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Unique mononuclear Mn^{II} complexes of end-off compartmental Schiff base ligand: experimental and theoretical study on their bio-relevant catalytic promiscuity†

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Table S1 Selected bond lengths [Å, °]

Compound **1**	
Mn1—O1	2.111(4)
Mn1—N2	2.226(5)
Mn1—N1	2.257(4)
N1—C11	1.273(7)
N3—C19	1.283(7)

Compound **2**	
Mn01—O1	2.0784(15)
Mn01—O3	2.1784(17)
Mn01—N5	2.223(2)
Mn01—O2	2.2247(18)
Mn01—N3	2.2306(16)
Mn01—N4	2.2408(18)
N1—C11	1.284(3)

N3—C19	1.274(3)

Compound **3**

Mn1—O1	2.073(2)
Mn1—N6	2.091(3)
Mn1—N5	2.111(3)
Mn1—N1	2.185(3)
Mn1—N2	2.249(3)
N1—C11	1.271(4)
N3—C19	1.280(4)

Table S2 Hydrogen bonds in studied compounds [Å, °].

D-H•••A	d(D-H)	d(H•••A)	d(D•••A)	<(DHA)
Compound **1**				
N3—H3N•••O1	0.79	1.99	2.607(5)	135.2
C13—H13•••O2^{vi}	0.93	2.60	3.421(10)	147.7
C16—H16•••O2	0.93	2.40	3.164(8)	139.0
Compound **2**				
O2—H2O•••N2^{iii}	0.81(3)	1.99(3)	2.791(3)	168(3)
O2—H2P•••O5'	0.89(4)	1.92(4)	2.752(5)	154(3)
O2—H2P•••O4	0.89(4)	2.21(4)	3.059(10)	158(3)
O2—H2P•••Cl02	0.89(4)	2.86(4)	3.647(2)	149(3)
O3—H3P•••O7	0.82(3)	2.06(3)	2.871(3)	171(3)
O3—H3P•••Cl02	0.82(3)	2.95(3)	3.706(2)	156(3)
O3—H3O•••N7^{ii}	0.83(3)	1.98(3)	2.801(3)	176(3)
N1—H1N•••O1	0.79(3)	1.91(3)	2.553(2)	138(3)
C11—H11•••O4' ^{iii}	0.93	2.33	3.220(5)	161.0
C12—H12B•••O5' ^{iv}	0.97	2.54	3.247(5)	130.2
C16—H16•••O6' ^{v}	0.93	2.50	3.421(5)	172.1
Compound **3**				
N3—H3N•••O1	0.81(4)	1.94(4)	2.578(4)	135(4)

Symmetry transformations used to generate equivalent atoms: (i) -x+2, -y, -z+2; (ii) -x+1, -y+1, -z; (iii) -x+1, -y, -z+1; (iv) x+1, y, z; (v) -x, -y+1, -z+1; (vi) -x+1.5, -y+0.5, z-1.

Table S3 Stacking interactions [Å, °]. Cg(1), Cg(2), Cg(3) indicates the centroids of six-membered aromatic rings (R) containing N2, N4, C8 atoms respectively, α is a dihedral angle between planes I and J, β is an angle between Cg(I)-Cg(J) vector and normal to plane I and d_p is a perpendicular distance of Cg(I) on ring J plane.

R(I)•••R(J)	Cg•••Cg	α	β	d_p
Compound **3**				
Cg(1)•••Cg(1)^{i}	3.970(3)	08.44	-3.927(2)	
Cg(1)•••Cg(3)^{ii}	3.960(2)	17.6(2)	17.27	3.9594(19)
Cg(2)•••Cg(3)^{iii}	4.003(3)	21.3(2)	24.16	-3.974(2)
Cg(3)•••Cg(1)^{ii}	3.960(2)	17.6(2)	0.64	3.7811(15)
Cg(3)•••Cg(2)^{iv}	4.003(3)	21.3(2)	6.86	3.6527(14)
Compound **1**				
Cg(1)•••Cg(3)^{iv}	3.6081(15)	6.21(12)	12.36	3.4484(11)
Cg(3)•••Cg(1)^{iv}	3.6081(15)	6.21(12)	17.11	3.5245(8)

Symmetry transformations used to generate rings: (i) -x+1.5, y+0.5, -z+2.5; (ii) -x+1.5, y-0.5, -z+2.5; (iii) -x+2, -y, -z+2; (iv) -x+1, -y, -z+1.

