

## Supporting Information

### Complete Reference 18

Gaussian 09, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, N. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, 2009.

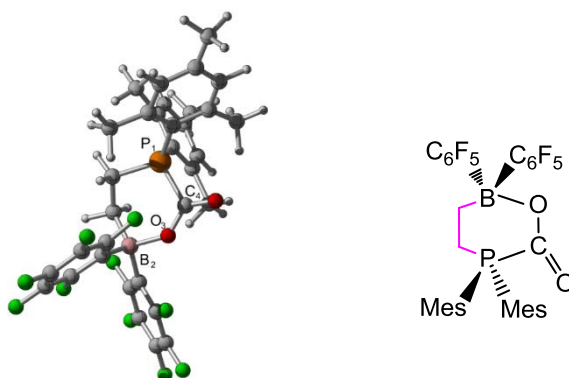
**Table S1.** The  $\Delta E_{\text{gas}}$ ,  $\Delta G_{\text{gas}}$ , and,  $\Delta E_{\text{sol}}$  of the species involved in  $\text{H}_2$  activation by FLPs A, B, C and D with density functionals B97D, B3LYP, wB97XD and BPW91.

	B97D			B3LYP			wB97XD			BPW91		
	$\Delta E_{\text{gas}}$	$\Delta G_{\text{gas}}$	$\Delta G_{\text{sol}}$	$\Delta E_{\text{gas}}$	$\Delta G_{\text{gas}}$	$\Delta G_{\text{sol}}$	$\Delta E_{\text{gas}}$	$\Delta G_{\text{gas}}$	$\Delta G_{\text{sol}}$	$\Delta E_{\text{gas}}$	$\Delta G_{\text{gas}}$	$\Delta G_{\text{sol}}$
A + $\text{H}_2$	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
A1	-2.0	4.5	6.0	1.9	7.9	12.9	-1.0	5.1	5.8	-0.4	4.0	5.1
TS12A	21.9	28.7	21.8	13.3	22.6	20.7	22.0	28.6	22.9	10.5	19.8	16.7
A2	4.6	12.7	-1.4	-3.6	7.4	-6.7	-1.2	5.2	-7.0	-4.3	7.3	-7.2
B + $\text{H}_2$	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
B1	4.5	9.2	7.1	1.0	6.4	8.7	4.5	11.0	9.3	0.7	6.3	5.9
TS12B	21.2	28.2	21.3	16.3	26.0	21.6	18.6	27.8	21.6	13.1	23.7	22.4
B2	0.9	10.4	-3.9	-4.6	7.5	-5.2	-6.4	3.7	-8.0	-5.3	8.6	-3.1
C + $\text{H}_2$	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C1	-1.1	5.2	4.4	0.8	6.0	6.4	-1.9	7.7	8.0	0.9	6.5	6.9
TS12C	14.1	22.9	17.3	16.1	24.8	20.4	12.3	24.5	19.1	14.3	21.4	17.4
C2	-1.0	8.4	-4.6	-6.2	5.8	-5.6	-8.5	3.2	-6.4	-4.8	6.9	-2.6
D + $\text{H}_2$	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
D1	-6.8	3.3	5.9	0.9	7.5	7.9	-8.7	3.1	4.9	1.8	12.0	14.2
TS12D	16.3	27.4	23.5	17.4	30.5	25.2	15.6	27.5	24.3	15.3	28.0	28.1
D2	-1.8	11.7	1.7	-1.2	11.1	-3.3	-7.5	6.0	-2.2	1.7	16.3	6.8

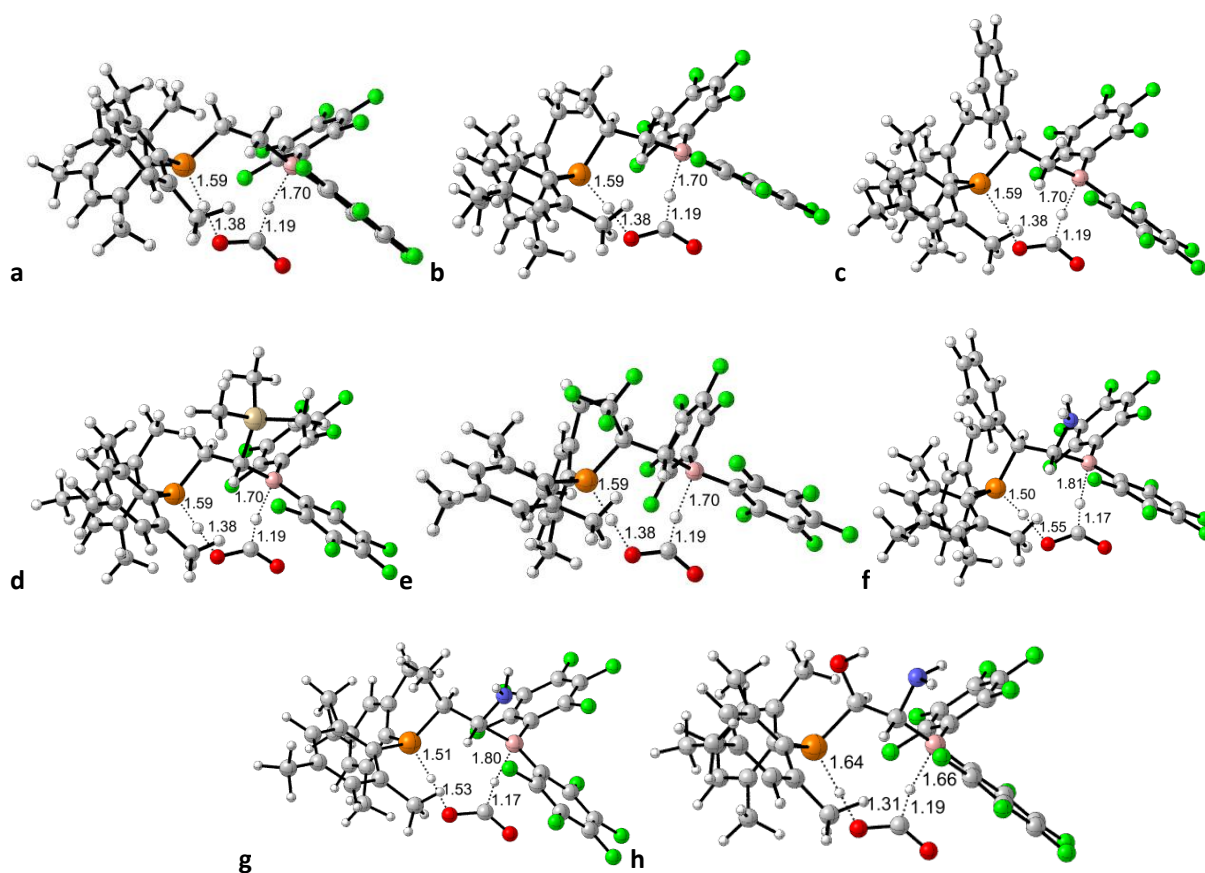
**Table S2.** The  $\Delta E_{\text{gas}}$ ,  $\Delta G_{\text{gas}}$ , and,  $\Delta E_{\text{sol}}$  of the species involved in the direct hydrogenation route when system L is used as the catalyst.

Species	$\Delta E_{\text{gas}}$	$\Delta G_{\text{gas}}$	$\Delta E_{\text{sol}}$
<b>L</b>	0.0	0.0	0.0
<b>L1</b>	20.2	12.8	12.8
<b>TSL12</b>	42.4	30.2	21.0
<b>L2</b>	17.9	4.0	-7.2
<b>L3</b>	23.4	1.2	-10.9
<b>TS34L</b>	54.2	29.5	-2.1
<b>L4</b>	20.7	-4.4	-20.6
<b>HCOOH</b>	18.5	6.0	-14.4

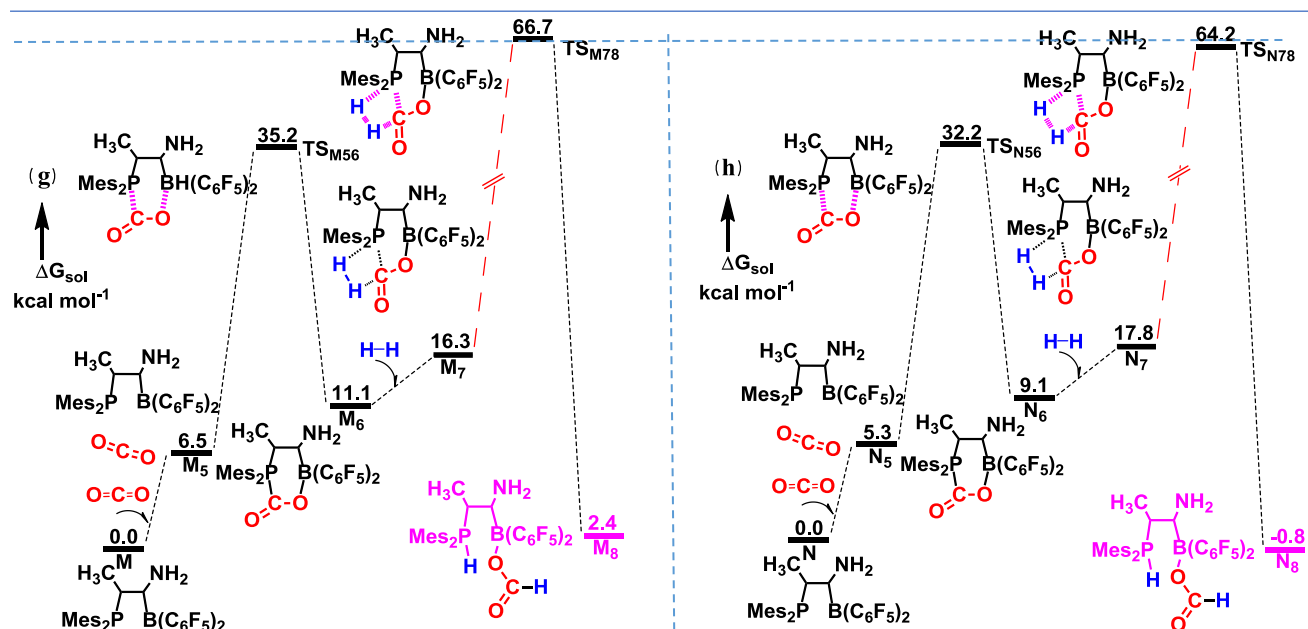
**Table S3.** Selected bond distances ( $\text{\AA}$ ) for  $\mathbf{A}_6$  from both experimental and theoretical investigations.



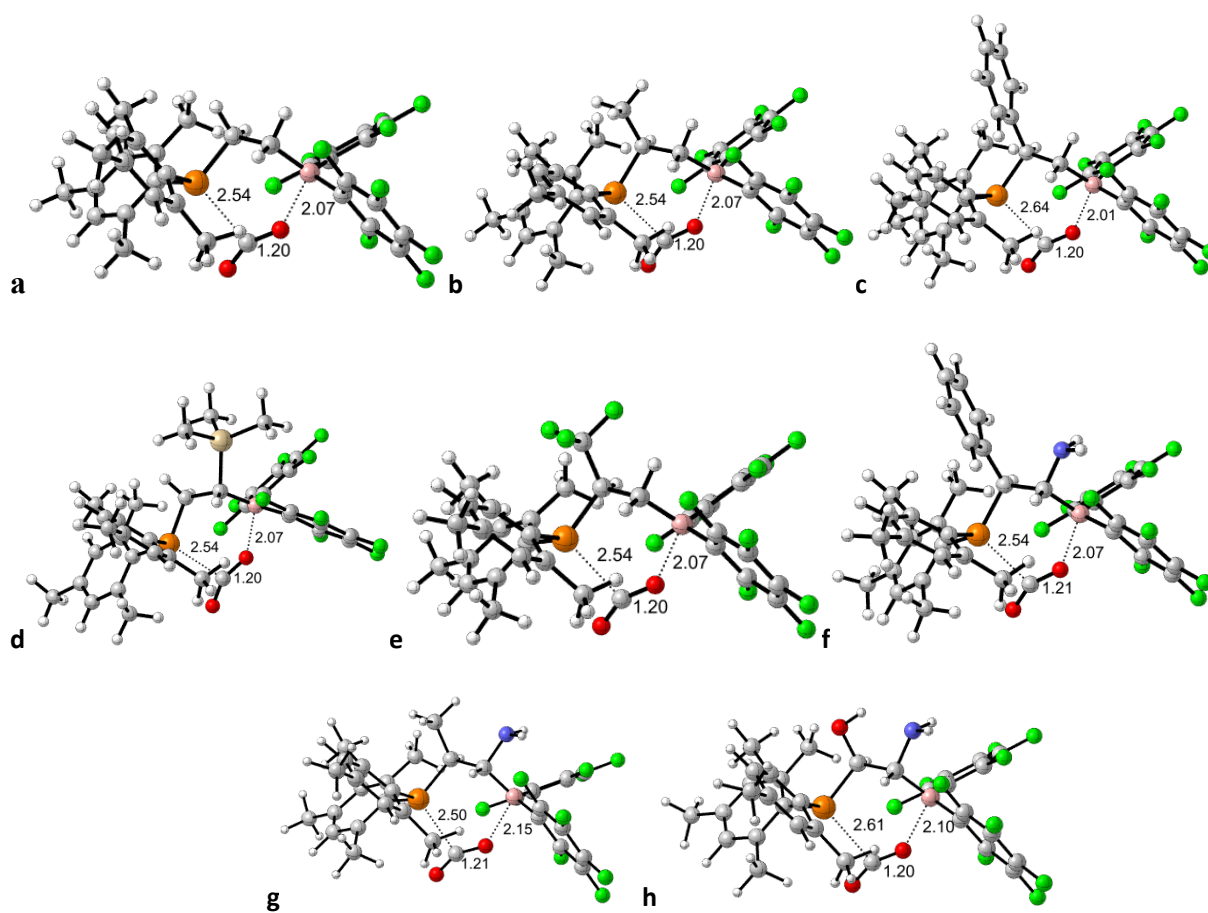
Ref 8	Parameters	$[\mathbf{A}_6]$	
		X-Ray <sup>a</sup>	Theoretical
Bond ( $\text{\AA}$ )	P1-C4	1.900	1.953
	B2-O3	1.550	1.564
	C4-O3	1.300	1.282



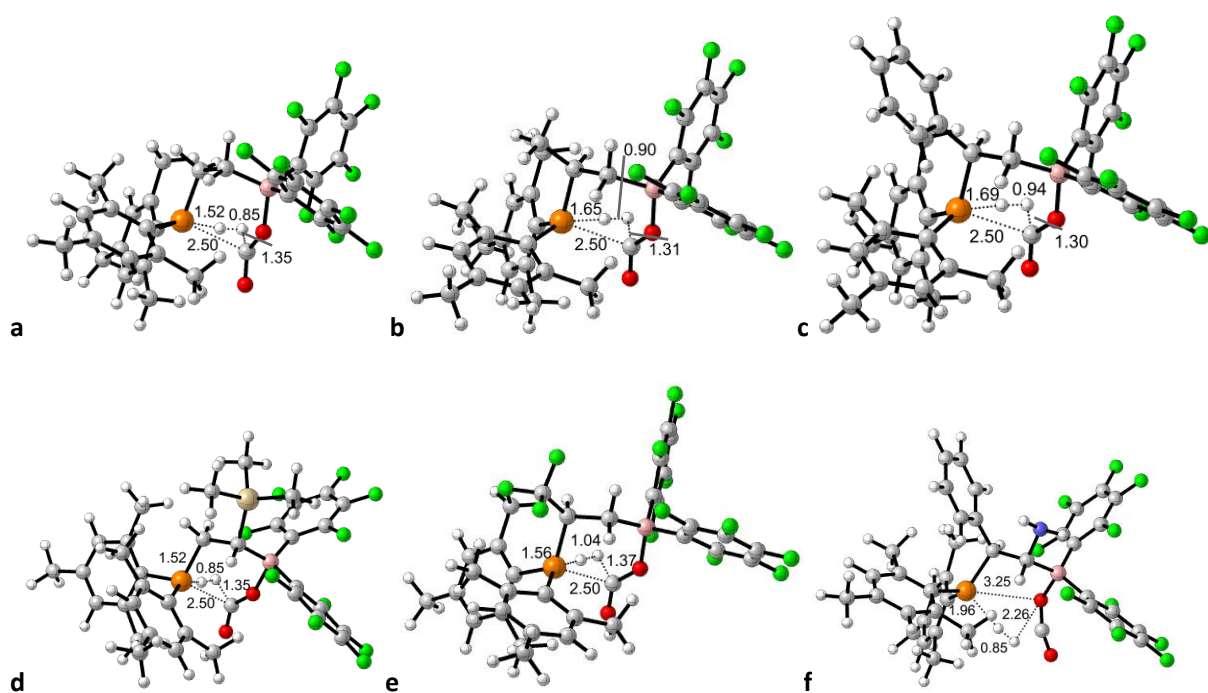
**Figure S1.** Optimized structure of reductive elimination TS (a) TS<sub>34A</sub>; (b) TS<sub>34B</sub>; (c) TS<sub>34C</sub>; (d) TS<sub>34D</sub>; (e) TS<sub>34E</sub>; (f) TS<sub>34L</sub>; (g) TS<sub>34M</sub>; (h) TS<sub>34N</sub>.

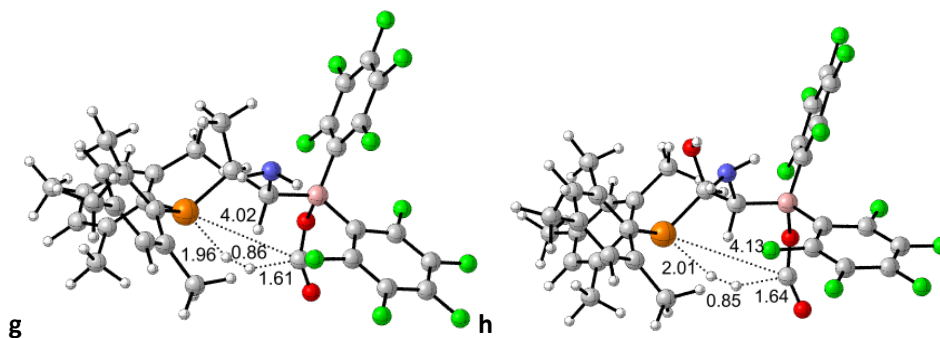


**Figure S2.** Energy profiles calculated for CO<sub>2</sub> reduction through transferring hydrogenation pathway catalyzed by systems **M** and **N**. The calculated solvent-corrected free energies are given in kcal/mol.

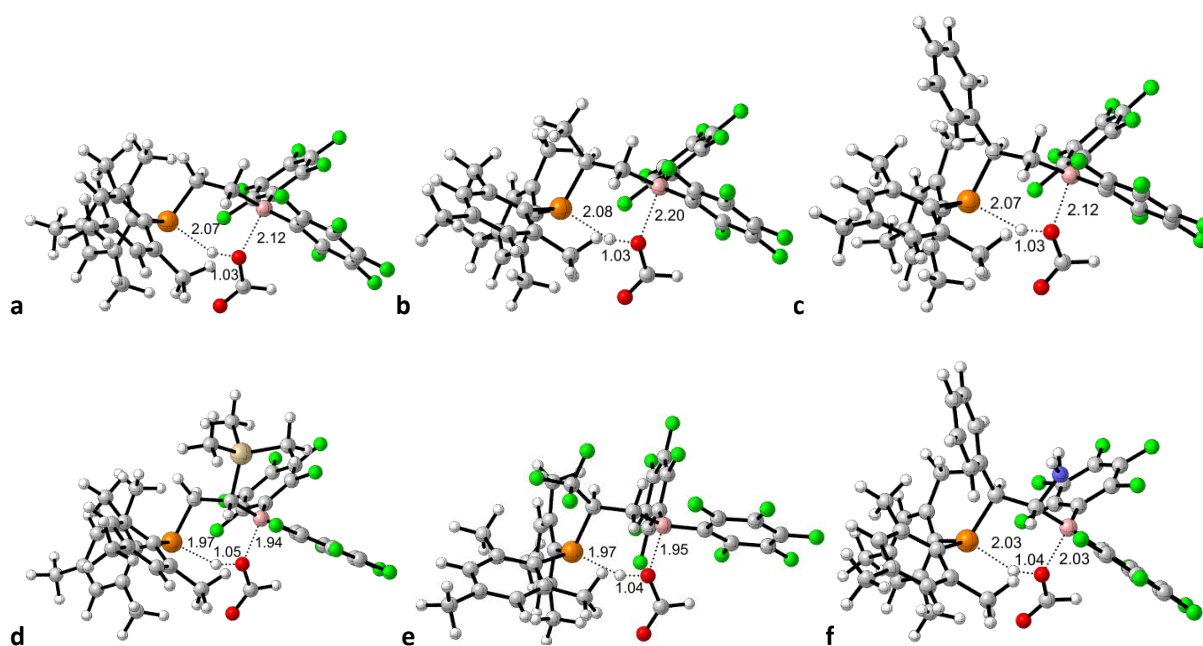


**Figure S3.** Optimized structure of reductive elimination TS (a) TSA34; (b) TSB34; (c) TSC34; (d) TSD34; (e) TSE34; (f) TSL34; (g) TSM34; (h) TSN34.

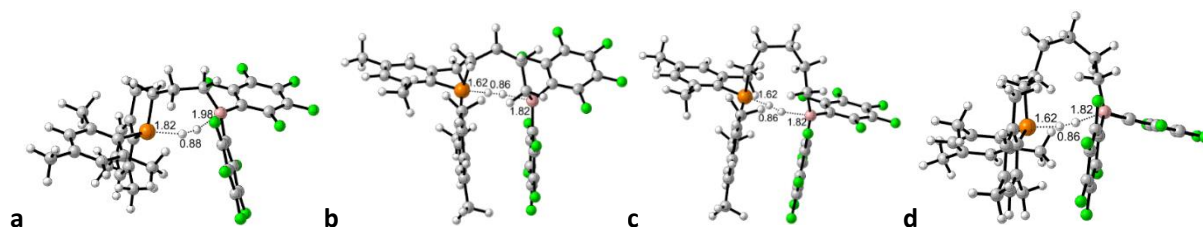




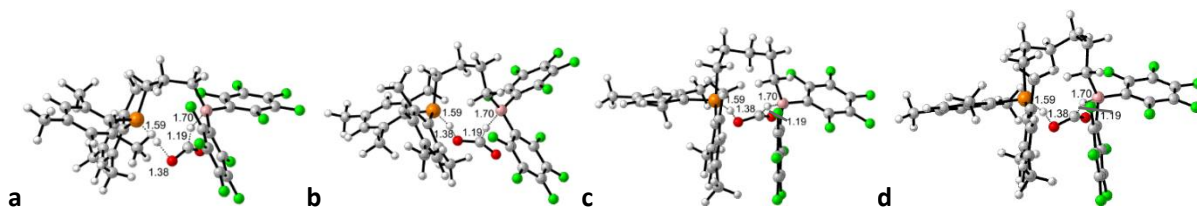
**Figure S4.** Optimized structure of reductive elimination TS (a)  $TS_{A34}$ ; (b)  $TS_{B34}$ ; (c)  $TS_{C34}$ ; (d)  $TS_{D34}$ ; (e)  $TS_{E34}$ ; (f)  $TS_{L34}$ ; (g)  $TS_{M34}$ ; (h)  $TS_{N34}$ .



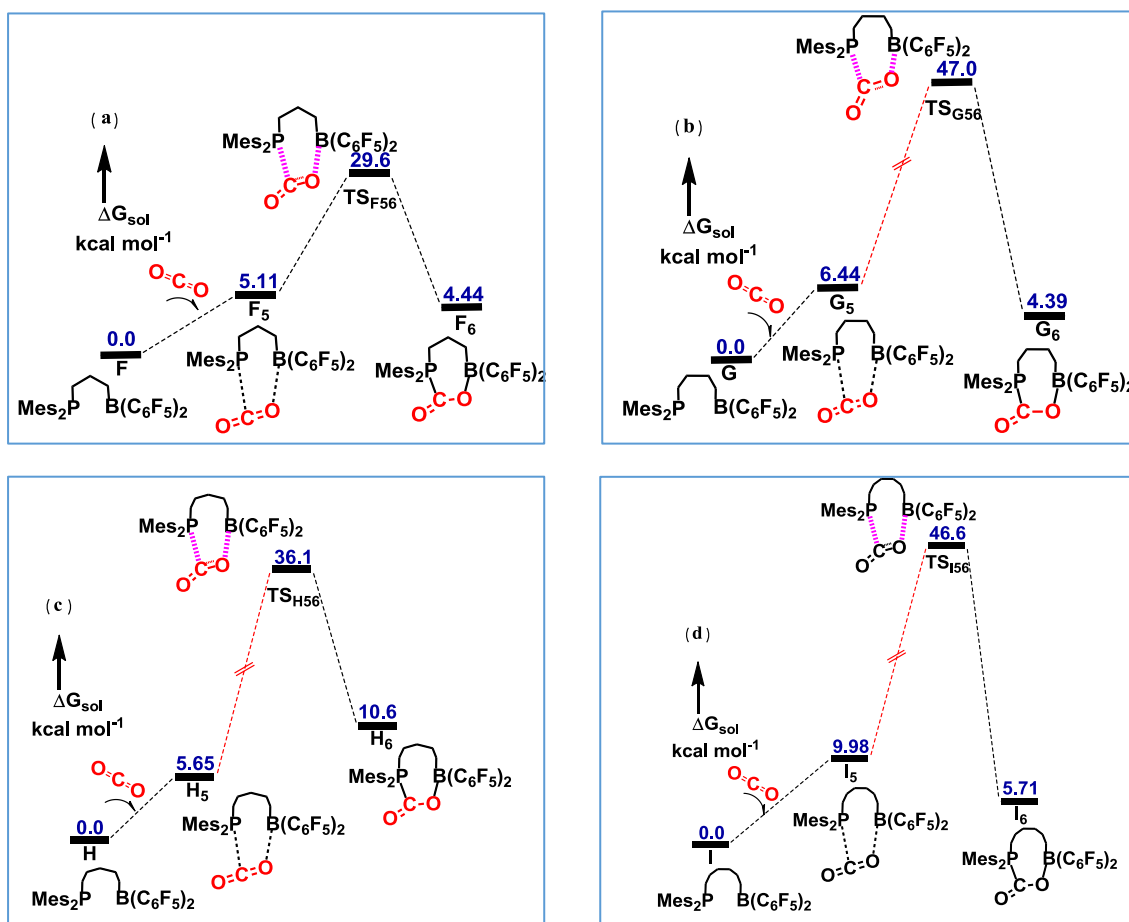
**Figure S4.** Optimized structure of reductive elimination TS (a)  $TS_{34A}$ ; (b)  $TS_{34B}$ ; (c)  $TS_{34C}$ ; (d)  $TS_{34D}$ ; (e)  $TS_{34E}$ ; (f)  $TS_{34L}$ .



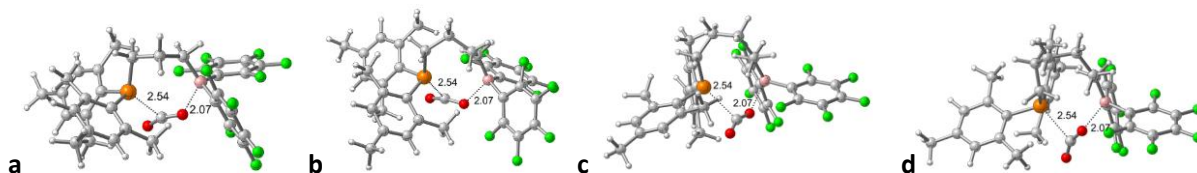
**Figure S5.** Optimized structure of H<sub>2</sub> activation TS (a)  $TS_{F12}$ ; (b)  $TS_{G12}$ ; (c)  $TS_{H12}$ ; (d)  $TS_{I12}$ .



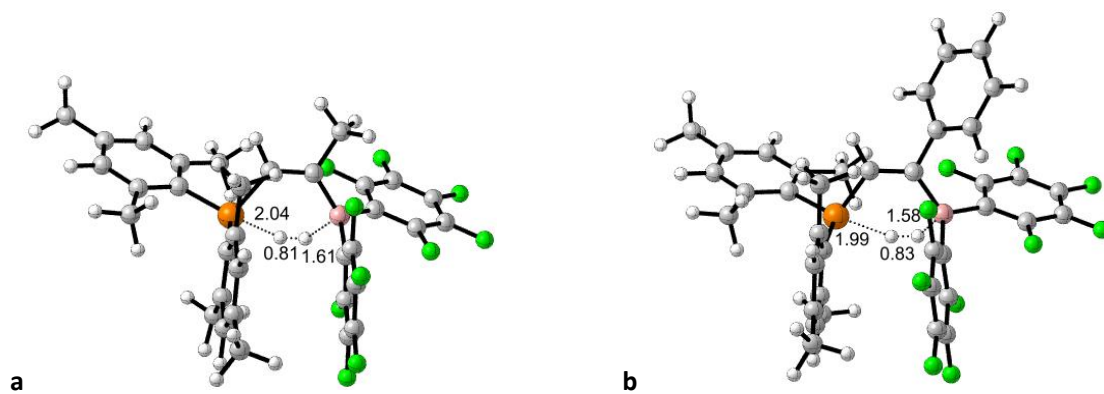
**Figure S6.** Optimized structure of reductive elimination TS (a)  $\text{TS}_{\text{F34}}$ ; (b)  $\text{TS}_{\text{G34}}$ ; (c)  $\text{TS}_{\text{H34}}$ ; (d)  $\text{TS}_{\text{I34}}$ .



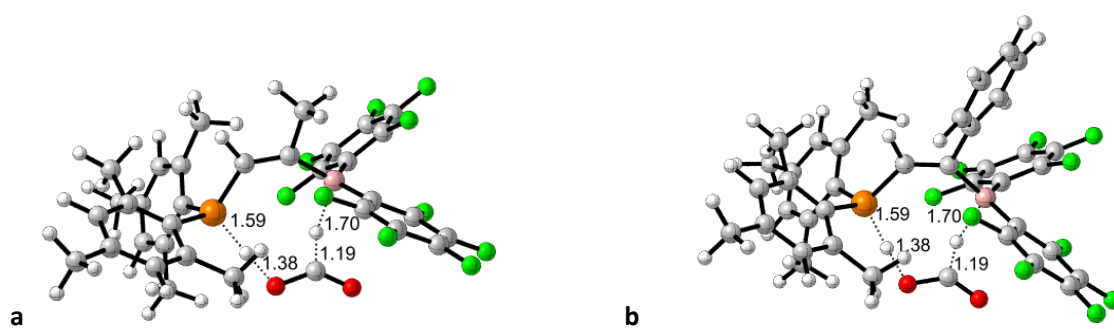
**Figure S7.** Energy profiles calculated for  $\text{CO}_2$  activation catalyzed by elongated alkyl chain-bridged FLPs. The calculated solvent-corrected free energies are given in kcal/mol.



**Figure S8.** Optimized structure of  $\text{CO}_2$  activation TS (a)  $\text{TS}_{\text{F56}}$ ; (b)  $\text{TS}_{\text{G56}}$ ; (c)  $\text{TS}_{\text{H56}}$ ; (d)  $\text{TS}_{\text{I56}}$ .



**Figure S9.** Optimized structure of H<sub>2</sub> activation TS (a) TS<sub>J12</sub>; (b) TS<sub>K12</sub>.



**Figure S10.** Optimized structure of reductive elimination TS (a) TS<sub>J34</sub>; (b) TS<sub>K34</sub>.



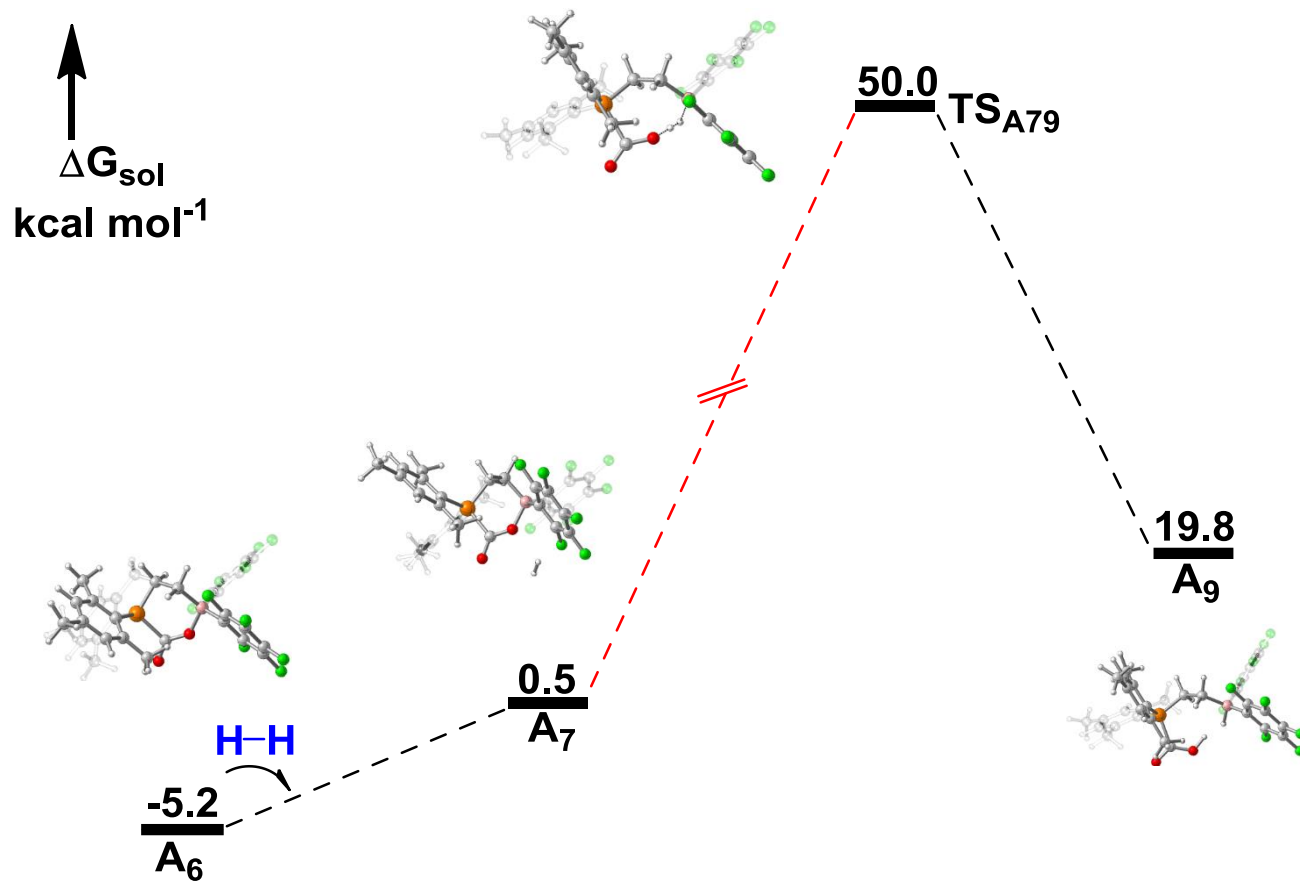


Figure S11. Energy profile for H<sub>2</sub> insertion into B-O bond in system A.

---

## Cartesian coordinates for all the species

calculated in this study:

### A

E= -2264.7253067au

C	2.231463	2.008357	0.476606
C	3.091848	2.899547	-0.217504
C	3.435070	4.122038	0.368413
H	4.097948	4.792420	-0.175942
C	2.953851	4.513145	1.620475
C	2.098838	3.637251	2.285687
H	1.704228	3.920176	3.259252
C	1.726837	2.398144	1.744907
C	3.655015	2.610708	-1.591406
H	2.861092	2.540852	-2.344337
H	4.215668	1.672736	-1.620065
H	4.326317	3.415974	-1.905446
C	3.350549	5.840163	2.223248
H	2.869104	5.999621	3.193237
H	3.071205	6.675436	1.568957
H	4.435780	5.901163	2.374188
C	0.780046	1.542910	2.566675
H	1.179691	0.540727	2.748202
H	-0.189785	1.413984	2.076838
H	0.597202	2.014556	3.537779
C	3.210216	-0.558246	-0.746761
C	3.573535	-0.928464	-2.069134
C	4.723257	-1.706020	-2.276922
H	4.981182	-1.978911	-3.298232
C	5.548079	-2.133666	-1.239732
C	5.178164	-1.774242	0.056465
H	5.790043	-2.103403	0.894271
C	4.034378	-1.017558	0.323452
C	2.820739	-0.530797	-3.323492
H	3.278547	-1.004391	-4.197052
H	2.849994	0.550485	-3.494233
H	1.771756	-0.835955	-3.306954
C	6.795379	-2.943241	-1.503324
H	6.883944	-3.782985	-0.804101
H	7.699780	-2.331357	-1.386301
H	6.802305	-3.348549	-2.520356
C	3.723739	-0.732851	1.778163

H	4.451179	-1.230166	2.427095
H	2.725369	-1.094681	2.052408
H	3.750616	0.338027	2.007405
C	-2.823371	0.526580	-0.861079
C	-2.832833	1.796316	-0.292092
F	-1.732591	2.257835	0.339323
C	-3.946368	2.631782	-0.333534
F	-3.914116	3.843593	0.231444
C	-5.104540	2.193928	-0.973124
F	-6.179323	2.985048	-1.027000
C	-5.137171	0.929804	-1.558658
F	-6.244213	0.504431	-2.177034
C	-4.002939	0.126826	-1.487173
C	-1.611622	-1.683253	0.133645
C	-1.254068	-2.989921	-0.228606
F	-0.919116	-3.273176	-1.498551
C	-1.265566	-4.052669	0.669028
F	-0.937840	-5.287964	0.273301
C	-1.627631	-3.821514	1.994258
F	-1.633510	-4.827296	2.869865
C	-1.983880	-2.538421	2.405289
F	-2.321450	-2.316548	3.679565
C	-1.982239	-1.505161	1.474689
F	-2.312197	-0.281337	1.924239
F	-4.047048	-1.093800	-2.065308
C	-0.470901	-0.289191	-1.970499
H	-0.948531	-0.001493	-2.919200
H	0.071386	-1.220939	-2.153624
C	0.538190	0.838750	-1.589675
H	1.068208	1.181963	-2.477608
H	0.008735	1.709525	-1.190318
B	-1.598111	-0.488830	-0.884196
P	1.658486	0.329410	-0.151784
H	-0.746648	-8.001696	2.216903
H	-0.876815	-7.293393	2.036653

### A<sub>1</sub>

= -2265.897779au

C	2.231463	2.008357	0.476606
C	3.091848	2.899547	-0.217504
C	3.435070	4.122038	0.368413
H	4.097948	4.792420	-0.175942
C	2.953851	4.513145	1.620475

---

C	2.098838	3.637251	2.285687
H	1.704228	3.920176	3.259252
C	1.726837	2.398144	1.744907
C	3.655015	2.610708	-1.591406
H	2.861092	2.540852	-2.344337
H	4.215668	1.672736	-1.620065
H	4.326317	3.415974	-1.905446
C	3.350549	5.840163	2.223248
H	2.869104	5.999621	3.193237
H	3.071205	6.675436	1.568957
H	4.435780	5.901163	2.374188
C	0.780046	1.542910	2.566675
H	1.179691	0.540727	2.748202
H	-0.189785	1.413984	2.076838
H	0.597202	2.014556	3.537779
C	3.210216	-0.558246	-0.746761
C	3.573535	-0.928464	-2.069134
C	4.723257	-1.706020	-2.276922
H	4.981182	-1.978911	-3.298232
C	5.548079	-2.133666	-1.239732
C	5.178164	-1.774242	0.056465
H	5.790043	-2.103403	0.894271
C	4.034378	-1.017558	0.323452
C	2.820739	-0.530797	-3.323492
H	3.278547	-1.004391	-4.197052
H	2.849994	0.550485	-3.494233
H	1.771756	-0.835955	-3.306954
C	6.795379	-2.943241	-1.503324
H	6.883944	-3.782985	-0.804101
H	7.699780	-2.331357	-1.386301
H	6.802305	-3.348549	-2.520356
C	3.723739	-0.732851	1.778163
H	4.451179	-1.230166	2.427095
H	2.725369	-1.094681	2.052408
H	3.750616	0.338027	2.007405
C	-2.823371	0.526580	-0.861079
C	-2.832833	1.796316	-0.292092
F	-1.732591	2.257835	0.339323
C	-3.946368	2.631782	-0.333534
F	-3.914116	3.843593	0.231444
C	-5.104540	2.193928	-0.973124
F	-6.179323	2.985048	-1.027000
C	-5.137171	0.929804	-1.558658

F	-6.244213	0.504431	-2.177034
C	-4.002939	0.126826	-1.487173
C	-1.611622	-1.683253	0.133645
C	-1.254068	-2.989921	-0.228606
F	-0.919116	-3.273176	-1.498551
C	-1.265566	-4.052669	0.669028
F	-0.937840	-5.287964	0.273301
C	-1.627631	-3.821514	1.994258
F	-1.633510	-4.827296	2.869865
C	-1.983880	-2.538421	2.405289
F	-2.321450	-2.316548	3.679565
C	-1.982239	-1.505161	1.474689
F	-2.312197	-0.281337	1.924239
F	-4.047048	-1.093800	-2.065308
C	-0.470901	-0.289191	-1.970499
H	-0.948531	-0.001493	-2.919200
H	0.071386	-1.220939	-2.153624
C	0.538190	0.838750	-1.589675
H	1.068208	1.181963	-2.477608
H	0.008735	1.709525	-1.190318
B	-1.598111	-0.488830	-0.884196
P	1.658486	0.329410	-0.151784
H	-0.746648	-8.001696	2.216903
H	-0.876815	-7.293393	2.036653

### TS<sub>12A</sub>

E= -2265.8796583au

C	3.145266	1.379973	0.276442
C	4.208689	1.725500	-0.597841
C	5.064658	2.776786	-0.257411
H	5.876726	3.026969	-0.937248
C	4.910602	3.513440	0.919314
C	3.862390	3.163500	1.768523
H	3.723361	3.720052	2.692616
C	2.975833	2.117489	1.478193
C	4.464977	1.017188	-1.907808
H	3.632364	1.156227	-2.607037
H	4.605924	-0.058770	-1.771267
H	5.362716	1.416200	-2.389252
C	5.836926	4.660489	1.245253
H	5.783290	4.930331	2.304713
H	5.576694	5.555102	0.664146
H	6.878229	4.414418	1.008496

C	1.872547	1.852677	2.484000
H	1.854558	0.812349	2.820645
H	0.884902	2.078575	2.073395
H	2.011969	2.484879	3.366315
C	2.898264	-1.576385	-0.389066
C	3.029784	-2.278989	-1.618482
C	3.728056	-3.495556	-1.635936
H	3.816574	-4.022208	-2.583625
C	4.313224	-4.053548	-0.501422
C	4.170026	-3.358096	0.699142
H	4.602189	-3.771327	1.608111
C	3.473065	-2.150336	0.781798
C	2.480158	-1.820898	-2.954780
H	2.731803	-2.552646	-3.727648
H	2.904066	-0.862970	-3.269499
H	1.392222	-1.719072	-2.951340
C	5.084510	-5.349697	-0.567888
H	4.892889	-5.974743	0.311436
H	6.166530	-5.165108	-0.602934
H	4.821793	-5.927983	-1.459541
C	3.357137	-1.514573	2.150147
H	3.829761	-2.148921	2.905895
H	2.308779	-1.375549	2.439335
H	3.840372	-0.532318	2.193070
C	-2.280344	1.372116	-0.477878
C	-1.795982	2.618362	-0.081828
F	-0.554182	2.725963	0.451254
C	-2.515503	3.804533	-0.203662
F	-1.992217	4.967966	0.204679
C	-3.788632	3.772045	-0.764413
F	-4.495840	4.898371	-0.898877
C	-4.312910	2.556870	-1.196098
F	-5.529756	2.515270	-1.752995
C	-3.558448	1.395548	-1.047327
C	-2.325734	-1.262288	0.216412
C	-2.674973	-2.388041	-0.533692
F	-2.301249	-2.489246	-1.824793
C	-3.426340	-3.443405	-0.021079
F	-3.733905	-4.499367	-0.786161
C	-3.866873	-3.392582	1.298236
F	-4.586311	-4.397926	1.806945
C	-3.553005	-2.287153	2.084560
F	-3.971858	-2.229312	3.355868

C	-2.806672	-1.251998	1.529183
F	-2.529089	-0.201868	2.331026
F	-4.110277	0.255284	-1.509027
C	-0.410277	-0.320020	-1.550919
H	-0.919230	-0.141200	-2.508127
H	-0.142236	-1.382111	-1.561157
C	0.891073	0.532949	-1.522949
H	1.407249	0.512772	-2.481982
H	0.666550	1.582545	-1.302950
B	-1.481058	-0.029839	-0.379801
P	1.935750	-0.002002	-0.065088
H	0.100723	0.081124	0.761085
H	-0.708534	0.241012	0.874069

## A<sub>2</sub>

E=-2265.9065622au

C	-3.570856	-2.051735	-0.157473
C	-3.218284	-0.855762	0.514518
C	-3.834028	-0.534696	1.756615
C	-4.806995	-1.393831	2.270109
C	-5.192213	-2.563685	1.611064
C	-4.556461	-2.869656	0.408767
P	-1.942787	0.330774	-0.083993
C	-3.466887	0.679803	2.581897
C	-6.266158	-3.457327	2.181116
C	-2.920779	-2.555467	-1.427014
C	-0.802976	-0.129571	-1.464189
C	0.544017	0.618126	-1.287167
B	1.469398	0.064807	-0.026543
C	1.760837	-1.529661	-0.319813
C	0.883667	-2.524814	0.107667
C	1.024033	-3.880103	-0.183334
C	2.114690	-4.301672	-0.934721
C	3.025693	-3.352765	-1.391587
C	2.824841	-2.007039	-1.090127
F	-0.234734	-2.196277	0.822265
F	3.729789	-1.143253	-1.598235
F	4.074696	-3.745002	-2.131779
F	2.275606	-5.599676	-1.232941
F	0.100275	-4.770510	0.226784
C	2.830159	0.941174	0.271240
C	3.863008	0.413106	1.057107
C	5.014693	1.107934	1.416320

C	5.178793	2.424325	0.997306
C	4.178343	3.011292	0.234240
C	3.045274	2.269681	-0.101649
F	3.774169	-0.850247	1.530139
F	5.963612	0.525529	2.168188
F	6.277321	3.117092	1.334667
F	4.303404	4.289202	-0.166599
F	2.113956	2.957015	-0.819264
C	-2.645236	1.989830	-0.440695
C	-3.712004	2.116115	-1.366344
C	-4.202945	3.391014	-1.658532
C	-3.677918	4.543421	-1.069849
C	-2.622079	4.394258	-0.168435
C	-2.084288	3.146292	0.165484
C	-4.350732	0.934645	-2.064149
C	-4.244419	5.906795	-1.382796
C	-0.924217	3.123842	1.140564
H	1.077803	0.477399	-2.238427
H	-0.655981	-1.208610	-1.449196
H	-5.271268	-1.141318	3.220536
H	-4.823879	-3.786529	-0.110510
H	-2.189790	5.280377	0.289763
H	-5.017740	3.483552	-2.372738
H	-4.093807	0.730791	3.475930
H	-2.424707	0.635411	2.923341
H	-3.597589	1.618189	2.033666
H	-2.783173	-1.780361	-2.184274
H	-1.940445	-2.991792	-1.203238
H	-3.532438	-3.344058	-1.873585
H	-6.158049	-3.567671	3.265602
H	-7.264085	-3.038522	1.996268
H	-6.238037	-4.454704	1.732259
H	-0.739960	4.133099	1.518242
H	-1.114411	2.484883	2.009722
H	0.003204	2.779003	0.673399
H	-3.464506	6.675167	-1.374457
H	-4.731435	5.923530	-2.362883
H	-4.996268	6.198295	-0.637468
H	-4.876520	0.276913	-1.364037
H	-5.077461	1.280005	-2.804582
H	-3.617090	0.321350	-2.600274
H	0.344426	1.692109	-1.237415
H	-1.313401	0.131192	-2.398893

H	-1.076804	0.502626	1.008102
H	0.833933	0.125944	1.021899

### A<sub>3</sub>

E= -2454.494348au

C	-3.926538	-1.681726	-0.861706
C	-3.464541	-0.674150	0.021956
C	-4.099206	-0.494659	1.283830
C	-5.179121	-1.313284	1.618674
C	-5.657212	-2.306973	0.761325
C	-5.014778	-2.469160	-0.465263
P	-2.026290	0.425687	-0.319120
C	0.441405	-1.289053	3.344842
O	1.248494	-2.129574	3.373590
C	-3.646086	0.524225	2.306796
C	-6.837867	-3.163118	1.148795
C	-3.316869	-2.003802	-2.209376
C	-0.888356	-0.023390	-1.700552
C	0.499763	0.644481	-1.542388
B	1.396872	0.039709	-0.295462
O	-0.385786	-0.457645	3.358817
C	1.692336	-1.561192	-0.544308
C	0.863440	-2.553595	-0.021166
C	1.064536	-3.921593	-0.188916
C	2.154897	-4.354602	-0.935763
C	3.007719	-3.410906	-1.501605
C	2.757532	-2.053526	-1.304082
F	-0.248631	-2.209742	0.699389
F	3.611343	-1.199014	-1.906134
F	4.052364	-3.819858	-2.238495
F	2.373228	-5.664786	-1.120462
F	0.218537	-4.818612	0.347132
C	2.763706	0.892950	0.008356
C	3.306284	0.913588	1.296823
C	4.442802	1.635984	1.654891
C	5.101476	2.389226	0.688759
C	4.610236	2.400295	-0.612390
C	3.471207	1.658480	-0.921156
F	2.726301	0.202503	2.294589
F	4.905650	1.616532	2.916868
F	6.195867	3.096706	1.008055
F	5.238954	3.123052	-1.555333
F	3.064911	1.718464	-2.210473

C	-2.490751	2.197224	-0.455146
C	-3.472029	2.609143	-1.392108
C	-3.777947	3.968111	-1.493034
C	-3.147182	4.933800	-0.704951
C	-2.175278	4.505260	0.200701
C	-1.824645	3.158735	0.351638
C	-4.201643	1.649763	-2.307047
C	-3.516843	6.392659	-0.817075
C	-0.749564	2.821605	1.364088
H	1.001884	0.485556	-2.503818
H	-0.788983	-1.111604	-1.686881
H	-5.656150	-1.170346	2.585424
H	-5.364844	-3.241765	-1.145230
H	-1.661010	5.242451	0.812322
H	-4.527719	4.279699	-2.216511
H	-4.341087	0.544166	3.150572
H	-2.656615	0.276828	2.709238
H	-3.600492	1.538057	1.896128
H	-3.124614	-1.117430	-2.817714
H	-2.370390	-2.545509	-2.102562
H	-3.992485	-2.648115	-2.778284
H	-6.746874	-3.521768	2.180064
H	-7.773840	-2.592960	1.086610
H	-6.935187	-4.033377	0.492936
H	-0.361756	3.740148	1.812462
H	-1.127616	2.197650	2.182359
H	0.096227	2.287860	0.920647
H	-2.664428	7.040184	-0.588285
H	-3.874941	6.639482	-1.821696
H	-4.319174	6.647741	-0.112053
H	-4.791266	0.913411	-1.751415
H	-4.885601	2.196347	-2.961979
H	-3.511918	1.098191	-2.956836
H	0.371619	1.734006	-1.467400
H	-1.386696	0.258130	-2.634884
H	-1.233289	0.332908	0.834469
H	0.743530	0.111952	0.730282

**TS34A**

**E= -2454.4562256au**

C	3.611934	2.175030	-0.208362
C	3.353096	0.942453	0.441411
C	4.101653	0.597878	1.602647

C	5.114203	1.455799	2.040215
C	5.408102	2.656328	1.392475
C	4.635370	2.995386	0.282407
P	2.032646	-0.282195	-0.002736
C	-0.797657	-0.262510	2.283124
O	-1.769115	-0.293395	3.004207
C	3.837586	-0.647673	2.423765
C	6.526658	3.549251	1.871885
C	2.824125	2.716907	-1.381616
C	0.885430	0.184407	-1.402569
C	-0.425766	-0.632200	-1.317872
B	-1.648735	-0.053030	-0.449067
O	0.451692	-0.377467	2.497943
C	-1.900517	1.526877	-0.588199
C	-1.097861	2.521491	-0.029046
C	-1.300625	3.883592	-0.236614
C	-2.357594	4.300224	-1.039323
C	-3.186720	3.346777	-1.625873
C	-2.944977	1.996418	-1.391812
F	-0.040577	2.188425	0.750671
F	-3.764841	1.116366	-2.000108
F	-4.198009	3.735908	-2.411491
F	-2.565949	5.601514	-1.259082
F	-0.473200	4.785249	0.309088
C	-2.877841	-0.974774	-0.050068
C	-3.931777	-0.484794	0.742844
C	-4.998936	-1.267873	1.172136
C	-5.047325	-2.612258	0.818618
C	-4.028081	-3.152410	0.039991
C	-2.976411	-2.338746	-0.367704
F	-3.958138	0.799572	1.124102
F	-5.975098	-0.741528	1.919548
F	-6.063323	-3.378784	1.219682
F	-4.066254	-4.445987	-0.307981
F	-2.028406	-2.948758	-1.113442
C	2.805479	-1.878427	-0.553141
C	3.829068	-1.892669	-1.538931
C	4.362992	-3.117839	-1.946906
C	3.931921	-4.335555	-1.415755
C	2.923109	-4.301609	-0.454660
C	2.344304	-3.106004	-0.008504
C	4.398449	-0.645717	-2.181142
C	4.553701	-5.639354	-1.854194

C	1.230081	-3.226970	1.011711
H	-0.844355	-0.667349	-2.339330
H	0.684871	1.252030	-1.365091
H	5.680289	1.176860	2.926080
H	4.825279	3.939202	-0.223584
H	2.562500	-5.237079	-0.033364
H	5.143010	-3.117307	-2.705252
H	4.542479	-0.702403	3.258191
H	2.827587	-0.639326	2.850075
H	3.949313	-1.567831	1.840567
H	2.689400	1.990417	-2.186704
H	1.832165	3.055053	-1.060252
H	3.335895	3.583854	-1.808710
H	6.606194	3.538914	2.964161
H	7.494367	3.216779	1.473032
H	6.378570	4.585113	1.550516
H	1.257784	-4.217679	1.474768
H	1.280661	-2.485313	1.810534
H	0.244111	-3.126623	0.540249
H	3.880124	-6.484022	-1.678620
H	4.810651	-5.622353	-2.918838
H	5.480701	-5.838234	-1.300119
H	5.019044	-0.073339	-1.483889
H	5.022583	-0.916381	-3.037672
H	3.622406	0.032477	-2.549062
H	-0.202457	-1.676150	-1.092940
H	1.403887	-0.020478	-2.344301
H	1.159730	-0.396324	1.316756
H	-1.020308	-0.113924	1.127485

#### A4

E= -2454.4826055au

C	3.282045	2.508094	-0.173215
C	3.095954	1.211647	0.372680
C	3.870404	0.841913	1.509636
C	4.829636	1.725181	2.016037
C	5.049020	2.986107	1.463241
C	4.251167	3.354694	0.380767
P	1.801501	-0.058801	-0.112075
C	-0.446337	0.528211	3.288830
O	-1.086397	0.474251	4.305736
C	3.699599	-0.476590	2.236313
C	6.110644	3.910681	2.009033

C	2.475484	3.083626	-1.318555
C	0.868324	0.391907	-1.699290
C	-0.363931	-0.537332	-1.833995
B	-1.622201	-0.173274	-0.948841
O	-0.183550	-0.555775	2.532814
C	-2.161635	1.324303	-0.980099
C	-1.606488	2.404053	-0.300595
C	-2.114965	3.696694	-0.382407
C	-3.233599	3.936779	-1.178043
C	-3.823238	2.885825	-1.877906
C	-3.281193	1.608840	-1.762041
F	-0.519214	2.214561	0.484888
F	-3.861070	0.608868	-2.459181
F	-4.891434	3.111375	-2.649383
F	-3.733664	5.170466	-1.274927
F	-1.539493	4.701821	0.285860
C	-2.450746	-1.235737	-0.154634
C	-3.127439	-0.914073	1.035492
C	-3.847355	-1.845866	1.775348
C	-3.929955	-3.158925	1.316174
C	-3.287120	-3.528002	0.135473
C	-2.559696	-2.574702	-0.566991
F	-3.067865	0.330249	1.531397
F	-4.460547	-1.498478	2.907389
F	-4.624515	-4.062559	2.004007
F	-3.379925	-4.785856	-0.308943
F	-1.977923	-2.979948	-1.708876
C	2.753743	-1.559355	-0.718892
C	3.836150	-1.483823	-1.633735
C	4.450282	-2.665570	-2.066729
C	4.043551	-3.925871	-1.627659
C	2.980608	-3.984458	-0.725771
C	2.332102	-2.835075	-0.258479
C	4.401392	-0.184419	-2.165903
C	4.744261	-5.180685	-2.091711
C	1.205752	-3.031710	0.736989
H	-0.734325	-0.440416	-2.872149
H	0.549359	1.431086	-1.652386
H	5.412610	1.415293	2.880990
H	4.380000	4.343414	-0.054837
H	2.641026	-4.954830	-0.369743
H	5.275673	-2.593252	-2.772240
H	4.315214	-0.491955	3.140522

H	2.660123	-0.638626	2.546340
H	3.990408	-1.334844	1.621346
H	2.481334	2.446934	-2.207547
H	1.431591	3.246662	-1.027649
H	2.882514	4.055518	-1.612271
H	6.251233	3.767661	3.085820
H	7.081157	3.728218	1.528016
H	5.854970	4.961447	1.836166
H	1.046372	-4.099165	0.918146
H	1.418041	-2.562234	1.702984
H	0.256277	-2.613467	0.389747
H	4.047205	-6.021392	-2.176263
H	5.223210	-5.035775	-3.065703
H	5.528538	-5.480154	-1.383569
H	4.952059	0.360234	-1.392374
H	5.090937	-0.382800	-2.992155
H	3.628985	0.494184	-2.538119
H	-0.061635	-1.583042	-1.738172
H	1.514548	0.281720	-2.574345
H	0.371326	-0.315601	1.745709
H	-0.018344	1.463109	2.884400

**B**

E= -2304.0320035au

C	-2.552061	1.998583	0.674407
C	-2.186491	0.959744	-0.221484
C	-2.195160	1.244426	-1.618843
C	-2.522083	2.526515	-2.070854
C	-2.827572	3.568644	-1.193480
C	-2.855690	3.270749	0.167948
P	-1.473329	-0.731535	0.166259
C	-1.837384	0.207984	-2.666863
C	-3.079563	4.971215	-1.692252
C	-2.667803	1.858710	2.180897
C	-0.814201	-0.766700	1.973681
C	0.691643	-1.128309	1.920573
B	1.620556	-0.334265	0.918047
C	1.335108	1.174404	0.545384
C	1.406152	1.629041	-0.776329
C	1.106238	2.934571	-1.147682
C	0.743712	3.854040	-0.166074
C	0.686618	3.456092	1.166379
C	0.978744	2.136723	1.492976

F	1.721415	0.766902	-1.761781
F	0.895061	1.798257	2.798564
F	0.319864	4.328937	2.113230
F	0.432478	5.108165	-0.505991
F	1.146054	3.311019	-2.430381
C	2.966874	-0.974865	0.389360
C	4.152283	-0.223714	0.319924
C	5.369633	-0.749995	-0.101058
C	5.434995	-2.083578	-0.495947
C	4.287605	-2.871334	-0.454112
C	3.092477	-2.314426	-0.008416
F	4.163916	1.064551	0.703746
F	6.471035	0.008353	-0.128411
F	6.590090	-2.604379	-0.909861
F	4.344052	-4.150953	-0.839587
F	2.025521	-3.132470	-0.009187
C	-2.848732	-2.010794	0.032849
C	-4.246987	-1.786160	0.150350
C	-5.136361	-2.843888	-0.085531
C	-4.712716	-4.127214	-0.426646
C	-3.338929	-4.339630	-0.536071
C	-2.407412	-3.318999	-0.319947
C	-4.874002	-0.462220	0.527747
C	-5.699516	-5.249268	-0.645742
C	-0.945646	-3.684626	-0.458040
H	1.125068	-0.932251	2.921083
H	-0.885889	0.252369	2.345398
H	-2.518433	2.718395	-3.141804
H	-3.127293	4.054877	0.872911
H	-2.973564	-5.328826	-0.805322
H	-6.203218	-2.650333	0.006805
H	-2.027019	0.604782	-3.669371
H	-0.778030	-0.068133	-2.606866
H	-2.416443	-0.715442	-2.559482
H	-2.910566	0.845371	2.502327
H	-1.744450	2.159169	2.692739
H	-3.458750	2.519278	2.551877
H	-3.829104	5.488258	-1.082946
H	-2.156352	5.564111	-1.645988
H	-3.422053	4.974896	-2.732274
H	-0.840298	-4.676675	-0.908629
H	-0.392216	-2.966150	-1.069016
H	-0.442326	-3.718873	0.515232



H	-6.697665	-4.865134	-0.880486
H	-5.385922	-5.904786	-1.466032
H	-5.792632	-5.876940	0.250809
H	-4.721002	0.305170	-0.236052
H	-5.952677	-0.585680	0.666088
H	-4.467971	-0.067814	1.462829
H	0.815388	-2.205715	1.772449
C	-1.580625	-1.686653	2.931991
H	-2.631629	-1.394953	3.028595
H	-1.564743	-2.727877	2.591845
H	-1.127280	-1.656600	3.931528

### B<sub>1</sub>

E= -2305.2058438au

C	-3.061191	0.887621	-0.033531
C	-4.368684	0.570453	0.418299
C	-5.417628	1.468168	0.176186
H	-6.412957	1.209565	0.532587
C	-5.234469	2.673632	-0.500310
C	-3.946929	2.971390	-0.948448
H	-3.774900	3.900341	-1.488740
C	-2.865752	2.110213	-0.733102
C	-4.722925	-0.706023	1.148672
H	-3.993432	-0.954479	1.921593
H	-4.771975	-1.563411	0.469119
H	-5.700765	-0.605729	1.630795
C	-6.380098	3.633143	-0.720146
H	-6.280418	4.164618	-1.672971
H	-6.417943	4.393370	0.071763
H	-7.344369	3.114131	-0.719396
C	-1.517143	2.545460	-1.269529
H	-1.628428	3.431143	-1.903345
H	-1.032341	1.759607	-1.856720
H	-0.823049	2.808330	-0.462660
C	-2.133942	-1.953268	-0.083178
C	-2.198088	-3.035464	0.829342
C	-2.583962	-4.304036	0.375712
H	-2.629736	-5.117301	1.097431
C	-2.914727	-4.562891	-0.952759
C	-2.835024	-3.496066	-1.847148
H	-3.074240	-3.663617	-2.895542
C	-2.439123	-2.213987	-1.452524
C	-1.906769	-2.922982	2.307542

H	-1.848990	-3.918295	2.758676
H	-2.696217	-2.376314	2.836016
H	-0.962349	-2.418333	2.512845
C	-3.303500	-5.947677	-1.413120
H	-2.437924	-6.490371	-1.816552
H	-4.058648	-5.909782	-2.206161
H	-3.706742	-6.545625	-0.588881
C	-2.353466	-1.161941	-2.540312
H	-2.508932	-1.620683	-3.521692
H	-1.372937	-0.671083	-2.548426
H	-3.104391	-0.373189	-2.419819
C	1.752484	1.672318	0.448482
C	2.099979	1.915233	-0.888959
F	2.246707	0.886877	-1.742271
C	2.287070	3.189447	-1.411328
F	2.608003	3.363389	-2.699118
C	2.140576	4.297236	-0.578622
F	2.324407	5.526579	-1.060921
C	1.798947	4.112586	0.758269
F	1.663205	5.170584	1.565554
C	1.602312	2.820153	1.239348
C	2.588091	-0.911145	0.553808
C	2.212670	-2.252861	0.390014
F	0.931442	-2.623174	0.551619
C	3.104733	-3.257612	0.026915
F	2.689105	-4.518818	-0.132708
C	4.446187	-2.939059	-0.168475
F	5.318048	-3.889465	-0.506242
C	4.874423	-1.623313	-0.007863
F	6.164521	-1.316810	-0.183953
C	3.949242	-0.643800	0.336851
F	4.429712	0.602788	0.492412
F	1.280732	2.715664	2.543455
B	1.567617	0.204852	1.008266
P	-1.535894	-0.190714	0.185729
C	0.514188	-0.103255	2.150836
H	0.895301	0.414775	3.047075
H	0.511511	-1.164570	2.407506
C	-0.926868	0.404268	1.902198
H	-0.836117	1.460885	1.611620
C	-1.806983	0.403307	3.158772
H	-2.811507	0.779010	2.940987
H	-1.895242	-0.584884	3.614511

---

H	-1.362665	1.070467	3.909624
H	3.630261	1.244675	-4.002782
H	4.025728	0.969188	-4.567529

### TS<sub>12B</sub>

E= -2305.1814753au

C	-3.432920	0.732512	0.193765
C	-4.655507	0.285675	0.758378
C	-5.793174	1.096153	0.654571
H	-6.723938	0.739031	1.090433
C	-5.774524	2.338541	0.020983
C	-4.563563	2.767079	-0.524369
H	-4.519293	3.731648	-1.025767
C	-3.398358	1.996437	-0.454732
C	-4.814923	-1.031253	1.482126
H	-4.028653	-1.180340	2.226533
H	-4.778374	-1.885451	0.798484
H	-5.775737	-1.061820	2.004977
C	-7.011109	3.202551	-0.047277
H	-7.050205	3.773140	-0.981524
H	-7.031111	3.928670	0.776460
H	-7.924325	2.602827	0.024484
C	-2.143186	2.573773	-1.069410
H	-2.379298	3.474445	-1.644276
H	-1.639310	1.869233	-1.734941
H	-1.412579	2.864328	-0.304010
C	-2.238583	-2.052438	-0.097880
C	-2.139595	-3.167753	0.772914
C	-2.371097	-4.455006	0.268307
H	-2.289716	-5.297432	0.951806
C	-2.708928	-4.697496	-1.061762
C	-2.812767	-3.592590	-1.906715
H	-3.077709	-3.746016	-2.950685
C	-2.573630	-2.287925	-1.465583
C	-1.825663	-3.081282	2.248609
H	-1.774380	-4.084083	2.682563
H	-2.596976	-2.531282	2.797260
H	-0.870197	-2.593086	2.450822
C	-2.925818	-6.100438	-1.575776
H	-2.007150	-6.503900	-2.022282
H	-3.700318	-6.128164	-2.349999
H	-3.223421	-6.781088	-0.771358
C	-2.695373	-1.182434	-2.495918

H	-2.916726	-1.607434	-3.479364
H	-1.769807	-0.601139	-2.585104
H	-3.494840	-0.473806	-2.253042
C	1.639304	1.635049	0.080511
C	1.357633	2.285215	-1.123749
F	0.735913	1.629436	-2.129071
C	1.670040	3.621513	-1.368307
F	1.354442	4.193218	-2.538247
C	2.316649	4.363600	-0.385415
F	2.626354	5.646349	-0.601191
C	2.638242	3.757141	0.825830
F	3.269347	4.457820	1.777049
C	2.301666	2.421308	1.028973
C	2.664942	-0.860450	0.156858
C	3.374245	-1.494452	1.182180
F	2.968640	-1.402950	2.464297
C	4.529767	-2.243973	0.962309
F	5.167145	-2.828487	1.985925
C	5.024814	-2.382335	-0.330110
F	6.128893	-3.101114	-0.557200
C	4.357531	-1.767637	-1.386294
F	4.820751	-1.895827	-2.636768
C	3.212742	-1.023293	-1.120621
F	2.602186	-0.451068	-2.180894
F	2.662917	1.882939	2.214073
B	1.350203	0.068872	0.399931
P	-1.845680	-0.253086	0.227975
C	0.489148	-0.262505	1.727127
H	1.042154	0.161605	2.572463
H	0.485131	-1.343007	1.905657
C	-0.953202	0.288683	1.786595
H	-0.899677	1.358860	1.527265
C	-1.602484	0.227449	3.173609
H	-2.623807	0.622862	3.157363
H	-1.625572	-0.782582	3.586165
H	-1.017833	0.846497	3.866439
H	-0.065348	-0.186481	-0.582153
H	0.739992	-0.363474	-0.794078

### B<sub>2</sub>

E= -2305.214788au

C	-3.174356	-2.372456	0.125207
C	-2.925275	-1.097300	0.688307

C	-3.414237	-0.791769	1.989710
C	-4.171361	-1.749421	2.668022
C	-4.456688	-3.001414	2.119527
C	-3.941365	-3.287439	0.856022
P	-1.940555	0.235635	-0.123348
C	-3.130531	0.509010	2.711172
C	-5.303723	-4.003536	2.864733
C	-2.621083	-2.862716	-1.194000
C	-0.788421	-0.132572	-1.564312
C	0.514546	0.675811	-1.307352
B	1.456690	0.164599	-0.046232
C	1.956699	-1.362658	-0.406198
C	1.212046	-2.482898	-0.042933
C	1.538094	-3.792276	-0.387852
C	2.690332	-4.030946	-1.128088
C	3.476843	-2.950250	-1.518604
C	3.092509	-1.657899	-1.164482
F	0.049033	-2.334933	0.657168
F	3.884327	-0.658278	-1.609788
F	4.585077	-3.165280	-2.245439
F	3.028496	-5.281291	-1.477373
F	0.733508	-4.814873	-0.039020
C	2.701752	1.165759	0.342112
C	3.673524	0.733546	1.254066
C	4.735866	1.513625	1.701233
C	4.866083	2.819828	1.239078
C	3.923780	3.310394	0.345041
C	2.879952	2.485261	-0.075932
F	3.605402	-0.516147	1.764747
F	5.631411	1.024262	2.575148
F	5.878227	3.594378	1.658867
F	4.020747	4.574586	-0.103900
F	2.002418	3.076247	-0.934003
C	-2.962936	1.732579	-0.447743
C	-4.195148	1.624560	-1.142575
C	-4.915469	2.788198	-1.425762
C	-4.471309	4.053091	-1.036719
C	-3.267363	4.133450	-0.334908
C	-2.495960	3.008162	-0.022395
C	-4.807804	0.307507	-1.568839
C	-5.281265	5.290737	-1.336604
C	-1.223775	3.246126	0.768631
H	1.085368	0.592627	-2.244690

H	-0.572361	-1.199978	-1.492600
H	-4.540332	-1.508523	3.662092
H	-4.128659	-4.265108	0.418770
H	-2.907239	5.108575	-0.016393
H	-5.853867	2.698526	-1.968085
H	-3.652670	0.526608	3.671368
H	-2.060166	0.624868	2.925786
H	-3.453594	1.388176	2.144629
H	-2.631579	-2.108933	-1.983139
H	-1.588107	-3.202889	-1.060702
H	-3.202795	-3.716950	-1.551473
H	-5.146379	-3.934123	3.946096
H	-6.371870	-3.828611	2.679275
H	-5.080367	-5.028175	2.551658
H	-1.182843	4.290471	1.089574
H	-1.171673	2.631351	1.673694
H	-0.314987	3.053516	0.191143
H	-4.638355	6.165856	-1.475257
H	-5.887247	5.163903	-2.239401
H	-5.968257	5.518248	-0.510724
H	-5.247997	-0.223526	-0.717162
H	-5.603705	0.481553	-2.298593
H	-4.087884	-0.370944	-2.032789
H	0.248217	1.734932	-1.250029
H	-1.037263	0.615933	0.881822
H	0.793945	0.088574	0.983701
C	-1.403209	0.185890	-2.936554
H	-2.278005	-0.422371	-3.190179
H	-1.685983	1.240467	-3.012327
H	-0.640768	-0.007525	-3.698404

### **B<sub>3</sub>**

**E= -2493.799371au**

C	2.797635	2.194650	-0.763993
C	2.626732	1.091596	0.108338
C	2.814717	1.257842	1.509442
C	3.113344	2.529736	1.999361
C	3.225409	3.644043	1.165414
C	3.097895	3.443390	-0.208988
P	1.978222	-0.550920	-0.410448
C	-1.524267	-1.835370	3.584466
O	-2.579889	-2.333489	3.595025
C	2.677138	0.132087	2.510685

C	3.438898	5.022749	1.736115	H	3.110871	0.429603	3.469485
C	2.659095	2.148805	-2.271069	H	1.622776	-0.105275	2.693526
C	0.922717	-0.602035	-1.972018	H	3.185608	-0.783489	2.191520
C	-0.495864	-1.161704	-1.682474	H	2.920705	1.183161	-2.705738
B	-1.332210	-0.515190	-0.415054	H	1.634785	2.389564	-2.581632
O	-0.450191	-1.368064	3.602927	H	3.313378	2.898978	-2.725721
C	-1.239251	1.134411	-0.410988	H	3.932860	5.686754	1.019654
C	-0.750805	1.879952	0.663939	H	2.469172	5.470530	1.989614
C	-0.654389	3.271493	0.663176	H	4.037518	4.993860	2.652443
C	-1.084476	3.985254	-0.449782	H	1.244872	-4.416529	1.133064
C	-1.597084	3.294453	-1.545348	H	1.204938	-2.767569	1.757717
C	-1.660910	1.902937	-1.499889	H	0.571891	-3.115390	0.152243
F	-0.303629	1.262549	1.783234	H	6.955578	-4.979091	0.002238
F	-2.156817	1.289001	-2.599403	H	5.699375	-5.929956	0.818609
F	-2.014737	3.974468	-2.626105	H	5.809269	-5.933887	-0.943614
F	-0.996776	5.324108	-0.472827	H	5.011975	0.306883	-0.762771
F	-0.137181	3.931303	1.716842	H	6.111841	-0.698403	-1.714588
C	-2.909487	-0.968165	-0.333666	H	4.522182	-0.290861	-2.349065
C	-3.629238	-0.666894	0.827805	H	-0.435909	-2.256027	-1.585135
C	-4.964728	-0.996324	1.035481	H	1.048346	-0.826476	0.606174
C	-5.659420	-1.664956	0.031585	H	-0.835344	-0.909370	0.629584
C	-4.997426	-1.989667	-1.146375	C	1.624851	-1.341574	-3.121656
C	-3.656217	-1.636778	-1.305261	H	2.580237	-0.893371	-3.418827
F	-3.011880	-0.018165	1.847493	H	1.808029	-2.390323	-2.866863
F	-5.587750	-0.677386	2.181596	H	0.963183	-1.322682	-3.994043
F	-6.948535	-1.995201	0.201451				
F	-5.654607	-2.639451	-2.122301				
F	-3.099590	-2.003262	-2.484762				
C	3.191930	-1.931656	-0.307931				
C	4.517281	-1.812028	-0.796867				
C	5.375267	-2.910213	-0.686993				
C	4.971359	-4.121724	-0.122255				
C	3.662631	-4.214984	0.354816				
C	2.757759	-3.151276	0.279736				
C	5.064732	-0.554834	-1.434503				
C	5.910654	-5.300894	-0.052130				
C	1.372071	-3.366901	0.854367				
H	-1.027894	-0.988790	-2.623606				
H	0.801648	0.450298	-2.235327				
H	3.240338	2.654272	3.071922				
H	3.217421	4.290302	-0.880905				
H	3.328440	-5.146609	0.805067				
H	6.392452	-2.812125	-1.058837				
				<b>TS<sub>34B</sub></b>			
				<b>E= -2493.76213au</b>			
C	3.299737	2.303376	-0.112392	C	3.299737	2.303376	-0.112392
C	3.128977	1.041667	0.511776	C	3.128977	1.041667	0.511776
C	3.820876	0.770086	1.726283	C	3.820876	0.770086	1.726283
C	4.683153	1.740425	2.249583	C	4.683153	1.740425	2.249583
C	4.878747	2.977812	1.639338	C	4.878747	2.977812	1.639338
C	4.170117	3.233940	0.465191	C	4.170117	3.233940	0.465191
P	1.987258	-0.323824	-0.031995	P	1.987258	-0.323824	-0.031995
C	-0.845150	-0.399288	2.308715	C	-0.845150	-0.399288	2.308715
O	-1.780554	-0.417907	3.075504	O	-1.780554	-0.417907	3.075504
C	3.671027	-0.514620	2.516228	C	3.671027	-0.514620	2.516228
C	5.826399	4.001334	2.216517	C	5.826399	4.001334	2.216517
C	2.577552	2.758691	-1.361558	C	2.577552	2.758691	-1.361558
C	0.819279	0.000889	-1.498265	C	0.819279	0.000889	-1.498265
C	-0.495210	-0.784771	-1.241739	C	-0.495210	-0.784771	-1.241739
B	-1.704159	-0.139270	-0.411033	B	-1.704159	-0.139270	-0.411033

O	0.401050	-0.617713	2.448399
C	-1.935529	1.437096	-0.586934
C	-1.105198	2.422116	-0.053028
C	-1.284644	3.784781	-0.274606
C	-2.345905	4.211435	-1.066793
C	-3.203511	3.267173	-1.626597
C	-2.985151	1.914968	-1.378667
F	-0.045649	2.072609	0.715353
F	-3.832122	1.044572	-1.961980
F	-4.219025	3.666485	-2.401370
F	-2.531082	5.513409	-1.301814
F	-0.428155	4.677052	0.241672
C	-2.953825	-1.034689	-0.009063
C	-3.979861	-0.525321	0.806711
C	-5.066087	-1.280660	1.236848
C	-5.163931	-2.615462	0.856766
C	-4.175251	-3.172744	0.051440
C	-3.101948	-2.386572	-0.355060
F	-3.953310	0.752516	1.211488
F	-6.013806	-0.738011	2.008811
F	-6.199313	-3.356025	1.257518
F	-4.263470	-4.456010	-0.324461
F	-2.189664	-3.007904	-1.135156
C	2.990284	-1.831577	-0.468401
C	4.200175	-1.733187	-1.210757
C	4.895296	-2.901344	-1.538003
C	4.456787	-4.169066	-1.152457
C	3.277809	-4.245318	-0.413975
C	2.532080	-3.113735	-0.057822
C	4.833386	-0.430273	-1.653659
C	5.248866	-5.407450	-1.495649
C	1.271565	-3.375004	0.744602
H	-0.957048	-0.948196	-2.231847
H	0.612983	1.070859	-1.489098
H	5.208631	1.516485	3.174886
H	4.290041	4.198046	-0.024289
H	2.915527	-5.220229	-0.095474
H	5.814708	-2.812134	-2.112611
H	4.314450	-0.483290	3.400117
H	2.642573	-0.655179	2.866121
H	3.953304	-1.399959	1.937350
H	2.551583	2.002758	-2.148867
H	1.546387	3.047071	-1.130399

H	3.069520	3.642187	-1.778267
H	5.389313	5.005943	2.195920
H	6.086997	3.765590	3.252946
H	6.760945	4.043960	1.641703
H	1.374250	-4.318018	1.290352
H	1.042242	-2.599262	1.476543
H	0.394108	-3.487074	0.094908
H	4.603333	-6.288505	-1.570225
H	5.781373	-5.291828	-2.445539
H	6.001356	-5.618351	-0.724157
H	5.362589	0.057506	-0.827680
H	5.561733	-0.621862	-2.447424
H	4.112875	0.293538	-2.037165
H	-0.261605	-1.795181	-0.904229
H	1.090007	-0.537056	1.258563
H	-1.106152	-0.151332	1.178428
C	1.403460	-0.384643	-2.868243
H	2.321742	0.152579	-3.119660
H	1.618483	-1.456287	-2.920198
H	0.665857	-0.152713	-3.645367

#### B<sub>4</sub>

E= -2493.7875877au

C	2.809352	2.699385	0.041192
C	2.764285	1.358649	0.504526
C	3.443799	1.044304	1.718570
C	4.172804	2.035668	2.385005
C	4.244688	3.349273	1.924475
C	3.549272	3.651219	0.754844
P	1.755778	-0.070641	-0.181256
C	-0.466846	0.402061	3.192080
O	-1.169109	0.353948	4.167297
C	3.430611	-0.331464	2.356295
C	5.010155	4.408629	2.680630
C	2.087000	3.213370	-1.185728
C	0.820919	0.298590	-1.825463
C	-0.403248	-0.662042	-1.851724
B	-1.647273	-0.334392	-0.933449
O	-0.318254	-0.639338	2.348647
C	-2.232299	1.145779	-0.995547
C	-1.718962	2.244128	-0.315190
C	-2.246809	3.525946	-0.431899
C	-3.347989	3.733012	-1.260496

C	-3.898531	2.660548	-1.959605
C	-3.334174	1.396279	-1.812193
F	-0.649644	2.083142	0.500148
F	-3.873763	0.375340	-2.512017
F	-4.950096	2.854208	-2.762448
F	-3.867757	4.955888	-1.390551
F	-1.702099	4.552478	0.230412
C	-2.437882	-1.406108	-0.113368
C	-3.190693	-1.061942	1.025560
C	-3.879488	-1.993862	1.794009
C	-3.851820	-3.335745	1.421465
C	-3.129029	-3.731259	0.297376
C	-2.439263	-2.774122	-0.436312
F	-3.241555	0.208468	1.447260
F	-4.567137	-1.618596	2.873569
F	-4.514823	-4.240992	2.137566
F	-3.110786	-5.018520	-0.065409
F	-1.773802	-3.220571	-1.518000
C	2.989540	-1.400721	-0.669190
C	4.245401	-1.139263	-1.285074
C	5.072099	-2.211545	-1.639618
C	4.723612	-3.541685	-1.400612
C	3.509011	-3.782244	-0.761808
C	2.639346	-2.749576	-0.385985
C	4.801828	0.245198	-1.545200
C	5.626430	-4.674632	-1.826630
C	1.366286	-3.172055	0.324096
H	-0.836559	-0.597666	-2.869635
H	0.457520	1.322667	-1.732320
H	4.693935	1.765118	3.300996
H	3.578150	4.670295	0.374453
H	3.223960	-4.807780	-0.536531
H	6.027193	-1.993608	-2.113677
H	3.913759	-0.294218	3.337101
H	2.412072	-0.706778	2.508614
H	3.956932	-1.078277	1.753424
H	2.251971	2.596205	-2.071521
H	1.007165	3.272904	-1.011078
H	2.427616	4.224644	-1.426431
H	5.405496	5.176117	2.006479
H	4.366081	4.917547	3.410252
H	5.850472	3.977338	3.235011
H	1.491078	-4.176820	0.740309

