132881	-2.741464
H	1.287560	-1.907102	3.664877	H	-1.120870	-1.974042	-3.290706
C	2.562296	0.961253	2.353138	C	-2.661143	0.594405	-1.705772
H	1.739907	0.436538	4.272486	H	-1.993159	0.306038	-3.728589
C	-4.001789	-0.566932	0.498137	C	4.449323	-0.310801	-0.613220
H	-4.413849	-0.399886	1.495995	H	4.754549	-0.150574	-1.649870
C	-3.312128	3.427946	-0.931636	C	3.725990	3.680740	0.804087
O	-3.080375	4.539717	-1.415260	O	3.498248	4.792735	1.288856
C	-3.760230	3.170951	0.429509	C	4.039257	3.411465	-0.592105
C	-3.967944	4.331436	1.362181	C	4.093098	4.557529	-1.563310
H	-4.303486	3.986180	2.344502	H	4.328395	4.203095	-2.571137
H	-3.040726	4.901416	1.494730	H	3.134435	5.088320	-1.599177
H	-4.718314	5.025791	0.965810	H	4.854821	5.288928	-1.268145
C	0.792958	-3.222355	0.101032	C	-0.110266	-3.331739	0.170483
O	1.099880	-3.418003	-1.062738	O	-0.311043	-3.583506	1.344874
O	3.566460	2.712053	0.300371	O	-2.539911	1.358088	1.553883
C	3.450275	1.407256	0.072786	C	-3.336112	0.812451	0.796619
C	3.995234	1.087918	-1.259338	C	-4.793313	0.737930	1.083070
C	3.709557	1.942624	-2.352220	C	-5.297273	1.411500	2.210574
C	4.868558	-0.006048	-1.461710	C	-5.671237	0.005483	0.266023
C	4.242709	1.679056	-3.613555	C	-6.655917	1.355263	2.511827
H	3.047433	2.790263	-2.207028	H	-4.613802	1.975287	2.837604
C	5.381124	-0.268504	-2.729131	C	-7.032532	-0.050697	0.570934
H	5.142453	-0.640720	-0.624926	H	-5.296189	-0.524165	-0.604573
C	5.074211	0.571405	-3.811195	C	-7.526047	0.623759	1.692041
H	4.001620	2.335570	-4.445327	H	-7.040044	1.879436	3.382495
H	6.034710	-1.124642	-2.874534	H	-7.705188	-0.619926	-0.064284
H	5.485505	0.364100	-4.795148	H	-8.585793	0.580040	1.928600
O	2.848169	2.269959	2.613731	N	-3.156993	1.937160	-2.005711
C	2.372202	2.863598	3.824711	O	-3.650921	2.592561	-1.080876
H	2.641457	3.918400	3.760736	O	-3.062714	2.358087	-3.161937
H	1.284481	2.760180	3.908474				
H	2.860498	2.412937	4.696295				

P-4- $S_{1,min}$

C	3.029724	3.994168	-0.935530
H	3.765975	3.948792	-1.744152
H	2.748644	5.041169	-0.781151
H	3.499748	3.629391	-0.017662
O	-0.491464	2.933737	-0.727486
C	-1.602119	2.908991	0.202938
H	-1.369396	2.233028	1.029463
H	-1.760353	3.919796	0.591476
O	-2.683824	1.053218	-0.887514
C	-4.122474	2.553018	0.276287
C	-4.960279	1.365576	-0.229319
H	-3.908128	2.445441	1.342747
H	-5.625326	1.717186	-1.024549
H	-5.569750	0.908584	0.552057
O	-4.702001	3.832662	0.018701
H	-5.347687	4.029569	0.715839
N	-3.765805	-0.902734	-0.126780
C	-3.471792	-0.917083	1.232164
O	-3.379864	0.095990	1.921040
N	-3.294476	-2.181524	1.761758
H	-3.086683	-2.208217	2.756039
C	-2.829023	2.441243	-0.548237
H	-2.948001	3.030051	-1.469037
C	-3.820905	-2.082232	-0.852017
H	-4.032249	-1.950229	-1.907658
C	1.798010	3.154087	-1.310160
H	1.350597	3.563457	-2.221779
C	2.142048	1.693356	-1.588603
C	2.669267	0.872920	-0.600132
C	1.948995	1.139115	-2.872537
C	3.025387	-0.480252	-0.820670
H	2.830960	1.285299	0.388543
C	2.299788	-0.166428	-3.151315
H	1.529064	1.751128	-3.666175
C	2.858549	-1.003110	-2.154078
H	2.163556	-0.570642	-4.145369
C	-3.938422	0.381719	-0.833438
H	-4.231247	0.095334	-1.846030
C	-3.350812	-3.412247	1.100283
O	-3.161848	-4.457739	1.728408
C	-3.637345	-3.317723	-0.324055
C	-3.713900	-4.579028	-1.138274