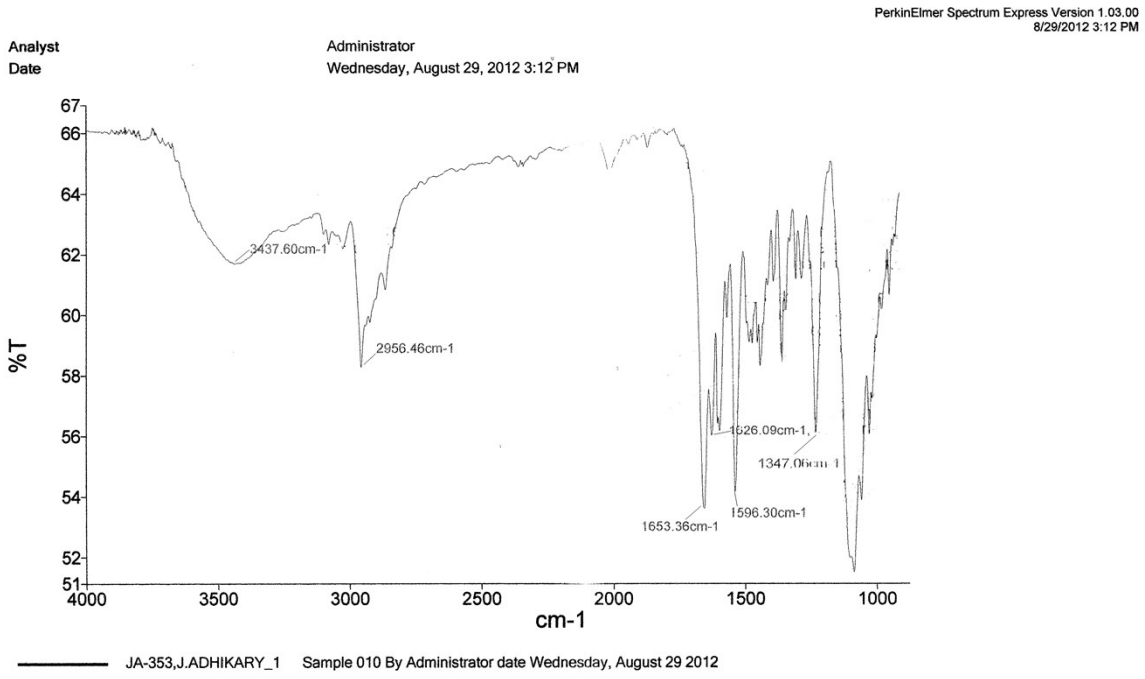

Fig. S1 FTIR spectrum of complex **1.**

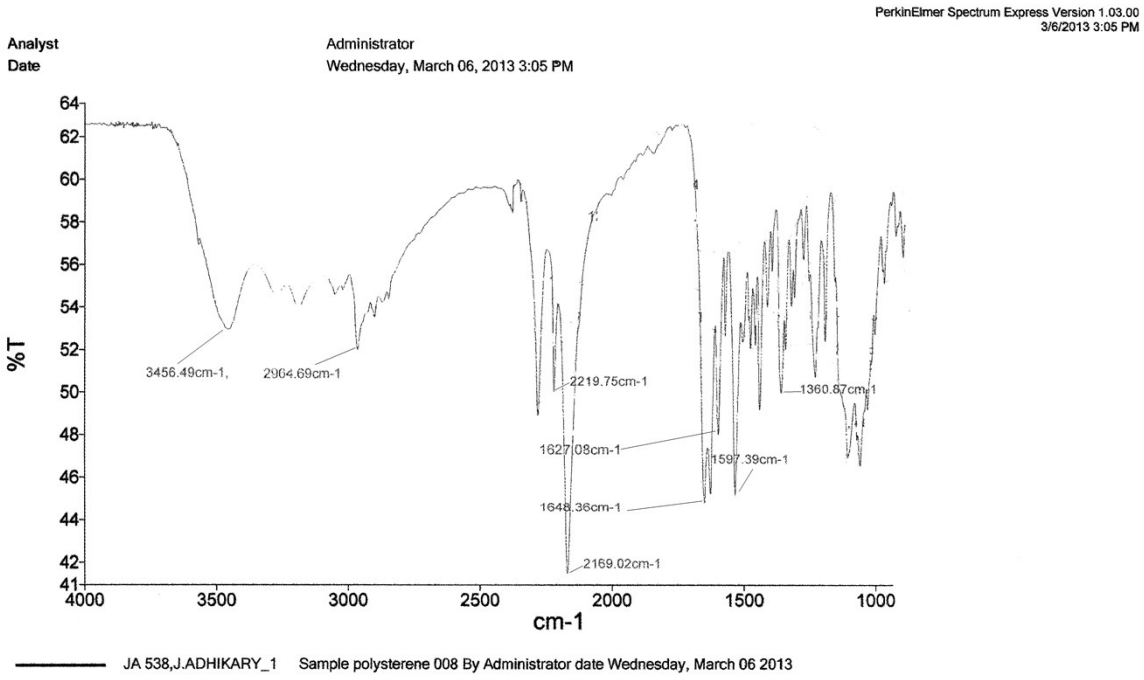

Fig. S2 FTIR spectrum of complex **2.**

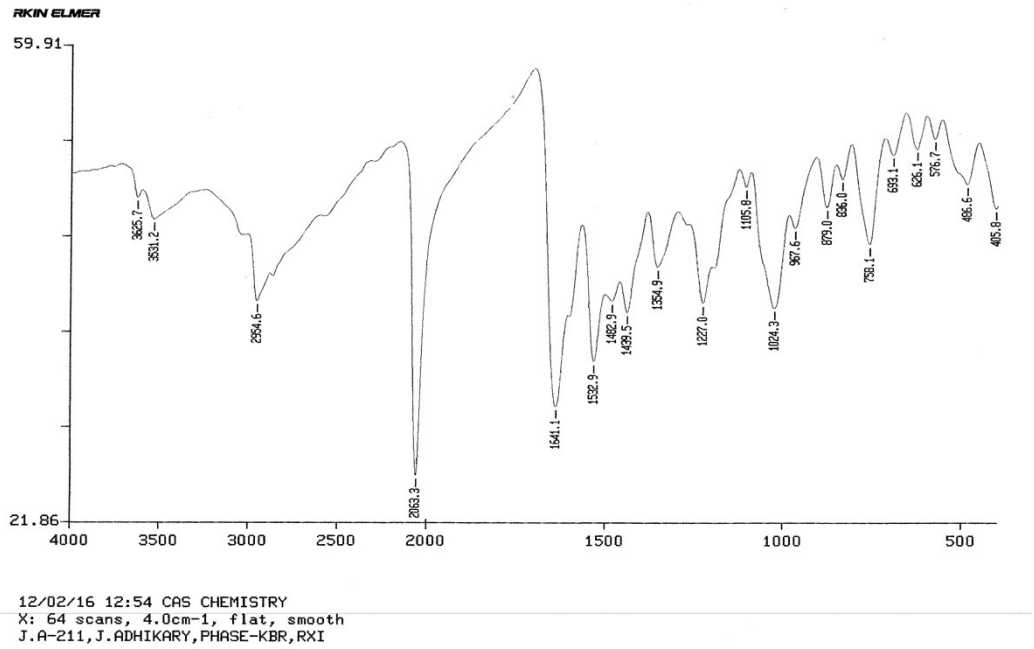

Fig. S3 FTIR spectrum of complex **3.**

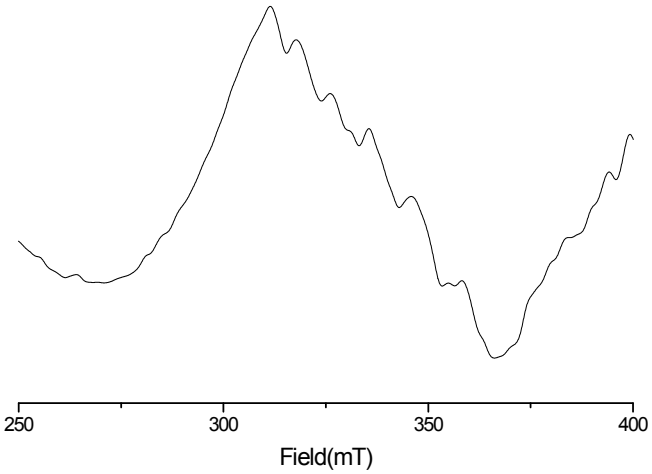

Fig. S4 EPR spectrum of complex **2** in methanol.

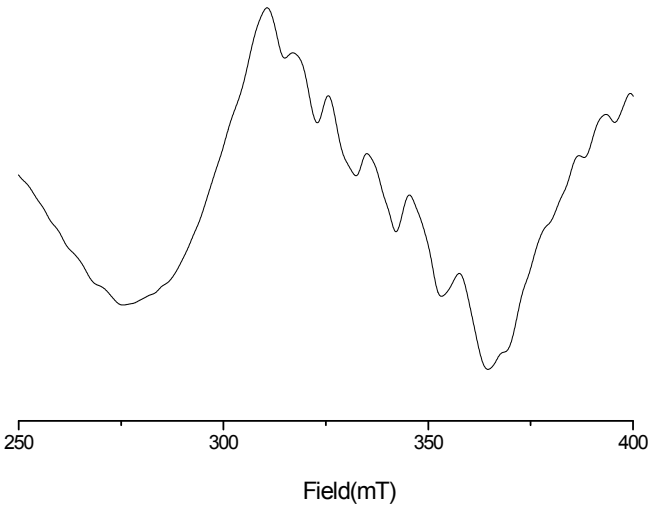

Fig. S5 EPR spectrum of complex **3** in methanol.

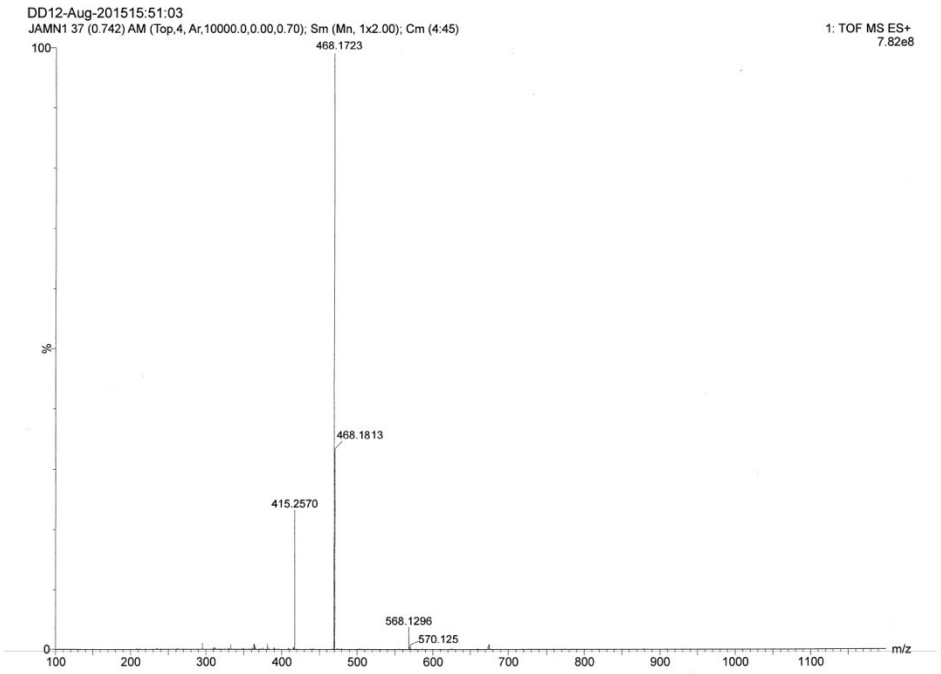

Fig. S6 ESI-MS spectrum of complex **1** in methanolic solution.