H	1.092554	-2.504886	1.144236
H	0.508855	-3.218527	-0.356755
H	6.683530	-4.406611	-1.722395
H	5.443725	-5.577218	-1.234373
H	5.461291	-4.936141	-2.880480
H	5.222422	0.680594	-0.631684
H	5.604678	0.192991	-2.287497
H	4.055346	0.950267	-1.909830
H	-0.059396	-1.693695	-1.762622
H	0.285190	-0.405335	1.594188
H	0.120141	1.291789	2.902048
C	1.607563	0.161088	-3.137295
H	2.454693	0.847533	-3.204357
H	1.994118	-0.855036	-3.262532
H	0.945972	0.374532	-3.986729

### C

E= -2495.7627907au

C	-1.927333	2.650876	0.362152
C	-1.583914	1.651758	-0.588565
C	-1.319448	2.069907	-1.927500
C	-1.375909	3.425181	-2.265593
C	-1.668772	4.415795	-1.327661
C	-1.959189	3.997420	-0.031176
P	-1.198177	-0.171514	-0.309655
C	-0.941155	1.103017	-3.030765
C	-1.631985	5.881268	-1.688319
C	-2.273864	2.400661	1.816998
C	-0.950176	-0.546318	1.578123
C	0.458238	-1.197718	1.684978
B	1.624874	-0.533003	0.840061
C	1.709635	1.037545	0.655401
C	2.046284	1.622125	-0.572522
C	2.054054	2.994043	-0.787837
C	1.742067	3.850722	0.266068
C	1.431471	3.320997	1.514028
C	1.419457	1.939702	1.682030
F	2.326583	0.836194	-1.630392
F	1.089830	1.484031	2.911068
F	1.113070	4.133761	2.529911
F	1.724646	5.172249	0.071850
F	2.340506	3.499530	-1.992774
C	2.841408	-1.413289	0.333502

C	4.155217	-0.909831	0.294137
C	5.257889	-1.661021	-0.101029
C	5.078201	-2.983426	-0.495956
C	3.800360	-3.534990	-0.479530
C	2.725065	-2.757669	-0.059793
F	4.418865	0.349905	0.679647
F	6.483655	-1.126241	-0.101659
F	6.121000	-3.716973	-0.883684
F	3.617452	-4.804538	-0.858871
F	1.529520	-3.378010	-0.075707
C	-2.659637	-1.133966	-0.996861
C	-4.030920	-0.859140	-0.749500
C	-5.013057	-1.621283	-1.391951
C	-4.701820	-2.657884	-2.272911
C	-3.353053	-2.928727	-2.498402
C	-2.329645	-2.192098	-1.888249
C	-4.507382	0.211093	0.202136
C	-5.788205	-3.440002	-2.971984
C	-0.905899	-2.583938	-2.233465
H	0.772006	-1.153568	2.743936
H	-0.885383	0.427860	2.054274
H	-1.164909	3.713045	-3.293290
H	-2.221113	4.743896	0.716660
H	-3.081116	-3.736996	-3.174023
H	-6.058290	-1.396616	-1.188603
H	-0.819621	1.638450	-3.977498
H	0.004977	0.597070	-2.806308
H	-1.699302	0.327429	-3.182924
H	-2.784277	1.452776	1.977915
H	-1.383712	2.421008	2.459646
H	-2.935399	3.194603	2.179080
H	-0.651346	6.311363	-1.443973
H	-1.802740	6.038300	-2.758428
H	-2.384756	6.452622	-1.134056
H	-0.908702	-3.458655	-2.891984
H	-0.374309	-1.778795	-2.751676
H	-0.310607	-2.835364	-1.353177
H	-6.155295	-2.902385	-3.856591
H	-5.425596	-4.416158	-3.310528
H	-6.649471	-3.605145	-2.315102
H	-4.121339	1.198214	-0.065180
H	-5.600441	0.265142	0.198932
H	-4.194080	-0.007328	1.228502

H	0.384800	-2.263120	1.459776
C	-1.992682	-1.361405	2.317951
C	-2.365385	-2.648468	1.896039
C	-2.558134	-0.871705	3.506900
C	-3.283583	-3.405799	2.622722
H	-1.940340	-3.063480	0.987288
C	-3.477759	-1.627756	4.237339
H	-2.263430	0.108011	3.874649
C	-3.847741	-2.898026	3.795290
H	-3.558870	-4.396442	2.270317
H	-3.898291	-1.223638	5.154661
H	-4.563099	-3.489464	4.360394

### C<sub>1</sub>

E= -2496.9368492au

C	2.425990	-1.123214	-1.221085
C	3.812735	-0.826064	-1.164887
C	4.703856	-1.577873	-1.940598
H	5.765308	-1.344789	-1.882077
C	4.283351	-2.615893	-2.773553
C	2.918335	-2.904084	-2.810734
H	2.564319	-3.714305	-3.444943
C	1.983329	-2.181049	-2.061224
C	4.402449	0.259847	-0.293446
H	3.990816	0.238063	0.718320
H	4.214304	1.258118	-0.701785
H	5.486348	0.130211	-0.212662
C	5.268463	-3.384906	-3.621618
H	4.922766	-4.406545	-3.811936
H	6.251990	-3.441279	-3.142785
H	5.410297	-2.902261	-4.598046
C	0.526880	-2.583394	-2.185947
H	-0.118629	-1.728117	-2.408817
H	0.145112	-3.035848	-1.263897
H	0.406314	-3.322376	-2.984464
C	1.556861	1.613020	-0.373251
C	1.891893	2.484434	0.690834
C	2.091841	3.847735	0.433209
H	2.357909	4.495505	1.266198
C	1.969199	4.398660	-0.840811
C	1.632129	3.532101	-1.882088
H	1.525928	3.929463	-2.889471
C	1.408374	2.166536	-1.680195

C	2.046806	2.034638	2.122523
H	2.591325	2.785950	2.703235
H	2.587884	1.092277	2.209125
H	1.073587	1.901121	2.609152
C	2.159344	5.877096	-1.082335
H	2.786939	6.332184	-0.308939
H	1.196383	6.405315	-1.074781
H	2.625021	6.068495	-2.055405
C	0.998163	1.350515	-2.889940
H	0.902963	1.999412	-3.765921
H	0.031051	0.859388	-2.733464
H	1.723877	0.567601	-3.132905
C	-2.584317	-1.444889	0.523587
C	-2.301346	-2.821795	0.504708
F	-1.080350	-3.279535	0.847598
C	-3.210758	-3.801869	0.122255
F	-2.858659	-5.092421	0.107931
C	-4.501461	-3.429085	-0.240167
F	-5.392093	-4.352094	-0.601163
C	-4.853055	-2.083244	-0.217458
F	-6.095730	-1.715338	-0.547492
C	-3.908189	-1.131590	0.156230
C	-1.806643	1.172352	0.631640
C	-1.731806	2.221562	1.555030
F	-1.498683	1.974270	2.862980
C	-1.905370	3.560847	1.212206
F	-1.824415	4.518389	2.144082
C	-2.165575	3.898916	-0.110891
F	-2.322075	5.177337	-0.462129
C	-2.260864	2.891072	-1.068804
F	-2.506930	3.206404	-2.347286
C	-2.099177	1.568964	-0.680920
F	-2.198411	0.638512	-1.652137
F	-4.352896	0.134901	0.177206
C	-0.380197	-0.713545	2.048022
H	-0.696167	-1.526462	2.715722
H	-0.211242	0.156566	2.683886
C	0.958212	-1.144103	1.392036
H	0.754921	-2.103628	0.906496
B	-1.538579	-0.349331	1.001598
P	1.092481	-0.200531	-0.285639
H	-3.527397	1.264967	-3.888839
H	-3.906828	1.051948	-4.490479

C	2.108099	-1.429084	2.347144
C	2.148995	-0.944595	3.664004
C	3.139163	-2.295063	1.939589
C	3.193365	-1.283139	4.527802
H	1.355195	-0.302684	4.030685
C	4.185804	-2.630131	2.797417
H	3.116625	-2.713466	0.938101
C	4.220952	-2.121955	4.097826
H	3.195382	-0.892865	5.542347
H	4.968710	-3.300057	2.451324
H	5.031881	-2.387491	4.770660

### TS<sub>12c</sub>

E= -2496.9126515au

C	3.080037	-0.963124	-0.976596
C	4.394031	-0.848129	-0.452435
C	5.430896	-1.571295	-1.053019
H	6.433264	-1.478642	-0.640151
C	5.223619	-2.413166	-2.147007
C	3.924000	-2.523731	-2.643327
H	3.734353	-3.178203	-3.491330
C	2.851259	-1.813079	-2.093007
C	4.739813	-0.002086	0.750581
H	4.140802	-0.287898	1.620726
H	4.572034	1.063425	0.569205
H	5.792209	-0.136191	1.018351
C	6.370300	-3.160170	-2.785225
H	6.031872	-4.090036	-3.254218
H	7.144085	-3.409527	-2.051339
H	6.847709	-2.555398	-3.567887
C	1.490939	-1.993995	-2.738058
H	1.093307	-1.046277	-3.118473
H	0.742215	-2.404053	-2.051929
H	1.565903	-2.685817	-3.582607
C	2.066760	1.734561	0.011222
C	2.203608	2.384596	1.259697
C	2.494608	3.755585	1.292350
H	2.602471	4.236461	2.262302
C	2.655887	4.516987	0.137112
C	2.508237	3.864771	-1.089554
H	2.622042	4.433506	-2.010077
C	2.203911	2.504816	-1.182313
C	2.039686	1.688763	2.586897



H	2.494582	2.277974	3.389233
H	2.493114	0.697862	2.599845
H	0.980866	1.562806	2.842382
C	2.959839	5.994543	0.200277
H	3.229186	6.305185	1.214619
H	2.091956	6.590875	-0.109949
H	3.787494	6.261326	-0.467385
C	2.015189	1.927464	-2.570557
H	2.197279	2.698109	-3.325687
H	0.991992	1.559154	-2.709949
H	2.696955	1.095349	-2.777168
C	-2.822954	-1.446025	-0.138871
C	-2.481073	-2.762453	-0.465499
F	-1.176286	-3.096111	-0.627286
C	-3.405027	-3.782217	-0.664294
F	-3.006272	-5.019169	-0.988241
C	-4.761406	-3.501762	-0.519559
F	-5.671196	-4.464186	-0.697487
C	-5.158678	-2.211326	-0.186087
F	-6.460094	-1.933959	-0.037589
C	-4.197157	-1.216676	-0.006320
C	-2.108975	1.227221	-0.108070
C	-2.589577	1.971619	0.972037
F	-2.739556	1.373088	2.173158
C	-2.943063	3.313895	0.888484
F	-3.399541	3.973325	1.961702
C	-2.822872	3.972654	-0.333021
F	-3.153168	5.264575	-0.437861
C	-2.356045	3.275342	-1.441778
F	-2.235112	3.898290	-2.622198
C	-2.022716	1.928052	-1.312012
F	-1.578699	1.313853	-2.434764
F	-4.665605	0.000524	0.324655
C	-0.639064	-0.599553	1.326516
H	-1.107129	-1.329387	2.000132
H	-0.541661	0.315805	1.918050
C	0.782563	-1.152188	1.009359
H	0.643237	-2.013317	0.342355
B	-1.688001	-0.317864	0.099251
P	1.605885	-0.040379	-0.318563
H	-0.246818	-0.316614	-1.054913
H	-1.030040	-0.585679	-1.157586
C	1.540593	-1.707576	2.207720

C	1.211561	-1.387279	3.533720
C	2.555518	-2.658168	1.997298
C	1.890528	-1.969388	4.606917
H	0.413305	-0.682274	3.738741
C	3.237044	-3.238309	3.066355
H	2.808809	-2.950553	0.982444
C	2.910103	-2.893197	4.379739
H	1.612744	-1.701840	5.623152
H	4.016293	-3.970607	2.871616
H	3.435503	-3.348451	5.214841

## C<sub>2</sub>

E= -2496.9481528au

C	-1.685053	2.529012	-2.074447
C	-1.798296	1.129642	-1.882405
C	-2.058992	0.282418	-2.996615
C	-2.213102	0.859014	-4.259226
C	-2.110054	2.234634	-4.472065
C	-1.851234	3.042723	-3.366118
P	-1.595499	0.277454	-0.255152
C	-2.146647	-1.225555	-2.908393
C	-2.249940	2.820914	-5.855357
C	-1.364772	3.531254	-0.988415
C	-0.601616	1.115156	1.129986
C	0.619459	0.204354	1.440541
B	1.608355	-0.063802	0.117880
C	3.021438	0.772878	0.240824
C	2.993283	2.168904	0.294200
C	4.114332	2.988807	0.365932
C	5.376452	2.404387	0.391300
C	5.473708	1.019263	0.341365
C	4.315208	0.243048	0.268576
F	1.795966	2.825564	0.275387
F	4.525030	-1.090073	0.217309
F	6.683646	0.437595	0.364766
F	6.478376	3.165609	0.464327
F	3.990666	4.326944	0.412031
C	1.786820	-1.676799	-0.123152
C	1.526707	-2.311924	-1.336557
C	1.597046	-3.693160	-1.526397
C	1.965489	-4.507962	-0.462743
C	2.247975	-3.926846	0.772080
C	2.154778	-2.545406	0.909123

F	1.143189	-1.593032	-2.424523
F	1.307904	-4.239256	-2.721061
F	2.040335	-5.837973	-0.619224
F	2.604995	-4.705359	1.806628
F	2.445972	-2.038307	2.127386
C	-3.183698	-0.468044	0.312868
C	-4.361018	0.310926	0.430736
C	-5.544651	-0.312819	0.834206
C	-5.604816	-1.674864	1.135215
C	-4.425606	-2.416976	1.041278
C	-3.210940	-1.851593	0.638978
C	-4.392731	1.798678	0.170771
C	-6.904640	-2.327989	1.537129
C	-2.000912	-2.764495	0.592100
H	1.155913	0.726337	2.243680
H	-0.201310	2.008308	0.659750
H	-2.416047	0.204681	-5.103649
H	-1.768521	4.117922	-3.505155
H	-4.445316	-3.474399	1.293919
H	-6.444566	0.290973	0.924133
H	-2.499673	-1.635929	-3.858263
H	-1.158434	-1.659305	-2.716291
H	-2.836313	-1.565968	-2.129894
H	-1.903029	3.344068	-0.057195
H	-0.291446	3.537543	-0.766820
H	-1.632676	4.538328	-1.320769
H	-1.303865	2.744683	-6.407028
H	-3.009400	2.291245	-6.440409
H	-2.522921	3.880121	-5.816968
H	-2.256784	-3.742082	1.009052
H	-1.645499	-2.935702	-0.431039
H	-1.152602	-2.379319	1.166716
H	-6.735820	-3.183034	2.199697
H	-7.566796	-1.622275	2.049079
H	-7.443349	-2.700244	0.655612
H	-4.125677	2.044513	-0.861765
H	-5.393349	2.197000	0.359883
H	-3.701683	2.329253	0.835854
H	0.268897	-0.727254	1.903858
H	-0.832004	-0.846445	-0.588914
H	1.047002	0.394643	-0.870454
C	-1.420765	1.526287	2.341032
C	-2.033182	0.587510	3.186387

C	-1.489314	2.882802	2.697730
C	-2.714820	0.994328	4.332814
H	-1.968286	-0.471312	2.957102
C	-2.167792	3.292214	3.847806
H	-0.980359	3.623045	2.086008
C	-2.789978	2.348943	4.665671
H	-3.181172	0.249554	4.972121
H	-2.200126	4.347208	4.106360
H	-3.317550	2.663659	5.561866

### C<sub>3</sub>

E= -2685.5331359au

C	-2.614260	2.392538	0.663351
C	-2.257519	1.497763	-0.375416
C	-2.213444	1.957435	-1.722656
C	-2.536413	3.289458	-1.989014
C	-2.888847	4.190446	-0.981515
C	-2.927200	3.715714	0.328797
P	-1.745225	-0.257402	-0.119153
C	2.396085	-0.612704	-3.869037
O	3.529648	-0.391587	-3.702326
C	-1.797626	1.091785	-2.892960
C	-3.186338	5.634956	-1.299246
C	-2.650173	2.046182	2.135869
C	-0.888569	-0.671180	1.519085
C	0.548916	-1.203533	1.225736
B	1.505104	-0.384035	0.153667
O	1.263804	-0.828291	-4.080647
C	1.482406	1.258309	0.304588
C	1.599956	2.075418	-0.825456
C	1.553052	3.467802	-0.798839
C	1.378307	4.119896	0.417148
C	1.252970	3.361372	1.575542
C	1.318006	1.971961	1.493977
F	1.734964	1.527733	-2.060211
F	1.151704	1.316600	2.671556
F	1.047184	3.971006	2.756272
F	1.311748	5.458416	0.468907
F	1.657214	4.183957	-1.930615
C	3.015895	-1.013005	0.218087
C	3.964018	-0.675846	1.186207
C	5.243077	-1.226046	1.244108
C	5.618067	-2.178685	0.301547

C	4.707665	-2.561506	-0.678154
C	3.441359	-1.981010	-0.693649
F	3.658194	0.228052	2.144631
F	6.111998	-0.856059	2.199317
F	6.841623	-2.726559	0.340936
F	5.055609	-3.486603	-1.588422
F	2.604742	-2.419138	-1.671461
C	-2.984398	-1.474632	-0.721912
C	-4.339349	-1.422265	-0.310612
C	-5.240157	-2.346688	-0.843951
C	-4.847324	-3.328042	-1.757185
C	-3.500216	-3.382103	-2.120260
C	-2.549222	-2.481241	-1.627450
C	-4.850612	-0.434449	0.710698
C	-5.850938	-4.292313	-2.340677
C	-1.116204	-2.653564	-2.091497
H	1.015007	-1.236087	2.219129
H	-0.768701	0.303955	1.988486
H	-2.501610	3.633334	-3.019867
H	-3.201979	4.397092	1.130542
H	-3.169522	-4.154332	-2.810559
H	-6.278967	-2.302591	-0.525308
H	-2.007948	1.608599	-3.833172
H	-0.720092	0.885521	-2.873560
H	-2.327713	0.134291	-2.922055
H	-2.958856	1.020175	2.338721
H	-1.665903	2.199103	2.597619
H	-3.350298	2.706560	2.656575
H	-2.257847	6.219105	-1.342574
H	-3.681339	5.738574	-2.270530
H	-3.825249	6.091135	-0.536546
H	-1.019214	-3.588033	-2.650822
H	-0.788184	-1.848205	-2.758455
H	-0.394760	-2.692463	-1.269487
H	-5.379837	-5.238079	-2.626674
H	-6.656333	-4.510163	-1.631618
H	-6.315901	-3.872839	-3.242736
H	-4.692241	0.602959	0.400182
H	-5.923217	-0.572593	0.872544
H	-4.354518	-0.579484	1.677434
H	0.480047	-2.251834	0.901765
H	-0.683989	-0.390632	-1.028114
H	1.107511	-0.607928	-0.974371

C	-1.686212	-1.559986	2.458475
C	-2.048287	-2.872726	2.115802
C	-1.990884	-1.104771	3.751169
C	-2.716823	-3.690990	3.025826
H	-1.797898	-3.265549	1.135545
C	-2.655158	-1.924906	4.665900
H	-1.680698	-0.108297	4.054250
C	-3.027604	-3.219363	4.303404
H	-2.988049	-4.703091	2.737708
H	-2.873055	-1.551450	5.662851
H	-3.544249	-3.860065	5.012665

### TS<sub>34C</sub>

E= -2685.4906024au

C	-3.068068	2.464898	-0.515270
C	-2.881060	1.192420	-1.104377
C	-3.462702	0.928704	-2.380833
C	-4.227819	1.923621	-2.995388
C	-4.431702	3.179987	-2.422730
C	-3.837668	3.423609	-1.187492
P	-1.828250	-0.199203	-0.441590
C	1.156351	-0.301133	-2.600387
O	2.133013	-0.330686	-3.313138
C	-3.295517	-0.370554	-3.142554
C	-5.269304	4.225700	-3.117977
C	-2.472705	2.893390	0.803863
C	-0.733818	0.092141	1.108434
C	0.548410	-0.772050	0.903168
B	1.835859	-0.160339	0.172482
O	-0.084312	-0.492855	-2.810701
C	2.137647	1.394229	0.422717
C	1.392080	2.441937	-0.117535
C	1.626995	3.784011	0.168234
C	2.662444	4.123589	1.033357
C	3.437017	3.114687	1.601555
C	3.163643	1.785973	1.289613
F	0.360301	2.178808	-0.955866
F	3.929746	0.851444	1.884180
F	4.426602	3.430458	2.445172
F	2.901182	5.404128	1.329523
F	0.848364	4.738642	-0.359264
C	3.060532	-1.110241	-0.182721
C	4.165709	-0.630643	-0.908148

C	5.237007	-1.429531	-1.294725
C	5.237436	-2.780561	-0.962165
C	4.166977	-3.310107	-0.248013
C	3.111642	-2.480272	0.116761
F	4.234553	0.659885	-1.265053
F	6.262309	-0.913223	-1.980794
F	6.257013	-3.562935	-1.321949
F	4.159416	-4.609115	0.080987
F	2.114641	-3.078904	0.805676
C	-2.921483	-1.668710	-0.132928
C	-4.155068	-1.526841	0.558989
C	-4.960155	-2.653198	0.751184
C	-4.598889	-3.919460	0.288270
C	-3.381091	-4.040656	-0.380384
C	-2.530433	-2.950820	-0.607309
C	-4.666389	-0.215381	1.113000
C	-5.506333	-5.109782	0.484348
C	-1.233351	-3.248656	-1.334526
H	0.937737	-0.995653	1.910228
H	-0.466208	1.146235	1.056525
H	-4.669146	1.705220	-3.965312
H	-3.969728	4.396362	-0.719564
H	-3.074075	-5.018128	-0.745256
H	-5.899451	-2.532428	1.286340
H	-3.856095	-0.322656	-4.080493
H	-2.247226	-0.554627	-3.399630
H	-3.665349	-1.236011	-2.584399
H	-2.574312	2.133350	1.579488
H	-1.409473	3.135604	0.692930
H	-2.969788	3.797879	1.166471
H	-4.955898	4.357474	-4.160134
H	-6.328596	3.938443	-3.134551
H	-5.195482	5.196033	-2.617445
H	-1.319745	-4.201198	-1.865743
H	-0.952956	-2.489041	-2.066498
H	-0.392376	-3.356347	-0.637531
H	-6.243162	-5.178715	-0.326957
H	-4.942147	-6.047895	0.492809
H	-6.064892	-5.037287	1.423632
H	-5.062158	0.433412	0.324574
H	-5.473170	-0.402367	1.827871
H	-3.888882	0.341269	1.641753
H	0.282956	-1.753719	0.509436

H	-0.835492	-0.422028	-1.658491
H	1.355339	-0.070548	-1.453920
C	-1.342934	-0.169974	2.480097
C	-1.752955	-1.452086	2.882921
C	-1.375321	0.860409	3.433613
C	-2.219273	-1.680888	4.177305
H	-1.700534	-2.281112	2.186232
C	-1.838601	0.632475	4.731208
H	-1.011153	1.849027	3.167711
C	-2.271973	-0.638903	5.105747
H	-2.534687	-2.681011	4.462115
H	-1.849301	1.448688	5.448524
H	-2.632499	-0.820822	6.114380

#### C<sub>4</sub>

E= -2685.5143616au

C	2.548011	2.469837	-0.203107
C	2.016305	1.491480	0.679962
C	1.693135	1.900891	2.008989
C	1.867927	3.232353	2.397597
C	2.340714	4.209133	1.520504
C	2.691157	3.794334	0.237640
P	1.435522	-0.260849	0.298941
C	-4.159691	-0.793783	2.743516
O	-4.907474	-1.720427	2.904515
C	1.131949	0.951485	3.047810
C	2.438074	5.658967	1.929691
C	2.998510	2.215418	-1.628178
C	1.334878	-0.563352	-1.615007
C	-0.111668	-1.069046	-1.873373
B	-1.294924	-0.292593	-1.161327
O	-4.565785	0.398539	2.261958
C	-1.208906	1.276837	-0.927192
C	-1.564376	1.876271	0.282712
C	-1.447510	3.232731	0.544492
C	-0.961804	4.073122	-0.455525
C	-0.610342	3.534281	-1.689063
C	-0.738151	2.163363	-1.898852
F	-1.997893	1.097651	1.314016
F	-0.360185	1.698969	-3.108773
F	-0.121885	4.324646	-2.651398
F	-0.818525	5.379323	-0.222653
F	-1.778339	3.730637	1.741413

C	-2.661726	-1.024047	-0.858559
C	-3.899393	-0.362221	-0.974285
C	-5.129362	-0.985447	-0.790688
C	-5.166640	-2.334326	-0.449670
C	-3.973532	-3.040780	-0.313218
C	-2.764231	-2.388802	-0.527319
F	-3.948689	0.939372	-1.310094
F	-6.267104	-0.303367	-0.938344
F	-6.330903	-2.947327	-0.267017
F	-4.000402	-4.335451	0.013775
F	-1.662652	-3.149314	-0.371030
C	2.685528	-1.424634	1.079244
C	4.097193	-1.315739	0.979608
C	4.907729	-2.227204	1.666863
C	4.383019	-3.254984	2.450472
C	2.994309	-3.359751	2.532759
C	2.137467	-2.470426	1.873649
C	4.794939	-0.273479	0.139640
C	5.284713	-4.204245	3.203103
C	0.647803	-2.690229	2.054510
H	-0.307412	-0.997390	-2.959481
H	1.410949	0.424798	-2.060728
H	1.610233	3.514004	3.416400
H	3.096544	4.525622	-0.459395
H	2.558039	-4.156545	3.131621
H	5.987774	-2.130097	1.577156
H	1.002087	1.469029	4.003329
H	0.155181	0.559855	2.740610
H	1.785829	0.090644	3.221489
H	3.420598	1.221954	-1.770548
H	2.180012	2.343212	-2.348957
H	3.769703	2.941767	-1.904959
H	1.540672	6.208937	1.615856
H	2.526569	5.766774	3.015707
H	3.299378	6.152127	1.465809
H	0.472618	-3.547614	2.712196
H	0.157582	-1.819062	2.501378
H	0.131886	-2.889650	1.111728
H	5.489654	-3.834396	4.216855
H	4.828159	-5.194539	3.306130
H	6.250201	-4.324259	2.700273
H	4.510039	0.742416	0.425330
H	5.880498	-0.361509	0.246355

H	4.559213	-0.402181	-0.921996
H	-0.171760	-2.136300	-1.651942
H	-3.787717	0.968905	2.129552
H	-3.077192	-0.832675	2.969378
C	2.356403	-1.460494	-2.287170
C	2.554073	-2.791643	-1.884106
C	3.076732	-0.998285	-3.400914
C	3.452972	-3.619973	-2.555415
H	2.006045	-3.186071	-1.034054
C	3.977695	-1.825391	-4.075442
H	2.918891	0.017050	-3.755927
C	4.172580	-3.140186	-3.652156
H	3.591003	-4.644234	-2.219180
H	4.520405	-1.441158	-4.935306
H	4.872461	-3.787084	-4.174145

## D

E= -2673.3952817au

C	-3.572699	2.435576	-0.189503
C	-3.388296	1.167337	-0.799794
C	-4.320180	0.770697	-1.800769
C	-5.425791	1.578736	-2.089666
C	-5.647868	2.796763	-1.449846
C	-4.693143	3.208303	-0.520497
P	-1.917113	0.005360	-0.598241
C	-4.169218	-0.498227	-2.613601
C	-6.867241	3.635741	-1.750040
C	-2.604362	3.058083	0.794799
C	-0.910551	0.406147	0.975373
C	0.351560	-0.502502	0.993829
B	1.597129	-0.004963	0.205477
C	1.987666	1.546803	0.259085
C	1.331541	2.539391	-0.465918
C	1.677391	3.887229	-0.400026
C	2.736706	4.280574	0.412944
C	3.432017	3.321433	1.146337
C	3.051748	1.987381	1.044975
F	0.312251	2.208562	-1.285668
F	3.755883	1.087193	1.770388
F	4.450899	3.687583	1.932978
F	3.081326	5.568572	0.494368
F	0.999476	4.799638	-1.106260
C	2.569130	-0.970360	-0.590844

C	3.547069	-0.487181	-1.485400
C	4.393642	-1.309126	-2.224505
C	4.298540	-2.690360	-2.090703
C	3.350750	-3.228547	-1.224985
C	2.515644	-2.376140	-0.510847
F	3.706984	0.827828	-1.696814
F	5.294734	-0.781929	-3.059362
F	5.104194	-3.490854	-2.785746
F	3.249265	-4.555023	-1.089124
F	1.631792	-2.993722	0.295779
C	-2.691152	-1.607992	0.003319
C	-3.666794	-1.705372	1.030680
C	-4.113631	-2.968835	1.437485
C	-3.643723	-4.151481	0.863340
C	-2.698085	-4.042709	-0.155836
C	-2.221411	-2.803047	-0.602288
C	-4.302830	-0.508433	1.707496
C	-4.166056	-5.496853	1.309762
C	-1.228524	-2.814881	-1.749847
H	-0.613783	1.452008	0.960777
H	-6.126647	1.243874	-2.852123
H	-4.815734	4.173640	-0.032999
H	-2.319504	-4.948196	-0.625872
H	-4.856495	-3.026396	2.231212
H	-4.864075	-0.491226	-3.459194
H	-3.153971	-0.596718	-3.017119
H	-4.368322	-1.399641	-2.024473
H	-2.470705	2.455825	1.698606
H	-1.618448	3.211028	0.342185
H	-2.969367	4.039739	1.111233
H	-7.214884	3.484537	-2.777791
H	-7.702308	3.378375	-1.084112
H	-6.663166	4.703523	-1.614774
H	-1.030388	-3.844220	-2.065947
H	-1.606817	-2.262647	-2.616555
H	-0.271719	-2.357394	-1.484990
H	-3.463518	-6.300677	1.066089
H	-4.346864	-5.518949	2.390246
H	-5.118905	-5.735517	0.818298
H	-5.011824	-0.004990	1.041881
H	-4.850195	-0.826665	2.600636
H	-3.576621	0.247992	2.015180
H	0.070667	-1.516359	0.695790

H	-1.527251	0.259967	1.866352
Si	0.831496	-0.832661	2.870567
C	-0.543401	-1.931988	3.569700
H	-0.617574	-2.874202	3.014684
H	-0.327782	-2.176791	4.617580
H	-1.528328	-1.454529	3.536776
C	0.910149	0.793282	3.840522
H	0.024010	1.419692	3.690518
H	0.977788	0.573024	4.913561
H	1.793299	1.382878	3.573997
C	2.480373	-1.740316	3.083698
H	2.670535	-1.886862	4.154703
H	2.472150	-2.727268	2.611192
H	3.321793	-1.170568	2.677334

### **D<sub>1</sub>**

**E= -2674.5693308au**

C	-2.198888	2.322283	-0.190840
C	-3.272151	2.871786	0.566074
C	-3.807949	4.108798	0.207170
H	-4.627476	4.513463	0.798159
C	-3.329199	4.843310	-0.883906
C	-2.286902	4.293181	-1.620240
H	-1.896950	4.838378	-2.478020
C	-1.709142	3.052765	-1.301755
C	-3.874100	2.177241	1.765685
H	-3.147900	2.073060	2.579946
H	-4.235827	1.175962	1.514835
H	-4.718929	2.752386	2.156525
C	-3.927567	6.184361	-1.236101
H	-3.746259	6.920635	-0.442592
H	-5.014528	6.115161	-1.366112
H	-3.502188	6.582268	-2.162705
C	-0.583746	2.605264	-2.215659
H	-0.924535	2.601037	-3.258093
H	-0.202693	1.612357	-1.981920
H	0.253283	3.310391	-2.154281
C	-2.703102	-0.622021	0.212557
C	-3.228567	-1.360074	1.308554
C	-4.158633	-2.382033	1.063576
H	-4.548030	-2.936105	1.915023
C	-4.605851	-2.713396	-0.213021
C	-4.078258	-1.987869	-1.280964

H	-4.396147	-2.226273	-2.294008
C	-3.140626	-0.967693	-1.100253
C	-2.880258	-1.135999	2.767183
H	-3.443456	-1.834572	3.392783
H	-3.132385	-0.127293	3.105231
H	-1.820663	-1.300396	2.980318
C	-5.631471	-3.799544	-0.432846
H	-5.687167	-4.477678	0.424868
H	-5.399311	-4.395637	-1.322614
H	-6.633358	-3.374987	-0.581834
C	-2.634184	-0.274868	-2.347885
H	-3.047476	-0.754044	-3.240617
H	-1.542881	-0.311626	-2.426410
H	-2.924139	0.781025	-2.375521
C	2.300081	0.562790	-0.047512
C	2.223408	1.953306	-0.180843
F	1.119709	2.624099	0.206453
C	3.232644	2.734587	-0.736832
F	3.065479	4.055719	-0.879616
C	4.420117	2.134287	-1.143130
F	5.405651	2.869557	-1.662200
C	4.571199	0.759108	-0.992030
F	5.716509	0.168835	-1.352938
C	3.523750	0.012297	-0.459915
C	0.971263	-1.784863	-0.210879
C	0.875813	-3.025378	0.431797
F	1.000273	-3.117067	1.773039
C	0.678471	-4.227436	-0.243556
F	0.608205	-5.383707	0.427262
C	0.558948	-4.222318	-1.629693
F	0.361291	-5.363706	-2.293564
C	0.644065	-3.014621	-2.318006
F	0.519954	-2.995154	-3.652090
C	0.861567	-1.840946	-1.606530
F	0.921606	-0.703572	-2.333764
F	3.755651	-1.308252	-0.313689
C	0.520950	-0.186900	1.998175
H	0.017322	-1.127467	2.246732
C	-0.576392	0.910431	1.939697
H	-1.241202	0.895093	2.804052
H	-0.136305	1.908290	1.884659
B	1.165412	-0.398080	0.550571
P	-1.362191	0.695322	0.239871

H	1.857969	-0.578474	-5.532447
H	1.572779	-0.882149	-4.917834
Si	1.766528	0.055716	3.443675
C	0.827510	-0.193962	5.074736
H	0.028612	0.546053	5.205820
H	0.371082	-1.190087	5.126649
H	1.505469	-0.098562	5.932209
C	2.516975	1.798173	3.438249
H	3.176852	1.959707	2.578959
H	1.750411	2.581839	3.421975
H	3.117384	1.946867	4.344619
C	3.160279	-1.225959	3.339158
H	3.700283	-1.179077	2.386094
H	3.890894	-1.062993	4.141208
H	2.772607	-2.245296	3.440652

### TS<sub>12D</sub>

E= -2674.5430382au

C	-3.172028	1.623689	-0.477171
C	-4.269202	1.957392	0.358263
C	-5.087474	3.039801	0.019941
H	-5.922764	3.283930	0.673307
C	-4.863930	3.817742	-1.117765
C	-3.774954	3.487042	-1.923183
H	-3.572482	4.084848	-2.809146
C	-2.925795	2.411000	-1.633580
C	-4.596467	1.211466	1.631153
H	-3.791770	1.308438	2.369311
H	-4.753660	0.144154	1.452595
H	-5.505242	1.614291	2.088169
C	-5.782580	4.962785	-1.471743
H	-6.148297	5.475171	-0.575180
H	-6.663292	4.606651	-2.022854
H	-5.278207	5.700725	-2.103910
C	-1.767897	2.171192	-2.582184
H	-1.751455	1.148560	-2.970865
H	-0.804663	2.352225	-2.096835
H	-1.836507	2.850696	-3.437267
C	-3.029500	-1.346437	0.099159
C	-3.228408	-2.088986	1.295731
C	-3.968559	-3.276372	1.248526
H	-4.108682	-3.831318	2.173995
C	-4.533481	-3.772148	0.072697

C	-4.328073	-3.038111	-1.092943
H	-4.747555	-3.400228	-2.028959
C	-3.584862	-1.852422	-1.109343
C	-2.696789	-1.689415	2.654259
H	-2.980663	-2.435885	3.401700
H	-3.097218	-0.728081	2.990005
H	-1.607869	-1.616382	2.670695
C	-5.329695	-5.055164	0.071730
H	-4.733063	-5.894948	0.448654
H	-5.671954	-5.312775	-0.935399
H	-6.214423	-4.975730	0.715895
C	-3.407190	-1.171543	-2.449344
H	-3.872020	-1.765357	-3.241990
H	-2.346797	-1.051321	-2.700608
H	-3.861258	-0.174730	-2.472285
C	2.353439	1.187332	-0.036757
C	1.939415	2.505245	-0.246611
F	0.615798	2.788458	-0.343550
C	2.802046	3.587958	-0.384063
F	2.325831	4.822226	-0.592329
C	4.175010	3.373947	-0.302588
F	5.027257	4.395897	-0.423478
C	4.647395	2.083101	-0.090148
F	5.964784	1.861673	-0.004078
C	3.742311	1.029249	0.027457
C	1.862504	-1.467140	-0.482175
C	1.924925	-2.685608	0.200597
F	1.526596	-2.792617	1.488694
C	2.401311	-3.866513	-0.369011
F	2.436029	-4.999205	0.345738
C	2.844009	-3.865836	-1.686397
F	3.300489	-4.989557	-2.247791
C	2.804061	-2.680443	-2.415329
F	3.222275	-2.662133	-3.687719
C	2.328023	-1.526628	-1.803136
F	2.311261	-0.409019	-2.562720
F	4.286555	-0.187717	0.239076
C	0.338957	-0.115524	1.412043
H	0.038524	-1.162271	1.529760
C	-0.981685	0.717621	1.346765
H	-1.529823	0.682021	2.288768
H	-0.771879	1.770985	1.141289
B	1.307529	-0.060331	0.112610

P	-2.004821	0.203506	-0.132300
H	-0.180367	0.195132	-0.982196
H	0.634787	0.324371	-1.105462
S	1.232285	0.285911	3.083433
C	0.137101	-0.300219	4.524239
H	-0.849268	0.177426	4.544710
H	-0.015345	-1.385877	4.506437
H	0.631538	-0.058632	5.473925
C	1.482117	2.156820	3.297838
H	2.247875	2.558604	2.626662
H	0.558817	2.723235	3.127051
H	1.805888	2.365340	4.325528
C	2.896364	-0.596520	3.286663
H	3.598288	-0.403775	2.471174
H	3.369743	-0.264596	4.219617
H	2.759373	-1.680767	3.348973

## D<sub>2</sub>

E= -2674.572727au

C	-3.696721	2.127178	0.039441
C	-3.364446	0.967496	-0.701346
C	-4.017610	0.710468	-1.939798
C	-5.002119	1.595195	-2.381686
C	-5.363662	2.733004	-1.655466
C	-4.696577	2.974306	-0.456190
P	-2.075111	-0.250332	-0.187344
C	-3.681382	-0.464743	-2.831552
C	-6.428513	3.671925	-2.167264
C	-3.013866	2.562095	1.317090
C	-0.888300	0.136496	1.188363
C	0.453813	-0.618248	0.973671
B	1.336282	0.047747	-0.290121
C	1.619196	1.642489	0.022016
C	0.704518	2.628234	-0.348333
C	0.844406	3.985901	-0.066031
C	1.976713	4.425361	0.608574
C	2.931308	3.489738	0.998661
C	2.729461	2.143645	0.705348
F	-0.448237	2.293066	-1.001324
F	3.688002	1.295934	1.147403
F	4.023573	3.894099	1.665421
F	2.137654	5.724780	0.897160
F	-0.115067	4.861848	-0.418946



C	2.664586	-0.802851	-0.775341
C	3.701508	-0.212688	-1.511899
C	4.795678	-0.903181	-2.029287
C	4.891628	-2.278030	-1.845848
C	3.880334	-2.926799	-1.149721
C	2.808883	-2.187172	-0.652529
F	3.682022	1.111224	-1.783080
F	5.751248	-0.255437	-2.715349
F	5.933134	-2.964428	-2.338754
F	3.935521	-4.258005	-0.968777
F	1.859845	-2.935939	-0.016277
C	-2.792980	-1.916211	0.110085
C	-3.818000	-2.074618	1.078899
C	-4.327484	-3.352263	1.318804
C	-3.863055	-4.479277	0.635848
C	-2.851605	-4.299744	-0.308317
C	-2.296961	-3.045991	-0.593510
C	-4.392228	-0.923109	1.875466
C	-4.452317	-5.843685	0.898474
C	-1.192684	-2.993489	-1.630214
H	-0.732031	1.213707	1.211576
H	-5.496685	1.388489	-3.328077
H	-4.950166	3.861085	0.119308
H	-2.468885	-5.165685	-0.842635
H	-5.108573	-3.468832	2.066519
H	-4.331952	-0.470367	-3.710101
H	-2.648438	-0.409805	-3.198268
H	-3.803888	-1.426672	-2.323935
H	-2.857936	1.747662	2.027943
H	-2.039245	3.009644	1.091767
H	-3.612556	3.325440	1.821453
H	-6.114069	4.148768	-3.103866
H	-7.362897	3.137472	-2.376105
H	-6.645209	4.464565	-1.445165
H	-1.053802	-3.984157	-2.071509
H	-1.417341	-2.305001	-2.451824
H	-0.232265	-2.695753	-1.199932
H	-3.755019	-6.640926	0.623147
H	-4.716330	-5.968842	1.953889
H	-5.369858	-5.992902	0.313965
H	-4.904231	-0.195233	1.237357
H	-5.117157	-1.292083	2.606143
H	-3.621772	-0.382288	2.437175

H	0.207435	-1.654871	0.711023
H	-1.409295	-0.140930	2.112604
H	-1.245853	-0.381971	-1.312346
H	0.628409	0.030430	-1.293749
Si	1.242502	-0.848270	2.716991
C	0.120759	-2.050956	3.684467
H	0.054410	-3.022725	3.179488
H	0.529234	-2.230618	4.687102
H	-0.903335	-1.679465	3.819391
C	1.301010	0.781428	3.696162
H	0.344530	1.319052	3.691407
H	1.549131	0.572481	4.744614
H	2.068081	1.458804	3.308134
C	2.975994	-1.602745	2.693670
H	3.344181	-1.704699	3.722746
H	2.977426	-2.597663	2.237478
H	3.681201	-0.973319	2.144642

### D<sub>3</sub>

E= -2863.15657au

C	3.840987	1.949993	-0.494244
C	3.477399	0.897430	0.382011
C	4.155330	0.747374	1.624717
C	5.186005	1.633936	1.941955
C	5.573506	2.667857	1.086402
C	4.885407	2.803952	-0.117987
P	2.119534	-0.305422	0.036742
C	-0.441515	1.290575	3.514305
O	-1.420661	1.917015	3.424452
C	3.800762	-0.309148	2.648074
C	6.704072	3.596486	1.456024
C	3.158616	2.256918	-1.809957
C	0.935889	0.020576	-1.353973
C	-0.410987	-0.724421	-1.142500
B	-1.320894	-0.006921	0.071453
O	0.541900	0.664884	3.646969
C	-1.562760	1.586197	-0.283274
C	-0.680633	2.576978	0.147029
C	-0.805664	3.934435	-0.144120
C	-1.881827	4.364156	-0.910951
C	-2.797569	3.422652	-1.373263
C	-2.618100	2.080035	-1.052914
F	0.417921	2.247462	0.895856

F -3.542666 1.226987 -1.553818  
 F -3.833228 3.818587 -2.128880  
 F -2.027027 5.661765 -1.214392  
 F 0.104520 4.820961 0.296819  
 C -2.683074 -0.815530 0.535373  
 C -3.748474 -0.183445 1.192221  
 C -4.873355 -0.842415 1.685521  
 C -4.972659 -2.223445 1.560471  
 C -3.934013 -2.911516 0.946763  
 C -2.832275 -2.203560 0.470677  
 F -3.728907 1.150445 1.405617  
 F -5.855665 -0.157474 2.292696  
 F -6.043477 -2.878852 2.031917  
 F -3.992496 -4.249252 0.825954  
 F -1.857825 -2.985009 -0.079657  
 C 2.738779 -2.030072 -0.097556  
 C 3.732563 -2.354443 -1.056288  
 C 4.166665 -3.678278 -1.155505  
 C 3.653037 -4.693147 -0.344825  
 C 2.669003 -4.351987 0.584197  
 C 2.191865 -3.044735 0.733933  
 C 4.344160 -1.339165 -1.997556  
 C 4.161226 -6.109945 -0.454935  
 C 1.107535 -2.812310 1.766728  
 H 0.780300 1.098331 -1.404180  
 H 5.697648 1.512564 2.893876  
 H 5.159823 3.609386 -0.794561  
 H 2.247263 -5.129608 1.216091  
 H 4.926336 -3.922234 -1.894422  
 H 4.499416 -0.267041 3.488034  
 H 2.796112 -0.148894 3.055989  
 H 3.842683 -1.322626 2.236718  
 H 3.002256 1.373585 -2.433480  
 H 2.183574 2.729449 -1.645523  
 H 3.763190 2.960702 -2.388364  
 H 6.585358 3.979720 2.475881  
 H 7.669551 3.075836 1.417765  
 H 6.760106 4.451993 0.776369  
 H 0.925291 -3.735211 2.323885  
 H 1.372957 -2.040786 2.496787  
 H 0.159623 -2.519484 1.305860  
 H 3.384441 -6.835069 -0.192098  
 H 4.509719 -6.333052 -1.468476

H 5.006895 -6.275994 0.225649  
 H 4.805495 -0.502652 -1.464007  
 H 5.117979 -1.809687 -2.610060  
 H 3.601756 -0.922263 -2.689210  
 H -0.175404 -1.749220 -0.828857  
 H 1.465955 -0.275951 -2.266564  
 H 1.321862 -0.279930 1.190126  
 H -0.640456 -0.022887 1.093462  
 Si -1.151668 -1.022233 -2.897316  
 C -0.006786 -2.266903 -3.781202  
 H 0.045099 -3.215345 -3.232256  
 H -0.388971 -2.490194 -4.785424  
 H 1.021047 -1.901864 -3.906057  
 C -1.172219 0.565685 -3.944367  
 H -0.214472 1.100841 -3.930307  
 H -1.387046 0.314809 -4.990998  
 H -1.949949 1.258516 -3.609114  
 C -2.887867 -1.770465 -2.895329  
 H -3.221679 -1.923221 -3.929807  
 H -2.909360 -2.741153 -2.390006  
 H -3.608026 -1.111772 -2.403003

### TS34D

E= -2863.1255568au

C -3.703898 2.286668 0.067697  
 C -3.462037 1.087118 -0.644651  
 C -4.241740 0.796618 -1.801563  
 C -5.266709 1.671064 -2.169151  
 C -5.543375 2.840588 -1.458156  
 C -4.743254 3.126955 -0.354162  
 P -2.131392 -0.159021 -0.289627  
 C 0.647253 0.039014 -2.586292  
 O 1.616470 0.116092 -3.309823  
 C -3.999382 -0.408008 -2.687620  
 C -6.656082 3.765809 -1.887996  
 C -2.882497 2.776817 1.240954  
 C -0.948617 0.236458 1.114795  
 C 0.368872 -0.585711 1.012948  
 B 1.555575 0.026130 0.130237  
 O -0.595918 -0.105040 -2.818691  
 C 1.835975 1.604944 0.315890  
 C 1.022033 2.627703 -0.172970  
 C 1.252912 3.981938 0.061034

C 2. 356277 4. 366121 0. 814174  
C 3. 204259 3. 386119 1. 325184  
C 2. 930694 2. 047591 1. 065838  
F -0. 077291 2. 339619 -0. 911496  
F 3. 783805 1. 145334 1. 598642  
F 4. 265339 3. 738931 2. 060792  
F 2. 593440 5. 657991 1. 057987  
F 0. 408091 4. 905625 -0. 416446  
C 2. 733665 -0. 884104 -0. 445918  
C 3. 803382 -0. 339985 -1. 182068  
C 4. 803757 -1. 105500 -1. 775845  
C 4. 761599 -2. 490538 -1. 674963  
C 3. 716607 -3. 088086 -0. 976935  
C 2. 738415 -2. 288116 -0. 398899  
F 3. 924832 0. 984177 -1. 348719  
F 5. 798931 -0. 517846 -2. 448430  
F 5. 710870 -3. 240545 -2. 237614  
F 3. 657595 -4. 422745 -0. 871755  
F 1. 753272 -2. 970850 0. 237759  
C -2. 906193 -1. 775075 0. 195305  
C -3. 901650 -1. 834906 1. 205203  
C -4. 438841 -3. 077887 1. 558945  
C -4. 036755 -4. 266021 0. 949340  
C -3. 059182 -4. 186569 -0. 043825  
C -2. 479414 -2. 975060 -0. 436865  
C -4. 449381 -0. 621251 1. 925919  
C -4. 633013 -5. 595526 1. 344791  
C -1. 404626 -3. 044910 -1. 503052  
H -0. 739860 1. 302322 1. 106999  
H -5. 859154 1. 431727 -3. 049521  
H -4. 922812 4. 042964 0. 203800  
H -2. 727794 -5. 099352 -0. 534040  
H -5. 199963 -3. 112333 2. 335152  
H -4. 717469 -0. 416269 -3. 512498  
H -2. 996145 -0. 383807 -3. 129086  
H -4. 108763 -1. 355218 -2. 149119  
H -2. 730303 2. 019276 2. 013992  
H -1. 897813 3. 122028 0. 905783  
H -3. 377196 3. 628904 1. 715508  
H -6. 468139 4. 171023 -2. 889995  
H -7. 617556 3. 239639 -1. 929791  
H -6. 763916 4. 610576 -1. 200773  
H -1. 452540 -4. 011539 -2. 013209

H -1. 482060 -2. 264655 -2. 262349  
H -0. 402567 -2. 967887 -1. 065056  
H -3. 862018 -6. 279584 1. 720087  
H -5. 389018 -5. 479839 2. 127364  
H -5. 108220 -6. 087644 0. 487411  
H -5. 088267 -0. 015247 1. 275231  
H -5. 049800 -0. 934341 2. 784959  
H -3. 663250 0. 038571 2. 305065  
H 0. 128873 -1. 598663 0. 679315  
H -1. 490838 0. 026130 2. 042216  
H -1. 290990 -0. 206978 -1. 634056  
H 0. 867512 0. 080996 -1. 421441  
S 0. 938227 -0. 937587 2. 852213  
C -0. 310821 -2. 182857 3. 554258  
H -0. 114023 -2. 357994 4. 619382  
H -1. 352551 -1. 854804 3. 462224  
H -0. 225138 -3. 147567 3. 039979  
C 0. 882179 0. 657854 3. 878194  
H -0. 087725 1. 166324 3. 832734  
H 1. 074452 0. 419265 4. 931889  
H 1. 650153 1. 372221 3. 562621  
C 2. 664428 -1. 689709 3. 022129  
H 2. 873879 -1. 852203 4. 087290  
H 2. 742628 -2. 657396 2. 517601  
H 3. 442823 -1. 030784 2. 628197

#### D<sub>4</sub>

E= -2863.1560119au

C 3. 441905 2. 525067 -0. 060363  
C 3. 281536 1. 285753 0. 612381  
C 4. 118151 1. 017252 1. 733417  
C 5. 111278 1. 933052 2. 097998  
C 5. 307086 3. 132621 1. 415900  
C 4. 447905 3. 407958 0. 352688  
P 1. 955998 -0. 014808 0. 321629  
C -0. 394655 0. 910564 3. 511897  
O -1. 244008 1. 054743 4. 352322  
C 3. 982004 -0. 223182 2. 592118  
C 6. 405632 4. 091892 1. 807109  
C 2. 566386 3. 004829 -1. 199448  
C 0. 937385 0. 275501 -1. 258107  
C -0. 308550 -0. 656176 -1. 229371

B	-1.573862	-0.143524	-0.471066
O	-0.315922	-0.182959	2.732365
C	-2.013709	1.387780	-0.637263
C	-1.365331	2.468223	-0.044999
C	-1.764295	3.791485	-0.213875
C	-2.877512	4.070569	-1.001258
C	-3.569906	3.022732	-1.604979
C	-3.132932	1.717787	-1.402911
F	-0.287873	2.258367	0.749622
F	-3.835238	0.731644	-2.005340
F	-4.639336	3.278218	-2.366477
F	-3.274681	5.332013	-1.183243
F	-1.083570	4.786689	0.365680
C	-2.512955	-1.077003	0.386539
C	-3.456225	-0.556710	1.296536
C	-4.258634	-1.347830	2.113361
C	-4.147470	-2.732815	2.048291
C	-3.229344	-3.306058	1.172354
C	-2.439843	-2.482470	0.379734
F	-3.618748	0.765003	1.443496
F	-5.132845	-0.789946	2.954013
F	-4.911851	-3.505951	2.816817
F	-3.113567	-4.637247	1.102682
F	-1.572684	-3.128029	-0.429151
C	2.889083	-1.567485	-0.179584
C	3.914884	-1.583399	-1.161881
C	4.512949	-2.800340	-1.510269
C	4.150209	-4.010541	-0.917195
C	3.150753	-3.978893	0.054737
C	2.516559	-2.790353	0.439202
C	4.442960	-0.344190	-1.853565
C	4.837450	-5.301794	-1.293106
C	1.448385	-2.897728	1.510338
H	0.626925	1.315723	-1.305280
H	5.742207	1.700202	2.953347
H	4.556305	4.350307	-0.180384
H	2.849389	-4.907741	0.534382
H	5.291954	-2.797355	-2.270314
H	4.629809	-0.148274	3.470503
H	2.954301	-0.356933	2.951914
H	4.253247	-1.137393	2.054008
H	2.521194	2.297630	-2.032541
H	1.542226	3.193207	-0.859450

H	2.951649	3.948293	-1.597042
H	6.646391	4.012360	2.872538
H	7.329192	3.886951	1.248840
H	6.124817	5.129907	1.598782
H	1.459600	-3.899309	1.951367
H	1.587973	-2.176581	2.319823
H	0.443303	-2.734126	1.109223
H	4.181126	-6.164927	-1.140231
H	5.155222	-5.296423	-2.341306
H	5.735833	-5.463507	-0.682345
H	5.081846	0.245265	-1.187134
H	5.041353	-0.625246	-2.725865
H	3.650640	0.324464	-2.198593
H	-0.008634	-1.645572	-0.873229
H	1.564217	0.084517	-2.133294
H	0.427481	-0.096435	2.078415
H	0.395548	1.656475	3.308092
Si	-0.766320	-1.081664	-3.092828
C	0.636306	-2.187044	-3.726368
H	0.693387	-3.118575	-3.151218
H	0.455403	-2.454352	-4.775225
H	1.619889	-1.707965	-3.672563
C	-0.851659	0.503479	-4.127671
H	0.041662	1.128429	-4.018254
H	-0.939116	0.240687	-5.189517
H	-1.724402	1.113403	-3.871616
C	-2.395188	-2.025346	-3.284773
H	-2.568062	-2.224499	-4.350235
H	-2.374276	-2.988696	-2.766566
H	-3.252370	-1.455117	-2.914634

## E

E= -2601.7559048au

C	-2.318510	2.248420	0.547335
C	-1.972465	1.241527	-0.392527
C	-1.899843	1.603278	-1.771102
C	-2.139005	2.923879	-2.161793
C	-2.430509	3.930891	-1.240124
C	-2.531832	3.560668	0.099517
P	-1.383545	-0.515528	-0.104391
C	-1.545446	0.612020	-2.863601
C	-2.590632	5.369424	-1.669019
C	-2.493987	2.043728	2.040495

C	-0.789280	-0.693221	1.724155
C	0.695002	-1.132944	1.712550
B	1.691173	-0.343906	0.770000
C	1.510035	1.193911	0.467525
C	1.676264	1.713024	-0.821945
C	1.471012	3.051550	-1.133611
C	1.110672	3.937843	-0.120751
C	0.961799	3.474744	1.183199
C	1.159359	2.124354	1.448658
F	1.993331	0.886983	-1.836790
F	0.985768	1.720593	2.726894
F	0.596423	4.316211	2.157516
F	0.888683	5.223607	-0.405350
F	1.598034	3.492230	-2.389474
C	3.006003	-1.050538	0.251758
C	4.237258	-0.372916	0.223890
C	5.428052	-0.963947	-0.186175
C	5.419595	-2.289370	-0.613045
C	4.225257	-3.005363	-0.613999
C	3.057633	-2.386027	-0.178284
F	4.321650	0.902411	0.639107
F	6.574097	-0.275486	-0.172967
F	6.548690	-2.869703	-1.017279
F	4.210338	-4.275578	-1.031085
F	1.942970	-3.136242	-0.223491
C	-2.819617	-1.684178	-0.427269
C	-4.204470	-1.380540	-0.324396
C	-5.145147	-2.327758	-0.748645
C	-4.786033	-3.573270	-1.262759
C	-3.425505	-3.863229	-1.350880
C	-2.441801	-2.953677	-0.949321
C	-4.760161	-0.090410	0.233317
C	-5.832043	-4.579451	-1.679245
C	-1.002675	-3.403785	-1.065645
H	1.102239	-1.010535	2.732397
H	-0.854087	0.288683	2.185128
H	-2.076798	3.173363	-3.218906
H	-2.790593	4.318838	0.836600
H	-3.111640	-4.827266	-1.745888
H	-6.200893	-2.077894	-0.665300
H	-1.663722	1.078756	-3.846532
H	-0.505602	0.275273	-2.774402
H	-2.177974	-0.281803	-2.843321

H	-2.832293	1.044309	2.308203
H	-1.564834	2.244878	2.589885
H	-3.235997	2.752419	2.422527
H	-3.320174	5.897758	-1.045627
H	-1.635489	5.903636	-1.577656
H	-2.912419	5.446430	-2.712796
H	-0.937651	-4.332247	-1.641625
H	-0.366271	-2.655302	-1.546050
H	-0.573890	-3.602617	-0.077918
H	-6.743240	-4.087059	-2.035556
H	-5.464015	-5.234333	-2.476375
H	-6.118604	-5.222968	-0.836475
H	-4.531866	0.771644	-0.399108
H	-5.848670	-0.160463	0.321868
H	-4.362696	0.117419	1.228504
H	0.760193	-2.203739	1.507636
C	-1.594460	-1.618616	2.617716
F	-1.580136	-2.900714	2.187456
F	-1.091837	-1.627733	3.878308
F	-2.892771	-1.248228	2.728354

**E<sub>1</sub>**

**E= -2602.9242087au**

C	3.015303	-0.627866	-0.452256
C	4.335982	-0.177940	-0.187289
C	5.420525	-0.954573	-0.614068
H	6.426060	-0.596870	-0.402239
C	5.263643	-2.164249	-1.290593
C	3.962146	-2.592301	-1.550856
H	3.807376	-3.526861	-2.086295
C	2.842759	-1.852484	-1.154616
C	4.664791	1.104017	0.542672
H	4.138286	1.166879	1.496992
H	4.400181	1.991149	-0.039824
H	5.737439	1.150517	0.754912
C	6.457756	-2.990244	-1.705615
H	6.256706	-3.553354	-2.623428
H	6.722603	-3.719902	-0.928559
H	7.339268	-2.363262	-1.876416
C	1.482366	-2.418690	-1.508002
H	1.593919	-3.298800	-2.149058
H	0.854553	-1.690538	-2.031170
H	0.924746	-2.736151	-0.618663

C	1.792366	2.118017	-0.308673
C	1.905625	3.169723	0.633330
C	2.091583	4.482115	0.181242
H	2.182761	5.273431	0.922479
C	2.172008	4.811134	-1.171089
C	2.051351	3.769239	-2.089739
H	2.104780	3.990676	-3.153729
C	1.847047	2.442388	-1.696499
C	1.848810	2.970038	2.126250
H	2.036240	3.916497	2.642418
H	2.592537	2.252882	2.477853
H	0.870663	2.611457	2.457548
C	2.348387	6.241149	-1.622960
H	1.377276	6.728402	-1.784174
H	2.900197	6.298440	-2.567479
H	2.888556	6.833656	-0.876758
C	1.691620	1.416292	-2.802212
H	1.716538	1.909429	-3.778732
H	0.739998	0.877082	-2.720851
H	2.488171	0.664111	-2.791035
C	-1.729708	-1.761475	0.285931
C	-2.071306	-2.001579	-1.052773
F	-2.259092	-0.966746	-1.890990
C	-2.204703	-3.276126	-1.589584
F	-2.519537	-3.450028	-2.878676
C	-2.006363	-4.385984	-0.769656
F	-2.137306	-5.615874	-1.266592
C	-1.667299	-4.203394	0.568328
F	-1.482710	-5.263692	1.361389
C	-1.525363	-2.909119	1.064298
C	-2.717489	0.761778	0.471467
C	-2.437853	2.131388	0.344607
F	-1.181992	2.583354	0.493361
C	-3.403508	3.082900	0.030731
F	-3.078633	4.373612	-0.095697
C	-4.723716	2.678798	-0.151394
F	-5.663784	3.576973	-0.443092
C	-5.058262	1.332212	-0.026646
F	-6.327177	0.943399	-0.190394
C	-4.061933	0.408037	0.269078
F	-4.453967	-0.871963	0.391852
F	-1.203666	-2.799860	2.366832
B	-1.616001	-0.295760	0.863716

P	1.432106	0.297350	-0.053331
C	-0.541033	0.054114	1.976189
H	-0.871909	-0.480334	2.880835
H	-0.555442	1.114571	2.229259
C	0.899545	-0.399939	1.653666
H	0.851608	-1.449729	1.337681
C	1.752409	-0.496484	2.918390
H	-3.271690	-1.332438	-4.340714
H	-3.556545	-1.047890	-4.964498
F	3.067987	-0.651940	2.664647
F	1.624349	0.558333	3.754413
F	1.362041	-1.585551	3.631288

### TS<sub>12E</sub>

E= -2602.899729au

C	3.396293	-0.558413	-0.162139
C	4.638547	0.007838	0.221471
C	5.815636	-0.715219	-0.012730
H	6.761900	-0.270255	0.286646
C	5.818960	-1.979307	-0.599633
C	4.586439	-2.527495	-0.960349
H	4.557004	-3.515093	-1.415954
C	3.381579	-1.848061	-0.762376
C	4.782300	1.350512	0.897916
H	4.144140	1.414262	1.782122
H	4.519217	2.182344	0.237757
H	5.815618	1.498076	1.225681
C	7.103727	-2.737775	-0.831753
H	7.977044	-2.144135	-0.544618
H	7.216939	-3.015826	-1.886718
H	7.125726	-3.668350	-0.250821
C	2.110880	-2.546403	-1.193405
H	2.348607	-3.470094	-1.729557
H	1.494128	-1.926531	-1.848880
H	1.485154	-2.828997	-0.337269
C	1.941041	2.126159	-0.377394
C	1.880825	3.237946	0.498949
C	1.948108	4.532137	-0.034740
H	1.903334	5.374134	0.652506
C	2.080306	4.781425	-1.399401
C	2.148363	3.677379	-2.250444
H	2.258952	3.838091	-3.320630
C	2.068606	2.364097	-1.779785

C	1.754477	3.131090	1.997746
H	1.914219	4.109687	2.459949
H	2.480798	2.441872	2.431218
H	0.763563	2.787614	2.306245
C	2.126231	6.189595	-1.941616
H	2.835585	6.276398	-2.772064
H	2.416927	6.907905	-1.168355
H	1.143421	6.497324	-2.322715
C	2.139024	1.255788	-2.813134
H	2.215681	1.684189	-3.816767
H	1.250631	0.612648	-2.794274
H	3.007823	0.604533	-2.664996
C	-1.651114	-1.680613	-0.113640
C	-1.371467	-2.271110	-1.348522
F	-0.792575	-1.552632	-2.338521
C	-1.639069	-3.607240	-1.639873
F	-1.328634	-4.120348	-2.837496
C	-2.236303	-4.410621	-0.673573
F	-2.503305	-5.693885	-0.934438
C	-2.552603	-3.865681	0.568165
F	-3.135589	-4.626553	1.502374
C	-2.261250	-2.526972	0.817671
C	-2.776260	0.766856	0.080768
C	-3.487188	1.328070	1.146462
F	-3.048694	1.199725	2.413832
C	-4.676300	2.037988	0.981131
F	-5.314173	2.552758	2.040306
C	-5.203583	2.209623	-0.294650
F	-6.339345	2.891703	-0.469495
C	-4.535126	1.667357	-1.389301
F	-5.028789	1.829115	-2.623678
C	-3.356420	0.959870	-1.177915
F	-2.743849	0.457887	-2.272277
F	-2.612706	-2.045819	2.029168
B	-1.422822	-0.117932	0.256610
P	1.753989	0.309978	-0.011093
C	-0.544269	0.212452	1.574998
H	-1.056266	-0.259863	2.418785
H	-0.564929	1.286197	1.782393
C	0.918761	-0.283932	1.566854
H	0.912097	-1.356596	1.327089
C	1.548040	-0.265958	2.959787
H	-0.061206	0.194132	-0.733567

H	-0.864640	0.394999	-0.930939
F	2.896876	-0.354733	2.934943
F	1.233099	0.823088	3.692778
F	1.097643	-1.335524	3.660040

## E<sub>2</sub>

E= -2602.936 4464au

C	1.806814	2.709879	0.855350
C	1.958463	1.343942	1.193536
C	2.132565	0.955188	2.550805
C	2.151305	1.946651	3.532515
C	1.996489	3.301116	3.227561
C	1.835690	3.653356	1.887733
P	1.924100	-0.034536	-0.011557
C	2.268868	-0.484251	3.000201
C	1.978800	4.345656	4.315838
C	1.581156	3.246023	-0.541503
C	0.840580	0.169649	-1.543357
C	-0.367792	-0.785577	-1.416253
B	-1.343932	-0.312779	-0.165733
C	-2.351814	0.893158	-0.647998
C	-2.291764	2.200185	-0.164053
C	-3.160007	3.217474	-0.560596
C	-4.158206	2.939482	-1.487386
C	-4.262329	1.652116	-2.008141
C	-3.367576	0.672929	-1.583663
F	-1.334714	2.564190	0.726968
F	-3.513371	-0.552609	-2.134271
F	-5.216466	1.374361	-2.910696
F	-5.003487	3.901897	-1.883959
F	-3.037060	4.460809	-0.062458
C	-2.191563	-1.539414	0.512948
C	-2.628877	-1.439147	1.837512
C	-3.353350	-2.431561	2.494365
C	-3.680869	-3.599635	1.812410
C	-3.275364	-3.749893	0.490691
C	-2.553203	-2.727767	-0.124758
F	-2.347033	-0.331547	2.558756
F	-3.735648	-2.276556	3.773995
F	-4.375641	-4.570632	2.424205
F	-3.582395	-4.875133	-0.176982
F	-2.192688	-2.954503	-1.409470
C	3.591834	-0.769248	-0.302986

C	4.764350	0.018474	-0.436698
C	5.993760	-0.632137	-0.580484
C	6.112006	-2.022328	-0.600685
C	4.942572	-2.776199	-0.487850
C	3.682624	-2.189403	-0.343576
C	4.778130	1.530009	-0.449290
C	7.459294	-2.689573	-0.726570
C	2.490727	-3.120683	-0.261219
H	-0.895470	-0.763198	-2.375852
H	0.472785	1.197036	-1.530822
H	2.284875	1.647389	4.569153
H	1.719268	4.702502	1.627302
H	5.006331	-3.860952	-0.522553
H	6.888736	-0.024312	-0.687795
H	2.553905	-0.522885	4.054731
H	1.315050	-1.020194	2.904759
H	3.028701	-1.037426	2.436854
H	2.083915	2.680594	-1.327201
H	0.507432	3.262044	-0.759262
H	1.937296	4.278320	-0.607182
H	0.959392	4.485978	4.698266
H	2.607738	4.053974	5.163295
H	2.325461	5.316286	3.947189
H	2.816284	-4.155481	-0.394239
H	1.976956	-3.070058	0.707020
H	1.754052	-2.909553	-1.041316
H	7.384957	-3.645585	-1.254812
H	8.172213	-2.055417	-1.262940
H	7.885926	-2.896748	0.263821
H	4.473769	1.957327	0.510619
H	5.786493	1.891683	-0.668188
H	4.116348	1.931643	-1.220638
H	-0.009488	-1.813898	-1.301614
H	1.251631	-1.055075	0.666614
H	-0.629557	0.144422	0.715143
C	1.630365	0.018816	-2.836356
F	2.694425	0.872835	-2.887529
F	2.119182	-1.226219	-3.008498
F	0.853906	0.304198	-3.894126

### E<sub>3</sub>

E= -2791.5217325au

C	1.594852	2.728430	0.468317
---	----------	----------	----------

C	1.711193	1.409762	0.974455
C	1.440722	1.138028	2.344514
C	1.003712	2.185195	3.155720
C	0.825780	3.483274	2.669333
C	1.161109	3.733955	1.338191
P	2.011217	-0.054679	-0.079029
C	-0.544389	-4.478096	2.658071
O	-1.441870	-5.215571	2.550292
C	1.565913	-0.236077	2.965727
C	0.244642	4.566539	3.542409
C	1.893099	3.156640	-0.955341
C	1.083743	0.066338	-1.714773
C	-0.237193	-0.733106	-1.628465
B	-1.236599	-0.316397	-0.378341
O	0.380452	-3.767491	2.777107
C	-1.716859	1.258439	-0.321858
C	-2.159502	1.787947	0.897004
C	-2.567137	3.107968	1.069262
C	-2.559115	3.976894	-0.017561
C	-2.136930	3.503059	-1.254132
C	-1.735434	2.172251	-1.374875
F	-2.186919	1.011507	2.000457
F	-1.290646	1.812268	-2.608019
F	-2.096333	4.332775	-2.311196
F	-2.935342	5.255930	0.131357
F	-2.937895	3.565889	2.281815
C	-2.544229	-1.299701	-0.381063
C	-2.804734	-2.221229	0.632160
C	-3.913634	-3.065635	0.647828
C	-4.830236	-3.001368	-0.396863
C	-4.619714	-2.097622	-1.435341
C	-3.495021	-1.276671	-1.403475
F	-1.952908	-2.345604	1.683960
F	-4.103793	-3.936124	1.652986
F	-5.904098	-3.804294	-0.406232
F	-5.498095	-2.031370	-2.448855
F	-3.340301	-0.419858	-2.439515
C	3.719282	-0.741996	-0.099698
C	4.888913	0.058865	-0.122627
C	6.133728	-0.572240	-0.040502
C	6.268721	-1.958487	0.043006
C	5.103557	-2.727740	0.044793
C	3.828671	-2.160607	-0.027255



C	4.883023	1.562135	-0.264804
C	7.629218	-2.608453	0.097293
C	2.646708	-3.109685	-0.024485
H	-0.729142	-0.598007	-2.596823
H	0.829477	1.116327	-1.849600
H	0.777298	1.973736	4.197649
H	1.063936	4.744917	0.948964
H	5.184306	-3.810445	0.102633
H	7.027335	0.047031	-0.049175
H	1.565841	-0.154633	4.056032
H	0.717755	-0.876563	2.689840
H	2.490915	-0.748811	2.678746
H	2.510062	2.455054	-1.515426
H	0.965655	3.312565	-1.519977
H	2.422644	4.115272	-0.947723
H	0.593412	5.559811	3.242098
H	-0.849542	4.558412	3.456732
H	0.495310	4.414389	4.597150
H	3.002309	-4.139106	-0.120389
H	2.065133	-3.059559	0.904213
H	1.966660	-2.925265	-0.860486
H	8.380699	-1.931776	0.516033
H	7.613478	-3.521268	0.701777
H	7.965840	-2.890454	-0.909052
H	4.198850	2.049818	0.433466
H	5.884179	1.963032	-0.084892
H	4.593696	1.852334	-1.280627
H	-0.000197	-1.802812	-1.544162
H	1.292239	-1.060264	0.571198
H	-0.648365	-0.512920	0.667610
C	1.964155	-0.292549	-2.902850
F	1.312981	-0.087152	-4.057382
F	2.371514	-1.580835	-2.886769
F	3.091460	0.476766	-2.939336

**TS<sub>34E</sub>**

E= -2791.4816022au

C	2.207427	2.463618	-0.311013
C	2.342643	1.371228	0.585649
C	2.692995	1.623066	1.943145
C	2.817873	2.945220	2.378467
C	2.603791	4.033462	1.533338
C	2.330690	3.763433	0.192705

P	1.962623	-0.407862	0.235992
C	-0.943219	-0.993981	2.422798
O	-1.895037	-1.178665	3.144651
C	2.963546	0.528564	2.955536
C	2.657842	5.451698	2.043561
C	1.958512	2.365149	-1.803886
C	0.809583	-0.611539	-1.279322
C	-0.541099	-1.311102	-0.961612
B	-1.718626	-0.469641	-0.262891
O	0.305767	-1.196070	2.562183
C	-1.749081	1.117304	-0.510539
C	-1.264495	2.123062	0.326586
C	-1.344942	3.476959	0.004970
C	-1.927947	3.865125	-1.198531
C	-2.421911	2.895318	-2.068215
C	-2.322187	1.554063	-1.707700
F	-0.680420	1.814668	1.499127
F	-2.802732	0.637360	-2.575361
F	-2.980660	3.256838	-3.229165
F	-2.005741	5.159975	-1.521190
F	-0.855427	4.406988	0.835861
C	-3.095470	-1.170025	0.079532
C	-4.027353	-0.544206	0.923830
C	-5.243278	-1.118476	1.279505
C	-5.571898	-2.377945	0.786631
C	-4.680974	-3.044359	-0.050757
C	-3.470681	-2.441307	-0.377111
F	-3.763388	0.666424	1.438332
F	-6.093589	-0.476342	2.087654
F	-6.735252	-2.944275	1.112817
F	-4.994703	-4.253852	-0.532440
F	-2.658563	-3.144265	-1.192532
C	3.478710	-1.468076	0.111910
C	4.746993	-0.978790	-0.296722
C	5.845240	-1.845981	-0.254472
C	5.744030	-3.170951	0.167884
C	4.483342	-3.636773	0.544760
C	3.348144	-2.822611	0.528843
C	5.011338	0.428072	-0.785372
C	6.955444	-4.068969	0.229172
C	2.032010	-3.456801	0.923501
H	-0.971476	-1.582923	-1.936827
H	0.590235	0.398387	-1.621682

H	3.080368	3.123705	3.418377	C	-2.068685	-3.113918	-1.046733
H	2.212574	4.595165	-0.498580	C	-0.817026	-0.123766	-1.529478
H	4.372342	-4.671631	0.859772	C	0.439810	0.789050	-1.514051
H	6.813494	-1.465689	-0.571287	B	1.739804	0.350325	-0.731710
H	3.395956	0.961219	3.862145	O	0.590150	0.584936	2.423161
H	2.047828	0.001981	3.245306	C	2.245592	-1.148902	-0.873344
H	3.671902	-0.218644	2.580785	C	1.689694	-2.246155	-0.224809
H	2.384601	1.472843	-2.261196	C	2.149828	-3.547506	-0.398454
H	0.887440	2.391554	-2.044274	C	3.221996	-3.777424	-1.258193
H	2.406540	3.229229	-2.304043	C	3.813290	-2.707782	-1.928373
H	1.642220	5.843450	2.184729	C	3.320055	-1.422760	-1.720810
H	3.175182	5.515122	3.005789	F	0.649425	-2.061781	0.622439
H	3.165862	6.115812	1.335474	F	3.900645	-0.407082	-2.391735
H	2.194944	-4.490300	1.241455	F	4.836756	-2.924129	-2.760109
H	1.528796	-2.935534	1.743272	F	3.675271	-5.018290	-1.445683
H	1.343967	-3.488910	0.071804	F	1.566989	-4.569274	0.237518
H	6.711672	-5.091002	-0.080378	C	2.662317	1.383617	-0.006465
H	7.761436	-3.700108	-0.412961	C	3.529214	0.992994	1.032070
H	7.349448	-4.126112	1.252492	C	4.331845	1.888466	1.730417
H	4.922338	1.168299	0.015288	C	4.303967	3.238129	1.386938
H	6.025994	0.494784	-1.188309	C	3.469898	3.678097	0.360797
H	4.323776	0.720424	-1.581772	C	2.669356	2.757667	-0.304139
H	-0.379280	-2.266763	-0.456729	F	3.588733	-0.286703	1.421040
H	1.061531	-0.854407	1.462654	F	5.127820	1.470940	2.716358
H	-1.185235	-0.556394	1.347112	F	5.074050	4.108065	2.036384
C	1.487280	-1.302071	-2.460819	F	3.451571	4.972291	0.024589
F	1.716834	-2.611177	-2.235233	F	1.900047	3.246460	-1.294970
F	2.679183	-0.736863	-2.781611	C	-3.040534	1.450583	-0.211252
F	0.714025	-1.216347	-3.564704	C	-4.362302	1.181312	-0.665288

#### E4

E= -2791.5067906au

C	-2.665127	-2.689926	0.278598	C	-2.667049	2.799573	0.043101
C	-2.629116	-1.373436	0.806480	C	-4.946228	-0.202379	-0.859345
C	-3.196091	-1.146588	2.096900	C	-5.816082	4.712887	-1.011870
C	-3.803796	-2.202281	2.784154	C	-1.321927	3.237666	0.593960
C	-3.861290	-3.496119	2.267883	H	0.829590	0.831471	-2.549630
C	-3.282677	-3.707750	1.018249	H	-0.518036	-1.170537	-1.568754
P	-1.746267	0.141110	0.142366	H	-4.239298	-1.999994	3.760523
C	0.754424	-0.448536	3.274779	H	-3.307768	-4.707826	0.590788
O	1.611493	-0.464724	4.117874	H	-3.277972	4.853415	-0.015639
C	-3.195587	0.202527	2.790457	H	-6.236198	2.030742	-1.256806
C	-4.492575	-4.625459	3.046029	H	-3.565328	0.096682	3.814455

H	-2.192847	0.641853	2.849390
H	-3.830702	0.934360	2.280750
H	-2.331870	-2.447232	-1.867844
H	-0.975865	-3.175309	-0.986522
H	-2.423416	-4.113798	-1.312906
H	-4.843696	-5.422486	2.382374
H	-3.773796	-5.074976	3.744168
H	-5.344663	-4.276447	3.639390
H	-1.436553	4.178314	1.142270
H	-0.874822	2.510866	1.275018
H	-0.593420	3.429548	-0.203437
H	-6.855930	4.424070	-0.824659
H	-5.594349	5.600435	-0.410076
H	-5.746365	5.008393	-2.067307
H	-5.251914	-0.640243	0.098110
H	-5.836544	-0.142747	-1.493190
H	-4.252390	-0.898754	-1.323548
H	0.140713	1.810595	-1.290500
H	-0.145273	0.405329	1.779740
H	0.025240	-1.264622	3.123333
C	-1.572564	0.146710	-2.828614
F	-2.724841	-0.555234	-2.946706
F	-1.880637	1.447133	-2.987303
F	-0.808174	-0.211440	-3.893858

## F

E= -2304.0372144au

C	-2.087484	2.552086	0.032208
C	-3.422731	2.887581	0.381547
C	-3.921409	4.156436	0.065584
H	-4.946330	4.395616	0.342988
C	-3.153250	5.120965	-0.588191
C	-1.844651	4.781017	-0.927665
H	-1.222923	5.514608	-1.436794
C	-1.297616	3.523620	-0.639336
C	-4.362265	1.941911	1.095143
H	-4.022998	1.719323	2.113563
H	-4.460523	0.988389	0.569945
H	-5.358730	2.386357	1.179248
C	-3.730138	6.471780	-0.939777
H	-2.946399	7.230996	-1.032016
H	-4.446016	6.811419	-0.183193
H	-4.264920	6.436584	-1.898531

C	0.133888	3.282086	-1.078228
H	0.217283	2.421226	-1.748665
H	0.805113	3.092417	-0.237202
H	0.513543	4.159436	-1.611923
C	-2.413330	-0.450480	-0.187202
C	-3.147417	-1.391086	0.587035
C	-3.783023	-2.464564	-0.054875
H	-4.336043	-3.174316	0.557583
C	-3.732748	-2.663076	-1.433330
C	-3.041985	-1.715528	-2.188625
H	-2.996415	-1.828336	-3.269717
C	-2.381654	-0.632098	-1.601606
C	-3.308288	-1.360707	2.095700
H	-4.196377	-1.933206	2.381498
H	-3.427041	-0.353956	2.494607
H	-2.458231	-1.827503	2.609184
C	-4.364230	-3.875348	-2.073559
H	-3.671138	-4.726705	-2.046054
H	-4.618342	-3.691630	-3.122723
H	-5.276092	-4.180272	-1.548537
C	-1.623124	0.295420	-2.527691
H	-1.757656	-0.013991	-3.568665
H	-0.548635	0.279252	-2.310695
H	-1.959403	1.334139	-2.442616
C	3.072175	0.186092	0.550100
C	3.468853	1.530106	0.496884
F	2.686637	2.492291	1.025715
C	4.646045	1.965357	-0.103561
F	4.955808	3.266585	-0.141686
C	5.512688	1.027707	-0.658455
F	6.652982	1.421001	-1.227359
C	5.182207	-0.324067	-0.612135
F	6.017309	-1.231790	-1.130508
C	3.984316	-0.714971	-0.022025
C	0.992104	-1.566988	0.785172
C	0.300020	-2.465377	1.612436
F	0.239049	-2.283455	2.948747
C	-0.379787	-3.584794	1.139215
F	-1.037935	-4.384152	1.988774
C	-0.407849	-3.845292	-0.225220
F	-1.079971	-4.896458	-0.699080
C	0.253989	-2.983946	-1.096543
F	0.209506	-3.207494	-2.414596

C	0.933983	-1.887901	-0.583983
F	1.509856	-1.078316	-1.491738
F	3.744209	-2.037592	0.003948
C	-1.138010	0.922116	2.296825
H	-1.237242	-0.090854	2.686037
H	-1.938313	1.525149	2.736531
C	0.232433	1.481300	2.722722
H	0.150916	1.836822	3.758601
H	0.490983	2.359672	2.122065
C	1.399577	0.453024	2.675196
H	2.292721	0.977338	3.035307
H	1.176982	-0.319547	3.419874
P	-1.255493	0.906445	0.413533
B	1.753967	-0.276998	1.304958