P-4- $T_{1,min}$

C	-2.716417	-3.891375	-1.305414
H	-3.379505	-3.779401	-2.168924
H	-2.418609	-4.942623	-1.231833
H	-3.274643	-3.631401	-0.401611
O	0.749626	-2.875405	-0.676015
C	1.759171	-2.900236	0.363811
H	1.490030	-2.183997	1.144445
H	1.804636	-3.906348	0.791490
O	3.069936	-1.168349	-0.681853
C	4.270267	-2.686511	0.708512
C	5.229760	-1.570259	0.260358
H	3.941663	-2.520325	1.737765
H	5.965312	-1.994586	-0.430367
H	5.765059	-1.107734	1.091300
O	4.798910	-4.006063	0.569667
H	5.346484	-4.206635	1.345270
N	4.169677	0.761284	0.116692
C	3.707065	0.859574	1.424231
O	3.469551	-0.111576	2.138154
N	3.538951	2.156722	1.871375
H	3.206841	2.244584	2.827691
C	3.087739	-2.542222	-0.264818
H	3.270935	-3.184164	-1.138296
C	4.390176	1.897985	-0.644295
H	4.727588	1.702024	-1.656372
C	-1.480421	-2.993084	-1.481271
H	-0.936918	-3.300929	-2.379873
C	-1.845435	-1.520263	-1.646682
C	-2.493857	-0.817630	-0.619188
C	-1.545778	-0.838938	-2.834596
C	-2.832306	0.534130	-0.736422
H	-2.711139	-1.323910	0.316332
C	-1.890675	0.497988	-3.001919
H	-1.048408	-1.360013	-3.647584
C	-2.533045	1.183529	-1.959510
H	-1.681955	1.010035	-3.934245
C	4.347487	-0.564915	-0.506311
H	4.774782	-0.347075	-1.487670
C	3.756507	3.347823	1.171774
O	3.554278	4.432451	1.724984
C	4.216982	3.166509	-0.197541
C	4.474214	4.379118	-1.047837

H	-3.938398	-4.354501	-2.185123	H	4.814055	4.090024	-2.046679
H	-2.767556	-5.131363	-1.099001	H	3.566729	4.985183	-1.154227
H	-4.492896	-5.248231	-0.754167	H	5.238914	5.021820	-0.595743
C	0.721206	3.227790	-0.227094	C	-0.514125	-3.142090	-0.305451
O	0.919103	3.494931	0.944980	O	-0.835118	-3.436574	0.832315
O	4.058902	-2.365829	0.241053	O	-2.798410	2.342774	0.782119
C	3.559984	-1.220610	0.307004	C	-3.328713	1.272354	0.476070
C	3.569878	-0.681171	1.707200	C	-4.405583	0.677010	1.313376
C	4.789952	-0.645849	2.403431	C	-4.529929	1.098581	2.650569
C	2.374573	-0.322433	2.352619	C	-5.331579	-0.243957	0.791231
C	4.818535	-0.200295	3.725354	C	-5.550216	0.595286	3.453930
H	5.705980	-0.945434	1.903883	H	-3.815569	1.813073	3.047399
C	2.411902	0.102987	3.680593	C	-6.363796	-0.732999	1.594257
H	1.427493	-0.381811	1.825382	H	-5.261558	-0.561382	-0.244398
C	3.631457	0.171161	4.364936	C	-6.470472	-0.320225	2.925982
H	5.764693	-0.150672	4.256212	H	-5.632131	0.914486	4.489138
H	1.488801	0.382607	4.179824	H	-7.082754	-1.434418	1.180606
H	3.654239	0.509003	5.397148	H	-7.269388	-0.708314	3.552078
N	3.211230	-2.279379	-2.562987	N	-2.850247	2.529528	-2.173317
O	3.801623	-3.131068	-1.765789	O	-3.764732	3.207120	-1.516548
O	2.999142	-2.689565	-3.746494	O	-2.725448	3.129144	-3.323574