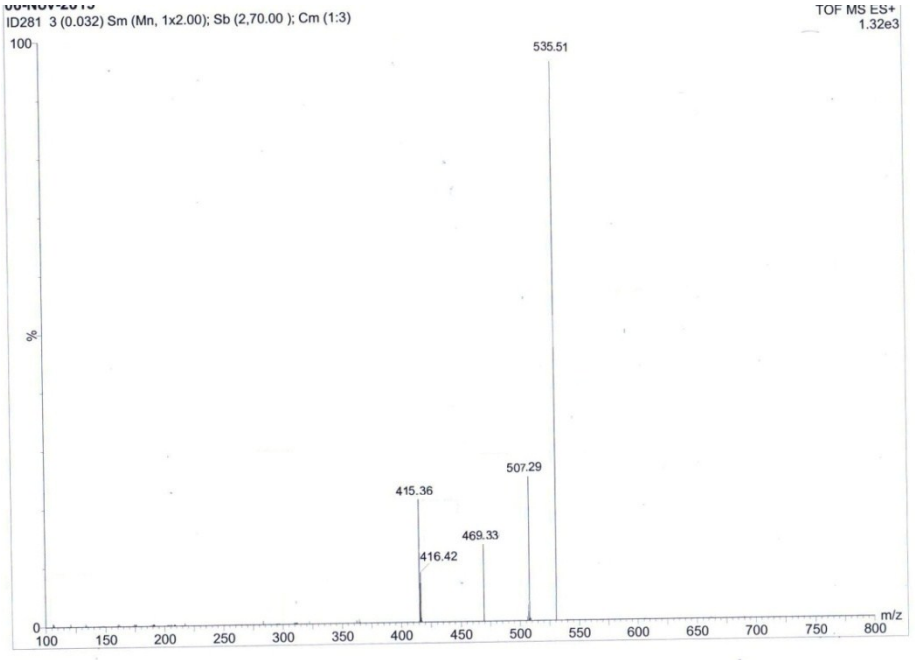

Fig. S7 ESI-MS spectrum of complex **2** in methanolic solution.

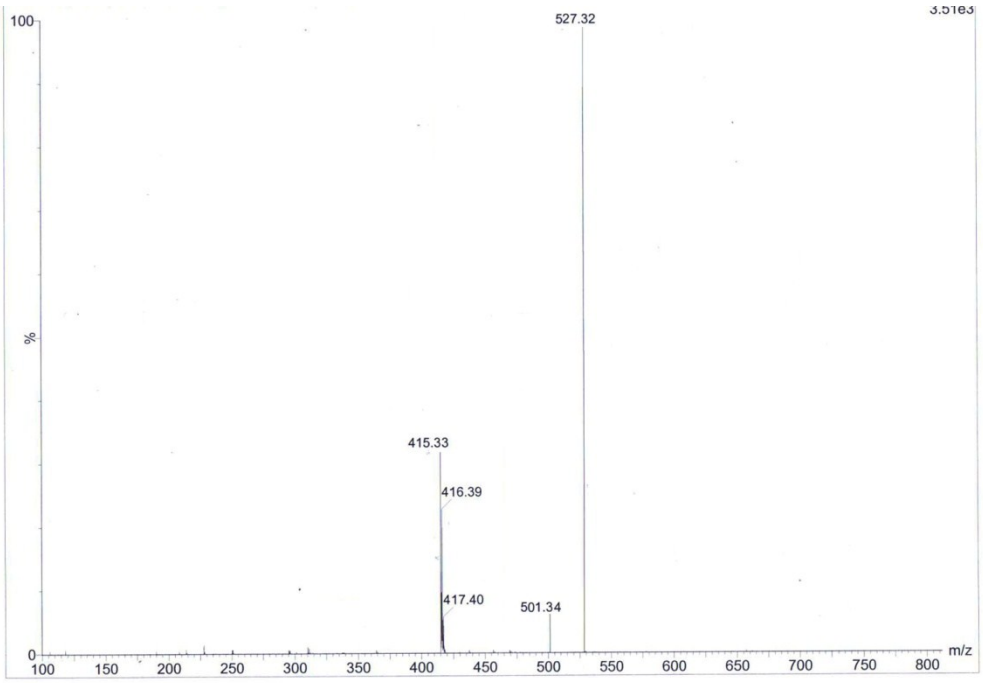

Fig. S8 ESI-MS spectrum of complex **3** in methanolic solution.