**F<sub>1</sub>**

**E= -2305.2153873au**

C	-1.694118	3.371602	0.635538
C	-1.622447	2.147518	-0.085988
C	-1.534120	2.212793	-1.505613
C	-1.558271	3.452615	-2.154801
C	-1.640165	4.656029	-1.458845
C	-1.704795	4.583388	-0.067591
P	-1.482475	0.391699	0.578835
C	-1.400694	0.985123	-2.382993
C	-1.634174	5.986548	-2.173077
C	-1.750333	3.496084	2.145099
B	1.536602	-0.742046	1.269009
C	2.497194	0.400676	0.729912
C	2.221462	1.760642	0.927121
C	3.061973	2.786976	0.509554
C	4.261824	2.470086	-0.120484
C	4.597440	1.134321	-0.324830
C	3.720717	0.137858	0.094128
F	1.079041	2.138609	1.531326
F	4.122162	-1.128930	-0.115779
F	5.756578	0.821811	-0.915447
F	5.084396	3.440045	-0.522522
F	2.730539	4.069442	0.709756
C	1.472914	-2.112523	0.476498
C	1.532179	-2.166286	-0.924870
C	1.527713	-3.348721	-1.653823
C	1.469425	-4.565224	-0.977040

C	1.405747	-4.573690	0.412461
C	1.396640	-3.364586	1.105622
F	1.563452	-1.027365	-1.642072
F	1.570184	-3.330993	-2.991143
F	1.467710	-5.712767	-1.656955
F	1.350931	-5.737548	1.070661
F	1.336786	-3.463504	2.447400
C	-3.149090	-0.409591	0.180010
C	-4.408859	0.168223	0.495528
C	-5.584973	-0.515878	0.165632
C	-5.578692	-1.758417	-0.469418
C	-4.338574	-2.320831	-0.765203
C	-3.133311	-1.676515	-0.457789
C	-4.572021	1.499195	1.193176
C	-6.866893	-2.454479	-0.839183
C	-1.855902	-2.401181	-0.821438
H	-1.502486	3.470251	-3.241281
H	-1.768834	-5.507747	0.503299
H	-4.299819	-3.294016	-1.250353
H	-6.538978	-0.057360	0.418946
H	-1.291985	1.279946	-3.431290
H	-0.522145	0.388673	-2.111222
H	-2.275127	0.328536	-2.315158
H	-2.487921	2.834091	2.601920
H	-0.778363	3.282266	2.602791
H	-2.015753	4.520486	2.423716
H	-1.874798	5.871894	-3.235001
H	-2.360104	6.680666	-1.733889
H	-0.649497	6.468636	-2.109156
H	-2.083475	-3.314213	-1.381075
H	-1.194172	-1.784991	-1.435714
H	-1.287081	-2.691650	0.067871
H	-6.723151	-3.534964	-0.943752
H	-7.644689	-2.285898	-0.086129
H	-7.257636	-2.082658	-1.795990
H	-4.150543	2.322922	0.610648
H	-5.631879	1.712210	1.362336
H	-4.079142	1.509457	2.170827
H	3.504169	6.299088	-1.595058
H	3.330178	5.797432	-1.076119
C	-0.581739	-0.875169	2.930487
C	-1.465149	0.302301	2.465634
C	0.929132	-0.607305	2.726532

H	-2.482699	0.183337	2.850767
H	-1.056135	1.220200	2.884658
H	-0.773818	-1.033870	4.000150
H	-0.879416	-1.804527	2.428660
H	1.172897	0.364003	3.169116
H	1.480236	-1.351647	3.321213

**TS<sub>F12</sub>**

**E= -2305.1795068au**

C	-1.946326	-3.403846	0.188499
C	-2.154807	-2.058138	0.589298
C	-2.604656	-1.813439	1.918065
C	-2.886869	-2.886543	2.769306
C	-2.715188	-4.213065	2.376570
C	-2.238606	-4.439812	1.086299
P	-1.751238	-0.491694	-0.363023
C	-2.787669	-0.420470	2.485242
C	-2.995760	-5.355926	3.323033
C	-1.400779	-3.833680	-1.158590
B	1.782839	0.469686	-0.987796
C	3.106703	-0.404078	-0.783752
C	3.136610	-1.779979	-1.047662
C	4.280723	-2.562351	-0.930747
C	5.479101	-1.961946	-0.552461
C	5.508645	-0.595079	-0.292685
C	4.336946	0.149053	-0.407301
F	2.006978	-2.426001	-1.411381
F	4.443241	1.468626	-0.160492
F	6.659136	-0.008547	0.059801
F	6.591659	-2.692254	-0.442924
F	4.240898	-3.877548	-1.179538
C	1.565255	1.735046	-0.047581
C	1.862248	1.696523	1.324252
C	1.711619	2.785407	2.175467
C	1.262605	3.999046	1.658575
C	0.965730	4.095941	0.303973
C	1.114809	2.975872	-0.511422
F	2.308552	0.559774	1.883916
F	1.999951	2.682946	3.478531
F	1.115927	5.057344	2.458730
F	0.522334	5.252991	-0.204595
F	0.789231	3.154190	-1.808388
C	-3.408307	0.357640	-0.674186

C	-4.552645	-0.320111	-1.169386
C	-5.733928	0.399619	-1.391460
C	-5.838519	1.766624	-1.136272
C	-4.708306	2.418910	-0.642336
C	-3.501914	1.749175	-0.407970
C	-4.593610	-1.804119	-1.462020
C	-7.126396	2.517585	-1.379130
C	-2.346778	2.583686	0.106914
H	-3.243124	-2.671342	3.774740
H	-2.084543	-5.465196	0.756314
H	-4.760728	3.485222	-0.430273
H	-6.601941	-0.133619	-1.773875
H	-3.019601	-0.474288	3.553149
H	-1.878165	0.182630	2.374020
H	-3.598718	0.128433	1.994933
H	-1.937749	-3.387430	-1.999538
H	-0.340109	-3.579027	-1.264901
H	-1.480031	-4.919884	-1.262899
H	-3.804407	-5.110002	4.019721
H	-3.277929	-6.265181	2.781573
H	-2.110130	-5.597884	3.925937
H	-2.721752	3.491601	0.590498
H	-1.725986	2.043551	0.825323
H	-1.688763	2.904883	-0.709607
H	-6.985125	3.327186	-2.105944
H	-7.909371	1.856064	-1.762804
H	-7.499211	2.977977	-0.455688
H	-4.586758	-2.398593	-0.542635
H	-5.502940	-2.054974	-2.016902
H	-3.741339	-2.138476	-2.059585
H	0.001923	-0.490149	0.140212
H	0.825968	-0.792831	0.201308
C	-0.415271	0.417690	-2.663083
C	-1.177700	-0.816891	-2.126463
C	1.108311	0.337070	-2.425015
H	-2.033103	-1.049723	-2.765939
H	-0.509034	-1.676651	-2.141875
H	-0.584873	0.469198	-3.746461
H	-0.830142	1.345914	-2.257377
H	1.468322	-0.577658	-2.909150
H	1.580956	1.161066	-2.986712

**F<sub>2</sub>**

---

**E= -2305.2136147au**

C	-1.099705	-3.137996	0.694927
C	-1.566022	-1.804081	0.815611
C	-1.861869	-1.269697	2.100090
C	-1.706336	-2.086704	3.222176
C	-1.261253	-3.405900	3.128933
C	-0.970441	-3.903847	1.858876
P	-1.804647	-0.655695	-0.603940
C	-2.312767	0.155664	2.334284
C	-1.068507	-4.253322	4.362208
C	-0.677053	-3.797998	-0.598522
B	1.420507	0.265384	-0.980066
C	2.991781	-0.202147	-0.888667
C	3.333674	-1.534039	-1.133449
C	4.633366	-2.030748	-1.103437
C	5.683691	-1.161831	-0.823452
C	5.405347	0.179814	-0.586765
C	4.084407	0.626495	-0.629443
F	2.364475	-2.440061	-1.443569
F	3.903521	1.948033	-0.403924
F	6.410585	1.032160	-0.325737
F	6.947501	-1.612514	-0.790691
F	4.884583	-3.329678	-1.346184
C	1.103974	1.591885	-0.050081
C	1.396923	1.553875	1.321571
C	1.155589	2.601420	2.206212
C	0.577986	3.777676	1.731563
C	0.257461	3.871054	0.383784
C	0.529681	2.794485	-0.463510
F	1.954075	0.446331	1.853631
F	1.469085	2.494307	3.508063
F	0.325085	4.796164	2.566587
F	-0.326733	4.984840	-0.092020
F	0.155482	2.983051	-1.757478
C	-3.579716	-0.199788	-0.828338
C	-4.546186	-1.216084	-1.042808
C	-5.879834	-0.852134	-1.242478
C	-6.294457	0.481558	-1.244765
C	-5.326569	1.465012	-1.036805
C	-3.974296	1.165353	-0.831147
C	-4.206223	-2.690382	-1.063752
C	-7.737791	0.847459	-1.491396
C	-3.034459	2.334709	-0.612653

H	-1.934520	-1.670590	4.200308
H	-0.615726	-4.927016	1.762528
H	-5.628954	2.509329	-1.033694
H	-6.615286	-1.637621	-1.400312
H	-2.526681	0.312104	3.394720
H	-1.531466	0.874828	2.058085
H	-3.220480	0.408015	1.776549
H	-1.394376	-3.658623	-1.411476
H	0.295463	-3.413913	-0.925262
H	-0.567129	-4.875351	-0.447175
H	-1.773754	-3.977858	5.153068
H	-1.196757	-5.317980	4.141974
H	-0.056432	-4.122701	4.767085
H	-2.561409	2.308513	0.375055
H	-2.232436	2.393020	-1.354100
H	-3.591310	3.273449	-0.673164
H	-7.988786	1.813207	-1.041640
H	-7.942946	0.924068	-2.567336
H	-8.417960	0.092046	-1.084258
H	-3.831362	-3.041131	-0.096707
H	-5.092437	-3.280974	-1.311417
H	-3.444540	-2.929186	-1.815434
H	-1.191679	0.544380	-0.214005
H	0.785425	-0.646998	-0.440531
C	-0.486928	0.188087	-2.941565
C	-1.133716	-1.058636	-2.284147
C	1.001160	0.338118	-2.572314
H	-1.984353	-1.429382	-2.865563
H	-0.388550	-1.846566	-2.201366
H	-0.605441	0.055424	-4.026290
H	-1.053208	1.093887	-2.697820
H	1.520536	-0.493874	-3.070693
H	1.379321	1.248311	-3.054245

**F<sub>3</sub>****E= -2493.7974752au**

C	-1.286384	-3.188087	0.417062
C	-1.692050	-1.842208	0.608457
C	-1.888322	-1.340830	1.924688
C	-1.697384	-2.199889	3.009258
C	-1.316530	-3.532262	2.846539
C	-1.122384	-3.998104	1.546043
P	-1.980190	-0.641107	-0.755073



B 1. 686573 0. 302771 -0. 864310  
 O -0. 148642 -0. 219996 1. 884293  
 C 2. 959125 -0. 682213 -0. 794259  
 C 2. 802110 -2. 060490 -0. 979466  
 C 3. 853278 -2. 969548 -0. 975774  
 C 5. 151071 -2. 499247 -0. 796403  
 C 5. 367532 -1. 135178 -0. 625212  
 C 4. 282144 -0. 262314 -0. 626198  
 F 1. 562716 -2. 571766 -1. 176389  
 F 4. 570825 1. 046545 -0. 481964  
 F 6. 615472 -0. 672507 -0. 471904  
 F 6. 181422 -3. 350567 -0. 798605  
 F 3. 632462 -4. 278953 -1. 150858  
 C 1. 759685 1. 667340 -0. 022569  
 C 2. 360934 1. 736920 1. 247298  
 C 2. 506396 2. 908871 1. 980751  
 C 2. 064146 4. 113035 1. 440728  
 C 1. 482295 4. 113335 0. 179262  
 C 1. 347431 2. 913004 -0. 514767  
 F 2. 844228 0. 627891 1. 824077  
 F 3. 081117 2. 892528 3. 188179  
 F 2. 196096 5. 251123 2. 125394  
 F 1. 041944 5. 259796 -0. 358530  
 F 0. 763598 3. 029306 -1. 730115  
 C -3. 345421 0. 783271 -0. 671792  
 C -4. 544223 0. 342179 -1. 293768  
 C -5. 558296 1. 273505 -1. 546273  
 C -5. 447635 2. 618823 -1. 194773  
 C -4. 272819 3. 027203 -0. 562649  
 C -3. 220401 2. 145557 -0. 293398  
 C -4. 839572 -1. 096283 -1. 667931  
 C -6. 560219 3. 600397 -1. 474459  
 C -1. 994121 2. 733960 0. 371785  
 H -4. 248439 -2. 526996 3. 414836  
 H -3. 030141 -5. 286825 0. 391563  
 H -4. 163045 4. 068601 -0. 267419  
 H -6. 470202 0. 927285 -2. 027375  
 H -3. 795872 -0. 384599 3. 374719  
 H -2. 301044 0. 098554 2. 579651  
 H -3. 869016 0. 427866 1. 811060  
 H -2. 254858 -3. 192734 -2. 171357  
 H -0. 774281 -3. 500367 -1. 244725  
 H -1. 990588 -4. 756476 -1. 414794

H -3. 595034 -5. 499761 3. 583356  
 H -5. 229145 -4. 894613 3. 302272  
 H -4. 505719 -6. 059283 2. 175942  
 H -2. 265786 3. 641650 0. 919327  
 H -1. 507203 2. 057552 1. 077457  
 H -1. 249596 3. 024710 -0. 375964  
 H -6. 954752 4. 027874 -0. 544339  
 H -6. 205349 4. 437994 -2. 087028  
 H -7. 391508 3. 124762 -2. 003590  
 H -5. 046091 -1. 705353 -0. 781544  
 H -5. 720804 -1. 139191 -2. 314671  
 H -4. 022614 -1. 587344 -2. 202868  
 H -0. 914122 0. 036860 0. 768523  
 H 0. 911004 -0. 710457 0. 256406  
 C -0. 472955 0. 478689 -2. 604618  
 C -1. 299849 -0. 709102 -2. 083989  
 C 1. 015387 0. 259240 -2. 318878  
 H -2. 168807 -0. 895010 -2. 719408  
 H -0. 681974 -1. 604344 -2. 084436  
 H -0. 623010 0. 538452 -3. 690137  
 H -0. 834577 1. 429261 -2. 204343  
 H 1. 302694 -0. 676243 -2. 812064  
 H 1. 587010 1. 042843 -2. 842825

**F<sub>4</sub>**

**E= -2493.7929935au**

C -3. 096792 -2. 944154 -0. 505405  
 C -2. 957067 -1. 718761 0. 199155  
 C -3. 534744 -1. 620316 1. 497721  
 C -4. 272216 -2. 690866 2. 015650  
 C -4. 444923 -3. 885200 1. 319079  
 C -3. 838691 -3. 985319 0. 067446  
 P -1. 944993 -0. 219414 -0. 312708  
 C 0. 663483 -1. 374350 2. 412298  
 O 1. 393195 -1. 628864 3. 334145  
 C -3. 388151 -0. 401049 2. 385326  
 C -5. 218873 -5. 038454 1. 911644  
 C -2. 476223 -3. 243699 -1. 855621  
 B 2. 013751 0. 354749 -1. 234655  
 O 0. 304462 -0. 120246 2. 078570  
 C 2. 827113 -0. 972629 -0. 950403  
 C 2. 197703 -2. 214207 -0. 840109  
 C 2. 885393 -3. 409123 -0. 659021



C	4.277413	-3.383679	-0.604110
C	4.953653	-2.169798	-0.716349
C	4.223310	-0.996464	-0.874773
F	0.844267	-2.280896	-0.862951
F	4.915048	0.152499	-0.982862
F	6.289514	-2.145298	-0.670359
F	4.960376	-4.517567	-0.443150
F	2.229931	-4.568463	-0.538371
C	2.281129	1.633451	-0.363490
C	2.841445	1.564478	0.928868
C	3.081247	2.684584	1.718331
C	2.781060	3.949468	1.219308
C	2.242519	4.079762	-0.058564
C	2.000427	2.938007	-0.813607
F	3.168245	0.387898	1.470683
F	3.604313	2.561487	2.939876
F	3.011225	5.032510	1.958794
F	1.964818	5.294667	-0.545237
F	1.493745	3.148459	-2.042037
C	-3.158640	1.208220	-0.424827
C	-4.405303	1.127807	-1.098473
C	-5.212393	2.268905	-1.182370
C	-4.841198	3.492538	-0.623236
C	-3.622005	3.551351	0.052101
C	-2.777588	2.440511	0.167954
C	-4.955567	-0.144368	-1.708411
C	-5.718521	4.713838	-0.762907
C	-1.498357	2.623922	0.961136
H	-4.715595	-2.583519	3.003382
H	-3.943075	-4.911618	-0.493933
H	-3.315086	4.489270	0.510019
H	-6.165859	2.192873	-1.701564
H	-3.816872	-0.600449	3.371799
H	-2.336072	-0.132936	2.537359
H	-3.891651	0.480074	1.974777
H	-2.771609	-2.530044	-2.629921
H	-1.381780	-3.251335	-1.806227
H	-2.787829	-4.235594	-2.195782
H	-5.991689	-4.688502	2.604264
H	-5.704852	-5.637195	1.133693
H	-4.558336	-5.711651	2.474445
H	-1.479559	2.001172	1.862179
H	-0.602838	2.368677	0.387210

H	-1.400018	3.666319	1.279907
H	-5.569681	5.411594	0.067856
H	-5.493032	5.258467	-1.689686
H	-6.779584	4.444147	-0.795716
H	-5.300675	-0.841350	-0.937151
H	-5.807468	0.085798	-2.355799
H	-4.220529	-0.684143	-2.310509
H	-0.314386	-0.138904	1.298770
H	0.221472	-2.144540	1.752268
C	-0.392811	0.826603	-2.476690
C	-1.387750	-0.308975	-2.112603
C	1.090802	0.366026	-2.520426
H	-2.255096	-0.258041	-2.775534
H	-0.903377	-1.268919	-2.279920
H	-0.661742	1.185276	-3.476992
H	-0.515979	1.692477	-1.819479
H	1.134499	-0.605574	-3.026656
H	1.626545	1.062488	-3.188090

## G

E= -2343.3430971au

C	2.627140	-2.816216	-1.282674
C	2.977271	-2.054432	-0.135482
C	4.284403	-2.183988	0.395310
C	5.205477	-3.028612	-0.237728
C	4.879943	-3.769534	-1.374060
C	3.582183	-3.650983	-1.874565
P	1.619836	-0.962582	0.577416
C	4.740143	-1.469886	1.647203
C	5.884280	-4.692578	-2.023346
C	1.244672	-2.785455	-1.905588
B	-1.829795	0.430272	0.729905
C	-3.076933	-0.522293	0.454165
C	-3.043615	-1.716386	-0.260394
C	-4.163839	-2.525286	-0.429375
C	-5.379228	-2.133010	0.128628
C	-5.457650	-0.943515	0.849207
C	-4.310101	-0.169500	0.998982
F	-1.885613	-2.128280	-0.815363
F	-4.408442	0.979615	1.704511
F	-6.621417	-0.559751	1.387210
F	-6.465215	-2.896213	-0.026692
F	-4.085356	-3.668704	-1.120630

C	-1.452030	1.534011	-0.327129
C	-1.737059	1.409710	-1.700062
C	-1.390013	2.371471	-2.643342
C	-0.736757	3.530379	-2.230096
C	-0.440685	3.711421	-0.882537
C	-0.795473	2.726068	0.033167
F	-2.349577	0.315896	-2.177213
F	-1.673369	2.193649	-3.938475
F	-0.397331	4.460744	-3.121890
F	0.183771	4.825427	-0.481280
F	-0.503015	2.987889	1.314805
C	2.412108	0.716091	0.896072
C	2.607293	1.389041	2.132728
C	2.988600	2.740335	2.132678
C	3.206637	3.467125	0.965813
C	3.056499	2.787190	-0.243642
C	2.658021	1.449774	-0.304462
C	2.451160	0.756272	3.501836
C	3.558756	4.934486	0.994807
C	2.496252	0.844642	-1.682899
H	6.207910	-3.111034	0.178111
H	3.299507	-4.224560	-2.755295
H	3.237609	3.317882	-1.176612
H	3.118404	3.237585	3.091737
H	5.777045	-1.729731	1.882012
H	4.676067	-0.382417	1.550471
H	4.128303	-1.755477	2.510998
H	0.956794	-1.780256	-2.229483
H	1.210072	-3.444124	-2.779467
H	0.467519	-3.117469	-1.209763
H	5.712496	-5.736686	-1.729029
H	5.818161	-4.651984	-3.116486
H	6.909061	-4.435934	-1.735637
H	2.662733	1.602712	-2.454508
H	3.202234	0.026372	-1.860021
H	1.490733	0.430529	-1.824582
H	4.409124	5.158767	0.339920
H	2.712086	5.539193	0.645029
H	3.812338	5.268060	2.006136
H	3.073528	-0.135942	3.617821
H	2.757415	1.466618	4.275613
H	1.417731	0.470513	3.722624
C	1.172956	-1.930161	2.155362

C	-1.141157	0.374000	2.145189
C	-0.350030	-2.122449	2.330729
C	-1.145604	-0.951049	2.935158
H	-0.782407	-2.403281	1.363727
H	-0.496612	-2.988320	2.991902
H	-0.763003	-0.755207	3.947195
H	-2.182258	-1.286299	3.069793
H	1.623398	-1.546720	3.069201
H	1.619063	-2.915576	1.980948
H	-0.136382	0.801402	2.104013
H	-1.718872	1.116187	2.730088

### G<sub>1</sub>

E= -2344.5201982au

C	2.610573	-2.816998	-1.287732
C	2.979262	-2.061249	-0.144641
C	4.294724	-2.197948	0.368141
C	5.203013	-3.042390	-0.279712
C	4.858527	-3.778380	-1.415710
C	3.555697	-3.653694	-1.896531
P	1.638552	-0.964794	0.591744
C	4.768795	-1.489399	1.616409
C	5.856131	-4.699405	-2.077942
C	1.220031	-2.781173	-1.892185
B	-1.794624	0.429762	0.781739
C	-3.052951	-0.512413	0.521517
C	-3.037976	-1.713774	-0.181353
C	-4.168667	-2.511020	-0.335667
C	-5.376062	-2.098831	0.225236
C	-5.436335	-0.901262	0.934162
C	-4.278900	-0.139493	1.069455
F	-1.888475	-2.145020	-0.739295
F	-4.359386	1.017989	1.763607
F	-6.592256	-0.498301	1.474873
F	-6.471704	-2.850758	0.083912
F	-4.107588	-3.662140	-1.015557
C	-1.418030	1.525635	-0.284451
C	-1.705537	1.391539	-1.655524
C	-1.360212	2.345804	-2.606348
C	-0.706733	3.508390	-2.203781
C	-0.407596	3.698746	-0.858211
C	-0.760422	2.719892	0.065530
F	-2.319372	0.292865	-2.122812

F	-1.646586	2.158325	-3.900494
F	-0.369404	4.431796	-3.103302
F	0.218338	4.815029	-0.466309
F	-0.464781	2.990396	1.344525
C	2.444840	0.709558	0.898911
C	2.659010	1.381878	2.132873
C	3.048138	2.730932	2.127543
C	3.256128	3.456159	0.957854
C	3.087567	2.776588	-0.249321
C	2.680710	1.441433	-0.304714
C	2.516317	0.750926	3.504327
C	3.616638	4.921577	0.982073
C	2.499970	0.836808	-1.680965
H	6.210835	-3.130024	0.122364
H	3.258958	-4.223215	-2.774995
H	3.260455	3.305738	-1.184717
H	3.192427	3.227774	3.084733
H	5.804186	-1.762001	1.843294
H	4.717595	-0.401168	1.519755
H	4.159896	-1.766825	2.484805
H	0.932081	-1.775649	-2.215243
H	1.170843	-3.441586	-2.764021
H	0.450847	-3.108145	-1.185426
H	5.959285	-5.640137	-1.520625
H	5.550075	-4.954917	-3.097623
H	6.851750	-4.243787	-2.126289
H	2.652318	1.595879	-2.454518
H	3.205872	0.020961	-1.869156
H	1.493971	0.419261	-1.807843
H	4.461831	5.140655	0.318778
H	2.769992	5.530768	0.640019
H	3.881873	5.254560	1.990596
H	3.136665	-0.143535	3.614017
H	2.834484	1.460796	4.273707
H	1.484466	0.469542	3.737733
H	-4.038147	0.089149	-4.990236
H	-3.531414	0.360987	-4.520637
C	1.213503	-1.931757	2.176234
C	-1.095053	0.376604	2.191580
C	-0.307107	-2.121447	2.373300
C	-1.093274	-0.947016	2.984245
H	-0.753266	-2.405258	1.413528
H	-0.445620	-2.984766	3.039539

H	-0.698995	-0.749592	3.991455
H	-2.129020	-1.279917	3.131062
H	1.677566	-1.548476	3.083286
H	1.655572	-2.917932	1.995980
H	-0.090654	0.804074	2.142590
H	-1.669281	1.119322	2.779296

## TS<sub>G12</sub>

E= -2344.4833002au

C	-3.278879	-2.523830	1.145305
C	-3.540889	-1.570719	0.126293
C	-4.876920	-1.319332	-0.266001
C	-5.915165	-2.001576	0.380609
C	-5.678844	-2.934209	1.391121
C	-4.351764	-3.183647	1.751661
P	-2.055241	-0.743529	-0.635614
C	-5.240315	-0.360793	-1.375763
C	-6.814422	-3.666313	2.065874
C	-1.876995	-2.862528	1.612575
B	1.607669	-0.123252	-0.687092
C	2.796004	-1.171743	-0.402318
C	2.678907	-2.479320	0.071723
C	3.774048	-3.319155	0.269948
C	5.055383	-2.859607	-0.017772
C	5.223601	-1.566255	-0.504131
C	4.102442	-0.760874	-0.682864
F	1.470715	-3.009279	0.368157
F	4.312149	0.482274	-1.170036
F	6.451009	-1.113787	-0.795663
F	6.114870	-3.657172	0.162698
F	3.602334	-4.566282	0.732645
C	1.660980	1.232730	0.169063
C	1.828168	1.199037	1.560414
C	1.863057	2.334535	2.364005
C	1.733942	3.589656	1.774853
C	1.571619	3.679453	0.397347
C	1.541245	2.518010	-0.372101
F	1.916179	0.014102	2.195832
F	2.006408	2.232592	3.693664
F	1.756352	4.696225	2.527463
F	1.430760	4.886011	-0.179512
F	1.386363	2.698359	-1.698630
C	-2.299529	1.096553	-0.704566

C	-2.422039	1.914986	-1.858140
C	-2.378050	3.307993	-1.709547
C	-2.230559	3.933813	-0.473063
C	-2.163630	3.116250	0.656847
C	-2.180503	1.722912	0.570635
C	-2.592056	1.403481	-3.273610
C	-2.103299	5.433104	-0.359629
C	-2.059553	0.942920	1.864566
H	-6.939883	-1.798307	0.076979
H	-4.141551	-3.912555	2.531599
H	-2.071497	3.574646	1.638987
H	-2.457877	3.922632	-2.603353
H	-6.323567	-0.339556	-1.527064
H	-4.907295	0.660131	-1.165544
H	-4.783578	-0.662499	-2.326073
H	-1.373821	-2.001850	2.066836
H	-1.909712	-3.656636	2.364492
H	-1.230531	-3.211299	0.800081
H	-7.786773	-3.271212	1.755999
H	-6.796187	-4.736371	1.822685
H	-6.748504	-3.584593	3.157313
H	-2.002000	1.629969	2.713796
H	-2.915838	0.280851	2.032676
H	-1.152797	0.326454	1.888623
H	-2.592008	5.812348	0.544488
H	-1.044905	5.718196	-0.305545
H	-2.539929	5.941828	-1.225129
H	-3.355936	0.625558	-3.352273
H	-2.895368	2.223971	-3.930363
H	-1.657151	1.000512	-3.680669
H	-0.573952	-0.856608	0.014224
H	0.248450	-0.872363	0.265234
C	-1.801914	-1.640260	-2.274707
C	0.992154	-0.087854	-2.161445
C	-0.408676	-2.307267	-2.380421
C	0.718506	-1.403639	-2.915377
H	-0.119778	-2.743323	-1.418741
H	-0.511936	-3.153972	-3.072486
H	0.482556	-1.162641	-3.963032
H	1.637383	-2.004029	-2.948355
H	-1.980683	-1.001611	-3.138506
H	-2.579213	-2.411729	-2.281525
H	0.101863	0.553314	-2.188516

H	1.731706	0.473469	-2.755019
---	----------	----------	-----------

## G<sub>2</sub>

E= -2344.5204083au

C	2.973067	-2.624527	-1.083006
C	3.369804	-1.740458	-0.044046
C	4.729273	-1.647503	0.340242
C	5.675002	-2.421952	-0.336547
C	5.317452	-3.290093	-1.370682
C	3.967018	-3.374697	-1.720295
P	2.099037	-0.748927	0.832225
C	5.201731	-0.747440	1.460634
C	6.351551	-4.136148	-2.072785
C	1.541491	-2.811192	-1.545410
B	-1.530825	-0.291467	0.459710
C	-2.969172	-1.050408	0.267265
C	-3.057220	-2.412222	-0.026899
C	-4.260671	-3.096714	-0.188670
C	-5.459703	-2.405941	-0.047612
C	-5.430904	-1.048369	0.257974
C	-4.201867	-0.409866	0.411928
F	-1.931959	-3.163361	-0.163889
F	-4.245051	0.904783	0.724664
F	-6.584631	-0.375425	0.405314
F	-6.631461	-3.043275	-0.195955
F	-4.276738	-4.411353	-0.473235
C	-1.458762	1.146917	-0.346633
C	-1.134470	1.173319	-1.705843
C	-0.935830	2.334839	-2.449316
C	-1.073876	3.569363	-1.825880
C	-1.411458	3.606891	-0.478153
C	-1.610444	2.416286	0.220350
F	-0.920570	0.012359	-2.379783
F	-0.570619	2.274476	-3.744023
F	-0.853916	4.707395	-2.505378
F	-1.505924	4.799142	0.145036
F	-1.930957	2.557445	1.523558
C	2.411747	1.064904	0.851829
C	2.512981	1.857057	2.022797
C	2.461347	3.249850	1.891084
C	2.315098	3.886336	0.659342
C	2.309530	3.086937	-0.486292
C	2.351449	1.693681	-0.426077

C	2. 655015	1. 322861	3. 432539
C	2. 122766	5. 378385	0. 560950
C	2. 326408	0. 935914	-1. 736094
H	6. 719431	-2. 343920	-0. 043945
H	3. 670554	-4. 049929	-2. 519409
H	2. 239565	3. 559958	-1. 462340
H	2. 515134	3. 853185	2. 793995
H	6. 274581	-0. 875556	1. 628378
H	5. 020929	0. 310981	1. 244064
H	4. 699423	-0. 978207	2. 408914
H	0. 867244	-3. 120629	-0. 740468
H	1. 109493	-1. 902874	-1. 979348
H	1. 499172	-3. 586852	-2. 314638
H	7. 359538	-3. 731279	-1. 940037
H	6. 352417	-5. 160374	-1. 677462
H	6. 148646	-4. 204880	-3. 146859
H	2. 310649	1. 639412	-2. 572491
H	3. 203710	0. 291935	-1. 856461
H	1. 432598	0. 313281	-1. 844638
H	2. 646953	5. 797783	-0. 304433
H	1. 055249	5. 604089	0. 438693
H	2. 472293	5. 892939	1. 461342
H	3. 325476	0. 462099	3. 500109
H	3. 065116	2. 102111	4. 081160
H	1. 684095	1. 036954	3. 854837
H	0. 905527	-0. 859724	0. 075555
H	-0. 718311	-1. 002143	-0. 121225
C	1. 675237	-1. 642134	2. 415649
C	-1. 117681	-0. 166150	2. 049351
C	0. 298688	-2. 357058	2. 349686
C	-0. 884558	-1. 486063	2. 810187
H	0. 104566	-2. 755274	1. 349194
H	0. 375329	-3. 229082	3. 012206
H	-0. 743368	-1. 281674	3. 884438
H	-1. 786259	-2. 109157	2. 742330
H	1. 694791	-0. 959917	3. 263147
H	2. 487168	-2. 364113	2. 552163
H	-0. 221569	0. 472134	2. 160683
H	-1. 895378	0. 382650	2. 594417

**G<sub>3</sub>**

E= -2533.1050986au

C	-3. 978709	-2. 430989	0. 341807
---	------------	------------	-----------

C	-4. 014341	-1. 126195	-0. 226187
C	-5. 235535	-0. 411680	-0. 289644
C	-6. 386918	-1. 010788	0. 234080
C	-6. 377346	-2. 282494	0. 807750
C	-5. 163223	-2. 973093	0. 845545
P	-2. 412087	-0. 460604	-0. 845463
C	0. 898770	-2. 575388	2. 963694
O	2. 028116	-2. 791810	3. 156727
C	-5. 383141	0. 966779	-0. 895403
C	-7. 638600	-2. 907990	1. 351411
C	-2. 721186	-3. 270769	0. 439279
B	1. 368047	-0. 108062	-0. 784514
O	-0. 246910	-2. 376380	2. 813231
C	2. 628005	-1. 157519	-0. 678474
C	2. 511611	-2. 459890	-0. 196921
C	3. 572138	-3. 358723	-0. 102760
C	4. 837318	-2. 958073	-0. 518286
C	5. 012943	-1. 670146	-1. 017837
C	3. 918282	-0. 811287	-1. 087780
F	1. 302290	-2. 937294	0. 222279
F	4. 152984	0. 423902	-1. 585963
F	6. 230562	-1. 276001	-1. 426621
F	5. 875919	-3. 804644	-0. 443908
F	3. 386075	-4. 601399	0. 375715
C	1. 710426	1. 264536	0. 067190
C	1. 778258	1. 204367	1. 462047
C	2. 000823	2. 295981	2. 297263
C	2. 174430	3. 553977	1. 729366
C	2. 124162	3. 675670	0. 346364
C	1. 906379	2. 548551	-0. 446842
F	1. 581546	0. 017606	2. 096325
F	2. 033443	2. 153043	3. 634368
F	2. 370617	4. 633545	2. 503647
F	2. 246773	4. 897322	-0. 214836
F	1. 860973	2. 783778	-1. 776421
C	-2. 192984	1. 341652	-0. 634736
C	-2. 232454	2. 286486	-1. 690590
C	-1. 936444	3. 619486	-1. 396889
C	-1. 606047	4. 052793	-0. 110303
C	-1. 625036	3. 110368	0. 919654
C	-1. 903012	1. 760115	0. 693146
C	-2. 553982	1. 961594	-3. 133933
C	-1. 206923	5. 483830	0. 147501

C	-1.858604	0.819269	1.878541
H	-7.322885	-0.459635	0.187388
H	-5.131992	-3.968379	1.282565
H	-1.394600	3.426857	1.933542
H	-1.953411	4.342571	-2.208646
H	-6.438242	1.252648	-0.920491
H	-4.843117	1.729810	-0.327033
H	-5.014345	1.007055	-1.925412
H	-1.990684	-2.854145	1.142785
H	-2.970827	-4.274140	0.794437
H	-2.213156	-3.390626	-0.523873
H	-7.990785	-3.714778	0.695870
H	-7.469202	-3.348186	2.340504
H	-8.445751	-2.174653	1.438540
H	-1.840691	1.393689	2.808640
H	-2.727326	0.153168	1.925228
H	-0.954568	0.198350	1.867984
H	-1.428748	5.785598	1.176084
H	-0.127330	5.604764	-0.006709
H	-1.716732	6.173158	-0.533644
H	-3.365919	1.236692	-3.246081
H	-2.859997	2.869773	-3.660728
H	-1.673730	1.567907	-3.655788
H	-1.442369	-0.996278	0.018654
H	0.436063	-0.619219	-0.176619
C	-2.013082	-1.262514	-2.482404
C	0.930888	0.143996	-2.348175
C	-0.629055	-1.962704	-2.566847
C	0.515561	-1.109391	-3.140783
H	-0.340413	-2.368158	-1.592219
H	-0.779033	-2.827699	-3.226919
H	0.245347	-0.838396	-4.175206
H	1.382233	-1.778606	-3.229076
H	-2.132082	-0.542158	-3.291488
H	-2.820994	-1.994698	-2.593436
H	0.115306	0.882871	-2.387238
H	1.750543	0.612115	-2.907098

### TSG34

E=-2264.7253067au

C	-3.542021	-2.639419	0.678757
C	-3.694226	-1.249204	0.415542
C	-4.908258	-0.613366	0.798825

C	-5.942494	-1.396398	1.327455
C	-5.832099	-2.771898	1.528571
C	-4.613563	-3.365077	1.212042
P	-2.185318	-0.403651	-0.337456
C	0.444217	-0.634761	2.107442
O	1.324882	-0.505774	2.923324
C	-5.192942	0.875485	0.734690
C	-6.971254	-3.568449	2.117762
C	-2.259488	-3.413554	0.446277
B	1.503575	0.018662	-0.471663
O	-0.785784	-0.953120	2.184758
C	2.464096	-1.287711	-0.541282
C	2.225696	-2.568591	-0.049352
C	3.113339	-3.633066	-0.200585
C	4.308288	-3.435812	-0.882733
C	4.589678	-2.177885	-1.409681
C	3.674755	-1.146362	-1.228684
F	1.071440	-2.855661	0.600423
F	3.994065	0.052484	-1.765849
F	5.730095	-1.973492	-2.081645
F	5.169632	-4.445414	-1.045777
F	2.817058	-4.841272	0.295676
C	2.158921	1.282327	0.279244
C	3.209549	1.156376	1.209561
C	3.798682	2.240598	1.856373
C	3.350238	3.529845	1.591654
C	2.319573	3.714848	0.676665
C	1.757846	2.607931	0.048490
F	3.736137	-0.038175	1.505505
F	4.799549	2.052325	2.723860
F	3.903680	4.578834	2.204839
F	1.873499	4.951529	0.408086
F	0.763118	2.886235	-0.822068
C	-2.579372	1.359911	-0.763880
C	-3.334798	1.713884	-1.912365
C	-3.471230	3.067949	-2.239700
C	-2.924306	4.087828	-1.461037
C	-2.276788	3.720733	-0.279929
C	-2.099868	2.385916	0.091834
C	-4.119944	0.740802	-2.775619
C	-3.046051	5.536278	-1.865256
C	-1.450568	2.114797	1.430773
H	-6.868724	-0.898866	1.606766

H	-4.474781	-4.427636	1.398607	C	5.394628	-3.144139	-0.832947
H	-1.893799	4.496315	0.378848	P	2.196039	-0.875722	0.346133
H	-4.051310	3.329836	-3.122445	C	-0.805428	-2.332490	-1.563424
H	-6.121978	1.087552	1.271697	O	-1.735246	-2.891742	-2.075586
H	-4.405369	1.472256	1.199664	C	5.110394	0.935511	0.480829
H	-5.316919	1.247597	-0.285832	C	7.886175	-2.871217	-1.134135
H	-2.126280	-3.711694	-0.600001	C	2.981777	-3.650257	-0.664792
H	-1.372390	-2.859519	0.759997	B	-1.885981	-0.071068	1.013077
H	-2.275743	-4.334588	1.035866	O	0.397108	-2.199436	-2.115455
H	-7.925716	-3.312320	1.643706	C	-3.172666	-0.911793	0.652830
H	-6.810878	-4.644519	1.998968	C	-3.251026	-2.307477	0.641345
H	-7.079960	-3.366950	3.191363	C	-4.387082	-3.008371	0.263372
H	-1.421839	3.034517	2.022303	C	-5.528463	-2.307598	-0.095898
H	-1.983137	1.361578	2.018951	C	-5.515637	-0.918344	-0.080613
H	-0.418474	1.770182	1.330106	C	-4.354466	-0.253588	0.280190
H	-3.195978	6.184338	-0.995129	F	-2.192934	-3.053854	0.968150
H	-2.131486	5.877111	-2.368028	F	-4.421234	1.081339	0.294860
H	-3.879536	5.692779	-2.557534	F	-6.613383	-0.241529	-0.405035
H	-4.366170	-0.188962	-2.257382	F	-6.628328	-2.957199	-0.444800
H	-5.065816	1.207161	-3.070452	F	-4.389917	-4.335587	0.252119
H	-3.598036	0.483943	-3.705687	C	-1.669455	1.290148	0.220154
H	-1.261520	-0.651545	0.927935	C	-1.685330	1.354372	-1.171074
H	0.727264	-0.399625	0.979723	C	-1.497686	2.531864	-1.880218
C	-1.928695	-1.337383	-1.953121	C	-1.332903	3.719869	-1.183434
C	0.668315	0.276991	-1.807679	C	-1.335143	3.709990	0.203133
C	-0.547281	-1.950045	-2.217859	C	-1.474158	2.505551	0.874798
C	0.436452	-0.910169	-2.754005	F	-1.861335	0.238947	-1.890426
H	-0.153513	-2.433599	-1.321602	F	-1.465179	2.529466	-3.209840
H	-0.678385	-2.744578	-2.964820	F	-1.133905	4.858694	-1.840555
H	0.055911	-0.534426	-3.715424	F	-1.164643	4.845785	0.876505
H	1.390662	-1.399751	-2.977181	F	-1.459680	2.562855	2.212495
H	-2.151722	-0.639910	-2.759684	C	2.088669	0.974905	0.467510
H	-2.712593	-2.097921	-1.967391	C	2.168885	1.784483	1.622093
H	-0.245126	0.861700	-1.672014	C	2.051450	3.171767	1.497307
H	1.331582	0.985551	-2.330981	C	1.902936	3.802978	0.269384
				C	1.841099	2.996411	-0.862929
				C	1.909489	1.607421	-0.789882
				C	2.440739	1.268827	3.017010
				C	1.828630	5.302696	0.151181
				C	1.817781	0.850009	-2.096699
				H	7.219509	-0.371350	-0.303362
				H	5.496752	-4.173847	-1.168995
				H	1.720559	3.464668	-1.837834

#### G<sub>4</sub>

E= -2532.4142868au

C	4.127762	-2.673610	-0.491161	C	1.828630	5.302696	0.151181
C	3.966335	-1.337107	-0.040899	C	1.817781	0.850009	-2.096699
C	5.108491	-0.505381	0.022908	H	7.219509	-0.371350	-0.303362
C	6.350839	-1.024543	-0.353438	H	5.496752	-4.173847	-1.168995
C	6.523798	-2.335671	-0.777163	H	1.720559	3.464668	-1.837834

H	2.106571	3.780236	2.397098	C	5.173765	-0.264507	0.633380
H	6.137248	1.309845	0.517879	C	6.170633	-4.528011	-1.797629
H	4.543293	1.589122	-0.187188	C	1.366459	-3.412497	-0.893709
H	4.686958	1.049456	1.480382	B	-2.027809	0.129371	0.961275
H	2.381228	-3.410369	-1.547935	C	-3.049886	-0.873836	0.271719
H	3.373982	-4.661052	-0.806963	C	-2.756786	-1.605898	-0.875097
H	2.297965	-3.692224	0.187645	C	-3.635433	-2.536760	-1.420108
H	8.359929	-3.339592	-0.262869	C	-4.866900	-2.751192	-0.802606
H	7.822754	-3.630073	-1.920249	C	-5.199961	-2.038347	0.346982
H	8.550965	-2.074507	-1.481700	C	-4.285515	-1.123141	0.862156
H	1.867822	1.548246	-2.936702	F	-1.574498	-1.414525	-1.499095
H	2.628718	0.125214	-2.224931	F	-4.623558	-0.447793	1.982553
H	0.871783	0.306576	-2.187326	F	-6.381750	-2.239830	0.942131
H	2.777969	5.708960	-0.217079	F	-5.725957	-3.638538	-1.313421
H	1.047478	5.603619	-0.552721	F	-3.314260	-3.221349	-2.524453
H	1.613054	5.769876	1.115657	C	-1.826489	1.579742	0.388100
H	3.259430	0.543634	3.035165	C	-2.253532	1.966424	-0.898935
H	2.724972	2.096886	3.671703	C	-1.997378	3.218729	-1.448690
H	1.560937	0.794239	3.465429	C	-1.297937	4.161947	-0.702054
H	0.977653	-1.749380	-1.451126	C	-0.873053	3.847712	0.584860
H	-0.860688	-1.866759	-0.562930	C	-1.141329	2.585357	1.100167
C	1.923407	-1.751781	1.991404	F	-2.927439	1.118291	-1.687962
C	-0.900929	-0.300127	2.215778	F	-2.411181	3.520545	-2.683771
C	0.552668	-2.444367	2.133246	F	-1.031197	5.362575	-1.218298
C	-0.519820	-1.632488	2.869094	F	-0.207937	4.755512	1.305934
H	0.183760	-2.751612	1.149768	F	-0.715653	2.372337	2.356588
H	0.701860	-3.372577	2.698317	C	2.276089	1.039935	0.153119
H	-0.134983	-1.416314	3.875501	C	2.590975	2.136628	0.999979
H	-1.404110	-2.258959	3.010606	C	2.699000	3.424447	0.454162
H	2.118798	-1.124260	2.857830	C	2.510782	3.691978	-0.900723
H	2.712020	-2.510231	2.000534	C	2.206060	2.609268	-1.725942
H	-0.000916	0.295776	2.035915	C	2.070232	1.307413	-1.233063
H	-1.448568	0.298394	2.971015	C	2.811919	2.042117	2.496765

## H

E= -2382.6569178au

C	2.818366	-2.998074	-0.739829	H	6.599879	-2.180409	-0.480280
C	3.227872	-1.804656	-0.087883	H	3.452243	-4.776690	-1.761226
C	4.616151	-1.516268	-0.007775	H	2.055360	2.778716	-2.790475
C	5.539399	-2.414242	-0.555504	H	2.941089	4.248104	1.122621
C	5.149417	-3.594044	-1.192176	H	6.264804	-0.324125	0.696925
C	3.784121	-3.863845	-1.270603	H	4.918365	0.632362	0.060507
P	1.861162	-0.732332	0.637427	H	4.793987	-0.109496	1.647437
				H	0.734755	-2.605795	-1.273349



H	1.288950	-4.260202	-1.582411	C	-3.016420	-0.973275	0.285540
H	0.927069	-3.729200	0.060005	C	-2.718316	-1.661930	-0.886551
H	6.463278	-4.197804	-2.803481	C	-3.577265	-2.601046	-1.448492
H	7.083919	-4.569536	-1.193655	C	-4.793688	-2.869275	-0.822268
H	5.777775	-5.545933	-1.890401	C	-5.131223	-2.201304	0.352736
H	1.520297	0.673563	-3.217530	C	-4.236171	-1.276251	0.884137
H	2.445324	-0.542634	-2.328640	F	-1.549873	-1.418937	-1.518407
H	0.751296	-0.268275	-1.930694	F	-4.577251	-0.646282	2.029654
H	2.955782	5.114285	-2.474359	F	-6.298555	-2.454825	0.956405
H	1.593412	5.570183	-1.446142	F	-5.633836	-3.765326	-1.348904
H	3.243577	5.730170	-0.836085	F	-3.251428	-3.242737	-2.576890
H	3.470697	1.219281	2.780132	C	-1.844751	1.503312	0.454276
H	3.265208	2.967247	2.865638	C	-2.299667	1.915302	-0.815282
H	1.865570	1.915852	3.035742	C	-2.074973	3.186344	-1.334733
C	2.144643	-1.038121	2.491001	C	-1.380534	4.122294	-0.575022
C	-1.262217	-0.379163	2.242349	C	-0.929345	3.783067	0.696307
C	1.488199	-2.365178	2.946893	C	-1.166090	2.502460	1.181756
C	-1.043790	-1.903832	2.365364	F	-2.971917	1.077029	-1.615750
C	0.017526	-2.305734	3.413428	F	-2.514731	3.512802	-2.555684
H	-0.310381	0.146908	2.325227	F	-1.143571	5.341195	-1.064099
H	-1.840416	-0.026388	3.116513	F	-0.270108	4.684090	1.430700
H	-0.756749	-2.321335	1.392708	F	-0.715832	2.264808	2.424729
H	-1.998784	-2.376638	2.627519	C	2.270300	1.045221	0.204174
H	-0.057333	-1.633882	4.281552	C	2.573405	2.116366	1.087437
H	-0.229760	-3.307190	3.791031	C	2.652624	3.424902	0.587550
H	1.589709	-3.123818	2.159877	C	2.447023	3.737720	-0.754844
H	2.076540	-2.746217	3.792619	C	2.155442	2.679743	-1.616400
H	1.722954	-0.213592	3.067739	C	2.048365	1.358699	-1.170003
H	3.214708	-1.072558	2.715224	C	2.812591	1.974110	2.577852

## H<sub>1</sub>

E= -2383.8339887au

C	2.873802	-2.952364	-0.828970	H	6.643343	-2.083689	-0.561446
C	3.268224	-1.775213	-0.139181	H	3.529774	-4.685309	-1.913032
C	4.652116	-1.467394	-0.056690	H	1.992868	2.884502	-2.672952
C	5.586288	-2.331833	-0.638826	H	2.885583	4.228294	1.283312
C	5.211351	-3.495783	-1.312532	H	6.285787	-0.268914	0.671909
C	3.849997	-3.784472	-1.393296	H	4.912858	0.682810	0.086411
P	1.888251	-0.750326	0.628235	H	4.822795	-0.118659	1.646477
C	5.193122	-0.228878	0.623033	H	0.780152	-2.572194	-1.329251
C	6.243671	-4.392494	-1.954409	H	1.357815	-4.203440	-1.711566
C	1.427634	-3.383824	-0.988909	H	1.002127	-3.746919	-0.045414
B	-2.012166	0.035105	0.993171	H	6.512823	-4.033510	-2.956982
				H	7.166982	-4.426544	-1.365494

H	5.872404	-5.416827	-2.064341	C	-3.895508	-3.082879	-0.962130
H	1.503462	0.785405	-3.174126	C	-5.169749	-2.679368	-0.575564
H	2.446820	-0.447314	-2.328838	C	-5.317428	-1.534441	0.202108
H	0.749904	-0.210425	-1.919406	C	-4.182402	-0.816711	0.568269
H	2.880858	5.225695	-2.269879	F	-1.585876	-2.801144	-0.979347
H	1.487336	5.608102	-1.254487	F	-4.368973	0.281318	1.334859
H	3.120406	5.791553	-0.605973	F	-6.538605	-1.140183	0.589980
H	3.487056	1.152815	2.826417	F	-6.243072	-3.390649	-0.941570
H	3.256360	2.893148	2.972653	F	-3.745247	-4.188805	-1.706391
H	1.874822	1.815529	3.123419	C	-1.664918	1.256538	0.207639
H	-1.770208	6.315487	-4.220369	C	-1.868954	1.550256	-1.147314
H	-1.804999	5.834726	-3.655727	C	-1.833431	2.838757	-1.670643
C	2.186880	-1.111014	2.469151	C	-1.588060	3.910969	-0.817712
C	-1.226301	-0.487404	2.256312	C	-1.380718	3.676521	0.536265
C	1.548324	-2.458271	2.890091	C	-1.426509	2.370482	1.018855
C	-0.995756	-2.011939	2.352787	F	-2.061137	0.549549	-2.028712
C	0.083512	-2.425630	3.377182	F	-2.009811	3.055981	-2.982059
H	-0.277048	0.044892	2.331493	F	-1.513062	5.158690	-1.304923
H	-1.792590	-0.150583	3.144312	F	-1.121445	4.703149	1.359652
H	-0.722016	-2.413407	1.369529	F	-1.206764	2.224988	2.344094
H	-1.943895	-2.494405	2.622313	C	2.216463	1.215227	0.216423
H	0.013260	-1.775149	4.261847	C	2.374181	2.310005	1.105937
H	-0.148508	-3.438248	3.734188	C	2.365101	3.613811	0.592196
H	1.645497	-3.191283	2.078566	C	2.202229	3.892825	-0.763543
H	2.150605	-2.860499	3.715932	C	2.062527	2.806313	-1.627463
H	1.759383	-0.309962	3.073878	C	2.051531	1.484223	-1.173554
H	3.258782	-1.139368	2.685238	C	2.520954	2.197703	2.609675

## TS<sub>H12</sub>

E= -2383.7935329au

C	3.090759	-2.749431	-0.782688	C	2.121065	5.311960	-1.271181
C	3.419953	-1.544376	-0.107529	C	1.852780	0.403120	-2.218380
C	4.776270	-1.142771	-0.022389	H	6.801107	-1.642691	-0.523476
C	5.762120	-1.957396	-0.594653	H	3.852407	-4.449035	-1.842868
C	5.459303	-3.150301	-1.251019	H	1.936885	2.988150	-2.692513
C	4.115908	-3.525121	-1.332299	H	2.478510	4.441314	1.288806
P	2.020791	-0.585047	0.674030	H	6.323190	0.149870	0.731790
C	5.233827	0.144116	0.630152	H	4.947469	1.019847	0.038178
C	6.540733	-4.005695	-1.866956	H	4.811049	0.288104	1.628970
C	1.666856	-3.239857	-0.948743	H	1.027232	-2.511420	-1.456186
B	-1.679267	-0.253566	0.737241	H	1.648949	-4.159632	-1.540804
C	-2.883106	-1.176604	0.200926	H	1.185664	-3.463003	0.009565
C	-2.785583	-2.335954	-0.569490	H	6.456777	-4.023403	-2.961050
				H	7.538568	-3.632978	-1.615934
				H	6.471338	-5.044694	-1.523446
				H	1.693123	0.858321	-3.199976

H	2.717746	-0.263167	-2.298870	C	-5.226224	-1.787405	0.255348
H	0.971196	-0.213378	-2.009002	C	-4.102440	-1.015829	0.542731
H	2.572722	5.410966	-2.264245	F	-1.515892	-2.948108	-1.082978
H	1.073440	5.628671	-1.355354	F	-4.307921	0.096225	1.284625
H	2.623221	6.010833	-0.594390	F	-6.445308	-1.428926	0.693549
H	3.284910	1.478307	2.914400	F	-6.143793	-3.714508	-0.780782
H	2.803787	3.167975	3.027651	F	-3.655856	-4.445799	-1.653986
H	1.573736	1.913296	3.083321	C	-1.754880	1.170079	0.054285
H	0.524922	-0.817025	0.092776	C	-1.716807	1.526767	-1.297027
H	-0.264069	-0.837054	-0.248825	C	-1.775422	2.836183	-1.766126
C	2.303639	-0.952669	2.505790	C	-1.914655	3.875705	-0.853726
C	-1.057339	-0.623977	2.155689	C	-1.992489	3.581354	0.501759
C	1.791119	-2.353265	2.926803	C	-1.922164	2.252091	0.921398
C	-0.757114	-2.126274	2.362007	F	-1.554252	0.569532	-2.243066
C	0.328937	-2.438196	3.409143	F	-1.659462	3.110220	-3.080023
H	-0.157211	-0.023028	2.322795	F	-1.924758	5.155879	-1.276096
H	-1.747324	-0.282270	2.942460	F	-2.117944	4.580472	1.393677
H	-0.472217	-2.593903	1.409834	F	-1.988970	2.066616	2.258813
H	-1.686666	-2.628471	2.658025	C	2.313414	1.368397	0.247272
H	0.199409	-1.780438	4.281200	C	2.546015	2.472821	1.106368
H	0.182010	-3.461742	3.779963	C	2.354790	3.763008	0.598008
H	1.957828	-3.078704	2.119983	C	1.939141	4.005872	-0.710974
H	2.433115	-2.686739	3.752634	C	1.760776	2.903364	-1.549759
H	1.816054	-0.192767	3.114077	C	1.933431	1.590878	-1.108140
H	3.378899	-0.887849	2.695846	C	2.969635	2.382693	2.557769

## H<sub>2</sub>

E= -2383.8302286au

C	3.203215	-2.611337	-0.735427	C	1.658532	5.403551	-1.203371
C	3.593032	-1.429680	-0.047354	C	1.685515	0.478868	-2.103669
C	4.960629	-1.057650	0.014920	H	6.955523	-1.583205	-0.560315
C	5.908227	-1.871572	-0.610436	H	3.905952	-4.289424	-1.861700
C	5.553845	-3.036536	-1.294806	H	1.445164	3.064345	-2.577481
C	4.202265	-3.383872	-1.338135	H	2.522809	4.607110	1.262191
P	2.318072	-0.394652	0.776042	H	6.536007	0.284722	0.605469
C	5.454199	0.183481	0.726636	H	4.988839	1.095072	0.338470
C	6.594726	-3.880599	-1.988587	H	5.258185	0.147331	1.805339
C	1.774056	-3.097480	-0.858064	H	1.108098	-2.372067	-1.334543
B	-1.518312	-0.399996	0.491074	H	1.740580	-4.009754	-1.459212
C	-2.810840	-1.332302	0.116123	H	1.329020	-3.336872	0.112947
C	-2.717484	-2.510897	-0.624742	H	6.680339	-3.601065	-3.046913
C	-3.810830	-3.317968	-0.936500	H	7.582771	-3.753008	-1.535272
C	-5.077419	-2.950858	-0.494344	H	6.335581	-4.943813	-1.954378
				H	1.491789	0.901676	-3.092501
				H	2.542932	-0.195758	-2.194243
				H	0.800241	-0.110281	-1.838937

H	2.081138	5.568591	-2.200794
H	0.576595	5.569747	-1.278111
H	2.067761	6.159613	-0.526455
H	3.742265	1.631631	2.736489
H	3.374608	3.344916	2.882823
H	2.121097	2.159240	3.215105
C	2.397575	-0.719086	2.601615
C	-1.033873	-0.621053	2.043909
C	1.923466	-2.138277	3.018117
C	-0.613510	-2.079995	2.337571
C	0.446204	-2.278989	3.439873
H	-0.197961	0.067269	2.253974
H	-1.803807	-0.328889	2.768249
H	-0.261413	-2.572487	1.418469
H	-1.510656	-2.644662	2.620844
H	0.246299	-1.589150	4.272546
H	0.352686	-3.291089	3.857851
H	2.160112	-2.867228	2.232152
H	2.549388	-2.424371	3.872688
H	1.803650	0.042032	3.108280
H	3.441387	-0.574220	2.893593
H	-0.595628	-0.787954	-0.230336
H	1.054634	-0.864998	0.339023

### H<sub>3</sub>

E= -2572.4225398au

C	-4.473454	-1.568881	0.422932
C	-4.160744	-0.320252	-0.182839
C	-5.189424	0.624028	-0.428971
C	-6.498086	0.312188	-0.051150
C	-6.829925	-0.901931	0.553092
C	-5.803310	-1.821586	0.776595
P	-2.412587	0.034922	-0.644060
C	2.320314	0.877639	3.885959
O	3.381933	0.500140	3.580733
C	-4.947310	1.958183	-1.098082
C	-8.255852	-1.223541	0.928097
C	-3.460881	-2.662095	0.705809
B	1.236341	-0.733804	-1.339865
O	1.263603	1.245649	4.232372
C	1.888208	-1.949069	-0.439508
C	1.228186	-2.609746	0.593064
C	1.783087	-3.635522	1.355143

C	3.085215	-4.045130	1.090444
C	3.798559	-3.420826	0.070427
C	3.192767	-2.400686	-0.660136
F	-0.062117	-2.280584	0.923485
F	3.940114	-1.832372	-1.631638
F	5.056280	-3.809391	-0.193391
F	3.644790	-5.032128	1.806282
F	1.078302	-4.229601	2.335617
C	2.099065	0.648026	-1.074268
C	2.095683	1.210449	0.205631
C	2.734026	2.397013	0.546174
C	3.446625	3.091520	-0.425148
C	3.498302	2.574364	-1.714276
C	2.836964	1.379052	-2.008329
F	1.419635	0.592749	1.212394
F	2.658040	2.893819	1.803365
F	4.064193	4.244340	-0.122338
F	4.180149	-3.233907	-2.666146
F	2.937982	0.965576	-3.290188
C	-1.759645	1.602634	0.051518
C	-1.432063	2.747419	-0.719642
C	-0.893606	3.857749	-0.060825
C	-0.643675	3.873957	1.311826
C	-0.976350	2.735603	2.048113
C	-1.522073	1.597099	1.453628
C	-1.572532	2.860302	-2.223020
C	0.015744	5.057545	1.973393
C	-1.774252	0.395982	2.337220
H	-7.280713	1.044084	-0.236244
H	-6.040536	-2.774142	1.244187
H	-0.775083	2.714777	3.115142
H	-0.640421	4.733935	-0.652658
H	-5.867960	2.547668	-1.116882
H	-4.184004	2.549320	-0.583760
H	-4.627411	1.836229	-2.140587
H	-3.962190	-3.520716	1.160190
H	-2.968494	-3.020782	-0.204013
H	-2.670541	-2.348843	1.395760
H	-8.845605	-0.314195	1.080275
H	-8.746334	-1.804538	0.135983
H	-8.303746	-1.820548	1.844751
H	-1.625235	0.663859	3.385847
H	-2.792153	0.002560	2.238049

H	-1.065411	-0.408454	2.107992
H	-0.406346	5.250734	2.965417
H	1.085780	4.856106	2.105143
H	-0.084070	5.966001	1.371309
H	-2.525399	2.484749	-2.601993
H	-1.496626	3.908634	-2.524212
H	-0.768883	2.320935	-2.737035
H	-1.679931	-0.972819	-0.010648
H	0.138996	-0.484355	-0.861336
C	-2.181044	-0.230234	-2.459335
C	1.052567	-1.168556	-2.911734
C	-2.270012	-1.712293	-2.889077
C	0.239300	-2.459403	-3.168111
C	-1.119994	-2.642866	-2.458094
H	-2.954786	0.350258	-2.970599
H	-1.207618	0.184393	-2.715477
H	-3.231172	-2.124398	-2.551385
H	-2.322806	-1.702377	-3.986456
H	-0.973167	-2.594243	-1.374039
H	-1.464101	-3.666309	-2.665048
H	0.855647	-3.314983	-2.859248
H	0.075842	-2.593300	-4.249937
H	2.029916	-1.319823	-3.385413
H	0.608800	-0.336193	-3.483780

### TS<sub>H34</sub>

E= -2572.3597376au

C	3.628937	-2.711483	-0.867052
C	3.641524	-1.497453	-0.124571
C	4.898624	-0.908346	0.190880
C	6.073046	-1.495946	-0.295553
C	6.073435	-2.658712	-1.063142
C	4.840054	-3.253146	-1.316866
P	2.005529	-0.762025	0.482236
C	-0.834575	-1.782478	-1.620270
O	-1.695297	-2.349017	-2.246157
C	5.096561	0.327307	1.045932
C	7.358347	-3.277218	-1.558866
C	2.390987	-3.504838	-1.232562
B	-1.679551	-0.324306	0.663559
O	0.383548	-1.502704	-1.861383
C	-3.183355	-0.851024	0.360392
C	-3.529912	-2.201047	0.213417

C	-4.824523	-2.648349	-0.035023
C	-5.860043	-1.725415	-0.130033
C	-5.579302	-0.372550	0.028935
C	-4.268426	0.032686	0.265866
F	-2.591952	-3.163710	0.316682
F	-4.093703	1.360308	0.439865
F	-6.569670	0.528076	-0.036316
F	-7.112173	-2.133722	-0.356859
F	-5.080128	-3.955665	-0.170212
C	-1.362939	1.131229	0.060059
C	-1.581429	1.466512	-1.285058
C	-1.421872	2.748590	-1.803923
C	-1.075614	3.789360	-0.949546
C	-0.898948	3.526055	0.402255
C	-1.034428	2.224258	0.873090
F	-1.983808	0.529180	-2.157925
F	-1.615876	2.988594	-3.106273
F	-0.900185	5.030024	-1.419985
F	-0.573315	4.524833	1.237330
F	-0.870014	2.075597	2.205875
C	2.198391	1.093444	0.473060
C	2.226106	1.944619	1.612194
C	2.353685	3.326100	1.420150
C	2.461631	3.911700	0.160124
C	2.475638	3.057926	-0.941633
C	2.343950	1.670292	-0.823305
C	2.146925	1.503325	3.061097
C	2.504382	5.409431	-0.011499
C	2.403566	0.873939	-2.110481
H	7.022796	-1.024844	-0.052370
H	4.805619	-4.179515	-1.886318
H	2.585188	3.480622	-1.937636
H	2.356374	3.968092	2.297110
H	6.148376	0.404786	1.336788
H	4.830127	1.248840	0.520550
H	4.510676	0.301637	1.968342
H	2.665117	-4.549466	-1.408285
H	1.624049	-3.499751	-0.456429
H	1.916633	-3.117779	-2.137860
H	8.186354	-2.562119	-1.525018
H	7.643601	-4.141963	-0.945341
H	7.257815	-3.633404	-2.590117
H	2.522892	1.553017	-2.959195

H	3.252151	0.181205	-2.123658
H	1.502182	0.281319	-2.287360
H	3.133737	5.700734	-0.859107
H	1.494194	5.792663	-0.203861
H	2.881172	5.908911	0.886721
H	2.889833	0.743769	3.319639
H	2.330376	2.362255	3.712071
H	1.157251	1.118916	3.323297
H	1.001741	-1.166426	-0.677478
H	-1.119604	-1.383398	-0.540155
C	1.996161	-1.527836	2.206159
C	-1.074507	-0.729346	2.078083
C	1.437652	-2.959774	2.283431
C	-1.020685	-2.179609	2.604285
C	-0.038835	-3.130273	1.894631
H	3.046812	-1.528900	2.511809
H	1.457535	-0.896129	2.902252
H	2.061475	-3.638322	1.690560
H	1.567810	-3.271745	3.329246
H	-0.161499	-3.038083	0.810960
H	-0.319876	-4.164735	2.129404
H	-2.021881	-2.614988	2.547628
H	-0.768783	-2.152994	3.675592
H	-1.767898	-0.178761	2.739177
H	-0.127369	-0.220989	2.240446

#### H<sub>4</sub>

E= -2572.4142556au

C	-2.785595	-3.164638	0.107831
C	-3.200157	-1.935554	-0.470370
C	-4.560689	-1.783892	-0.845066
C	-5.451415	-2.845680	-0.645318
C	-5.053765	-4.062392	-0.089014
C	-3.716070	-4.196716	0.282118
P	-1.866579	-0.626359	-0.700879
C	1.361709	-2.604914	3.604446
O	1.028476	-3.157588	4.616808
C	-5.128181	-0.514322	-1.441254
C	-6.032551	-5.199782	0.083623
C	-1.363871	-3.427528	0.565942
B	2.128206	0.616909	-1.280618
O	0.702196	-1.536410	3.102576
C	3.363507	-0.228313	-0.727970

C	3.275693	-1.342046	0.098414
C	4.382040	-2.067968	0.524431
C	5.652718	-1.674982	0.107975
C	5.791097	-0.566177	-0.724737
C	4.651637	0.128310	-1.124820
F	2.055262	-1.757960	0.531743
F	4.814282	1.200535	-1.928466
F	7.005144	-0.180957	-1.128187
F	6.728993	-2.355492	0.505509
F	4.236628	-3.127283	1.332351
C	1.513622	1.760162	-0.396328
C	1.541768	1.752416	1.010569
C	0.955764	2.734788	1.799735
C	0.318491	3.809831	1.184101
C	0.274442	3.883240	-0.204895
C	0.860464	2.873160	-0.958878
F	2.125649	0.737433	1.679574
F	0.999259	-2.659317	3.131227
F	-0.242686	4.764858	1.922513
F	-0.329972	4.914989	-0.799161
F	0.792136	3.023278	-2.293575
C	-2.622542	1.011908	-0.160019
C	-2.848645	2.177820	-0.940968
C	-3.230701	3.370922	-0.309317
C	-3.407377	3.476528	1.069264
C	-3.203847	2.322440	1.825714
C	-2.810421	1.109009	1.251121
C	-2.706269	2.260107	-2.448720
C	-3.767455	4.791420	1.718528
C	-2.600984	-0.057935	2.192884
H	-6.492033	-2.712431	-0.935307
H	-3.381357	-5.130824	0.728622
H	-3.346135	2.362118	2.903795
H	-3.397443	4.250059	-0.928414
H	-6.160299	-0.676687	-1.767213
H	-5.127918	0.309170	-0.720493
H	-4.559407	-0.172630	-2.311033
H	-1.295819	-4.415266	1.033088
H	-0.650117	-3.407037	-0.264970
H	-1.023316	-2.687429	1.296441
H	-7.047697	-4.831236	0.266611
H	-6.072833	-5.828446	-0.816331
H	-5.750002	-5.848180	0.919806

H	-2.762326	0.254918	3.228711
H	-3.287118	-0.885477	1.984544
H	-1.584516	-0.463574	2.130105
H	-4.350295	4.642024	2.633761
H	-2.861706	5.347171	1.993813
H	-4.349485	5.427929	1.043355
H	-3.189645	1.430284	-2.967092
H	-3.164855	3.184087	-2.813670
H	-1.656909	2.284384	-2.764561
H	1.135145	-1.245391	2.280915
H	2.229301	-2.909736	2.991406
C	-1.665098	-0.691384	-2.584222
C	1.676885	0.344474	-2.765845
C	-0.859339	-1.932650	-3.030430
C	1.644643	-1.124053	-3.251477
C	0.611422	-2.055536	-2.580828
H	-2.633884	-0.715310	-3.092144
H	-1.156449	0.216470	-2.906776
H	-1.394553	-2.829163	-2.691370
H	-0.890820	-1.968838	-4.129344
H	0.674961	-1.953628	-1.491547
H	0.919819	-3.086294	-2.803254
H	2.639596	-1.562204	-3.100050
H	1.476977	-1.132381	-4.337512
H	2.449776	0.873822	-3.357449
H	0.745798	0.853649	-3.014309

## I

E= -242 1.9670401au

C	-4.484364	-1.918813	1.882839
C	-4.482554	-1.413665	0.555026
C	-5.598835	-1.686551	-0.276495
C	-6.661683	-2.448828	0.225962
C	-6.669905	-2.958987	1.524361
C	-5.570121	-2.677822	2.335898
P	-2.953323	-0.447433	0.028955
C	-5.736960	-1.174237	-1.694503
C	-7.816032	-3.805908	2.025560
C	-3.353889	-1.667985	2.863474
B	2.723665	0.018611	-0.282816
C	4.102875	-0.747071	-0.484110
C	4.594725	-1.720370	0.379972
C	5.785346	-2.402020	0.146877

C	6.526556	-2.103857	-0.995784
C	6.069289	-1.135279	-1.886736
C	4.870256	-0.481457	-1.615215
F	3.898464	-2.024603	1.494962
F	4.440218	0.452585	-2.492254
F	6.777368	-0.846157	-2.984560
F	7.672975	-2.746653	-1.236004
F	6.223370	-3.332295	1.002722
C	2.691437	1.334048	0.577715
C	3.604578	1.594690	1.617082
C	3.576897	2.754723	2.384624
C	2.620531	3.730433	2.114101
C	1.700807	3.532056	1.087102
C	1.745046	2.351724	0.352237
F	4.547431	0.698747	1.942358
F	4.456193	2.941080	3.374058
F	2.586288	4.849800	2.834167
F	0.791582	4.473092	0.816943
F	0.843881	2.238720	-0.634639
C	-3.618620	1.039715	-0.915121
C	-3.364110	1.401247	-2.264631
C	-3.872143	2.607566	-2.765127
C	-4.617366	3.495505	-1.990622
C	-4.833012	3.148760	-0.658109
C	-4.341044	1.961705	-0.104521
C	-2.549952	0.575232	-3.240549
C	-5.131463	4.796855	-2.559583
C	-4.606329	1.730520	1.368449
H	-7.511190	-2.648089	-0.424819
H	-5.554159	-3.055741	3.356405
H	-5.394853	3.825737	-0.017151
H	-3.674895	2.857140	-3.806005
H	-6.541856	-1.706084	-2.212071
H	-5.974690	-0.105264	-1.715913
H	-4.823376	-1.303220	-2.279575
H	-2.406298	-2.103363	2.528748
H	-3.169742	-0.598745	3.010902
H	-3.594585	-2.107711	3.836918
H	-8.749645	-3.565550	1.505818
H	-7.619790	-4.874689	1.864726
H	-7.978826	-3.665555	3.099782
H	-5.011191	2.637260	1.828586
H	-5.321497	0.919213	1.542033

H	-3.686104	1.464055	1.902803
H	-6.070712	5.098952	-2.083472
H	-4.412226	5.612439	-2.403686
H	-5.306852	4.721418	-3.638269
H	-2.939661	-0.437979	-3.371249
H	-2.550751	1.052774	-4.224980
H	-1.502902	0.487434	-2.928774
C	-2.185381	-1.718833	-1.152574
C	1.460853	-0.487951	-1.075759
C	-1.612215	-2.923152	-0.370858
C	1.346366	-1.988290	-1.415341
C	-0.352940	-2.648280	0.483175
H	-2.911323	-2.085365	-1.884261
H	-1.384076	-1.224826	-1.703472
H	1.546712	0.079332	-2.024485
H	0.531600	-0.120529	-0.629037
C	0.999134	-2.892423	-0.217017
H	-2.405077	-3.331875	0.267021
H	-1.384175	-3.717028	-1.096718
H	-0.397290	-1.628227	0.886373
H	-0.377134	-3.310463	1.358745
H	1.024847	-3.936737	-0.560170
H	1.793514	-2.804577	0.535638
H	0.593400	-2.123487	-2.202613
H	2.291738	-2.339069	-1.848583

## I<sub>1</sub>

E= -2423.1430285au

C	-4.732555	-2.107528	1.719327
C	-4.623395	-1.454415	0.463703
C	-5.645344	-1.654781	-0.500311
C	-6.721632	-2.497159	-0.194544
C	-6.833931	-3.155155	1.031517
C	-5.828506	-2.941485	1.974501
P	-3.079855	-0.407644	0.192880
C	-5.666778	-0.978826	-1.855077
C	-7.991019	-4.083871	1.315704
C	-3.711189	-1.939106	2.828690
B	2.803917	-0.011919	-0.328938
C	4.134093	-0.873593	-0.449208
C	4.564654	-1.778240	0.516181
C	5.708856	-2.554928	0.362788
C	6.465005	-2.427825	-0.801898

C	6.068094	-1.533174	-1.793437
C	4.913503	-0.779230	-1.598790
F	3.850821	-1.915875	1.653044
F	4.541044	0.080853	-2.572284
F	6.790741	-1.407951	-2.912490
F	7.567811	-3.163813	-0.966438
F	6.089043	-3.414454	1.314794
C	2.847046	1.384270	0.392665
C	3.801573	1.710826	1.375055
C	3.843086	2.942798	2.020189
C	2.916196	3.924610	1.678965
C	1.956453	3.661424	0.704417
C	1.932485	2.412346	0.092972
F	4.720319	0.815335	1.763414
F	4.761031	3.192454	2.958994
F	2.948108	5.111175	2.281473
F	1.074313	4.606217	0.366683
F	0.992283	2.239008	-0.849505
C	-3.695182	1.163230	-0.641989
C	-3.294424	1.689262	-1.898785
C	-3.788825	2.931053	-2.318341
C	-4.657660	3.700947	-1.545636
C	-5.014383	3.194708	-0.297508
C	-4.543359	1.964229	0.174422
C	-2.328563	1.008464	-2.847413
C	-5.153093	5.045652	-2.022841
C	-4.969225	1.558231	1.569984
H	-7.497918	-2.641324	-0.944084
H	-5.896194	-3.434286	2.942397
H	-5.674364	3.776737	0.343112
H	-3.478138	3.307207	-3.291365
H	-6.406850	-1.456997	-2.504767
H	-5.929739	0.080952	-1.770788
H	-4.700753	-1.020631	-2.364486
H	-2.719436	-2.306282	2.543711
H	-3.583664	-0.888841	3.110490
H	-4.026005	-2.492671	3.719365
H	-8.917008	-3.725682	0.852405
H	-7.799031	-5.089819	0.918497
H	-8.167236	-4.187157	2.391602
H	-5.442764	2.401738	2.081970
H	-5.682287	0.726858	1.565517
H	-4.110941	1.239198	2.173751



H	-6.122758	5.295598	-1.578957	C	-5.759146	-1.060618	-1.049173
H	-4.454183	5.848112	-1.750174	C	-5.542910	0.248856	-0.630249
H	-5.262588	5.069278	-3.112721	C	-4.324028	0.580451	-0.044644
H	-2.648885	0.002965	-3.133056	F	-2.640970	-2.620616	-0.120143
H	-2.233822	1.593372	-3.767281	F	-4.171565	1.860296	0.360873
H	-1.323846	0.927184	-2.415724	F	-6.503789	1.169789	-0.789112
C	-2.186613	-1.543922	-1.039565	F	-6.921738	-1.405956	-1.614945
C	1.505240	-0.521465	-1.058746	F	-4.958867	-3.274984	-1.263333
C	-1.636990	-2.798588	-0.322500	C	-1.231698	1.450730	0.227551
C	1.329001	-2.030569	-1.318232	C	-0.966612	1.516722	-1.146978
C	-0.404532	-2.559997	0.582302	C	-0.338878	2.594293	-1.762385
H	-2.848565	-1.853881	-1.853754	C	0.051958	3.685917	-0.993750
H	-1.358054	-0.989112	-1.480621	C	-0.194478	3.678542	0.374481
H	1.571800	-0.002558	-2.035856	C	-0.819955	2.576020	0.951732
H	0.605187	-0.100338	-0.599099	F	-1.269342	0.469911	-1.944687
C	0.958767	-2.859890	-0.074580	F	-0.069611	2.571852	-3.076620
H	-2.445032	-3.257418	0.259246	F	0.680865	4.720226	-1.560924
H	-1.378827	-3.539746	-1.092408	F	0.187009	4.720700	1.125960
H	-0.427191	-1.532934	0.969721	F	-1.006219	2.641822	2.287556
H	-0.479983	-3.205896	1.466589	C	2.546984	0.848703	0.249067
H	0.974696	-3.921821	-0.358824	C	2.889738	1.742728	1.299863
H	1.741887	-2.739476	0.685468	C	3.517102	2.953486	0.985651
H	0.560221	-2.175704	-2.088489	C	3.820010	3.334153	-0.323171
H	2.254117	-2.438944	-1.744622	C	3.444243	2.463895	-1.344300
H	-0.603106	1.316188	3.223992	C	2.803602	1.244484	-1.093511
H	-1.031226	0.994040	2.707678	C	2.591065	1.506615	2.766330

## TS<sub>112</sub>

E= -2423.1022492au

C	2.074595	-3.011453	-1.228491	H	5.838091	-3.417784	-0.367562
C	2.692695	-2.103366	-0.330699	H	2.352370	-4.739687	-2.467050
C	4.070278	-2.253123	-0.027127	H	3.634252	2.744430	-2.377766
C	4.781964	-3.310108	-0.606362	H	3.771562	3.626987	1.801177
C	4.187011	-4.224118	-1.477972	H	5.816474	-1.738146	1.121334
C	2.835285	-4.049930	-1.778215	H	5.018736	-0.344071	0.380146
P	1.630680	-0.769125	0.429351	H	4.324431	-1.093523	1.808210
C	4.842394	-1.308024	0.869334	H	0.345653	-1.919254	-2.000650
C	4.973901	-5.373447	-2.061335	H	0.409152	-3.625795	-2.446121
C	0.618715	-2.916263	-1.640055	H	-0.068444	-3.149007	-0.819622
B	-1.936049	0.168986	0.879568	H	6.036896	-5.127023	-2.153380
C	-3.283712	-0.332400	0.154310	H	4.899866	-6.265036	-1.424308
C	-3.555941	-1.635275	-0.268957	H	4.600927	-5.651842	-3.052659
C	-4.757874	-2.009651	-0.866779	H	2.500711	1.019405	-3.210678
				H	3.012625	-0.476699	-2.416116

H	1.353692	0.099803	-2.245673
H	5.587322	4.581608	-0.370162
H	4.435061	4.910461	-1.671458
H	4.095803	5.459081	-0.021143
H	3.003624	0.566312	3.140966
H	3.023362	2.311531	3.367295
H	1.513199	1.506298	2.966185
H	0.036047	-0.892355	0.162421
H	-0.805686	-1.068574	0.168025
C	1.470020	-1.372408	2.200122
C	-1.805765	-0.088165	2.449964
C	0.669608	-2.694239	2.226797
C	-2.094908	-1.505631	3.028126
C	-1.054495	-1.982342	4.078355
C	-0.004833	-3.001635	3.576526
H	0.935502	-0.602694	2.754107
H	2.442713	-1.508049	2.679852
H	-0.111156	-2.681098	1.461065
H	1.338993	-3.521195	1.963140
H	-0.493064	-3.980122	3.468965
H	0.761549	-3.130483	4.354262
H	-0.548225	-1.105815	4.505157
H	-1.570356	-2.454786	4.924245
H	-3.085243	-1.497270	3.497900
H	-2.164983	-2.248286	2.226301
H	-0.830000	0.261731	2.801342
H	-2.503814	0.627845	2.913933

## I<sub>2</sub>

E= -2423.1341229au

C	-3.341257	-2.351650	1.258009
C	-3.622205	-1.492061	0.162173
C	-4.963768	-1.257021	-0.237316
C	-5.994489	-1.880696	0.468857
C	-5.747949	-2.730336	1.550384
C	-4.420139	-2.945799	1.923174
P	-2.254101	-0.684766	-0.756625
C	-5.341439	-0.357144	-1.394804
C	-6.881051	-3.412068	2.277343
C	-1.949101	-2.682834	1.756038
B	1.663025	-0.363495	-0.436748
C	3.166683	-0.950589	-0.130729
C	3.393816	-2.182919	0.485548

C	4.662065	-2.685889	0.774423
C	5.785478	-1.937676	0.440353
C	5.618468	-0.704348	-0.182289
C	4.330341	-0.246635	-0.451335
F	2.356028	-2.986972	0.826234
F	4.240382	0.958827	-1.058083
F	6.697246	0.026082	-0.514352
F	7.016052	-2.402338	0.708967
F	4.811438	-3.884232	1.367907
C	1.474499	1.105206	0.316753
C	1.068712	1.148704	1.655102
C	0.823445	2.317082	2.372917
C	0.991204	3.545537	1.746484
C	1.407464	3.568956	0.421966
C	1.642982	2.371886	-0.255511
F	0.820506	-0.002093	2.335409
F	0.367067	2.269226	3.640516
F	0.710633	4.689580	2.394770
F	1.531838	4.755610	-0.208097
F	2.020021	2.515410	-1.543053
C	-2.382255	1.149000	-0.823700
C	-2.392313	1.909137	-2.021425
C	-2.292153	3.301799	-1.924738
C	-2.178786	3.968509	-0.705368
C	-2.235973	3.201890	0.460670
C	-2.331055	1.809954	0.437692
C	-2.479965	1.338897	-3.421343
C	-1.946925	5.456485	-0.639302
C	-2.366410	1.091624	1.769139
H	-7.021337	-1.693439	0.163828
H	-4.208094	-3.599048	2.765819
H	-2.170643	3.699783	1.424556
H	-2.280030	3.880544	-2.844880
H	-6.429075	-0.290086	-1.482898
H	-4.954242	0.659238	-1.272376
H	-4.968703	-0.738789	-2.353499
H	-1.377101	-3.259082	1.021906
H	-1.349042	-1.801915	2.004862
H	-2.014813	-3.291841	2.661316
H	-7.790469	-2.802686	2.263829
H	-7.124801	-4.372772	1.804825
H	-6.621352	-3.618550	3.320378
H	-2.247516	1.809654	2.584037