P-5-S₀

C	2.915282	-3.751657	1.088619
H	3.456566	-3.825898	2.037213
H	2.737753	-4.764619	0.711553
H	3.548801	-3.226149	0.368207
O	-0.538154	-2.811608	0.265468
C	-1.410692	-2.642763	-0.878350
H	-1.113024	-1.747489	-1.430661
H	-1.319874	-3.518267	-1.528423
O	-2.984660	-1.278749	0.335719
C	-3.874007	-2.502529	-1.501865
C	-4.982236	-1.595726	-0.938812
H	-3.447259	-2.068608	-2.410022
H	-5.744768	-2.223040	-0.466537
H	-5.464586	-0.985189	-1.703915
O	-4.284105	-3.848386	-1.746855
H	-4.719285	-3.889415	-2.613209
N	-4.184168	0.701173	-0.122087
C	-3.604635	1.149633	-1.304048

P-5-S_{1,min}

C	-3.120028	4.032006	0.633809
H	-3.653107	4.267998	1.560581
H	-2.955490	4.964614	0.082690
H	-3.756469	3.383338	0.024900
O	0.326453	2.923085	-0.033112
C	1.187962	2.570459	-1.141049
H	0.860358	1.618767	-1.567981
H	1.124559	3.351560	-1.905021
O	2.728271	1.320005	0.229758
C	3.648622	2.291709	-1.735995
C	4.740195	1.447520	-1.055696
H	3.215748	1.750955	-2.581949
H	5.509153	2.118670	-0.660054
H	5.217679	0.738498	-1.733953
O	4.081494	3.587841	-2.150841
H	4.524123	3.509421	-3.010821
N	3.905772	-0.716388	0.040168
C	3.332417	-1.305567	-1.081461

O	-3.201624	0.403170	-2.192547	O	2.945969	-0.674299	-2.061800
N	-3.521950	2.525547	-1.409327	N	3.235693	-2.682939	-1.012430
H	-3.105026	2.868784	-2.270088	H	2.824718	-3.128461	-1.827965
C	-2.830644	-2.518550	-0.371867	C	2.604950	2.470368	-0.621013
H	-3.058074	-3.354725	0.304961	H	2.854332	3.375749	-0.048823
C	-4.591291	1.598117	0.852431	C	4.295377	-1.486755	1.123776
H	-5.007463	1.135899	1.740994	H	4.709096	-0.920538	1.951080
C	1.585022	-3.013083	1.309823	C	-1.784082	3.349839	0.968672
H	0.975777	-3.578322	2.022533	H	-1.171091	4.038450	1.560020
C	1.780416	-1.609181	1.884429	C	-1.961648	2.071822	1.793546
C	2.440969	-0.615368	1.148150	C	-2.598518	0.961288	1.250239
C	1.313708	-1.297791	3.167916	C	-1.489545	2.026701	3.121325
C	2.616029	0.675086	1.671176	C	-2.790931	-0.233216	2.013480
H	2.795333	-0.839089	0.146277	H	-2.959015	0.994233	0.225003
C	1.491724	-0.016833	3.703257	C	-1.673107	0.862365	3.888871
H	0.805799	-2.059785	3.754087	H	-0.987001	2.889840	3.548944
C	2.126363	0.971615	2.954976	C	-2.307083	-0.251414	3.361964
H	1.127443	0.206363	4.702317	H	-1.309000	0.835732	4.913575
H	2.255485	1.972554	3.355024	H	-2.442023	-1.146032	3.962704
C	-4.291616	-0.745824	0.146637	C	4.029825	0.751526	0.123218
H	-4.839440	-0.805514	1.089911	H	4.571133	0.925036	1.056175
C	-3.923271	3.490035	-0.479874	C	3.620078	-3.525991	0.034747
O	-3.772740	4.688723	-0.732796	O	3.460371	-4.745778	-0.066834
C	-4.499700	2.946471	0.741600	C	4.191068	-2.837455	1.183321
C	-4.958900	3.892591	1.815688	C	4.631478	-3.642996	2.373613
H	-5.364507	3.344645	2.671261	H	5.035320	-2.993310	3.155671
H	-4.131179	4.519283	2.168173	H	3.794551	-4.211877	2.795652
H	-5.735812	4.568523	1.439110	H	5.404759	-4.368335	2.094023
C	0.779111	-2.924463	0.015827	C	-0.990249	3.038253	-0.295419
O	1.249602	-2.928405	-1.108551	O	-1.461374	2.890533	-1.410596
O	2.828302	2.933927	1.005565	O	-3.675557	-2.506084	2.032515
C	3.241225	1.777776	0.870257	C	-3.432577	-1.358328	1.465024
C	4.351987	1.483961	-0.081549	C	-3.996002	-1.540289	0.097798
C	4.543960	2.337330	-1.185002	C	-3.199342	-2.096685	-0.938243
C	5.259369	0.430576	0.118077	C	-5.365298	-1.262054	-0.157310
C	5.595901	2.126306	-2.069597	C	-3.719516	-2.235734	-2.212265
H	3.852269	3.159471	-1.342540	H	-2.171051	-2.373063	-0.727138
C	6.326951	0.239069	-0.761816	C	-5.873979	-1.405283	-1.435561
H	5.153729	-0.226811	0.975490	H	-5.993265	-0.900801	0.651035
C	6.509637	1.073372	-1.873784	C	-5.063936	-1.890988	-2.489681
H	5.717092	2.786951	-2.925299	H	-3.093659	-2.620226	-3.012667