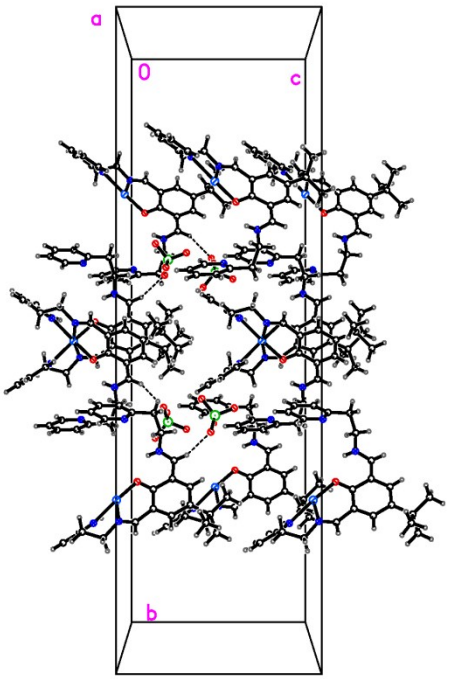

Fig. S9 Packing diagram of complex **1.**

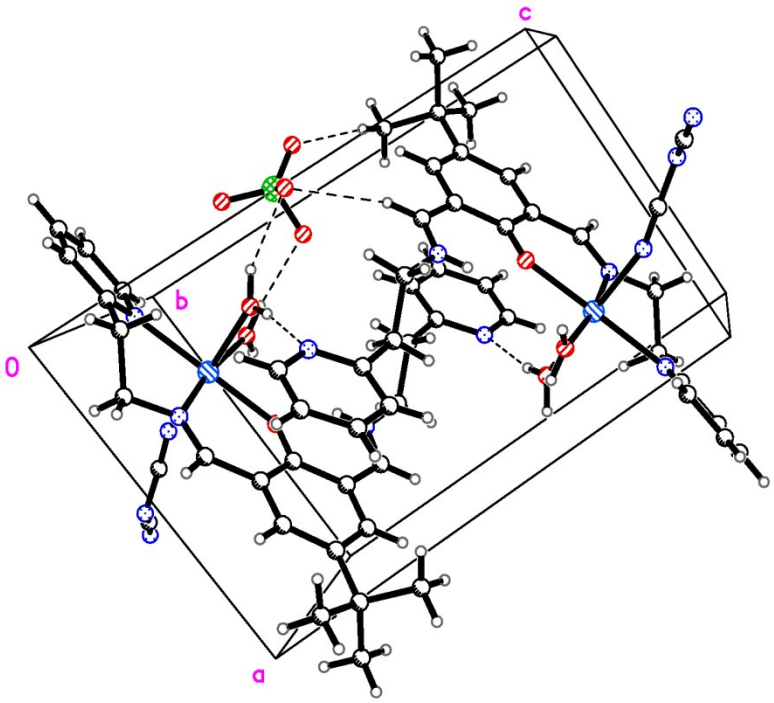

Fig. S10 Packing diagram of complex **2.**

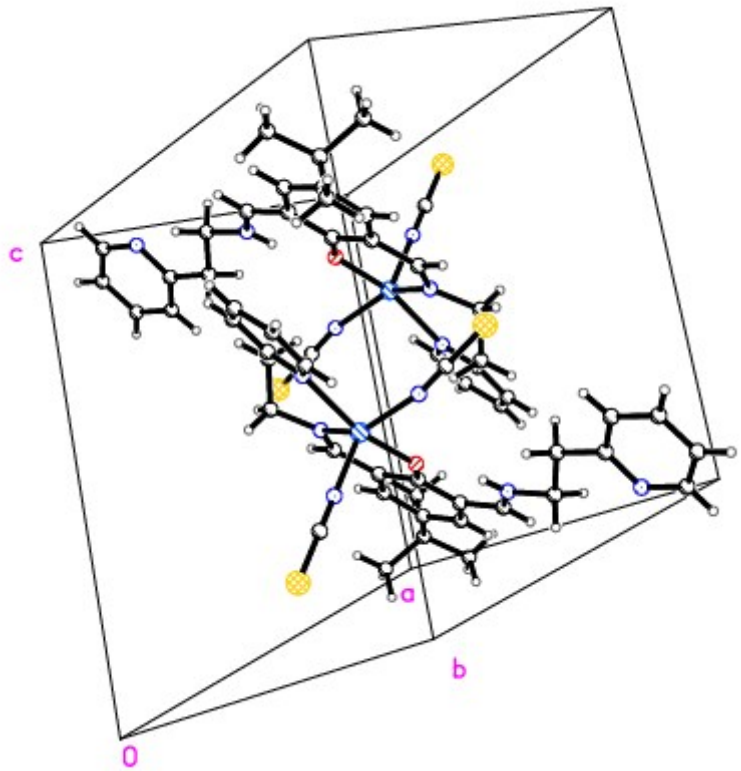

Fig. S11 Packing diagram of complex **3.**

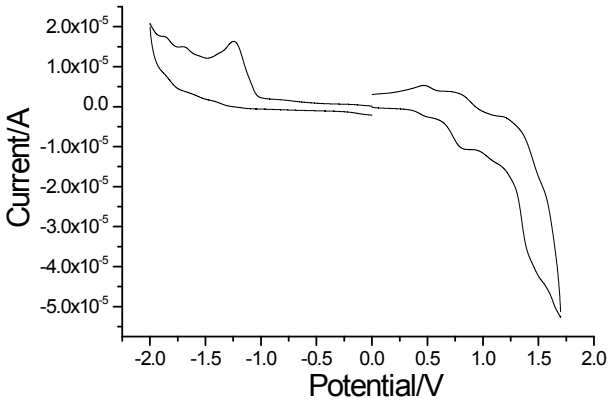

Fig. S12 Cyclic voltammogram of complex **1**.

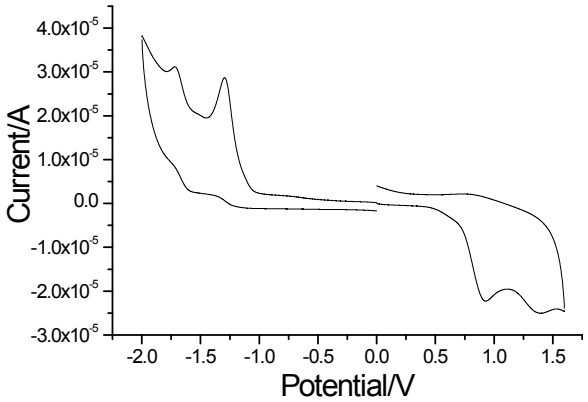

Fig. S13 Cyclic voltammogram of complex **2**.

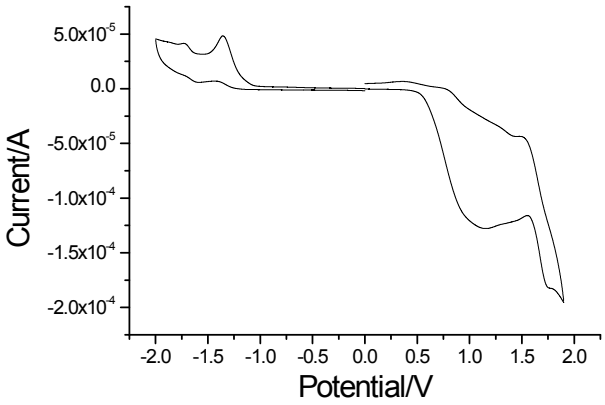

Fig. S14 Cyclic voltammogram of complex **3**.

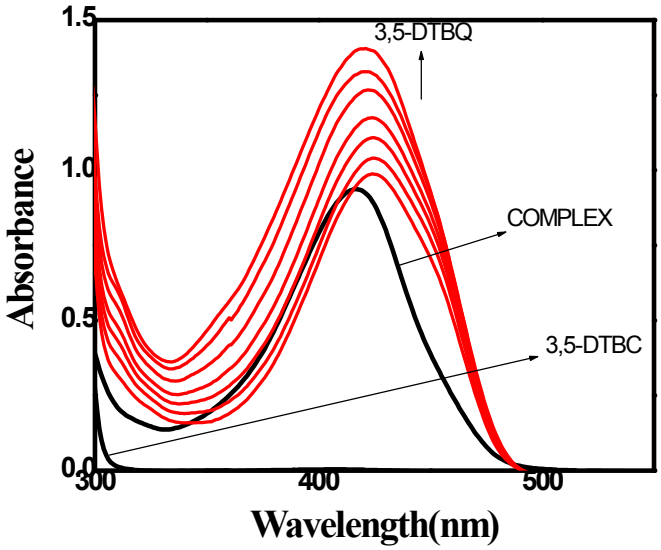

Fig. S15 UV−vis spectra of (i) Complex **2**, (ii) 3,5-DTBC, and (iii) changes in UV−vis spectra of Complex **2** upon addition of 3,5-DTBC observed after each 5 min interval.

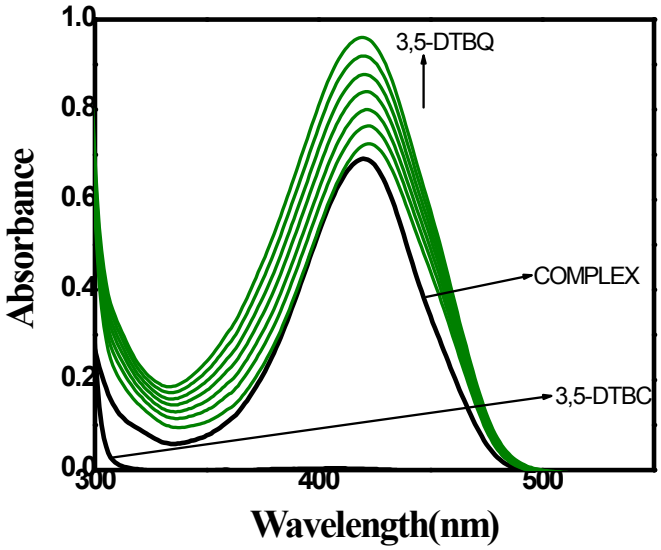

Fig. S16 UV−vis spectra of (i) Complex **3**, (ii) 3,5-DTBC, and (iii) changes in UV−vis spectra of Complex **3** upon addition of 3,5-DTBC observed after each 5 min interval.