H	-3.310238	0.558616	1.923732
H	-1.548260	0.373445	1.880752
H	-2.496928	5.914657	0.189615
H	-0.879905	5.653371	-0.474461
H	-2.240380	5.954433	-1.568524
H	-3.234904	0.554688	-3.519498
H	-2.746774	2.132260	-4.124638
H	-1.518142	0.930804	-3.752171
C	-2.002121	-1.582197	-2.361998
C	1.270235	-0.303660	-2.034836
C	-1.547091	-3.047667	-2.178211
C	1.367696	-1.575821	-2.922525
C	-0.172617	-3.277399	-1.523768
H	-2.947099	-1.553086	-2.911174
H	-1.261281	-1.020770	-2.928492
H	1.865135	0.460317	-2.546286
H	0.241203	0.097610	-2.085712
C	1.099090	-2.984520	-2.342258
H	-2.316664	-3.584982	-1.608259
H	-1.554752	-3.492086	-3.183109
H	-0.096790	-2.727365	-0.583582
H	-0.134547	-4.340052	-1.246689
H	1.142857	-3.696330	-3.181239
H	1.931119	-3.249264	-1.681792
H	0.740318	-1.440015	-3.820310
H	2.391480	-1.627170	-3.317900
H	0.872040	-1.098575	0.138905
H	-1.063482	-0.918894	-0.033155

### I<sub>3</sub>

E= -2611.7194462au

C	-3.642947	-2.400536	0.883762
C	-3.877947	-1.392677	-0.090238
C	-5.203654	-1.063853	-0.474390
C	-6.265292	-1.744207	0.126304
C	-6.064398	-2.739241	1.086026
C	-4.750485	-3.045316	1.445848
P	-2.464733	-0.523650	-0.875737
C	1.772343	-2.581482	3.050942
O	2.858645	-2.208987	3.261009
C	-5.532281	-0.008261	-1.507777
C	-7.229474	-3.477326	1.698276
C	-2.269916	-2.822730	1.361742

B	1.577120	-0.142581	-0.669648
O	0.681000	-2.973273	2.885803
C	3.111278	-0.720371	-0.535751
C	3.410902	-1.985952	-0.031530
C	4.703044	-2.489646	0.106211
C	5.782548	-1.704888	-0.283379
C	5.545167	-0.434680	-0.800819
C	4.233737	0.021518	-0.914076
F	2.414016	-2.828375	0.357692
F	4.076527	1.264853	-1.422059
F	6.580357	0.332308	-1.183957
F	7.037129	-2.167296	-0.166004
F	4.915392	-3.721384	0.602119
C	1.431460	1.254991	0.218481
C	1.121927	1.181072	1.580284
C	0.922433	2.278193	2.414745
C	1.043731	3.558096	1.888436
C	1.363808	-3.699474	0.544599
C	1.552308	2.568600	-0.251096
F	0.922507	-0.027636	2.176351
F	0.560825	2.113727	3.702174
F	0.811036	4.639121	2.652874
F	1.440551	4.937503	0.013488
F	1.833271	2.828718	-1.544755
C	-2.518808	1.304385	-0.713280
C	-2.567945	2.206578	-1.806311
C	-2.448761	3.575461	-1.542406
C	-2.277335	4.084086	-0.255012
C	-2.282010	3.177640	0.807938
C	-2.390478	1.799798	0.616419
C	-2.705144	1.809528	-3.260659
C	-2.039903	5.553221	-0.014927
C	-2.342747	0.915980	1.844111
H	-7.280215	-1.485763	-0.166191
H	-4.572719	-3.813015	2.194740
H	-2.166427	3.551087	1.822028
H	-2.469426	4.264381	-2.383087
H	-6.615479	0.097376	-1.610840
H	-5.125771	0.972838	-1.242578
H	-5.143339	-0.269485	-2.499637
H	-1.651879	-3.235079	0.558238
H	-1.701727	-2.003369	1.812508
H	-2.360149	-3.599289	2.125061

H	-8.141641	-2.872620	1.680428	O	-1.539262	-2.343722	-2.462030
H	-7.438559	-4.402716	1.145474	C	5.053968	0.214259	1.342050
H	-7.024069	-3.758878	2.736097	C	7.514814	-2.873248	-1.700511
H	-2.261171	1.531759	2.743338	C	2.538406	-3.159044	-1.742798
H	-3.238246	0.293930	1.945511	B	-1.673079	-0.316258	0.504717
H	-1.466470	0.258402	1.847221	O	0.369948	-1.212142	-1.963906
H	-2.530571	5.896560	0.901950	C	-3.223494	-0.744695	0.268910
H	-0.964280	5.738242	0.098487	C	-3.667433	-2.047418	0.015294
H	-2.397707	6.163131	-0.850146	C	-5.006307	-2.391665	-0.155084
H	-3.449915	1.027671	-3.426716	C	-5.983704	-1.407988	-0.050006
H	-3.010254	2.676681	-3.852558	C	-5.602261	-0.099758	0.228517
H	-1.749742	1.462805	-3.671224	C	-4.251356	0.201870	0.381102
H	-1.311117	-0.883670	-0.152025	F	-2.786149	-3.061548	-0.073861
H	0.838080	-0.938723	-0.108561	F	-3.969034	1.487671	0.685265
C	-2.195901	-1.235432	-2.567923	F	-6.533471	0.855447	0.356600
C	1.074450	0.046676	-2.226374	F	-7.275301	-1.717699	-0.199678
C	-1.716573	-2.704583	-2.530362	F	-5.358019	-3.659253	-0.404419
C	1.153511	-1.141994	-3.221898	C	-1.327446	1.121052	-0.137877
C	-0.325578	-2.971828	-1.926382	C	-1.612305	1.432322	-1.476809
H	-3.144330	-1.166904	-3.108613	C	-1.463407	2.700576	-2.032006
H	-1.466697	-0.605354	-3.073789	C	-1.069712	3.758643	-1.220240
H	1.608943	0.871765	-2.708798	C	-0.834748	3.522441	0.128170
H	0.032234	0.409068	-2.171357	C	-0.956225	2.231837	0.633623
C	0.920502	-2.596473	-2.750921	F	-2.083864	0.487323	-2.304886
H	-2.468137	-3.305317	-2.001052	F	-1.726751	2.914110	-3.326596
H	-1.736496	-3.053496	-3.572023	F	-0.930745	4.987992	-1.725327
H	-0.230461	-2.504105	-0.943121	F	-0.490282	4.540598	0.933309
H	-0.270641	-4.053491	-1.741185	F	-0.747645	2.119730	1.963408
H	0.948342	-3.238140	-3.645286	C	2.213873	1.076914	0.636154
H	1.774414	-2.901794	-2.137494	C	2.199740	1.796415	1.861530
H	0.492664	-0.940429	-4.082974	C	2.398394	3.181258	1.833288
H	2.163270	-1.145112	-3.655028	C	2.612104	3.893636	0.653794

### TS134

E= -2611.65799au

C	3.741328	-2.447237	-1.161978	C	2.759375	5.394370	0.662078
C	3.689145	-1.390305	-0.208212	C	2.507054	1.132903	-1.946540
C	4.917085	-0.861884	0.282866	H	7.054020	-0.927729	0.159689
C	6.128315	-1.351011	-0.223749	H	5.001204	-3.698079	-2.356167
C	6.193537	-2.355490	-1.185609	H	2.812727	3.692824	-1.472683
C	4.986028	-2.893344	-1.624572	H	2.376891	3.722784	2.775826
P	2.014448	-0.765765	0.438514	H	6.077772	0.216806	1.727746
C	-0.793240	-1.693169	-1.774594	H	4.846825	1.213845	0.948740

H	4.391561	0.061498	2.196566	C	-5.988688	-4.254048	0.340975
H	1.799027	-3.436582	-0.988079	C	-4.976045	-4.020906	1.273024
H	2.012685	-2.546201	-2.478424	P	-3.134255	-0.512102	0.087990
H	2.859054	-4.082811	-2.232846	C	-0.779578	1.785726	1.965243
H	8.334491	-2.188393	-1.461551	O	0.048708	2.490164	2.489582
H	7.757495	-3.847417	-1.256168	C	-5.663189	-1.228420	-1.932896
H	7.492745	-3.011927	-2.787227	C	-6.855068	-5.488612	0.421723
H	2.633811	1.900189	-2.715453	C	-3.082874	-2.747308	2.277670
H	3.354972	0.444259	-2.027941	B	3.299460	-0.125048	-1.024756
H	1.604711	0.567124	-2.193085	O	-1.220689	0.638474	2.493825
H	3.351156	5.746853	-0.188891	C	4.670261	-0.742802	-0.503260
H	1.771172	5.866945	0.598962	C	4.869553	-1.099564	0.830018
H	3.234662	5.748166	1.583052	C	6.032112	-1.711684	1.285714
H	2.715047	0.408141	3.472399	C	7.060384	-1.972184	0.380781
H	2.106609	1.971271	3.997152	C	6.908372	-1.624906	-0.959306
H	0.988240	0.779638	3.356742	C	5.720287	-1.028047	-1.374800
H	1.002357	-1.028307	-0.754303	F	3.893487	-0.855033	1.728983
H	-1.162347	-1.419692	-0.680919	F	5.611240	-0.698319	-2.679954
C	2.003453	-1.749142	2.056197	F	7.895664	-1.867181	-1.829889
C	-1.066914	-0.695248	1.915234	F	8.187724	-2.554154	0.798720
C	1.682143	-3.241008	1.856042	F	6.174433	-2.048404	2.572464
C	-1.306103	-1.977595	2.750519	C	2.861722	1.318194	-0.582827
C	0.286629	-3.574712	1.308863	C	3.670343	2.143338	0.231343
H	3.019730	-1.654172	2.449437	C	3.278199	3.392599	0.702377
H	1.330472	-1.314492	2.787189	C	2.020771	3.887963	0.372792
H	-1.560307	0.100181	2.501221	C	1.188767	3.133444	-0.448598
H	-0.024313	-0.394068	1.960660	C	1.615121	1.896988	-0.910035
C	-0.916663	-3.392053	2.246924	F	4.900094	1.758579	0.596850
H	2.444124	-3.682202	1.203194	F	4.097116	4.115632	1.470452
H	1.812359	-3.723358	2.835199	F	1.625364	5.070581	0.822480
H	0.105074	-3.021583	0.381184	F	-0.033853	3.585343	-0.761050
H	0.299592	-4.631941	1.012681	F	0.723025	1.257934	-1.695789
H	-0.762805	-4.021081	3.135646	C	-4.173184	1.013868	-0.257797
H	-1.773612	-3.820802	1.725203	C	-4.065166	1.903421	-1.359473
H	-0.802103	-1.803087	3.712343	C	-4.882118	3.041223	-1.405147
H	-2.373616	-2.019021	3.001921	C	-5.797824	3.358409	-0.403167

#### I<sub>4</sub>

E= -2611.7318037au

C	-4.142273	-2.898919	1.203032	C	-5.067651	1.355581	0.797671
C	-4.321067	-1.960649	0.152982	C	-3.093707	1.743539	-2.512372
C	-5.350831	-2.179234	-0.797174	C	-6.646666	4.605088	-0.479340
C	-6.157100	-3.318467	-0.680582	C	-5.192728	0.546087	2.072376
				H	-6.944643	-3.474601	-1.415341
				H	-4.828203	-4.730523	2.084564

H	-6.553038	2.727369	1.504934	C	2.838942	-2.178883	-0.319948
H	-4.792644	3.704002	-2.263461	C	4.239422	-1.975643	-0.443463
H	-6.300947	-1.720912	-2.673670	C	5.088003	-3.090119	-0.510260
H	-6.191863	-0.337429	-1.576912	H	6.158549	-2.915247	-0.597464
H	-4.767181	-0.875052	-2.449148	C	4.622871	-4.403604	-0.477123
H	-2.067444	-2.770507	1.867885	C	3.242749	-4.588867	-0.414293
H	-3.181146	-1.804804	2.826793	H	2.839826	-5.599909	-0.430357
H	-3.160635	-3.563126	3.003037	C	2.348131	-3.515717	-0.350841
H	-7.832183	-5.323978	-0.044303	C	4.918770	-0.623713	-0.539061
H	-6.385367	-6.335933	-0.095728	H	4.828471	-0.039852	0.380369
H	-7.020287	-5.795427	1.460154	H	4.513020	-0.006129	-1.344941
H	-5.856522	1.053933	2.778240	H	5.986344	-0.762780	-0.736294
H	-5.594659	-0.457434	1.898924	C	5.573154	-5.576906	-0.511506
H	-4.220559	0.425513	2.567039	H	5.150531	-6.419539	-1.070186
H	-7.621344	4.456526	-0.002013	H	5.794397	-5.939808	0.501502
H	-6.160593	5.447281	0.031233	H	6.527734	-5.306703	-0.975512
H	-6.819145	4.909925	-1.516998	C	0.871977	-3.852264	-0.341329
H	-3.167154	0.770031	-3.003862	H	0.303676	-3.216554	-1.029855
H	-3.292342	2.504920	-3.272393	H	0.418587	-3.721830	0.646212
H	-2.053510	1.880102	-2.191858	H	0.720248	-4.894583	-0.639394
H	-1.838513	0.202074	1.845769	C	2.254528	0.840203	-0.129526
H	-1.242432	2.031227	0.990571	C	2.739092	1.434607	1.060924
C	-2.077040	-1.010570	-1.395466	C	3.123859	2.781755	1.048005
C	2.474414	-1.070492	-1.987320	H	3.486877	3.228706	1.971530
C	-1.052391	-2.112364	-1.044706	C	3.061162	3.566021	-0.104952
C	2.143954	-2.480876	-1.417775	C	2.628971	2.953057	-1.283730
C	0.056037	-1.646286	-0.084409	H	2.597006	3.534935	-2.202912
H	-2.707473	-1.345475	-2.224915	C	2.216936	1.616215	-1.318508
H	-1.522736	-0.132699	-1.730322	C	2.888615	0.681245	2.364616
H	3.132723	-1.229926	-2.857757	H	3.592838	1.199638	3.023716
H	1.567012	-0.609462	-2.374820	H	3.258611	-0.337221	2.210587
C	1.338306	-2.495477	-0.101634	H	1.932305	0.607647	2.892935
H	-1.558216	-3.000901	-0.644348	C	3.403068	5.036332	-0.073278
H	-0.603003	-2.429084	-1.995215	H	3.888903	5.358754	-1.000807
H	0.314147	-0.610315	-0.327690	H	4.066322	5.278692	0.763491
H	-0.326228	-1.615480	0.942357	H	2.491081	5.636626	0.043255
H	1.091568	-3.539114	0.140815	C	1.753568	1.053457	-2.649535
H	1.983369	-2.142607	0.713688	H	1.855353	1.808436	-3.435809
H	1.603250	-3.039709	-2.192675	H	0.705786	0.734017	-2.618118
H	3.077370	-3.032076	-1.248717	H	2.336722	0.176795	-2.954898
				C	-2.918710	-0.829518	0.378911
				C	-3.065943	-2.225048	0.283831
				F	-2.033808	-3.039818	0.547821

**J**

E= -2302.8152858au

C	-4.252439	-2.847767	-0.091318
F	-4.329030	-4.179841	-0.178377
C	-5.371938	-2.068798	-0.371081
F	-6.518645	-2.647362	-0.722464
C	-5.289370	-0.681567	-0.275283
F	-6.367726	0.067373	-0.528142
C	-4.082583	-0.093193	0.086888
C	-1.251826	1.332257	0.377603
C	-0.669892	2.234899	1.277615
F	-0.425072	1.860788	2.547155
C	-0.345462	3.543131	0.935634
F	0.218489	4.368689	1.824672
C	-0.585724	3.984360	-0.361404
F	-0.242330	5.224808	-0.716038
C	-1.162946	3.125270	-1.294580
F	-1.371540	3.545040	-2.548060
C	-1.489158	1.831333	-0.910473
F	-2.010639	1.027555	-1.854773
F	-4.088571	1.245365	0.179395
B	-1.556862	-0.153287	0.794178
P	1.491510	-0.864063	-0.279897
C	-0.538873	-0.911797	1.724156
C	0.734904	-1.200631	1.383944
H	1.339983	-1.772326	2.090146
C	-1.064717	-1.327190	3.089659
H	-1.937129	-1.985711	2.996790
H	-0.298517	-1.856099	3.667021
H	-1.380853	-0.453461	3.674091

### **J<sub>1</sub>**

**E= -2303.9915418au**

C	2.853773	-2.179949	-0.308033
C	4.254670	-1.980848	-0.434977
C	5.099904	-3.097619	-0.501512
H	6.170740	-2.925864	-0.591684
C	4.630875	-4.409880	-0.464861
C	3.250517	-4.591005	-0.399187
H	2.844776	-5.600915	-0.412967
C	2.358908	-3.515091	-0.336045
C	4.936747	-0.630680	-0.535663
H	4.848799	-0.043461	0.381817
H	4.531104	-0.015086	-1.343236
H	6.003743	-0.772506	-0.734047

C	5.578222	-5.585577	-0.498160
H	6.514597	-5.332570	-1.007052
H	5.133501	-6.444680	-1.012563
H	5.838719	-5.915649	0.516772
C	0.881695	-3.847167	-0.325105
H	0.315352	-3.212015	-1.015764
H	0.428530	-3.712434	0.661988
H	0.726852	-4.889912	-0.620035
C	2.278602	0.841041	-0.113339
C	2.763801	1.430720	1.079353
C	3.147603	2.778091	1.071843
H	3.510437	3.221496	1.997152
C	3.083659	3.567275	-0.077746
C	2.653181	2.958494	-1.259230
H	2.621483	3.543834	-2.176212
C	2.242786	1.621261	-1.299593
C	2.916228	0.671761	2.379459
H	3.623843	1.186167	3.038064
H	3.283784	-0.346722	2.220010
H	1.961745	0.598041	2.911012
C	3.421688	5.038261	-0.039161
H	3.898033	5.368518	-0.968804
H	4.091715	5.276960	0.793281
H	2.508896	5.634741	0.090102
C	1.786458	1.061349	-2.633894
H	1.863535	1.826453	-3.413094
H	0.748824	0.711569	-2.599570
H	2.391999	0.203981	-2.951263
C	-2.910550	-0.815153	0.420467
C	-3.061952	-2.209927	0.322285
F	-2.026354	-3.027183	0.564156
C	-4.256322	-2.828560	-0.034087
F	-4.337459	-4.160030	-0.125350
C	-5.378881	-2.046005	-0.290827
F	-6.532882	-2.620816	-0.624020
C	-5.291757	-0.659281	-0.191216
F	-6.372810	0.092866	-0.421995
C	-4.077377	-0.074993	0.151508
C	-1.234763	1.338780	0.387529
C	-0.636468	2.243161	1.275329
F	-0.375658	1.873763	2.542704
C	-0.313448	3.549153	0.923505
F	0.265481	4.376787	1.800880

C	-0.570590	3.986055	-0.371692
F	-0.228772	5.223977	-0.735788
C	-1.165512	3.125776	-1.292774
F	-1.394653	3.542666	-2.543390
C	-1.491222	1.834970	-0.897968
F	-2.039643	1.033024	-1.830223
F	-4.077595	1.263388	0.249059
B	-1.540878	-0.143148	0.816361
P	1.510882	-0.860822	-0.268132
C	-0.518474	-0.902883	1.740005
C	0.753433	-1.195642	1.395674
H	1.357665	-1.770394	2.100110
C	-1.039589	-1.318166	3.107627
H	-1.914513	-1.973830	3.018521
H	-0.272366	-1.849837	3.681071
H	-1.350293	-0.443995	3.694435
H	-2.125768	-1.270905	-4.216625
H	-2.106538	-0.755245	-3.682627

## TS<sub>J12</sub>

E= -2303.9745912au

C	3.266201	-1.898362	-0.198671
C	4.638429	-1.542926	-0.124601
C	5.603160	-2.557799	-0.164958
H	6.651605	-2.273052	-0.104129
C	5.276739	-3.909286	-0.280164
C	3.926032	-4.236960	-0.394427
H	3.641029	-5.279345	-0.521025
C	2.918025	-3.267700	-0.373745
C	5.156431	-0.123273	-0.019247
H	4.838166	0.370395	0.902681
H	4.820276	0.507434	-0.847215
H	6.250613	-0.127852	-0.028792
C	6.345520	-4.975996	-0.276746
H	7.274382	-4.615678	-0.731941
H	6.022572	-5.868689	-0.822819
H	6.587035	-5.290719	0.747531
C	1.492466	-3.741939	-0.572705
H	0.995912	-3.198930	-1.385778
H	0.870356	-3.606284	0.316977
H	1.481838	-4.805780	-0.828083
C	2.274621	1.060747	-0.125719
C	2.517904	1.776320	1.072157
C	2.687994	3.165078	1.009574

H	2.864445	3.709406	1.934916
C	2.631060	3.872611	-0.192702
C	2.436736	3.143952	-1.369236
H	2.414482	3.670017	-2.321513
C	2.248661	1.758563	-1.361540
C	2.601217	1.125826	2.435748
H	3.140410	1.776255	3.132090
H	3.116456	0.160913	2.408136
H	1.602629	0.949818	2.848012
C	2.727164	5.379020	-0.220555
H	3.255878	5.733813	-1.112010
H	3.243853	5.767660	0.662926
H	1.722946	5.822964	-0.238079
C	2.011565	1.064659	-2.688855
H	2.205582	1.754376	-3.516184
H	0.975712	0.716190	-2.783854
H	2.657032	0.190363	-2.826570
C	-2.855607	-1.154256	0.205010
C	-2.909826	-2.540540	0.004817
F	-1.770768	-3.262123	0.016227
C	-4.088427	-3.241762	-0.224844
F	-4.074407	-4.567088	-0.415666
C	-5.295736	-2.547248	-0.253542
F	-6.441136	-3.199483	-0.466508
C	-5.299642	-1.170275	-0.054092
F	-6.457764	-0.499089	-0.071780
C	-4.095334	-0.503102	0.163588
C	-1.382944	1.171331	0.182231
C	-1.062891	2.070550	1.201611
F	-0.849709	1.628141	2.459390
C	-0.938464	3.442254	0.998729
F	-0.596532	4.256580	2.005772
C	-1.153418	3.964538	-0.271639
F	-1.003578	5.276851	-0.491370
C	-1.501094	3.113448	-1.317087
F	-1.705058	3.610105	-2.544230
C	-1.619550	1.750116	-1.068400
F	-1.941494	0.965029	-2.117388
F	-4.182380	0.824479	0.360475
B	-1.459168	-0.407260	0.438974
P	1.808742	-0.735538	-0.203118
C	-0.440156	-1.040030	1.488179
C	0.900158	-1.156507	1.326133



H	1.478377	-1.656811	2.104460
C	-1.047738	-1.553323	2.782095
H	-1.745835	-2.376673	2.589212
H	-0.277934	-1.914621	3.473271
H	-1.615068	-0.764514	3.291062
H	-0.052983	-0.881175	-1.020056
H	-0.865151	-0.887096	-0.984012

## **J<sub>2</sub>**

**E= -2304.0109466au**

C	2.513374	1.705203	-1.269249
C	2.466567	0.828739	-0.156862
C	2.926638	1.257751	1.115328
C	3.414516	2.560406	1.248548
C	3.445770	3.453761	0.175703
C	3.011656	2.996745	-1.071159
P	1.704060	-0.839743	-0.235838
C	2.858998	0.391631	2.356253
C	3.873844	4.887393	0.366932
C	2.028927	1.350796	-2.659237
C	0.540767	-1.184498	-1.547049
C	-0.802827	-1.029547	-1.404899
B	-1.531334	-0.444137	-0.052869
C	-1.148279	1.135879	0.165725
C	-0.710842	1.632702	1.394474
C	-0.281870	2.944760	1.593227
C	-0.297651	3.835059	0.526969
C	-0.742650	3.398478	-0.717895
C	-1.153725	2.078035	-0.864132
F	-0.617030	0.816914	2.473867
F	-1.526874	1.701920	-2.111988
F	-0.737376	4.243533	-1.762072
F	0.150622	5.091695	0.684777
F	0.181038	3.343209	2.790289
C	-3.131522	-0.785978	-0.000215
C	-4.192094	0.114126	-0.114682
C	-5.533373	-0.253459	0.007649
C	-5.863147	-1.583000	0.244029
C	-4.844400	-2.525882	0.351736
C	-3.522819	-2.109334	0.226247
F	-3.966512	1.424113	-0.356422
F	-6.507566	0.663425	-0.107287
F	-7.146088	-1.955090	0.358856

F	-5.146716	-3.817025	0.567737
F	-2.578542	-3.079283	0.317103
C	2.901201	-2.228652	-0.094024
C	4.202037	-2.199592	-0.652495
C	5.017283	-3.326315	-0.503292
C	4.594051	-4.474192	0.169717
C	3.299593	-4.485434	0.693611
C	2.436951	-3.391400	0.579328
C	4.766734	-1.022396	-1.417822
C	5.510903	-5.661540	0.337393
C	1.053191	-3.509721	1.183965
H	3.754878	2.890934	2.226870
H	3.039312	3.675520	-1.920284
H	2.941389	-5.375757	1.205128
H	6.014653	-3.304757	-0.936286
H	3.466644	0.827231	3.154200
H	1.828619	0.330232	2.729546
H	3.220950	-0.628138	2.186573
H	2.405566	0.384961	-3.010529
H	0.936463	1.303377	-2.703991
H	2.360707	2.110670	-3.372599
H	2.992436	5.513113	0.558948
H	4.551319	4.998313	1.219467
H	4.370671	5.284075	-0.524639
H	0.871478	-4.538849	1.505243
H	0.938515	-2.871066	2.069349
H	0.254889	-3.234872	0.487114
H	4.952784	-6.603526	0.324202
H	6.266482	-5.699806	-0.453741
H	6.043044	-5.612355	1.296658
H	4.929205	-0.150535	-0.776391
H	5.728113	-1.292871	-1.863551
H	4.109918	-0.705388	-2.234328
H	0.950184	-0.895111	0.948884
H	-1.048760	-1.048210	0.886983
H	0.987095	-1.600638	-2.449633
C	-1.647258	-1.477367	-2.573604
H	-2.278717	-2.320458	-2.268876
H	-2.325772	-0.671538	-2.875132
H	-1.054144	-1.787356	-3.442317

## **J<sub>3</sub>**

**E= -2492.5959905au**

C	2.579894	2.014722	-1.097561
C	2.500169	1.015162	-0.096818
C	2.747472	1.336608	1.262911
C	3.047804	2.660840	1.593608
C	3.095123	3.673284	0.632459
C	2.884954	3.320865	-0.703268
P	1.932076	-0.692000	-0.453547
C	-1.400573	-1.795228	3.413578
O	-2.521050	-1.544191	3.619191
C	2.653328	0.322455	2.384105
C	3.302934	5.114351	1.027136
C	2.319037	1.773945	-2.569556
C	0.856183	-0.927503	-1.864142
C	-0.497223	-0.810368	-1.793200
B	-1.316814	-0.384894	-0.439090
O	-0.269706	-2.056172	3.248742
C	-1.152769	1.216066	-0.099531
C	-1.026487	1.665372	1.217395
C	-0.806423	2.995498	1.570221
C	-0.711509	3.956733	0.570464
C	-0.845376	3.569587	-0.758466
C	-1.066999	2.227830	-1.057323
F	-1.061196	0.787612	2.251403
F	-1.134173	1.922843	-2.376698
F	-0.728315	4.484468	-1.734915
F	-0.453288	5.237998	0.882572
F	-0.655936	3.352206	2.856334
C	-2.881374	-0.871271	-0.448392
C	-3.918586	-0.195076	-1.093935
C	-5.250901	-0.601375	-1.061729
C	-5.594258	-1.751104	-0.356617
C	-4.599264	-2.471265	0.296594
C	-3.281046	-2.023651	0.233292
F	-3.651792	0.917229	-1.817455
F	-6.200715	0.094909	-1.706085
F	-6.868318	-2.164626	-0.314310
F	-4.917085	-3.587772	0.971166
F	-2.368973	-2.789010	0.884068
C	3.244208	-1.980537	-0.434283
C	4.590780	-1.747742	-0.806712
C	5.490909	-2.817322	-0.755074
C	5.110153	-4.100431	-0.357712
C	3.776066	-4.305396	-0.000316

C	2.828017	-3.278591	-0.027871
C	5.127812	-0.406753	-1.258436
C	6.101921	-5.238337	-0.344094
C	1.410474	-3.608292	0.391241
H	3.224766	2.909180	2.637373
H	2.934363	4.093204	-1.467235
H	3.455999	-5.296683	0.312074
H	6.525017	-2.637002	-1.039279
H	3.098041	0.727804	3.297170
H	1.607336	0.079907	2.612999
H	3.171344	-0.615451	2.155043
H	2.774011	0.851709	-2.943659
H	1.246054	1.710344	-2.775122
H	2.724060	2.602252	-3.158489
H	3.841813	5.201681	1.975844
H	3.856298	5.668317	0.261587
H	2.329564	5.607218	1.150701
H	1.291964	-4.690656	0.491460
H	1.151617	-3.163469	1.359960
H	0.665555	-3.258058	-0.330209
H	7.125920	-4.876616	-0.206477
H	5.880142	-5.952717	0.455512
H	6.074717	-5.792317	-1.291796
H	5.124670	0.332643	-0.451386
H	6.158827	-0.516138	-1.606359
H	4.549754	0.016016	-2.085514
H	1.134325	-0.985481	0.664473
H	-0.792119	-0.973191	0.481643
H	1.367487	-1.231966	-2.776906
C	-1.263966	-1.149549	-3.049390
H	-1.930542	-2.000075	-2.859135
H	-1.909311	-0.308914	-3.325687
H	-0.617483	-1.398032	-3.899587

### TS<sub>J34</sub>

E= -2492.5438518au

C	2.909362	2.437670	-0.584057
C	2.960737	1.305210	0.267121
C	3.686545	1.373912	1.485737
C	4.369106	2.553641	1.802832
C	4.343316	3.674956	0.974787
C	3.602217	3.592103	-0.206382
P	2.049171	-0.283804	0.003024

C	-0.760217	-0.374831	2.227085
O	-1.770526	-0.398803	2.892274
C	3.748158	0.233733	2.482242
C	5.095811	4.934136	1.331998
C	2.146321	2.491545	-1.889574
C	0.926409	-0.313173	-1.441158
C	-0.424167	-0.332820	-1.513567
B	-1.631025	-0.105906	-0.475319
O	0.475618	-0.510874	2.499925
C	-2.090591	1.427092	-0.446954
C	-1.309792	2.442034	0.110347
C	-1.674049	3.786044	0.091904
C	-2.860502	4.159646	-0.532756
C	-3.660067	3.186964	-1.128846
C	-3.263701	1.854675	-1.075929
F	-0.136975	2.140064	0.707256
F	-4.055966	0.955806	-1.693885
F	-4.791365	3.541678	-1.749973
F	-3.223311	5.444455	-0.573280
F	-0.891894	4.715520	0.653874
C	-2.652535	-1.267640	-0.144018
C	-3.827073	-1.054762	0.600687
C	-4.692148	-2.081227	0.970427
C	-4.394287	-3.393105	0.616628
C	-3.234513	-3.663004	-0.105254
C	-2.396235	-2.612396	-0.457081
F	-4.182949	0.174910	0.988932
F	-5.802745	-1.818192	1.666483
F	-5.212586	-4.386828	0.964915
F	-2.935236	-4.923230	-0.446074
F	-1.277980	-2.956511	-1.134184
C	3.228318	-1.676059	-0.327587
C	4.422355	-1.525410	-1.076395
C	5.251682	-2.638835	-1.254592
C	4.944597	-3.894227	-0.728638
C	3.746438	-4.028425	-0.024870
C	2.877997	-2.953260	0.186487
C	4.862555	-0.228128	-1.720494
C	5.878885	-5.066562	-0.907249
C	1.581903	-3.224816	0.919469
H	4.926360	2.594220	2.735836
H	3.555233	4.459150	-0.861780
H	3.469420	-5.003094	0.370367

H	6.165513	-2.516176	-1.831842
H	4.414073	0.494252	3.309902
H	2.761398	0.020707	2.909541
H	4.125918	-0.693579	2.037469
H	2.503347	1.751478	-2.614739
H	1.078798	2.308910	-1.745824
H	2.261883	3.477368	-2.349315
H	5.398960	4.934631	2.383544
H	6.005029	5.037176	0.725147
H	4.486275	5.827126	1.153667
H	1.538597	-4.272953	1.229185
H	1.459000	-2.608057	1.814660
H	0.714945	-3.040255	0.274694
H	6.504886	-4.949105	-1.797769
H	6.551704	-5.167028	-0.045162
H	5.327308	-6.008307	-0.998523
H	5.216478	0.501383	-0.985155
H	5.680384	-0.419126	-2.421661
H	4.055868	0.250096	-2.284366
H	1.217744	-0.475187	1.340248
H	-0.918867	-0.212966	1.062704
H	1.475212	-0.430116	-2.376313
C	-1.018949	-0.487320	-2.915527
H	-1.467498	-1.480775	-3.021843
H	-1.816359	0.241531	-3.101205
H	-0.259039	-0.370520	-3.695311

#### J<sub>4</sub>

E= -2492.5679332au

C	2.698806	2.793842	-0.481235
C	2.747034	1.607288	0.294442
C	3.451562	1.631191	1.529709
C	4.113832	2.795586	1.931613
C	4.086445	3.965375	1.172645
C	3.368807	3.935848	-0.022707
P	1.834245	0.002942	-0.034549
C	-0.755027	-0.799206	3.157479
O	-1.791580	-1.056537	3.713221
C	3.525382	0.436378	2.458334
C	4.775394	5.223508	1.644924
C	1.978798	2.925311	-1.806790
C	1.002825	0.021188	-1.676945
C	-0.322690	-0.103095	-1.883347

B	-1.549370	-0.122877	-0.886909
O	-0.679651	-0.001798	2.081063
C	-2.311048	1.255031	-0.704069
C	-1.711997	2.384613	-0.145440
C	-2.369880	3.605015	-0.016925
C	-3.677993	3.723718	-0.479635
C	-4.312763	2.624533	-1.055580
C	-3.626073	1.419278	-1.148504
F	-0.448792	2.316347	0.315243
F	-4.270967	0.377772	-1.710818
F	-5.566530	2.738899	-1.508520
F	-4.321644	4.888311	-0.375977
F	-1.759709	4.658257	0.537530
C	-2.175306	-1.446321	-0.337186
C	-3.181830	-1.458068	0.652398
C	-3.730066	-2.629126	1.165165
C	-3.289553	-3.859365	0.683369
C	-2.300242	-3.907197	-0.296436
C	-1.765474	-2.718809	-0.778160
F	-3.649777	-0.320962	1.168101
F	-4.676143	-2.586918	2.104004
F	-3.809829	-4.988374	1.159149
F	-1.873094	-5.088533	-0.757571
F	-0.806964	-2.842681	-1.712860
C	3.166720	-1.284418	-0.370294
C	4.353850	-1.045707	-1.107370
C	5.278634	-2.086226	-1.272500
C	5.076866	-3.361621	-0.747062
C	3.893064	-3.589067	-0.042791
C	2.938686	-2.585909	0.149843
C	4.701627	0.280796	-1.746543
C	6.082050	-4.468418	-0.960409
C	1.671999	-2.960670	0.889227
H	4.658181	2.784784	2.873929
H	3.326136	4.836293	-0.632195
H	3.700564	-4.578460	0.367353
H	6.186845	-1.886352	-1.837772
H	4.052858	0.701849	3.379261
H	2.525578	0.083077	2.742481
H	4.046527	-0.414470	2.006687
H	2.436131	2.310469	-2.590514
H	0.931219	2.630247	-1.736737
H	2.015655	3.963815	-2.149910

H	5.689930	4.994867	2.203075
H	5.043417	5.873483	0.805279
H	4.125025	5.804786	2.312310
H	1.718097	-4.001439	1.224242
H	1.504596	-2.332788	1.770409
H	0.794658	-2.859205	0.242754
H	7.069619	-4.069849	-1.214215
H	6.186518	-5.092247	-0.065652
H	5.774221	-5.130403	-1.780826
H	5.034761	1.018714	-1.009633
H	5.508972	0.146891	-2.473339
H	3.852442	0.721153	-2.274966
H	0.218984	-0.027237	1.658584
H	0.224833	-1.194253	3.488608
H	1.651389	0.029208	-2.553763
C	-0.834360	-0.171020	-3.322414
H	-1.376395	-1.106357	-3.506135
H	-1.528513	0.651272	-3.538907
H	-0.006669	-0.115487	-4.037262

## K

E= -2494.5525787au

C	-1.835375	2.483823	-0.581159
C	-2.740181	3.306971	0.139290
C	-2.911866	4.640292	-0.249944
H	-3.605589	5.261173	0.314081
C	-2.226311	5.199498	-1.330491
C	-1.332656	4.382725	-2.021817
H	-0.775274	4.796971	-2.859647
C	-1.120037	3.043333	-1.671405
C	-3.553835	2.824689	1.320258
H	-2.946576	2.286226	2.053309
H	-4.353664	2.143745	1.012182
H	-4.014713	3.674175	1.834091
C	-2.460721	6.633013	-1.744897
H	-2.622603	7.280448	-0.875837
H	-3.350227	6.721225	-2.383216
H	-1.612090	7.030277	-2.311495
C	-0.083244	2.276332	-2.467898
H	-0.397631	1.257411	-2.708797
H	0.851735	2.195424	-1.902213
H	0.143297	2.800380	-3.402112
C	-3.161857	-0.097814	0.171614

C	-3.568625	-0.699783	1.390981
C	-4.806168	-1.355748	1.450018
H	-5.105834	-1.804891	2.394834
C	-5.666800	-1.449765	0.356940
C	-5.248210	-0.867051	-0.839519
H	-5.891283	-0.929799	-1.715486
C	-4.018729	-0.212209	-0.959421
C	-2.761876	-0.674382	2.673621
H	-3.270088	-1.262405	3.444284
H	-2.647850	0.340809	3.069604
H	-1.757842	-1.088201	2.554371
C	-6.983358	-2.183832	0.453051
H	-7.337789	-2.237098	1.487857
H	-6.892113	-3.214962	0.085704
H	-7.759577	-1.695700	-0.146912
C	-3.659908	0.351154	-2.319174
H	-4.375422	0.009685	-3.073529
H	-2.659643	0.033328	-2.639013
H	-3.661454	1.446781	-2.328651
C	2.760190	-0.210359	-0.292289
C	3.197371	1.120814	-0.396118
F	2.391463	2.130517	-0.028519
C	4.437240	1.482065	-0.912294
F	4.792411	2.767757	-1.008005
C	5.315557	0.486077	-1.331920
F	6.511944	0.810916	-1.820044
C	4.937773	-0.851582	-1.242110
F	5.783931	-1.809396	-1.636104
C	3.682049	-1.173467	-0.738256
C	0.649548	-1.923120	-0.130903
C	0.070891	-2.805184	0.786522
F	0.159826	-2.556747	2.110004
C	-0.586131	-3.973359	0.410457
F	-1.109801	-4.792431	1.329374
C	-0.687032	-4.287251	-0.941830
F	-1.315720	-5.399171	-1.326326
C	-0.126345	-3.437589	-1.895955
F	-0.231973	-3.737493	-3.195682
C	0.535517	-2.290451	-1.478591
F	1.045327	-1.491289	-2.432122
F	3.393692	-2.482802	-0.660996
B	1.357053	-0.588723	0.316157
P	-1.495343	0.671483	-0.206326

C	0.732991	0.324172	1.442927
C	-0.509163	0.855194	1.344727
H	-0.861186	1.506297	2.144371
C	1.589590	0.655392	2.620488
C	2.326551	-0.350586	3.270512
C	1.692900	1.972808	3.100621
C	3.125598	-0.052654	4.374267
H	2.241097	-1.379874	2.933493
C	2.494373	2.270585	4.201953
H	1.159484	2.767576	2.587392
C	3.213193	1.259250	4.843817
H	3.676525	-0.847607	4.869978
H	2.564795	3.296492	4.553941
H	3.839070	1.492729	5.700873

### **K<sub>1</sub>**

**E= -2495.7329386au**

C	-0.670962	2.978729	0.145937
C	-1.299901	3.887675	1.043342
C	-1.183564	5.259790	0.817157
H	-1.670422	5.942966	1.510237
C	-0.467555	5.783374	-0.264469
C	0.122238	4.880039	-1.141957
H	0.671551	5.256484	-2.002890
C	0.035733	3.490313	-0.966432
C	-2.105239	3.452185	2.247892
H	-1.469685	3.027567	3.033511
H	-2.859834	2.704281	1.989517
H	-2.623808	4.310191	2.685644
C	-0.336339	7.274790	-0.459174
H	0.019980	7.517958	-1.465075
H	0.376774	7.704185	0.256709
H	-1.294002	7.785041	-0.304479
C	0.700837	2.651841	-2.036944
H	0.635722	1.579962	-1.859899
H	1.760632	2.916126	-2.118418
H	0.243402	2.855091	-3.012865
C	-2.567049	0.654358	0.327442
C	-3.325354	0.072423	1.380842
C	-4.651309	-0.307397	1.131025
H	-5.222358	-0.742798	1.948043
C	-5.263404	-0.155832	-0.112065
C	-4.500973	0.402397	-1.137181

H	-4.945863	0.530833	-2.121604
C	-3.173590	0.800183	-0.950233
C	-2.817106	-0.185371	2.785817
H	-3.625244	-0.597173	3.397808
H	-2.469032	0.726085	3.279778
H	-1.992810	-0.902175	2.798941
C	-6.684199	-0.608573	-0.347963
H	-7.268698	-0.593067	0.577810
H	-6.711099	-1.636324	-0.733980
H	-7.190754	0.026621	-1.082569
C	-2.453352	1.370501	-2.151790
H	-3.076951	1.274261	-3.045444
H	-1.514142	0.848112	-2.355441
H	-2.221630	2.432180	-2.021759
C	2.122118	-0.325534	-0.510417
C	2.843743	0.865556	-0.370181
F	2.313908	1.898868	0.315037
C	4.098238	1.087176	-0.930360
F	4.708195	2.272823	-0.789382
C	4.718193	0.066304	-1.643275
F	5.926170	0.254779	-2.183464
C	4.065828	-1.154126	-1.781408
F	4.658827	-2.157317	-2.442343
C	2.803478	-1.325822	-1.217158
C	-0.223191	-1.759512	-0.339553
C	-0.866786	-2.712193	0.454620
F	-0.691616	-2.723146	1.793461
C	-1.715458	-3.694135	-0.056725
F	-2.298665	-4.583386	0.758336
C	-1.956417	-3.746543	-1.424567
F	-2.769313	-4.677719	-1.934158
C	-1.348174	-2.811851	-2.260317
F	-1.582222	-2.844209	-3.580499
C	-0.507015	-1.856626	-1.706400
F	0.040591	-0.961333	-2.563636
F	2.271426	-2.559056	-1.350609
B	0.708191	-0.577141	0.230989
P	-0.758760	1.137450	0.471561
C	0.771098	-0.287655	1.823915
C	-0.052489	0.752111	2.094190
H	-0.232536	1.227110	3.052981
C	1.633768	-0.990636	2.793731
C	2.296698	-2.173343	2.417484

C	1.831917	-0.509501	4.102027
C	3.114860	-2.855602	3.316601
H	2.166825	-2.566376	1.413706
C	2.651668	-1.187575	4.999706
H	1.349835	0.412040	4.415400
C	3.295522	-2.366129	4.611165
H	3.612945	-3.769518	3.004470
H	2.792840	-0.795366	6.003435
H	3.936214	-2.894987	5.311636
H	0.018124	-1.058953	-5.889763
H	-0.170295	-1.273881	-5.204430

### TS<sub>K12</sub>

E= -2495.7079755au

C	3.170009	-2.121578	-0.550345
C	4.558486	-2.029719	-0.272283
C	5.358108	-3.167162	-0.445117
H	6.420590	-3.087230	-0.225235
C	4.851343	-4.389542	-0.886223
C	3.492104	-4.449765	-1.195103
H	3.073802	-5.379647	-1.574784
C	2.645933	-3.345944	-1.054480
C	5.263865	-0.771209	0.188409
H	4.903048	-0.421115	1.158973
H	5.139482	0.058063	-0.513880
H	6.336290	-0.964193	0.287664
C	5.739364	-5.603277	-1.020193
H	5.412303	-6.251271	-1.840578
H	5.723056	-6.207944	-0.103372
H	6.781082	-5.320133	-1.204192
C	1.203184	-3.513360	-1.487286
H	0.916190	-2.758976	-2.229524
H	0.492579	-3.421348	-0.660473
H	1.057605	-4.498103	-1.941119
C	2.625715	0.908028	-0.010425
C	2.823717	1.381807	1.309968
C	3.181774	2.722225	1.497670
H	3.318476	3.086153	2.513683
C	3.356996	3.607520	0.432275
C	3.214513	3.105713	-0.864173
H	3.376323	3.768995	-1.711313
C	2.845910	1.779523	-1.108392
C	2.666239	0.524428	2.546588

H	3.229055	0.958736	3.379303
H	3.023394	-0.498387	2.396686
H	1.616999	0.462080	2.850166
C	3.635638	5.071373	0.672533
H	4.138902	5.235527	1.630907
H	2.692985	5.634051	0.694447
H	4.255955	5.501564	-0.121002
C	2.687501	1.333774	-2.548532
H	3.063264	2.105088	-3.227878
H	1.636587	1.150029	-2.803874
H	3.234179	0.408276	-2.761704
C	-2.763015	-0.467039	-0.487450
C	-3.002948	-1.783795	-0.900036
F	-1.983921	-2.665729	-0.954223
C	-4.253032	-2.251947	-1.289709
F	-4.419492	-3.520688	-1.685621
C	-5.341461	-1.383297	-1.265734
F	-6.552566	-1.813539	-1.630602
C	-5.158488	-0.066030	-0.856534
F	-6.202526	0.772388	-0.821163
C	-3.887726	0.365871	-0.482648
C	-0.956776	1.573889	-0.121111
C	-0.525460	2.316449	0.979676
F	-0.423852	1.741417	2.196688
C	-0.181256	3.663827	0.906452
F	0.266062	4.318158	1.987450
C	-0.276834	4.327621	-0.310508
F	0.083024	5.613962	-0.401821
C	-0.725484	3.640182	-1.435203
F	-0.815858	4.271139	-2.613412
C	-1.059007	2.295237	-1.316325
F	-1.466544	1.668562	-2.438799
F	-3.790151	1.646514	-0.076954
B	-1.297099	0.008303	-0.049601
P	1.914587	-0.752330	-0.429860
C	-0.521786	-0.933841	0.987905
C	0.796046	-1.262683	0.917761
H	1.198926	-1.977393	1.634616
C	-1.334333	-1.571041	2.071402
C	-2.239129	-0.812758	2.835572
C	-1.228544	-2.946227	2.344667
C	-2.993690	-1.404218	3.848386
H	-2.329275	0.253548	2.655677

C	-1.988375	-3.539554	3.352315
H	-0.561266	-3.558311	1.744684
C	-2.873127	-2.770344	4.110665
H	-3.677015	-0.794844	4.434086
H	-1.895839	-4.606536	3.538077
H	-3.466803	-3.232167	4.894957
H	0.196795	-0.492218	-1.399793
H	-0.624416	-0.397318	-1.419820

## **K<sub>2</sub>**

**E= -2495.7387255 au**

C	-1.668821	3.175157	0.278661
C	-2.174981	2.047372	-0.411493
C	-2.823099	2.205880	-1.666183
C	-2.975692	3.493261	-2.184906
C	-2.505098	4.625465	-1.515286
C	-1.855951	4.438427	-0.294828
P	-2.023452	0.322725	0.206025
C	-3.331164	1.045739	-2.497638
C	-2.708812	6.007383	-2.087021
C	-0.888501	3.118087	1.572671
C	-0.931002	-0.098489	1.563313
C	0.404846	-0.285322	1.405229
B	1.122331	0.033374	-0.042032
C	2.663072	0.560837	0.082180
C	3.000490	1.911758	-0.013759
C	4.309638	2.386828	0.050459
C	5.354573	1.483622	0.218784
C	5.071715	0.124940	0.327421
C	3.747255	-0.301755	0.261384
F	2.036444	2.850955	-0.164001
F	3.534243	-1.628047	0.392324
F	6.072751	-0.752207	0.500977
F	6.620803	1.918892	0.284363
F	4.572033	3.700822	-0.047695
C	1.044068	-1.212432	-1.116506
C	1.321744	-0.947716	-2.463812
C	1.290850	-1.913341	-3.467512
C	0.964124	-3.227150	-3.141845
C	0.673532	-3.543493	-1.819823
C	0.728528	-2.543155	-0.849768
F	1.637860	0.305355	-2.848786
F	1.565057	-1.592461	-4.741972

F	0.918388	-4.170813	-4.092614
F	0.337243	-4.801792	-1.489794
F	0.412183	-2.934808	0.410942
C	-3.665808	-0.404759	0.614373
C	-4.628111	0.308418	1.370029
C	-5.848363	-0.311200	1.657866
C	-6.148305	-1.606704	1.231951
C	-5.170005	-2.302053	0.518216
C	-3.930333	-1.737529	0.202366
C	-4.404429	1.706363	1.905361
C	-7.489140	-2.233375	1.528039
C	-2.929320	-2.597105	-0.541331
H	-3.470955	3.610769	-3.145970
H	-1.465902	5.304749	0.234035
H	-5.368938	-3.323643	0.203136
H	-6.583243	0.237847	2.242228
H	-3.889784	1.417881	-3.360602
H	-2.503494	0.439003	-2.888416
H	-3.996877	0.380132	-1.938023
H	-1.285145	2.403193	2.296176
H	0.149214	2.833873	1.370039
H	-0.878924	4.105460	2.043774
H	-2.677862	5.995667	-3.181483
H	-3.685695	6.414055	-1.793025
H	-1.943463	6.703975	-1.730839
H	-3.319283	-3.611920	-0.657152
H	-2.721493	-2.217773	-1.549994
H	-1.972932	-2.674533	-0.014333
H	-7.413973	-3.322690	1.607037
H	-7.913634	-1.850614	2.461895
H	-8.208743	-2.013177	0.728314
H	-4.435209	2.461396	1.113098
H	-5.179899	1.956747	2.634844
H	-3.439297	1.807698	2.412805
H	-1.612247	-0.393021	-0.930579
H	0.466116	0.929788	-0.541195
H	-1.452145	-0.285021	2.501332
C	1.120659	-0.751744	2.628998
C	2.161063	0.007102	3.193286
C	0.728857	-1.933302	3.283465
C	2.780259	-0.399409	4.375400
H	2.470342	0.930797	2.717471
C	1.364054	-2.348781	4.453250

H	-0.059270	-2.540642	2.851055
C	2.390387	-1.581578	5.007037
H	3.573798	0.209737	4.800379
H	1.055619	-3.274905	4.931538
H	2.883724	-1.903103	5.920370

### **K<sub>3</sub>**

**E= -2684.3246198 au**

C	-2.978734	1.566152	1.398029
C	-2.844981	0.782340	0.226709
C	-3.326478	1.261499	-1.019743
C	-3.916237	2.527402	-1.065874
C	-4.030925	3.335267	0.068090
C	-3.578815	2.824173	1.287140
P	-1.952858	-0.820703	0.202620
C	1.281779	-0.877159	-4.053006
O	2.331277	-0.384602	-4.186841
C	-3.190548	0.487462	-2.314998
C	-4.566169	4.742070	-0.029572
C	-2.473472	1.150429	2.762723
C	-0.696583	-1.148606	1.439414
C	0.626982	-0.892447	1.240302
B	1.225048	-0.109501	-0.079886
O	0.225172	-1.374500	-3.957751
C	0.685135	1.442166	-0.139325
C	0.281875	2.029073	-1.340791
C	-0.238589	3.317729	-1.443544
C	-0.363408	4.092942	-0.296673
C	0.035086	3.564803	0.926929
C	0.549258	2.272350	0.974910
F	0.319995	1.322900	-2.500413
F	0.867566	1.808773	2.207070
F	-0.113279	4.290933	2.047014
F	-0.902764	5.321306	-0.363135
F	-0.649746	3.803624	-2.626127
C	2.845980	-0.208853	-0.271050
C	3.778493	0.653843	0.309563
C	5.151195	0.579532	0.078577
C	5.650374	-0.406813	-0.765802
C	4.767585	-1.302705	-1.360284
C	3.405162	-1.184794	-1.099285
F	3.372926	1.627810	1.151547
F	5.994711	1.443908	0.664430



F	6.967335	-0.498606	-0.997189
F	5.236129	-2.270036	-2.165692
F	2.609056	-2.116447	-1.687048
C	-3.041956	-2.293094	0.024402
C	-4.340114	-2.384984	0.586208
C	-5.074510	-3.556729	0.379504
C	-4.576304	-4.635724	-0.354159
C	-3.287034	-4.529535	-0.877867
C	-2.501428	-3.385240	-0.708119
C	-4.986780	-1.295849	1.414545
C	-5.411825	-5.871287	-0.584707
C	-1.115756	-3.380527	-1.317820
H	-4.274007	2.899930	-2.022682
H	-3.672722	3.433428	2.183004
H	-2.869698	-5.364653	-1.435377
H	-6.068696	-3.627085	0.814647
H	-3.808330	0.944214	-3.093025
H	-2.154283	0.497171	-2.677534
H	-3.502809	-0.558259	-2.219539
H	-2.671739	0.100617	2.996326
H	-1.392073	1.298928	2.841823
H	-2.950857	1.756583	3.538319
H	-5.085265	5.042968	0.886328
H	-3.734078	5.441796	-0.182333
H	-5.254929	4.857074	-0.872508
H	-0.858656	-4.384011	-1.667820
H	-1.042502	-2.710270	-2.182726
H	-0.344023	-3.070577	-0.606336
H	-4.785914	-6.760090	-0.713616
H	-6.098277	-6.053036	0.248743
H	-6.021281	-5.766670	-1.492161
H	-5.196775	-0.396915	0.827264
H	-5.934208	-1.654111	1.826852
H	-4.361527	-0.992245	2.260211
H	-1.245293	-0.761901	-1.009731
H	0.739445	-0.669960	-1.041402
H	-1.050645	-1.704968	2.305608
C	1.524391	-1.444065	2.299714
C	1.443189	-1.001613	3.629467
C	2.449013	-2.454351	1.982844
C	2.268158	-1.548511	4.613843
H	0.749527	-0.206939	3.885081
C	3.256415	-3.013635	2.972377

H	2.516168	-2.815732	0.961581
C	3.174237	-2.559215	4.290751
H	2.200951	-1.181787	5.634928
H	3.955507	-3.803588	2.710350
H	3.813690	-2.987500	5.057936

### TS<sub>K34</sub>

E= -2684.2736413au

C	3.016871	2.465807	-0.637465
C	3.115839	1.416501	0.307909
C	3.921851	1.586370	1.467747
C	4.630139	2.779182	1.631446
C	4.556736	3.823087	0.706589
C	3.742736	3.642305	-0.410664
P	2.181886	-0.181190	0.247098
C	-0.491243	-0.040724	2.599779
O	-1.472447	0.024773	3.304933
C	4.044341	0.537748	2.555253
C	5.331913	5.101405	0.917568
C	2.170860	2.417017	-1.891294
C	0.991274	-0.325034	-1.133542
C	-0.363808	-0.323667	-1.150334
B	-1.518238	-0.032004	-0.054757
O	0.753905	-0.152617	2.839197
C	-2.017407	1.490448	-0.042485
C	-1.193923	2.540687	0.371193
C	-1.588395	3.876271	0.366575
C	-2.858410	4.206426	-0.095654
C	-3.709279	3.198447	-0.544378
C	-3.279756	1.875801	-0.510533
F	0.055222	2.284124	0.815507
F	-4.129210	0.949865	-0.989692
F	-4.924401	3.511221	-1.010393
F	-3.255008	5.481248	-0.121402
F	-0.757664	4.836828	0.788872
C	-2.472093	-1.197564	0.441495
C	-3.605180	-0.974814	1.247490
C	-4.411113	-2.001358	1.733385
C	-4.089320	-3.324408	1.451049
C	-2.959937	-3.604256	0.687361
C	-2.181895	-2.553387	0.217827
F	-3.981927	0.261473	1.591585
F	-5.486653	-1.725269	2.478378

F	-4.849326	-4.317590	1.914634
F	-2.624020	-4.874649	0.426634
F	-1.073952	-2.912862	-0.465408
C	3.334676	-1.608660	-0.017940
C	4.462926	-1.544685	-0.873887
C	5.284496	-2.671394	-0.992945
C	5.031750	-3.858938	-0.305078
C	3.896101	-3.911511	0.505045
C	3.037966	-2.818929	0.664236
C	4.837715	-0.327375	-1.691437
C	5.958673	-5.044388	-0.425609
C	1.808048	-3.007468	1.526137
H	5.248775	2.896636	2.518473
H	3.662310	4.445820	-1.138913
H	3.660530	-4.835140	1.028834
H	6.147656	-2.615019	-1.652560
H	4.747060	0.875011	3.322478
H	3.082848	0.355693	3.049326
H	4.411477	-0.421548	2.173572
H	2.457805	1.600762	-2.563061
H	1.111477	2.283575	-1.660683
H	2.279773	3.350464	-2.450942
H	5.108362	5.838767	0.140652
H	5.095377	5.552650	1.888581
H	6.413582	4.917091	0.903903
H	1.797117	-4.016992	1.947032
H	1.752909	-2.300001	2.358837
H	0.890391	-2.890728	0.938537
H	5.410708	-5.990234	-0.358718
H	6.505235	-5.031958	-1.374222
H	6.703651	-5.043325	0.381226
H	5.226261	0.485100	-1.069626
H	5.610489	-0.590559	-2.419697
H	3.987508	0.074393	-2.251532
H	1.431226	-0.240291	1.643193
H	-0.697058	-0.019347	1.431731
H	1.491513	-0.529253	-2.079570
C	-0.958984	-0.609545	-2.511602
C	-1.784368	0.318468	-3.168573
C	-0.658306	-1.814912	-3.172263
C	-2.290111	0.051233	-4.441576
H	-2.003881	1.271260	-2.702395
C	-1.171113	-2.083148	-4.440516

H	-0.030752	-2.547980	-2.677572
C	-1.991852	-1.152254	-5.080656
H	-2.917383	0.790156	-4.932816
H	-0.929199	-3.024063	-4.927706
H	-2.392591	-1.362505	-6.068446

#### **K<sub>4</sub>**

**E= -2684.3051123 au**

C	-2.083816	3.092164	0.350603
C	-2.434030	1.912987	-0.357552
C	-3.220259	2.034794	-1.537191
C	-3.644197	3.299878	-1.959861
C	-3.305561	4.466614	-1.276760
C	-2.527495	4.331806	-0.126833
P	-1.838773	0.165206	-0.005777
C	0.158869	0.502905	-3.571582
O	0.601893	0.456791	-4.687969
C	-3.650684	0.848345	-2.376174
C	-3.737160	5.824802	-1.775960
C	-1.269739	3.121457	1.626977
C	-0.898594	0.073500	1.572394
C	0.419571	-0.221646	1.654526
B	1.425177	-0.413824	0.447606
O	-0.341221	-0.580596	-2.939024
C	2.459731	0.765050	0.194447
C	2.089135	2.012111	-0.302052
C	2.991745	3.052844	-0.497784
C	4.332932	2.852885	-0.177854
C	4.750948	1.618673	0.316514
C	3.816282	0.601096	0.480557
F	0.800737	2.230952	-0.651702
F	4.257507	-0.583863	0.947694
F	6.038098	1.423874	0.621927
F	5.215898	3.839049	-0.347972
F	2.587687	4.229392	-0.987516
C	1.576580	-1.731571	-0.374296
C	2.241651	-1.774228	-1.617203
C	2.399470	-2.939182	-2.357999
C	1.894705	-4.137513	-1.857604
C	1.230786	-4.155230	-0.632261
C	1.078104	-2.969224	0.074317
F	2.727972	-0.654730	-2.167602
F	3.025594	-2.922701	-3.535092

F	2.041959	-5.263580	-2.549770
F	0.740945	-5.304146	-0.155391
F	0.425302	-3.055536	1.244491
C	-3.382910	-0.805507	0.457359
C	-4.418141	-0.310113	1.291598
C	-5.533819	-1.116579	1.550163
C	-5.673624	-2.398019	1.017369
C	-4.636906	-2.880863	0.218080
C	-3.499695	-2.118563	-0.069601
C	-4.401946	1.056343	1.940587
C	-6.906598	-3.227797	1.285189
C	-2.418493	-2.772289	-0.903279
H	-4.253576	3.368333	-2.858541
H	-2.253460	5.225818	0.429605
H	-4.707144	-3.886078	-0.192186
H	-6.317593	-0.724912	2.195512
H	-4.171308	1.190858	-3.275235
H	-2.799560	0.241933	-2.705742
H	-4.327425	0.181130	-1.832062
H	-1.779200	2.610140	2.451592
H	-0.292352	2.652041	1.507806
H	-1.107369	4.156857	1.941740
H	-3.914944	6.519011	-0.947330
H	-2.965953	6.274436	-2.415683
H	-4.655148	5.760600	-2.369603
H	-2.755430	-3.748922	-1.264268
H	-2.127788	-2.177833	-1.774446
H	-1.519139	-2.938581	-0.302387
H	-6.668880	-4.296037	1.331635
H	-7.384089	-2.943447	2.228729
H	-7.652042	-3.095951	0.489409
H	-4.596357	1.856253	1.219102
H	-5.170858	1.112293	2.717390
H	-3.442084	1.280217	2.413098
H	-0.677706	-0.336618	-2.039983
H	0.121631	1.422794	-2.961105
H	-1.458832	0.179748	2.500679
C	1.082057	-0.263073	2.997714
C	0.731219	0.648249	4.011297
C	2.094196	-1.200666	3.274453
C	1.352950	0.609469	5.257813
H	-0.020413	1.405354	3.811438
C	2.717339	-1.238181	4.521705

H	2.383141	-1.925089	2.520374
C	2.348352	-0.335100	5.519276
H	1.066078	1.325367	6.023540
H	3.489900	-1.977767	4.713192
H	2.835228	-0.362622	6.490153

## L

E= -2551.119303au

C	-2.53697300	2.68662000	-0.37170800
C	-2.52208200	1.46666300	-1.09343300
C	-3.04141700	1.47136900	-2.42328400
C	-3.57421500	2.64604800	-2.96136100
C	-3.59616300	3.84935600	-2.25612000
C	-3.07094600	3.83879400	-0.96674200
P	-1.74404400	-0.18710300	-0.64528000
C	-3.04627400	0.24813600	-3.31756500
C	-4.14249600	5.11280800	-2.87703700
C	-2.01160500	2.85885300	1.03543600
C	-0.76101700	-0.14938400	1.03594800
C	0.49118100	-0.98016200	0.71595200
B	1.97146900	-0.44927100	0.51003900
C	2.35639800	1.09668400	0.69411100
C	1.79501000	2.13639700	-0.04790700
C	2.19357000	3.46582300	0.08451200
C	3.20084100	3.78995100	0.98959200
C	3.79451500	2.78504300	1.74995100
C	3.36398400	1.47137400	1.58599300
F	0.80835600	1.88339000	-0.92799600
F	3.96511600	0.52667500	2.34178500
F	4.76213200	3.09118000	2.62466500
F	3.59271100	5.06016400	1.13271500
F	1.61246200	4.43146300	-0.63904700
C	2.98438000	-1.33113700	-0.37094000
C	3.18135700	-1.00072200	-1.71501800
C	4.03886100	-1.69990800	-2.55954400
C	4.74182900	-2.79500000	-2.06185200
C	4.57564900	-3.16783800	-0.73187600
C	3.71224600	-2.43263200	0.07799400
F	2.51893800	0.04704400	-2.24113800
F	4.19029100	-1.33681700	-3.83942000
F	5.56789100	-3.48343900	-2.85671900
F	5.24402500	-4.22084400	-0.24213500
F	3.59811000	-2.85700100	1.36497000

C	-3.19398000	-1.35345000	-0.37001300
C	-4.39263400	-1.04541700	0.32596100
C	-5.41464400	-2.00063200	0.39304100
C	-5.30524400	-3.26005700	-0.19730100
C	-4.11988900	-3.55675000	-0.87087500
C	-3.07081600	-2.63522000	-0.97555500
C	-4.63294600	0.26901100	1.03025500
C	-6.43871900	-4.25609500	-0.13103000
C	-1.83806800	-3.08197200	-1.74008900
H	-0.44620400	0.88706400	1.14942300
H	-3.97497800	2.61650700	-3.97272900
H	-3.07638200	4.76089400	-0.38890400
H	-4.00557700	-4.53360600	-1.33665900
H	-6.32491800	-1.74884900	0.93371800
H	-3.41833400	0.50976200	-4.31293900
H	-2.03792000	-0.16699300	-3.43318300
H	-3.68159400	-0.55406700	-2.92622200
H	-2.32866300	2.05584800	1.70297600
H	-0.91558500	2.90480500	1.05328200
H	-2.37318600	3.80057900	1.46006700
H	-3.41633900	5.56188100	-3.56778100
H	-5.05447100	4.91605900	-3.45228600
H	-4.37740700	5.86419800	-2.11591900
H	-2.02070700	-4.04986600	-2.21788800
H	-1.54827900	-2.36532200	-2.51329000
H	-0.96518000	-3.20440600	-1.08740000
H	-6.07035000	-5.28698400	-0.16759300
H	-7.02515600	-4.13557000	0.78619300
H	-7.12837600	-4.12754600	-0.97620000
H	-4.67018600	1.10842800	0.33033900
H	-5.58146000	0.24022700	1.57546700
H	-3.84282100	0.48267800	1.75625100
H	0.26861900	-1.96552500	0.31139300
N	1.47248500	-1.14174400	1.86444500
C	-1.39486100	-0.59926600	2.34243600
C	-1.36328200	0.25144200	3.46178000
C	-1.90774700	-1.89612600	2.52213500
C	-1.85618900	-0.16002000	4.70346400
H	-0.94756800	1.25130000	3.36192300
C	-2.40051800	-2.30843500	3.75973500
H	-1.93300000	-2.58743600	1.68658000
C	-2.38218600	-1.44212600	4.85603300
H	-1.82212800	0.52277200	5.54842100

H	-2.80013400	-3.31337900	3.86750600
H	-2.76728900	-1.76710400	5.81861700
H	1.77486700	-2.08044800	2.10625600
H	1.27686900	-0.57926700	2.68887100

## L1

E= -2552.274441au

C	2.52123200	-0.92998200	-1.25533200
C	3.88301700	-0.54979200	-1.12423800
C	4.85472700	-1.21488800	-1.88235600
H	5.89445200	-0.91396400	-1.77000000
C	4.53944800	-2.24381900	-2.77050700
C	3.19641400	-2.60005500	-2.89683100
H	2.92108900	-3.39058500	-3.59209900
C	2.18368600	-1.96846800	-2.16521200
C	4.36220800	0.54967700	-0.20400300
H	3.92742500	0.46270200	0.79415600
H	4.10637300	1.54222200	-0.58879100
H	5.45021900	0.50269800	-0.09464800
C	5.61512300	-2.96129500	-3.55118800
H	5.98104700	-3.84094100	-3.00450900
H	6.47756200	-2.31217100	-3.73610000
H	5.24050000	-3.31431500	-4.51801400
C	0.76298500	-2.44217600	-2.39789000
H	0.72193300	-3.09292200	-3.27715600
H	0.07028700	-1.61043800	-2.55550900
H	0.38124000	-3.01711500	-1.54856900
C	1.41987200	1.72513700	-0.46992400
C	1.69235000	2.65546000	0.56127800
C	1.79875300	4.01973000	0.25629900
H	2.01538600	4.71280500	1.06670800
C	1.64291500	4.51551900	-1.03607800
C	1.35147900	3.59311200	-2.04244300
H	1.20575600	3.94838400	-3.06057800
C	1.22250100	2.22325900	-1.79314500
C	1.87313600	2.26895600	2.00744500
H	2.35177500	3.08050000	2.56464500
H	2.49084400	1.37879000	2.12288400
H	0.91194300	2.07147200	2.49620600
C	1.79746400	5.98604300	-1.34253100
H	1.66913400	6.59831600	-0.44400000
H	1.06621500	6.31898900	-2.08761500

H	2.79429900	6.20422600	-1.74881700
C	0.85243700	1.34486700	-2.97107600
H	0.68694600	1.96001000	-3.86075600
H	-0.06925900	0.78512000	-2.77865000
H	1.63342500	0.61633200	-3.21124500
C	-2.43153800	-1.58206600	0.43298700
C	-2.05146500	-2.91442700	0.22191500
F	-0.77215200	-3.30654400	0.43714700
C	-2.90660100	-3.91868600	-0.21574400
F	-2.45537600	-5.16292900	-0.41360600
C	-4.24760600	-3.61904200	-0.43603400
F	-5.09157600	-4.56606100	-0.84594500
C	-4.69719700	-2.32175100	-0.21508200
F	-5.98695900	-2.02377100	-0.40456700
C	-3.80024300	-1.34355400	0.20723100
C	-1.84652400	1.06558400	0.61110100
C	-1.85981700	2.10659700	1.54762700
F	-1.57341100	1.87336100	2.84664800
C	-2.17824600	3.42483700	1.22725100
F	-2.17501600	4.37381300	2.17129100
C	-2.50343900	3.75137900	-0.08422000
F	-2.80305800	5.00994700	-0.41205500
C	-2.51376300	2.75137100	-1.05447100
F	-2.82343700	3.05409600	-2.32219200
C	-2.20810200	1.44838400	-0.68892400
F	-2.24014600	0.52522700	-1.67258200
F	-4.33688400	-0.13095500	0.42046500
C	-0.28785800	-0.73386400	2.03363800
H	-0.17915900	0.18896900	2.60523700
C	1.08969900	-1.04655400	1.37001200
H	0.96280300	-2.02537300	0.89322800
B	-1.45171900	-0.43694600	0.94936800
P	1.11014400	-0.12135000	-0.32254000
H	-4.07432700	0.80222800	-4.44975600
H	-3.69698200	1.04901600	-3.85982900
N	-0.75005700	-1.74193900	3.00576600
H	-0.73503100	-2.66558900	2.57937100
H	-0.10607800	-1.78509800	3.79465300
C	2.26564600	-1.22095700	2.31708200
C	3.30286700	-2.10248700	1.96264400
C	2.32973400	-0.62112300	3.58635200
C	4.37795800	-2.34080800	2.81779800
H	3.26390000	-2.60547600	1.00076700

C	3.40050300	-0.86520600	4.44992500
H	1.53749400	0.04459700	3.91432300
C	4.43374500	-1.72053800	4.06789000
H	5.16703300	-3.02228000	2.51063100
H	3.41986700	-0.38698300	5.42580400
H	5.26584200	-1.91147200	4.74003500

## TS12L

E= -2552.246582au

C	2.99937400	-1.15220900	-1.01753200
C	4.28580600	-1.03786600	-0.42843200
C	5.36008400	-1.73741300	-0.99188400
H	6.33998100	-1.64099900	-0.52865500
C	5.21828500	-2.56100400	-2.10940300
C	3.94478400	-2.67947100	-2.66744300
H	3.80327300	-3.32123700	-3.53461200
C	2.83964000	-1.98946100	-2.15592400
C	4.56881300	-0.21670300	0.80812300
H	3.92852000	-0.52046300	1.64193300
H	4.40721100	0.85184900	0.64133000
H	5.60711500	-0.35507100	1.12487900
C	6.40478100	-3.27976900	-2.70627400
H	7.13956100	-3.54659100	-1.93896800
H	6.91986400	-2.64806300	-3.44246900
H	6.10107700	-4.19719300	-3.22149300
C	1.51241100	-2.18490500	-2.86373900
H	1.09278300	-1.23659100	-3.21586000
H	0.75369400	-2.64884700	-2.22131600
H	1.64059700	-2.84011400	-3.73097800
C	1.95787300	1.50120100	-0.00967600
C	1.99127800	2.12918000	1.25735900
C	2.23756600	3.50642400	1.34295600
H	2.25447900	3.96712300	2.32866100
C	2.45249900	4.30164000	0.21882900
C	2.43615400	3.66953800	-1.02599600
H	2.60631500	4.26129700	-1.92298100
C	2.17784800	2.30303400	-1.17010900
C	1.75035500	1.39745600	2.55298700
H	2.16119300	1.96254800	3.39592200
H	2.20846600	0.40931800	2.55845700
H	0.67884400	1.27098900	2.74707100
C	2.63878700	5.79515200	0.33414200
H	3.03239700	6.07822400	1.31597500

H	1. 67795500	6. 31061600	0. 20311400
H	3. 32153600	6. 17788700	-0. 43227600
C	2. 11391200	1. 75939600	-2. 58382100
H	2. 33349200	2. 55484800	-3. 30241500
H	1. 11542100	1. 36817300	-2. 81380900
H	2. 82878700	0. 94818300	-2. 75726400
C	-3. 22284200	-1. 05114200	-0. 12481900
C	-3. 40196600	-2. 33031400	-0. 65921400
F	-2. 31451200	-3. 06993100	-0. 99293400
C	-4. 64343400	-2. 90525400	-0. 89850800
F	-4. 74491900	-4. 13039400	-1. 42877200
C	-5. 79255400	-2. 18721800	-0. 57427700
F	-6. 99882900	-2. 71871900	-0. 78793100
C	-5. 67265300	-0. 91532600	-0. 02413600
F	-6. 77150600	-0. 22333700	0. 29958800
C	-4. 40567000	-0. 37235100	0. 18629900
C	-1. 62382600	1. 16253500	-0. 03878600
C	-1. 60568700	2. 03017900	1. 05797800
F	-1. 75603000	1. 54372600	2. 31129400
C	-1. 43459900	3. 40635900	0. 95380100
F	-1. 39901100	4. 17472100	2. 04926100
C	-1. 28585100	3. 98017200	-0. 30412600
F	-1. 08631700	5. 29669400	-0. 42632600
C	-1. 33557700	3. 16843500	-1. 43128400
F	-1. 18818500	3. 70431600	-2. 64962400
C	-1. 52249600	1. 79680000	-1. 28185200
F	-1. 55095300	1. 07860800	-2. 42515300
F	-4. 36846100	0. 85307400	0. 74040900
C	-0. 80584800	-1. 16366100	1. 24721100
H	-0. 76152900	-0. 44248100	2. 06841700
C	0. 67639500	-1. 49341500	0. 82304000
H	0. 57153700	-2. 28992100	0. 06838000
B	-1. 77540700	-0. 42636800	0. 16542200
P	1. 46515300	-0. 25284400	-0. 44553200
H	-0. 55159400	-0. 72773900	-1. 25877800
H	-1. 25997300	-1. 05148900	-1. 29815100
C	1. 50691500	-2. 12186000	1. 93649200
C	2. 43077800	-3. 13208800	1. 61435000
C	1. 35176300	-1. 79776300	3. 29578100
C	3. 19506400	-3. 76003400	2. 59779900
H	2. 55300200	-3. 43011500	0. 57740700
C	2. 10932000	-2. 43042300	4. 28411700
H	0. 62632500	-1. 04897500	3. 59701800

C	3. 04155100	-3. 40947900	3. 94023600
H	3. 90349700	-4. 53341500	2. 31265000
H	1. 96230900	-2. 15733900	5. 32580300
H	3. 63044600	-3. 90220200	4. 70897500
N	-1. 47973400	-2. 35069400	1. 80670100
H	-1. 51149900	-3. 09230900	1. 10973500
H	-0. 94290200	-2. 71959900	2. 58938000

## L2

E= -2552.288464au

C	-1. 75203200	-2. 74115300	1. 53708900
C	-1. 75429700	-1. 33078500	1. 66644600
C	-1. 79128800	-0. 73806000	2. 96012400
C	-1. 84673100	-1. 56948700	4. 07978100
C	-1. 85630600	-2. 96219000	3. 97732600
C	-1. 81330800	-3. 51829700	2. 70028500
P	-1. 68427900	-0. 15955700	0. 24484700
C	-1. 72849100	0. 75403000	3. 20378600
C	-1. 88426400	-3. 83207400	5. 20989600
C	-1. 64567800	-3. 49760900	0. 23159100
C	-0. 76792900	-0. 70566300	-1. 31897700
C	0. 44542200	0. 28021800	-1. 50668000
B	1. 46728100	0. 19596200	-0. 18718900
C	2. 68758300	-0. 88203400	-0. 41181400
C	2. 58913800	-2. 19629700	0. 04941700
C	3. 59634000	-3. 15011400	-0. 07748800
C	4. 78890500	-2. 80179200	-0. 70232800
C	4. 93880500	-1. 51109900	-1. 19861300
C	3. 89711800	-0. 59811700	-1. 04837400
F	1. 45075400	-2. 62957800	0. 65456000
F	4. 10290300	0. 62539900	-1. 59416700
F	6. 07652300	-1. 16356200	-1. 82156900
F	5. 77405500	-3. 70183600	-0. 83715100
F	3. 42740800	-4. 39877100	0. 39256600
C	1. 98709700	1. 68116600	0. 29232500
C	2. 09407300	2. 00556300	1. 64835200
C	2. 49925400	3. 25127700	2. 12612000
C	2. 82876100	4. 25394400	1. 22078900
C	2. 73364500	3. 99164800	-0. 14231100
C	2. 31983200	2. 73123600	-0. 56834200
F	1. 76603200	1. 09613200	2. 59991300
F	2. 56768500	3. 49454800	3. 44648400
F	3. 21906500	5. 46121300	1. 65536200

F	3.03591200	4.95458300	-1.02893600
F	2.23277700	2.56710800	-1.90943200
C	-3.30815700	0.67883400	-0.02377800
C	-4.51210800	-0.04849800	-0.19800400
C	-5.71376700	0.65241800	-0.32897900
C	-5.77124600	2.04701300	-0.30613300
C	-4.57072000	2.74550100	-0.16699300
C	-3.33612300	2.10204800	-0.02647200
C	-4.56121400	-1.55507400	-0.28382600
C	-7.08841400	2.77517600	-0.41688200
C	-2.11011300	2.98830400	0.09483900
H	-0.33464300	-1.67317600	-1.06565200
H	-1.87742200	-1.10937300	5.06449000
H	-1.81750100	-4.60053800	2.59448300
H	-4.58890200	3.83267600	-0.17160000
H	-6.63224500	0.08580600	-0.46245500
H	-1.91689600	0.96984200	4.25888100
H	-0.72926100	1.14186900	2.96780100
H	-2.46910100	1.31152300	2.62103600
H	-2.15920900	-3.01632400	-0.60094300
H	-0.59193000	-3.62085300	-0.04168900
H	-2.07402700	-4.49829800	0.34332600
H	-0.87425800	-3.95165400	5.62317300
H	-2.50665700	-3.39283200	5.99689600
H	-2.26764600	-4.83266700	4.98677000
H	-2.39031700	4.03169900	-0.07236900
H	-1.64932700	2.93700500	1.08873900
H	-1.33121500	2.74077200	-0.63394100
H	-6.96454700	3.76171700	-0.87502400
H	-7.81094200	2.20827400	-1.01292200
H	-7.53372300	2.92969000	0.57491600
H	-4.18688200	-2.03449900	0.62592300
H	-5.58923800	-1.89455200	-0.43785500
H	-3.96862600	-1.92022700	-1.13018800
H	0.02064700	1.30002600	-1.58198600
H	-0.91399100	0.89479700	0.73687100
H	0.83585600	-0.24971300	0.75091000
N	1.09333200	-0.12502400	-2.75759800
H	2.01736100	0.29575500	-2.80074300
H	0.57648400	0.21355400	-3.56798100
C	-1.65874800	-0.86186600	-2.53964600
C	-1.73134600	-2.10372700	-3.19016900
C	-2.34498100	0.22371700	-3.10785100

C	-2.48914900	-2.26589700	-4.35157700
H	-1.16554900	-2.94392700	-2.79786100
C	-3.10288800	0.06437800	-4.26833500
H	-2.28173800	1.20569600	-2.64958600
C	-3.18416000	-1.18295800	-4.89113500
H	-2.52480300	-3.23641800	-4.83907000
H	-3.62564000	0.91914200	-4.68916200
H	-3.77277300	-1.30529700	-5.79619500

### L3

E= -2740.87038au

C	-2.15794500	2.87931800	-0.48566100
C	-2.09968600	1.62513100	-1.14154600
C	-2.20137500	1.56431600	-2.56025700
C	-2.37215300	2.75161500	-3.27481500
C	-2.44536600	3.99753400	-2.64929600
C	-2.33365600	4.03210900	-1.26026500
P	-1.88272600	0.00525700	-0.28486900
C	1.87233800	2.26539100	-2.93622100
O	2.72275500	2.92036400	-2.47685200
C	-2.10409200	0.28281100	-3.35800800
C	-2.66004600	5.25891300	-3.44929500
C	-2.00226200	3.08761900	1.00287400
C	-0.98252100	-0.04805600	1.37804200
C	0.22670300	-1.06307000	1.25202300
B	1.38892900	-0.48430700	0.21636500
O	1.01564500	1.63760800	-3.42927100
C	2.30018700	0.67055700	0.95247300
C	2.06301600	2.03248100	0.77802800
C	2.81259500	3.04484300	1.37242500
C	3.88049000	2.70214700	2.19397900
C	4.16532500	1.35624900	2.40923900
C	3.37763100	0.38714200	1.79400000
F	1.02378400	2.45306900	-0.00056800
F	3.70219900	-0.90276900	2.06408800
F	5.18682700	1.01197500	3.20931800
F	4.61871000	3.65496600	2.78179900
F	2.51077700	4.33862700	1.16715900
C	2.33943400	-1.63717500	-0.47285500
C	3.15256600	-1.27919000	-1.55357700
C	3.96927300	-2.16422900	-2.25177000
C	4.00686600	-3.50109800	-1.86658800
C	3.22698600	-3.91475900	-0.79328400