H	7.027658	-0.572225	-0.579729	H	-6.910502	-1.149624	-1.636598
C	7.646659	0.853250	-2.842113	C	-5.617559	-2.029951	-3.876987
H	7.268450	0.560349	-3.829986	H	-5.458702	-1.095530	-4.435145
H	8.230967	1.770740	-2.981860	H	-5.116868	-2.828423	-4.432916
H	8.323090	0.066646	-2.494091	H	-6.694978	-2.220661	-3.864240

P-5- $T_{1,min}$

C	2.886266	-3.936985	1.052710
H	3.396330	-4.066861	2.012674
H	2.699246	-4.927588	0.623828
H	3.553072	-3.393070	0.377402
O	-0.515351	-2.859884	0.172946
C	-1.347233	-2.616898	-0.986814
H	-1.008190	-1.708032	-1.491248
H	-1.262031	-3.465652	-1.672205
O	-2.920510	-1.256921	0.232014
C	-3.791495	-2.387034	-1.667948
C	-4.903769	-1.499682	-1.081929
H	-3.338110	-1.908700	-2.540510
H	-5.681305	-2.142852	-0.657760
H	-5.364247	-0.845905	-1.824272
O	-4.208285	-3.712983	-1.995013
H	-4.628162	-3.701887	-2.869776
N	-4.114456	0.745269	-0.122854
C	-3.526095	1.261136	-1.272752
O	-3.120982	0.567687	-2.202092
N	-3.437758	2.640682	-1.294916
H	-3.015413	3.033040	-2.131695
C	-2.777346	-2.474041	-0.515438
H	-3.043772	-3.329180	0.122798
C	-4.524078	1.584003	0.901184
H	-4.948042	1.071319	1.757810
C	1.567102	-3.177789	1.268558
H	0.922404	-3.763181	1.932361
C	1.773516	-1.808454	1.920829
C	2.468487	-0.800417	1.252355
C	1.260778	-1.558645	3.206892
C	2.690197	0.465936	1.853529
H	2.829718	-0.979472	0.243860

P-6- S_0

C	2.446081	-4.094884	0.891287
H	2.937037	-4.303205	1.847272
H	2.251702	-5.047761	0.387316
H	3.132523	-3.513749	0.268637
O	-0.923817	-2.893635	0.039593
C	-1.733137	-2.559824	-1.114354
H	-1.348547	-1.645802	-1.574340
H	-1.679477	-3.380710	-1.836071
O	-3.253214	-1.183357	0.152862
C	-4.154941	-2.189786	-1.806343
C	-5.218646	-1.254246	-1.206006
H	-3.664934	-1.715833	-2.660981
H	-6.037801	-1.861671	-0.808155
H	-5.631613	-0.553605	-1.933567
O	-4.647119	-3.478786	-2.175035
H	-5.052185	-3.418758	-3.054817
N	-4.291640	0.908930	-0.184147
C	-3.642167	1.404960	-1.309309
O	-3.262032	0.702593	-2.242662
N	-3.460447	2.775365	-1.301957
H	-2.992242	3.153375	-2.120754
C	-3.159803	-2.371642	-0.647992
H	-3.472365	-3.239537	-0.049578
C	-4.667351	1.754326	0.847172
H	-5.144422	1.255714	1.683923
C	1.133662	-3.333755	1.140270
H	0.470406	-3.954342	1.751602
C	1.351305	-2.018486	1.889518
C	2.064454	-0.964474	1.300690
C	0.854645	-1.852383	3.188674
C	2.262071	0.245243	1.983806
H	2.442643	-1.074832	0.288474