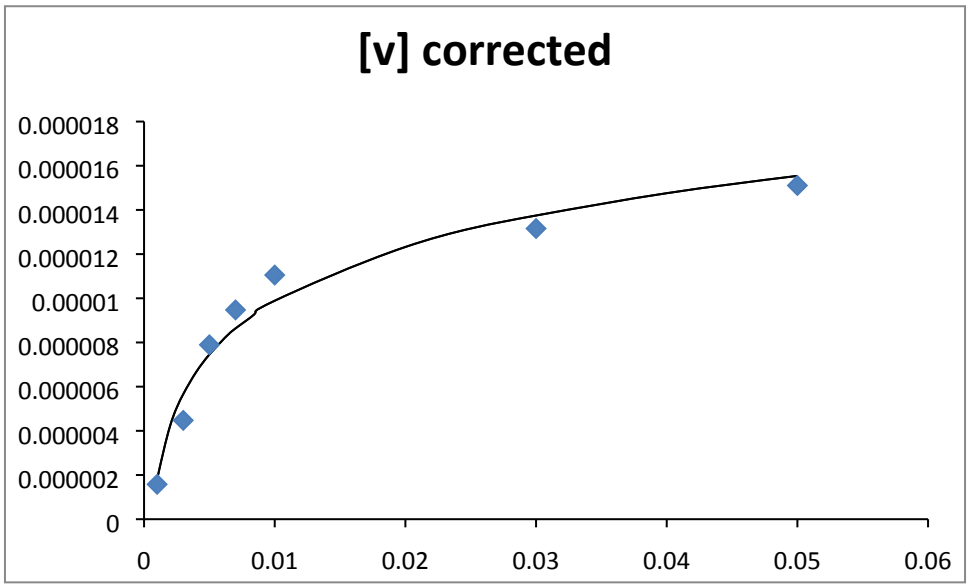

Fig. S17 Plot of rate vs concentration for complex **1.**

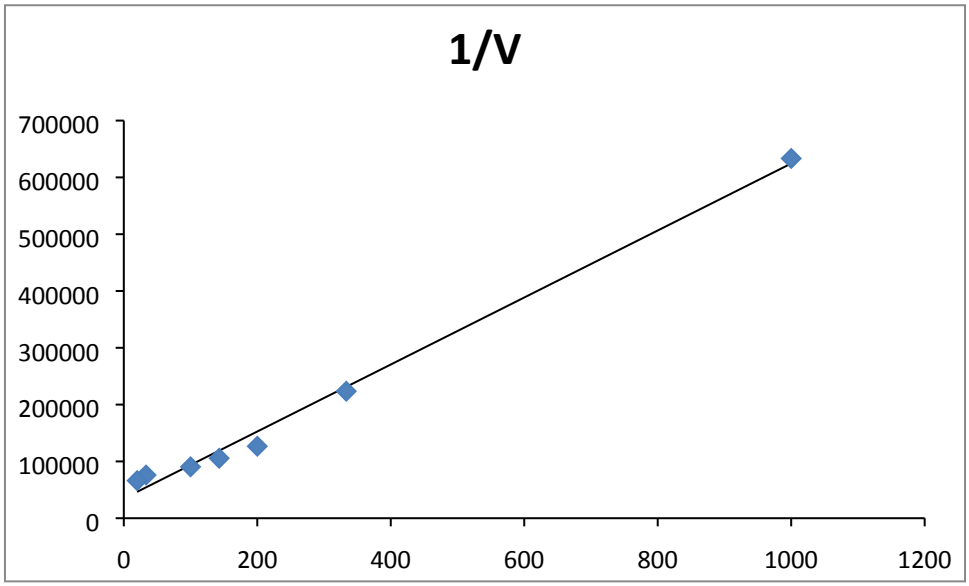

Fig. S18 Lineweaver–Burk plot of complex **1.**

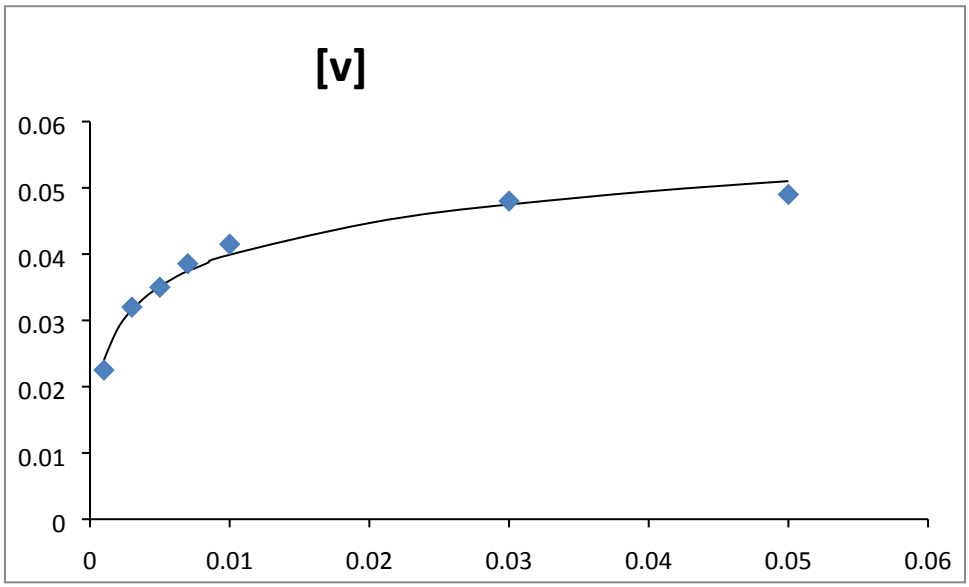

Fig. S19 Plot of rate vs concentration for complex **2.**

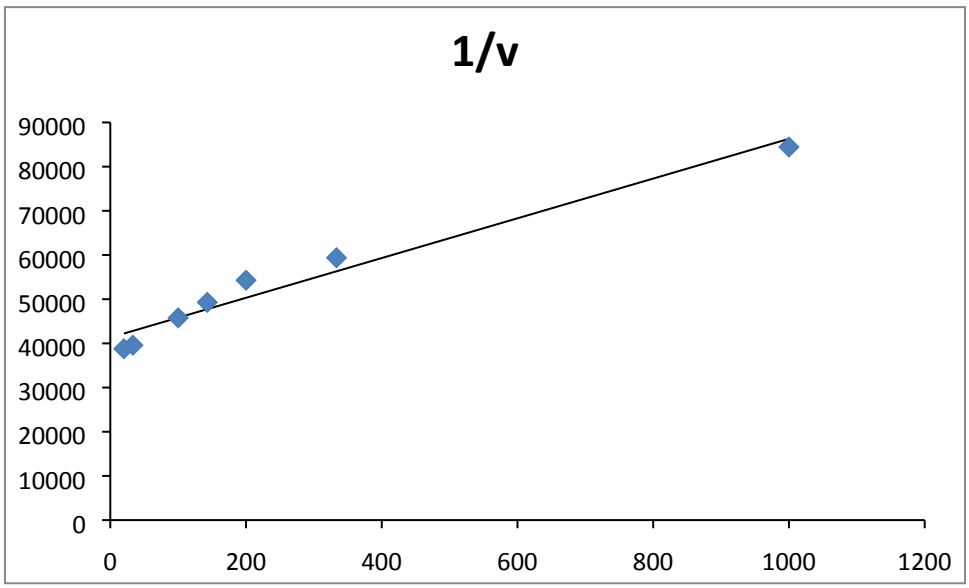

Fig. S20 Lineweaver–Burk plot of complexes **2.**

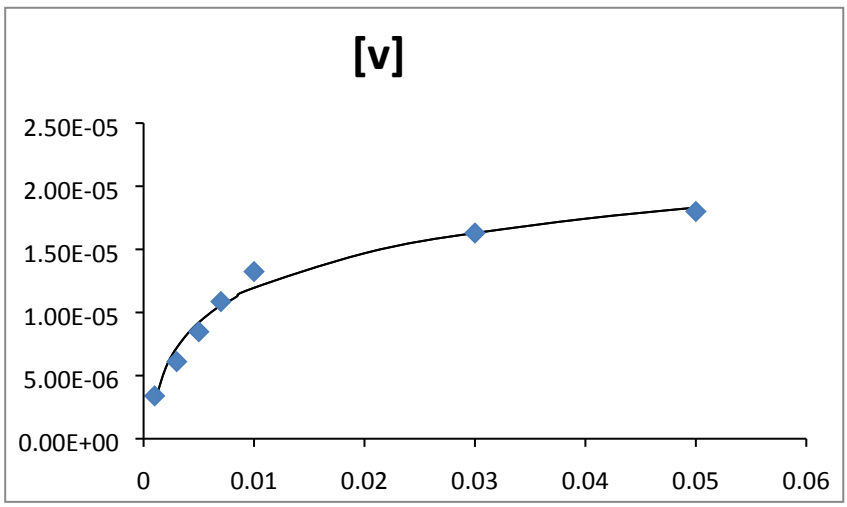