C	2.42757800	-2.98608900	-0.12648400
F	3.17650000	0.00707500	-1.98018900
F	4.71690900	-1.74643000	-3.28661700
F	4.78271900	-4.37651900	-2.52283400
F	3.25214200	-5.20160400	-0.40602600
F	1.70947100	-3.48322400	0.91327400
C	-3.42133000	-1.00713000	-0.38819300
C	-4.66859800	-0.50143500	0.05656500
C	-5.80868100	-1.29753200	-0.08376200
C	-5.76202500	-2.57708800	-0.63955000
C	-4.51946600	-3.06450600	-1.04998900
C	-3.34239800	-2.31623100	-0.94063300
C	-4.82743100	0.85319400	0.70551700
C	-7.01408000	-3.40325100	-0.80473500
C	-2.06014200	-2.97438900	-1.41335000
H	-0.54626800	0.94537700	1.48895600
H	-2.44210600	2.69631700	-4.35830800
H	-2.37521100	4.99120100	-0.74961100
H	-4.45726200	-4.06674400	-1.46717500
H	-6.76102000	-0.90391400	0.26336400
H	-2.31925600	0.48072300	-4.41126700
H	-1.09028800	-0.13362600	-3.31220700
H	-2.81072900	-0.48067700	-3.01722000
H	-2.47602200	2.31220200	1.60582000
H	-0.93912100	3.12439200	1.26430400
H	-2.44424100	4.04460500	1.29545700
H	-2.15949800	5.20498900	-4.42173500
H	-3.72855000	5.42345100	-3.64222900
H	-2.28333200	6.13889200	-2.91875000
H	-2.25941700	-4.01010000	-1.70055800
H	-1.63204800	-2.47541300	-2.29099400
H	-1.28389600	-2.99527200	-0.64160300
H	-6.80372400	-4.47340500	-0.70810000
H	-7.77288100	-3.13431200	-0.06300500
H	-7.45696800	-3.24707200	-1.79732800
H	-4.55712400	1.66959400	0.02838500
H	-5.86522800	1.00752400	1.01351800
H	-4.20652000	0.93732100	1.60416300
H	-0.18553200	-2.00810800	0.85486100
H	-1.01313400	-0.67768200	-1.14080900
H	0.83588700	0.06556400	-0.72087600
N	0.73240700	-1.22706500	2.61734100
H	0.17456700	-1.89116400	3.15013900

H	1.68270000	-1.58228900	2.59113800
C	-1.89701700	-0.32266700	2.56214900
C	-1.96731400	0.60359600	3.61412800
C	-2.60003600	-1.53092700	2.69698700
C	-2.74304200	0.35095100	4.74684100
H	-1.38417400	1.51813900	3.55785900
C	-3.37570900	-1.78631000	3.82862700
H	-2.53533600	-2.28598300	1.91984100
C	-3.45727000	-0.84294300	4.85490600
H	-2.77617300	1.08277500	5.54940900
H	-3.91087100	-2.72863900	3.91003900
H	-4.05947600	-1.04385000	5.73668200

### TS34L

E= -2740.825368au

C	-3.02352700	2.58632800	-0.56997500
C	-2.82996200	1.31171000	-1.15495000
C	-3.33182300	1.06296800	-2.46747800
C	-4.01411700	2.08680800	-3.13167900
C	-4.20766200	3.35087500	-2.57480400
C	-3.70721700	3.57075600	-1.29360000
P	-1.87571200	-0.10747700	-0.41790100
C	1.16807400	-0.27608900	-2.59962000
O	2.15766600	-0.31447100	-3.30655500
C	-3.16956500	-0.24460600	-3.21410500
C	-4.91118400	4.44255700	-3.34341400
C	-2.52881800	2.99014100	0.79792700
C	-0.82928200	0.18298900	1.15984000
C	0.51130100	-0.63831200	1.04747400
B	1.83338000	-0.14699200	0.26194100
O	-0.06006400	-0.50929100	-2.82206500
C	2.24004600	1.38895700	0.47564400
C	1.48125100	2.45956200	0.00058500
C	1.79248600	3.79562200	0.23585500
C	2.92997100	4.10675400	0.97370500
C	3.72893000	3.07628700	1.46363900
C	3.37748300	1.75322300	1.20795600
F	0.36051400	2.23011000	-0.72776300
F	4.18534800	0.80778100	1.71328100
F	4.82192900	3.36707600	2.17972200
F	3.24697700	5.38111700	1.21974500
F	0.99622000	4.77180400	-0.22348500
C	2.94194000	-1.19998000	-0.17557100





F	4.52905600	3.25473000	2.99423800	H	-4.88099500	1.00208600	0.31907700
F	3.39994200	5.17010500	1.40454900	H	-5.56518100	0.17296400	1.72475000
F	1.53552900	4.46079700	-0.46390700	H	-3.85431200	0.60414100	1.69557400
C	2.98193100	-1.29900000	-0.00371600	H	0.22511400	-1.90581600	0.59795500
C	3.44560400	-0.88141200	-1.25528000	H	-0.10388700	-0.60173600	-2.19376700
C	4.33976300	-1.60937900	-2.03494700	H	0.68281400	1.11770800	-3.19789900
C	4.80872900	-2.83337700	-1.56460800	N	1.36580800	-1.02256300	2.15712600
C	4.37407100	-3.30112200	-0.32849300	H	1.14075500	-0.42735800	2.95040700
C	3.48323200	-2.53269900	0.41618000	H	1.64173300	-1.95817100	2.43826900
F	3.01643300	0.29244200	-1.76487500	C	-1.49480500	-0.43539000	2.51911100
F	4.74894000	-1.14833400	-3.21892000	C	-1.50276500	0.48258600	3.58412600
F	5.66732700	-3.55316200	-2.29223400	C	-1.99546500	-1.72632400	2.76375700
F	4.81559300	-4.47684800	0.13739700	C	-2.02467700	0.14111600	4.83506400
F	3.10651900	-3.06720400	1.61282500	H	-1.09366500	1.47904800	3.43586100
C	-3.16307700	-1.40550300	-0.20212400	C	-2.51744300	-2.06841400	4.01086900
C	-4.37775300	-1.10402600	0.46684000	H	-1.98676100	-2.46906400	1.97336400
C	-5.36098500	-2.09471200	0.58139500	C	-2.53992100	-1.13613600	5.05145000
C	-5.19487000	-3.37912700	0.06349600	H	-2.02077900	0.87409300	5.63742800
C	-3.99170400	-3.66501700	-0.58421500	H	-2.90658600	-3.07052100	4.16993100
C	-2.97877700	-2.71090600	-0.73632300	H	-2.94699700	-1.40692100	6.02165500
C	-4.68262900	0.24219300	1.08140300				
C	-6.28539400	-4.41731200	0.17949800				
C	-1.73144400	-3.14523300	-1.48210100				
H	-0.51256000	0.98420900	1.27308400				
H	-4.21484500	2.33013700	-3.91400700				
H	-3.24883800	4.72774300	-0.51376000				
H	-3.83408600	-4.66110400	-0.99239600				
H	-6.28502300	-1.85003100	1.10128700				
H	-3.60543900	0.23451000	-4.14896300				
H	-2.19480500	-0.37681200	-3.28469600				
H	-3.81433700	-0.74489000	-2.69367500				
H	-2.36611400	2.22218000	1.72748200				
H	-0.96533900	2.98474100	0.95168600				
H	-2.39166000	3.93855400	1.33562700				
H	-3.79421200	5.24998100	-3.78493100				
H	-5.40578500	4.63811500	-3.41019300				
H	-4.57563100	5.70811900	-2.26624300				
H	-1.82138800	-4.19296500	-1.78484300				
H	-1.55575300	-2.55388900	-2.38558600				
H	-0.82276100	-3.06225700	-0.87640800				
H	-5.87121300	-5.42915500	0.24506300				
H	-6.91016400	-4.24576500	1.06237100				
H	-6.94686900	-4.39397800	-0.69692000				
				<b>M</b>			
				<b>E= -2359.387324 au</b>			
				C	2.85240800	2.40275700	-0.16370400
				C	2.82633600	1.16481300	0.52896100
				C	3.46777400	1.09715900	1.80165700
				C	4.12382000	2.21954800	2.31572000
				C	4.15432900	3.43998700	1.64157200
				C	3.51136900	3.50053900	0.40733500
				P	1.90552000	-0.41807200	0.11856300
				C	3.48182200	-0.15637300	2.65352200
				C	4.83242500	4.65040700	2.23782800
				C	2.22170200	2.65658400	-1.51765500
				C	0.85036800	-0.25723500	-1.49408000
				C	-0.45880600	-0.97341000	-1.17015100
				B	-1.85721500	-0.34861400	-0.76586400
				C	-2.10942900	1.23556500	-0.72169000
				C	-1.42322300	2.11471900	0.11759800
				C	-1.71373500	3.47681500	0.19005600
				C	-2.73003700	4.00258900	-0.60366400
				C	-3.44215200	3.16401800	-1.45797000
				C	-3.12022800	1.81033300	-1.49575500
				F	-0.42579900	1.66426500	0.89898600

F	-3.83471800	1.03073800	-2.33834300
F	-4.41777300	3.66418000	-2.22827600
F	-3.01810500	5.30705200	-0.54965200
F	-1.02463700	4.28290100	1.00735000
C	-2.88752400	-1.25646100	0.07019700
C	-2.96700700	-1.09999300	1.45724600
C	-3.82968600	-1.83552400	2.26515400
C	-4.66124900	-2.78991200	1.68340000
C	-4.61491100	-2.98895600	0.30740900
C	-3.74088700	-2.22317400	-0.46155200
F	-2.17811400	-0.19472200	2.06610300
F	-3.86423000	-1.64055800	3.58932500
F	-5.49468600	-3.51026000	2.44128300
F	-5.40645400	-3.90594200	-0.26517100
F	-3.74997700	-2.47905900	-1.79841600
C	3.22097400	-1.68688800	-0.33798500
C	4.45553200	-1.42249600	-0.99196400
C	5.35063100	-2.47261600	-1.22935300
C	5.08914000	-3.78709100	-0.83986600
C	3.88098700	-4.03602900	-0.19159600
C	2.95049200	-3.02234600	0.07203800
C	4.89746100	-0.04859300	-1.44606600
C	6.09283200	-4.88877300	-1.08542300
C	1.68028300	-3.43905100	0.79028900
H	0.62634800	0.80320800	-1.61095100
H	4.61635900	2.13466700	3.28242400
H	3.52469900	4.43806700	-0.14519600
H	3.65070900	-5.05040800	0.12841600
H	6.28647600	-2.25059700	-1.73918100
H	3.94611100	0.05018400	3.62277500
H	2.46635200	-0.52810900	2.83546800
H	4.04109400	-0.97413900	2.18494100
H	2.43088700	1.86552100	-2.24271400
H	1.13243200	2.76715800	-1.44767400
H	2.60535300	3.59070000	-1.93927900
H	4.17417100	5.16190700	2.95293600
H	5.74406500	4.37411400	2.77941500
H	5.10349700	5.37891800	1.46627900
H	1.82261600	-4.40830500	1.27914100
H	1.36956400	-2.71013100	1.54315700
H	0.83737600	-3.55546700	0.09646100
H	5.61516300	-5.87410500	-1.08629800
H	6.60522800	-4.75791800	-2.04511100

H	6.86628900	-4.90099200	-0.30576300
H	5.24899800	0.56004600	-0.60606900
H	5.72102600	-0.13514300	-2.16223000
H	4.09527600	0.51532700	-1.92445200
H	-0.32074600	-2.02456700	-0.92205700
N	-1.53756000	-0.88400700	-2.24311200
H	-1.96173700	-1.74179200	-2.58189600
H	-1.38709800	-0.20516200	-2.98309600
C	1.48870400	-0.79646600	-2.78414600
H	2.39724900	-0.25154700	-3.05348200
H	1.75956400	-1.85216700	-2.68263500
H	0.79621200	-0.71109000	-3.63354900

### M1

E= -2360.543716 au

C	-2.23163100	2.33273500	-0.16294200
C	-3.57872200	2.51517900	0.24618600
C	-4.24775900	3.69543900	-0.10236000
H	-5.27871000	3.82192600	0.22267000
C	-3.64452000	4.70767000	-0.84952000
C	-2.32935800	4.50447100	-1.26735200
H	-1.83997200	5.26827900	-1.86829100
C	-1.61398700	3.34467800	-0.94660600
C	-4.36567400	1.48975200	1.03141900
H	-3.80927800	1.11317500	1.89244100
H	-4.62764200	0.62271100	0.41638900
H	-5.29624000	1.93008200	1.40336200
C	-4.38272700	5.98364700	-1.17802000
H	-4.24883200	6.73316800	-0.38626600
H	-5.45931700	5.80996500	-1.28056700
H	-4.01894400	6.42854100	-2.11032500
C	-0.19762000	3.23579700	-1.47542200
H	0.00329100	4.04638000	-2.18330100
H	-0.02468600	2.28466700	-1.98789700
H	0.54749500	3.30687800	-0.67740600
C	-2.28118900	-0.66148700	0.00852400
C	-2.74255600	-1.59914700	0.96609800
C	-3.46953200	-2.72157500	0.54317600
H	-3.81110600	-3.42779800	1.29714500
C	-3.77558000	-2.96322300	-0.79410900
C	-3.30314700	-2.04365300	-1.73146800
H	-3.50450800	-2.21208200	-2.78747800
C	-2.55635500	-0.91856400	-1.36890800

C	-2.53224900	-1.47005500	2.45675200
H	-2.86197700	-2.38055200	2.96601100
H	-3.11171500	-0.63955600	2.87405000
H	-1.48689600	-1.31134200	2.72649900
C	-4.59045100	-4.16311500	-1.21420800
H	-4.60192200	-4.93204700	-0.43499600
H	-4.19502800	-4.61509300	-2.13088400
H	-5.63328900	-3.88398500	-1.41629800
C	-2.05434900	-0.03805900	-2.49602400
H	-2.35295500	-0.45742100	-3.46159800
H	-0.96100200	0.03469800	-2.48770800
H	-2.44999700	0.98137100	-2.44007200
C	2.76859400	0.51478800	0.44833800
C	2.98760300	1.89931900	0.46493800
F	2.05870100	2.73540100	0.98697800
C	4.12032800	2.52175200	-0.04481300
F	4.24386000	3.85361600	-0.01027200
C	5.13667900	1.74080600	-0.58780700
F	6.23733300	2.31327800	-1.07499200
C	4.99261000	0.35756800	-0.61161000
F	5.96861300	-0.40407300	-1.11697900
C	3.83213300	-0.22243200	-0.10497300
C	1.09561400	-1.62601600	0.48895400
C	0.81128200	-2.72762400	1.30514200
F	0.90705500	-2.63168200	2.64732400
C	0.44634800	-3.97632000	0.80622200
F	0.19455700	-4.99499200	1.63777900
C	0.34522300	-4.16062400	-0.56840700
F	-0.01344600	-5.34624600	-1.06548700
C	0.62308900	-3.09697400	-1.42453500
F	0.52512500	-3.26427100	-2.74998500
C	1.00525000	-1.87578500	-0.88747200
F	1.26602100	-0.88456500	-1.76353200
F	3.79483100	-1.56398500	-0.14901700
C	0.69569800	0.37815200	2.33954200
H	0.28830700	-0.50108400	2.84402700
C	-0.50873800	1.30720100	1.97800200
H	-0.05042500	2.24302100	1.63161900
B	1.47733300	-0.18934400	1.04702300
P	-1.17469500	0.83632700	0.25713700
H	2.19332200	-1.38211800	-4.94234400
H	1.87190500	-1.55781500	-4.29647400
N	1.65467800	0.95166800	3.30548700

H	1.93134100	1.88725600	3.01785200
H	1.22688900	1.04071900	4.22524600
C	-1.39087000	1.69341300	3.16984200
H	-1.86918200	0.83440900	3.64521500
H	-0.77632400	2.18989900	3.93219600
H	-2.16609100	2.40525700	2.87077800

### TS12M

E= -2360.516336 au

C	2.93692200	-2.03793900	-0.13489800
C	4.19612600	-2.02333400	0.51900200
C	5.11846700	-3.04383500	0.25331800
H	6.07713300	-3.02193100	0.76790400
C	4.85231100	-4.08399100	-0.63724500
C	3.61019900	-4.08728800	-1.27310400
H	3.37438600	-4.88786900	-1.97123700
C	2.65544900	-3.08892100	-1.05108000
C	4.61900500	-0.95517200	1.50178600
H	3.85014700	-0.76427900	2.25450200
H	4.82414000	-0.00124600	1.00545000
H	5.52932300	-1.26263600	2.02599900
C	5.88130600	-5.15195300	-0.92312800
H	5.40912400	-6.10074800	-1.19940000
H	6.52463100	-5.33170800	-0.05512300
H	6.53451200	-4.85920900	-1.75625400
C	1.35435000	-3.18970500	-1.82346800
H	1.15065200	-2.27925100	-2.39718500
H	0.48630700	-3.35738300	-1.17376700
H	1.39554100	-4.02932000	-2.52433200
C	2.39137600	0.91712000	0.26732800
C	2.44536100	1.76583300	1.40108400
C	3.00959100	3.04318800	1.28039100
H	3.04102600	3.67856300	2.16303800
C	3.53247000	3.52734300	0.08235800
C	3.46933000	2.68635500	-1.02917900
H	3.85890800	3.03693600	-1.98265600
C	2.89652100	1.41187300	-0.97192900
C	1.94528900	1.38399400	2.77467500
H	1.99136800	2.24519500	3.44766900
H	2.55341000	0.59060900	3.22294700
H	0.90980900	1.03990200	2.76294200
C	4.10156000	4.92214300	-0.02056600
H	4.45232300	5.28522200	0.95117900

H	3.34312200	5.63044600	-0.38013400
H	4.94114700	4.96275000	-0.72315900
C	2.82308800	0.62946400	-2.26891600
H	3.27174300	1.20720500	-3.08281400
H	1.78324100	0.41397700	-2.54363800
H	3.34827400	-0.33029400	-2.21463300
C	-3.16208700	-0.78241600	0.13957600
C	-3.47978200	-2.13377400	-0.03022000
F	-2.48680200	-3.05845200	-0.00901400
C	-4.76626900	-2.60817600	-0.24914100
F	-4.99923100	-3.91553400	-0.42004800
C	-5.82239100	-1.69976600	-0.28700600
F	-7.07034800	-2.12966000	-0.48956900
C	-5.56562200	-0.34433400	-0.11063300
F	-6.57481700	0.53417500	-0.13755900
C	-4.25558300	0.08889900	0.09313000
C	-1.26730100	1.18394600	-0.09662100
C	-1.22871000	2.25974300	0.79738400
F	-1.55785700	2.07237000	2.09454400
C	-0.87845100	3.55582100	0.43367200
F	-0.85670400	4.53800200	1.34314000
C	-0.55145700	3.82690700	-0.89112800
F	-0.19894700	5.06187800	-1.26047300
C	-0.59631700	2.79851200	-1.82559100
F	-0.28320100	3.04120600	-3.10498600
C	-0.96719200	1.51838300	-1.42168900
F	-0.98618500	0.57955600	-2.39178100
F	-4.09057100	1.41165400	0.27107200
C	-0.86672800	-0.87189400	1.71799900
H	-0.70592000	0.01586400	2.33704000
C	0.54250500	-1.53393500	1.48178600
H	0.32597800	-2.46769700	0.93510300
B	-1.66483300	-0.28744000	0.42096700
P	1.58331700	-0.76022600	0.07533600
H	-0.42919200	-1.06060800	-0.80119300
H	-1.17795500	-1.27413600	-0.83680500
N	-1.75973900	-1.72763900	2.52369000
H	-1.85880600	-2.64376200	2.09152700
H	-1.37305900	-1.87897100	3.45237600
C	1.22795200	-1.97250600	2.78618600
H	1.35158700	-1.14791500	3.49237100
H	0.63311500	-2.74661300	3.28477300
H	2.21081100	-2.40727600	2.58409300

## M2

E= -2360.558095 au

C	-1.92210700	-2.96474500	0.44229500
C	-2.04035700	-1.60014300	0.80218100
C	-2.24814100	-1.23785700	2.16176700
C	-2.34857500	-2.24919200	3.11843000
C	-2.24154300	-3.60212500	2.78844600
C	-2.03544800	-3.93043500	1.44918700
P	-1.91561100	-0.21030100	-0.39505500
C	-2.31815600	0.19423000	2.64667000
C	-2.31987000	-4.66921200	3.85243100
C	-1.63980400	-3.47883600	-0.95294900
C	-0.83049200	-0.41740800	-1.91673100
C	0.37727400	0.57345100	-1.77637900
B	1.24351000	0.23727000	-0.39103600
C	2.49995000	-0.79553900	-0.64556200
C	2.41100100	-2.15509600	-0.33715800
C	3.45504400	-3.06474600	-0.49438200
C	4.67790100	-2.62253900	-0.98644100
C	4.82366900	-1.28073300	-1.32313200
C	3.74617000	-0.41569800	-1.14847600
F	1.25207700	-2.68224300	0.13624300
F	3.95519900	0.86946100	-1.53093500
F	5.99178700	-0.83823900	-1.81537500
F	5.69669300	-3.47944300	-1.14671600
F	3.29219300	-4.36102700	-0.17659700
C	1.69868400	1.59898700	0.41319500
C	1.66675900	1.65232400	1.81037500
C	2.01677500	2.77457400	2.55984900
C	2.43145900	3.92873200	1.90425000
C	2.47430500	3.93781900	0.51384800
C	2.11078500	2.79097000	-0.18946400
F	1.24765900	0.58039500	2.52765100
F	1.95056200	2.75574600	3.90253800
F	2.77201500	5.02259600	2.60146800
F	2.85871400	5.05091500	-0.13285800
F	2.15583600	2.89427100	-1.53846200
C	-3.56451000	0.54891200	-0.76378100
C	-4.70936600	-0.21742100	-1.10324200
C	-5.91789400	0.44166800	-1.34765100
C	-6.04332900	1.82975700	-1.27626800
C	-4.90333800	2.56738800	-0.95602200

C -3.66648100 1.96734100 -0.69553000  
 C -4.70632500 -1.72330900 -1.23600400  
 C -7.36968600 2.50778200 -1.51779100  
 C -2.51536800 2.89447800 -0.35508800  
 H -0.41613100 -1.42460500 -1.85958100  
 H -2.50871900 -1.96651400 4.15611100  
 H -1.94865100 -4.97753500 1.16904000  
 H -4.97178400 3.65147200 -0.90707100  
 H -6.78876800 -0.15534600 -1.60786700  
 H -2.65131200 0.22254100 3.68760900  
 H -1.32412000 0.65855200 2.61157700  
 H -3.01387700 0.80965600 2.06594500  
 H -2.09954600 -2.88651400 -1.74562000  
 H -0.55916500 -3.49923500 -1.12742500  
 H -2.00936700 -4.50345400 -1.05686100  
 H -1.34472400 -4.80372000 4.33841600  
 H -3.03843500 -4.40342800 4.63512400  
 H -2.61213000 -5.63625800 3.43124700  
 H -2.82825200 3.93482500 -0.47668700  
 H -2.18126400 2.78090800 0.68392300  
 H -1.64035200 2.74165900 -0.99463100  
 H -7.23639100 3.51720000 -1.92002100  
 H -7.98946900 1.93860600 -2.21817200  
 H -7.93683400 2.60164800 -0.58219200  
 H -4.37388400 -2.22116800 -0.32128000  
 H -5.71271100 -2.08416700 -1.46527000  
 H -4.05453000 -2.05889400 -2.05043600  
 H -0.05371800 1.58830700 -1.69080700  
 H -1.30556300 0.80708900 0.34223700  
 H 0.50152300 -0.35758600 0.36754000  
 N 1.15779600 0.44993600 -3.01702900  
 H 2.11371300 0.74320200 -2.83973400  
 H 0.80264900 1.07881900 -3.73539100  
 C -1.63304300 -0.26654900 -3.21691400  
 H -2.44018000 -1.00105000 -3.31513100  
 H -2.07651600 0.73106300 -3.31231600  
 H -0.93974700 -0.42032600 -4.04842700

**M3**

E= -2549.140375 au

C -2.38248400 -2.73328800 -0.01662800  
 C -2.43141500 -1.44603800 0.57174300  
 C -2.72679900 -1.30936500 1.95772400

C -2.96658300 -2.45909300 2.71138900  
 C -2.92646100 -3.73934000 2.15350800  
 C -2.63526300 -3.84643100 0.79466800  
 P -2.11576000 0.12294100 -0.33676900  
 C 1.15258300 -1.95381100 2.99267700  
 O 1.94865200 -2.75531600 2.69802600  
 C -2.76595900 0.02065300 2.67851700  
 C -3.21070300 -4.96040400 2.99362900  
 C -2.04290300 -3.02447000 -1.46220600  
 C -1.03120800 0.10098400 -1.86859500  
 C 0.19164000 1.07071700 -1.62435800  
 B 1.19963900 0.48727300 -0.44442600  
 O 0.34132600 -1.17631600 3.32260200  
 C 2.16160300 -0.72303600 -1.01300100  
 C 1.88985000 -2.06987300 -0.77547900  
 C 2.68705700 -3.12314600 -1.21781600  
 C 3.84445600 -2.84304000 -1.93542700  
 C 4.17225700 -1.51631800 -2.20055200  
 C 3.33480000 -0.50477200 -1.73826800  
 F 0.77366700 -2.43343600 -0.08420400  
 F 3.71380200 0.76473100 -2.04290900  
 F 5.28319600 -1.23091800 -2.89762700  
 F 4.62813900 -3.83734300 -2.37661000  
 F 2.34714400 -4.39850500 -0.96440800  
 C 2.10357100 1.63196800 0.31954300  
 C 2.81542600 1.26863700 1.46800100  
 C 3.57985400 2.14476100 2.23289200  
 C 3.66826700 3.47983000 1.84961100  
 C 2.98900500 3.89934200 0.71238400  
 C 2.23774500 2.97921200 -0.01973900  
 F 2.78510100 -0.01707700 1.89768000  
 F 4.22923900 1.72039300 3.32941700  
 F 4.39536700 4.34762500 2.56869900  
 F 3.06325100 5.18464800 0.32610100  
 F 1.61784100 3.48740000 -1.11602700  
 C -3.66566100 1.10923800 -0.54765800  
 C -4.86089300 0.53283900 -1.05292100  
 C -5.99635000 1.33666500 -1.18308700  
 C -6.00253600 2.68825100 -0.83213900  
 C -4.81820400 3.23551900 -0.33973500  
 C -3.64713200 2.48429700 -0.18391200  
 C -4.99078400 -0.91793800 -1.46000700  
 C -7.25522500 3.51975800 -0.96174800

C	-2.43983500	3.20841100	0.37943600	P	2.03841800	-0.23379400	-0.06383200
H	-0.63172300	-0.91172700	-1.94178500	C	-0.79428200	-0.32628500	2.33798600
H	-3.18504200	-2.34701800	3.77061500	O	-1.73489700	-0.33426100	3.10862700
H	-2.59280300	-4.83295500	0.33961000	C	3.61750000	-0.41258800	2.55857500
H	-4.79654200	4.28724700	-0.06519800	C	5.67980600	4.14721600	2.38074500
H	-6.90582300	0.88761600	-1.57550900	C	2.66002000	2.84886100	-1.37405600
H	-3.15165800	-0.11370300	3.69254000	C	0.91082100	0.09584800	-1.55527500
H	-1.75893500	0.44514800	2.77271400	C	-0.46124700	-0.63523800	-1.37241400
H	-3.40767700	0.75384600	2.17883400	B	-1.68438100	-0.10472100	-0.45959000
H	-2.40847100	-2.27235100	-2.16275300	O	0.44069800	-0.58737300	2.48126900
H	-0.95751300	-3.10106400	-1.58218900	C	-2.02586900	1.45599400	-0.59578100
H	-2.47471900	-3.98419100	-1.76098800	C	-1.17693600	2.46980000	-0.15044700
H	-2.71503200	-4.89675200	3.96853600	C	-1.43391000	3.82704400	-0.32036000
H	-4.28691900	-5.06422200	3.18448700	C	-2.60609100	4.22063100	-0.95769200
H	-2.87229100	-5.87548800	2.49851200	C	-3.49359000	3.24922300	-1.41482000
H	-2.67229100	4.26798700	0.51426700	C	-3.19418800	1.90211600	-1.22723000
H	-2.14257000	2.81889700	1.36092000	F	-0.01917600	2.15874700	0.48200500
H	-1.56292700	3.14970400	-0.27228400	F	-4.08685600	1.01638000	-1.69828000
H	-7.02566300	4.58933300	-0.99015300	F	-4.62056600	3.61918400	-2.03527700
H	-7.81260500	3.26497100	-1.86960200	F	-2.87251300	5.51693700	-1.14019600
H	-7.92744000	3.34944400	-0.11051800	F	-0.55244200	4.74502100	0.10196500
H	-4.87860200	-1.59579300	-0.60815800	C	-2.81445100	-1.11040900	0.02978200
H	-5.97482900	-1.09764800	-1.90149200	C	-3.83786500	-0.67876300	0.89101000
H	-4.24677600	-1.20702300	-2.20848400	C	-4.82889300	-1.51717100	1.39289300
H	-0.23044300	2.03066700	-1.28643200	C	-4.83063600	-2.86206800	1.04142500
H	-1.39540400	0.88315700	0.59162800	C	-3.84035100	-3.34471700	0.19154800
H	0.50733900	-0.00843100	0.43120000	C	-2.86575900	-2.47581100	-0.28691300
N	0.84997800	1.24106400	-2.92847500	F	-3.91166000	0.60572800	1.26861100
H	0.50741200	2.06864500	-3.41097600	F	-5.77910100	-1.03997200	2.20451000
H	1.84711800	1.37575100	-2.80060100	F	-5.77431700	-3.68351500	1.50969100
C	-1.83880400	0.42639000	-3.13481100	F	-3.83297300	-4.63892800	-0.16091800
H	-2.62364500	-0.30738300	-3.34744000	F	-1.94651500	-3.04257600	-1.10727300
H	-2.30860600	1.41471000	-3.07816500	C	3.04770300	-1.74307600	-0.44713500
H	-1.13456000	0.42344200	-3.96998600	C	4.29810000	-1.65498500	-1.12030100

### TSM34

E= -2549.095113 au

C	3.32058900	2.40240600	-0.08792700	C	4.51897700	-4.09379800	-1.05383000
C	3.13157300	1.14418400	0.53585900	C	3.30318700	-4.15718500	-0.37658800
C	3.77748600	0.87613300	1.77835400	C	2.55035600	-3.01795400	-0.06019200
C	4.60550600	1.85649500	2.33416400	C	4.97121300	-0.35691000	-1.51741900
C	4.80944400	3.09821500	1.73288200	C	5.28912200	-5.34355500	-1.40494400
C	4.15742200	3.34233700	0.52537400	C	1.24972500	-3.25702700	0.68211700
				H	0.73667600	1.17150200	-1.56280800
				H	5.09919900	1.63622900	3.27769700

H	4.29685200	4.30310600	0.03520400	C	3.50616500	-0.22503200	2.49356700
H	2.91752900	-5.12740300	-0.07245300	C	4.72890600	4.62961100	2.39150700
H	5.95216300	-2.75101300	-1.92273700	C	2.21953400	2.80866700	-1.51932900
H	4.23979100	-0.37940000	3.45731100	C	0.90993100	-0.13260900	-1.70617400
H	2.58058000	-0.55959200	2.88008100	C	-0.39565300	-0.88073300	-1.44673000
H	3.92224400	-1.29307300	1.98344700	B	-1.81669000	-0.29524300	-1.04849100
H	2.66810400	2.08539900	-2.15453500	O	-0.10753000	-1.21384400	2.50017400
H	1.62094000	3.14435900	-1.19181600	C	-2.07745700	1.28968300	-1.00728200
H	3.17680400	3.72531300	-1.77500300	C	-1.42095000	2.16833500	-0.14688200
H	6.51793200	3.69481300	2.92141400	C	-1.69688600	3.53188100	-0.08583400
H	6.08575300	4.84541700	1.64160200	C	-2.67607400	4.06515000	-0.92127500
H	5.10525100	4.73679600	3.10726400	C	-3.35994300	3.22981100	-1.80084900
H	1.28856000	-4.23117100	1.17886700	C	-3.04893600	1.87223000	-1.82402100
H	1.03080300	-2.50943700	1.44776600	F	-0.45589400	1.70651200	0.67970900
H	0.38999800	-3.29266600	0.00163000	F	-3.73328000	1.10048200	-2.69752700
H	5.11940100	-5.62805500	-2.45183100	F	-4.29772100	3.73540600	-2.61181400
H	6.36772100	-5.19744700	-1.28092400	F	-2.95238200	5.37175400	-0.88288100
H	4.98492800	-6.18999700	-0.78151900	F	-1.02948000	4.33127100	0.75483900
H	5.44830200	0.12616600	-0.65742400	C	-2.84049200	-1.23950300	-0.24425300
H	5.74937600	-0.55432300	-2.26080900	C	-3.26450300	-0.89058900	1.04231800
H	4.28508700	0.37466700	-1.94800100	C	-4.12735300	-1.66500700	1.81359200
H	-0.25746400	-1.68494800	-1.17491800	C	-4.60403200	-2.86786100	1.30049200
H	1.17273400	-0.48123800	1.14704900	C	-4.20417900	-3.27177800	0.03047800
H	-1.04451100	-0.05119400	1.22455300	C	-3.34311000	-2.45994000	-0.70172100
N	-1.29849300	-0.60691900	-2.59268500	F	-2.82335700	0.25311800	1.60660900
H	-1.28328900	0.28876200	-3.06928600	F	-4.49856000	-1.26548100	3.03185600
H	-1.11646700	-1.35929400	-3.24928100	F	-5.43427300	-3.62901000	2.01856000
C	1.57429900	-0.32131400	-2.88112300	F	-4.64901300	-4.42841600	-0.47805500
H	2.52073100	0.19298300	-3.06300400	F	-2.99257700	-2.93975500	-1.93111200
H	1.77266800	-1.39746900	-2.90605100	C	3.25145300	-1.60025300	-0.52894800
H	0.91200400	-0.08294300	-3.71834000	C	4.48604600	-1.29453500	-1.16065400
				C	5.39487400	-2.32658800	-1.43016500
				C	5.14330100	-3.65595700	-1.09413700
				C	3.93136100	-3.94253100	-0.46483000
				C	2.98849800	-2.95191600	-0.16761400
				C	4.92162800	0.10068700	-1.55253400
				C	6.15494200	-4.74182100	-1.37317900
				C	1.72626500	-3.40402600	0.54172300
				H	0.67416900	0.92828300	-1.78606100
				H	4.55878400	2.05232400	3.27729500
				H	3.46088200	4.53283400	-0.02220500
				H	3.70962000	-4.97081400	-0.18699400
				H	6.33257800	-2.07540600	-1.92195600

## M4

E= -2549.147538 au

C	2.83308600	2.48930100	-0.17131600	C	2.98849800	-2.95191600	-0.16761400
C	2.82116400	1.21482900	0.45057600	C	4.92162800	0.10068700	-1.55253400
C	3.45329600	1.07970600	1.72308000	C	6.15494200	-4.74182100	-1.37317900
C	4.07510500	2.18461500	2.31170900	C	1.72626500	-3.40402600	0.54172300
C	4.08521700	3.44437800	1.71280000	H	0.67416900	0.92828300	-1.78606100
C	3.46056500	3.56442400	0.47382700	H	4.55878400	2.05232400	3.27729500
P	1.92727000	-0.34583400	-0.07843900	H	3.46088200	4.53283400	-0.02220500
C	-0.51223900	-0.25199800	3.35614900	H	3.70962000	-4.97081400	-0.18699400
O	-1.05099800	-0.50099400	4.40191700	H	6.33257800	-2.07540600	-1.92195600



H	3.96703500	-0.06531500	3.47276300	B	-1.76484400	0.20170400	-0.67907900
H	2.50920200	-0.64649000	2.66432300	C	-1.92462600	1.75592400	-0.31417600
H	4.09107000	-0.99152400	1.97335900	C	-1.32028300	2.36152600	0.79017400
H	2.46341200	2.07000700	-2.28783400	C	-1.53121900	3.69767500	1.12963000
H	1.12707600	2.88724800	-1.46352000	C	-2.37479300	4.47995000	0.34513600
H	2.58573200	3.77617000	-1.87557600	C	-2.99788700	3.91980400	-0.76760100
H	4.08758100	5.02368800	3.19090100	C	-2.76328200	2.58123400	-1.06734200
H	5.68584400	4.35787500	2.85147600	F	-0.49026300	1.65835000	1.57553700
H	4.91126500	5.44594300	1.68507900	F	-3.38508700	2.07710300	-2.15961700
H	1.80666200	-4.46185800	0.81013500	F	-3.80620800	4.66689100	-1.53103500
H	1.53129200	-2.84262900	1.45952300	F	-2.58275400	5.76292200	0.65521300
H	0.83195600	-3.30363300	-0.08391100	F	-0.92865200	4.23575300	2.19652700
H	5.66753000	-5.68192900	-1.65387000	C	-2.91716700	-0.78541100	-0.14502100
H	6.83677300	-4.45684500	-2.18113300	C	-3.06145300	-1.00823900	1.22696800
H	6.76769900	-4.94810800	-0.48547800	C	-4.04392600	-1.82739500	1.77561900
H	5.26926500	0.67133300	-0.68460200	C	-4.94297100	-2.47195900	0.92881000
H	5.74755000	0.04933700	-2.26901600	C	-4.83977900	-2.28725500	-0.44632600
H	4.12025000	0.68378000	-2.00851700	C	-3.84229200	-1.45369100	-0.94790000
H	-0.24775100	-1.93813500	-1.23340400	F	-2.20863500	-0.41329800	2.08386900
H	0.34950000	-0.82326800	1.71600100	F	-4.13017800	-2.00431500	3.09913200
H	-0.29995300	0.77106800	3.00118800	F	-5.89321500	-3.26490900	1.43260200
N	-1.44919000	-0.77899800	-2.53794500	F	-5.69424900	-2.90484900	-1.27194400
H	-1.30446800	-0.07195300	-3.25188100	F	-3.80163300	-1.32592100	-2.30156000
H	-1.82620100	-1.64681500	-2.90481600	C	2.37349800	-1.95383700	-0.06685500
C	1.59321900	-0.60725500	-2.99861400	C	3.32171400	-2.45784800	-0.99679400
H	2.49166200	-0.02897400	-3.22866100	C	3.42980700	-3.84331400	-1.17226800
H	1.88753200	-1.65908500	-2.93177300	C	2.64636600	-4.75709600	-0.46483800
H	0.91573200	-0.50487700	-3.85740500	C	1.73613100	-4.24831900	0.46093600
				C	1.59505900	-2.87296400	0.68715400
				C	4.26793600	-1.58888300	-1.79609800
				C	2.80683200	-6.24504400	-0.67137600
				C	0.63186500	-2.44639100	1.78083700
				H	0.80418800	1.35746200	-1.22679700
				H	6.51972900	0.62430900	2.09704800
				H	5.49709500	3.35294600	-1.02758800
				H	1.12344000	-4.93845000	1.03761500
				H	4.15462700	-4.21806400	-1.89273100
				H	5.03280100	-0.77297700	3.00613000
				H	3.30388800	-0.68125600	2.64393500
				H	4.33695500	-1.77005000	1.72139800
				H	2.72977700	1.82478400	-2.33831200
				H	2.20415500	2.98664500	-1.10522000
				H	3.60629200	3.34410400	-2.10515600

## N

E= -2395.284211 au

C	3.99995700	1.89117900	-0.56937900	C	0.63186500	-2.44639100	1.78083700
C	3.66272900	0.76002200	0.21825500	H	0.80418800	1.35746200	-1.22679700
C	4.58782400	0.33938300	1.21765500	H	6.51972900	0.62430900	2.09704800
C	5.82570800	0.97859100	1.33708300	H	5.49709500	3.35294600	-1.02758800
C	6.19051900	2.05556500	0.53004100	H	1.12344000	-4.93845000	1.03761500
C	5.25299400	2.49688600	-0.40143200	H	4.15462700	-4.21806400	-1.89273100
P	2.01865500	-0.14223900	0.28825200	H	5.03280100	-0.77297700	3.00613000
C	4.29936400	-0.78274500	2.19391200	H	3.30388800	-0.68125600	2.64393500
C	7.52426200	2.74503500	0.69489900	H	4.33695500	-1.77005000	1.72139800
C	3.08205700	2.53553100	-1.58676200	H	2.72977700	1.82478400	-2.33831200
C	0.96931600	0.27301700	-1.25633500	H	2.20415500	2.98664500	-1.10522000
C	-0.37291300	-0.42185100	-1.12230600	H	3.60629200	3.34410400	-2.10515600

H	7.49838000	3.47338300	1.51678100	C	-3.45811000	-2.74103300	0.74544700
H	8.32058100	2.02826800	0.92509600	H	-3.76974200	-3.39241400	1.55984500
H	7.80923000	3.28799800	-0.21251100	C	-3.81254800	-3.07452400	-0.55814500
H	0.09014100	-3.31710700	2.16482500	C	-3.39164100	-2.21544600	-1.57786400
H	1.16796400	-1.99280800	2.62334000	H	-3.64487200	-2.45097300	-2.60973400
H	-0.10421100	-1.70594400	1.46051100	C	-2.64231100	-1.06639300	-1.32099400
H	1.91867000	-6.79401800	-0.34134800	C	-2.39899700	-1.39712400	2.53148700
H	2.98491700	-6.48723000	-1.72519500	H	-3.21418100	-1.79350600	3.14706900
H	3.66193100	-6.63439800	-0.10259600	H	-2.23919300	-0.35643500	2.81094700
H	5.06308200	-1.17926900	-1.16322600	H	-1.49706900	-1.95580000	2.81334100
H	4.74496900	-2.18125900	-2.58414300	C	-4.60971500	-4.31899400	-0.86908100
H	3.75164500	-0.74995800	-2.26184300	H	-4.91112300	-4.83963800	0.04525800
H	-0.28129300	-1.50690700	-1.10830400	H	-4.02742900	-5.02296200	-1.47722600
N	-1.36529600	-0.03482800	-2.21637200	H	-5.51803900	-4.08115000	-1.43638900
H	-1.82950000	-0.76455600	-2.74858500	C	-2.20191100	-0.24174200	-2.51444800
H	-1.17085600	0.79496500	-2.76956500	H	-2.54988500	-0.70506000	-3.44281100
O	1.61093100	-0.09296200	-2.48421100	H	-1.10917200	-0.16660200	-2.56778600
H	0.93521100	-0.17208400	-3.17796700	H	-2.59679100	0.78001400	-2.48646200

## N1

E= -2396.447552 au

C	-2.32628500	2.28512600	-0.21181500	C	2.82059400	0.55580800	0.48497900
C	-3.62874100	2.47495300	0.32007800	C	3.00073000	1.94498300	0.43666500
C	-4.32714200	3.65099700	0.01540700	F	2.01498200	2.77835400	0.84425200
H	-5.32208000	3.78675200	0.43509000	C	4.15066700	2.56744500	-0.03346200
C	-3.79569800	4.64874000	-0.80255100	F	4.24192200	3.90141200	-0.06901100
C	-2.51590500	4.44712100	-1.32181300	C	5.21770200	1.78384500	-0.46490800
H	-2.07666500	5.21050700	-1.96085000	F	6.33435900	2.35784700	-0.91082700
C	-1.77396300	3.29211600	-1.04988000	C	5.10824000	0.39725600	-0.42317600
C	-4.33103700	1.46405600	1.20126400	F	6.13177200	-0.36304100	-0.82460500
H	-3.69783000	1.11652300	2.02095400	C	3.93010600	-0.18463800	0.03727000
H	-4.63102300	0.57553300	0.63635300	C	1.15137200	-1.57749000	0.42509300
H	-5.23385700	1.90397800	1.63665100	C	0.84617600	-2.69635500	1.20871400
C	-4.58762200	5.89084100	-1.13620100	F	0.90532500	-2.62550200	2.55408100
H	-5.31120700	6.12857500	-0.34928600	C	0.49047600	-3.93142000	0.67244700
H	-5.15228800	5.76090700	-2.06923600	F	0.21283100	-4.96745100	1.47225100
H	-3.93392200	6.75919400	-1.27207900	C	0.42708900	-4.08277900	-0.70893700
C	-0.39348300	3.18585700	-1.66885300	F	0.07755400	-5.25455000	-1.24273900
H	-0.23852500	3.99734900	-2.38713600	C	0.72952800	-3.00063300	-1.53302100
H	-0.24915200	2.23455100	-2.19031000	F	0.66050500	-3.13545700	-2.86387100
H	0.40111000	3.25597900	-0.91844300	C	1.10047100	-1.79234300	-0.95911100
C	-2.30901200	-0.72220900	0.02485700	F	1.37172100	-0.77790900	-1.80415500
C	-2.71633000	-1.59169300	1.06491300	F	3.91515600	-1.52679800	0.06103500
				C	0.65602100	0.40623300	2.26539300
				H	0.20269700	-0.46480400	2.74417300
				C	-0.51505100	1.31629000	1.81899700

H	-0.06864300	2.26575400	1.49468000
B	1.51615600	-0.15950800	1.02929200
P	-1.22824200	0.80234400	0.13460100
H	2.33016000	-1.16671800	-4.98421100
H	2.00424500	-1.36589100	-4.34748600
N	1.51502500	1.01773700	3.29555500
H	1.88040300	1.90531600	2.95520200
H	0.93398900	1.24657900	4.10173300
O	-1.34581700	1.57479300	2.94950100
H	-1.91284100	2.33104300	2.72755300

## TSN12

E= -2396.447552 au

C	2.93861900	-2.00871100	-0.16705100
C	4.14693400	-2.03740400	0.57397500
C	5.04671400	-3.09253500	0.36680600
H	5.97207700	-3.10409900	0.93896300
C	4.79839200	-4.12258400	-0.53991800
C	3.60253400	-4.07913900	-1.26167700
H	3.38689000	-4.86864700	-1.97876100
C	2.67159000	-3.04922500	-1.09965600
C	4.53757200	-0.97529700	1.57889700
H	3.72472300	-0.74145700	2.27108700
H	4.81468200	-0.03623800	1.08854200
H	5.39580200	-1.31054100	2.16947900
C	5.77600700	-5.25841000	-0.72689400
H	6.74734700	-5.02941600	-0.27754800
H	5.93627700	-5.47676600	-1.78895400
H	5.40529500	-6.18113500	-0.26152200
C	1.41085000	-3.10007500	-1.94126000
H	1.26704900	-2.18001300	-2.51781300
H	0.50485900	-3.24182800	-1.33868000
H	1.46100800	-3.93567500	-2.64610800
C	2.41664300	0.97411500	0.19113000
C	2.46511100	1.79753200	1.34005600
C	3.06749100	3.06189200	1.24331200
H	3.10420000	3.68175000	2.13685100
C	3.61625500	3.54944700	0.06057400
C	3.53712100	2.73344800	-1.07255800
H	3.94087200	3.09321000	-2.01674100
C	2.93986800	1.47302600	-1.03950600
C	1.88336700	1.43642800	2.68839200
H	2.47015000	1.90151200	3.48807900

H	1.84186200	0.36329500	2.87658600
H	0.86124800	1.82588400	2.78428500
C	4.27035100	4.90874900	-0.00618000
H	4.17170200	5.44750200	0.94127000
H	3.82319900	5.52772500	-0.79341600
H	5.34077700	4.82451400	-0.23349400
C	2.85549100	0.69992600	-2.34073500
H	3.31353500	1.27380900	-3.15195400
H	1.81249100	0.50331900	-2.61796100
H	3.36799200	-0.26760700	-2.29069300
C	-3.05787600	-0.86599700	0.14256300
C	-3.25151700	-2.23533600	-0.05705600
F	-2.17363400	-3.06446100	-0.05888500
C	-4.49263800	-2.82396000	-0.26422400
F	-4.60759900	-4.14406900	-0.45915700
C	-5.62763500	-2.01608600	-0.26483600
F	-6.83474000	-2.55484300	-0.45838800
C	-5.49390900	-0.64665100	-0.05898500
F	-6.58131200	0.13374400	-0.05102200
C	-4.22646700	-0.09842800	0.13647400
C	-1.33716200	1.26933500	-0.09171400
C	-1.41615600	2.33299100	0.81285100
F	-1.72494200	2.09748400	2.10564100
C	-1.19314200	3.66138700	0.46431200
F	-1.27930500	4.63253800	1.38222400
C	-0.88135300	3.97815900	-0.85464100
F	-0.65983300	5.24753200	-1.20980900
C	-0.80189900	2.95969200	-1.79758400
F	-0.49941000	3.24627900	-3.07093400
C	-1.04280800	1.64478500	-1.40626300
F	-0.94614800	0.71276400	-2.38225500
F	-4.17774600	1.22987600	0.33988100
C	-0.76231300	-0.75405300	1.71153700
H	-0.54147700	0.14955400	2.28359700
C	0.60171800	-1.44146200	1.43157100
H	0.36840300	-2.40832400	0.94997100
B	-1.58924500	-0.25289600	0.38457300
P	1.62014100	-0.69790100	0.00835000
H	-0.25958500	-0.88024300	-0.73301100
H	-1.06271400	-1.03001500	-0.77830200
N	-1.59659000	-1.58119700	2.59953300
H	-1.81453100	-2.46492600	2.14224200
H	-1.04993100	-1.81905600	3.42608200

---

O	1.23879500	-1.69961600	2.67848100
H	1.98118500	-2.30273600	2.50932800

## N2

E= -2396.470743 au

C	-3.73031400	-2.17526000	-0.15278000
C	-3.40841300	-0.98681700	0.54996700
C	-4.10705300	-0.65657300	1.74608300
C	-5.12947000	-1.49858600	2.18511400
C	-5.48367000	-2.66154100	1.49652700
C	-4.77010000	-2.97428400	0.34094400
P	-2.08325700	0.18675400	0.04075500
C	-3.78670300	0.55617900	2.59327200
C	-6.57930300	-3.56389500	2.00892700
C	-3.00321500	-2.68589700	-1.37657400
C	-0.89284800	-0.34820400	-1.30465500
C	0.44007800	0.47473800	-1.21709600
B	1.41983500	-0.02443000	0.01109200
C	1.95275300	-1.55601800	-0.27725400
C	1.26506800	-2.67804600	0.18985400
C	1.68731700	-3.99109200	-0.00146100
C	2.86587900	-4.23042600	-0.70183100
C	3.58433300	-3.15222100	-1.20884400
C	3.11256200	-1.85777500	-0.99444100
F	0.08439400	-2.53085200	0.85231100
F	3.84240800	-0.85852900	-1.54756000
F	4.71006600	-3.36989500	-1.90598300
F	3.29115300	-5.48518900	-0.90320400
F	0.96872700	-5.02354800	0.47078000
C	2.65655600	0.99441700	0.37856200
C	3.44953700	0.69657600	1.49466100
C	4.50107400	1.48976300	1.94453500
C	4.80802500	2.66525600	1.26460000
C	4.05180300	3.01625900	0.15364700
C	3.00928300	2.18480100	-0.25690900
F	3.20158700	-0.42290300	2.20753100
F	5.21688700	1.13943300	3.02515700
F	5.81358100	3.44920700	1.67972200
F	4.32623300	4.15082600	-0.51237700
F	2.32613300	2.63039400	-1.35103100
C	-2.69085300	1.88327900	-0.28927000
C	-3.73876100	2.09548000	-1.21961400
C	-4.14353000	3.40940900	-1.47609600

C	-3.55109900	4.50941400	-0.85453500
C	-2.52032900	4.27130000	0.05887200
C	-2.07158300	2.98384700	0.36513100
C	-4.44024500	0.97390600	-1.95163900
C	-4.01423600	5.91658600	-1.14350300
C	-0.96493200	2.85290000	1.39288100
H	-0.69061800	-1.40450400	-1.09793300
H	-5.66158700	-1.23634500	3.09656200
H	-5.02034300	-3.88132800	-0.20377900
H	-2.04348700	5.11568900	0.55086600
H	-4.94406800	3.57329400	-2.19327200
H	-4.45092700	0.59551800	3.46062300
H	-2.75945900	0.52217500	2.97861300
H	-3.90314500	1.49594500	2.04419300
H	-2.76323900	-1.91045600	-2.10694600
H	-2.06190200	-3.16666000	-1.08038900
H	-3.60829300	-3.44728000	-1.87678600
H	-6.19929100	-4.23212500	2.79277900
H	-7.40170800	-2.98722800	2.44565000
H	-6.98681700	-4.19254600	1.21127500
H	-0.61257000	3.84507300	1.68692300
H	-1.31307900	2.35302000	2.30563700
H	-0.09730500	2.29507900	1.02874400
H	-3.16449300	6.58901700	-1.30600900
H	-4.65374300	5.95463300	-2.03040100
H	-4.58939800	6.32168500	-0.30082200
H	-4.99899700	0.32649500	-1.26668700
H	-5.15220000	1.38306600	-2.67409300
H	-3.72123200	0.35666200	-2.49840700
H	0.15731700	1.52646200	-1.08689200
H	-1.26687800	0.28713600	1.17872400
H	0.74468500	-0.07728500	1.02794100
N	0.96803400	0.40526500	-2.61142700
H	1.61844800	-0.37530700	-2.69462300
H	1.51236000	1.24471100	-2.78862200
O	-1.50722800	-0.17035700	-2.55591400
H	-0.71295600	0.11690000	-3.10292200

## N3

E= -2585.055757 au

C	-3.75202900	-2.13193100	-0.47922400
C	-3.41754500	-0.99181300	0.29397400
C	-4.09111900	-0.74435200	1.52473800

C	-5.10829000	-1.61267400	1.92278700	C	-0.99333500	2.81682000	1.31382200
C	-5.48186700	-2.72264100	1.16066400	H	-0.71116800	-1.28799200	-1.39375900
C	-4.78420800	-2.96213600	-0.02163200	H	-5.61796000	-1.41672000	2.86324300
P	-2.10904200	0.22392600	-0.15795200	H	-5.04014900	-3.83467400	-0.61764300
C	0.48560300	-1.62354200	3.27623000	H	-2.12278100	5.11227400	0.63753800
O	1.33392600	-2.42116600	3.33655200	H	-5.05541900	3.69719700	-2.14112100
C	-3.73696700	0.39472800	2.45670500	H	-4.41490400	0.40262700	3.31444700
C	-6.60812300	-3.62414500	1.60341500	H	-2.71937100	0.28413600	2.85134300
C	-3.04208700	-2.56675200	-1.74211100	H	-3.80791800	1.37402200	1.97303200
C	-0.93433800	-0.22501300	-1.54808400	H	-2.81630100	-1.74953800	-2.43006000
C	0.39412000	0.60614200	-1.46544000	H	-2.09348600	-3.05923700	-1.49123100
B	1.38954300	0.08161200	-0.26253800	H	-3.65170800	-3.30134100	-2.27578700
O	-0.38153000	-0.83441700	3.25424400	H	-6.57529800	-3.80283400	2.68372300
C	1.99381500	-1.40647100	-0.61816400	H	-7.58309600	-3.17140700	1.37992600
C	1.37609100	-2.58036500	-0.18375000	H	-6.57023800	-4.59256100	1.09540800
C	1.86371200	-3.86105600	-0.42855000	H	-0.65939900	3.79315800	1.67496600
C	3.03974600	-4.00900400	-1.15820000	H	-1.30536900	2.23793400	2.19184900
C	3.69180400	-2.87547400	-1.63421700	H	-0.12112700	2.31162800	0.88876600
C	3.15676200	-1.61688300	-1.36270600	H	-3.32254200	6.70234100	-0.95048600
F	0.20202800	-2.52005000	0.51026700	H	-4.69011400	6.09518900	-1.90341000
F	3.82403100	-0.55846500	-1.88200100	H	-4.83413700	6.26677500	-0.15005000
F	4.81476200	-3.00694100	-2.35628900	H	-5.06739300	0.41417700	-1.40804300
F	3.52759500	-5.23004400	-1.41462200	H	-5.23303500	1.53855700	-2.76096700
F	1.21233300	-4.94696200	0.01756800	H	-3.79951700	0.50700100	-2.64643700
C	2.57092700	1.12679400	0.19510000	H	0.10644900	1.65320000	-1.30454000
C	3.23612900	0.88074000	1.40253200	H	-1.29048800	0.26900000	0.98092400
C	4.22993400	1.69827500	1.93288200	H	0.70266200	-0.05367800	0.73273100
C	4.60688800	2.84591200	1.24079200	N	0.89066000	0.57112900	-2.87256600
C	3.97685900	3.14592000	0.03909300	H	1.45610100	1.39962800	-3.03326600
C	2.98861900	2.29105700	-0.44922800	H	1.51810700	-0.22339600	-2.99383900
F	2.91490300	-0.21302400	2.13280600	O	-1.58179300	-0.00014500	-2.77575800
F	4.82173600	1.39866800	3.10009400	H	-0.80303200	0.30917100	-3.33243600
F	5.55898600	3.65292800	1.73002800				
F	4.32137900	4.25371700	-0.63810100				
F	2.42611500	2.68219100	-1.62688500				
C	-2.74179800	1.92803600	-0.38751300				
C	-3.81162000	2.18110400	-1.28238000				
C	-4.23884000	3.50165100	-1.45028600				
C	-3.65028600	4.57045800	-0.77197300				
C	-2.59777900	4.29267100	0.10377100				
C	-2.12472000	2.99522800	0.32097400				
C	-4.51509500	1.09544800	-2.06495500				
C	-4.14824800	5.98296200	-0.95923200				
				<b>TSN34</b>			
				<b>E= -2585.01026 au</b>			
C	3.58516000	2.24933500	-0.16051900				
C	3.35447100	1.02724500	0.51797200				
C	4.11712000	0.72143200	1.68269900				
C	5.10982400	1.60940400	2.10092000				
C	5.36958500	2.80734000	1.43143500				
C	4.59167300	3.10239900	0.31459000				
P	2.06183800	-0.23669000	0.10171200				
C	-0.77005600	-0.16971200	2.36855500				

O	-1.74071900	-0.19654300	3.08621900	H	5.29643600	-3.14717500	-2.38366700
C	3.89553400	-0.52275100	2.51886800	H	4.60145600	-0.54347000	3.35408900
C	6.43814200	3.75512200	1.92058900	H	2.88625200	-0.54484800	2.94641800
C	2.79626600	2.74589200	-1.35308800	H	4.03766000	-1.44514100	1.94615100
C	0.90266400	0.24544200	-1.31589300	H	2.61064800	1.97983400	-2.10902000
C	-0.41103200	-0.60544200	-1.23703900	H	1.82538100	3.14390600	-1.03015500
B	-1.63221500	-0.04992000	-0.33528300	H	3.33034600	3.57008900	-1.83510200
O	0.48229200	-0.24506400	2.58622600	H	6.14542900	4.22362800	2.86900500
C	-1.95226300	1.51640300	-0.50966400	H	7.38479100	3.23187300	2.09947200
C	-1.22820700	2.55265600	0.08301300	H	6.62473200	4.55633400	1.19876900
C	-1.52377500	3.90110400	-0.10150400	H	1.17880300	-4.13905500	1.57790200
C	-2.58835600	4.25996600	-0.92304300	H	1.31502600	-2.42594800	1.97355800
C	-3.33174000	3.26507900	-1.55379900	H	0.24333100	-2.95530900	0.67943800
C	-3.00163700	1.93170100	-1.33483500	H	4.00741700	-6.07537500	-2.42857400
F	-0.16757400	2.27496600	0.87502500	H	5.61097100	-5.54767800	-1.90850600
F	-3.73423300	1.00445600	-1.99453100	H	4.53557700	-6.38510600	-0.77268000
F	-4.34302600	3.59745600	-2.36408300	H	5.09521900	-0.05114900	-1.21579500
F	-2.88230900	5.54689900	-1.12126600	H	5.28074100	-0.95850200	-2.72018600
F	-0.78426500	4.84717600	0.48815800	H	3.80615300	-0.02696300	-2.43108500
C	-2.83336800	-1.00722300	0.07951000	H	-0.13008400	-1.62443600	-0.97080500
C	-3.89325000	-0.53723000	0.87671500	H	1.15733900	-0.29996600	1.46328600
C	-4.93396900	-1.34494700	1.32712700	H	-0.99023300	-0.07195800	1.19959700
C	-4.95183000	-2.69356900	0.98797200	N	-0.92516500	-0.70860300	-2.63856100
C	-3.92829800	-3.21400500	0.20060000	H	-1.59353900	0.02897900	-2.85704700
C	-2.90431400	-2.37549100	-0.22398300	H	-1.40511300	-1.59652100	-2.75880100
F	-3.95301000	0.75003700	1.24237800	O	1.53003000	0.05164500	-2.55970900
F	-5.91419700	-0.83593800	2.07938700	H	0.80123300	-0.31646600	-3.12331900
F	-5.94220600	-3.48202400	1.40723000				
F	-3.93741200	-4.50911000	-0.13966900				
F	-1.95098600	-2.96978700	-0.98627300				
C	2.84909000	-1.83801000	-0.40760600				
C	3.92990300	-1.88122300	-1.32915400				
C	4.46821700	-3.12429600	-1.67901100				
C	3.98681500	-4.32644600	-1.15982000				
C	2.93599800	-4.26180600	-0.24504400				
C	2.35469400	-3.05030600	0.14679500				
C	4.55979000	-0.65666800	-1.95428100				
C	4.57000500	-5.65214100	-1.58570500				
C	1.21893800	-3.13397300	1.14790600				
H	0.66590400	1.30166400	-1.16500200				
H	5.69052100	1.35733100	2.98564700				
H	4.76494600	4.03568800	-0.21623000				
H	2.55172000	-5.18326800	0.18654600				
				<b>N4</b>			
				<b>E= -2585.04727 au</b>			
				C	-3.93343100	-1.96310200	-0.61087200
				C	-3.81674500	-0.62163800	-0.15069600
				C	-5.01102300	0.06673900	0.20689300
				C	-6.25063800	-0.51468900	-0.07899800
				C	-6.37759400	-1.77485400	-0.66563700
				C	-5.20342100	-2.49154100	-0.88260100
				P	-2.13287400	0.11780300	0.23415000
				C	-0.48324800	-1.24058000	4.03624300
				O	-0.39227700	-1.61954400	5.17432000
				C	-5.04013400	1.38292300	0.95947700
				C	-7.73082800	-2.35106500	-1.00478500
				C	-2.77002700	-2.93341700	-0.73783600
				C	-1.01015900	-0.45707200	-1.21785300

C	0.25364100	0.37771700	-1.22880200	H	-2.06861300	-2.84313500	0.09886400
B	1.72044900	-0.16244000	-0.93714100	H	-3.15019300	-3.95872100	-0.72716600
O	-1.66038900	-1.17284400	3.38380700	H	-8.48452400	-2.06761900	-0.26195300
C	2.04212400	-1.70261900	-0.62538500	H	-8.08399100	-1.98660800	-1.97889000
C	1.44329200	-2.45849600	0.38057000	H	-7.69958700	-3.44426700	-1.05711400
C	1.80069600	-3.77372800	0.66917600	H	-0.65681900	2.91356400	2.95390100
C	2.81215500	-4.37934200	-0.07212500	H	-1.67657300	1.48113800	2.80389400
C	3.44585200	-3.66493000	-1.08712300	H	-0.08810800	1.51578800	2.04228700
C	3.05225100	-2.35375200	-1.33890700	H	-1.19207900	6.73621100	0.33503100
F	0.44210100	-1.92663800	1.12063600	H	-1.91065400	6.67418500	-1.28585200
F	3.69213200	-1.69412300	-2.32726800	H	-2.94728800	6.76301800	0.14004000
F	4.41659500	-4.24305600	-1.80469400	H	-4.10774500	1.21093800	-2.00255100
F	3.16989400	-5.64022300	0.18398100	H	-3.95508400	2.72013600	-2.90891900
F	1.18105200	-4.45591200	1.63844700	H	-2.66481600	1.50761000	-2.96629700
C	2.81917500	0.89375500	-0.44204800	H	0.07982300	1.44908000	-1.16566000
C	2.97435700	1.12073700	0.92628600	H	-1.53520400	-0.83988300	2.46711200
C	3.90940800	2.00209800	1.45891100	H	0.38060900	-0.91538500	3.42992100
C	4.74425200	2.70589200	0.59218300	N	1.15473900	0.08635500	-2.40740200
C	4.62481700	2.51858600	-0.78197300	H	0.84537900	-0.68435900	-2.99388600
C	3.67509600	1.62119300	-1.26689300	H	1.46792800	0.87892100	-2.95978800
F	2.17560400	0.46061000	1.79718500	O	-1.56450400	-0.45114500	-2.53838300
F	4.01276100	2.18347000	2.78036600	H	-2.47812100	-0.77750800	-2.48616500
F	5.64939000	3.56046000	1.07812300				
F	5.41797500	3.19649500	-1.62094700				
F	3.59779900	1.49015000	-2.61446800				
C	-2.18638200	1.97798200	-0.02026900	H	0.000000	0.000000	0.371400
C	-2.73087700	2.66367000	-1.14045400	H	0.000000	0.000000	-0.371400
C	-2.65390300	4.06095600	-1.18827900				
C	-2.05719100	4.81842300	-0.17867600				
C	-1.52571000	4.13283600	0.91235400				
C	-1.58086100	2.73732300	1.01839400				
C	-3.40222600	1.98518300	-2.31589700				
C	-2.01955900	6.32606700	-0.25297400				
C	-0.97226100	2.12322800	2.26583200				
H	-0.74161700	-1.48233300	-0.95904000				
H	-7.15018800	0.03398200	0.19288900				
H	-5.26784300	-3.51496200	-1.24646000				
H	-1.05633400	4.69727300	1.71494600				
H	-3.07918000	4.57284600	-2.04927500				
H	-6.01529800	1.50398000	1.44120800				
H	-4.28008600	1.42408000	1.74583200				
H	-4.87978900	2.25115800	0.31338900				
H	-2.20206600	-2.81818200	-1.66865700				

## H<sub>2</sub> (hydrogen)

E= -1.1754824 au

H	0.000000	0.000000	0.371400
H	0.000000	0.000000	-0.371400

## A<sub>5</sub>

E= -2453.3042293 au

C	3.236260	-1.668440	-1.672379
C	2.092176	-1.368097	-0.931829
C	1.500987	-2.437490	-0.262970
C	2.004535	-3.734772	-0.321747
C	3.146577	-3.990241	-1.077894
C	3.770305	-2.950008	-1.763846
B	1.584075	0.139766	-0.938392
C	2.436967	1.196201	-0.147808
C	2.997893	0.916660	1.106886
C	3.733927	1.844272	1.835527
C	3.958626	3.108343	1.293609
C	3.436377	3.431761	0.042599
C	2.684687	2.484732	-0.645509

F	2.801977	-0.285038	1.682141
F	4.226348	1.537068	3.039259
F	4.671333	4.007039	1.971124
F	3.663518	4.640363	-0.481240
F	2.219982	2.840128	-1.854249
F	0.396649	-2.237043	0.484548
F	1.402356	-4.732028	0.334092
F	3.638830	-5.229357	-1.149596
F	4.862839	-3.189949	-2.497273
F	3.850121	-0.676267	-2.353568
O	0.354312	0.424594	3.411812
C	0.560149	-0.727994	3.415166
O	0.762485	-1.878212	3.439216
C	0.377049	0.550536	-1.866454
C	-0.889641	-0.331561	-1.768397
P	-1.760607	0.073171	-0.128040
C	-2.624265	1.667767	-0.635702
C	-3.703111	1.740760	-1.554141
C	-4.237935	2.991506	-1.889310
C	-3.753535	4.182693	-1.348380
C	-2.703067	4.096873	-0.433811
C	-2.131891	2.872571	-0.066336
C	-4.356147	0.528912	-2.185042
C	-4.329726	5.518885	-1.753562
C	-1.005628	2.908711	0.949043
C	-3.158469	-1.128054	0.249000
C	-3.930851	-0.778229	1.392570
C	-4.964924	-1.617020	1.823573
C	-5.259321	-2.823191	1.191168
C	-4.465060	-3.180276	0.101611
C	-3.423602	-2.375014	-0.376274
C	-3.679010	0.474388	2.205527
C	-2.629658	-2.937001	-1.536972
C	-6.359937	-3.728937	1.690792
H	-0.605816	-1.382960	-1.774414
H	-1.532876	-0.155731	-2.635447
H	0.110542	1.606749	-1.769590
H	0.778871	0.446652	-2.892656
H	-4.657348	-4.125919	-0.401814
H	-5.548339	-1.315263	2.691420
H	-1.598376	-3.162542	-1.241655
H	-2.590971	-2.260508	-2.395237
H	-3.078002	-3.874108	-1.880113

H	-5.968453	-4.487697	2.381911
H	-6.845097	-4.263357	0.866456
H	-7.129381	-3.165193	2.228926
H	-3.942505	1.387894	1.661743
H	-2.622620	0.562293	2.487370
H	-4.268905	0.453632	3.127168
H	-5.064885	3.030294	-2.595991
H	-2.313844	5.009637	0.013097
H	-4.985036	0.833949	-3.027577
H	-4.992396	-0.002519	-1.468858
H	-3.631707	-0.198580	-2.558610
H	-5.366288	5.422689	-2.093549
H	-3.756103	5.964207	-2.577667
H	-4.308961	6.232970	-0.923009
H	-0.839206	3.935757	1.290101
H	-0.061446	2.539902	0.536261
H	-1.216469	2.290571	1.826696

### TS<sub>A56</sub>

E= -2453.2901708au

C	3.729335	-2.131710	0.349958
C	3.479404	-0.904641	-0.318981
C	4.378956	-0.491311	-1.341619
C	5.511271	-1.263795	-1.620218
C	5.786787	-2.454389	-0.949530
C	4.876266	-2.865707	0.023397
P	1.986569	0.197512	-0.096993
C	0.375504	-0.182998	-2.027987
O	1.054232	-0.459344	-2.953614
C	4.176595	0.758925	-2.171584
C	6.999128	-3.287108	-1.290891
C	2.824787	-2.743096	1.399331
C	0.893867	-0.244715	1.369024
C	-0.426474	0.554819	1.279382
B	-1.595232	-0.003445	0.350654
O	-0.695738	0.017763	-1.514837
C	-1.984298	-1.559736	0.491377
C	-1.246438	-2.658328	0.044480
C	-1.635464	-3.981603	0.238892
C	-2.814961	-4.255550	0.923378
C	-3.579624	-3.198804	1.408171
C	-3.155400	-1.891628	1.184927
F	-0.068634	-2.491683	-0.606064



F	-3.927546	-0.915268	1.704101
F	-4.707756	-3.444673	2.084514
F	-3.200068	-5.518079	1.126814
F	-0.875808	-4.986186	-0.215531
C	-2.777201	0.971987	-0.100931
C	-3.625476	0.637310	-1.165816
C	-4.663375	1.453084	-1.604962
C	-4.902551	2.661277	-0.954896
C	-4.099283	3.032513	0.118054
C	-3.061864	2.193062	0.519960
F	-3.451433	-0.519612	-1.827359
F	-5.433880	1.087580	-2.637148
F	-5.896921	3.456387	-1.358130
F	-4.327482	4.188524	0.755278
F	-2.339927	2.614718	1.577230
C	2.620089	1.877855	0.439918
C	3.555873	2.033692	1.495854
C	3.935558	3.323998	1.884893
C	3.430781	4.471120	1.271416
C	2.526368	4.299328	0.222928
C	2.112568	3.033705	-0.208517
C	4.209244	0.877150	2.222506
C	3.831863	5.849929	1.738346
C	1.148194	2.980121	-1.376285
H	-0.875335	0.557409	2.287001
H	0.691108	-1.312716	1.356894
H	6.192336	-0.921404	-2.396486
H	5.058275	-3.798051	0.553820
H	2.128377	5.176677	-0.282333
H	4.652462	3.430526	2.696474
H	4.905308	0.790421	-2.987049
H	3.179696	0.778221	-2.624230
H	4.296251	1.674619	-1.583179
H	2.633698	-2.071306	2.240918
H	1.859278	-3.034606	0.972392
H	3.284032	-3.648600	1.805970
H	7.348711	-3.860248	-0.425512
H	6.771470	-4.007594	-2.087865
H	7.827412	-2.663639	-1.644017
H	0.928428	3.991905	-1.729813
H	1.563969	2.419223	-2.220398
H	0.195530	2.510127	-1.115049
H	3.844103	6.565938	0.909652

H	3.125860	6.232706	2.487431
H	4.824988	5.844756	2.199517
H	4.923991	0.352191	1.580774
H	4.750317	1.241653	3.100863
H	3.488520	0.130608	2.567862
H	-0.215678	1.610533	1.083180
H	1.411490	-0.016070	2.305215

### A<sub>6</sub>

E= -2453.3110813 au

P	1.928982	-0.125583	-0.081329
B	-1.369310	0.013398	-0.125745
O	-0.531295	0.043955	1.194582
O	1.256918	0.070632	2.537781
C	0.850948	0.343972	-1.514691
H	0.622668	1.407502	-1.468492
H	1.388732	0.147192	-2.447708
C	-0.443753	-0.486692	-1.374129
H	-0.196026	-1.552723	-1.331217
H	-1.008928	-0.365051	-2.305777
C	0.723667	0.004315	1.450968
C	3.386048	0.928800	0.363019
C	3.578744	2.234337	-0.162681
C	4.713406	2.954990	0.225197
H	4.853391	3.952126	-0.184669
C	5.658378	2.451777	1.117966
C	5.437605	1.177024	1.638270
H	6.150429	0.764872	2.348519
C	4.325581	0.401691	1.295136
C	2.631608	2.940436	-1.109632
H	1.649834	3.091714	-0.651731
H	2.495304	2.402423	-2.053151
H	3.027418	3.928459	-1.358573
C	6.854689	3.270622	1.536348
H	6.645177	3.820758	2.463114
H	7.123573	4.007304	0.772639
H	7.727724	2.637156	1.725468
C	4.217606	-0.955151	1.959791
H	4.465381	-1.773388	1.275907
H	3.216684	-1.123230	2.360646
H	4.916230	-1.006195	2.799770
C	2.498315	-1.837471	-0.504874
C	3.488652	-1.959443	-1.517299

C 3. 887193 -3. 239327 -1. 917440  
H 4. 639016 -3. 325379 -2. 698470  
C 3. 355148 -4. 399445 -1. 355302  
C 2. 387155 -4. 252369 -0. 360953  
H 1. 952947 -5. 142059 0. 088412  
C 1. 941621 -3. 003307 0. 084990  
C 4. 187566 -0. 791250 -2. 185998  
H 4. 701042 -1. 135173 -3. 088258  
H 4. 937796 -0. 342723 -1. 526225  
H 3. 509583 0. 011848 -2. 488075  
C 3. 820555 -5. 767264 -1. 791323  
H 4. 284421 -5. 736421 -2. 782113  
H 2. 989272 -6. 479449 -1. 824627  
H 4. 564603 -6. 169770 -1. 091392  
C 0. 897216 -2. 999726 1. 180202  
H 0. 643063 -4. 027402 1. 452341  
H -0. 030547 -2. 508292 0. 874817  
H 1. 249096 -2. 498154 2. 086882  
C -2. 618457 -0. 971129 0. 274342  
C -3. 380058 -0. 690305 1. 415320  
F -3. 105812 0. 401004 2. 155125  
C -4. 443645 -1. 478280 1. 848413  
F -5. 131988 -1. 158464 2. 954434  
C -4. 796619 -2. 608383 1. 116679  
F -5. 814882 -3. 381912 1. 514431  
C -4. 081126 -2. 924191 -0. 032331  
F -4. 413339 -4. 009573 -0. 749724  
C -3. 022376 -2. 107280 -0. 428418  
F -2. 392323 -2. 483583 -1. 565230  
C -1. 902235 1. 547778 -0. 411872  
C -3. 010566 1. 763370 -1. 237667  
F -3. 634906 0. 713037 -1. 813559  
C -3. 524277 3. 022785 -1. 537968  
F -4. 594997 3. 156093 -2. 333533  
C -2. 908058 4. 154484 -1. 011583  
F -3. 377549 5. 376020 -1. 293626  
C -1. 783439 3. 999948 -0. 209283  
F -1. 151596 5. 080040 0. 275775  
C -1. 311075 2. 717655 0. 065580  
F -0. 172292 2. 669151 0. 810245

P 1. 92806600 -0. 15664900 -0. 09619200  
B -1. 36983800 -0. 01155000 -0. 13689300  
O -0. 52939100 0. 04140900 1. 18028600  
O 1. 26035600 0. 06871300 2. 52148300  
C 0. 84826500 0. 29716300 -1. 53328600  
H 0. 62129700 1. 36151400 -1. 50012200  
H 1. 38401000 0. 08820900 -2. 46485900  
C -0. 44706200 -0. 53008300 -1. 37961600  
H -0. 20045200 -1. 59561900 -1. 32197700  
H -1. 01368300 -0. 42111400 -2. 31187600  
C 0. 72575400 -0. 00532700 1. 43588700  
C 3. 38684400 0. 90157500 0. 33282100  
C 3. 57752700 2. 20185600 -0. 20628000  
C 4. 71414200 2. 92575300 0. 16955000  
H 4. 85246900 3. 91901400 -0. 25013500  
C 5. 66267100 2. 43083800 1. 06318100  
C 5. 44313000 1. 16172900 1. 59772500  
H 6. 15831600 0. 75669600 2. 30969800  
C 4. 32921300 0. 38369700 1. 26722000  
C 2. 62557800 2. 89923800 -1. 15477800  
H 1. 64449600 3. 05030200 -0. 69519000  
H 2. 48853100 2. 35523700 -2. 09480000  
H 3. 01733300 3. 88712500 -1. 41044900  
C 6. 86118400 3. 25305300 1. 46838200  
H 6. 65705800 3. 80967800 2. 39246400  
H 7. 12515300 3. 98434400 0. 69782500  
H 7. 73557100 2. 62120400 1. 65674400  
C 4. 22183800 -0. 96541700 1. 94758300  
H 4. 46856600 -1. 79163900 1. 27296400  
H 3. 22145100 -1. 12871900 2. 35184200  
H 4. 92160000 -1. 00679900 2. 78715700  
C 2. 49373500 -1. 87444300 -0. 49979300  
C 3. 48317100 -2. 01049000 -1. 51120300  
C 3. 87957200 -3. 29594900 -1. 89545800  
H 4. 63083500 -3. 39300000 -2. 67572600  
C 3. 34628500 -4. 44804900 -1. 31829700  
C 2. 37913000 -4. 28707800 -0. 32517400  
H 1. 94405000 -5. 17040800 0. 13577300  
C 1. 93575000 -3. 03192100 0. 10526400  
C 4. 18308100 -0. 85155400 -2. 19469700  
H 4. 69627700 -1. 20719700 -3. 09255700  
H 4. 93349500 -0. 39525700 -1. 54050000  
H 3. 50553800 -0. 05187000 -2. 50674600

## A7

E= -2454.488293au

C	3.80899700	-5.82211800	-1.73719000	H	0.11686800	1.33877900	-1.20182600
H	4.28690700	-5.80201600	-2.72151700	H	0.87875300	0.16076600	-2.21759100
H	2.97356900	-6.52920700	-1.77680600	C	-0.44919700	-0.49760600	1.85508500
H	4.54016200	-6.22404700	-1.02352400	C	-3.67462500	-1.02822300	0.13971000
C	0.89215000	-3.01274800	1.20108000	C	-4.03251500	-2.13017400	-0.68269600
H	0.63671700	-4.03644300	1.48668300	C	-5.22214000	-2.81872200	-0.41349600
H	-0.03523300	-2.52417700	0.88984900	H	-5.48889600	-3.65425900	-1.05690400
H	1.24536100	-2.49984800	2.10082600	C	-6.07369100	-2.47842400	0.63743500
C	-2.61790800	-0.99054400	0.28019400	C	-5.69933900	-1.40499400	1.44493400
C	-3.37720300	-0.69376800	1.41865800	H	-6.33849800	-1.11820200	2.27688900
F	-3.10146300	0.40783900	2.14244700	C	-4.51958500	-0.68515200	1.23368700
C	-4.43978800	-1.47569200	1.86501800	C	-3.22265500	-2.64399600	-1.85606100
F	-5.12581800	-1.14041400	2.96783700	H	-2.27244400	-3.08941000	-1.54217400
C	-4.79423200	-2.61591000	1.14984000	H	-2.99545800	-1.86648000	-2.58924400
F	-5.81161500	-3.38377900	1.56044300	H	-3.78142300	-3.42603800	-2.37745300
C	-4.08113800	-2.94772300	0.00383900	C	-7.33356500	-3.26387500	0.90919200
F	-4.41478300	-4.04305100	-0.69755600	H	-7.13312300	-4.10682300	1.58385800
C	-3.02332400	-2.13638000	-0.40593700	H	-7.75416000	-3.67893500	-0.01275700
F	-2.39562300	-2.52865400	-1.53862800	H	-8.09900700	-2.64194000	1.38471200
C	-1.90697000	1.51719000	-0.44656600	C	-4.20920400	0.43596700	2.20380100
C	-3.00986300	1.71485600	-1.28422000	H	-4.22227800	1.41783300	1.71884900
F	-3.62146300	0.65294100	-1.85220700	H	-3.22845800	0.30525200	2.67397100
C	-3.53091200	2.96647100	-1.60400200	H	-4.95193000	0.45431400	3.00656000
F	-4.59561700	3.08168600	-2.41013500	C	-2.56893600	1.75321000	-0.35919700
C	-2.92873100	4.10926100	-1.08533700	C	-2.04987400	2.80710900	0.43248900
F	-3.40541900	5.32360900	-1.38461000	C	-2.38789700	4.12745200	0.11218200
C	-1.80972600	3.97191900	-0.27226400	H	-1.98363400	4.92812800	0.72708300
F	-1.19211900	5.06392300	0.20760000	C	-3.21837000	4.44656100	-0.96125600
C	-1.32897800	2.69723300	0.02160600	C	-3.72825800	3.39244300	-1.72087600
F	-0.19613500	2.66651700	0.77734300	H	-4.38697500	3.61492600	-2.55735900
H	0.88914700	5.12268900	2.78218400	C	-3.42818700	2.05278300	-1.45046600
H	0.47934000	4.82247600	2.24065500	C	-1.13206400	2.59228900	1.61372900