C	1.452929	-0.306921	3.807580	C	1.055245	-0.653995	3.883350
H	0.711263	-2.336065	3.731310	H	0.305422	-2.662987	3.661686
C	2.153338	0.697655	3.150137	C	1.742251	0.397328	3.280695
H	1.054345	-0.120909	4.801893	H	0.667076	-0.543175	4.892192
H	2.311262	1.659262	3.629154	H	1.888143	1.336624	3.805221
C	-4.226325	-0.713721	0.059488	C	-4.511124	-0.542673	-0.035195
H	-4.785727	-0.828575	0.990870	H	-5.097247	-0.633921	0.882156
C	-3.840329	3.549415	-0.311455	C	-3.824843	3.691241	-0.310130
O	-3.683174	4.760523	-0.490851	O	-3.582696	4.892009	-0.462192
C	-4.426309	2.936101	0.871833	C	-4.478593	3.097107	0.847165
C	-4.888183	3.817795	1.998242	C	-4.908235	3.986445	1.980362
H	-5.297993	3.220668	2.818124	H	-5.379573	3.402858	2.776611
H	-4.060708	4.420619	2.390605	H	-4.052172	4.523054	2.406239
H	-5.662434	4.516401	1.659501	H	-5.623779	4.743264	1.637460
C	0.805463	-3.007431	-0.042724	C	0.394989	-3.060820	-0.168003
O	1.307113	-2.982660	-1.153629	O	0.915256	-2.978138	-1.267111
O	3.326493	2.765714	1.617987	O	2.529897	2.559398	1.584501
C	3.375753	1.522549	1.159729	C	2.940537	1.418761	1.339785
C	4.288870	1.439065	0.026247	C	4.088886	1.211314	0.418723
C	4.359411	2.514931	-0.905747	C	4.377364	2.198774	-0.538913
C	5.201162	0.359524	-0.131469	C	4.947765	0.095692	0.505523
C	5.249576	2.471352	-1.972780	C	5.464683	2.082553	-1.401112
H	3.684148	3.356246	-0.793103	H	3.727710	3.065566	-0.612113
C	6.064501	0.325545	-1.212237	C	6.048297	-0.023199	-0.332087
H	5.215662	-0.443829	0.598043	H	4.771975	-0.671837	1.252352
C	6.113664	1.379578	-2.159317	C	6.311212	0.964782	-1.297878
H	5.268975	3.295046	-2.682261	H	5.644734	2.854866	-2.139700
H	6.733577	-0.523917	-1.330791	H	6.719367	-0.873421	-0.254633
C	7.065312	1.313575	-3.324011	O	7.401146	0.753892	-2.079615
H	6.779424	0.512296	-4.019025	C	7.738776	1.724202	-3.078639
H	7.082121	2.253949	-3.882947	H	8.636033	1.341241	-3.565226
H	8.086681	1.092502	-2.989314	H	6.933854	1.824265	-3.815067
				H	7.952675	2.697068	-2.622491