Fig. S21 Plot of rate vs concentration for complex **3.**

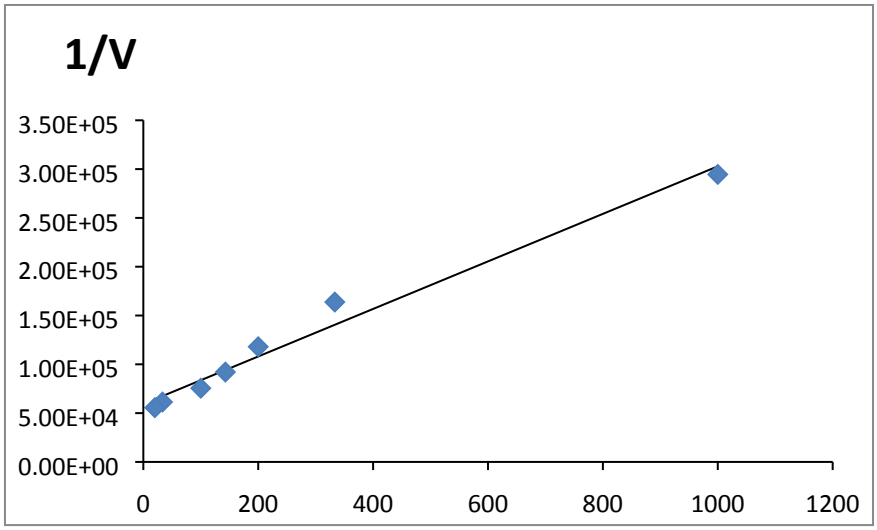

Fig. S22 Lineweaver–Burk plot of complexes **3.**

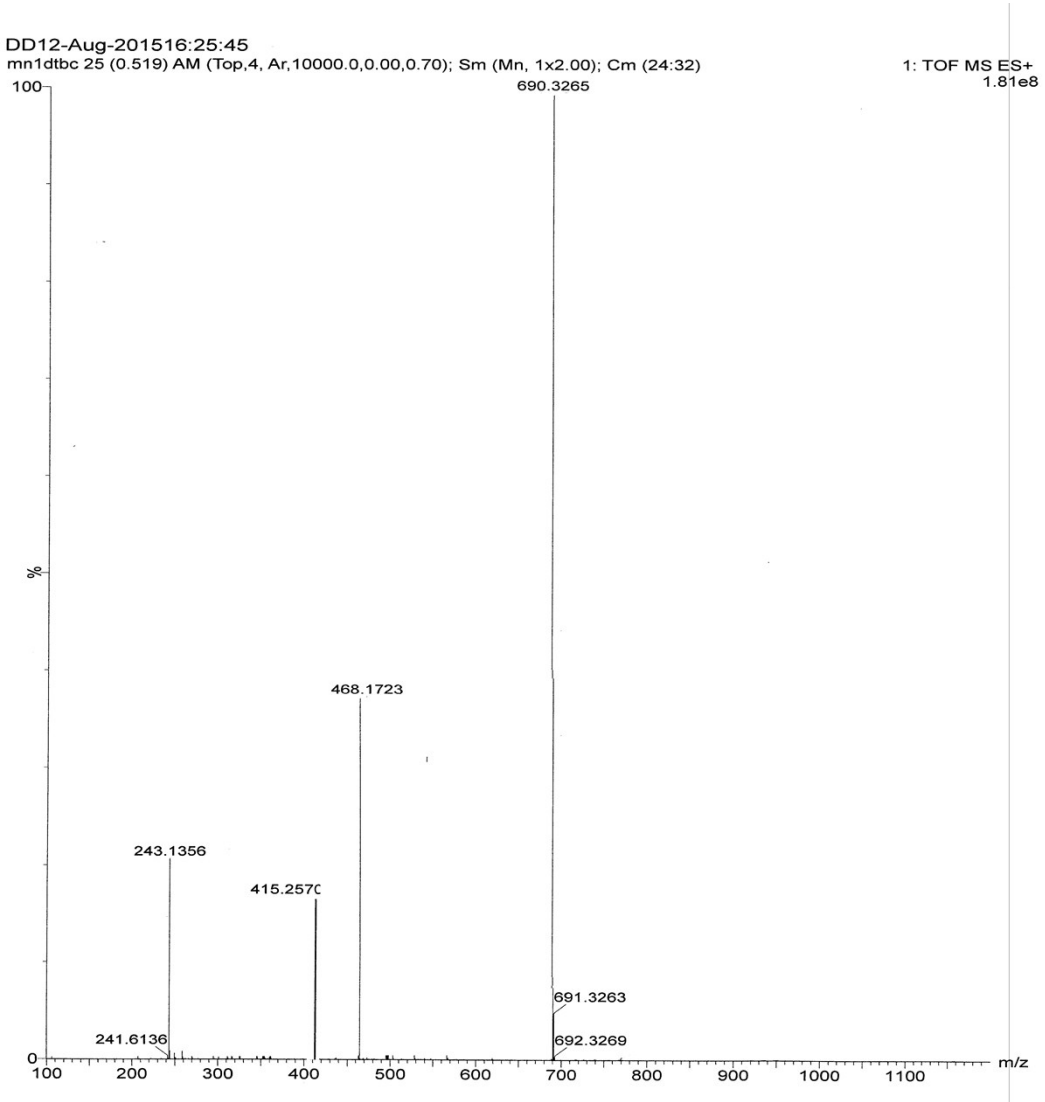

Fig. S23 ESI MS spectrum of 1: 50 mixture of the complex 1(most active) and 3,5-DTBC in methanol.

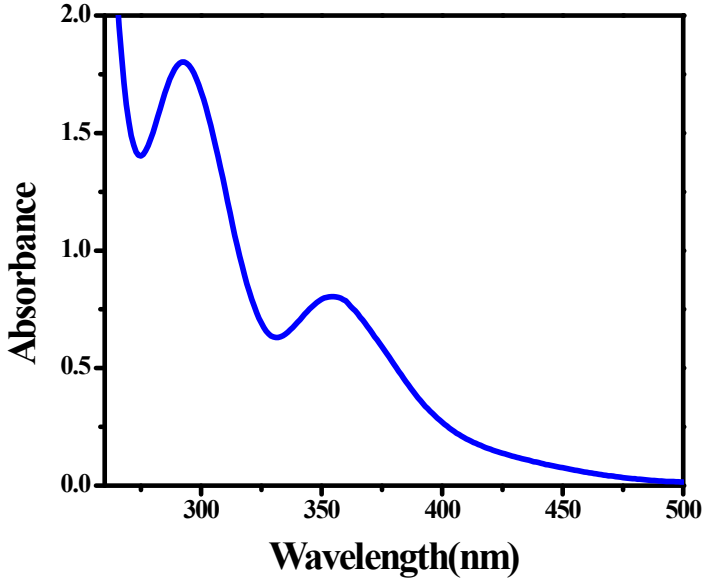

Fig. S24 Electronic spectra of the formation of I_3^- ion in presence of H_2O_2 (detection of H_2O_2 was achieved as described in the text).