## TSA78

E= -2454.354627au

P	-2.09655300	-0.02100200	0.03600100	C	-3.53691800	5.88148600	-1.30482900
B	1.41373200	-0.13819400	-0.08192000	H	-3.52606000	6.51890000	-0.41466800
O	0.61163100	-0.10170400	1.32082100	H	-4.51961100	5.97211800	-1.77931200
O	-0.96355100	-0.43699800	2.93620200	H	-2.79695600	6.28902300	-2.00634700
C	-0.95928600	-0.52359700	-1.37034700	C	-4.06986300	1.01542000	-2.34548900
H	-0.76982400	-1.59907400	-1.28785400	H	-4.59090100	1.50554700	-3.17280700
H	-1.43662800	-0.35371300	-2.33727700	H	-4.80013300	0.40370700	-1.80659800
C	0.35957900	0.27211900	-1.25965000	H	-3.33795300	0.33243700	-2.78593400

C	2.53918300	1.02570800	0.17744100
C	3.33166400	0.96066300	1.33168200
F	3.15538100	-0.04902300	2.20776600
C	4.32310100	1.88471100	1.64870300
F	5.03757000	1.76941100	2.77729600
C	4.57751100	2.93402800	0.77045200
F	5.52515700	3.83623200	1.05070600
C	3.83762000	3.03191200	-0.40180700
F	4.07904800	4.03357900	-1.26102100
C	2.84990400	2.08552900	-0.67865100
F	2.20048800	2.25892100	-1.84914100
C	2.09659000	-1.60867200	-0.28799400
C	2.93755300	-1.78347700	-1.39406500
F	3.13711600	-0.75655400	-2.25019900
C	3.60686600	-2.96823400	-1.68549300
F	4.39512500	-3.06476200	-2.76468900
C	3.45106100	-4.06236800	-0.83892000
F	4.07921900	-5.21448400	-1.09913800
C	2.62934700	-3.94409500	0.27583600
F	2.46376500	-4.99005800	1.09750300
C	1.98127500	-2.73474100	0.52838700
F	1.19708600	-2.72026300	1.63409200
H	-0.83921900	-1.63242600	1.22940500
H	-1.35168300	-1.06045800	0.86508100

## A8

E= -2454.514926au

P	-2.08653600	0.42378000	-0.16212500
B	1.48940100	0.15878800	-0.06177000
O	0.68770300	0.42265800	1.21472500
O	-0.01731500	0.15211400	3.30312200
C	-0.82771200	0.03982600	-1.46977700
H	-0.68801500	-1.04279600	-1.46581500
H	-1.28035000	0.30764100	-2.43118500
C	0.52374400	0.77135300	-1.25131200
H	0.33408900	1.83857400	-1.09714300
H	1.04905800	0.71330000	-2.21366900
C	0.82278300	-0.04243800	2.44163300
C	-3.31342300	-0.89084300	0.23241600
C	-3.64355800	-1.97145000	-0.62336300
C	-4.57512900	-2.91592600	-0.17723900
H	-4.82990800	-3.74018500	-0.83906600
C	-5.17445700	-2.84639300	1.08028900

C	-4.82357900	-1.78000600	1.91043700
H	-5.27406500	-1.70473200	2.89712200
C	-3.90443000	-0.80201900	1.52413800
C	-3.03120000	-2.22152500	-1.98561600
H	-2.05184500	-2.70618900	-1.89244200
H	-2.89719700	-1.31577500	-2.57906100
H	-3.66814800	-2.89811000	-2.56243200
C	-6.14698600	-3.90376800	1.54189400
H	-5.63511800	-4.66550600	2.14442900
H	-6.61573900	-4.41596100	0.69574400
H	-6.93853700	-3.47522700	2.16573900
C	-3.56933500	0.28537600	2.52215500
H	-3.71597900	1.28894800	2.10752300
H	-2.53117600	0.20949500	2.87323100
H	-4.21592300	0.19925500	3.39960300
C	-2.83889900	2.07818400	-0.44072200
C	-3.84273300	2.26425100	-1.42604500
C	-4.39335900	3.53524300	-1.59794500
H	-5.16148600	3.67157900	-2.35571100
C	-3.98483300	4.63204000	-0.83438000
C	-2.98292700	4.42967300	0.11482700
H	-2.63875200	5.27414000	0.70659400
C	-2.39110800	3.17999100	0.33814100
C	-4.33668600	1.15236500	-2.32364100
H	-5.14217300	1.51287100	-2.96924800
H	-4.72306400	0.29993000	-1.75644400
H	-3.54219900	0.78203200	-2.98320400
C	-4.62044100	5.98793400	-1.02181600
H	-4.86096800	6.17560000	-2.07367700
H	-3.96340000	6.79021000	-0.67219800
H	-5.55866900	6.06096400	-0.45605800
C	-1.30092100	3.10318500	1.38742900
H	-1.11744900	4.09874700	1.80030000
H	-0.35487100	2.73107200	0.98514000
H	-1.55595300	2.44530200	2.22528500
C	2.93860900	0.94180600	0.10496800
C	3.95011300	0.40721200	0.90981200
F	3.76982700	-0.79363100	1.51531600
C	5.17364000	1.02342800	1.15410300
F	6.09349100	0.44309000	1.93926700
C	5.43878200	2.25809800	0.57030800
F	6.60680500	2.87600500	0.78775400
C	4.47161300	2.84106600	-0.23874500

F	4.70859800	4.03371400	-0.80792600
C	3.25994400	2.18221500	-0.45123000
F	2.38954700	2.83844800	-1.25468400
C	1.69565100	-1.46116700	-0.35040600
C	2.69951200	-1.93370000	-1.20278000
F	3.55872000	-1.06925100	-1.78373600
C	2.88343400	-3.27731000	-1.52212500
F	3.87382900	-3.65852400	-2.34171500
C	2.02062500	-4.23209100	-0.99232200
F	2.17439600	-5.52840300	-1.29167600
C	0.98481200	-3.81755800	-0.16357400
F	0.12058500	-4.71813900	0.33220300
C	0.84447100	-2.46041900	0.12540900
F	-0.22700300	-2.14229000	0.90408200
H	-1.33582600	0.55750400	1.01166600
H	1.74634000	-0.61047500	2.63344400

## TSA8

E= -2454.486696au

P	-2.03851100	0.29349300	0.02016800
B	1.59661300	0.05795200	-0.37729600
O	0.61043900	0.17673800	1.49858200
O	-0.16020200	-0.32366400	3.56344400
C	-0.91603400	-0.10514100	-1.44313800
H	-0.74135200	-1.18028600	-1.46140700
H	-1.38631000	0.16631100	-2.39238100
C	0.41990000	0.66097900	-1.27706400
H	0.21803800	1.70931600	-1.03229600
H	0.89163700	0.71468400	-2.27361300
C	0.74836200	-0.25759000	2.77656900
C	-3.43107100	-0.93181800	0.26057100
C	-3.75016400	-2.05339500	-0.54747200
C	-4.79787200	-2.89994900	-0.16130200
H	-5.03002500	-3.75342700	-0.79516600
C	-5.54726800	-2.69424900	0.99634900
C	-5.20193100	-1.60673800	1.79835700
H	-5.74985500	-1.43299000	2.72202800
C	-4.15973700	-0.73557100	1.46773800
C	-3.01051000	-2.44134600	-1.81060900
H	-2.02952200	-2.87379700	-1.57991300
H	-2.85271600	-1.59949100	-2.48741700
H	-3.57461500	-3.20256600	-2.35773200
C	-6.69522600	-3.60519300	1.36009400

H	-7.63819300	-3.24767100	0.92467300
H	-6.83756300	-3.65573100	2.44483800
H	-6.53258800	-4.62327100	0.99048000
C	-3.83838900	0.37088000	2.45049900
H	-3.94835600	1.36702200	2.00758100
H	-2.81132900	0.28155100	2.82621200
H	-4.51138800	0.31863200	3.31169500
C	-2.79833700	1.93978700	-0.44832900
C	-3.74640400	2.10821500	-1.49192000
C	-4.24644100	3.38542500	-1.76622300
H	-4.97129300	3.49790800	-2.57017000
C	-3.84731400	4.51518100	-1.04948600
C	-2.90996900	4.33757600	-0.03290700
H	-2.57698800	5.20292100	0.53608100
C	-2.37941600	3.08082000	0.28651200
C	-4.24993200	0.97073800	-2.35171900
H	-5.02816800	1.32467200	-3.03453200
H	-4.66928900	0.15744400	-1.75414900
H	-3.45171300	0.54261900	-2.96959600
C	-4.42931000	5.87547600	-1.35169000
H	-5.40196000	6.00727200	-0.85898400
H	-4.59121300	6.01242700	-2.42657500
H	-3.77371500	6.67908500	-1.00093800
C	-1.36821000	3.02845100	1.41651300
H	-1.25461900	4.02147100	1.86235100
H	-0.37731300	2.71105500	1.07526500
H	-1.66798300	2.33985500	2.21278500
C	2.83551300	0.99739300	0.00664300
C	3.77173200	0.61203200	0.97536400
F	3.62647800	-0.56660700	1.62274300
C	4.86655900	1.38165800	1.35100300
F	5.71227100	0.95748700	2.29752000
C	5.08024200	2.60707100	0.72454200
F	6.12679200	3.36257100	1.06323200
C	4.19209700	3.03469900	-0.25585800
F	4.39119100	4.20674500	-0.87055200
C	3.09930000	2.23612400	-0.59192200
F	2.30323800	2.72207600	-1.56280700
C	1.90850600	-1.51306200	-0.51941600
C	3.03737300	-1.91495400	-1.24475500
F	3.85681500	-0.98745200	-1.78122800
C	3.37234900	-3.24558000	-1.47965500
F	4.46459300	-3.56110600	-2.18542300

C	2.55542800	-4.25255200	-0.97433800
F	2.85716600	-5.53615800	-1.18557700
C	1.41455400	-3.90758400	-0.25656000
F	0.61193100	-4.86561900	0.22288800
C	1.11195100	-2.56259600	-0.05269200
F	-0.02326400	-2.31562300	0.63857800
H	-0.38858300	0.27779000	1.26673100
H	1.79277700	-0.51751900	2.98534600

## B<sub>5</sub>

E= -2492.6143853au

C	-2.769027	-2.120701	-0.668452
C	-2.346271	-1.081271	0.203117
C	-2.191160	-1.390778	1.587268
C	-2.422605	-2.690560	2.046539
C	-2.789600	-3.728482	1.188519
C	-2.975248	-3.409963	-0.155326
P	-1.733795	0.642474	-0.225699
C	4.419111	-1.595054	2.126902
O	4.271249	-2.681208	1.720726
C	-1.748062	-0.363411	2.610032
C	-2.940829	-5.146058	1.685096
C	-3.032982	-1.968942	-2.154384
C	-1.357407	0.794106	-2.106358
C	0.121696	1.244989	-2.230837
B	1.183996	0.560406	-1.271060
O	4.577382	-0.514051	2.544416
C	1.064763	-0.984380	-0.932856
C	1.277894	-1.489903	0.355406
C	1.084662	-2.819353	0.703250
C	0.679361	-3.725278	-0.274195
C	0.483581	-3.283048	-1.578122
C	0.675705	-1.937926	-1.879025
F	1.661570	-0.656590	1.346872
F	0.450664	-1.572417	-3.160191
F	0.076492	-4.138927	-2.524451
F	0.468025	-5.005156	0.042618
F	1.274900	-3.232056	1.960761
C	2.469799	1.356891	-0.790602
C	3.694536	0.717019	-0.521027
C	4.853875	1.380634	-0.135929
C	4.833883	2.763733	0.007936
C	3.653259	3.456013	-0.243797

C	2.516906	2.756574	-0.640281
F	3.817993	-0.618878	-0.637114
F	5.978749	0.698161	0.102482
F	5.931513	3.418586	0.381521
F	3.619938	4.786067	-0.108148
F	1.431342	3.523501	-0.854101
C	-3.105427	1.855276	0.214320
C	-4.500863	1.675780	0.009363
C	-5.392971	2.669585	0.430141
C	-4.971859	3.845504	1.051822
C	-3.603014	4.009443	1.255191
C	-2.667561	3.043784	0.862918
C	-5.111421	0.461879	-0.652882
C	-5.965849	4.883702	1.515357
C	-1.213194	3.334945	1.177589
H	0.458552	1.027447	-3.261616
H	-1.430349	-0.207943	-2.520926
H	-2.292619	-2.899056	3.106408
H	-3.294278	-4.191986	-0.842342
H	-3.244489	4.913891	1.742185
H	-6.456920	2.515141	0.260970
H	-1.770251	-0.796391	3.615123
H	-0.724992	-0.022522	2.411545
H	-2.389773	0.524251	2.616292
H	-3.390489	-0.976364	-2.425613
H	-2.138090	-2.180097	-2.753689
H	-3.795386	-2.689513	-2.468486
H	-3.730392	-5.681215	1.146080
H	-2.007432	-5.705297	1.535690
H	-3.175230	-5.176494	2.754273
H	-1.130142	4.281955	1.720964
H	-0.766046	2.549821	1.796467
H	-0.594326	3.417838	0.280951
H	-6.380642	4.623633	2.498573
H	-5.500650	5.870587	1.608472
H	-6.809892	4.969145	0.821941
H	-4.817945	-0.468704	-0.161943
H	-6.203506	0.527178	-0.629179
H	-4.817576	0.379904	-1.704606
H	0.172873	2.331749	-2.141800
C	-2.279812	1.727060	-2.900429
H	-3.312247	1.365789	-2.931514
H	-2.298278	2.733699	-2.468650

---

H -1.925476 1.815009 -3.935737

**TS<sub>B56</sub>**

E= -2492.5945752au

C -3.559769 -2.272909 -0.198398  
C -3.379960 -0.985252 0.374846  
C -4.282717 -0.563832 1.392799  
C -5.362177 -1.384080 1.740907  
C -5.580077 -2.626946 1.150728  
C -4.657161 -3.048460 0.194219  
P -1.954761 0.181869 0.053373  
C -0.374288 -0.165165 2.015700  
O -1.079782 -0.440418 2.922903  
C -4.151714 0.740342 2.153704  
C -6.737277 -3.504566 1.563474  
C -2.621552 -2.915832 -1.198461  
C -0.837637 -0.223926 -1.447605  
C 0.480499 0.576016 -1.252959  
B 1.639324 0.028600 -0.305975  
O 0.717906 0.035807 1.548893  
C 2.056440 -1.518706 -0.456611  
C 1.344411 -2.631180 -0.004960  
C 1.752267 -3.946638 -0.212255  
C 2.927352 -4.196753 -0.913315  
C 3.667889 -3.124488 -1.401915  
C 3.224152 -1.825900 -1.166421  
F 0.172585 -2.485124 0.660051  
F 3.971344 -0.832415 -1.690152  
F 4.791202 -3.347653 -2.094074  
F 3.330818 -5.451496 -1.129381  
F 1.013896 -4.965933 0.244633  
C 2.805554 1.017798 0.159368  
C 3.646721 0.686406 1.230974  
C 4.674454 1.508761 1.681962  
C 4.909982 2.721063 1.038387  
C 4.113121 3.089727 -0.040153  
C 3.086026 2.243552 -0.454150  
F 3.476375 -0.474164 1.886737  
F 5.438723 1.145465 2.719520  
F 5.894591 3.522501 1.452959  
F 4.337427 4.249841 -0.671361  
F 2.370095 2.664539 -1.516166  
C -2.685861 1.848471 -0.395901

C -3.788157 2.003714 -1.279751  
C -4.207755 3.293826 -1.627063  
C -3.600342 4.443915 -1.122679  
C -2.548408 4.274472 -0.223139  
C -2.086946 3.010098 0.162501  
C -4.609195 0.861331 -1.841124  
C -4.090720 5.818874 -1.509159  
C -0.995162 2.974017 1.213857  
H 0.978182 0.602547 -2.238343  
H -0.619839 -1.288408 -1.359679  
H -6.046789 -1.035283 2.511211  
H -4.785449 -4.026232 -0.265331  
H -2.071043 5.153718 0.203535  
H -5.043697 3.396422 -2.316422  
H -4.804624 0.723356 3.031555  
H -3.130676 0.897073 2.513637  
H -4.430166 1.609804 1.549497  
H -2.485798 -2.320969 -2.104935  
H -1.635882 -3.096222 -0.759013  
H -3.017425 -3.887138 -1.508496  
H -7.115428 -4.092368 0.719928  
H -6.435791 -4.215341 2.344514  
H -7.566322 -2.912324 1.964694  
H -0.728433 3.992727 1.510569  
H -1.328523 2.447512 2.115674  
H -0.080462 2.482115 0.875422  
H -4.984732 6.095961 -0.934785  
H -3.330207 6.583215 -1.320492  
H -4.362499 5.863207 -2.569631  
H -5.389394 0.559622 -1.131576  
H -5.106804 1.173447 -2.764944  
H -4.025308 -0.031136 -2.056600  
H 0.249171 1.627594 -1.060080  
C -1.407102 0.060064 -2.846554  
H -2.303896 -0.519524 -3.078585  
H -1.650747 1.120322 -2.966989  
H -0.650467 -0.194785 -3.599434

**B<sub>6</sub>**

E= -2492.609743au

P -1.868054 -0.143870 -0.176015  
B 1.484489 -0.246848 -0.170734  
O 0.593111 -0.376519 1.106844

O -1.203822 -0.932300 2.316511  
 C -0.774766 0.108881 -1.708565  
 H -1.304925 -0.351552 -2.548403  
 C 0.582398 -0.603055 -1.491797  
 H 1.174020 -0.420892 -2.393200  
 H 0.402218 -1.678779 -1.477401  
 C -0.660351 -0.547522 1.302195  
 C -3.092545 -1.553247 -0.148806  
 C -3.000726 -2.683847 -1.008062  
 C -4.020862 -3.641249 -0.978255  
 H -3.939431 -4.496791 -1.643921  
 C -5.114050 -3.556439 -0.118505  
 C -5.139834 -2.487178 0.773583  
 H -5.947227 -2.425056 1.499197  
 C -4.158676 -1.488972 0.797025  
 C -1.830711 -3.009796 -1.911468  
 H -2.032517 -3.937295 -2.453530  
 H -0.921468 -3.172021 -1.324887  
 H -1.620109 -2.245023 -2.661896  
 C -6.214757 -4.587842 -0.142882  
 H -5.839153 -5.567630 -0.455357  
 H -7.004960 -4.300843 -0.849488  
 H -6.682038 -4.697896 0.841047  
 C -4.327610 -0.437093 1.877001  
 H -3.376247 -0.176423 2.340432  
 H -4.971356 -0.839493 2.664893  
 H -4.802060 0.474990 1.501398  
 C -2.821494 1.433815 0.034011  
 C -3.877327 1.677196 -0.885753  
 C -4.605890 2.865948 -0.775966  
 H -5.414194 3.044545 -1.481400  
 C -4.328148 3.826793 0.196816  
 C -3.271440 3.574294 1.071624  
 H -3.026174 4.313824 1.830052  
 C -2.501694 2.406325 1.016622  
 C -4.293455 0.725691 -1.991176  
 H -3.445777 0.274110 -2.514547  
 H -4.882326 1.264500 -2.739091  
 H -4.910680 -0.094861 -1.610410  
 C -5.115095 5.112092 0.276628  
 H -5.277290 5.417291 1.315882  
 H -6.091599 5.015567 -0.208190  
 H -4.579199 5.930795 -0.221263

C -1.391629 2.276061 2.035654  
 H -1.617123 1.520130 2.794715  
 H -1.249356 3.229077 2.551954  
 H -0.430971 2.005518 1.594392  
 C 2.152771 1.262094 -0.126349  
 C 2.333578 2.001143 1.049219  
 F 1.927536 1.523486 2.244690  
 C 2.922544 3.266257 1.092937  
 F 3.040071 3.921587 2.258048  
 C 3.394624 3.846681 -0.076797  
 F 3.961786 5.059159 -0.056960  
 C 3.264051 3.147477 -1.272043  
 F 3.717621 3.685509 -2.414581  
 C 2.666085 1.891335 -1.266649  
 F 2.608734 1.281373 -2.476150  
 C 2.600888 -1.448081 0.026749  
 C 3.987342 -1.320385 -0.095032  
 F 4.558020 -0.134278 -0.390774  
 C 4.879829 -2.381198 0.069586  
 F 6.200186 -2.185842 -0.060294  
 C 4.396752 -3.649007 0.368776  
 F 5.238662 -4.677547 0.528321  
 C 3.023626 -3.836488 0.492720  
 F 2.535234 -5.055205 0.769764  
 C 2.173451 -2.749332 0.317854  
 F 0.847138 -3.025106 0.434403  
 C -0.625901 1.607804 -2.031829  
 H -0.257488 2.186518 -1.181655  
 H 0.112995 1.700858 -2.833695  
 H -1.562283 2.056512 -2.371198

**B7**

**E= -2493.795986au**

P -1.92177000 0.12647400 -0.08892800  
 B 1.37837000 0.04330900 -0.07613700  
 O 0.53534700 -0.05359800 1.22632100  
 O -1.27976300 -0.04438300 2.53091400  
 C -0.81306800 -0.30303700 -1.54842200  
 H -0.54249300 -1.35091800 -1.40823800  
 C 0.45465000 0.55633000 -1.32030600  
 H 0.17747500 1.61492300 -1.26297800  
 H 1.05303500 0.47899400 -2.23638500  
 C -0.72455300 0.00616100 1.45397700



C	-3.31945400	-0.99543500	0.39892400
C	-3.41177100	-2.33818900	-0.05616200
C	-4.50616100	-3.11230600	0.34507900
H	-4.56915600	-4.13677700	-0.01319900
C	-5.49959200	-2.63070100	1.19556900
C	-5.36207200	-1.32687000	1.66936000
H	-6.10461100	-0.93542900	2.36080900
C	-4.29584400	-0.49613500	1.30872200
C	-2.38219200	-3.04024400	-0.91695000
H	-1.40463600	-3.06490100	-0.42645100
H	-2.26607400	-2.58568900	-1.90508300
H	-2.68471400	-4.07817400	-1.07844400
C	-6.65070400	-3.50386800	1.63076100
H	-6.41958300	-4.01018000	2.57716600
H	-6.86820100	-4.27972100	0.88978100
H	-7.56098200	-2.91653200	1.79081600
C	-4.27818300	0.87877700	1.94718900
H	-4.64024300	1.65899900	1.26974500
H	-3.28016800	1.15089100	2.29196900
H	-4.93308900	0.87644600	2.82331900
C	-2.56026600	1.83670900	-0.42425900
C	-3.65944300	1.98010300	-1.31505200
C	-4.08570800	3.26778500	-1.66068800
H	-4.92362900	3.36561300	-2.34719600
C	-3.48398700	4.41832800	-1.15442500
C	-2.43088700	4.25245000	-0.25410200
H	-1.95927500	5.13397600	0.17282400
C	-1.95121700	2.99636800	0.13211300
C	-4.48050600	0.83783900	-1.88141000
H	-4.95019700	1.14769100	-2.81979400
H	-5.28153300	0.55592600	-1.18762100
H	-3.90879600	-0.06657000	-2.08273000
C	-3.94187700	5.79375900	-1.57300500
H	-4.96745000	5.77693200	-1.95501100
H	-3.30010500	6.19288400	-2.36937500
H	-3.89835500	6.50109100	-0.73802100
C	-0.83993700	2.98691500	1.16039000
H	-0.55486100	4.01377300	1.40317300
H	0.06172900	2.47782200	0.81401500
H	-1.15061400	2.50422100	2.09245700
C	2.60820900	1.04190800	0.35550300
C	3.37509500	0.73886500	1.48732500
F	3.11386800	-0.37490900	2.19777400

C	4.43122200	1.52609500	1.93961600
F	5.12574100	1.18365000	3.03485800
C	4.77055500	2.67926900	1.23788800
F	5.78167000	3.45231100	1.65411200
C	4.04855000	3.01892700	0.09983100
F	4.36654300	4.12767700	-0.58762000
C	2.99754600	2.20183900	-0.31608300
F	2.35757200	2.60551300	-1.43794300
C	1.97025300	-1.45951400	-0.41617400
C	3.01317200	-1.59340400	-1.33896300
F	3.50317300	-0.49711400	-1.96002800
C	3.59165400	-2.80997900	-1.69164600
F	4.59187700	-2.86340100	-2.58269100
C	3.11448500	-3.98337100	-1.11419100
F	3.64816100	-5.16656200	-1.44139700
C	2.06083100	-3.91082500	-0.21046700
F	1.56599800	-5.03578700	0.33114100
C	1.51747100	-2.66817500	0.11298900
F	0.45651600	-2.70320300	0.96260700
H	-0.40658100	-5.20878300	2.99159600
H	-0.04211000	-4.87653100	2.43648900
C	-1.40727800	-0.11619400	-2.95022300
H	-2.23936100	-0.79332500	-3.16815200
H	-1.74317800	0.91241900	-3.11272800
H	-0.61625000	-0.32354800	-3.67957800

## TSB78

E= -2493.666824au

P	2.05313600	0.05866900	0.04241800
B	-1.44693900	-0.05219500	0.01117400
O	-0.67007100	-0.00743300	-1.40546100
O	1.02942400	-0.42695200	-2.87065400
C	0.89892300	-0.30074600	1.51905500
H	0.71251200	-1.37933000	1.49521900
C	-0.42022600	0.44941500	1.18779100
H	-0.17721900	1.50903800	1.04845800
H	-1.00421700	0.43540400	2.11434000
C	0.45155500	-0.43729100	-1.81202600
C	3.50680100	-1.08954700	-0.23143300
C	3.73693000	-2.31603500	0.44776300
C	4.84340800	-3.09519400	0.08833700
H	5.01359500	-4.02537500	0.62577500
C	5.72565400	-2.73274100	-0.92879400

C	5.45881300	-1.54925500	-1.61620400
H	6.11331900	-1.25091500	-2.43208600
C	4.36652300	-0.73128200	-1.31067800
C	2.85715900	-2.88141800	1.54372900
H	1.85637300	-3.13901500	1.17849900
H	2.73646600	-2.19922000	2.38797700
H	3.29581400	-3.80375900	1.93393000
C	6.89415900	-3.61155000	-1.30340900
H	6.60755400	-4.33790600	-2.07548000
H	7.26117600	-4.17977700	-0.44236200
H	7.72565900	-3.02268800	-1.70444600
C	4.17021500	0.49809800	-2.17462200
H	4.41077600	1.42511500	-1.64436100
H	3.14249800	0.57303000	-2.54213100
H	4.82022000	0.43997900	-3.05257500
C	2.69108200	1.79191600	0.32126000
C	2.07505700	2.87495700	-0.35590600
C	2.49346500	4.17863900	-0.06558300
H	2.01224500	5.00363100	-0.58538500
C	3.50793200	4.45241900	0.85162500
C	4.13680200	3.36771700	1.46504000
H	4.95483500	3.55316400	2.15775500
C	3.76379000	2.04121900	1.21932200
C	1.00639200	2.70702200	-1.41273200
H	0.83293900	3.65848300	-1.92370500
H	0.04831900	2.38438400	-0.99558300
H	1.28991300	1.97637200	-2.17653700
C	3.90835800	5.87141300	1.17475800
H	3.72038300	6.54303200	0.33087000
H	4.96926100	5.93971800	1.43761600
H	3.33545600	6.25384000	2.02993200
C	4.59589700	0.96670700	1.88711200
H	5.13390800	1.38670600	2.74235600
H	5.34097300	0.56115700	1.19254900
H	4.00871700	0.12167400	2.24530700
C	-2.62297200	1.06442100	-0.25972500
C	-3.44569300	0.89882100	-1.38336700
F	-3.25769300	-0.15779100	-2.19927200
C	-4.48070100	1.76296500	-1.72802000
F	-5.22221100	1.54832800	-2.82427000
C	-4.75034800	2.85721000	-0.91154000
F	-5.73970700	3.70445300	-1.21865800
C	-3.98088600	3.05701700	0.22773400

F	-4.23409100	4.10336000	1.02872400
C	-2.95026500	2.16665200	0.53427500
F	-2.27696000	2.44609300	1.67188500
C	-2.08436000	-1.53717600	0.28016200
C	-2.89013100	-1.70716400	1.41363900
F	-3.09762100	-0.66701100	2.25213400
C	-3.52136300	-2.90079500	1.75153800
F	-4.27504500	-2.99011200	2.85575600
C	-3.36523100	-4.01077100	0.92622200
F	-3.95691400	-5.17090900	1.23176100
C	-2.58162900	-3.89802100	-0.21614200
F	-2.41619300	-4.95707500	-1.02066900
C	-1.97250600	-2.67903500	-0.51403900
F	-1.22597000	-2.67085900	-1.64746800
H	0.62285000	-1.61436100	-1.25183800
H	1.12708700	-1.02465100	-0.79578000
C	1.39173300	0.09763300	2.91765300
H	2.27011200	-0.45958200	3.25381700
H	1.62934500	1.16530800	2.96011600
H	0.58758400	-0.09103100	3.63846900

## B8

E= -2493.822617au

P	-2.04989900	0.35752700	-0.16609400
B	1.49521700	0.20925300	-0.02731400
O	0.65982300	0.28693700	1.24606400
O	0.23089900	-0.08170500	3.40068200
C	-0.79422100	0.02238700	-1.54294800
H	-0.61138200	-1.05332500	-1.49564400
C	0.52528500	0.78541500	-1.23451800
H	0.28746400	1.84385900	-1.11101900
H	1.10583600	0.74136300	-2.16786600
C	0.96976500	-0.18618100	2.44066400
C	-2.95504700	-1.05593600	0.59515600
C	-3.17680700	-2.31091800	-0.02029600
C	-3.89112700	-3.28567100	0.68591600
H	-4.06354900	-4.24611800	0.20596600
C	-4.37312700	-3.07681600	1.97722200
C	-4.12161700	-1.83927300	2.57310600
H	-4.47442200	-1.65503300	3.58502200
C	-3.41597100	-0.82471100	1.92314900
C	-2.64927100	-2.72285200	-1.37645500
H	-1.63384400	-3.12441100	-1.27583300

H	-2.62054100	-1.91384600	-2.10709200
H	-3.26982900	-3.51979100	-1.79652800
C	-5.11251700	-4.16045200	2.72296700
H	-4.44356100	-4.67304100	3.42633000
H	-5.51450400	-4.91606900	2.04094200
H	-5.94256700	-3.74918100	3.30766800
C	-3.13980100	0.44427700	2.70050700
H	-3.42144000	1.34978900	2.15256500
H	-2.07552900	0.50613100	2.97025800
H	-3.71057500	0.44081600	3.63319900
C	-3.15341200	1.77908100	-0.55836600
C	-4.36077100	1.60570800	-1.28188400
C	-5.13296300	2.73018200	-1.58613700
H	-6.05333000	2.59114500	-2.14851800
C	-4.76386400	4.01750300	-1.19202100
C	-3.58303000	4.16233400	-0.46209800
H	-3.28202400	5.15546100	-0.13785800
C	-2.76426000	3.07844700	-0.12540400
C	-4.89168500	0.25781300	-1.71811900
H	-5.73163600	0.38806000	-2.40625200
H	-5.24775800	-0.32894100	-0.86441100
H	-4.14299500	-0.34827200	-2.23501500
C	-5.62980200	5.21063600	-1.51522300
H	-6.21094400	5.04852500	-2.42866000
H	-5.02972800	6.11686500	-1.64657800
H	-6.34329100	5.40707100	-0.70397500
C	-1.53113300	3.37858700	0.70614300
H	-1.50344500	4.44432700	0.94833800
H	-0.59202300	3.14252000	0.19840700
H	-1.52810900	2.83277700	1.65648500
C	2.84676700	1.13469400	0.24269800
C	3.98763600	0.60869200	0.86023600
F	4.02905700	-0.69815700	1.21671300
C	5.12804100	1.34460300	1.17084500
F	6.18445200	0.76126200	1.75603300
C	5.16300600	2.70292600	0.87476400
F	6.24616400	3.43493800	1.16349000
C	4.05028500	3.28946600	0.28531700
F	4.05510400	4.60288600	0.00710700
C	2.93217500	2.50767700	-0.00463400
F	1.89543500	3.19312300	-0.55194100
C	1.86102400	-1.35234000	-0.45099900
C	2.87850700	-1.64296600	-1.36648000

F	3.64939000	-0.64749400	-1.85656200
C	3.16036200	-2.92035600	-1.84393100
F	4.16065200	-3.12332700	-2.71391300
C	2.37899300	-3.99480300	-1.42750800
F	2.61623100	-5.22916000	-1.89027200
C	1.33517600	-3.76008600	-0.54156800
F	0.52720900	-4.76831600	-0.16821200
C	1.10552400	-2.46460300	-0.07906000
F	0.03380800	-2.32983900	0.74817600
H	-1.24163700	0.80911600	0.88292000
H	1.95247600	-0.68296700	2.50180200
C	-1.33682900	0.39048200	-2.93492300
H	-2.24614400	-0.15015800	-3.21726100
H	-1.54446800	1.46257300	-3.00816600
H	-0.56912500	0.14882200	-3.67750400

### TSB8

E= -2493.791851au

P	1.96321300	-0.35459500	-0.01745000
B	-1.67145700	-0.15167000	-0.39343200
O	-0.65550700	-0.29270700	1.54902800
O	0.17166400	0.22024400	3.59120900
C	0.84360600	-0.09765000	-1.56120100
H	0.67414000	0.97820900	-1.62439000
C	-0.51363700	-0.80192000	-1.27492000
H	-0.33328200	-1.84575800	-0.99922300
H	-1.02913900	-0.88795300	-2.24975000
C	-0.75370500	0.15071400	2.82251200
C	3.17223900	1.02696800	0.34680200
C	3.39016900	2.22300100	-0.38575200
C	4.30886100	3.16395300	0.09286600
H	4.46472000	4.07179000	-0.48692700
C	5.02619200	2.98588100	1.27647500
C	4.77943100	1.82337900	2.00275200
H	5.30442900	1.66346400	2.94190500
C	3.86165600	0.85400900	1.58021700
C	2.66707300	2.59497100	-1.66214100
H	1.63187200	2.88970900	-1.45522500
H	2.64540000	1.78744700	-2.39675600
H	3.15448300	3.45266300	-2.13524600
C	6.01827700	4.02119500	1.75038300
H	6.83899500	4.14674600	1.03268700
H	6.45708900	3.74204300	2.71339500

H	5.54428500	5.00325400	1.86997700
C	3.63411900	-0.32643800	2.50288000
H	3.86603300	-1.28572700	2.02818200
H	2.59290700	-0.36232600	2.84622200
H	4.26897900	-0.23636800	3.38961300
C	2.97417500	-1.88748100	-0.38691700
C	4.16104500	-1.90575400	-1.16775400
C	4.80333800	-3.12617600	-1.40849700
H	5.70408100	-3.12550700	-2.01936400
C	4.33521800	-4.33600500	-0.89399400
C	3.19092700	-4.29859100	-0.09815900
H	2.81579700	-5.22453000	0.33244300
C	2.50960800	-3.10674000	0.17776800
C	4.82732900	-0.66820000	-1.72965100
H	5.56203100	-0.94853800	-2.49106300
H	5.35382900	-0.11329900	-0.94542100
H	4.12405000	0.02906700	-2.18627700
C	5.06552100	-5.63104800	-1.15912800
H	5.92419900	-5.74631300	-0.48424400
H	5.45308500	-5.66995400	-2.18322200
H	4.41297300	-6.49719800	-1.00904600
C	1.32202800	-3.19848700	1.11798600
H	1.21029900	-4.22575900	1.47845600
H	0.37529100	-2.91585500	0.64813400
H	1.45052200	-2.55122100	1.99234100
C	-2.91711700	-1.05919800	0.03165100
C	-3.81844200	-0.64077200	1.02005600
F	-3.62817100	0.53951000	1.65064600
C	-4.91965000	-1.38154900	1.43290500
F	-5.73023700	-0.92818300	2.39629100
C	-5.17713700	-2.60889800	0.82688400
F	-6.23137200	-3.33590100	1.20149200
C	-4.32425800	-3.06886700	-0.17015800
F	-4.56521900	-4.24351600	-0.76443800
C	-3.22248200	-2.29982900	-0.54308800
F	-2.46073300	-2.81606500	-1.52624900
C	-1.94682100	1.42098900	-0.54098600
C	-3.08384600	1.85318500	-1.23581300
F	-3.95175400	0.94955600	-1.73436000
C	-3.37644600	3.19230200	-1.47952000
F	-4.47728300	3.53905400	-2.15637100
C	-2.50635700	4.17504900	-1.01630200
F	-2.76486500	5.46542800	-1.24130900

C	-1.35770800	3.79786100	-0.32744200
F	-0.49867100	4.72956100	0.10382400
C	-1.10184000	2.44611300	-0.10890400
F	0.03886600	2.16350300	0.55713500
H	0.33202600	-0.40279500	1.27781200
H	-1.79102100	0.42001800	3.05675500
C	1.39781200	-0.59717000	-2.90521000
H	2.33166400	-0.10878200	-3.19334500
H	1.58255900	-1.67587200	-2.87977800
H	0.66740500	-0.40296600	-3.70116900

## C<sub>5</sub>

E= -2684.3457682au

C	-0.617427	3.026240	0.438339
C	-0.724119	1.955174	-0.486440
C	-0.418137	2.201009	-1.854242
C	-0.044207	3.487741	-2.255552
C	0.063638	4.551931	-1.360035
C	-0.229181	4.291025	-0.022663
P	-1.144145	0.180149	-0.052174
C	3.387871	3.054130	-2.798439
O	3.567068	4.094958	-2.294594
C	-0.485683	1.142126	-2.932115
C	0.506103	5.919686	-1.819053
C	-0.912559	2.925490	1.919208
C	-1.571744	-0.277029	1.773664
C	-0.734517	-1.577743	1.705665
B	0.485126	-1.142386	0.717761
O	3.212890	2.026790	-3.327308
C	1.540091	-0.030816	1.282806
C	2.365600	0.699901	0.418159
C	3.361184	1.573262	0.842407
C	3.575633	1.757038	2.204673
C	2.784272	1.060740	3.111480
C	1.797098	0.192997	2.642403
F	2.213623	0.576961	-0.914404
F	1.078451	-0.430448	3.599167
F	2.975657	1.225293	4.427480
F	4.526119	2.591694	2.635002
F	4.114032	2.239249	-0.048364
C	1.281465	-2.326819	-0.056136
C	1.677889	-2.410067	-1.392246
C	2.424841	-3.463751	-1.917563

C	2.836779	-4.497475	-1.084640
C	2.487145	-4.459165	0.261213
C	1.732249	-3.391149	0.739084
F	1.319586	-1.463427	-2.287893
F	2.747556	-3.485328	-3.218106
F	3.557717	-5.513937	-1.570016
F	2.881502	-5.440672	1.083514
F	1.456341	-3.407377	2.060544
C	-2.676886	-0.231209	-1.055367
C	-3.787584	0.657538	-1.040379
C	-4.925515	0.338463	-1.790397
C	-5.024525	-0.827002	-2.549295
C	-3.937945	-1.700360	-2.528449
C	-2.769778	-1.431837	-1.804998
C	-3.842731	1.946967	-0.250813
C	-6.255768	-1.125217	-3.370329
C	-1.667452	-2.461434	-1.887567
H	-0.454217	-1.927728	2.701022
H	-1.018122	0.424733	2.394271
H	0.167482	3.656051	-3.309695
H	-0.157589	5.101830	0.698679
H	-3.992381	-2.627092	-3.095196
H	-5.767440	1.026947	-1.765776
H	0.047705	1.482445	-3.824419
H	-0.018566	0.208503	-2.616956
H	-1.519040	0.921501	-3.221339
H	-1.897014	2.496290	2.121418
H	-0.167400	2.320892	2.447490
H	-0.893772	3.921364	2.371138
H	1.593455	5.944687	-1.962824
H	0.044210	6.189157	-2.775652
H	0.248912	6.691616	-1.086813
H	-2.015772	-3.342576	-2.434546
H	-0.792706	-2.071479	-2.411813
H	-1.330871	-2.798740	-0.904178
H	-6.180511	-0.676331	-4.369817
H	-6.395100	-2.202571	-3.507647
H	-7.158675	-0.720560	-2.900771
H	-3.235814	2.734455	-0.707955
H	-4.874661	2.306815	-0.201192
H	-3.498170	1.815702	0.777805
H	-1.327119	-2.379542	1.246797
C	-2.983508	-0.371944	2.297499

C	-3.912876	-1.295551	1.791478
C	-3.378897	0.431047	3.380671
C	-5.193476	-1.395486	2.334765
H	-3.636660	-1.943979	0.966825
C	-4.659185	0.332297	3.927703
H	-2.667048	1.127245	3.817371
C	-5.574818	-0.579880	3.402411
H	-5.894334	-2.117260	1.923582
H	-4.935105	0.962166	4.769359
H	-6.572087	-0.662120	3.826085

### TSc<sub>56</sub>

E= -2684.3224687au

C	-3.281287	2.405352	-0.344252
C	-3.083238	1.137483	-0.946711
C	-3.841340	0.818895	-2.111704
C	-4.781353	1.735874	-2.595030
C	-4.999748	2.975987	-1.998039
C	-4.232420	3.284231	-0.876746
P	-1.772358	-0.128674	-0.496573
C	0.029552	0.282065	-2.385776
O	-0.620935	0.642417	-3.296433
C	-3.714745	-0.477856	-2.884757
C	-5.997606	3.956925	-2.565486
C	-2.522388	2.894948	0.865101
C	-0.719940	0.145561	1.112098
C	0.587146	-0.677224	0.890116
B	1.794716	-0.091743	0.028993
O	1.054575	-0.011159	-1.832659
C	2.209467	1.443366	0.292195
C	1.510956	2.576781	-0.126877
C	1.893257	3.880796	0.176692
C	3.030901	4.096497	0.947512
C	3.757404	3.001789	1.406527
C	3.338700	1.715610	1.074817
F	0.373072	2.459545	-0.856832
F	4.071477	0.700958	1.575295
F	4.844502	3.191411	2.163122
F	3.411486	5.338717	1.256797
F	1.165793	4.919479	-0.253133
C	2.995685	-1.071956	-0.378814
C	3.926528	-0.694692	-1.357006
C	4.987968	-1.498626	-1.759769

C	5.165079	-2.743465	-1.161219
C	4.277337	-3.160156	-0.175574
C	3.219916	-2.329282	0.191952
F	3.814585	0.498721	-1.967503
F	5.838491	-1.087818	-2.708831
F	6.179243	-3.529874	-1.530982
F	4.442287	-4.352776	0.411639
F	2.413947	-2.803579	1.162919
C	-2.694203	-1.728516	-0.203711
C	-3.882632	-1.799194	0.568009
C	-4.505302	-3.042418	0.745820
C	-4.003105	-4.219837	0.194347
C	-2.839593	-4.130456	-0.573881
C	-2.183564	-2.915842	-0.796941
C	-4.549001	-0.602623	1.211448
C	-4.693882	-5.546370	0.403939
C	-0.981576	-2.945349	-1.721012
H	1.049230	-0.796206	1.883700
H	-0.471593	1.206552	1.087941
H	-5.354940	1.464989	-3.479142
H	-4.371813	4.246778	-0.389248
H	-2.432735	-5.032662	-1.025937
H	-5.411593	-3.085353	1.346105
H	-4.203093	-0.376848	-3.858723
H	-2.671418	-0.743635	-3.072749
H	-4.183061	-1.318812	-2.363121
H	-2.575258	2.187657	1.694686
H	-1.468082	3.074938	0.630155
H	-2.940151	3.843213	1.216175
H	-5.547498	4.561193	-3.364481
H	-6.863667	3.443523	-2.997343
H	-6.359991	4.649366	-1.798419
H	-0.718494	-3.979470	-1.963218
H	-1.197690	-2.434165	-2.667483
H	-0.094300	-2.470201	-1.298161
H	-5.111104	-5.929429	-0.536185
H	-3.995813	-6.305289	0.777077
H	-5.515607	-5.461178	1.121724
H	-5.108116	-0.012433	0.477089
H	-5.254327	-0.935186	1.979350
H	-3.832766	0.066694	1.691791
H	0.337630	-1.702518	0.602892
C	-1.293953	-0.172015	2.486571

C	-1.620153	-1.483416	2.873851
C	-1.372609	0.835075	3.462777
C	-2.055529	-1.762489	4.169160
H	-1.528659	-2.295512	2.161832
C	-1.805431	0.557825	4.761385
H	-1.065988	1.847435	3.214106
C	-2.159322	-0.742954	5.117920
H	-2.306731	-2.784962	4.438916
H	-1.853361	1.359275	5.493961
H	-2.496150	-0.963987	6.127069

## C<sub>6</sub>

E= -2684.3337121au

P	1.809161	-0.160522	-0.004016
B	-1.585826	-0.285802	0.020611
O	-0.654313	-0.246613	-1.226983
O	0.982644	-1.274441	-2.357836
C	0.713376	0.433968	1.454885
H	1.223740	0.062392	2.343065
C	-0.709058	-0.205527	1.422894
H	-1.282284	0.354242	2.168276
H	-0.622233	-1.210000	1.842498
C	0.548031	-0.667037	-1.405783
C	2.898191	-1.662363	0.238670
C	2.827045	-2.523420	1.370379
C	3.654664	-3.649612	1.419511
H	3.579344	-4.301772	2.286293
C	4.558524	-3.970919	0.408515
C	4.622153	-3.111081	-0.683451
H	5.314997	-3.335022	-1.490610
C	3.825361	-1.965170	-0.802572
C	1.938632	-2.325927	2.579130
H	1.986514	-3.210881	3.218828
H	0.892853	-2.183157	2.311583
H	2.262442	-1.477275	3.194139
C	5.439388	-5.191919	0.506571
H	4.875848	-6.061718	0.861845
H	6.262390	-5.028594	1.214714
H	5.881668	-5.444913	-0.461742
C	4.067104	-1.137559	-2.049727
H	3.138220	-0.839427	-2.533142
H	4.631081	-1.733435	-2.773006
H	4.657092	-0.241438	-1.831310

C	2.914122	1.254413	-0.476272
C	3.981737	1.555101	0.413352
C	4.839922	2.614609	0.107293
H	5.653020	2.836313	0.794732
C	4.684631	3.395271	-1.038230
C	3.624728	3.087524	-1.889336
H	3.480474	3.684803	-2.786134
C	2.727252	2.040893	-1.643708
C	4.280034	0.790200	1.687161
H	3.384638	0.581514	2.278696
H	4.949096	1.377998	2.322101
H	4.769958	-0.167589	1.483411
C	5.608714	4.553321	-1.325294
H	5.660981	4.768178	-2.397396
H	6.623840	4.355280	-0.965265
H	5.258147	5.465869	-0.825243
C	1.644465	1.832478	-2.680808
H	1.805046	0.919869	-3.263129
H	1.644004	2.671413	-3.381854
H	0.639384	1.771034	-2.259188
C	-2.626659	0.976552	-0.106797
C	-2.680293	1.929527	-1.124549
F	-1.808080	1.904687	-2.161633
C	-3.580877	2.996376	-1.140868
F	-3.559606	3.889050	-2.144043
C	-4.499232	3.138028	-0.108785
F	-5.371071	4.154840	-0.108049
C	-4.494403	2.211597	0.930390
F	-5.374930	2.328425	1.935549
C	-3.574262	1.170530	0.903732
F	-3.637566	0.289819	1.929851
C	-2.323640	-1.764404	-0.115168
C	-3.676406	-2.019315	-0.362391
F	-4.566799	-1.019202	-0.510792
C	-4.212015	-3.303317	-0.483309
F	-5.522206	-3.473395	-0.710860
C	-3.383783	-4.413615	-0.375793
F	-3.883871	-5.649749	-0.491474
C	-2.024787	-4.220610	-0.150443
F	-1.200843	-5.275108	-0.051650
C	-1.543131	-2.921934	-0.032872
F	-0.197261	-2.817170	0.166245
C	0.709614	1.951333	1.584225

C	1.205465	2.521491	2.766458
C	0.166783	2.805407	0.614261
C	1.162978	3.900699	2.976681
H	1.613866	1.878124	3.542796
C	0.126647	4.184240	0.819408
H	-0.238414	2.399847	-0.303510
C	0.624031	4.738565	2.000455
H	1.545965	4.315947	3.905042
H	-0.302741	4.824933	0.054134
H	0.585947	5.812607	2.159906

## C7

E= -2685.52347au

P	-1.74276200	-0.05204400	-0.41406000
B	1.55649000	-0.08977300	-0.16268000
O	0.82908200	0.06087200	-1.52391600
O	-0.88069900	0.08979100	-2.96218000
C	-0.73563800	0.25639800	1.18304600
H	-0.43049800	1.30221800	1.12559000
C	0.52288000	-0.63042100	0.97736300
H	0.21926000	-1.67051100	0.81890000
H	1.04785700	-0.64098700	1.93843300
C	-0.41073500	0.02915000	-1.84582300
C	-3.02353300	1.14525300	-1.04837900
C	-3.04758000	2.50627600	-0.64735100
C	-4.04911500	3.34579800	-1.14619400
H	-4.05823900	4.38354900	-0.82222900
C	-5.01393600	2.90862600	-2.05080500
C	-4.93125800	1.58639000	-2.48420200
H	-5.64320000	1.22959000	-3.22481900
C	-3.95598400	0.69244200	-2.02792600
C	-2.02791000	3.15201000	0.26265200
H	-1.00986600	3.02080800	-0.11441400
H	-2.08152400	2.76499400	1.28228800
H	-2.20960100	4.22862300	0.31829100
C	-6.06796200	3.84469800	-2.58908800
H	-5.73541200	4.30888600	-3.52686900
H	-6.28428200	4.65297300	-1.88323400
H	-7.00263400	3.31541900	-2.80223300
C	-3.97889300	-0.68359600	-2.66519700
H	-4.44735000	-1.43819700	-2.02577400
H	-2.97602000	-1.02148700	-2.92675300
H	-4.55622100	-0.63626500	-3.59310800

C	-2.52151000	-1.71813600	-0.21055300
C	-3.71120500	-1.79774400	0.56381100
C	-4.28538000	-3.05446000	0.78689500
H	-5.19343600	-3.10702100	1.38310600
C	-3.73706800	-4.23069700	0.27828300
C	-2.57772300	-4.12438400	-0.49203700
H	-2.14003900	-5.02643100	-0.91231000
C	-1.95230500	-2.90170000	-0.75821700
C	-4.45639300	-0.60945000	1.13950100
H	-5.05056400	-0.93026200	1.99985800
H	-5.14272400	-0.18030900	0.39998100
H	-3.80463800	0.19433900	1.48367200
C	-4.35961400	-5.57524700	0.56452100
H	-5.41340500	-5.47853000	0.84390300
H	-3.84334700	-6.07645400	1.39382400
H	-4.29460900	-6.23920500	-0.30409400
C	-0.73844000	-2.94886300	-1.66272700
H	-0.48114200	-3.98890200	-1.87929700
H	0.14771600	-2.48520600	-1.22451700
H	-0.92643700	-2.45060300	-2.61923300
C	2.79848800	-1.10610800	-0.51747100
C	3.67422400	-0.77620000	-1.55937400
F	3.50017200	0.36888000	-2.24665000
C	4.75388300	-1.56780400	-1.94283900
F	5.55527900	-1.19761200	-2.95269200
C	5.00411900	-2.75509500	-1.26083700
F	6.03567400	-3.53329800	-1.61203100
C	4.17094900	-3.12391700	-0.21135700
F	4.40132900	-4.26621800	0.45567400
C	3.09977300	-2.30128100	0.13705200
F	2.34504300	-2.73924600	1.17167700
C	2.16270300	1.37999700	0.27706600
C	3.07581800	1.44913200	1.33508400
F	3.41886500	0.32190500	1.99796000
C	3.66867100	2.62837700	1.77836300
F	4.53869500	2.62061000	2.79822600
C	3.34525600	3.82907100	1.15243100
F	3.89570800	4.97802100	1.56328200
C	2.42798700	3.82076000	0.10813600
F	2.08555600	4.97401900	-0.48888900
C	1.86458500	2.61310200	-0.30292000
F	0.95017100	2.71030700	-1.30226600
H	0.42702600	5.30250000	-3.33210600

H	0.71195100	4.93763700	-2.75151600
C	-1.41657600	0.02030800	2.52232900
C	-1.70403900	1.10052200	3.37140900
C	-1.66584400	-1.27697700	3.00150400
C	-2.26009700	0.90039800	4.63645200
H	-1.45892800	2.11185000	3.06084600
C	-2.22386000	-1.47930700	4.26349600
H	-1.40919400	-2.13690800	2.39360600
C	-2.53237200	-0.39209800	5.08402000
H	-2.46543100	1.75593000	5.27406900
H	-2.40610700	-2.49276400	4.61079200
H	-2.96165900	-0.55266100	6.06909200

## TSC78

E= -2685.395691au

P	1.88713100	-0.05125600	-0.40036600
B	-1.61921700	-0.05031900	-0.23589900
O	-0.91624100	-0.05906300	-1.69127800
O	0.68199700	-0.57134700	-3.23609200
C	0.80075900	-0.33901900	1.17105900
H	0.58475100	-1.41238400	1.15349300
C	-0.51550700	0.44391600	0.87379800
H	-0.24791600	1.48952400	0.68838400
H	-1.04836500	0.47565200	1.82832900
C	0.16567200	-0.54573800	-2.14451800
C	3.29688700	-1.23350500	-0.78849000
C	3.58624000	-2.43287600	-0.08781600
C	4.59977700	-3.27600400	-0.55830500
H	4.81127700	-4.18583800	-0.00105600
C	5.34264400	-2.99456900	-1.70349300
C	5.03518100	-1.82150900	-2.39133400
H	5.59035900	-1.57617400	-3.29387300
C	4.02714500	-0.94351800	-1.97905700
C	2.87671900	-2.87579000	1.16941500
H	1.82786200	-3.13802800	0.98585200
H	2.89729500	-2.10806700	1.94533600
H	3.35743600	-3.76879200	1.57880200
C	6.41098900	-3.93824900	-2.19955000
H	5.99214700	-4.67190400	-2.90111000
H	6.86553500	-4.49844300	-1.37580400
H	7.20586400	-3.40132600	-2.72769500
C	3.80046500	0.27778200	-2.84685200
H	4.16523200	1.19504300	-2.37369600



H 2.74455600 0.41444200 -3.09245200  
H 4.33410900 0.15901000 -3.79432800  
C 2.61626400 1.66232200 -0.28200200  
C 2.02013000 2.74144100 -0.97932400  
C 2.57672700 4.01987300 -0.84326700  
H 2.10962200 4.84573900 -1.37400800  
C 3.70764300 4.26536100 -0.06596800  
C 4.29460200 3.17953100 0.58854500  
H 5.18280900 3.34343200 1.19515300  
C 3.78350600 1.88109700 0.50117500  
C 0.82805900 2.59575700 -1.89750600  
H 0.60292000 3.55300400 -2.37621300  
H -0.07489200 2.27576400 -1.37163700  
H 1.00906400 1.86845700 -2.69590200  
C 4.29142100 5.65203700 0.05848300  
H 3.68265100 6.39204900 -0.46946000  
H 5.30593500 5.69341300 -0.35722600  
H 4.36215000 5.96026700 1.10858600  
C 4.53709500 0.79440100 1.23688400  
H 5.18500600 1.24089200 1.99686100  
H 5.16984600 0.21680800 0.55422400  
H 3.87374200 0.09252300 1.74568800  
C -2.76001000 1.11349000 -0.46146400  
C -3.64782400 0.96403600 -1.53703100  
F -3.54753300 -0.11339700 -2.34126800  
C -4.66301100 1.86497400 -1.84420400  
F -5.46926400 1.66296600 -2.89625100  
C -4.84407900 2.98321200 -1.03591000  
F -5.81243900 3.86606900 -1.30732500  
C -4.00775900 3.16951400 0.05743800  
F -4.17517100 4.23889800 0.85043600  
C -2.99967700 2.24203300 0.32741000  
F -2.25732500 2.51426000 1.42279300  
C -2.29802800 -1.50312500 0.09479800  
C -3.03533700 -1.62807100 1.27978300  
F -3.14498800 -0.57272200 2.11668100  
C -3.69452000 -2.79029000 1.67012900  
F -4.37850900 -2.83756600 2.82118500  
C -3.64104700 -3.91242200 0.84827000  
F -4.26139400 -5.04286700 1.20402700  
C -2.92920600 -3.84356600 -0.34354400  
F -2.86230500 -4.91530000 -1.14557400  
C -2.28849300 -2.65510600 -0.69339500

F -1.61645000 -2.68971100 -1.87211400  
H 0.27194700 -1.72240700 -1.61097900  
H 0.88370700 -1.18800400 -1.14673400  
C 1.31453400 0.01761100 2.55809700  
C 1.36166400 -0.96402500 3.56130400  
C 1.60504200 1.34332600 2.92308800  
C 1.72822600 -0.64634300 4.87083200  
H 1.08296800 -1.98731500 3.32372900  
C 1.97704800 1.66164200 4.22880300  
H 1.52982400 2.13548000 2.18712300  
C 2.04829000 0.66830300 5.20798600  
H 1.75124100 -1.42708700 5.62638100  
H 2.20024300 2.69431300 4.48354600  
H 2.33317900 0.92042600 6.22570500

### C8

E= -2685.55267au

P -1.91799200 -0.23628500 -0.34277000  
B 1.64193100 -0.21739100 -0.20094800  
O 0.89593400 -0.18291000 -1.53009000  
O 0.68804100 0.24753100 -3.70704400  
C -0.74238500 0.09466000 1.12023400  
H -0.49083100 1.15002100 1.00189000  
C 0.54883600 -0.76295300 0.91267500  
H 0.25607000 -1.79955700 0.73653400  
H 1.04615200 -0.77756400 1.89148700  
C 1.33702600 0.29797700 -2.68027800  
C -2.65805900 1.19533400 -1.24606800  
C -2.90012300 2.47233900 -0.68612700  
C -3.47404400 3.46206600 -1.49246300  
H -3.66140100 4.43885300 -1.05300400  
C -3.79822100 3.24566400 -2.83041700  
C -3.53333300 1.98414500 -3.36688200  
H -3.76791000 1.79132400 -4.41090700  
C -2.96375700 0.95340800 -2.61648200  
C -2.53640300 2.87819400 0.72218600  
H -1.49102000 3.20887000 0.75788100  
H -2.66794100 2.08200000 1.45492900  
H -3.15219300 3.72364100 1.04329200  
C -4.38942300 4.34207200 -3.68205600  
H -3.62812700 4.77246500 -4.34540300  
H -4.79089900 5.15500300 -3.06921000  
H -5.19572500 3.96280500 -4.31961400

C	-2.66381500	-0.34435900	-3.33301000
H	-3.04795700	-1.22135800	-2.80244500
H	-1.58003800	-0.45285600	-3.48186200
H	-3.12721200	-0.33786500	-4.32339900
C	-3.13656900	-1.58501700	-0.05227600
C	-4.37184100	-1.33413100	0.59803700
C	-5.26922500	-2.39030100	0.77144000
H	-6.21315900	-2.19193500	1.27366700
C	-4.99087800	-3.68542200	0.32946000
C	-3.76617300	-3.91093300	-0.30094400
H	-3.52842100	-4.91385000	-0.64671400
C	-2.82452400	-2.89624800	-0.50995800
C	-4.76407000	0.02331000	1.13334800
H	-5.74832200	-0.02563300	1.60726900
H	-4.81257500	0.77873200	0.34293500
H	-4.05662800	0.37307000	1.89298800
C	-5.99297900	-4.79996700	0.50663600
H	-6.57245100	-4.67498000	1.42728900
H	-5.50335900	-5.77838900	0.53925800
H	-6.70718500	-4.81875900	-0.32721100
C	-1.53963300	-3.28510900	-1.21762100
H	-1.56628400	-4.34926100	-1.46683300
H	-0.64318700	-3.12215000	-0.61232700
H	-1.39698500	-2.73959200	-2.15693500
C	2.93679300	-1.23449400	-0.41753100
C	4.14658500	-0.77582300	-0.95255700
F	4.30236300	0.53451400	-1.26168800
C	5.24806900	-1.58307000	-1.22338200
F	6.37426400	-1.06069900	-1.73059400
C	5.17042900	-2.94792800	-0.96835500
F	6.21378100	-3.74841700	-1.21952500
C	3.98748000	-3.46786900	-0.45863700
F	3.88412400	-4.78496800	-0.22013400
C	2.91223900	-2.61590800	-0.20618100
F	1.80250100	-3.24091700	0.26638900
C	2.09292500	1.29502300	0.31107500
C	3.07504400	1.47746400	1.29102000
F	3.74523600	0.41257400	1.78173700
C	3.41890500	2.71339900	1.83281000
F	4.38010300	2.81205200	2.76271600
C	2.74251300	3.85677600	1.41583400
F	3.04158900	5.05326300	1.93838000
C	1.73754000	3.73157300	0.46507300

F	1.03119100	4.80961200	0.08224400
C	1.44361300	2.47312000	-0.05901100
F	0.41224000	2.44619100	-0.94681800
H	-1.03610700	-0.76553300	-1.29018900
H	2.34215300	0.74910200	-2.63885100
C	-1.34688100	-0.10972500	2.50140300
C	-1.36341400	0.95430500	3.41697700
C	-1.78391000	-1.36973000	2.94219100
C	-1.82814100	0.77589400	4.72184300
H	-0.98603700	1.92721500	3.11384100
C	-2.25390000	-1.54795700	4.24310600
H	-1.74714500	-2.22142100	2.27128800
C	-2.28372200	-0.47515700	5.13723000
H	-1.82480100	1.61473100	5.41253500
H	-2.58843100	-2.53172800	4.56111500
H	-2.64560100	-0.61772300	6.15167300

## TSC8

E= -2685.521236au

P	-1.80787000	-0.17682800	-0.47546400
B	1.80052300	-0.16773200	0.11059200
O	0.91588400	-0.10148700	-1.81777300
O	0.29381800	0.62749400	-3.86644400
C	-0.76292900	-0.04602600	1.15931700
H	-0.53375200	1.01718900	1.23875200
C	0.56768500	-0.82217600	0.88845700
H	0.34157500	-1.82548400	0.51553600
H	1.01792200	-1.01684900	1.87683900
C	1.14288600	0.46047400	-3.02932200
C	-2.91960100	1.27473200	-0.89690000
C	-3.16896300	2.44146600	-0.13513700
C	-3.98370500	3.45201300	-0.66392300
H	-4.16322800	4.33755500	-0.05784300
C	-4.56672300	3.36604900	-1.92568800
C	-4.28775100	2.22654000	-2.68060700
H	-4.70464400	2.13853800	-3.68171300
C	-3.47088300	1.19416100	-2.21026100
C	-2.58906400	2.69967800	1.23418600
H	-1.52562400	2.96020900	1.16917000
H	-2.68762600	1.84071800	1.89874500
H	-3.09651500	3.54457600	1.70969200
C	-5.46921700	4.45480700	-2.45490500
H	-6.52709900	4.17515800	-2.36021300

H	-5.28170100	4.64883700	-3.51704500
H	-5.32795400	5.39306700	-1.90860400
C	-3.19306700	0.05274100	-3.16697900
H	-3.51751400	-0.91671900	-2.77557300
H	-2.12347100	-0.01267600	-3.39970500
H	-3.72238800	0.21942500	-4.11005400
C	-2.92662800	-1.66220600	-0.30359600
C	-4.14413800	-1.65710500	0.42298700
C	-4.91240700	-2.82801300	0.47639200
H	-5.84213300	-2.81204400	1.04105400
C	-4.52667500	-4.00749700	-0.15809200
C	-3.33099500	-3.99406700	-0.88096700
H	-3.01314800	-4.89818000	-1.39629900
C	-2.52983300	-2.85203300	-0.97640300
C	-4.67711700	-0.44700600	1.15424100
H	-5.52764200	-0.72911800	1.78221000
H	-5.01249700	0.32960100	0.45983600
H	-3.92151000	-0.00110600	1.80597200
C	-5.36505200	-5.26062800	-0.07014000
H	-5.61713300	-5.64292500	-1.06680200
H	-6.30093000	-5.07934200	0.46736500
H	-4.82843600	-6.06190600	0.45373600
C	-1.28223600	-2.95313300	-1.83393700
H	-1.18884600	-3.96439500	-2.24176400
H	-0.36361000	-2.73989000	-1.27966500
H	-1.31423600	-2.25629100	-2.67879600
C	3.03160200	-1.10794700	-0.29903200
C	4.03716500	-0.65135100	-1.16192300
F	3.96685400	0.59705100	-1.67788300
C	5.13008500	-1.41295000	-1.55836300
F	6.04602100	-0.91567600	-2.39783100
C	5.26721600	-2.70864000	-1.06625800
F	6.30933900	-3.45919200	-1.42846700
C	4.30664000	-3.21142800	-0.19621000
F	4.42954700	-4.45321500	0.28747500
C	3.21977700	-2.41589100	0.16572000
F	2.34948000	-2.98172300	1.02345000
C	2.14704600	1.36860000	0.42824600
C	3.25217100	1.67074600	1.23420200
F	4.04164700	0.67937500	1.69390600
C	3.59035700	2.96282100	1.62756100
F	4.65819400	3.18267100	2.40316900
C	2.80120800	4.03137500	1.21163700

F	3.10348500	5.27821900	1.58156200
C	1.68606800	3.78433600	0.41725100
F	0.90191400	4.79707400	0.02775900
C	1.38414000	2.47544000	0.04852200
F	0.27640700	2.31983600	-0.71079900
H	-0.09274700	-0.19961200	-1.63056700
H	2.20236700	0.72054700	-3.14000300
C	-1.35067400	-0.49967800	2.48849000
C	-1.40449100	0.39351900	3.57153800
C	-1.72931500	-1.83304200	2.72141000
C	-1.85637900	-0.01390400	4.82851800
H	-1.07008800	1.41874600	3.43617700
C	-2.18233000	-2.24226500	3.97561700
H	-1.66908200	-2.56022400	1.91925800
C	-2.25522800	-1.33433700	5.03425900
H	-1.88617600	0.70131200	5.64643200
H	-2.47491900	-3.27820900	4.12554700
H	-2.60722000	-1.65631400	6.01055900

**D<sub>5</sub>**

**E= -2861.977578au**

C	-3.686122	-2.315910	-0.189180
C	-3.451218	-1.102289	0.507977
C	-4.365752	-0.738200	1.537205
C	-5.503359	-1.518565	1.770971
C	-5.774035	-2.679676	1.048862
C	-4.837002	-3.064069	0.090701
P	-1.939418	0.013412	0.377848
C	-0.076584	-0.876134	3.454303
O	-1.047189	-1.420976	3.809100
C	-4.160258	0.460390	2.439920
C	-7.027018	-3.486311	1.293977
C	-2.745198	-2.906354	-1.219385
C	-0.933581	-0.339153	-1.205735
C	0.341507	0.549949	-1.190695
B	1.575431	0.025964	-0.399473
O	0.908115	-0.328894	3.135446
C	1.974781	-1.523642	-0.493404
C	1.296147	-2.565449	0.135601
C	1.674872	-3.901943	0.028884
C	2.789984	-4.236385	-0.733544
C	3.507743	-3.229428	-1.375351
C	3.094246	-1.909366	-1.232579

F	0.213271	-2.307297	0.904300
F	3.824642	-0.963759	-1.867271
F	4.580322	-3.537384	-2.113407
F	3.166140	-5.512028	-0.854286
F	0.975220	-4.859046	0.649221
C	2.544283	0.972427	0.420771
C	3.488396	0.468454	1.338810
C	4.329834	1.272192	2.102417
C	4.262206	2.655340	1.972300
C	3.345275	3.213599	1.086514
C	2.513256	2.378740	0.348456
F	3.613810	-0.849265	1.551718
F	5.198693	0.726254	2.959525
F	5.064098	3.439129	2.691211
F	3.268724	4.542792	0.955190
F	1.656096	3.014744	-0.473364
C	-2.634827	1.691181	-0.130136
C	-3.594841	1.890737	-1.155959
C	-3.975741	3.195472	-1.496762
C	-3.449671	4.320487	-0.860799
C	-2.526147	4.110434	0.164142
C	-2.114919	2.827464	0.545493
C	-4.285059	0.763342	-1.895686
C	-3.851619	5.715983	-1.276388
C	-1.143653	2.726538	1.707026
H	-0.654818	-1.389842	-1.226904
H	-6.190480	-1.209826	2.556458
H	-4.999226	-3.986766	-0.463127
H	-2.114498	4.969084	0.691010
H	-4.712293	3.332241	-2.286371
H	-4.895256	0.453243	3.250671
H	-3.163315	0.445878	2.897163
H	-4.259923	1.411630	1.906938
H	-2.581246	-2.244445	-2.075069
H	-1.767989	-3.139560	-0.781966
H	-3.155321	-3.842775	-1.609087
H	-7.860342	-3.126513	0.675003
H	-6.877381	-4.544194	1.052417
H	-7.348697	-3.419395	2.339061
H	-0.870459	3.726947	2.057901
H	-1.585345	2.184595	2.550899
H	-0.221991	2.198754	1.448566
H	-3.879301	6.397592	-0.419117

H	-3.139045	6.135028	-1.999644
H	-4.839019	5.725024	-1.749851
H	-5.008255	0.249944	-1.253675
H	-4.825235	1.155289	-2.763483
H	-3.591827	-0.001793	-2.254627
H	0.070219	1.561202	-0.875510
H	-1.546182	-0.150510	-2.091442
Si	0.843256	0.897577	-3.058636
C	2.500447	1.792616	-3.256512
H	3.335049	1.218017	-2.843726
H	2.699388	1.938054	-4.326108
H	2.494804	2.779223	-2.783476
C	0.912409	-0.722631	-4.039184
H	0.005005	-1.325369	-3.922451
H	1.021024	-0.497439	-5.107744
H	1.768762	-1.340466	-3.749052
C	-0.515156	2.014612	-3.763232
H	-0.280083	2.274567	-4.803236
H	-1.502933	1.541954	-3.755638
H	-0.593558	2.948534	-3.194927

### TS<sub>D56</sub>

E= -2861.9573406au

C	-3.806625	2.285588	0.075996
C	-3.567929	1.057727	-0.598883
C	-4.473407	0.655551	-1.618742
C	-5.600448	1.440164	-1.892528
C	-5.864492	2.629014	-1.217324
C	-4.946046	3.030744	-0.245742
P	-2.080952	-0.058020	-0.388227
C	-0.488352	0.340925	-2.330783
O	-1.172050	0.566003	-3.267449
C	-4.286756	-0.594551	-2.452746
C	-7.083426	3.464183	-1.528481
C	-2.895573	2.883366	1.128002
C	-0.965925	0.382012	1.070106
C	0.350789	-0.449868	1.016183
B	1.505592	0.063867	0.049858
O	0.584817	0.209028	-1.799655
C	1.974411	1.608907	0.190904
C	1.231718	2.737605	-0.168410
C	1.662593	4.048677	0.027437
C	2.901329	4.285190	0.611057

C	3.687072	3.199815	0.986663
C	3.217475	1.909143	0.763479
F	0.008017	2.624705	-0.741747
F	4.046082	0.909772	1.139641
F	4.885125	3.403078	1.547249
F	3.328696	5.534129	0.814031
F	0.885556	5.076728	-0.336721
C	2.586429	-0.964331	-0.555211
C	3.551935	-0.540720	-1.485211
C	4.488488	-1.384161	-2.074279
C	4.488049	-2.738258	-1.754182
C	3.544179	-3.219666	-0.855558
C	2.619274	-2.340998	-0.293959
F	3.608050	0.744755	-1.874961
F	5.381541	-0.907190	-2.949862
F	5.378332	-3.564106	-2.308161
F	3.518971	-4.522458	-0.544579
F	1.731320	-2.922274	0.544732
C	-2.730566	-1.728846	0.158943
C	-3.667315	-1.872592	1.216115
C	-4.058327	-3.157792	1.610454
C	-3.565147	-4.311926	1.000287
C	-2.661770	-4.152225	-0.050747
C	-2.236597	-2.891769	-0.487197
C	-4.312927	-0.708172	1.937402
C	-3.979269	-5.684792	1.473399
C	-1.273175	-2.851563	-1.656364
H	-0.746789	1.444236	1.036367
H	-6.285655	1.107585	-2.669174
H	-5.116944	3.964362	0.286567
H	-2.273759	-5.034903	-0.554417
H	-4.775862	-3.254721	2.422726
H	-5.020585	-0.617765	-3.263951
H	-3.292680	-0.622603	-2.910852
H	-4.412009	-1.510145	-1.865191
H	-2.706598	2.202521	1.962960
H	-1.929103	3.173956	0.703500
H	-3.349859	3.786790	1.544848
H	-7.700566	3.618319	-0.634618
H	-6.801645	4.457851	-1.898747
H	-7.709453	2.989286	-2.290261
H	-1.089356	-3.864430	-2.027080
H	-1.668033	-2.260892	-2.489494

H	-0.304057	-2.422996	-1.384726
H	-3.970437	-6.410917	0.653642
H	-3.293895	-6.058509	2.245885
H	-4.984175	-5.673441	1.908450
H	-5.028862	-0.185707	1.294996
H	-4.851300	-1.064366	2.820897
H	-3.588855	0.039175	2.273575
H	0.093533	-1.484770	0.771173
H	-1.517254	0.197092	1.996757
S	0.938435	-0.626708	2.869164
C	2.671267	-1.347095	3.117723
H	3.453223	-0.740049	2.654730
H	2.879588	-1.391355	4.194637
H	2.747417	-2.364614	2.723734
C	0.870934	1.063461	3.732695
H	-0.119649	1.528356	3.670646
H	1.108168	0.942356	4.797139
H	1.597235	-1.769869	3.315263
C	-0.287730	-1.806508	3.710256
H	-0.048277	-1.899822	4.777097
H	-1.330410	-1.478203	3.635141
H	-0.227072	-2.808602	3.269327

## D<sub>6</sub>

E= -2861.97531au

C	-3.775909	2.296241	0.026141
C	-3.529799	1.037879	-0.586906
C	-4.437356	0.547382	-1.569078
C	-5.555947	1.319808	-1.897623
C	-5.817408	2.556046	-1.308775
C	-4.915223	3.016003	-0.350595
P	-2.047845	-0.006332	-0.187861
C	-0.851408	0.191336	-1.714387
O	-1.375854	0.329305	-2.799204
C	-4.293134	-0.774535	-2.293390
C	-7.015623	3.378789	-1.713915
C	-2.894642	2.949678	1.069995
C	-0.955935	0.455748	1.241933
C	0.349519	-0.379075	1.135752
B	1.278149	0.096684	-0.139446
O	0.403727	0.204317	-1.452187
C	1.894392	1.622482	0.069430
C	1.175642	2.787113	-0.209044

C	1.656485	4.081479	-0.023474
C	2.945558	4.265088	0.460588
C	3.716780	3.144445	0.751452
C	3.184807	1.872779	0.548934
F	-0.104801	2.723714	-0.676640
F	4.014639	0.847756	0.849629
F	4.964914	3.297013	1.214632
F	3.433339	5.496144	0.652039
F	0.882432	5.142255	-0.298999
C	2.416207	-0.984464	-0.654626
C	3.316489	-0.616193	-1.665528
C	4.266433	-1.470433	-2.217457
C	4.342291	-2.787270	-1.774096
C	3.461608	-3.216070	-0.790445
C	2.524934	-2.322343	-0.269809
F	3.301919	0.636131	-2.162274
F	5.102473	-1.041200	-3.173488
F	5.245160	-3.627938	-2.292852
F	3.503911	-4.486688	-0.358764
F	1.690788	-2.864480	0.657554
C	-2.597231	-1.736063	0.192495
C	-3.566224	-1.900490	1.220471
C	-3.946707	-3.195764	1.586113
C	-3.416163	-4.332862	0.976750
C	-2.482824	-4.144812	-0.042811
C	-2.056063	-2.877671	-0.455833
C	-4.265977	-0.761108	1.935668
C	-3.819195	-5.718392	1.418339
C	-1.053135	-2.829403	-1.587360
H	-0.745384	1.520124	1.188073
H	-6.242203	0.935415	-2.648382
H	-5.096236	3.976502	0.125630
H	-2.063221	-5.014897	-0.541608
H	-4.685271	-3.313544	2.375592
H	-4.994230	-0.811543	-3.132005
H	-3.289410	-0.894748	-2.703971
H	-4.512837	-1.627376	-1.642849
H	-2.725109	2.310192	1.941147
H	-1.921872	3.231108	0.657170
H	-3.370185	3.864895	1.432199
H	-7.363946	4.012584	-0.891895
H	-6.767076	4.040785	-2.553880
H	-7.848064	2.744228	-2.035130

H	-0.814649	-3.844902	-1.913983
H	-1.434211	-2.285746	-2.457035
H	-0.113450	-2.357654	-1.292422
H	-3.842115	-6.416526	0.575021
H	-3.104758	-6.117106	2.150498
H	-4.806697	-5.718458	1.890658
H	-5.003717	-0.274653	1.289117
H	-4.792861	-1.143523	2.814333
H	-3.584985	0.019880	2.285499
H	0.059649	-1.426245	0.989529
H	-1.515190	0.272229	2.164840
Si	1.090156	-0.425555	2.920418
C	2.811454	-1.191747	3.078102
H	3.558835	-0.658685	2.486433
H	3.121834	-1.149205	4.130191
H	2.815923	-2.241245	2.769723
C	1.132255	1.319801	3.672052
H	0.141507	1.789039	3.709393
H	1.502616	1.269787	4.703714
H	1.796707	1.991468	3.117953
C	-0.089959	-1.490294	3.968729
H	0.250585	-1.518216	5.011459
H	-1.123388	-1.122391	3.977971
H	-0.111749	-2.524232	3.603166

## D7

E= -2863.152431au

P	-2.04552100	-0.03839300	-0.17372700
B	1.27940100	0.08325900	-0.13096600
O	0.40207300	0.21195300	-1.43885200
O	-1.38080700	0.33673100	-2.78160800
C	-0.95164500	0.40705300	1.26009400
H	-0.74440300	1.47295400	1.22163100
H	-1.50743800	0.20841400	2.18194900
C	0.35564500	-0.42228700	1.13594900
H	0.06857700	-1.46681500	0.96700300
C	-0.85356100	0.18947400	-1.69953100
C	-3.53433100	1.00273100	-0.55256700
C	-3.78504300	2.25042800	0.07979700
C	-4.92876600	2.97014600	-0.28340100
H	-5.11314000	3.92267800	0.20728300
C	-5.83070900	2.52010400	-1.24648700
C	-5.56480600	1.29385100	-1.85413500



C	5. 41316700	-2. 82822300	0. 00647200	C	-3. 79756400	3. 40065600	-1. 26012900
H	5. 71021200	-3. 68188200	0. 61124600	F	-4. 51745200	4. 45438800	-1. 66010800
C	6. 24812100	-2. 41575100	-1. 02926500	C	-3. 03810800	3. 46430400	-0. 10009800
C	5. 82954900	-1. 32619000	-1. 79441600	F	-3. 02024600	4. 59143500	0. 62697800
H	6. 45029600	-0. 98592600	-2. 62062600	C	-2. 28805300	2. 35624700	0. 29986900
C	4. 62734600	-0. 65893600	-1. 54901300	F	-1. 58607900	2. 54531200	1. 44358600
C	3. 41665800	-2. 78597900	1. 46295000	C	-2. 20957900	-1. 59219700	-0. 08184500
H	2. 45636900	-3. 20435000	1. 14508400	C	-3. 58033400	-1. 65433700	0. 20243700
H	3. 21618100	-2. 05774800	2. 25311500	F	-4. 27811500	-0. 53802700	0. 50362000
H	3. 98600500	-3. 60314600	1. 91430100	C	-4. 32522700	-2. 83277000	0. 22013300
C	7. 54629900	-3. 12546900	-1. 32904800	F	-5. 63233300	-2. 80470800	0. 50800000
H	7. 52314700	-3. 59070500	-2. 32250000	C	-3. 70614800	-4. 04265800	-0. 07089000
H	7. 75144500	-3. 91223400	-0. 59668200	F	-4. 40135800	-5. 18378700	-0. 06413600
H	8. 39248100	-2. 42781900	-1. 32144600	C	-2. 34657600	-4. 04531100	-0. 36125600
C	4. 26602400	0. 47860800	-2. 48147800	F	-1. 72090900	-5. 19728600	-0. 63881300
H	4. 21896900	1. 44130700	-1. 96203900	C	-1. 64756600	-2. 84171700	-0. 35470600
H	3. 29798000	0. 31274100	-2. 96783100	F	-0. 31966100	-2. 95576800	-0. 63449100
H	5. 01406400	0. 56721300	-3. 27465000	H	1. 05100400	-1. 68418700	-1. 72811800
C	2. 57363200	1. 64257700	0. 13549100	H	1. 55017900	-1. 12345600	-1. 32949100
C	2. 06063500	2. 71846100	-0. 63133300	Si	-0. 95892400	-0. 33290100	2. 94595500
C	2. 35150100	4. 03247900	-0. 24392700	C	-0. 95269100	-2. 19824200	3. 31492300
H	1. 95185700	4. 84733100	-0. 84299600	H	-1. 23624400	-2. 36857200	4. 36125900
C	3. 12989000	4. 32798500	0. 87348100	H	-1. 66810000	-2. 74399000	2. 69000600
C	3. 63644200	3. 25533500	1. 60809500	H	0. 03334600	-2. 65525100	3. 16870200
H	4. 25852800	3. 45792700	2. 47709300	C	0. 21619900	0. 51462400	4. 17932800
C	3. 37955400	1. 92079900	1. 27434400	H	-0. 16441800	0. 39813000	5. 20192000
C	1. 19543400	2. 53895200	-1. 85652600	H	1. 23148200	0. 09977700	4. 16747000
H	1. 07604000	3. 49281800	-2. 37849600	H	0. 29293900	1. 58998400	3. 97790900
H	0. 19381100	2. 18487200	-1. 59353900	C	-2. 69625300	0. 33235900	3. 30055900
H	1. 61317400	1. 82617700	-2. 57145600	H	-2. 70714200	1. 42623700	3. 31232400
C	3. 39983400	5. 75446000	1. 28658300	H	-3. 44631900	0. 00195700	2. 57776900
H	3. 39545400	6. 42950500	0. 42458500	H	-3. 01202600	-0. 01683200	4. 29211500
H	4. 36676900	5. 84997000	1. 79170400				
H	2. 63076600	6. 11174200	1. 98418400				
C	3. 99574000	0. 87077600	2. 17344700				
H	4. 67318500	1. 34415200	2. 88972500				
H	4. 56698100	0. 12620700	1. 61502100				
H	3. 23797200	0. 33868500	2. 75962700				
C	-2. 25403200	1. 14633200	-0. 39898000				
C	-3. 03952200	1. 14353100	-1. 56264800				
F	-3. 09526100	0. 03503500	-2. 32790000				
C	-3. 79791400	2. 22265000	-2. 00181100				
F	-4. 52494500	2. 14079100	-3. 12440200				
				<b>D8</b>			
				<b>E= -2863.178768au</b>			
				P	2. 20081700	0. 29580400	-0. 09513300
				B	-1. 36587500	-0. 02924200	-0. 22534700
				O	-0. 48972300	0. 12583000	-1. 47637100
				O	0. 12520400	-0. 23012000	-3. 58279000
				C	0. 92400700	-0. 11513200	1. 19721400
				H	0. 78544100	-1. 19613600	1. 16531300
				H	1. 39685900	0. 11450100	2. 15865900
				C	-0. 43168500	0. 63233900	0. 99372000