P-6-S_{1,min}

C	-3.086389	4.066248	0.699863
H	-3.590832	4.311447	1.640221
H	-2.942794	4.992991	0.132960
H	-3.739425	3.407602	0.119737

P-6-T_{1,min}

C	2.345660	-4.389434	0.680251
H	2.782644	-4.711492	1.631029
H	2.135410	-5.279771	0.077346
H	3.084633	-3.783321	0.148089

O	0.340357	2.946136	-0.057144	O	-0.922970	-2.936615	-0.184063
C	1.165222	2.570554	-1.184740	C	-1.658783	-2.448195	-1.330858
H	0.815257	1.617081	-1.589562	H	-1.215034	-1.509599	-1.673586
H	1.088524	3.342126	-1.957188	H	-1.603434	-3.190227	-2.133376
O	2.727560	1.330148	0.170062	O	-3.184755	-1.145214	0.006233
C	3.599787	2.237278	-1.849120	C	-4.022841	-1.892514	-2.092145
C	4.694246	1.380708	-1.188671	C	-5.075264	-0.973363	-1.447576
H	3.128399	1.691214	-2.670634	H	-3.467965	-1.356637	-2.866880
H	5.492037	2.040688	-0.833418	H	-5.943236	-1.576526	-1.163098
H	5.131343	0.647204	-1.868124	H	-5.412550	-0.177435	-2.113516
O	4.047506	3.515541	-2.302481	O	-4.550689	-3.110043	-2.620256
H	4.449445	3.413503	-3.179767	H	-4.897283	-2.940609	-3.510627
N	3.843881	-0.739361	-0.018561	N	-4.117328	1.016721	-0.141490
C	3.221811	-1.336346	-1.109601	C	-3.387528	1.603012	-1.169919
O	2.824277	-0.715708	-2.092380	O	-2.988259	0.991761	-2.157801
N	3.089305	-2.708588	-1.006802	N	-3.147645	2.953544	-0.997355
H	2.643994	-3.160256	-1.800612	H	-2.620469	3.397708	-1.743896
C	2.596014	2.460570	-0.705661	C	-3.098663	-2.243963	-0.914096
H	2.877709	3.375338	-0.164420	H	-3.477867	-3.155280	-0.429647
C	4.236548	-1.495555	1.074160	C	-4.510782	1.759007	0.960319
H	4.685389	-0.922397	1.878207	H	-5.053371	1.194586	1.710933
C	-1.739099	3.390320	1.001290	C	1.058391	-3.593349	0.948746
H	-1.110096	4.086803	1.566386	H	0.340433	-4.239161	1.465359
C	-1.892003	2.122098	1.846469	C	1.295839	-2.369634	1.837628
C	-2.486141	0.982814	1.313293	C	2.064472	-1.298614	1.381487
C	-1.445750	2.118365	3.183834	C	0.739876	-2.322769	3.129131
C	-2.661493	-0.204610	2.092823	C	2.314176	-0.163688	2.198967
H	-2.825648	0.989161	0.280155	H	2.462882	-1.322591	0.370845
C	-1.614288	0.962529	3.969225	C	0.962911	-1.204097	3.945306
H	-0.976271	3.003455	3.604253	H	0.134044	-3.150109	3.489712
C	-2.205350	-0.178611	3.450970	C	1.732433	-0.137040	3.497529
H	-1.271301	0.965270	5.001834	H	0.530067	-1.172247	4.942507
H	-2.327468	-1.065115	4.066188	H	1.905631	0.722000	4.138833
C	4.009392	0.726229	0.028353	C	-4.403866	-0.430650	-0.169690
H	4.589170	0.903657	0.937035	H	-5.042552	-0.596936	0.700859
C	3.477124	-3.538631	0.049524	C	-3.524954	3.769525	0.073630
O	3.281772	-4.755442	-0.020316	O	-3.223745	4.966555	0.071002
C	4.094947	-2.840913	1.168009	C	-4.264323	3.082514	1.122867
C	4.540416	-3.632224	2.365956	C	-4.714213	3.859666	2.328486
H	4.982302	-2.978001	3.123236	H	-5.254574	3.215268	3.028147
H	3.697629	-4.166159	2.820728	H	-3.859113	4.299740	2.855073

H	5.284853	-4.386537	2.084778	H	-5.374432	4.686252	2.040219
C	-0.983227	3.066425	-0.281997	C	0.394626	-3.158521	-0.354085
O	-1.485804	2.912963	-1.382853	O	0.963703	-3.004079	-1.421424
O	-3.476370	-2.500391	2.145800	O	3.141664	2.091198	2.408346
C	-3.259599	-1.363140	1.552879	C	3.070271	0.962564	1.728760
C	-3.769031	-1.549278	0.166326	C	3.990352	1.028676	0.595437
C	-5.141554	-1.319057	-0.134637	C	4.100852	2.240742	-0.152120
C	-2.928204	-2.091373	-0.848108	C	4.888483	-0.032969	0.276946
C	-5.634631	-1.499134	-1.410233	C	4.989684	2.363944	-1.207582
H	-5.798579	-0.961913	0.651911	H	3.447859	3.068964	0.099172
C	-3.402966	-2.276906	-2.123756	C	5.760089	0.077555	-0.783254
H	-1.893924	-2.319268	-0.611294	H	4.875103	-0.942435	0.868430
C	-4.763414	-1.978425	-2.423171	C	5.824234	1.278444	-1.541428
H	-6.671824	-1.277237	-1.628876	H	5.024147	3.288616	-1.771521
H	-2.767979	-2.644993	-2.922708	H	6.422286	-0.739918	-1.052376
O	-5.285766	-2.177171	-3.057738	O	6.717689	1.276628	-2.548527
C	-6.651738	-1.893413	-3.433237	C	6.879948	2.455555	-3.354773
H	-6.740963	-2.247637	-4.458504	H	7.654401	2.205343	-4.078948
H	-7.341934	-2.437289	-2.783657	H	5.947116	2.696989	-3.874030
H	-6.838501	-0.817622	-3.387232	H	7.202468	3.301017	-2.739009