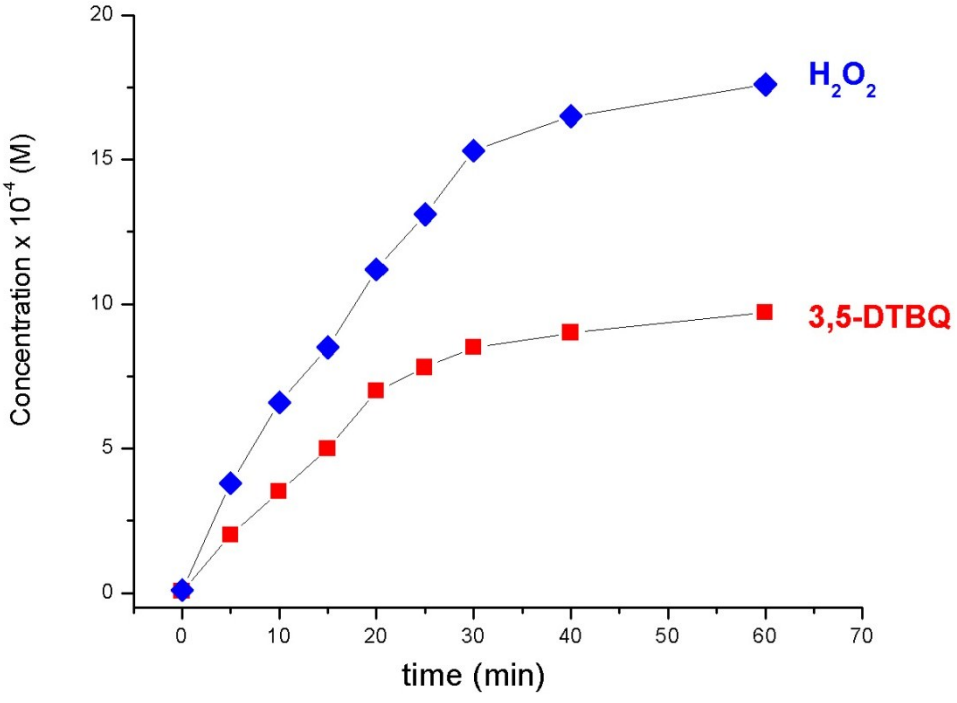

Fig.S25 Course of 3,5-DTBQ and H_2O_2 formation during the catalytic reaction for compounds **1**.

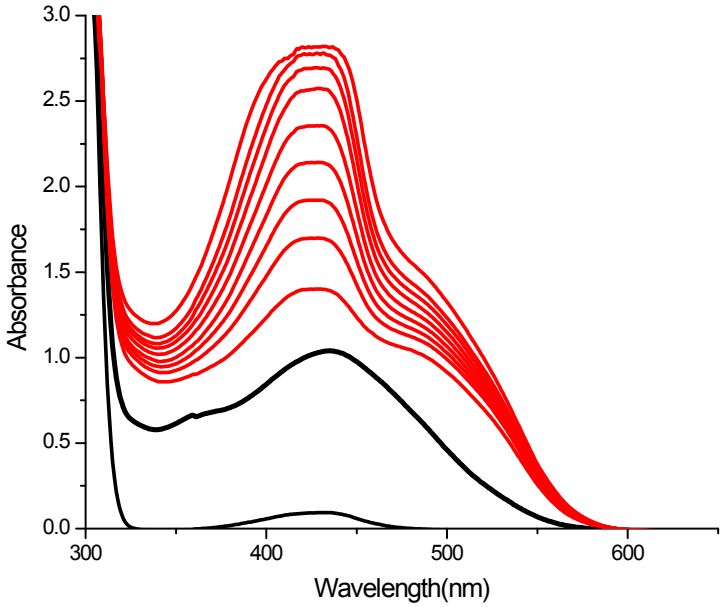

Fig. S26 UV–Vis spectral scans showing the increase in phenoxazinone chromophore band at 420 nm after the addition of o-aminophenol (0.001 M) to a solution of Complex **2** (1×10^{-4} M) in methanol at 25°C. The spectra were recorded for the period of 30minute.

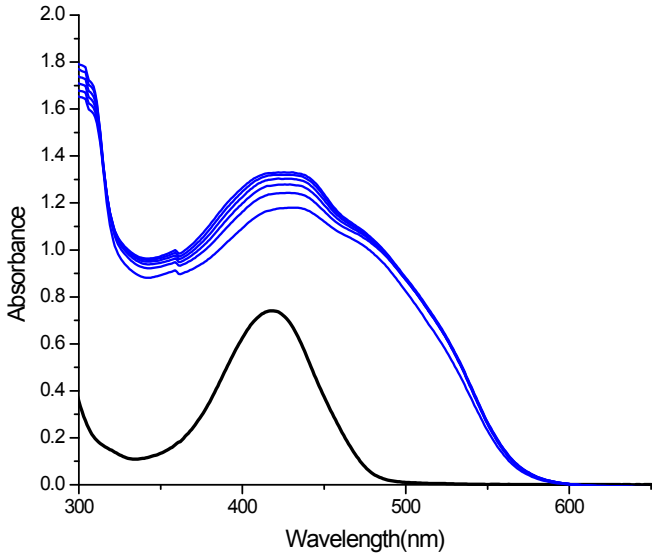

Fig. S27 UV–Vis spectral scans showing the increase in phenoxazinone chromophore band at 420 nm after the addition of o-aminophenol (0.001 M) to a solution of Complex **3** (1×10^{-4} M) in methanol at 25°C. The spectra were recorded for the period of 30minute.

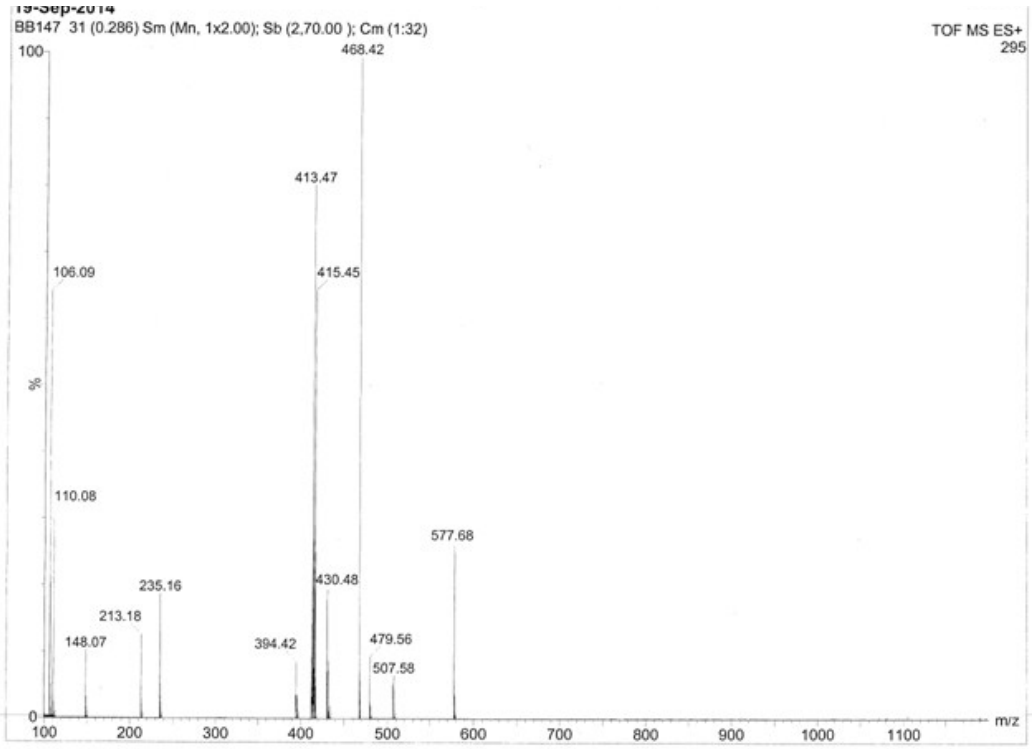

Fig. S28 ESI MS spectrum of 1: 50 mixture of the complex **1**(most active) and OAPH in methanol.