H	-0.19691900	1.66075300	0.69482100	C	-3.83967500	0.22809000	-1.25437300
C	-0.68151100	-0.37278000	-2.68185400	F	-3.84252100	-1.09668700	-1.53442500
C	3.45588100	-0.99020800	-0.50521000	C	-4.96891400	0.92225400	-1.68383300
C	3.80315500	-2.07524300	0.33727700	F	-5.98020700	0.27933800	-2.28541000
C	4.76650800	-2.98700900	-0.10920400	C	-5.03588800	2.29863100	-1.50037200
H	5.03539500	-3.81385100	0.54383500	F	-6.10813300	2.98921600	-1.90630400
C	5.37871900	-2.88270900	-1.35827200	C	-3.96362200	2.94598800	-0.89907900
C	5.00265400	-1.81901100	-2.18073800	F	-3.99521300	4.27665600	-0.72591800
H	5.45775000	-1.72094600	-3.16334400	C	-2.85759800	2.20377200	-0.48987600
C	4.05138800	-0.87282300	-1.79239300	F	-1.85394400	2.94512600	0.05266600
C	3.16736200	-2.36592100	1.67996900	C	-1.62631400	-1.63602600	0.10484100
H	2.19502200	-2.85572900	1.54910800	C	-2.70835800	-2.08415800	0.86780900
H	3.01241800	-1.47701900	2.29399900	F	-3.61971000	-1.19895500	1.33511400
H	3.79739100	-3.05234400	2.25270000	C	-2.92812800	-3.41118600	1.22358500
C	6.38845500	-3.90425200	-1.82107200	F	-3.98872800	-3.75446700	1.96838100
H	5.90498000	-4.68205400	-2.42660600	C	-2.02664700	-4.38772600	0.81071000
H	6.87333300	-4.40201600	-0.97534000	F	-2.21084500	-5.67048300	1.14663800
H	7.16578800	-3.44658500	-2.44203500	C	-0.92161000	-4.00411900	0.06176300
C	3.68269600	0.20646100	-2.78737500	F	-0.01985000	-4.92148000	-0.32375400
H	3.78537600	1.21333900	-2.36829000	C	-0.74968500	-2.65894100	-0.26671700
H	2.65089800	0.08695400	-3.14583300	F	0.38226300	-2.38571700	-0.97347900
H	4.33831900	0.14997200	-3.66058900	H	1.45986700	0.43172700	-1.27177800
C	2.93137100	1.95735700	0.20167300	H	-1.62610400	-0.92820800	-2.81470900
C	3.92458200	2.14570000	1.19724400	Si	-1.15907500	0.90470000	2.76270200
C	4.46801800	3.41822000	1.37954900	C	-1.21433200	-0.70906700	3.76764400
H	5.22753600	3.55532800	2.14580700	H	-0.28724200	-1.29148700	3.70053500
C	4.06359400	4.51522600	0.61426800	H	-1.37345200	-0.47499400	4.82795400
C	3.07298900	4.31112500	-0.34623400	H	-2.03937600	-1.35436600	3.45031700
H	2.73286700	5.15597500	-0.93986000	C	-2.87429200	1.70120000	2.82103700
C	2.48631600	3.06022000	-0.57804400	H	-2.87918100	2.69469300	2.36167000
C	4.41540000	1.03138400	2.09351000	H	-3.62883600	1.08767200	2.32209300
H	5.20201900	1.39587300	2.75982900	H	-3.17695100	1.81769400	3.86975800
H	4.82553900	0.19092700	1.52497000	C	0.02784500	2.09705200	3.65981800
H	3.61255500	0.64262300	2.73191500	H	-0.34828500	2.31601800	4.66719000
C	4.69254000	5.87302100	0.81053200	H	1.04395200	1.70012600	3.77950100
H	4.92357100	6.05872500	1.86485800	H	0.10843400	3.05205200	3.12606900
H	4.03534200	6.67377800	0.45763900				
H	5.63513300	5.95129900	0.25275000				
C	1.39423100	2.99396400	-1.62801700				
H	1.31123600	3.96195500	-2.12972700				
H	0.41679400	2.76996600	-1.19044300				
H	1.57372100	2.24220700	-2.40261000				
C	-2.74592700	0.81536100	-0.60658600				

## TSD8

E= -2863.152738au

P	-2.12574100	-0.17304100	-0.28815000
B	1.45386000	0.03935600	0.00054300
O	0.46268700	0.05525400	-1.67183300
O	-0.17547500	0.70947900	-3.73518900

C	-0.98824200	0.22406900	1.16936200	H	-1.37226700	-3.90489800	-2.13982900
H	-0.81009600	1.29672800	1.17894000	H	-0.41327400	-2.72426600	-1.25231200
H	-1.49239000	-0.02294900	2.10781800	H	-1.63588900	-2.17733400	-2.40061300
C	0.35605200	-0.55838000	1.01717300	C	2.64283400	-0.92117100	-0.54973400
H	0.11037300	-1.58320400	0.72009600	C	3.68574800	-0.42601400	-1.34803000
C	0.67195000	0.62744200	-2.88637600	F	3.72382200	0.88284700	-1.68940900
C	-3.51378000	1.04833900	-0.56029700	C	4.71479800	-1.20141600	-1.87267900
C	-3.83049600	2.18406300	0.22584100	F	5.67462600	-0.64613400	-2.62213600
C	-4.88425500	3.01895000	-0.17144400	C	4.73244300	-2.56973400	-1.62247800
H	-5.11697800	3.88364200	0.44655300	F	5.70834900	-3.33602700	-2.11418400
C	-5.63732800	2.78797700	-1.32112800	C	3.71062200	-3.12692800	-0.86380600
C	-5.28855100	1.68842900	-2.10686300	F	3.69696900	-4.44436500	-0.62557100
H	-5.83718300	1.49714000	-3.02678100	C	2.69763700	-2.30926600	-0.36478800
C	-4.24191500	0.82852600	-1.76454700	F	1.74047500	-2.96733200	0.32922400
C	-3.07601400	2.60338600	1.46949800	C	1.82650900	1.60760800	0.22412300
H	-2.09780500	3.02539500	1.21063000	C	3.01305800	1.97411400	0.87123000
H	-2.91140600	1.77982800	2.16749100	F	3.90136800	1.02515200	1.24048000
H	-3.63071700	3.38090500	2.00306100	C	3.36500900	3.28469000	1.17930700
C	-6.78954500	3.68641300	-1.70207800	F	4.51884400	3.55311200	1.80210500
H	-6.73286900	4.65133100	-1.18798000	C	2.50634200	4.32243400	0.82827000
H	-7.75272200	3.22925200	-1.43855900	F	2.82103900	5.58864400	1.11440400
H	-6.80853000	3.87693700	-2.78107500	C	1.31464500	4.01963000	0.18075100
C	-3.90989100	-0.28757000	-2.73296500	F	0.46642100	4.99919000	-0.15757300
H	-3.99414300	-1.27935500	-2.27565700	C	1.00524300	2.69028000	-0.10417000
H	-2.88844100	-0.18205800	-3.12010000	F	-0.17873100	2.50102200	-0.73708200
H	-4.59127500	-0.26109800	-3.58867600	H	-0.56171500	-0.10162400	-1.47622600
C	-2.88722500	-1.81569100	0.17710500	H	1.70730200	0.98026500	-2.97834100
C	-3.85561500	-1.96807700	1.20509300	Si	1.00814300	-0.84319000	2.83030100
C	-4.35672900	-3.24180400	1.49153100	C	0.95164500	0.77950100	3.81567500
H	-5.09532900	-3.34341500	2.28426000	H	-0.04441400	1.23653100	3.82165700
C	-3.94297700	-4.38194200	0.79915600	H	1.22726800	0.58463100	4.85971800
C	-2.99062400	-4.21819800	-0.20531400	H	1.65635500	1.52277700	3.42646300
H	-2.64760800	-5.09135700	-0.75599500	C	2.75671000	-1.55508500	2.99006000
C	-2.45467100	-2.96585400	-0.53438600	H	2.84107100	-2.54437300	2.53021900
C	-4.38665200	-0.81563600	2.02852700	H	3.51973100	-0.90506100	2.55458900
H	-5.11644700	-1.17575700	2.75980200	H	2.98714500	-1.66695900	4.05755700
H	-4.87590000	-0.05936100	1.40827200	C	-0.17262800	-2.09818100	3.62889100
H	-3.59279900	-0.30918700	2.58894000	H	0.08018300	-2.23729400	4.68755300
C	-4.52631200	-5.73856500	1.11483900	H	-1.22591300	-1.79984600	3.57951700
H	-4.68025600	-5.86753000	2.19195800	H	-0.08651300	-3.07546100	3.13875100
H	-3.87536300	-6.54615500	0.76487000				
H	-5.50322400	-5.87097400	0.63090900				
C	-1.41637700	-2.93220800	-1.64006800				

**E<sub>5</sub>**

**E= -2790.338086au**

C	-2.276087	2.492454	0.508553
C	-1.972414	1.454684	-0.412603
C	-1.696705	1.813575	-1.765489
C	-1.705044	3.158083	-2.149142
C	-1.955150	4.188170	-1.241454
C	-2.254254	3.824681	0.070662
P	-1.680140	-0.371914	-0.105882
C	4.935590	1.311031	-1.895970
O	4.873375	2.374864	-1.415243
C	-1.363327	0.790251	-2.834374
C	-1.866984	5.639214	-1.648482
C	-2.641449	2.303431	1.969613
C	-1.346746	-0.660902	1.773031
C	0.050705	-1.313503	1.920700
B	1.229719	-0.688193	1.061082
O	5.007422	0.251303	-2.385467
C	1.313667	0.875881	0.839859
C	1.668153	1.443154	-0.390478
C	1.675628	2.809970	-0.631848
C	1.340111	3.684000	0.399468
C	1.010135	3.174833	1.651302
C	0.999784	1.797340	1.843952
F	1.997108	0.643947	-1.427797
F	0.650398	1.364345	3.075519
F	0.664460	4.003233	2.644286
F	1.319006	5.000690	0.181702
F	1.991888	3.290017	-1.838304
C	2.433111	-1.596024	0.578820
C	3.747158	-1.102465	0.473594
C	4.840969	-1.875991	0.103278
C	4.654635	-3.220831	-0.200584
C	3.376410	-3.766504	-0.123035
C	2.308402	-2.962835	0.265122
F	4.024907	0.186445	0.748403
F	6.060770	-1.334192	0.028772
F	5.687014	-3.978294	-0.564606
F	3.184203	-5.055363	-0.421121
F	1.113546	-3.577502	0.294974
C	-3.219545	-1.305516	-0.645036
C	-4.546866	-0.799790	-0.691464
C	-5.557783	-1.584395	-1.261062
C	-5.323432	-2.853756	-1.788911
C	-4.021012	-3.346211	-1.722040

C	-2.971466	-2.605220	-1.169405
C	-4.970533	0.544493	-0.146440
C	-6.434212	-3.654576	-2.425127
C	-1.612230	-3.265819	-1.123587
H	0.364583	-1.221273	2.974913
H	-1.324225	0.313217	2.253299
H	-1.490075	3.404443	-3.186670
H	-2.484749	4.605812	0.793023
H	-3.807758	-4.340463	-2.109167
H	-6.569467	-1.184262	-1.282161
H	-1.280313	1.278871	-3.810183
H	-0.409263	0.292344	-2.624254
H	-2.124297	0.007041	-2.919338
H	-3.155437	1.365839	2.175048
H	-1.758779	2.354644	2.621082
H	-3.304367	3.114266	2.288586
H	-2.620623	6.248329	-1.137211
H	-0.883031	6.050096	-1.385869
H	-2.000024	5.764752	-2.727896
H	-1.616151	-4.192019	-1.706759
H	-0.819625	-2.618881	-1.511251
H	-1.339845	-3.527472	-0.096705
H	-6.530686	-3.417583	-3.493368
H	-6.248142	-4.730970	-2.346793
H	-7.401371	-3.440775	-1.957477
H	-4.582630	1.376036	-0.741747
H	-6.062418	0.618253	-0.143055
H	-4.627760	0.686349	0.879372
H	-0.026405	-2.385023	1.736025
C	-2.383246	-1.467001	2.533435
F	-2.514007	-2.726985	2.060174
F	-2.043522	-1.577686	3.842117
F	-3.614196	-0.900284	2.504539

**TS<sub>E56</sub>**

**E= -2790.3130418au**

C	3.447562	-2.334257	-0.205099
C	3.297646	-0.999518	-0.674384
C	4.214056	-0.516281	-1.650962
C	5.305854	-1.310284	-2.023293
C	5.517357	-2.584257	-1.504325
C	4.559778	-3.076512	-0.617342
P	1.879540	0.160027	-0.295509



C	-4.156362	4.127952	0.412239
C	-4.344741	3.235300	-0.639928
H	-5.000156	3.517171	-1.459938
C	-3.729365	1.980098	-0.693972
C	-2.019728	2.126441	2.801189
H	-2.153681	2.951466	3.505048
H	-0.944462	1.974179	2.697835
H	-2.449497	1.237384	3.276888
C	-4.784057	5.498993	0.402663
H	-4.989576	5.854737	1.417537
H	-5.722010	5.507375	-0.162021
H	-4.112192	6.227918	-0.069194
C	-4.137217	1.101764	-1.861645
H	-3.286914	0.656582	-2.374436
H	-4.677025	1.705635	-2.596263
H	-4.809233	0.301242	-1.533413
C	-3.025315	-1.355295	-0.289107
C	-4.116373	-1.569078	0.599463
C	-5.028453	-2.586755	0.311402
H	-5.860674	-2.743438	0.993447
C	-4.900410	-3.413424	-0.805971
C	-3.806459	-3.203134	-1.643174
H	-3.675237	-3.844725	-2.510844
C	-2.855587	-2.199943	-1.418025
C	-4.358873	-0.776513	1.867032
H	-3.473346	-0.753231	2.509867
H	-5.157479	-1.244935	2.448732
H	-4.656659	0.256674	1.665787
C	-5.887194	-4.523333	-1.072515
H	-5.970699	-4.736560	-2.142978
H	-6.883435	-4.273961	-0.692875
H	-5.572077	-5.451770	-0.578233
C	-1.728852	-2.103005	-2.422269
H	-1.833230	-1.228400	-3.072130
H	-1.734334	-2.988135	-3.063904
H	-0.742650	-2.053023	-1.958654
C	2.413859	-1.200710	-0.010228
C	2.401289	-2.174811	-1.010453
F	1.631442	-2.043029	-2.113997
C	3.153502	-3.349489	-0.954591
F	3.082600	-4.249459	-1.948133
C	3.978878	-3.588806	0.136302
F	4.706916	-4.710629	0.205830

C	4.038849	-2.644408	1.156921
F	4.837548	-2.850404	2.215036
C	3.269102	-1.491549	1.057635
F	3.402344	-0.600688	2.069344
C	2.420614	1.554544	-0.215491
C	3.808580	1.642007	-0.364230
F	4.591745	0.546957	-0.321605
C	4.489593	2.843041	-0.573801
F	5.823902	2.853469	-0.702902
C	3.780885	4.035051	-0.655828
F	4.418739	5.194075	-0.857782
C	2.395989	4.007115	-0.526459
F	1.690882	5.146058	-0.605441
C	1.763542	2.786920	-0.315374
F	0.407215	2.845978	-0.206648
C	-0.534384	-1.966012	1.598305
F	-1.644348	-2.550399	2.110375
F	-0.285226	-2.559626	0.411656
F	0.477725	-2.271692	2.429563

## E7

E= -2791.512644au

P	1.86144900	0.12593000	-0.16610100
B	-1.46174500	0.05907700	-0.08342200
O	-0.64896800	-0.04733300	-1.40417000
O	1.13803600	-0.02500700	-2.75123800
C	0.75945200	-0.33926400	1.29190300
H	0.47298200	-1.38147000	1.14316700
C	-0.49553000	0.55292000	1.13923800
H	-0.19446600	1.60276000	1.08136300
C	0.60218700	0.01542800	-1.66512900
C	3.21680900	-1.01704500	-0.70851600
C	3.25549000	-2.38991300	-0.34008400
C	4.34169300	-3.16494000	-0.76067100
H	4.36898000	-4.21073500	-0.46513900
C	5.36734100	-2.66080900	-1.55826000
C	5.26128200	-1.33551400	-1.97707500
H	6.01684900	-0.93117800	-2.64657200
C	4.20734300	-0.49987200	-1.59359500
C	2.17392000	-3.12610100	0.42381500
H	1.19602500	-3.01021900	-0.05282500
H	2.10496500	-2.81464100	1.46806600
H	2.39460000	-4.19669000	0.42429600

C	6. 51058600	-3. 53594600	-2. 00943900
H	6. 27322800	-4. 02640600	-2. 96263900
H	6. 72276300	-4. 32469100	-1. 28061000
H	7. 42502800	-2. 95345800	-2. 16184800
C	4. 20544000	0. 88791900	-2. 20547400
H	4. 59327000	1. 65229700	-1. 52501200
H	3. 20729000	1. 18493800	-2. 52965900
H	4. 84434100	0. 88559900	-3. 09329000
C	2. 50260300	1. 83548000	0. 15553000
C	3. 64588200	1. 99050100	0. 98775900
C	4. 07763400	3. 28291100	1. 30251800
H	4. 94806500	3. 39016600	1. 94560200
C	3. 44141400	4. 42681700	0. 82367400
C	2. 34855300	4. 24875500	-0. 02422500
H	1. 85110000	5. 12439300	-0. 43298100
C	1. 86040100	2. 98744000	-0. 38195100
C	4. 50795600	0. 86339100	1. 51944400
H	4. 99751300	1. 18065000	2. 44482700
H	5. 29594100	0. 61313000	0. 79870000
H	3. 97215100	-0. 05651800	1. 73656300
C	3. 90705400	5. 80617000	1. 21861200
H	4. 97765200	5. 81861100	1. 44689100
H	3. 37682300	6. 15213000	2. 11561300
H	3. 71537000	6. 53632600	0. 42569700
C	0. 70841300	2. 97449200	-1. 36489000
H	0. 40763300	4. 00099900	-1. 58875100
H	-0. 17692800	2. 45905400	-0. 98859200
H	0. 98614100	2. 50231200	-2. 31265800
C	-2. 68181800	1. 08338100	-0. 47201100
C	-3. 48448000	0. 80242300	-1. 58474600
F	-3. 25660300	-0. 30579000	-2. 31479900
C	-4. 54330600	1. 60776700	-1. 99652600
F	-5. 27335500	1. 28717400	-3. 07457300
C	-4. 84755500	2. 75643300	-1. 27137800
F	-5. 85999900	3. 54636400	-1. 64902300
C	-4. 08871700	3. 07431500	-0. 15092700
F	-4. 37215800	4. 17838800	0. 55750700
C	-3. 03616100	2. 23986200	0. 22433500
F	-2. 35536500	2. 62181100	1. 32915400
C	-2. 07621000	-1. 43087400	0. 26290100
C	-3. 05454600	-1. 54512600	1. 25687500
F	-3. 44547700	-0. 44519500	1. 93843500
C	-3. 66569200	-2. 74324700	1. 61594600

F	-4. 59898100	-2. 77869700	2. 57662700
C	-3. 29289600	-3. 91734600	0. 96703100
F	-3. 86000400	-5. 08332100	1. 29683700
C	-2. 30914800	-3. 86491800	-0. 01368400
F	-1. 91924500	-4. 99232100	-0. 62922500
C	-1. 72875100	-2. 63981200	-0. 34094300
F	-0. 74704100	-2. 69452500	-1. 27807800
H	-0. 07350800	-5. 20112900	-3. 37602000
H	-0. 39987900	-4. 86569100	-2. 79953400
H	-1. 06754700	0. 47078300	2. 06807200
C	1. 33481200	-0. 26432400	2. 70195700
F	0. 40977000	-0. 67500300	3. 59058700
F	1. 71414800	0. 97751100	3. 05232200
F	2. 41423700	-1. 07806700	2. 87501400

### TSE78

E= -2791.384007au

P	1. 97198200	-0. 01540300	-0. 18009500
B	-1. 54109900	-0. 08996600	-0. 14390100
O	-0. 78175100	-0. 01851200	-1. 56891600
O	0. 89279200	-0. 46916100	-3. 05120700
C	0. 84521000	-0. 37532900	1. 31868700
H	0. 66170200	-1. 45238200	1. 31779300
C	-0. 47715800	0. 38466700	1. 02521800
H	-0. 22628800	1. 44065000	0. 88745700
H	-1. 04450500	0. 35907500	1. 95776200
C	0. 31689100	-0. 49013000	-1. 99263800
C	3. 43645800	-1. 13925700	-0. 49447700
C	3. 61818900	-2. 41963700	0. 09494500
C	4. 74730000	-3. 16907000	-0. 25649600
H	4. 88608500	-4. 13904300	0. 21510000
C	5. 68365100	-2. 73480500	-1. 19362000
C	5. 43485100	-1. 51942000	-1. 82947000
H	6. 11519500	-1. 17846100	-2. 60657500
C	4. 32567900	-0. 72287400	-1. 52717900
C	2. 65261100	-3. 08748500	1. 05351000
H	1. 65608700	-3. 20618400	0. 61141100
H	2. 54764700	-2. 54940100	1. 99570000
H	3. 00666700	-4. 09419700	1. 29062500
C	6. 87971400	-3. 58015600	-1. 55783900
H	6. 65053700	-4. 24073200	-2. 40449200
H	7. 18996900	-4. 21623000	-0. 72254700
H	7. 73319200	-2. 96021100	-1. 85148100

C	4.13993400	0.52467600	-2.36923300
H	4.41170500	1.44137100	-1.83728900
H	3.10871500	0.62711900	-2.72020100
H	4.77234600	0.45829400	-3.25922500
C	2.55917700	1.75546600	-0.00970000
C	1.90069800	2.80660400	-0.69751000
C	2.31640800	4.12325200	-0.46863900
H	1.80043400	4.92316300	-0.99365100
C	3.36613700	4.44125900	0.39148600
C	4.03688000	3.38469600	1.00734300
H	4.88351400	3.60137900	1.65457700
C	3.67366600	2.04583900	0.82569600
C	0.79375600	2.60788200	-1.70552800
H	0.58957400	3.54923900	-2.22314400
H	-0.14242200	2.28340200	-1.24525100
H	1.05547400	1.87035900	-2.47014500
C	3.75986800	5.87448200	0.65056900
H	3.51851800	6.51728900	-0.20207600
H	4.83116900	5.96610100	0.85775900
H	3.22378500	6.27284000	1.52206100
C	4.56586800	1.01885900	1.48963200
H	5.11682000	1.48614800	2.31098800
H	5.30236300	0.62809000	0.77762700
H	4.03078300	0.16573000	1.89801300
C	-2.67163900	1.09053500	-0.33883300
C	-3.51401400	1.00710300	-1.45785400
F	-3.37383600	-0.01709100	-2.32298300
C	-4.52117100	1.92184800	-1.74970600
F	-5.28133200	1.78393100	-2.84504900
C	-4.74324300	2.98525200	-0.87987700
F	-5.70450200	3.88002900	-1.13501000
C	-3.95518600	3.10354400	0.25783800
F	-4.16258800	4.11854700	1.10989200
C	-2.95347900	2.16433100	0.51102200
F	-2.26203000	2.36916200	1.65331500
C	-2.21530600	-1.55765900	0.09355600
C	-2.94243900	-1.76789900	1.27263500
F	-3.04182200	-0.77700400	2.18684800
C	-3.60541800	-2.95247800	1.58019300
F	-4.27889700	-3.08286900	2.73071300
C	-3.56845300	-4.00729100	0.67293900
F	-4.19298900	-5.15776100	0.94647700
C	-2.87141100	-3.84994000	-0.51943300

F	-2.82568100	-4.85612000	-1.40331900
C	-2.22571300	-2.64258800	-0.78680500
F	-1.57677000	-2.58546200	-1.97251100
H	0.45354900	-1.72782800	-1.42138400
H	1.06241500	-1.04312300	-0.92538600
C	1.32204800	-0.03672000	2.73019000
F	0.38524800	-0.39524400	3.63276800
F	2.45587100	-0.70157400	3.09147200
F	1.56824100	1.27417300	2.89673900

## E8

E= -2791.542659au

P	-1.98238100	0.16475100	-0.02095600
B	1.56177000	0.24936000	0.03314600
O	0.61510300	0.02870700	1.20431700
O	0.25022300	-0.06481700	3.40791000
C	-0.67951200	-0.26431100	-1.32798400
H	-0.37007900	-1.29034000	-1.12334900
C	0.56055700	0.66072400	-1.21884000
H	0.23977300	1.70231200	-1.15887800
C	1.01082800	-0.09387600	2.46333900
C	-2.35876700	-1.10206000	1.24955100
C	-2.23236000	-2.50039600	1.06903400
C	-2.57785300	-3.33851600	2.13407600
H	-2.48332900	-4.41252800	1.99329700
C	-3.03026200	-2.85264400	3.36069800
C	-3.14345300	-1.46987700	3.51184000
H	-3.48603300	-1.06432100	4.46045500
C	-2.80821000	-0.57768000	2.49259500
C	-1.72232500	-3.18277000	-0.18181300
H	-0.62742700	-3.22581900	-0.16366500
H	-2.03516000	-2.70458700	-1.11097400
H	-2.08014300	-4.21583600	-0.21461800
C	-3.35929200	-3.78782600	4.49790000
H	-2.50950400	-3.86876900	5.18801000
H	-3.58719100	-4.79581500	4.13723800
H	-4.21541300	-3.42796100	5.07858100
C	-2.89103900	0.90052500	2.79952400
H	-3.39798400	1.48144300	2.02175000
H	-1.87743100	1.29430900	2.94511500
H	-3.43933600	1.05986500	3.73182900
C	-3.51488100	0.94930400	-0.69104100
C	-4.70760100	0.21722300	-0.92512000

C	-5.84381200	0.91037500	-1.35633600
H	-6.75334600	0.34393100	-1.54048900
C	-5.85117300	2.28954000	-1.56346100
C	-4.66157300	2.98621700	-1.34281700
H	-4.63591200	4.05909300	-1.51711400
C	-3.49052600	2.35500300	-0.91638100
C	-4.84657700	-1.27726500	-0.74225500
H	-5.79404900	-1.61588700	-1.17059000
H	-4.83691700	-1.56389900	0.31347900
H	-4.04876800	-1.82749500	-1.24471600
C	-7.10361200	3.00937700	-1.99915700
H	-7.80752700	2.32959000	-2.48915100
H	-6.87494200	3.82513500	-2.69309700
H	-7.61947500	3.45202100	-1.13683000
C	-2.25892400	3.21952600	-0.75199300
H	-2.49261700	4.25450000	-1.01469800
H	-1.44922200	2.89288800	-1.41072800
H	-1.86789300	3.22977400	0.27125300
C	2.55521600	1.51451700	0.42520200
C	3.95062800	1.49483300	0.51798500
F	4.64942200	0.36283400	0.29829400
C	4.72271400	2.60689800	0.85869200
F	6.05871800	2.51413200	0.92129200
C	4.10123500	3.81493000	1.15030100
F	4.82447600	4.89081500	1.48282400
C	2.71291200	3.88735600	1.10087600
F	2.09010800	5.03983600	1.39324000
C	1.98735900	2.75212500	0.75366700
F	0.63494600	2.90739000	0.75859300
C	2.33538200	-1.14566100	-0.40358600
C	3.18642900	-1.14455100	-1.51593600
F	3.42716000	0.01657600	-2.16641900
C	3.82803800	-2.27096200	-2.01709700
F	4.63651300	-2.18799200	-3.08343500
C	3.61920500	-3.50236700	-1.40010800
F	4.21784600	-4.60515600	-1.86684600
C	2.77311300	-3.56941500	-0.30152000
F	2.54113400	-4.74976000	0.29542300
C	2.15698700	-2.40667200	0.16730400
F	1.32984100	-2.59059700	1.22880800
H	-1.36142000	1.20515600	0.67323200
H	2.10115800	-0.21870500	2.58659500
H	1.10788800	0.56467500	-2.16128500

C	-1.26786900	-0.28025800	-2.73424100
F	-2.37014100	-1.07857600	-2.82148800
F	-1.63531500	0.94476800	-3.15963700
F	-0.37129800	-0.76428200	-3.61145700

## TSE8

E= -2791.513647au

P	-1.84183600	-0.43143400	-0.22210900
B	1.65463600	-0.46856800	0.10013500
O	0.73614800	-0.74574400	-1.59752600
O	0.18633700	-0.60696100	-3.78050600
C	-0.75803900	-0.66804700	1.35288200
H	-0.58109300	0.32577000	1.75818100
C	0.62114400	-1.29709900	1.01139300
H	0.48802600	-2.30969300	0.62033600
C	1.01404700	-0.53147900	-2.91202200
C	-2.43529900	1.32829700	-0.40566200
C	-2.39033600	2.38366400	0.54336300
C	-2.73880900	3.67847400	0.13687400
H	-2.69118000	4.47776500	0.87375500
C	-3.15634800	3.98056000	-1.15844700
C	-3.22884000	2.92773500	-2.06955000
H	-3.56224900	3.12672000	-3.08555000
C	-2.87282300	1.61888000	-1.73085100
C	-2.00491100	2.24266800	2.00296300
H	-0.91715600	2.28567900	2.14787800
H	-2.36687500	1.31995800	2.45730400
H	-2.42508900	3.07441700	2.57642700
C	-3.54862300	5.38629100	-1.54517500
H	-4.57188800	5.61609500	-1.21923400
H	-3.51071200	5.52749800	-2.63002800
H	-2.88749500	6.12724600	-1.08261700
C	-2.99171000	0.56702300	-2.81552200
H	-3.65466300	-0.25536900	-2.52456900
H	-2.02226200	0.12949400	-3.08000500
H	-3.40448800	1.01395400	-3.72487500
C	-3.30375200	-1.59081200	-0.15964300
C	-4.58798100	-1.26240400	0.34490800
C	-5.61423500	-2.21230000	0.25216900
H	-6.59501400	-1.95057400	0.64335000
C	-5.42734200	-3.47238600	-0.31319500
C	-4.15872900	-3.77615100	-0.81072200
H	-3.98485300	-4.75010300	-1.26307500



C	-3.09952300	-2.86740900	-0.75264200
C	-4.94867900	0.06528900	0.97259000
H	-5.91514300	-0.01389300	1.47969900
H	-5.02926100	0.86279600	0.22663000
H	-4.21226600	0.38197000	1.71115300
C	-6.54759800	-4.48308300	-0.36624100
H	-7.52731600	-4.00050200	-0.29040000
H	-6.47023300	-5.20083500	0.46131700
H	-6.52263600	-5.06034300	-1.29714700
C	-1.77263300	-3.30930800	-1.33390100
H	-1.85739200	-4.32206300	-1.73916000
H	-0.98327000	-3.33048300	-0.57516800
H	-1.43727400	-2.65534600	-2.14658300
C	3.09002900	-1.12430000	-0.21482200
C	4.01186400	-0.48668700	-1.05617300
F	3.66486900	0.65502900	-1.69430900
C	5.28791000	-0.96966700	-1.32619200
F	6.10991500	-0.31231100	-2.15253200
C	5.70355700	-2.15546700	-0.72642500
F	6.92303600	-2.64022300	-0.96735800
C	4.83112700	-2.83325000	0.11825000
F	5.21809500	-3.97515200	0.69781500
C	3.55688100	-2.31722700	0.35279600
F	2.78381700	-3.03965500	1.18389200
C	1.68717200	1.12789700	0.35452500
C	2.25163100	1.52824600	1.57126400
F	2.73046600	0.58589800	2.41461300
C	2.35681700	2.85418400	1.98056500
F	2.91207900	3.16855700	3.15682700
C	1.87600000	3.85810500	1.14354800
F	1.96122600	5.14028800	1.51059900
C	1.30608700	3.51298600	-0.07775800
F	0.83918200	4.47031100	-0.88738500
C	1.22644300	2.17101700	-0.45050000
F	0.66566400	1.93127800	-1.65365100
H	-0.27640600	-0.72467500	-1.38156500
H	2.07416100	-0.30201400	-3.05980600
H	1.14037000	-1.43190600	1.96866600
C	-1.40722600	-1.46616600	2.47556400
F	-0.62480600	-1.46485600	3.58139900
F	-2.60512800	-0.95933400	2.86119000
F	-1.61013700	-2.75694200	2.13790500

**F<sub>5</sub>**

**E= -2492.6203926au**

C	-2.697326	-2.974156	-0.453818
C	-2.283032	-1.776374	0.188916
C	-2.057585	-1.816261	1.595998
C	-2.278314	-2.998162	2.309542
C	-2.695175	-4.175637	1.690081
C	-2.894482	-4.132609	0.312039
P	-1.831527	-0.118628	-0.582458
C	3.746411	0.314935	3.262899
O	3.021995	0.131898	4.161937
C	-1.569188	-0.620871	2.387727
C	-2.894860	-5.449363	2.476412
C	-2.948530	-3.129463	-1.940362
C	-0.955681	0.849337	-3.084383
B	1.272084	0.285462	-1.675141
O	4.485663	0.484545	2.372188
C	2.025114	-1.029651	-1.207768
C	1.445806	-2.300859	-1.324335
C	2.092511	-3.479618	-0.968314
C	3.398365	-3.418652	-0.488631
C	4.031082	-2.183862	-0.369081
C	3.343673	-1.027318	-0.725264
F	0.184533	-2.429699	-1.780348
F	4.025618	0.125153	-0.611136
F	5.289976	-2.121209	0.077942
F	4.039904	-4.537685	-0.148226
F	1.478749	-4.662452	-1.086643
C	1.597308	1.645117	-0.928236
C	1.836245	1.695744	0.452580
C	2.189717	2.850988	1.135186
C	2.321127	4.046041	0.431625
C	2.084432	4.059649	-0.939133
C	1.721690	2.878666	-1.585222
F	1.700676	0.581525	1.201786
F	2.402058	2.827378	2.459234
F	2.662578	5.167050	1.067583
F	2.206117	5.201709	-1.625083
F	1.520161	2.979198	-2.912487
C	-3.225917	1.053363	-0.072634
C	-4.609055	0.767212	-0.234798
C	-5.561381	1.710186	0.169820
C	-5.211660	2.939339	0.730245

C	-3.853679	3.209687	0.885703
C	-2.861353	2.299981	0.497631
C	-5.139410	-0.515811	-0.833146
C	-6.265826	3.944498	1.129076
C	-1.424089	2.724430	0.708365
H	-1.240157	1.019787	-4.131408
H	-2.110383	-2.993589	3.384704
H	-3.221783	-5.035996	-0.198842
H	-3.548484	4.157672	1.324019
H	-6.615041	1.469688	0.041576
H	-1.423487	-0.895534	3.436933
H	-0.611763	-0.249256	2.005028
H	-2.278725	0.213454	2.361246
H	-3.559289	-2.326771	-2.356611
H	-2.010597	-3.165747	-2.505028
H	-3.472907	-4.070616	-2.132069
H	-3.567081	-6.140112	1.956548
H	-1.942580	-5.974503	2.630714
H	-3.315616	-5.246900	3.467662
H	-1.384163	3.656339	1.281591
H	-0.845779	1.970116	1.247334
H	-0.910327	2.900968	-0.242655
H	-7.160242	3.451515	1.525708
H	-5.892475	4.636713	1.890994
H	-6.584010	4.547431	0.267867
H	-4.837472	-1.394835	-0.257734
H	-6.232837	-0.494400	-0.868379
H	-4.785960	-0.664457	-1.858913
H	-0.986312	1.832958	-2.599183
C	0.478093	0.268901	-3.044854
C	-2.003250	-0.099255	-2.463295
H	0.457790	-0.737067	-3.476453
H	1.097790	0.873090	-3.725039
H	-3.009926	0.218576	-2.751065
H	-1.840982	-1.097579	-2.865995

**TS<sub>F56</sub>**

**E= -2492.5814068au**

C	3.399524	-2.648177	0.611002
C	3.283975	-1.401174	-0.060084
C	4.130253	-1.163673	-1.179152
C	5.131746	-2.089339	-1.497173
C	5.317701	-3.271710	-0.784489

C	4.420038	-3.535790	0.247997
P	1.938023	-0.141202	0.332357
C	0.352262	-0.938224	-1.489503
O	1.072397	-1.573360	-2.167251
C	4.016870	0.030072	-2.108293
C	6.395046	-4.260167	-1.162399
C	2.457313	-3.146316	1.691334
C	0.303634	0.642394	2.438337
B	-1.665160	-0.125084	0.627113
O	-0.687816	-0.417946	-1.175281
C	-2.585062	-1.436820	0.399417
C	-2.030237	-2.709897	0.239304
C	-2.777918	-3.875472	0.110571
C	-4.167137	-3.797186	0.162385
C	-4.772981	-2.558007	0.340768
C	-3.982165	-1.415416	0.454638
F	-0.682277	-2.858933	0.192248
F	-4.643676	-0.258075	0.652400
F	-6.107360	-2.471101	0.406720
F	-4.908558	-4.902939	0.049499
F	-2.178880	-5.061912	-0.053047
C	-2.299984	1.276629	0.151128
C	-2.930046	1.422775	-1.097720
C	-3.500424	2.610752	-1.542314
C	-3.500329	3.726537	-0.709667
C	-2.935161	3.626621	0.555016
C	-2.362143	2.420712	0.958366
F	-3.030517	0.380230	-1.937970
F	-4.068058	2.684679	-2.752765
F	-4.049478	4.873094	-1.117789
F	-2.949473	4.681163	1.381147
F	-1.885462	2.413957	2.220410
C	2.807569	1.535144	0.229762
C	4.039198	1.787971	0.893022
C	4.570401	3.084722	0.871415
C	3.947366	4.144535	0.213126
C	2.757781	3.870815	-0.461759
C	2.181648	2.595435	-0.472221
C	4.897050	0.737291	1.573684
C	4.528361	5.537928	0.243345
C	0.919488	2.415907	-1.285896
H	0.229586	0.849137	3.513719
H	5.776774	-1.878549	-2.347958

H	4.498339	-4.478210	0.786760	C	-0.271731	0.568699	-2.380668
H	2.258347	4.671529	-1.003077	B	1.613577	-0.159695	-0.523819
H	5.512442	3.264394	1.385888	O	0.548929	-0.414944	0.620930
H	4.496883	-0.206611	-3.063023	C	2.675577	-1.401703	-0.351182
H	2.977771	0.288622	-2.328466	C	2.244607	-2.709337	-0.114838
H	4.500236	0.926725	-1.708218	C	3.097070	-3.804973	-0.008892
H	2.698163	-2.743677	2.682653	C	4.467087	-3.617061	-0.160910
H	1.410226	-2.919535	1.473754	C	4.949653	-2.339629	-0.422622
H	2.535196	-4.234987	1.768326	C	4.056368	-1.272856	-0.516415
H	6.790396	-4.778472	-0.281896	F	0.920171	-2.985351	0.008788
H	6.007025	-5.028985	-1.843991	F	4.604905	-0.070990	-0.797498
H	7.230554	-3.766784	-1.670048	F	6.266630	-2.145598	-0.587634
H	0.586358	3.377862	-1.687180	F	5.308348	-4.655410	-0.069027
H	1.081354	1.747370	-2.140901	F	2.610820	-5.034495	0.224580
H	0.096894	1.996419	-0.704503	C	2.264067	1.285416	-0.073696
H	5.611271	5.517859	0.404272	C	2.758831	1.448527	1.228093
H	4.332421	6.074527	-0.691292	C	3.324517	2.629033	1.702023
H	4.088175	6.131318	1.055882	C	3.430844	3.725461	0.851080
H	5.544356	0.237033	0.843415	C	2.970649	3.614594	-0.454736
H	5.544930	1.209347	2.319261	C	2.407817	2.412397	-0.885806
H	4.332846	-0.052549	2.068981	F	2.718931	0.421903	2.097437
H	0.299401	1.619742	1.947836	F	3.774294	2.719250	2.962395
C	-0.877031	-0.236523	1.997440	F	3.968888	4.871769	1.286610
C	1.629959	-0.074358	2.188936	F	3.066386	4.662018	-1.289463
H	-0.632240	-1.284392	2.207346	F	2.000576	2.404490	-2.177747
H	-1.734398	-0.024861	2.662039	C	-2.932164	1.469054	-0.263266
H	2.455439	0.461656	2.660606	C	-4.153445	1.645455	-0.972597
H	1.584303	-1.071460	2.619516	C	-4.727566	2.920501	-1.016171
				C	-4.153824	4.025056	-0.386685
				C	-2.964171	3.823132	0.312062
				C	-2.332587	2.576414	0.392063
				C	-4.947701	0.539165	-1.644273
				C	-4.781748	5.394180	-0.478335
				C	-1.053409	2.513140	1.196656
				H	-0.273224	0.808590	-3.452053
				H	-5.914376	-2.097567	2.253277
				H	-4.119127	-4.773055	-0.548367
				H	-2.498642	4.666125	0.816581
				H	-5.660872	3.046896	-1.560123
				H	-4.901105	-0.250193	2.919846
				H	-3.337372	0.292373	2.318933
				H	-4.828974	0.794259	1.500849
				H	-2.355534	-3.045231	-2.439132

## F<sub>6</sub>

E= -2492.6043251au

C	-3.229145	-2.829972	-0.447457	C	-4.947701	0.539165	-1.644273
C	-3.304969	-1.537708	0.136920	C	-4.781748	5.394180	-0.478335
C	-4.260861	-1.292272	1.164219	C	-1.053409	2.513140	1.196656
C	-5.187468	-2.294279	1.468676	H	-0.273224	0.808590	-3.452053
C	-5.195085	-3.537184	0.834555	H	-5.914376	-2.097567	2.253277
C	-4.186951	-3.787565	-0.093683	H	-4.119127	-4.773055	-0.548367
P	-2.117044	-0.198110	-0.351298	H	-2.498642	4.666125	0.816581
C	-0.668589	-0.445345	0.960674	H	-5.660872	3.046896	-1.560123
O	-1.140191	-0.643665	2.064435	H	-4.901105	-0.250193	2.919846
C	-4.331157	-0.036287	2.010917	H	-3.337372	0.292373	2.318933
C	-6.236581	-4.577694	1.164558	H	-4.828974	0.794259	1.500849
C	-2.143323	-3.304203	-1.394647	H	-2.355534	-3.045231	-2.439132

H	-1.151435	-2.927344	-1.134478
H	-2.080589	-4.395135	-1.350894
H	-5.877070	-5.588224	0.946200
H	-6.522674	-4.536816	2.220830
H	-7.149040	-4.419407	0.574339
H	-0.785008	3.513898	1.544845
H	-1.154090	1.871881	2.077361
H	-0.205423	2.140959	0.615139
H	-5.854707	5.331128	-0.685497
H	-4.644005	5.959698	0.449196
H	-4.324609	5.980090	-1.286503
H	-5.572124	0.007430	-0.916951
H	-5.613765	0.969491	-2.397740
H	-4.340524	-0.220063	-2.140766
H	-0.299751	1.538828	-1.871700
C	0.991935	-0.239112	-2.022591
C	-1.578813	-0.213849	-2.135631
H	0.802701	-1.293004	-2.276387
H	1.798107	0.068475	-2.698597
H	-2.403709	0.244159	-2.687574
H	-1.461126	-1.232683	-2.495307

## G5

E= -2531.9269925au

C	4.643415	0.286798	-2.311229
C	3.982911	0.343008	-1.056084
C	4.421270	1.321407	-0.115218
C	5.493707	2.162776	-0.422283
C	6.157906	2.104806	-1.647714
C	5.704986	1.166133	-2.571966
P	2.449063	-0.582939	-0.490725
C	0.918014	3.796578	2.061989
O	1.599129	4.607944	1.569356
C	3.767117	1.507515	1.238106
C	7.317970	3.022102	-1.953755
C	4.307854	-0.683479	-3.426331
C	0.889178	-1.373706	-2.838186
C	-0.580811	-1.226034	-2.396353
B	-2.294136	0.191583	-0.905716
O	0.248782	2.982314	2.571330
C	-2.798985	1.565951	-0.327142
C	-1.931818	2.635648	-0.039231
C	-2.360719	3.843445	0.498610

C	-3.715120	4.038690	0.754719
C	-4.621896	3.020365	0.471894
C	-4.156210	1.816397	-0.047898
F	-0.610376	2.524226	-0.251788
F	-5.090815	0.889158	-0.303438
F	-5.924961	3.206682	0.703740
F	-4.141055	5.193343	1.262140
F	-1.483134	4.818160	0.776192
C	-3.189138	-1.099145	-0.686057
C	-3.308607	-1.697196	0.565542
C	-4.057484	-2.850914	0.781235
C	-4.731957	-3.430226	-0.291934
C	-4.642390	-2.858809	-1.560668
C	-3.872171	-1.712860	-1.732516
F	-2.657218	-1.156438	1.617740
F	-4.135886	-3.403229	1.997330
F	-5.460807	-4.534225	-0.106049
F	-5.292639	-3.412661	-2.590595
F	-3.806393	-1.169561	-2.966425
C	3.018373	-1.719434	0.898457
C	4.218268	-2.474695	0.909994
C	4.514989	-3.279567	2.017104
C	3.667293	-3.375910	3.121538
C	2.480398	-2.643478	3.090391
C	2.140147	-1.819353	2.010765
C	5.214985	-2.473894	-0.227569
C	4.030578	-4.228827	4.314207
C	0.816127	-1.083370	2.089773
H	-1.215002	-1.243546	-3.291287
H	1.229687	-0.420787	-3.265412
H	5.806470	2.896022	0.318841
H	6.197409	1.104667	-3.540489
H	1.793235	-2.712194	3.931408
H	5.438448	-3.855877	2.007619
H	4.142017	2.415835	1.719910
H	2.677670	1.592001	1.146053
H	3.960239	0.664631	1.911598
H	4.521851	-1.721873	-3.149613
H	3.260807	-0.634464	-3.733428
H	4.913664	-0.458796	-4.309395
H	7.606682	2.963853	-3.008168
H	7.072723	4.066960	-1.728531
H	8.200646	2.763803	-1.353986

H	0.333713	-1.273106	3.053870
H	0.934009	-0.000403	1.979480
H	0.114159	-1.405124	1.311717
H	3.137909	-4.586462	4.838408
H	4.623619	-5.101062	4.018367
H	4.628617	-3.661455	5.040186
H	5.752901	-1.523583	-0.302508
H	5.954746	-3.268078	-0.085011
H	4.731401	-2.643789	-1.193819
H	-0.863164	-2.113797	-1.814093
H	0.920714	-2.099136	-3.662429
C	-0.894609	0.051242	-1.596738
C	1.871376	-1.873793	-1.750332
H	-0.181997	0.134618	-0.752228
H	-0.656354	0.940374	-2.196959
H	1.352970	-2.607826	-1.119445
H	2.701528	-2.415405	-2.207037

### TSG56

E= -2531.8653487au

C	-3.359853	-2.315438	-1.096675
C	-3.250028	-1.210501	-0.210899
C	-4.074363	-1.202094	0.947741
C	-5.048227	-2.196563	1.107948
C	-5.235244	-3.227522	0.189982
C	-4.354473	-3.278869	-0.888519
P	-1.929447	0.134290	-0.477272
C	-0.516036	-0.916804	1.357538
O	-1.284542	-1.658558	1.840693
C	-3.989052	-0.200637	2.086490
C	-6.324793	-4.256999	0.369738
C	-2.419997	-2.582578	-2.256225
C	-0.931246	0.408500	-3.334872
C	0.401517	0.747138	-2.675312
B	1.666358	-0.240205	-0.474102
O	0.525328	-0.320382	1.252518
C	2.460602	-1.570270	0.019011
C	1.836302	-2.824188	0.060236
C	2.472449	-4.008472	0.412510
C	3.825600	-3.977797	0.740080
C	4.500797	-2.763868	0.715170
C	3.818242	-1.597331	0.365545
F	0.514527	-2.929249	-0.225322

F	4.565017	-0.477552	0.368038
F	5.801814	-2.718785	1.026702
F	4.462977	-5.102027	1.076163
F	1.803325	-5.167591	0.438178
C	2.449195	1.156779	-0.228968
C	2.593604	1.894190	0.953653
C	3.344634	3.066434	1.044278
C	4.050837	3.527848	-0.059326
C	3.992314	2.802096	-1.243597
C	3.217501	1.648251	-1.295228
F	1.997982	1.520760	2.100581
F	3.401549	3.740730	2.200865
F	4.781744	4.643464	0.018801
F	4.692101	3.202445	-2.313132
F	3.282026	0.958448	-2.456543
C	-2.857011	1.724457	0.063402
C	-4.195137	2.018483	-0.320426
C	-4.761525	3.246319	0.056980
C	-4.073607	4.207839	0.791816
C	-2.757292	3.913920	1.144643
C	-2.142350	2.706732	0.796920
C	-5.140080	1.105576	-1.083053
C	-4.712965	5.520909	1.175679
C	-0.713503	2.524577	1.246583
H	1.149641	0.991377	-3.433231
H	-0.883790	-0.607022	-3.745404
H	-5.670868	-2.165066	2.000312
H	-4.420999	-4.110852	-1.586883
H	-2.179957	4.646314	1.705328
H	-5.787384	3.450369	-0.244014
H	-4.271005	-0.696456	3.021153
H	-2.991746	0.213721	2.229328
H	-4.669504	0.645825	1.944202
H	-2.644578	-1.984322	-3.145342
H	-1.375294	-2.405224	-1.989660
H	-2.493328	-3.632691	-2.554258
H	-6.041262	-5.221592	-0.064812
H	-6.555444	-4.415965	1.428602
H	-7.254922	-3.940246	-0.121367
H	-0.293403	3.478368	1.579969
H	-0.626205	1.828034	2.086021
H	-0.072510	2.144303	0.448919
H	-4.184144	6.369119	0.723005

H	-5.757511	5.567541	0.852093
H	-4.690331	5.672706	2.261798
H	-5.749290	0.511113	-0.391947
H	-5.827377	1.710039	-1.684403
H	-4.650280	0.398369	-1.746538
H	0.284688	1.655210	-2.067357
H	-1.127160	1.074639	-4.186253
C	0.891390	-0.446482	-1.832178
C	-2.103218	0.570678	-2.364608
H	0.087213	-1.168916	-1.690215
H	1.622536	-1.007342	-2.435456
H	-2.347238	1.633989	-2.317897
H	-2.992363	0.061165	-2.737131

## G<sub>6</sub>

E= -2531.9099149au

C	-2.618828	2.044444	1.834660
C	-2.211544	1.449040	0.612650
C	-1.607844	2.255556	-0.390996
C	-1.272969	3.572267	-0.071973
C	-1.514148	4.128614	1.185957
C	-2.239927	3.364392	2.099526
P	-2.322667	-0.377943	0.374947
C	-0.919142	-0.957204	-0.902868
O	-1.376667	-1.489194	-1.893275
C	-1.343706	1.811611	-1.815950
C	-1.017428	5.512902	1.515414
C	-3.531562	1.383834	2.853182
C	-0.766388	-2.141745	2.118155
C	0.460568	-1.415136	2.690020
B	1.416614	-0.293977	0.415780
O	0.290910	-0.696732	-0.630461
C	2.003767	1.092607	-0.263028
C	1.939301	2.371355	0.295367
C	2.417395	3.518243	-0.338351
C	3.004885	3.420741	-1.592994
C	3.101316	2.169713	-2.195030
C	2.604107	1.050725	-1.529272
F	1.379537	2.586983	1.507088
F	2.725023	-0.121060	-2.181602
F	3.664317	2.055591	-3.407049
F	3.463086	4.513917	-2.216714
F	2.292468	4.724423	0.250141

C	2.536729	-1.496498	0.337127
C	2.312418	-2.806765	-0.090728
C	3.299672	-3.791924	-0.111379
C	4.584056	-3.487244	0.324583
C	4.855205	-2.202850	0.785187
C	3.837527	-1.252360	0.786817
F	1.084640	-3.213252	-0.498437
F	3.017506	-5.033526	-0.537054
F	5.543661	-4.422272	0.315841
F	6.085093	-1.895541	1.225097
F	4.163589	-0.030014	1.267541
C	-3.946620	-0.992762	-0.277001
C	-4.999476	-0.127344	-0.688818
C	-6.199194	-0.694945	-1.136802
C	-6.407943	-2.069917	-1.212313
C	-5.352945	-2.899706	-0.835917
C	-4.130212	-2.404979	-0.374334
C	-4.952391	1.388416	-0.712258
C	-7.724474	-2.641397	-1.677479
C	-3.087236	-3.446361	-0.020827
H	1.295727	-2.125864	2.711532
H	-0.790826	4.180279	-0.834047
H	-2.532644	3.807234	3.049350
H	-5.474850	-3.977564	-0.911409
H	-6.996891	-0.025508	-1.448628
H	-1.464236	2.668812	-2.485875
H	-0.321851	1.441504	-1.944458
H	-2.022946	1.029579	-2.162915
H	-4.055507	0.508854	2.459343
H	-3.000204	1.081283	3.763559
H	-4.297883	2.102497	3.163701
H	-1.327009	5.828512	2.516120
H	0.077873	5.529732	1.471177
H	-1.383234	6.253365	0.793865
H	-2.974929	-3.580241	1.060712
H	-3.389393	-4.415492	-0.426757
H	-2.108280	-3.218793	-0.444118
H	-7.577178	-3.545043	-2.278457
H	-8.355033	-2.919551	-0.822617
H	-8.285758	-1.918714	-2.277933
H	-4.136722	1.773163	-1.328764
H	-5.885872	1.770770	-1.134088
H	-4.839507	1.827690	0.281809

H	-1.032783	-2.973036	2.783860
C	0.877369	-0.137230	1.940558
C	-2.007315	-1.221729	2.022382
H	0.071412	0.604771	2.009196
H	1.702320	0.314682	2.506830
H	-2.930620	-1.761774	2.246415
H	-1.913472	-0.433366	2.767784
H	0.246063	-1.167779	3.741335
H	-0.521186	-2.599000	1.156994

## H<sub>5</sub>

E= -2571.2391624au

C	2.839991	2.404641	-1.031268
C	2.470456	1.226670	-0.327499
C	1.997532	1.369465	1.011055
C	1.900458	2.638787	1.590360
C	2.224518	3.803410	0.893545
C	2.696576	3.654032	-0.410001
P	2.294609	-0.529367	-0.971381
C	-1.406333	-2.403116	3.382504
O	-0.324629	-2.842784	3.318364
C	1.579952	0.186381	1.860553
C	2.042729	5.169177	1.513375
C	3.429850	2.424505	-2.426785
C	1.666141	-0.317843	-3.841900
C	-0.606959	-1.155432	-2.787831
B	-2.018169	0.398356	-1.179076
O	-2.485213	-1.959845	3.467833
C	-1.986227	1.685221	-0.280112
C	-1.539738	2.927384	-0.770119
C	-1.416903	4.060754	0.024109
C	-1.741779	3.985471	1.375338
C	-2.199338	2.786040	1.913260
C	-2.321817	1.672597	1.087324
F	-1.228759	3.076878	-2.066146
F	-2.745932	0.547727	1.681075
F	-2.505366	2.711682	3.212507
F	-1.600831	5.059619	2.151921
F	-0.972370	5.215372	-0.485303
C	-2.972317	-0.812470	-0.794145
C	-2.571392	-1.853291	0.034812
C	-3.385302	-2.937831	0.337714
C	-4.664050	-2.999438	-0.213890

C	-5.104142	-1.979663	-1.055582
C	-4.252989	-0.910929	-1.328388
F	-1.337028	-1.811309	0.593102
F	-2.956518	-3.910413	1.153978
F	-5.464219	-4.032803	0.062681
F	-6.329525	-2.034817	-1.589523
F	-4.696672	0.066454	-2.147916
C	3.660748	-1.560450	-0.189874
C	4.997750	-1.149747	0.043075
C	5.888963	-2.028317	0.671696
C	5.519294	-3.314927	1.066303
C	4.207705	-3.716026	0.812748
C	3.274312	-2.871473	0.199819
C	5.539674	0.198229	-0.375758
C	6.512937	-4.249248	1.715761
C	1.879617	-3.424640	-0.025363
H	1.550453	2.714405	2.618327
H	2.980073	4.543125	-0.969922
H	3.893149	-4.715418	1.106621
H	6.909041	-1.693195	0.850915
H	0.773727	-0.386194	1.386764
H	2.404350	-0.514877	2.029886
H	1.228185	0.525972	2.840067
H	4.342532	1.825009	-2.493344
H	2.739567	2.054151	-3.188840
H	3.695105	3.448851	-2.705198
H	1.032951	5.556815	1.325602
H	2.183699	5.139297	2.599291
H	2.750089	5.895213	1.098346
H	1.605490	-3.435812	-1.087156
H	1.821342	-4.455882	0.337826
H	1.110289	-2.842797	0.491717
H	7.092098	-4.800159	0.962221
H	7.229885	-3.702902	2.338345
H	6.011719	-4.991165	2.346407
H	5.022115	1.028109	0.113188
H	6.604311	0.273186	-0.133259
H	5.441582	0.347843	-1.456738
C	-1.123324	0.263923	-2.467313
C	2.744048	-0.706351	-2.803434
H	-0.288422	0.966729	-2.406527
H	-1.736746	0.630599	-3.312364
C	0.409493	-1.207476	-3.946087

H	-0.152350	-1.581082	-1.888073
H	-1.453481	-1.804201	-3.048482
H	0.725241	-2.251650	-4.085519
H	-0.109362	-0.924044	-4.873529
H	2.156365	-0.342202	-4.825213
H	1.357283	0.724080	-3.701998
H	3.690138	-0.220036	-3.054687
H	2.934204	-1.785646	-2.883554

**TS<sub>H56</sub>**

**E= -2571.1884628au**

C	-1.880913	2.251070	1.358022
C	-1.949321	1.265890	0.332085
C	-1.883660	1.712380	-1.019923
C	-1.703502	3.073694	-1.298480
C	-1.584123	4.036985	-0.301581
C	-1.697754	3.596075	1.016155
P	-2.043407	-0.607028	0.571240
C	-0.549244	-1.549974	-1.258346
O	-1.205528	-2.347576	-1.821585
C	-2.040109	0.834076	-2.249171
C	-1.327283	5.488576	-0.625336
C	-2.012031	1.986429	2.842616
C	-1.523816	-1.287671	3.565193
C	0.459963	-2.182665	2.177423
B	1.563658	-0.368474	0.523864
O	0.417923	-0.842449	-1.135122
C	1.755436	1.162970	0.084558
C	1.541150	2.250276	0.936479
C	1.722555	3.576586	0.553143
C	2.146454	3.864138	-0.736888
C	2.400712	2.820045	-1.620984
C	2.216028	1.508209	-1.195602
F	1.144161	2.065579	2.213655
F	2.503146	0.551286	-2.095019
F	2.819146	3.085329	-2.865652
F	2.282615	5.136885	-1.130616
F	1.453222	4.577474	1.404890
C	2.800076	-1.341493	0.133680
C	2.695000	-2.660806	-0.317165
C	3.792793	-3.473053	-0.592847
C	5.078131	-2.979502	-0.395058
C	5.240248	-1.681859	0.078345

C	4.114568	-0.901008	0.329188
F	1.486149	-3.234878	-0.512259
F	3.619159	-4.726081	-1.033919
F	6.143211	-3.747808	-0.643906
F	6.469840	-1.195975	0.292689
F	4.349821	0.337667	0.812294
C	-3.756649	-1.136984	-0.073747
C	-4.870206	-0.276993	-0.286148
C	-6.024950	-0.788868	-0.893861
C	-6.154812	-2.123775	-1.273394
C	-5.095698	-2.975273	-0.968974
C	-3.919762	-2.521421	-0.360983
C	-4.955026	1.173091	0.151231
C	-7.414817	-2.639915	-1.926922
C	-2.945640	-3.615473	0.041690
H	-1.664424	3.382429	-2.341408
H	-1.643160	4.326795	1.819458
H	-5.182321	-4.036743	-1.195677
H	-6.859790	-0.111514	-1.062462
H	-1.064055	0.580182	-2.678383
H	-2.591580	-0.089253	-2.074152
H	-2.588021	1.385343	-3.020505
H	-2.851476	1.335198	3.091098
H	-1.100931	1.545560	3.255123
H	-2.169760	2.930772	3.371129
H	-0.252876	5.709792	-0.594802
H	-1.687813	5.746648	-1.626464
H	-1.814809	6.152592	0.096606
H	-3.356180	-4.176923	0.892232
H	-2.800619	-4.325925	-0.777511
H	-1.959194	-3.258183	0.330953
H	-8.056531	-3.157894	-1.201677
H	-8.002758	-1.825299	-2.361891
H	-7.186243	-3.356592	-2.723706
H	-4.457478	1.861587	-0.538385
H	-6.006990	1.470301	0.209574
H	-4.512728	1.336517	1.136457
C	0.835083	-0.725168	1.872651
C	-2.484279	-1.166144	2.368995
H	-0.011802	-0.059840	2.040588
H	1.571002	-0.385967	2.624474
C	-0.400874	-2.329693	3.443077
H	-0.079230	-2.617251	1.330558



H	1.366833	-2.789850	2.283599
H	-0.828898	-3.341338	3.468715
H	0.232145	-2.243233	4.336916
H	-2.152504	-1.564575	4.423599
H	-1.095622	-0.319152	3.826592
H	-3.358045	-0.572523	2.651961
H	-2.877058	-2.165488	2.159006

## H<sub>6</sub>

E= -2571.2254381 au

C	-2.023701	3.078924	0.663534
C	-2.097059	1.909596	-0.136424
C	-1.863628	2.009552	-1.538779
C	-1.435719	3.230294	-2.063839
C	-1.233944	4.360819	-1.271971
C	-1.580680	4.268846	0.075147
P	-2.295392	0.198661	0.541810
C	-0.680755	-0.677822	-0.140090
O	-0.658262	-1.327025	-1.156628
C	-2.063914	0.891122	-2.542335
C	-0.660479	5.625235	-1.858978
C	-2.443023	3.189178	2.114916
C	-1.010402	0.550040	3.221307
C	0.683513	-1.469179	3.293594
B	1.763297	-0.606250	0.925073
O	0.208784	-0.336598	0.716382
C	2.466672	0.792339	0.393301
C	3.560104	1.386353	1.033143
C	4.110256	2.611353	0.660812
C	3.573454	3.305929	-0.418309
C	2.511175	2.744316	-1.114217
C	2.005305	1.509439	-0.712654
F	4.163949	0.771238	2.070589
F	1.004529	1.018196	-1.482730
F	1.980601	3.395539	-2.169263
F	4.076284	4.493678	-0.784198
F	5.151792	3.127292	1.332096
C	2.259144	-1.946561	0.106783
C	1.536290	-3.142964	0.080623
C	1.953291	-4.305127	-0.560653
C	3.182070	-4.320937	-1.210638
C	3.959033	-3.169631	-1.200730
C	3.492810	-2.026256	-0.550758

F	0.333247	-3.237653	0.704424
F	1.185793	-5.407697	-0.549498
F	3.610937	-5.429018	-1.829469
F	5.153302	-3.166272	-1.812673
F	4.333152	-0.970232	-0.586564
C	-3.882596	-0.626853	0.060323
C	-5.063872	0.130920	-0.180224
C	-6.234342	-0.542851	-0.540265
C	-6.296638	-1.931536	-0.664088
C	-5.141913	-2.656325	-0.376741
C	-3.934625	-2.047412	-0.013619
C	-5.171157	1.637284	-0.052543
C	-7.568508	-2.620365	-1.093514
C	-2.775835	-2.981481	0.263133
H	-1.239059	3.287296	-3.131903
H	-1.512760	5.156277	0.700751
H	-5.171308	-3.741878	-0.430856
H	-7.132090	0.043918	-0.720025
H	-1.105827	0.456341	-2.838921
H	-2.689003	0.074018	-2.180972
H	-2.540745	1.300394	-3.439615
H	-3.133013	2.406585	2.431699
H	-1.581541	3.171239	2.789097
H	-2.951255	4.146516	2.269871
H	0.413263	5.492362	-2.039905
H	-1.124831	5.869803	-2.820938
H	-0.788370	6.479595	-1.187304
H	-2.159463	-2.685337	1.115096
H	-3.155956	-3.983690	0.479489
H	-2.104244	-3.048537	-0.595797
H	-8.455020	-2.073066	-0.756363
H	-7.623998	-2.687779	-2.188067
H	-7.624616	-3.640699	-0.701103
H	-4.646268	2.162909	-0.855555
H	-6.223224	1.933226	-0.094156
H	-4.768159	2.010258	0.893367
C	1.867343	-0.778160	2.559167
C	-2.194279	-0.026801	2.395400
H	2.014403	0.206025	3.024830
H	2.791244	-1.323860	2.786788
C	-0.249112	-0.503745	4.050579
H	0.098483	-2.088934	2.608186
H	1.075500	-2.165962	4.047013

H	-0.979604	-1.084154	4.635138
H	0.353407	0.046724	4.786597
H	-1.426616	1.284145	3.918277
H	-0.305830	1.084974	2.582315
H	-3.162044	0.291415	2.796363
H	-2.199194	-1.120645	2.469277

**I<sub>s</sub>**

**E= -2610.5495016au**

C	3.722451	3.022674	0.427551
C	4.393710	1.803672	0.709475
C	5.657075	1.874186	1.360634
C	6.256711	3.119489	1.586030
C	5.643388	4.319697	1.232986
C	4.366676	4.240411	0.675838
P	3.645733	0.090696	0.571738
C	0.845316	-0.457649	2.757970
O	1.038036	-1.602585	2.892752
C	6.401172	0.654725	1.866141
C	6.301398	5.653251	1.498829
C	2.297811	3.106123	-0.079429
C	2.388162	0.137115	-2.178425
C	-1.088819	-0.133249	-1.811769
B	-3.549733	0.143445	-0.783266
O	0.638184	0.687842	2.635601
C	-4.834847	1.003500	-0.498409
C	-5.203357	2.108156	-1.290991
C	-6.339438	2.875668	-1.057632
C	-7.163418	2.563996	0.021068
C	-6.844624	1.488072	0.845753
C	-5.708322	0.732517	0.574429
F	-4.463194	2.468904	-2.350087
F	-5.465769	-0.277519	1.421828
F	-7.630069	1.192237	1.885613
F	-8.249860	3.293018	0.263691
F	-6.644647	3.905494	-1.853103
C	-3.433256	-1.296083	-0.128820
C	-2.532374	-1.578458	0.893402
C	-2.406712	-2.839751	1.466611
C	-3.207855	-3.878214	0.993690
C	-4.121304	-3.640046	-0.032112
C	-4.222019	-2.358072	-0.564890
F	-1.755752	-0.580823	1.377427

F	-1.537224	-3.061472	2.457553
F	-3.100861	-5.099344	1.523130
F	-4.888536	-4.636359	-0.488111
F	-5.117211	-2.148140	-1.552487
C	4.882512	-0.990645	-0.339910
C	5.745879	-0.576753	-1.388928
C	6.592619	-1.517093	-1.989741
C	6.622825	-2.857842	-1.600906
C	5.768534	-3.250424	-0.571298
C	4.906389	-2.350007	0.067096
C	5.839842	0.847489	-1.897102
C	7.542887	-3.844050	-2.281767
C	4.033482	-2.892556	1.183145
H	7.232594	3.143854	2.067772
H	3.839442	5.161399	0.433169
H	5.771701	-4.289228	-0.247394
H	7.248119	-1.185058	-2.793314
H	7.182357	0.958711	2.570094
H	5.732017	-0.038748	2.390087
H	6.879317	0.085795	1.062165
H	2.166798	2.648119	-1.063303
H	1.598402	2.620153	0.611107
H	1.991342	4.153083	-0.165783
H	5.915213	6.114415	2.417965
H	7.385008	5.548149	1.617080
H	6.117547	6.361070	0.682386
H	4.256295	-3.950361	1.356790
H	4.186516	-2.352833	2.123569
H	2.963285	-2.816995	0.958666
H	7.274719	-3.976754	-3.337857
H	8.585201	-3.503112	-2.256881
H	7.500160	-4.827243	-1.802410
H	6.464985	1.467933	-1.244566
H	6.289273	0.860725	-2.895654
H	4.868460	1.340658	-1.955159
C	-2.411988	0.648332	-1.748354
C	2.201690	-0.028487	-0.663375
C	-0.130825	0.418235	-2.880308
C	1.200991	-0.349431	-3.036194
H	-2.877103	0.648096	-2.751903
H	-2.214122	1.715594	-1.570193
H	-0.608849	-0.120198	-0.827696
H	-1.294360	-1.189217	-2.035197

H	-0.661287	0.402222	-3.843046
H	0.077350	1.479491	-2.676461
H	1.030085	-1.419352	-2.845373
H	1.519283	-0.282903	-4.085122
H	3.274421	-0.427554	-2.487357
H	2.591779	1.186857	-2.426325
H	1.870850	-1.060279	-0.473212
H	1.400034	0.608834	-0.284029

### TS156

E= -2610.4860317au

C	-2.126757	1.675298	1.796263
C	-2.210671	1.026566	0.535201
C	-2.555056	1.816470	-0.604187
C	-2.733237	3.197694	-0.459976
C	-2.593769	3.852877	0.760852
C	-2.312821	3.061529	1.872066
P	-1.880246	-0.780860	0.078046
C	-0.056500	-1.109368	-1.664105
O	-0.421751	-0.748976	-2.725666
C	-2.828467	1.263693	-1.988827
C	-2.705701	5.352738	0.872288
C	-1.899217	0.987568	3.120907
C	-1.611019	-2.357399	2.780255
C	1.601022	-2.315463	2.356910
B	1.692563	-0.388246	0.466583
O	0.751621	-1.604733	-0.920639
C	1.357899	1.084171	-0.082486
C	1.011480	2.146479	0.761176
C	0.888122	3.463756	0.329103
C	1.104687	3.771093	-1.008680
C	1.479413	2.759651	-1.887972
C	1.622373	1.461670	-1.407835
F	0.830651	1.947314	2.081593
F	2.050747	0.543840	-2.295553
F	1.719547	3.045694	-3.173093
F	0.965354	5.026936	-1.441846
F	0.563238	4.438402	1.191542
C	3.198604	-0.870387	0.062618
C	3.599298	-2.148961	-0.347153
C	4.923656	-2.489435	-0.621385
C	5.930079	-1.543857	-0.462288
C	5.592562	-0.269138	-0.022615

C	4.256849	0.033816	0.229099
F	2.712807	-3.152496	-0.496289
F	5.233166	-3.729450	-1.024807
F	7.204678	-1.860406	-0.712082
F	6.547663	0.652130	0.161985
F	4.019351	1.283002	0.688990
C	-3.596710	-1.431135	-0.446758
C	-4.821149	-1.005532	0.140389
C	-6.034106	-1.500491	-0.355089
C	-6.104620	-2.430765	-1.391041
C	-4.898291	-2.893010	-1.908924
C	-3.655382	-2.424344	-1.462098
C	-4.933354	-0.070286	1.325708
C	-7.431886	-2.953474	-1.886591
C	-2.447755	-3.055883	-2.128243
H	-2.991011	3.775990	-1.344396
H	-2.228989	3.536465	2.846525
H	-4.913501	-3.648612	-2.691750
H	-6.957138	-1.153648	0.105573
H	-2.879578	2.084468	-2.710498
H	-2.068953	0.567086	-2.342297
H	-3.789831	0.738408	-2.018858
H	-2.643577	0.209264	3.309096
H	-0.907177	0.539028	3.195285
H	-1.979584	1.713305	3.935070
H	-1.709639	5.810026	0.816838
H	-3.310947	5.774133	0.063085
H	-3.150366	5.654303	1.826959
H	-2.723607	-4.029941	-2.543726
H	-2.075455	-2.442499	-2.953704
H	-1.613248	-3.230390	-1.443546
H	-7.854535	-3.689783	-1.190112
H	-8.166724	-2.146670	-1.986798
H	-7.330706	-3.443029	-2.860466
H	-4.784567	0.979082	1.055585
H	-5.929190	-0.159761	1.770921
H	-4.206414	-0.313026	2.104107
C	1.252505	-0.872644	1.910783
C	-1.429198	-2.208334	1.257697
C	0.826877	-2.817894	3.595805
C	-0.597457	-3.367379	3.359915
H	1.813960	-0.179159	2.559394
H	0.213840	-0.632286	2.127414

H	1.467127	-3.030115	1.537655
H	2.673342	-2.346418	2.586251
H	1.408740	-3.625088	4.060718
H	0.781102	-2.012816	4.344546
H	-0.544230	-4.251451	2.707755
H	-0.980680	-3.726663	4.324361
H	-2.636463	-2.686927	2.988685
H	-1.479628	-1.417013	3.308571
H	-2.005336	-3.005814	0.777421
H	-0.393776	-2.400694	0.992510

## I<sub>6</sub>

E= -2610.5432795au

C	-2.752074	2.069011	1.179387
C	-2.613388	1.075097	0.174144
C	-2.696079	1.448912	-1.200656
C	-2.810052	2.805515	-1.517678
C	-2.853920	3.807123	-0.547520
C	-2.868141	3.406750	0.787733
P	-2.131707	-0.682385	0.520181
C	-0.290243	-0.644797	-0.158928
O	-0.043486	-0.686004	-1.341796
C	-2.731293	0.476933	-2.364295
C	-2.841914	5.266031	-0.926365
C	-2.806939	1.805474	2.668282
C	-0.960813	-0.919044	3.259677
C	2.559408	-1.109312	3.253776
B	1.940555	0.126858	0.876235
O	0.449959	-0.448129	0.867666
C	1.727936	1.613910	0.177596
C	0.963335	2.594411	0.823301
C	0.688847	3.851932	0.294180
C	1.158844	4.177669	-0.971033
C	1.904527	3.239553	-1.672773
C	2.159562	1.991630	-1.100098
F	0.395825	2.354464	2.034682
F	2.846481	1.142181	-1.884456
F	2.349462	3.529355	-2.904745
F	0.868016	5.372747	-1.510998
F	-0.061359	4.740230	0.974177
C	2.968230	-0.891505	0.103144
C	2.728770	-2.231454	-0.196004
C	3.676010	-3.088893	-0.755732

C	4.954739	-2.616013	-1.019259
C	5.261476	-1.293585	-0.709926
C	4.279867	-0.479413	-0.155024
F	1.525028	-2.806311	0.072985
F	3.364487	-4.368180	-1.024954
F	5.882656	-3.422752	-1.552869
F	6.496341	-0.823153	-0.943554
F	4.650611	0.786587	0.140374
C	-3.294979	-1.875414	-0.280996
C	-4.693074	-1.615582	-0.283127
C	-5.545223	-2.547336	-0.881762
C	-5.078289	-3.729594	-1.461859
C	-3.709805	-3.985296	-1.398585
C	-2.802237	-3.095287	-0.811318
C	-5.344735	-0.395094	0.337316
C	-6.033610	-4.714053	-2.091468
C	-1.349454	-3.512149	-0.772939
H	-2.849623	3.084648	-2.567637
H	-2.946205	4.162796	1.564015
H	-3.324176	-4.913686	-1.812699
H	-6.613546	-2.342432	-0.885021
H	-2.612576	1.026760	-3.302026
H	-1.936979	-0.268835	-2.324797
H	-3.692585	-0.048307	-2.410327
H	-3.547139	1.044209	2.934442
H	-1.838845	1.498228	3.066898
H	-3.091251	2.722201	3.191325
H	-1.806314	5.625079	-0.982507
H	-3.305785	5.434937	-1.903528
H	-3.361692	5.880541	-0.184160
H	-1.261734	-4.579626	-0.992744
H	-0.745020	-2.967830	-1.503018
H	-0.886202	-3.349728	0.205130
H	-6.598576	-5.259871	-1.324650
H	-6.764892	-4.206682	-2.730568
H	-5.503704	-5.452529	-2.700399
H	-5.225497	0.500324	-0.281224
H	-6.416963	-0.573891	0.458927
H	-4.943462	-0.155063	1.326772
C	2.400643	0.207481	2.444979
C	-2.115157	-1.287327	2.292789
C	1.374828	-1.573830	4.130406
C	0.096511	-2.029977	3.391044

H	3.388521	0.689641	2.411477
H	1.775109	0.898850	3.019931
H	2.835859	-1.937503	2.586969
H	3.411330	-0.995867	3.938969
H	1.735977	-2.413400	4.739359
H	1.117724	-0.779389	4.847595
H	0.373804	-2.404369	2.400261
H	-0.361077	-2.874215	3.926699
H	-1.402931	-0.733045	4.247105
H	-0.471758	0.004008	2.954998
H	-3.097395	-1.028358	2.699078
H	-2.141980	-2.374425	2.146297

**J<sub>5</sub>**

**E= -2491.3971203au**

C	-2.784658	-2.272601	0.110108
C	-4.196762	-2.185027	0.237703
C	-4.952543	-3.364839	0.284100
H	-6.033476	-3.278374	0.376014
C	-4.382428	-4.635824	0.223480
C	-2.992714	-4.707716	0.149263
H	-2.509831	-5.683165	0.138700
C	-2.186635	-3.564970	0.105420
C	-4.980173	-0.892553	0.353566
H	-4.923776	-0.283009	-0.551963
H	-4.632276	-0.263544	1.177617
H	-6.035995	-1.117582	0.534050
C	-5.236005	-5.881707	0.236792
H	-6.168904	-5.723471	0.788613
H	-4.708171	-6.724425	0.696493
H	-5.509527	-6.187574	-0.782281
C	-0.688524	-3.783967	0.070968
H	-0.155991	-3.131691	0.771868
H	-0.259461	-3.587500	-0.916661
H	-0.453299	-4.820549	0.332390
C	-2.449257	0.792955	-0.030477
C	-2.947552	1.374410	-1.222276
C	-3.413046	2.695435	-1.198420
H	-3.782581	3.133501	-2.123620
C	-3.421491	3.465167	-0.034071
C	-2.988472	2.857465	1.146730
H	-3.019556	3.422060	2.076511
C	-2.499979	1.546279	1.172437

C	-3.036138	0.634122	-2.538961
H	-3.772020	1.113566	-3.192958
H	-3.336002	-0.409626	-2.403848
H	-2.075331	0.636430	-3.063752
C	-3.842171	4.914722	-0.056346
H	-4.320375	5.212364	0.883096
H	-4.538026	5.120946	-0.876363
H	-2.966030	5.561280	-0.197868
C	-2.065466	0.980700	2.510239
H	-2.245697	1.708569	3.307693
H	-1.002720	0.719071	2.526431
H	-2.612695	0.066282	2.768716
C	2.900105	-0.519377	-0.721060
C	3.155920	-1.901255	-0.677890
F	2.172826	-2.783477	-0.906568
C	4.405950	-2.439581	-0.389844
F	4.588611	-3.763222	-0.347925
C	5.477198	-1.583810	-0.148443
F	6.683133	-2.081417	0.120258
C	5.284911	-0.204630	-0.194672
F	6.316191	0.618854	0.022529
C	4.017842	0.297476	-0.469128
C	1.066924	1.483498	-0.486887
C	0.390953	2.399517	-1.303610
F	0.128286	2.091748	-2.586889
C	-0.003473	3.658361	-0.863656
F	-0.649566	4.502621	-1.676229
C	0.255634	4.029361	0.451775
F	-0.151544	5.218674	0.899403
C	0.927487	3.154326	1.304161
F	1.165417	3.509214	2.571724
C	1.325812	1.915188	0.820234
F	1.960288	1.096918	1.684769
F	3.911926	1.635156	-0.515831
B	1.467066	0.059151	-1.021696
P	-1.551294	-0.848672	0.099710
C	0.464800	-0.729815	-1.938994
C	-0.781859	-1.100365	-1.574349
H	-1.360968	-1.699898	-2.279105
O	1.872387	-2.022428	2.345028
C	1.321297	-1.369842	3.145049
O	0.778211	-0.731181	3.959171
C	0.971537	-1.091648	-3.327402

H	1.215071	-0.190245	-3.905028
H	1.884490	-1.696760	-3.275080
H	0.220218	-1.655787	-3.890833

**TS<sub>J56</sub>**

**E= -2491.3792704au**

C	-3.478479	-1.565016	0.149743
C	-4.780105	-1.015265	0.298546
C	-5.892150	-1.853865	0.147029
H	-6.882777	-1.417314	0.255176
C	-5.781301	-3.216802	-0.123307
C	-4.495976	-3.753927	-0.185970
H	-4.375821	-4.824630	-0.336740
C	-3.345767	-2.972354	-0.034870
C	-5.080693	0.427771	0.654162
H	-4.875561	1.120795	-0.166838
H	-4.502615	0.774599	1.514662
H	-6.140082	0.526099	0.909766
C	-7.003518	-4.078926	-0.328121
H	-7.869622	-3.682309	0.212152
H	-6.831318	-5.106102	0.010784
H	-7.277548	-4.129207	-1.390627
C	-2.020544	-3.709394	-0.008463
H	-1.493814	-3.538840	0.936139
H	-1.338532	-3.420171	-0.812082
H	-2.194421	-4.785991	-0.095134
C	-2.156412	1.243451	0.193669
C	-2.481772	1.903529	-1.018974
C	-2.496843	3.302184	-1.048856
H	-2.736594	3.799081	-1.986438
C	-2.210989	4.077447	0.077175
C	-1.961725	3.409418	1.277072
H	-1.780878	3.990012	2.179386
C	-1.928460	2.012776	1.362570
C	-2.838634	1.180083	-2.299610
H	-3.451698	1.825738	-2.936764
H	-3.400498	0.259369	-2.117006
H	-1.939041	0.916598	-2.864514
C	-2.138163	5.582589	-0.006432
H	-2.446366	6.055026	0.932278
H	-2.768427	5.973320	-0.811983
H	-1.107891	5.900538	-0.212792
C	-1.646767	1.409893	2.724141