P-7-S₀

C	2.330848	-4.012457	1.131040
H	2.779371	-4.199508	2.111905
H	2.182189	-4.974663	0.629451
H	3.033522	-3.422797	0.535119
O	-1.020302	-2.907392	0.102038
C	-1.781260	-2.593888	-1.090144
H	-1.387103	-1.679560	-1.541157
H	-1.686166	-3.420872	-1.800546
O	-3.367066	-1.228726	0.104716
C	-4.173256	-2.247505	-1.890179
C	-5.267318	-1.314121	-1.342935
H	-3.648660	-1.775841	-2.725270
H	-6.101083	-1.923692	-0.980260
H	-5.649599	-0.618528	-2.091744
O	-4.642375	-3.540980	-2.272819
H	-5.009155	-3.487531	-3.169663
N	-4.396940	0.857592	-0.289175

P-7-S_{1,min}

C	4.815756	-2.903624	-0.835644
H	5.549631	-3.172967	-0.069428
H	4.878962	-3.634849	-1.648483
H	5.079301	-1.920325	-1.236923
O	1.119409	-2.951199	-0.858349
C	0.009433	-2.613024	-1.725005
H	-0.014728	-1.529900	-1.871772
H	0.146598	-3.107147	-2.691517
O	-1.524140	-2.338322	0.116214
C	-2.502959	-2.917452	-1.969395
C	-3.635130	-2.689064	-0.952915
H	-2.382369	-2.041299	-2.612877
H	-4.129166	-3.645006	-0.752206
H	-4.386815	-1.980466	-1.304473
O	-2.654182	-4.093506	-2.764468
H	-3.250636	-3.896716	-3.504354
N	-3.221443	-0.831319	0.764741

C	-3.698852	1.351590	-1.385739	C	-3.043595	0.230870	-0.114912
O	-3.276987	0.647345	-2.299539	O	-2.660210	0.100799	-1.275325
N	-3.519097	2.722230	-1.373941	N	-3.340942	1.468882	0.423477
H	-3.016726	3.098819	-2.172903	H	-3.229779	2.254720	-0.210921
C	-3.229005	-2.417957	-0.688158	C	-1.266020	-3.098611	-1.073753
H	-3.560244	-3.286936	-0.101589	H	-1.170535	-4.163254	-0.815170
C	-4.816810	1.704861	0.723493	C	-3.623064	-0.608819	2.072207
H	-5.329357	1.207662	1.539861	H	-3.706717	-1.506883	2.674508
C	0.990694	-3.279956	1.307196	C	3.406623	-2.892621	-0.219750
H	0.312315	-3.909722	1.891687	H	3.176710	-3.892161	0.165903
C	1.139788	-1.952369	2.051071	C	3.297930	-1.912302	0.948216
C	1.869932	-0.893605	1.494148	C	3.190009	-0.533511	0.724024
C	0.558430	-1.776783	3.313458	C	3.335742	-2.377128	2.269474
C	2.001426	0.328068	2.173812	C	3.131665	0.371232	1.795309
H	2.312127	-1.011786	0.509378	H	3.170130	-0.157598	-0.295154
C	0.692339	-0.566389	4.004210	C	3.291157	-1.482603	3.345042
H	-0.005155	-2.591157	3.762119	H	3.403622	-3.445301	2.461300
C	1.398732	0.488743	3.434370	C	3.199862	-0.111807	3.113072
H	0.238658	-0.451270	4.984582	H	3.322776	-1.860743	4.363105
H	1.499063	1.435783	3.955007	H	3.165476	0.589956	3.940695
C	-4.617565	-0.594317	-0.144276	C	-2.926698	-2.209783	0.331194
H	-5.244789	-0.684034	0.745578	H	-3.214951	-2.829972	1.183253
C	-3.925790	3.639853	-0.400305	C	-3.764588	1.769471	1.721849
O	-3.677858	4.840414	-0.544279	O	-3.986272	2.941011	2.040807
C	-4.627919	3.047631	0.729365	C	-3.903205	0.611418	2.592976
C	-5.105142	3.939071	1.841689	C	-4.343167	0.815681	4.015799
H	-5.606511	3.356573	2.620198	H	-4.403112	-0.139230	4.546178
H	-4.268203	4.479184	2.299884	H	-3.644289	1.466327	4.554676
H	-5.808345	4.692968	1.468206	H	-5.327652	1.296492	4.057924
C	0.311241	-3.034112	-0.038576	C	2.344488	-2.574233	-1.268742
O	0.885014	-2.936478	-1.109343	O	2.551494	-2.025921	-2.337292
O	2.396945	2.646711	1.870611	O	3.635445	2.621889	2.341734
C	2.707946	1.494838	1.568129	C	3.057994	1.848605	1.571829
C	3.821222	1.278708	0.578309	C	2.276559	2.394148	0.421853
C	3.967382	2.198113	-0.474225	C	2.638283	3.655553	-0.100261
C	4.753863	0.239395	0.727259	C	1.151095	1.728663	-0.108879
C	5.013306	2.074265	-1.382518	C	1.926835	4.233464	-1.134901
H	3.251550	3.006493	-0.579293	H	3.496995	4.170707	0.317025
C	5.820878	0.115836	-0.160521	C	0.403852	2.288938	-1.132402
H	4.665438	-0.464305	1.548071	H	0.839725	0.773600	0.299738
C	5.927115	1.031924	-1.207187	C	0.802983	3.542548	-1.650914

H	5.125544	2.768172	-2.206376	H	2.215801	5.193736	-1.547706
H	6.553515	-0.673457	-0.046426	H	-0.470103	1.780217	-1.526230
N	7.041373	0.898135	-2.155225	N	0.086561	4.101198	-2.666945
O	7.842282	-0.025872	-1.987351	O	-0.964513	3.610248	-3.251949
O	7.124985	1.715940	-3.075802	O	0.306073	5.238836	-3.253650

P-7-T_{1,min}

C	2.276165	-4.066789	1.071355
H	2.729254	-4.265412	2.047858
H	2.115497	-5.023734	0.563381
H	2.980368	-3.478715	0.475622
O	-1.070716	-2.913904	0.074990
C	-1.835551	-2.584248	-1.110235
H	-1.433050	-1.672288	-1.558718
H	-1.755457	-3.408170	-1.826041
O	-3.397273	-1.206557	0.102589
C	-4.227652	-2.203895	-1.893523
C	-5.306179	-1.259267	-1.335030
H	-3.701985	-1.734829	-2.729372
H	-6.145382	-1.859868	-0.969918
H	-5.684331	-0.555281	-2.078103
O	-4.715901	-3.489201	-2.279883
H	-5.085415	-3.426772	-3.175015
N	-4.399757	0.895895	-0.277910
C	-3.700131	1.384278	-1.375954
O	-3.291536	0.677503	-2.293837
N	-3.502212	2.752378	-1.360509
H	-2.997944	3.124868	-2.160196
C	-3.278457	-2.392723	-0.698121
H	-3.616795	-3.260929	-0.114478
C	-4.804845	1.745428	0.738800
H	-5.320338	1.252369	1.555816
C	0.944274	-3.322833	1.261998
H	0.264293	-3.950148	1.847381
C	1.112595	-2.002215	2.014238
C	1.832837	-0.940022	1.450317
C	0.560963	-1.837603	3.291286
C	1.983606	0.275157	2.136831
H	2.250681	-1.049266	0.453752

C	0.714395	-0.633759	3.988963
H	0.005140	-2.654492	3.745186
C	1.409678	0.425353	3.411493
H	0.283490	-0.525700	4.980449
H	1.521730	1.368236	3.937542
C	-4.639834	-0.553486	-0.137184
H	-5.263442	-0.637633	0.755753
C	-3.893518	3.672254	-0.382693
O	-3.630723	4.869965	-0.524120
C	-4.599012	3.085700	0.747820
C	-5.060904	3.979662	1.864594
H	-5.567345	3.401147	2.642798
H	-4.215532	4.507305	2.321847
H	-5.755453	4.743874	1.495909
C	0.257495	-3.062410	-0.077037
O	0.823216	-2.971929	-1.152765
O	2.298662	2.596597	1.788375
C	2.671223	1.451457	1.519818
C	3.814278	1.252619	0.575785
C	4.042936	2.229949	-0.415455
C	4.709967	0.171129	0.692956
C	5.113998	2.129306	-1.287316
H	3.358599	3.067770	-0.497380
C	5.805562	0.056839	-0.151740
H	4.566924	-0.575086	1.466978
C	5.995796	1.036174	-1.146786
H	5.279105	2.870758	-2.061594
H	6.504424	-0.766537	-0.051836
N	7.069973	0.926165	-1.998936
O	7.974571	-0.014479	-2.014406
O	7.398304	1.735899	-2.968093