H	-1.864141	2.140242	3.509694
H	-0.591521	1.130593	2.824748
H	-2.241497	0.515317	2.929609
C	2.752860	-1.282760	-0.368567
C	2.604424	-2.649690	-0.093765
F	1.375815	-3.190095	0.002695
C	3.677811	-3.512665	0.099717
F	3.477776	-4.807981	0.370372
C	4.975807	-3.016498	0.001380
F	6.018836	-3.830426	0.174498
C	5.177857	-1.669776	-0.285186
F	6.422678	-1.190081	-0.393399
C	4.076892	-0.834727	-0.459855
C	1.603290	1.217741	-0.340636
C	1.049264	2.153301	-1.223408
F	0.468297	1.755653	-2.371891
C	1.081966	3.526271	-0.998685
F	0.518040	4.378617	-1.866271
C	1.684594	4.014278	0.154213
F	1.688863	5.328317	0.399071
C	2.277122	3.128455	1.051264
F	2.872803	3.596808	2.154834
C	2.240359	1.763622	0.784592
F	2.842657	0.962606	1.674652
F	4.348104	0.449216	-0.753329
B	1.489082	-0.344645	-0.582532
P	-1.886526	-0.600697	0.289271
C	0.325304	-0.905239	-1.504540
C	-0.996561	-1.012565	-1.263578
H	-1.628962	-1.437732	-2.043179
O	0.739142	-0.824329	1.526073
C	-0.269644	-1.322423	1.961558
O	-0.834792	-1.968717	2.781433
C	0.833151	-1.347666	-2.871931
H	1.379205	-0.538502	-3.373376
H	1.527240	-2.191874	-2.779932
H	0.008823	-1.649822	-3.526983

**J<sub>6</sub>**

**E= -2491.4063814au**

C	0.733574	-1.078380	-1.340408
O	1.206227	-1.606304	-2.323735
O	-0.515297	-0.869903	-1.092167

C	3.494412	-1.451030	-0.069593
C	4.776645	-0.850011	-0.204783
C	5.904507	-1.678416	-0.225580
H	6.881466	-1.212979	-0.330258
C	5.825914	-3.066603	-0.123645
C	4.557056	-3.635818	-0.022826
H	4.464442	-4.718019	0.029425
C	3.385951	-2.872680	-0.003880
C	5.044548	0.634844	-0.351852
H	4.764260	1.207737	0.536235
H	4.510751	1.074210	-1.198148
H	6.113238	0.794402	-0.519768
C	7.067916	-3.923465	-0.113765
H	7.916030	-3.406185	-0.573242
H	6.908391	-4.864366	-0.650989
H	7.357131	-4.181600	0.913622
C	2.082304	-3.643599	0.018755
H	1.627690	-3.652440	-0.977455
H	1.338180	-3.236550	0.705740
H	2.270194	-4.681023	0.309033
C	2.080941	1.353700	-0.012208
C	2.269690	2.064614	1.202421
C	2.170076	3.457755	1.188199
H	2.302153	3.995787	2.123900
C	1.896093	4.175877	0.022227
C	1.805252	3.460576	-1.172669
H	1.649803	4.001864	-2.103060
C	1.896303	2.065533	-1.225971
C	2.598894	1.413465	2.529303
H	3.143959	2.120995	3.161917
H	3.224807	0.521139	2.424347
H	1.686466	1.126707	3.060654
C	1.675618	5.667261	0.057941
H	1.964651	6.141957	-0.885274
H	2.237286	6.139479	0.870480
H	0.612406	5.882820	0.225136
C	1.802551	1.423915	-2.594252
H	2.088830	2.152252	-3.358757
H	0.779777	1.102742	-2.823661
H	2.446342	0.548535	-2.708305
C	-2.592487	-1.436601	0.174196
C	-2.451368	-2.813122	-0.028260
F	-1.214597	-3.357379	-0.118261

C	-3.520493	-3.698431	-0.122763
F	-3.315743	-5.009612	-0.317652
C	-4.818053	-3.209099	0.001722
F	-5.863633	-4.040564	-0.080644
C	-5.013883	-1.851110	0.224713
F	-6.258316	-1.370013	0.359866
C	-3.911039	-1.000091	0.310181
C	-1.551131	1.119788	0.110193
C	-1.248576	2.075124	1.078837
F	-0.740836	1.713574	2.282360
C	-1.415856	3.446097	0.890685
F	-1.043973	4.320352	1.842146
C	-1.928226	3.914437	-0.310733
F	-2.055642	5.233415	-0.518684
C	-2.280974	3.002317	-1.301361
F	-2.786535	3.441557	-2.463086
C	-2.091795	1.642322	-1.071618
F	-2.459042	0.812402	-2.065463
F	-4.192771	0.297544	0.549533
B	-1.249819	-0.492215	0.226293
P	1.929117	-0.488146	0.048541
C	-0.342925	-0.889839	1.526540
C	1.004926	-0.956383	1.522334
H	1.582400	-1.265587	2.391514
C	-1.060046	-1.251111	2.807246
H	-1.614063	-2.188526	2.679242
H	-0.372773	-1.369995	3.652439
H	-1.797030	-0.482922	3.065872

## J7

E= -2492.583573au

C	-0.73076900	-1.07766300	1.30182300
O	-1.20139200	-1.61852500	2.28108800
O	0.51640100	-0.86357200	1.05641900
C	-3.49163900	-1.45071500	0.03652500
C	-4.77605600	-0.85651200	0.18081000
C	-5.90012300	-1.69015700	0.19705600
H	-6.87884300	-1.23011400	0.30867500
C	-5.81562700	-3.07697500	0.08211800
C	-4.54456800	-3.63962200	-0.02811400
H	-4.44736100	-4.72085100	-0.09098200
C	-3.37692400	-2.87125100	-0.04347500
C	-5.05015300	0.62575100	0.34196100

H	-4.77341600	1.20809400	-0.54108800
H	-4.51735800	1.05952500	1.19177800
H	-6.11931600	0.77915800	0.51248600
C	-7.05365400	-3.93947300	0.06855100
H	-7.90531300	-3.42636500	0.52606100
H	-6.89112100	-4.87986600	0.60581300
H	-7.33877500	-4.19863700	-0.95969900
C	-2.07006200	-3.63621300	-0.07817600
H	-1.61368000	-3.65635600	0.91707800
H	-1.32883300	-3.21723600	-0.76104500
H	-2.25402700	-4.67057000	-0.38154000
C	-2.08929500	1.36088400	0.00591500
C	-2.28266600	2.08424000	-1.20067900
C	-2.18766500	3.47743600	-1.17140600
H	-2.32302100	4.02512900	-2.10098800
C	-1.91410500	4.18371100	0.00189100
C	-1.81924500	3.45578500	1.18883000
H	-1.66431000	3.98746500	2.12481400
C	-1.90548600	2.05992600	1.22721900
C	-2.61265100	1.44649200	-2.53387200
H	-3.16105000	2.15928400	-3.15761100
H	-3.23611300	0.55147300	-2.43730600
H	-1.70062300	1.16810700	-3.07032300
C	-1.69859700	5.67610100	-0.01794500
H	-1.98811800	6.13960000	0.93066400
H	-2.26271400	6.15520700	-0.82472300
H	-0.63627200	5.89694000	-0.18392600
C	-1.80823200	1.40405800	2.58846100
H	-2.09654000	2.12313100	3.36088500
H	-0.78417900	1.08420600	2.81401600
H	-2.44898700	0.52535500	2.69366800
C	2.59412600	-1.40965400	-0.21863700
C	2.45698500	-2.78888900	-0.03260100
F	1.22157700	-3.33752500	0.05007500
C	3.52857400	-3.67211500	0.05216400
F	3.32757600	-4.98603000	0.23086900
C	4.82473700	-3.17731900	-0.06528800
F	5.87271000	-4.00649000	0.00791300
C	5.01669900	-1.81615500	-0.27176700
F	6.25973200	-1.32971200	-0.39995200
C	3.91145100	-0.96742400	-0.34800500
C	1.54342400	1.14235000	-0.12758100
C	1.23534100	2.10620300	-1.08603400

F	0.72766500	1.75461800	-2.29254800
C	1.39655300	3.47587900	-0.88384500
F	1.01915000	4.35823900	-1.82555500
C	1.90823600	3.93404000	0.32179900
F	2.02939000	5.25137900	0.54332600
C	2.26639000	3.01340100	1.30256300
F	2.77107200	3.44285900	2.46819200
C	2.08318100	1.65497500	1.05901900
F	2.45482800	0.81647700	2.04368100
F	4.18941500	0.33386900	-0.57115700
B	1.24903400	-0.46921000	-0.26020000
P	-1.93154700	-0.47945800	-0.07637900
C	0.34024800	-0.85714500	-1.56196100
C	-1.00738700	-0.92882500	-1.55581200
H	-1.58552300	-1.23165400	-2.42676000
C	1.05600300	-1.20317500	-2.84759500
H	1.61122700	-2.14129100	-2.73045000
H	0.36768700	-1.31364900	-3.69304900
H	1.79173300	-0.43134900	-3.09873600
H	0.89769200	-2.77890200	4.58395500
H	0.47482300	-2.50197200	4.03789300

**TSJ78**

**E= -2492.43955au**

P	-1.98720100	0.07288100	0.03509700
B	1.42621300	-0.00892400	-0.08966000
O	0.61163000	0.17115300	1.23309800
O	-0.94152500	0.02869800	2.88931200
C	-0.90138800	0.04111000	-1.41671400
C	0.45118500	0.05499500	-1.38975600
C	-0.46667200	-0.22483200	1.80197700
C	-3.14299300	-1.40476900	0.13352600
C	-3.04193500	-2.57833500	-0.66217000
C	-3.92183300	-3.63751900	-0.41258600
H	-3.84475900	-4.52740600	-1.03319500
C	-4.88368800	-3.59988400	0.59807800
C	-4.94506000	-2.45245600	1.38956300
H	-5.67468100	-2.40144400	2.19464300
C	-4.08975900	-1.36318000	1.19788900
C	-2.03905000	-2.77890800	-1.77934600
H	-1.00856300	-2.67834500	-1.42978900
H	-2.17382700	-2.06184400	-2.59512800
H	-2.15184500	-3.78169100	-2.20134500



C	-5.79360400	-4.77653900	0.85389600
H	-5.32613500	-5.49035000	1.54516500
H	-6.01721000	-5.31919800	-0.07057700
H	-6.74056900	-4.46052600	1.30347400
C	-4.24176700	-0.18462300	2.13913000
H	-4.70888800	0.67456400	1.64584100
H	-3.28201300	0.14730600	2.54806000
H	-4.87328200	-0.46601700	2.98691700
C	-3.03209200	1.59805700	-0.23062200
C	-2.66284000	2.78245400	0.44584900
C	-3.41131600	3.94553400	0.23003700
H	-3.12263300	4.85272000	0.75544100
C	-4.50047900	3.97834600	-0.63990700
C	-4.82388600	2.80304800	-1.32361300
H	-5.65498600	2.81049700	-2.02608600
C	-4.11452500	1.61058000	-1.14829500
C	-1.45961400	2.86061500	1.35585900
H	-1.40165400	3.84482500	1.82993600
H	-0.53541400	2.72060400	0.78364100
H	-1.47832600	2.11146000	2.15358700
C	-5.29702900	5.24247700	-0.85756100
H	-4.91932400	6.06447700	-0.24218300
H	-6.35501700	5.09394500	-0.60871600
H	-5.25562600	5.56168400	-1.90631600
C	-4.55876400	0.41493400	-1.96510300
H	-5.21485100	0.74371700	-2.77660400
H	-5.11326400	-0.31301700	-1.36335500
H	-3.71963900	-0.12028100	-2.41968400
C	2.41095300	1.30167700	0.07650300
C	3.51352000	1.28496100	0.93751100
F	3.85335100	0.15099200	1.58394800
C	4.31790300	2.39288100	1.18860700
F	5.36941300	2.30332300	2.01514700
C	4.01911300	3.60738300	0.57796400
F	4.77780400	4.68549100	0.80663300
C	2.91692800	3.68760000	-0.26424500
F	2.59952700	4.85491200	-0.84477100
C	2.14003900	2.55054500	-0.48390900
F	1.05806200	2.72976700	-1.27901300
C	2.26777400	-1.43520600	-0.16731700
C	3.51061900	-1.51433400	-0.81103600
F	4.06633500	-0.41767200	-1.36677500
C	4.24859500	-2.68800800	-0.94409900

F	5.43604900	-2.67836900	-1.56326600
C	3.74330000	-3.88072000	-0.43661300
F	4.43472400	-5.01868100	-0.55671800
C	2.49841600	-3.87084700	0.17975100
F	1.96990700	-5.00866100	0.65171100
C	1.80241600	-2.66851900	0.28218500
F	0.56401700	-2.77737600	0.84759400
H	-0.68341500	-1.42558200	1.50226700
H	-1.22929500	-1.00884000	1.00142500
H	-1.41469300	0.12565600	-2.37535200
C	1.15512900	0.07484000	-2.73368800
H	0.46356400	0.27813500	-3.55835600
H	1.95467400	0.82057500	-2.75934700
H	1.62951700	-0.89673500	-2.92264600

## J8

E= -2492.612566au

P	2.16573300	-0.13871700	-0.08476400
B	-1.31548500	-0.22351100	-0.17670100
O	-0.38020800	0.08752300	0.96817700
O	0.08989400	0.44752100	3.11797500
C	1.02522100	-0.35264900	-1.46358200
H	1.58041600	-0.50271800	-2.39037700
C	-0.32630900	-0.44693000	-1.46368700
C	-0.72073100	0.37056200	2.21689200
C	2.53717200	1.55180500	0.52103000
C	2.25048100	2.72782000	-0.21540400
C	2.58250500	3.96074100	0.35409400
H	2.36675300	4.86451100	-0.21090000
C	3.17065000	4.07383700	1.61586000
C	3.43976900	2.89947000	2.31971300
H	3.89633200	2.96160800	3.30462900
C	3.13055900	1.63655700	1.80747800
C	1.59271900	2.75257800	-1.57787700
H	0.53055700	2.50815900	-1.50190700
H	2.03374300	2.04671600	-2.28687300
H	1.67648300	3.75313000	-2.01218400
C	3.47948700	5.42631000	2.21017000
H	2.60844000	5.82107200	2.74949300
H	3.74029600	6.15579100	1.43617500
H	4.30785300	5.37157800	2.92394700
C	3.40652800	0.42889100	2.67562300
H	3.94304500	-0.36589900	2.14537100

H	2.45775700	0.02919400	3.05584500
H	4.01596800	0.71466100	3.53753300
C	3.68891400	-1.07970500	-0.53776400
C	4.79699000	-0.50469000	-1.20656200
C	5.89647400	-1.31584000	-1.50709800
H	6.74289000	-0.86974400	-2.02425200
C	5.94096500	-2.67097200	-1.17553200
C	4.82936100	-3.22175100	-0.53532800
H	4.83152300	-4.28020300	-0.28550700
C	3.70177000	-2.46251400	-0.20805700
C	4.86534000	0.94609200	-1.62989400
H	5.74334300	1.11147000	-2.26075600
H	4.93683300	1.62249900	-0.77263000
H	3.98870700	1.25026900	-2.21004000
C	7.15559300	-3.51121700	-1.48753900
H	7.70241000	-3.12022200	-2.35158800
H	6.88078500	-4.55016000	-1.69737300
H	7.85168300	-3.52384500	-0.63833400
C	2.55148200	-3.17377800	0.47715000
H	2.73651800	-4.25136400	0.49271600
H	1.59264400	-3.01594700	-0.02620700
H	2.43446500	-2.85458300	1.52119200
C	-2.15378200	-1.59667800	0.23100600
C	-3.29687200	-1.56048200	1.03665300
F	-3.79561900	-0.37560700	1.46016200
C	-3.98651300	-2.69040300	1.46909400
F	-5.07727900	-2.57539800	2.23893500
C	-3.53109200	-3.95135600	1.09731200
F	-4.17529000	-5.05215700	1.50135800
C	-2.39274100	-4.05047500	0.30616100
F	-1.93195000	-5.25727800	-0.05668300
C	-1.73872700	-2.88806300	-0.09936800
F	-0.63367700	-3.08542900	-0.86369500
C	-2.31788000	1.04947000	-0.53070600
C	-3.49782100	0.88754300	-1.26463200
F	-3.86787600	-0.34160200	-1.69127200
C	-4.35347100	1.93029500	-1.60901400
F	-5.46997100	1.69828200	-2.31431500
C	-4.03962700	3.22809300	-1.21690000
F	-4.84412600	4.24782000	-1.53980900
C	-2.87384300	3.45048000	-0.49441100
F	-2.54791400	4.69645200	-0.11768100
C	-2.04667300	2.37339600	-0.17460100

F	-0.92453400	2.69271800	0.51342800
H	1.71408300	-0.82052600	1.04561000
H	-1.79929800	0.52715100	2.37626100
C	-0.96983300	-0.73285600	-2.80382000
H	-1.54541700	0.13864600	-3.13856200
H	-0.23580100	-0.97449000	-3.58002200
H	-1.68133500	-1.56050600	-2.72811000

## TSJ8

E= -2492.57257au

P	-1.96984400	0.13505500	0.01373700
B	1.56830400	0.10335500	-0.51242300
O	0.61709100	0.01558500	1.51241300
O	-0.05777300	-0.93376400	3.45433500
C	-0.96169400	0.14067600	-1.52096700
H	-1.50479200	0.21163000	-2.46405100
C	0.38571400	0.17235800	-1.57882400
C	0.81187000	-0.65594300	2.66866000
C	-2.95866500	-1.43542200	0.21022600
C	-2.97644200	-2.55109700	-0.66340600
C	-3.71982900	-3.68306900	-0.30478500
H	-3.72375400	-4.53330500	-0.98392100
C	-4.45071500	-3.76215100	0.88065200
C	-4.40008600	-2.66581600	1.74233300
H	-4.93733500	-2.70631700	2.68769100
C	-3.65951700	-1.51780500	1.44498900
C	-2.23242600	-2.61715900	-1.97993700
H	-1.15923800	-2.46504100	-1.84594000
H	-2.58063900	-1.86456200	-2.69614800
H	-2.37891300	-3.59743500	-2.44388700
C	-5.27364400	-4.98340000	1.21541000
H	-6.31946200	-4.85525900	0.90469200
H	-5.27884500	-5.17947300	2.29320000
H	-4.89074400	-5.87594400	0.70954700
C	-3.61248700	-0.42019400	2.48883200
H	-3.93198800	0.55149500	2.09697200
H	-2.59632500	-0.30552100	2.88704500
H	-4.26878000	-0.66899400	3.32844100
C	-3.16466700	1.53949800	-0.30623600
C	-4.36031900	1.43809500	-1.05961200
C	-5.18264600	2.56496300	-1.18985500
H	-6.10013500	2.47228800	-1.76761400
C	-4.86586000	3.79555300	-0.61515600

C	-3.67297700	3.88591600	0.10468200
H	-3.39409900	4.83734200	0.55310900
C	-2.81850200	2.79155200	0.26853600
C	-4.81159500	0.17295300	-1.75542600
H	-5.63120300	0.39554400	-2.44579600
H	-5.16355600	-0.58495000	-1.04866200
H	-4.00588400	-0.28407700	-2.33725000
C	-5.76101500	4.99858700	-0.79538200
H	-5.78746300	5.61762000	0.10827200
H	-6.78755500	4.70226700	-1.03463800
H	-5.40528500	5.63799500	-1.61447400
C	-1.53064200	3.01343100	1.03439400
H	-1.48056000	4.04300900	1.40230100
H	-0.65705100	2.84892000	0.39426000
H	-1.43619300	2.34401800	1.89616500
C	2.34457600	1.42964000	-0.10213500
C	3.35361100	1.42250300	0.87389700
F	3.68527400	0.27379600	1.49591000
C	4.04463900	2.55692600	1.27997800
F	4.99539500	2.48259900	2.21807100
C	3.73470000	3.78648600	0.70156800
F	4.38714700	4.88736700	1.07618500
C	2.73361700	3.85624900	-0.26048000
F	2.41802500	5.03341800	-0.81279600
C	2.05811500	2.69486800	-0.63269400
F	1.08582500	2.85579400	-1.54903700
C	2.32290700	-1.30588500	-0.48650600
C	3.66029900	-1.45075900	-0.87318900
F	4.38623400	-0.37100100	-1.21988200
C	4.30496000	-2.68265500	-0.94578200
F	5.58537300	-2.76311700	-1.32580800
C	3.60316500	-3.84060400	-0.62170600
F	4.20549400	-5.02994000	-0.68173300
C	2.26716100	-3.75069400	-0.23952600
F	1.58521000	-4.85913100	0.06955300
C	1.65634500	-2.50041600	-0.19147500
F	0.36048600	-2.47728000	0.17780400
H	-0.38259600	0.14091200	1.30979800
H	1.87778800	-0.88934600	2.79613000
C	1.02223600	0.20984500	-2.97307000
H	1.82997400	0.94649600	-3.04546900
H	1.45754900	-0.76623800	-3.22332100
H	0.27737300	0.45503700	-3.73682600

## K<sub>5</sub>

E= -2683.1350491au

C	1.896643	-2.440081	-0.806324
C	2.801508	-3.376337	-0.244966
C	2.999549	-4.606367	-0.885305
H	3.700688	-5.313390	-0.445870
C	2.332720	-4.955023	-2.060245
C	1.438813	-4.027307	-2.596816
H	0.903980	-4.274489	-3.511857
C	1.204144	-2.784856	-1.997257
C	3.591601	-3.125427	1.020581
H	2.962584	-2.759394	1.836986
H	4.379950	-2.380860	0.870852
H	4.064977	-4.051888	1.360751
C	2.547564	-6.300309	-2.712902
H	3.534720	-6.709449	-2.473290
H	2.461442	-6.234922	-3.803051
H	1.800519	-7.030121	-2.372496
C	0.185683	-1.873541	-2.652085
H	0.569027	-0.862389	-2.817490
H	-0.711094	-1.781133	-2.030232
H	-0.124400	-2.285625	-3.617950
C	3.171746	-0.029725	0.450440
C	3.559562	0.316783	1.771232
C	4.782017	0.971724	1.975078
H	5.066899	1.224247	2.994662
C	5.646692	1.303395	0.932437
C	5.248904	0.965795	-0.361232
H	5.896781	1.214969	-1.199513
C	4.033197	0.327111	-0.624985
C	2.748306	0.010404	3.013834
H	3.225130	0.461014	3.889974
H	2.679624	-1.066287	3.206193
H	1.727670	0.394553	2.961235
C	6.945474	2.030084	1.190213
H	7.716411	1.742203	0.467006
H	7.328087	1.822854	2.195335
H	6.815866	3.117922	1.109428
C	3.690292	0.049518	-2.073734
H	4.448059	0.482694	-2.733829
H	2.722136	0.483685	-2.351718
H	3.634599	-1.023293	-2.288092

C	-2.786063	0.094976	0.034037
C	-3.197684	-1.184804	-0.372621
F	-2.359606	-2.230031	-0.274891
C	-4.445564	-1.445509	-0.928825
F	-4.778025	-2.680401	-1.319516
C	-5.356420	-0.402103	-1.076363
F	-6.560425	-0.634173	-1.597482
C	-5.003433	0.885789	-0.679743
F	-5.880065	1.886807	-0.811937
C	-3.739258	1.111487	-0.145970
C	-0.688486	1.764759	0.502523
C	-0.070106	2.437878	1.561425
F	-0.115356	1.921667	2.806328
C	0.582130	3.658856	1.413017
F	1.145954	4.266913	2.461818
C	0.634261	4.250635	0.153988
F	1.257418	5.416984	-0.014720
C	0.022893	3.622257	-0.930621
F	0.073870	4.191765	-2.143861
C	-0.631084	2.413912	-0.737548
F	-1.196047	1.841199	-1.818543
F	-3.471202	2.371529	0.234974
B	-1.374807	0.358185	0.682990
P	1.521954	-0.735507	-0.096615
C	-0.722435	-0.758909	1.584480
C	0.526154	-1.241670	1.377388
H	0.882368	-2.044195	2.022640
C	-1.567895	-1.343900	2.668566
C	-2.282514	-0.506626	3.543491
C	-1.679687	-2.735147	2.835708
C	-3.067736	-1.042519	4.564212
H	-2.189921	0.571764	3.447944
C	-2.467899	-3.270239	3.854023
H	-1.162346	-3.394861	2.145319
C	-3.163899	-2.426372	4.722824
H	-3.601324	-0.377673	5.238338
H	-2.545028	-4.348812	3.963915
H	-3.778754	-2.844411	5.515260
O	-0.967590	2.801182	-4.837947
C	0.009191	2.335268	-4.397693
O	0.994357	1.860751	-3.980966

E= -2683.1119051au

C	3.431065	-1.723844	-0.493152
C	4.796166	-1.331843	-0.441620
C	5.783862	-2.323373	-0.376693
H	6.824139	-2.008497	-0.329393
C	5.490865	-3.686115	-0.379871
C	4.152047	-4.051879	-0.513505
H	3.895095	-5.106799	-0.580212
C	3.120326	-3.111212	-0.597195
C	5.297573	0.098268	-0.494144
H	5.107952	0.651912	0.429762
H	4.842904	0.670562	-1.306712
H	6.379236	0.097116	-0.659002
C	6.579897	-4.724024	-0.255882
H	7.527976	-4.362429	-0.667891
H	6.312774	-5.649794	-0.776490
H	6.759906	-4.982966	0.796272
C	1.734276	-3.651286	-0.891191
H	1.426623	-3.378562	-1.906906
H	0.957597	-3.285411	-0.216717
H	1.737625	-4.743590	-0.830470
C	2.456858	1.194029	-0.106586
C	2.757083	1.585768	1.223722
C	2.977302	2.939441	1.497401
H	3.199550	3.232745	2.521108
C	2.921625	3.922366	0.506404
C	2.684173	3.508506	-0.805172
H	2.675988	4.249847	-1.601439
C	2.449828	2.168818	-1.135736
C	2.881816	0.615122	2.377910
H	3.486067	1.057360	3.176425
H	3.357097	-0.325234	2.082181
H	1.901083	0.374876	2.800124
C	3.078689	5.383644	0.848068
H	3.469146	5.957571	0.001365
H	3.749271	5.529051	1.701630
H	2.105433	5.812347	1.119706
C	2.203545	1.848013	-2.595966
H	2.559659	2.669472	-3.225117
H	1.134112	1.722298	-2.801739
H	2.706847	0.935036	-2.926945
C	-2.738382	-0.754931	-0.324800
C	-2.730425	-2.086118	-0.763495

TSK56

F -1.571869 -2.764449 -0.855058  
 C -3.879689 -2.776229 -1.133676  
 F -3.811728 -4.044279 -1.557687  
 C -5.113945 -2.136249 -1.053505  
 F -6.229717 -2.783744 -1.396504  
 C -5.177845 -0.819429 -0.608066  
 F -6.362902 -0.203290 -0.515284  
 C -4.003469 -0.158544 -0.258677  
 C -1.297675 1.559584 0.041675  
 C -0.701225 2.324814 1.052210  
 F -0.239194 1.741044 2.174952  
 C -0.579513 3.709998 0.992677  
 F 0.000660 4.392204 1.991003  
 C -1.050168 4.388576 -0.124837  
 F -0.915704 5.714590 -0.208278  
 C -1.665849 3.677805 -1.152654  
 F -2.133450 4.329685 -2.224108  
 C -1.790861 2.296416 -1.047954  
 F -2.412108 1.675625 -2.059271  
 F -4.142655 1.103816 0.187676  
 B -1.400451 -0.020413 0.110971  
 P 1.979029 -0.552398 -0.545511  
 C -0.404547 -0.869814 1.020274  
 C 0.914471 -1.111107 0.842293  
 H 1.418642 -1.757842 1.559222  
 C -1.068096 -1.521503 2.198953  
 C -1.944774 -0.795177 3.024875  
 C -0.855100 -2.879717 2.493057  
 C -2.568408 -1.399743 4.116107  
 H -2.117938 0.258741 2.831881  
 C -1.481757 -3.485125 3.582043  
 H -0.210920 -3.470541 1.848904  
 C -2.340192 -2.747507 4.399627  
 H -3.232432 -0.814312 4.746506  
 H -1.306143 -4.538335 3.785162  
 H -2.830310 -3.219834 5.246563  
 O -0.511863 -0.330903 -2.000808  
 C 0.516724 -0.805506 -2.421789  
 O 1.115641 -1.326964 -3.308407

**K<sub>6</sub>**

E= -2683.1382899au

C 0.919176 -0.796548 -1.723855

O 1.406838 -1.252489 -2.735363  
 O -0.311829 -0.461984 -1.533221  
 C 3.492992 -1.669525 -0.311977  
 C 4.843119 -1.223537 -0.266986  
 C 5.864816 -2.179226 -0.310019  
 H 6.894452 -1.831946 -0.274852  
 C 5.617723 -3.548173 -0.399923  
 C 4.287898 -3.960344 -0.476541  
 H 4.066695 -5.020227 -0.576918  
 C 3.216180 -3.063301 -0.447447  
 C 5.294882 0.221809 -0.194961  
 H 5.000491 0.713265 0.736024  
 H 4.899120 0.825619 -1.015407  
 H 6.385959 0.262623 -0.254990  
 C 6.746391 -4.549556 -0.405148  
 H 7.692276 -4.086553 -0.703269  
 H 6.540909 -5.380205 -1.088801  
 H 6.891203 -4.980793 0.594256  
 C 1.836858 -3.660337 -0.632161  
 H 1.482839 -3.493401 -1.654896  
 H 1.080550 -3.246579 0.036901  
 H 1.873927 -4.740258 -0.464234  
 C 2.414299 1.262396 0.007235  
 C 2.584728 1.788023 1.315663  
 C 2.666143 3.172722 1.476795  
 H 2.783096 3.570981 2.481807  
 C 2.589230 4.057210 0.398423  
 C 2.510954 3.511088 -0.883152  
 H 2.508127 4.177080 -1.742898  
 C 2.428900 2.133395 -1.112815  
 C 2.711513 0.940431 2.563972  
 H 3.253368 1.497542 3.334453  
 H 3.258857 0.007408 2.392069  
 H 1.727526 0.685395 2.968206  
 C 2.560507 5.548947 0.615862  
 H 2.938715 6.092996 -0.255414  
 H 3.150546 5.841558 1.490702  
 H 1.528159 5.877383 0.792294  
 C 2.381796 1.681037 -2.556935  
 H 2.818367 2.454700 -3.195409  
 H 1.353367 1.522656 -2.901533  
 H 2.926578 0.751414 -2.737767  
 C -2.538462 -0.957528 -0.534004

C -2. 501465 -2. 308148 -0. 891828  
 F -1. 316212 -2. 960256 -0. 946143  
 C -3. 630598 -3. 065154 -1. 188065  
 F -3. 523045 -4. 358805 -1. 526404  
 C -4. 885115 -2. 466405 -1. 120227  
 F -5. 988219 -3. 172869 -1. 396538  
 C -4. 980192 -1. 129835 -0. 749573  
 F -6. 184377 -0. 545180 -0. 663858  
 C -3. 819704 -0. 410917 -0. 465127  
 C -1. 245768 1. 469173 -0. 184546  
 C -0. 859983 2. 283435 0. 879844  
 F -0. 436767 1. 750737 2. 050242  
 C -0. 866051 3. 676860 0. 827914  
 F -0. 435355 4. 404091 1. 874368  
 C -1. 280018 4. 318167 -0. 330605  
 F -1. 256428 5. 656364 -0. 404571  
 C -1. 702547 3. 554462 -1. 415619  
 F -2. 115992 4. 161501 -2. 537277  
 C -1. 679017 2. 165982 -1. 320671  
 F -2. 104354 1. 486886 -2. 401180  
 F -4. 005094 0. 870874 -0. 076843  
 B -1. 128484 -0. 170551 -0. 237768  
 P 2. 044429 -0. 537467 -0. 188547  
 C -0. 389741 -0. 842582 1. 069163  
 C 0. 945358 -1. 065451 1. 135948  
 H 1. 418679 -1. 535117 1. 994195  
 C -1. 213408 -1. 306578 2. 223378  
 C -2. 336023 -0. 574168 2. 652328  
 C -0. 901102 -2. 494520 2. 910163  
 C -3. 089837 -0. 994769 3. 746463  
 H -2. 622952 0. 332810 2. 132955  
 C -1. 663865 -2. 922877 3. 995700  
 H -0. 071744 -3. 107938 2. 569655  
 C -2. 757797 -2. 169421 4. 424612  
 H -3. 945075 -0. 404835 4. 064815  
 H -1. 408326 -3. 851393 4. 499486  
 H -3. 353829 -2. 501147 5. 270442

**K7**

**E= -2684.314811au**

C 0. 93486000 -0. 79210700 -1. 67436800  
 O 1. 43921900 -1. 25129000 -2. 67696200  
 O -0. 30275100 -0. 47611800 -1. 50092400

C 3. 50374600 -1. 61507900 -0. 22710200  
 C 4. 84770300 -1. 15195900 -0. 17148500  
 C 5. 88124700 -2. 09558800 -0. 19294500  
 H 6. 90616000 -1. 73563500 -0. 14968400  
 C 5. 65173100 -3. 46824200 -0. 27146200  
 C 4. 32787100 -3. 89759600 -0. 35777400  
 H 4. 12064300 -4. 96114400 -0. 44885900  
 C 3. 24518800 -3. 01358500 -0. 34974100  
 C 5. 28102800 0. 29947800 -0. 10949300  
 H 4. 96616500 0. 79854600 0. 81066700  
 H 4. 89132900 0. 88863500 -0. 94344500  
 H 6. 37234200 0. 35275100 -0. 15291500  
 C 6. 79213200 -4. 45610100 -0. 25510000  
 H 7. 73970700 -3. 97972200 -0. 52519500  
 H 6. 61408900 -5. 28342500 -0. 95049700  
 H 6. 91591500 -4. 89410600 0. 74414100  
 C 1. 87518800 -3. 62983000 -0. 54127000  
 H 1. 53260900 -3. 48644100 -1. 57149400  
 H 1. 10526100 -3. 21295100 0. 11006300  
 H 1. 92240000 -4. 70599300 -0. 35303200  
 C 2. 38441300 1. 30756700 0. 04193900  
 C 2. 52956800 1. 85479600 1. 34452100  
 C 2. 58741800 3. 24290600 1. 48614300  
 H 2. 68454100 3. 65747400 2. 48663900  
 C 2. 51147600 4. 11022000 0. 39389500  
 C 2. 46045400 3. 54404000 -0. 88046000  
 H 2. 46028200 4. 19700200 -1. 75015200  
 C 2. 40248500 2. 16215600 -1. 09068400  
 C 2. 65311800 1. 02770400 2. 60683600  
 H 3. 17803600 1. 60375400 3. 37511900  
 H 3. 21545600 0. 10006400 2. 45538800  
 H 1. 66805500 0. 76491300 3. 00336200  
 C 2. 45490100 5. 60435100 0. 58777700  
 H 2. 85324400 6. 14098900 -0. 27915800  
 H 3. 01208200 5. 91832400 1. 47654700  
 H 1. 41284400 5. 92031600 0. 72563600  
 C 2. 38425700 1. 68782200 -2. 52833800  
 H 2. 82197300 2. 45711100 -3. 17129200  
 H 1. 36366700 1. 51174500 -2. 88731600  
 H 2. 94325100 0. 76251300 -2. 68600300  
 C -2. 53393600 -0. 98568200 -0. 51925100  
 C -2. 47746900 -2. 33919700 -0. 86327700  
 F -1. 28411800 -2. 97760500 -0. 90040300

C	-3.59491600	-3.11234300	-1.16223100	O	1.28417400	-0.43604200	-3.16962600
F	-3.46911800	-4.40778500	-1.48682500	C	0.98148600	-0.38976800	1.10906200
C	-4.85702400	-2.52796300	-1.11161300	H	1.40337000	-0.47995400	2.10550200
F	-5.94895300	-3.25035900	-1.39078900	C	-0.36348800	-0.30279200	0.98750800
C	-4.97140800	-1.18904500	-0.75503400	C	0.66266900	-0.59904600	-2.15101000
F	-6.18308000	-0.61791400	-0.68589800	C	3.53506600	-1.53907000	-0.15343700
C	-3.82213900	-0.45365500	-0.46739400	C	3.54750100	-2.66033100	0.71564500
C	-1.27579800	1.46093900	-0.18939600	C	4.60254400	-3.57869900	0.61675100
C	-0.91491900	2.29459800	0.86864200	H	4.60438500	-4.43225300	1.29072600
F	-0.50194800	1.78354000	2.05226500	C	5.63749600	-3.44723500	-0.30642700
C	-0.93661200	3.68695100	0.79672500	C	5.58249500	-2.36229000	-1.18360200
F	-0.52832400	4.43390400	1.83816700	H	6.35707000	-2.25008900	-1.93926100
C	-1.34173600	4.30673800	-0.37650300	C	4.55317100	-1.41891800	-1.14324100
F	-1.33113200	5.64396800	-0.46960500	C	2.50374600	-2.96213200	1.77260600
C	-1.74045900	3.52295600	-1.45616000	H	1.48029300	-2.85555600	1.40752000
F	-2.14508000	4.10926700	-2.59191000	H	2.60277400	-2.30797400	2.64712400
C	-1.70202800	2.13630900	-1.34104700	H	2.62550700	-3.98935700	2.12796100
F	-2.10446800	1.43680100	-2.41732100	C	6.76936300	-4.44397800	-0.37123400
F	-4.02585900	0.82964300	-0.09330900	H	6.91842500	-4.81226700	-1.39302300
B	-1.13746300	-0.17755000	-0.21795600	H	6.58196500	-5.30679100	0.27527200
P	2.04091700	-0.49976600	-0.13167800	H	7.71583200	-3.98845700	-0.05284500
C	-0.40288800	-0.82203900	1.10510900	C	4.58446800	-0.31569400	-2.18225200
C	0.93458500	-1.02506600	1.18785000	H	4.84917100	0.65421900	-1.74823300
H	1.40599400	-1.47665000	2.05675400	H	3.62188500	-0.20161400	-2.69216700
C	-1.23172300	-1.28306300	2.25675900	H	5.32756500	-0.54931100	-2.95029500
C	-2.37085800	-0.56303600	2.66260400	C	2.96304200	1.42793100	-0.03981800
C	-0.90809200	-2.45584900	2.96411600	C	2.65352100	2.51186100	-0.89493900
C	-3.13026400	-0.98035600	3.75410000	C	3.22447700	3.76272400	-0.63469900
H	-2.66648500	0.33184300	2.12742300	H	2.98071900	4.58764300	-1.29982900
C	-1.67621400	-2.88115800	4.04705500	C	4.08207000	3.98636300	0.44138600
H	-0.06505700	-3.06054400	2.64208000	C	4.37030900	2.90334800	1.27154500
C	-2.78712400	-2.13972600	4.45267500	H	5.03770400	3.04884200	2.11809800
H	-3.99852100	-0.40001500	4.05431100	C	3.83278400	1.62695600	1.06628700
H	-1.41145900	-3.79812400	4.56696200	C	1.73479000	2.40264000	-2.08556600
H	-3.38745800	-2.46916400	5.29634900	H	1.69855600	3.35264300	-2.62618200
H	2.82255700	-2.55198400	-5.42130400	H	0.71202100	2.15842200	-1.78441700
H	2.47436300	-2.26529500	-4.83011400	H	2.05321900	1.63158700	-2.79122900

## TSK78

E= -2684.172729au

P	2.16272800	-0.26245800	-0.27095600	H	4.65165300	5.35689000	0.71602400
B	-1.25978400	-0.08795700	-0.36650500	H	4.80537700	5.91985500	-0.21056400
O	-0.33392000	0.00597500	-1.63830700	H	5.60965600	5.29627300	1.24274300
				H	3.96931000	5.94482000	1.34405500
				C	4.25637300	0.55554100	2.05015800
				H	4.73255200	1.02104100	2.91791800

H	4.97642200	-0.14205900	1.61028200	O	-0.42595200	0.82236500	-3.34655800
H	3.41911500	-0.03812800	2.42439200	C	-1.00374000	-0.07974600	1.26035300
C	-1.97699900	1.39383400	-0.46771800	H	-1.47775300	-0.14007200	2.23921700
C	-3.12490000	1.62821000	-1.23553600	C	0.34414100	-0.21877500	1.16186000
F	-3.72914700	0.62338800	-1.89915700	C	0.44758300	0.68472800	-2.51480500
C	-3.71727400	2.88075700	-1.38350700	C	-2.74816700	1.64809500	-0.70754400
F	-4.82413500	3.02828900	-2.12419200	C	-2.47400800	2.87754000	-0.05718800
C	-3.14492100	3.98898600	-0.76868900	C	-2.91550300	4.05877900	-0.66236600
F	-3.69643300	5.20013100	-0.90193800	H	-2.70977800	5.00161700	-0.16112200
C	-1.98359100	3.82107000	-0.02457500	C	-3.59510800	4.07295800	-1.88194300
F	-1.39905300	4.87999900	0.55608200	C	-3.84393700	2.84946500	-2.50432800
C	-1.42574400	2.54956200	0.09200900	H	-4.36775400	2.83306300	-3.45701500
F	-0.26509200	2.49277700	0.79005200	C	-3.43137800	1.63454200	-1.95172200
C	-2.33795700	-1.32858800	-0.50360800	C	-1.70781600	3.01557700	1.23993800
C	-3.53666200	-1.29982900	0.22221600	H	-0.64438900	2.82728700	1.07716900
F	-3.83455200	-0.23430200	0.99080700	H	-2.05004600	2.33071100	2.01854700
C	-4.48686900	-2.31573300	0.19914900	H	-1.81296600	4.03369500	1.62640900
F	-5.61086800	-2.21677100	0.92143600	C	-4.01931500	5.37311300	-2.52002800
C	-4.26528600	-3.44422700	-0.58430800	H	-3.21437300	5.77804400	-3.14733200
F	-5.16396100	-4.43447800	-0.61888000	H	-4.25752400	6.13162800	-1.76697300
C	-3.09498700	-3.52642400	-1.32745400	H	-4.89631900	5.23844000	-3.16141300
F	-2.85651400	-4.60355900	-2.08965100	C	-3.69450000	0.37229000	-2.74085800
C	-2.17196700	-2.48245600	-1.26918500	H	-4.16336600	-0.41640700	-2.14247900
F	-1.06046400	-2.66533300	-2.02982100	H	-2.74910100	-0.00055500	-3.15488300
H	0.85951200	-1.76346000	-1.58861000	H	-4.36178300	0.58361600	-3.58105800
H	1.42883100	-1.22627400	-1.14441800	C	-3.70515600	-0.95772200	0.56001000
C	-1.09786600	-0.43589200	2.29662400	C	-4.65964200	-0.42182800	1.45995100
C	-1.53363800	-1.69801700	2.73058400	C	-5.73995800	-1.21710800	1.85443100
C	-1.31329000	0.67183400	3.12993400	H	-6.46707200	-0.79801500	2.54615800
C	-2.17846000	-1.84690000	3.95922400	C	-5.91105600	-2.52485600	1.39794400
H	-1.36537300	-2.56771400	2.10143400	C	-4.94555000	-3.04320700	0.53357800
C	-1.95974500	0.52048700	4.35786600	H	-5.04440600	-4.06798700	0.18351300
H	-0.96530000	1.64961400	2.81716100	C	-3.84296100	-2.29762000	0.10336700
C	-2.39759600	-0.73673600	4.77636900	C	-4.56040000	0.96565600	2.05207800
H	-2.50816400	-2.83269300	4.27698900	H	-5.42331700	1.16782000	2.69256900
H	-2.11857700	1.39103000	4.98908000	H	-4.52296500	1.74493100	1.28586900
H	-2.90259500	-0.85154700	5.73163100	H	-3.66650100	1.07333100	2.67803700

## K8

E= -2684.341644au

P	-2.24854700	0.00963000	-0.03994300	H	-7.49936100	-3.02368200	2.78231800
B	1.22068900	-0.11984700	-0.23385600	H	-6.85447600	-4.41130800	1.88440200
O	0.19909000	0.30742200	-1.26798200	H	-7.91944800	-3.25414900	1.08188800
				C	-2.85249800	-2.99025200	-0.81277100
				H	-3.14062400	-4.03665600	-0.94529700



H	-1.83649100	-2.98258100	-0.40742600	O	-0.29136800	0.90479600	-3.78560900
H	-2.82035700	-2.53951600	-1.81256800	C	-1.01828900	-0.20397400	1.18614300
C	1.82200500	-1.56768900	-0.77830800	H	-1.49539400	-0.34442800	2.15523200
C	2.83095000	-1.63437400	-1.74623400	C	0.33562200	-0.22135000	1.16682400
F	3.42758300	-0.50491800	-2.18955100	C	0.58241700	0.67086400	-2.99227200
C	3.28246700	-2.81774900	-2.32510200	C	-3.16123200	1.43666200	-0.29135000
F	4.25725200	-2.80252000	-3.24403000	C	-3.13181900	2.49262400	0.65377000
C	2.70811300	-4.02741900	-1.94653600	C	-3.91591400	3.63057800	0.42282200
F	3.12303800	-5.17641800	-2.49192600	H	-3.88467700	4.43496400	1.15475700
C	1.69329000	-4.02243000	-0.99740500	C	-4.72899400	3.77288400	-0.70148700
F	1.11775600	-5.17523300	-0.62253300	C	-4.72241200	2.73725100	-1.63658100
C	1.28014100	-2.81018000	-0.44694900	H	-5.32449700	2.83048700	-2.53805200
F	0.28108700	-2.90420100	0.46922300	C	-3.94753000	1.58611400	-1.46703300
C	2.38488600	1.03201200	0.00947600	C	-2.29319000	2.49067400	1.91428300
C	3.67055000	0.74066700	0.47754700	H	-1.23179600	2.35419700	1.69618400
F	4.04878400	-0.53808800	0.69004200	H	-2.58404000	1.69683000	2.61095200
C	4.63729700	1.70484800	0.75086000	H	-2.40983900	3.44201600	2.44225300
F	5.85182200	1.35010900	1.19451300	C	-5.59080800	4.99763900	-0.89654900
C	4.33773300	3.04964300	0.55914600	H	-6.61501200	4.82326800	-0.53988000
F	5.25156000	3.99289100	0.81772300	H	-5.66030600	5.27414500	-1.95435700
C	3.07384900	3.39895000	0.09936800	H	-5.19589300	5.85767000	-0.34571200
F	2.76081400	4.69081800	-0.08648900	C	-3.95851100	0.55947900	-2.58168400
C	2.13962300	2.39718400	-0.15912300	H	-4.26837100	-0.43363600	-2.23808500
F	0.92948700	2.83277100	-0.59118300	H	-2.96386400	0.46066000	-3.03521600
H	-1.84009700	-0.71950800	-1.15485000	H	-4.65139900	0.86614800	-3.37110100
H	1.51200700	0.86114500	-2.73704200	C	-3.27220900	-1.57341500	0.03238400
C	1.05004100	-0.35190200	2.47517300	C	-4.36483000	-1.57300900	0.93668000
C	1.99239600	-1.36665800	2.71506700	C	-5.14924800	-2.72505100	1.05957300
C	0.77762800	0.55491100	3.51669200	H	-5.98669100	-2.71019800	1.75455700
C	2.61970400	-1.47974100	3.95536700	C	-4.89343200	-3.88764200	0.32944800
H	2.23063900	-2.07833100	1.93553300	C	-3.80622100	-3.87746300	-0.54389600
C	1.41723900	0.45103200	4.75134500	H	-3.57918600	-4.77298800	-1.11841100
H	0.07741700	1.36735100	3.34375000	C	-2.99092400	-2.75124700	-0.70705000
C	2.33807600	-0.57287300	4.97843600	C	-4.73864700	-0.38596900	1.79585200
H	3.33582800	-2.28046300	4.11939500	H	-5.48505100	-0.67897200	2.54056900
H	1.19841100	1.17365600	5.53329200	H	-5.15714900	0.43446900	1.20469200
H	2.83672700	-0.65898300	5.94002600	H	-3.87690200	0.01727600	2.33599500

## TSK8

E= -2684.302431au

P	-2.13604900	-0.12055300	-0.27061600	H	-5.60130200	-5.82994000	-0.31503400
B	1.44331100	-0.04160500	0.00864500	C	-1.81919700	-2.86617400	-1.66108000
O	0.38288100	0.04828400	-1.80534000	H	-1.81358500	-3.85257100	-2.13520000

H	-0.86494200	-2.74845500	-1.13627300	C	-4.11680600	3.59864600	-2.11282200
H	-1.85391600	-2.11330400	-2.45599600	C	-3.47827200	3.70674300	-0.87858700
C	2.28566500	-1.30898800	-0.48893700	P	-1.75017000	-0.15366600	-0.48488900
C	3.32688800	-1.19714700	-1.42504200	C	0.75577200	0.45539500	-3.73445500
F	3.63681900	0.00153600	-1.96323600	O	0.90160200	1.61331500	-3.77548600
C	4.07619200	-2.27175800	-1.88879200	C	-3.28495600	0.02667100	-3.08043000
F	5.06193200	-2.08699700	-2.77460100	C	-4.84103700	4.77170400	-2.72918000
C	3.78207000	-3.55505200	-1.43474000	C	-2.12697000	2.93940300	1.04115900
F	4.48569500	-4.60108900	-1.87039000	C	-0.79648800	-0.04169900	1.21231500
C	2.73264300	-3.73398400	-0.54174400	C	0.45566200	-0.89171700	0.94277000
F	2.41269900	-4.96424500	-0.12306200	B	1.95016300	-0.39006000	0.75748200
C	2.00468500	-2.62749700	-0.10666900	O	0.59942400	-0.70523300	-3.72257400
F	0.96447200	-2.90705000	0.69952500	C	2.34517100	1.15495600	0.92687800
C	2.11826100	1.41801900	-0.01353400	C	1.79371900	2.18965200	0.17123200
C	3.46201400	1.63905200	0.31487000	C	2.17998700	3.52154400	0.30679100
F	4.26247900	0.60348300	0.62396000	C	3.17144000	3.85332100	1.22689000
C	4.03623300	2.90533200	0.37763300	C	3.75820800	2.85356900	1.99915300
F	5.32656800	3.05525000	0.69927600	C	3.33595000	1.53712000	1.83384400
C	3.25413300	4.02631900	0.11087000	F	0.82322000	1.92754100	-0.72725000
F	3.78986200	5.24771300	0.16425900	F	3.92590000	0.59858000	2.60587500
C	1.90878600	3.86254000	-0.20443500	F	4.71024800	3.16690600	2.88807300
F	1.14479500	4.93182300	-0.45495500	F	3.55366200	5.12584900	1.37331600
C	1.37123300	2.57791200	-0.24766000	F	1.60154000	4.48154400	-0.42530800
F	0.05881100	2.49199500	-0.54551700	C	2.95878600	-1.30988700	-0.09256700
H	-0.61832200	-0.06983600	-1.59167600	C	3.31087600	-0.92596500	-1.38934800
H	1.64673300	0.90511400	-3.12739600	C	4.14680100	-1.66650300	-2.21878100
C	0.97990500	-0.43337000	2.52134300	C	4.67738100	-2.86645700	-1.75222800
C	1.84425200	0.51144100	3.10093400	C	4.35789000	-3.29792400	-0.46883500
C	0.66738900	-1.58420500	3.26978600	C	3.51819300	-2.51867500	0.32438500
C	2.38012900	0.31107500	4.37445600	F	2.82328700	0.22790400	-1.89663100
H	2.07284900	1.43010300	2.57466700	F	4.43983000	-1.23956900	-3.45294600
C	1.20647000	-1.78550300	4.53931000	F	5.48247900	-3.59728100	-2.52953400
H	0.00280200	-2.32698000	2.84308600	F	4.85895200	-4.45031500	-0.00535900
C	2.07018300	-0.84061000	5.09707500	F	3.25308900	-3.01557100	1.56341400
H	3.03707400	1.06403800	4.80177400	C	-3.06078900	-1.46764800	-0.20183400
H	0.95082300	-2.68533100	5.09279500	C	-4.29532000	-1.25826200	0.47159400
H	2.49201400	-0.99854800	6.08591000	C	-5.21293500	-2.30916000	0.56930900

## L5

E= -2739.70154au

C	-2.78005300	2.64512900	-0.28958100	C	-4.96592700	-3.57358300	0.02925900
C	-2.71502100	1.39231100	-0.95114800	C	-3.75390100	-3.76745900	-0.63066700
C	-3.33252300	1.28185700	-2.23222300	C	-2.80010700	-2.74791400	-0.76153600
C	-4.02610400	2.37261500	-2.76839500	C	-4.68939800	0.05836800	1.10048500
				C	-5.97501500	-4.68894400	0.16834300
				C	-1.52257000	-3.10522700	-1.50001500

H	-0.48135400	0.99879000	1.27945300	C	-3.74341700	0.88563100	-2.19632900
H	-4.50139200	2.25514200	-3.74025300	C	-4.65318000	1.80332900	-2.73322300
H	-3.52178800	4.65376300	-0.34402800	C	-4.87861200	3.05870100	-2.17221300
H	-3.53962800	-4.74048200	-1.06844200	C	-4.14001700	3.38715400	-1.03812900
H	-6.15256800	-2.13081600	1.08912700	P	-1.73607400	-0.04293500	-0.49144700
H	-3.67011700	0.23630000	-4.08313000	C	0.00345000	0.31566100	-2.30971100
H	-2.26291900	-0.35550400	-3.18689100	O	-0.61908200	0.68350300	-3.24373000
H	-3.88416100	-0.78670800	-2.65760300	C	-3.62174300	-0.43190700	-2.93600000
H	-2.37660700	2.19786800	1.80340000	C	-5.88741500	4.01428300	-2.76246600
H	-1.03524000	2.98160600	0.94787000	C	-2.49741400	3.02680700	0.76983700
H	-2.45251500	3.91486900	1.41524400	C	-0.78302300	0.23388300	1.18174300
H	-5.62045500	4.44121600	-3.42408400	C	0.55994900	-0.57457600	1.07368900
H	-5.31171100	5.39952700	-1.96449200	B	1.77727200	-0.08559300	0.15462900
H	-4.15087200	5.41252300	-3.29439600	O	1.04880300	0.03066300	-1.78117200
H	-1.68850700	-3.97905100	-2.13851000	C	2.28135100	1.43517900	0.35895000
H	-1.14349800	-2.28986800	-2.11998100	C	1.60715800	2.58043300	-0.07031300
H	-0.71509500	-3.37383600	-0.80519000	C	2.06911800	3.87791600	0.13679700
H	-5.72023600	-5.54154300	-0.46915700	C	3.26769100	4.07662200	0.81384300
H	-6.02619000	-5.05262900	1.20313200	C	3.97709600	2.97194300	1.27597300
H	-6.98280500	-4.35287100	-0.10258600	C	3.47727900	1.69377000	1.04169600
H	-4.99805600	0.79190000	0.34844500	F	0.42168400	2.48575000	-0.71960900
H	-5.52688500	-0.08799800	1.79004900	F	4.20540400	0.66979200	1.53449500
H	-3.86660500	0.50107000	1.66574100	F	5.12362400	3.14558200	1.94342100
H	0.23167400	-1.88434500	0.55813600	F	3.72381700	5.31226900	1.03141100
N	1.40740400	-1.03991600	2.11640700	F	1.36178600	4.92780200	-0.29781200
H	1.67600900	-1.98064300	2.38725200	C	2.89863500	-1.14278500	-0.30580200
H	1.20331500	-0.45006900	2.91935700	C	3.86196400	-0.77587800	-1.25969500
C	-1.43952600	-0.42818400	2.53584500	C	4.84040800	-1.63792000	-1.74510900
C	-1.43652600	0.48651700	3.60403500	C	4.89784700	-2.94514100	-1.27099200
C	-1.92456100	-1.72416700	2.78811200	C	3.97206600	-3.36256800	-0.32205300
C	-1.93358100	0.13851100	4.86323100	C	3.00259500	-2.46909700	0.12912900
H	-1.03666600	1.48604000	3.45144400	F	3.87033800	0.46782200	-1.76997200
C	-2.42150000	-2.07309600	4.04355600	F	5.72398600	-1.22199600	-2.66024800
H	-1.92229500	-2.46517600	1.99618100	F	5.83050200	-3.78741200	-1.72175900
C	-2.43414900	-1.14337600	5.08662200	F	4.01347900	-4.61570700	0.14879500
H	-1.92110300	0.87009500	5.66692500	F	2.15111300	-2.97164100	1.05644600
H	-2.79898700	-3.07905300	4.20727200	C	-2.67586700	-1.64005000	-0.25298300
H	-2.82173000	-1.41948900	6.06337200	C	-3.92364000	-1.70069800	0.42317100
				C	-4.56151600	-2.94021400	0.55784900
				C	-4.01702000	-4.12489700	0.06164400
				C	-2.79722400	-4.04418500	-0.61175200
				C	-2.12138600	-2.83184500	-0.79089000
				C	-4.63790800	-0.49968400	1.00447300

## TSL56

E= -2739.655471au

C	-3.21828100	2.51075700	-0.45198700
C	-3.01837100	1.22500500	-1.01530900

C -4.71103700 -5.45046300 0.26535700  
 C -0.84730800 -2.87172600 -1.61106000  
 H -0.54324400 1.29754900 1.17780000  
 H -5.19593900 1.51975200 -3.63265700  
 H -4.27739900 4.36587800 -0.58368100  
 H -2.35944000 -4.95035900 -1.02470700  
 H -5.51561300 -2.97591900 1.07967400  
 H -4.04142200 -0.32780400 -3.94115200  
 H -2.58392100 -0.74936500 -3.05315800  
 H -4.16326600 -1.23876700 -2.43140200  
 H -2.60855600 2.35261700 1.62047500  
 H -1.42974900 3.17140600 0.57804500  
 H -2.90596500 3.99731300 1.06657300  
 H -6.90491400 3.77616200 -2.42423600  
 H -5.67917400 5.04825100 -2.46864900  
 H -5.89179600 3.96622300 -3.85700100  
 H -0.57585300 -3.90816800 -1.83312000  
 H -0.97478200 -2.35619800 -2.57104500  
 H 0.00716300 -2.40849400 -1.11342800  
 H -4.49057100 -6.14831500 -0.54935300  
 H -4.38368000 -5.92719800 1.19905700  
 H -5.79765600 -5.32897100 0.32654000  
 H -5.14881900 0.07799700 0.22665300  
 H -5.39121600 -0.82837700 1.72694800  
 H -3.95885400 0.17839800 1.52442800  
 H 0.29609600 -1.61295900 0.86624400  
 N 1.20573300 -0.60255300 2.41526500  
 C -1.48542700 -0.08926600 2.49531100  
 C -1.67555100 0.91788900 3.45362800  
 C -1.85501400 -1.39817800 2.84507100  
 C -2.26209800 0.64610500 4.69166100  
 H -1.33375000 1.92810500 3.24536900  
 C -2.43969600 -1.67473400 4.07974200  
 H -1.67502900 -2.21403400 2.15482600  
 C -2.65761900 -0.65291000 5.00672200  
 H -2.39569300 1.45001500 5.41093700  
 H -2.71810400 -2.69729700 4.32139200  
 H -3.11345000 -0.87140500 5.96870300  
 H 1.84409900 -1.38741200 2.49244800  
 H 1.71483100 0.25349600 2.62029000

C -3.12728800 2.50173100 -0.53328100  
 C -2.97878400 1.18725900 -1.04944000  
 C -3.76053400 0.78997200 -2.17638200  
 C -4.64544400 1.71872800 -2.73638200  
 C -4.79860600 3.01524500 -2.25038000  
 C -4.03306300 3.37551200 -1.14448800  
 P -1.72669300 -0.03624300 -0.39430600  
 C -0.37002000 0.02608900 -1.80707100  
 O -0.79489100 0.10822100 -2.93844700  
 C -3.77023000 -0.57993500 -2.82877800  
 C -5.73640500 3.99540600 -2.91055900  
 C -2.38497700 3.05455100 0.66023000  
 C -0.75282800 0.27521800 1.21899500  
 C 0.59335800 -0.53632300 1.11307500  
 B 1.59452400 -0.05075200 -0.09987600  
 O 0.86281700 0.00337300 -1.45603400  
 C 2.17815400 1.46037300 0.21366900  
 C 1.55911300 2.63511900 -0.20869900  
 C 2.02917200 3.91704100 0.06724300  
 C 3.19563300 4.06717900 0.80726200  
 C 3.85381500 2.92960100 1.26552700  
 C 3.33668000 1.67232500 0.96590100  
 F 0.38719800 2.58859100 -0.90530100  
 F 4.02764500 0.61931800 1.46434500  
 F 4.97273300 3.05553600 1.99289900  
 F 3.66885900 5.28701800 1.09078200  
 F 1.35708500 4.99788100 -0.35984200  
 C 2.82299000 -1.10342500 -0.43808000  
 C 3.72750300 -0.76826900 -1.45480900  
 C 4.77005100 -1.59091300 -1.87202200  
 C 4.95018500 -2.82796200 -1.26007600  
 C 4.08253400 -3.21174600 -0.24569500  
 C 3.05015700 -2.35470200 0.13729100  
 F 3.61752100 0.41443700 -2.08958500  
 F 5.59998200 -1.20567700 -2.85212000  
 F 5.94437100 -3.63742000 -1.64535800  
 F 4.23847600 -4.40251100 0.35477700  
 F 2.25808000 -2.82494700 1.13402300  
 C -2.56053700 -1.68623000 -0.25490500  
 C -3.81542500 -1.74174900 0.41234000  
 C -4.44959600 -2.98202900 0.54883600  
 C -3.89838900 -4.16595700 0.06154500  
 C -2.66623500 -4.08547500 -0.58913600

**L6**

E= -2739.681707au

C	-1.97974600	-2.87955700	-0.76630300
C	-4.55363600	-0.54621700	0.98128900
C	-4.59230900	-5.49276300	0.25058200
C	-0.67456700	-2.95199200	-1.52969000
H	-0.49309000	1.33341800	1.19813400
H	-5.23492900	1.40554200	-3.59469600
H	-4.13403200	4.37709300	-0.73408500
H	-2.21717400	-4.99396800	-0.98291200
H	-5.40775000	-3.01628600	1.06211300
H	-4.20954100	-0.49641500	-3.82697300
H	-2.77191600	-0.99273600	-2.95361800
H	-4.37807100	-1.29352500	-2.26193600
H	-2.48855300	2.41367000	1.53704000
H	-1.32242700	3.19147100	0.44406800
H	-2.78959400	4.03465600	0.92689700
H	-6.12693400	4.72360000	-2.19217100
H	-5.21895700	4.55902100	-3.69804200
H	-6.58489100	3.48595200	-3.37897500
H	-0.41919600	-3.99670000	-1.72541100
H	-0.73867100	-2.44470600	-2.49796600
H	0.16430200	-2.51442500	-0.98457100
H	-4.49632200	-6.12384400	-0.63954300
H	-4.15316500	-6.04865500	1.08935500
H	-5.65766300	-5.36185200	0.46415200
H	-5.10928300	-0.01150800	0.20346600
H	-5.27335300	-0.88473600	1.73221500
H	-3.89657500	0.17420000	1.47203400
H	0.31989000	-1.59231000	0.96813800
N	1.27390500	-0.32245000	2.39972800
H	2.26343700	-0.53317000	2.31208700
H	0.90170200	-0.94036500	3.11689600
C	-1.47214000	-0.02921500	2.52776300
C	-1.66540200	0.99100200	3.47244000
C	-1.81943100	-1.33995500	2.89763500
C	-2.24127300	0.72739700	4.71655000
H	-1.32628500	1.99805300	3.25018600
C	-2.39319300	-1.60648200	4.14152200
H	-1.62956300	-2.16318500	2.21832000
C	-2.61905100	-0.57265500	5.05238400
H	-2.37564400	1.53779200	5.42779000
H	-2.65422500	-2.62895900	4.40133900
H	-3.06344200	-0.78250400	6.02139300

## L7

E= -2740.858829au

P	-1.72962600	-0.04592600	-0.38096100
B	1.59255000	-0.07152300	-0.08696400
O	0.85998400	0.02034700	-1.44023500
O	-0.79734200	0.14558000	-2.92160700
C	-0.75437200	0.23100800	1.23814900
H	-0.49255600	1.28892100	1.23952600
C	0.58978900	-0.58086400	1.11458700
H	0.31365500	-1.63262300	0.94564500
C	-0.37280200	0.04387900	-1.79172800
C	-2.98165100	1.19077300	-1.01095100
C	-3.12731700	2.49524900	-0.46991200
C	-4.03729600	3.37974000	-1.05912500
H	-4.13579200	4.37369700	-0.63008300
C	-4.80902300	3.03951700	-2.16696100
C	-4.65666900	1.75290800	-2.67922200
H	-5.24977500	1.45602500	-3.54085600
C	-3.76785400	0.81453900	-2.14219000
C	-2.37613700	3.02571200	0.72796600
H	-1.31261800	3.15364800	0.51122100
H	-2.48484400	2.37511700	1.59707400
H	-2.76908300	4.00694900	1.00749900
C	-5.75177700	4.03065100	-2.80331700
H	-5.24546900	4.59393800	-3.59822000
H	-6.12214400	4.75803800	-2.07365600
H	-6.61339900	3.53032400	-3.25755100
C	-3.77639200	-0.54147100	-2.82274100
H	-4.37732700	-1.26961100	-2.26729500
H	-2.77673500	-0.94650200	-2.96221100
H	-4.22224100	-0.43903800	-3.81626300
C	-2.56474400	-1.69723300	-0.27330200
C	-3.81768100	-1.76501800	0.39636100
C	-4.45264900	-3.00732900	0.50946500
H	-5.40929300	-3.05120000	1.02479000
C	-3.90418500	-4.18149700	-0.00371500
C	-2.67382200	-4.08894400	-0.65627400
H	-2.22695900	-4.98967300	-1.06991200
C	-1.98658500	-2.88042300	-0.81079000
C	-4.55333400	-0.58066900	0.99164600
H	-5.27185700	-0.93401500	1.73686200
H	-5.11036800	-0.02927500	0.22650600
H	-3.89466400	0.12884500	1.49618100

C	-4.59897700	-5.51132600	0.15904000
H	-5.66067500	-5.38389900	0.39188100
H	-4.14878500	-6.09147900	0.97517600
H	-4.51795900	-6.11756100	-0.74971100
C	-0.68414000	-2.93846500	-1.58002200
H	-0.42990900	-3.97926200	-1.79692400
H	0.15722500	-2.51195800	-1.02993400
H	-0.75169000	-2.41236100	-2.53792000
C	2.81497300	-1.12272400	-0.45112900
C	3.71752100	-0.77023000	-1.46379400
F	3.61014300	0.42569200	-2.07373300
C	4.75575500	-1.58804700	-1.90086100
F	5.58398500	-1.18616800	-2.87563700
C	4.93342100	-2.83772500	-1.31439600
F	5.92339600	-3.64275200	-1.71919300
C	4.06790900	-3.23864700	-0.30480400
F	4.22187400	-4.44156200	0.27140300
C	3.03995900	-2.38579500	0.09883800
F	2.25055200	-2.87240700	1.08983000
C	2.18824800	1.42783500	0.26121500
C	3.34625100	1.61173600	1.02205700
F	4.02355400	0.54161400	1.50194400
C	3.87757000	2.85654400	1.34807400
F	4.99486200	2.95431200	2.08198900
C	3.23643200	4.01105400	0.90834900
F	3.72399000	5.21920000	1.21539200
C	2.07105200	3.88821300	0.16191400
F	1.41604600	4.98618400	-0.25159200
C	1.58561500	2.61828700	-0.14019000
F	0.41679000	2.60115700	-0.84440400
H	-0.29358500	5.03461300	-3.08767100
H	0.01743900	4.75841000	-2.47266000
N	1.27019300	-0.39741200	2.40604900
H	2.25779400	-0.61547500	2.31520800
H	0.89179000	-1.02621400	3.11045200
C	-1.47443700	-0.09961300	2.54023400
C	-1.67187400	0.90189500	3.50385200
C	-1.81935000	-1.41805100	2.88427100
C	-2.24953300	0.61320800	4.74154100
H	-1.33480900	1.91382400	3.30154100
C	-2.39464500	-1.70967500	4.12179400
H	-1.62683100	-2.22769000	2.18950100
C	-2.62468500	-0.69394700	5.05178600

H	-2.38731900	1.40953200	5.46785800
H	-2.65375900	-2.73752800	4.36150300
H	-3.07039600	-0.92331300	6.01574400

## TSL78

E= -2740.792738au

P	-2.01204800	0.32944700	0.43153700
B	1.66977000	0.18909300	-0.02414800
O	0.99539200	-0.13942000	1.56405300
O	1.27132500	0.87510800	3.63661400
C	-0.83809600	-0.48966400	-0.86834200
H	-0.49640700	-1.40626700	-0.38896600
C	0.40765700	0.48159800	-1.03312500
H	0.03887800	1.50517100	-0.87451100
C	0.95697300	0.58003200	2.54500200
C	-2.72057700	-0.81701200	1.72799100
C	-2.66447400	-2.23397800	1.75295100
C	-3.11818900	-2.91933200	2.88912500
H	-3.06713900	-4.00607000	2.88588200
C	-3.63837500	-2.27138400	4.00604200
C	-3.72337700	-0.87919300	3.95477600
H	-4.15094600	-0.34298000	4.79928800
C	-3.27658900	-0.14018600	2.85639700
C	-2.16620200	-3.09751100	0.61722600
H	-1.07727400	-3.20949500	0.64072300
H	-2.44543600	-2.70350000	-0.35978300
H	-2.59217700	-4.10247300	0.69972000
C	-4.08497200	-3.03897900	5.22670600
H	-4.29799700	-4.08556300	4.98622300
H	-4.98596100	-2.60048200	5.67005500
H	-3.30736700	-3.03254500	6.00206100
C	-3.45223300	1.36340400	2.93345700
H	-4.11065200	1.74262500	2.14505800
H	-2.50155300	1.90060900	2.84962100
H	-3.89445800	1.63896600	3.89528300
C	-3.44070300	1.19316600	-0.40091400
C	-3.35499600	2.60632600	-0.53484500
C	-4.42174900	3.30506800	-1.11104200
H	-4.34100100	4.38491500	-1.21467300
C	-5.58341500	2.66596900	-1.54774600
C	-5.65120800	1.27954800	-1.40811300
H	-6.54050400	0.75658900	-1.75332000
C	-4.61033700	0.52674200	-0.85165600

C	-2.16421600	3.42473800	-0.07474100
H	-2.31243900	4.47830400	-0.33015600
H	-1.22323100	3.10779500	-0.53572400
H	-2.02381700	3.36659900	1.01011100
C	-6.73459900	3.45069900	-2.12977200
H	-7.42599200	3.77839600	-1.34185200
H	-7.31246600	2.84867200	-2.83882400
H	-6.38557900	4.34947100	-2.64914600
C	-4.79621700	-0.97113300	-0.78854400
H	-5.72620900	-1.25834300	-1.28820000
H	-4.84125300	-1.33858600	0.24118400
H	-3.97805800	-1.49431900	-1.29211700
C	2.67827000	1.42828100	0.30295700
C	3.70632400	1.25997000	1.24272700
F	3.82279500	0.08851000	1.90152500
C	4.62988800	2.24631400	1.57541800
F	5.57864200	2.01727100	2.49065600
C	4.55795300	3.48399400	0.94293700
F	5.43219000	4.44788600	1.24283100
C	3.56283900	3.70611700	-0.00230200
F	3.48332600	4.89095500	-0.62197100
C	2.65512000	2.69061400	-0.29980900
F	1.74142900	2.99797000	-1.24775000
C	2.45280300	-1.19390600	-0.36311000
C	3.51900900	-1.16706400	-1.26864600
F	3.90751600	0.00332000	-1.82373700
C	4.23413400	-2.29373700	-1.66147800
F	5.24559000	-2.19234500	-2.53400800
C	3.88960700	-3.53676700	-1.13940900
F	4.56131900	-4.63465200	-1.50311800
C	2.83247000	-3.62216300	-0.24154400
F	2.47875000	-4.81155500	0.26696700
C	2.14441200	-2.46537300	0.12190400
F	1.11833300	-2.64882700	0.98866700
H	-0.24508700	1.66111800	2.12809900
H	-0.85166900	1.41622600	1.58353700
N	0.97461100	0.31430000	-2.38828400
C	-1.46841000	-0.86843600	-2.20092200
C	-1.35193700	-2.18563700	-2.67326900
C	-2.09275200	0.07284900	-3.03760800
C	-1.87183700	-2.56116600	-3.91287800
H	-0.82691600	-2.92234100	-2.07207300
C	-2.60877500	-0.29820700	-4.28053500

H	-2.17997000	1.10638100	-2.71984500
C	-2.50912200	-1.61897800	-4.72100500
H	-1.76569900	-3.58883500	-4.25021200
H	-3.08860100	0.45077900	-4.90508100
H	-2.91255000	-1.90715000	-5.68787700
H	1.79884200	0.90188100	-2.48633200
H	0.31291900	0.63113200	-3.09392800

## L8

E= -2740.888473au

P	-1.94522200	-0.19117600	-0.36015700
B	1.64013200	-0.22404900	-0.16766200
O	0.86441300	-0.13415700	-1.47556000
O	0.66867200	0.29984100	-3.65392400
C	-0.79362900	0.09610900	1.12404300
H	-0.51998300	1.14813800	1.03229100
C	0.54596600	-0.79114300	0.95755900
H	0.21236600	-1.78245300	0.64857900
C	1.32054000	0.32780300	-2.62801500
C	-2.61635600	1.26636700	-1.27864800
C	-2.84037800	2.54708400	-0.71757800
C	-3.36562300	3.55526400	-1.53355400
H	-3.53935000	4.53447200	-1.09357300
C	-3.66044800	3.35437400	-2.88105500
C	-3.42235800	2.08722800	-3.41518500
H	-3.64065300	1.90378400	-4.46435500
C	-2.90180200	1.03700800	-2.65514700
C	-2.51266700	2.93915700	0.70404800
H	-1.46712100	3.26258500	0.77106500
H	-2.66962800	2.13818000	1.42604300
H	-3.13294700	3.78553500	1.01423600
C	-4.19159400	4.47456900	-3.74121800
H	-3.37563200	4.96162800	-4.29098500
H	-4.68610100	5.24360100	-3.13927800
H	-4.90736100	4.10577000	-4.48362800
C	-2.63556300	-0.26967700	-3.36833400
H	-3.06265900	-1.13271800	-2.84786300
H	-1.55365600	-0.41491400	-3.49482100
H	-3.07799500	-0.24414600	-4.36797700
C	-3.23015100	-1.48772700	-0.11026400
C	-4.47792100	-1.18856800	0.49419100
C	-5.42435200	-2.20735900	0.62848900
H	-6.37782000	-1.97117200	1.09505700

C	-5.18383100	-3.51181600	0.19277800
C	-3.94558200	-3.78657700	-0.38984800
H	-3.73538700	-4.79791200	-0.72899000
C	-2.95594800	-2.81094300	-0.55902500
C	-4.83628200	0.18057500	1.02297800
H	-5.83337900	0.16449900	1.47173200
H	-4.83885300	0.93903100	0.23408300
H	-4.13656400	0.50477700	1.80059300
C	-6.23698500	-4.58450500	0.32699200
H	-6.87167900	-4.41531500	1.20294900
H	-5.78788200	-5.57893300	0.41518400
H	-6.89345100	-4.59945300	-0.55313100
C	-1.66199500	-3.25384100	-1.21673300
H	-1.71906400	-4.31891600	-1.45677700
H	-0.78024100	-3.11860200	-0.58310100
H	-1.46680700	-2.72475800	-2.15624200
C	2.88626200	-1.28546400	-0.43799800
C	4.10119400	-0.86679000	-0.99225900
F	4.30454700	0.44279000	-1.28312300
C	5.16547600	-1.70971000	-1.30121300
F	6.30027000	-1.21962500	-1.82301300
C	5.03941500	-3.07442500	-1.07058900
F	6.04414100	-3.91163700	-1.35967900
C	3.84598400	-3.55638800	-0.54789900
F	3.69424800	-4.87425500	-0.33824700
C	2.80908600	-2.67044300	-0.25698600
F	1.68404400	-3.26732400	0.20898800
C	2.15103300	1.27700600	0.34038600
C	3.23677700	1.47477500	1.20375400
F	3.97661200	0.42791600	1.62245300
C	3.62909500	2.71874000	1.69596100
F	4.68367000	2.82766800	2.51665700
C	2.91079300	3.85709000	1.34339200
F	3.25764700	5.05825300	1.82226000
C	1.81600900	3.72056200	0.49958100
F	1.07554200	4.79381800	0.17232700
C	1.47509800	2.45704900	0.02055500
F	0.37453300	2.43104500	-0.77985000
H	-1.07855900	-0.76347400	-1.29467000
H	2.34075200	0.74277700	-2.58974000
N	1.24762800	-0.97654400	2.21678000
C	-1.46243000	-0.11255100	2.47278100
C	-1.47782800	0.93203700	3.41133800

C	-1.96708800	-1.36261900	2.87156400
C	-2.01066900	0.75002600	4.68929200
H	-1.05285600	1.89580000	3.14366000
C	-2.50014900	-1.54685500	4.14791800
H	-1.93459800	-2.20348000	2.18661400
C	-2.53127200	-0.48986000	5.06030500
H	-2.00918500	1.57647700	5.39476000
H	-2.88450900	-2.52297200	4.43105000
H	-2.94449600	-0.63622900	6.05430900
H	1.64743300	-0.10959600	2.56428300
H	0.66120700	-1.36500400	2.95063000

## TSL8

E= -2740.857704au

P	-1.80894400	-0.11203800	-0.46064900
B	1.76726300	-0.13933000	0.12914700
O	0.91656500	-0.01736400	-1.71315100
O	0.40635700	0.72777900	-3.78577600
C	-0.84045100	0.11051300	1.20193600
H	-0.62832500	1.17944100	1.24556300
C	0.52976800	-0.65536300	1.04083700
H	0.28943300	-1.68758900	0.79061700
C	1.20840200	0.56027900	-2.90400100
C	-2.87717100	1.32436900	-1.01862700
C	-3.16197500	2.52669000	-0.32739900
C	-3.93989900	3.51291300	-0.94926000
H	-4.15284700	4.42479800	-0.39521700
C	-4.44988900	3.36903800	-2.23701500
C	-4.14376800	2.18966700	-2.91667300
H	-4.51424400	2.04994700	-3.93008400
C	-3.35872000	1.17926800	-2.35359800
C	-2.66510800	2.84763200	1.06128800
H	-1.60292700	3.12044000	1.04512600
H	-2.79194300	2.01445300	1.75319000
H	-3.20988000	3.70332300	1.47168100
C	-5.27277500	4.45605900	-2.88601400
H	-4.66630700	5.04821600	-3.58414900
H	-5.68318400	5.14629400	-2.14178200
H	-6.10800900	4.03849100	-3.45964000
C	-3.04085900	-0.01160600	-3.23470400
H	-3.36476500	-0.96237400	-2.80031200
H	-1.96395200	-0.07351000	-3.43186200
H	-3.54231800	0.09559000	-4.20133500



C	-2.94005200	-1.58427500	-0.27830000
C	-4.20587500	-1.53177100	0.36124800
C	-4.99062900	-2.68969300	0.41793500
H	-5.95592000	-2.63753700	0.91735800
C	-4.57811700	-3.90273100	-0.13397800
C	-3.33041400	-3.93956300	-0.75883100
H	-2.98482400	-4.87382600	-1.19614400
C	-2.50669600	-2.81167100	-0.85154600
C	-4.76828700	-0.28343900	1.00066000
H	-5.63677600	-0.53403700	1.61742100
H	-5.08776600	0.44816000	0.25147700
H	-4.03628500	0.20713700	1.64696200
C	-5.46109800	-5.12666700	-0.08243100
H	-6.09073800	-5.19617000	-0.97962500
H	-6.13126100	-5.10177700	0.78329500
H	-4.86937900	-6.04685700	-0.03026000
C	-1.18437900	-2.98250300	-1.57575900
H	-1.12949000	-3.98098500	-2.02049200
H	-0.32082800	-2.88234000	-0.90927800
H	-1.05806200	-2.25326900	-2.38235500
C	2.89300200	-1.20237100	-0.31290500
C	3.97303400	-0.81268900	-1.11673900
F	4.06996000	0.46827200	-1.54757400
C	4.98587000	-1.66412400	-1.54397200
F	5.98217700	-1.21061900	-2.31525700
C	4.95335100	-3.00123000	-1.16130300
F	5.91279900	-3.84241300	-1.55603600
C	3.90188300	-3.45034200	-0.37137300
F	3.84744300	-4.73735500	-0.00372200
C	2.90368600	-2.56166200	0.02696100
F	1.92323700	-3.11393900	0.77156200
C	2.23690300	1.37839500	0.41418300
C	3.42022700	1.64939400	1.11539800
F	4.23148300	0.64734100	1.49353000
C	3.82889000	2.93418700	1.46661500
F	4.96906100	3.12593800	2.14121400
C	3.04171900	4.02662400	1.11409900
F	3.41542100	5.26497300	1.44757700
C	1.85734900	3.81241100	0.41753000
F	1.07580600	4.84784200	0.08306700
C	1.48623300	2.51107400	0.08738700
F	0.31476800	2.39217100	-0.58336500
H	-0.10489300	-0.13356100	-1.56106100

H	2.27028000	0.83075900	-2.95013300
C	-1.49861300	-0.29905200	2.51123300
C	-1.61847700	0.62868400	3.55989800
C	-1.88190900	-1.62700400	2.77013200
C	-2.13999100	0.26154500	4.80255200
H	-1.28841700	1.65299600	3.40686900
C	-2.40117100	-1.99764000	4.01112700
H	-1.77620600	-2.38100200	1.99791500
C	-2.54018400	-1.05464400	5.03190200
H	-2.22240400	1.00451200	5.59154600
H	-2.69482200	-3.03034200	4.17981500
H	-2.94474400	-1.34602800	5.99728000
N	1.31858400	-0.71759900	2.29302800
H	0.95604100	-1.41630000	2.93704600
H	1.30789000	0.17795300	2.77484300

## CO<sub>2</sub>

E= -188.5775705au

O	0.000000	0.000000	1.169592
C	0.000000	0.000000	0.000000
O	0.000000	0.000000	-1.169592

## HCOOH

E= -189.743482au

C	0.131235	0.361721	-0.000054
O	1.179170	-0.219022	0.000019
O	-1.059436	-0.281621	0.000002
H	-1.781119	0.369489	0.000067
H	0.035839	1.465330	0.000088