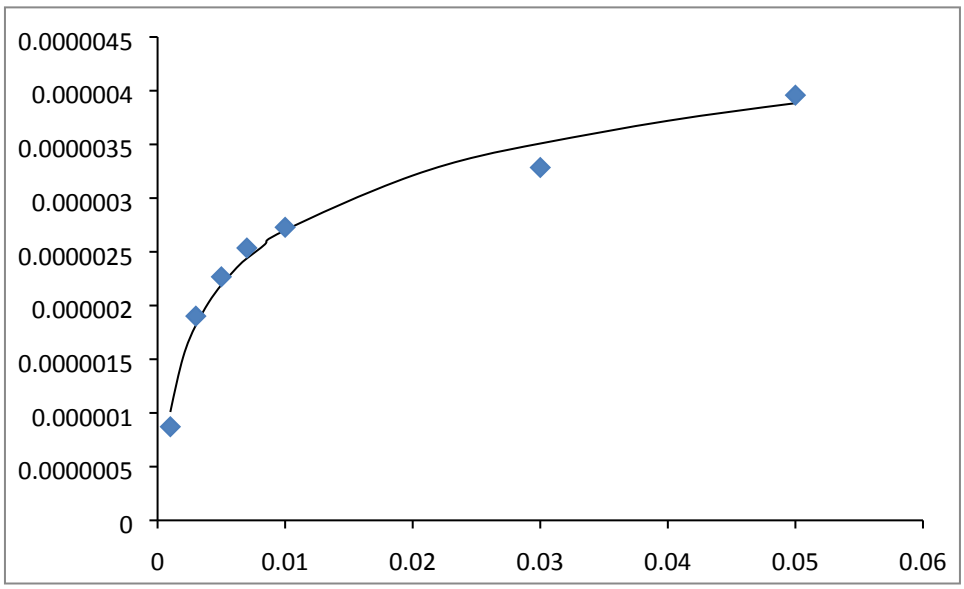

Fig. S29. Plot of rate vs concentration for complex **1.**

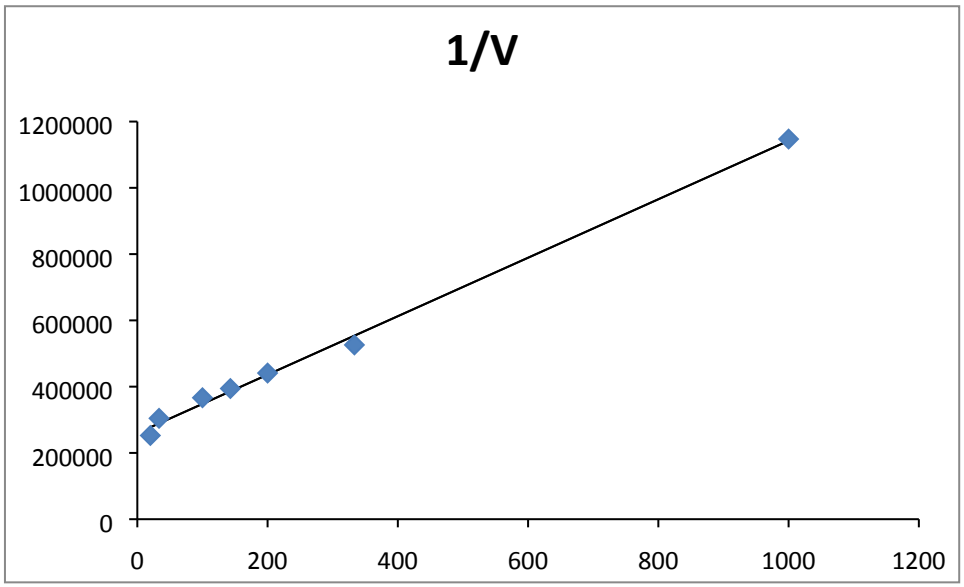

Fig. S30. Linewear-Burk plot of phenoxazinone synthase activity for complex **1.**

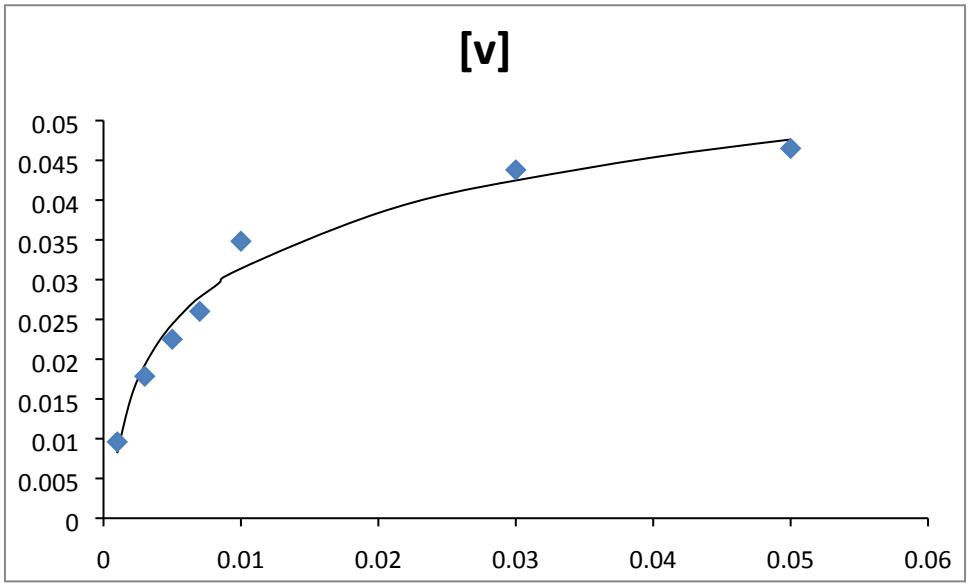

Fig. S31. Plot of rate vs concentration for complex **2.**

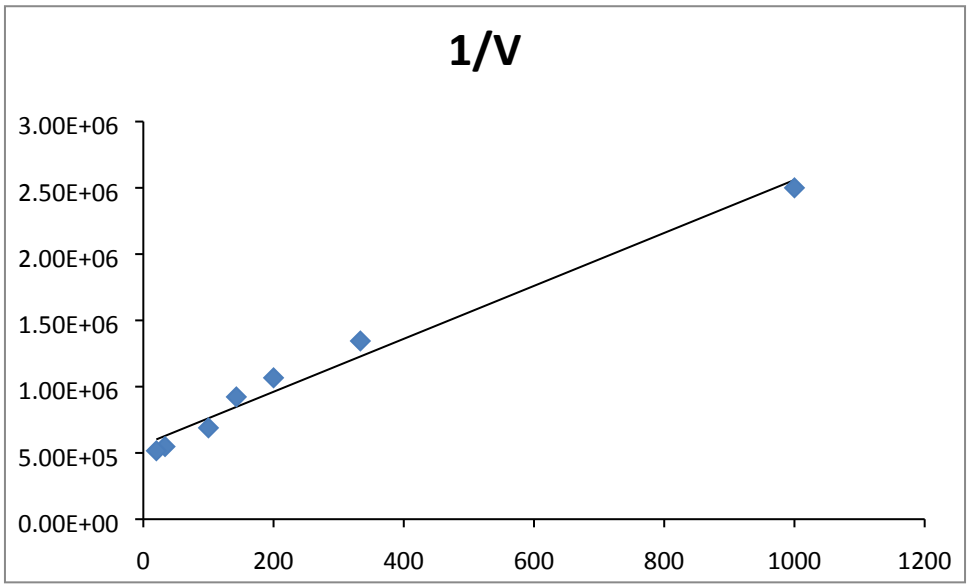

Fig. S32. Linewear-Burk plot of phenoxazinone synthase activity for complex **2.**

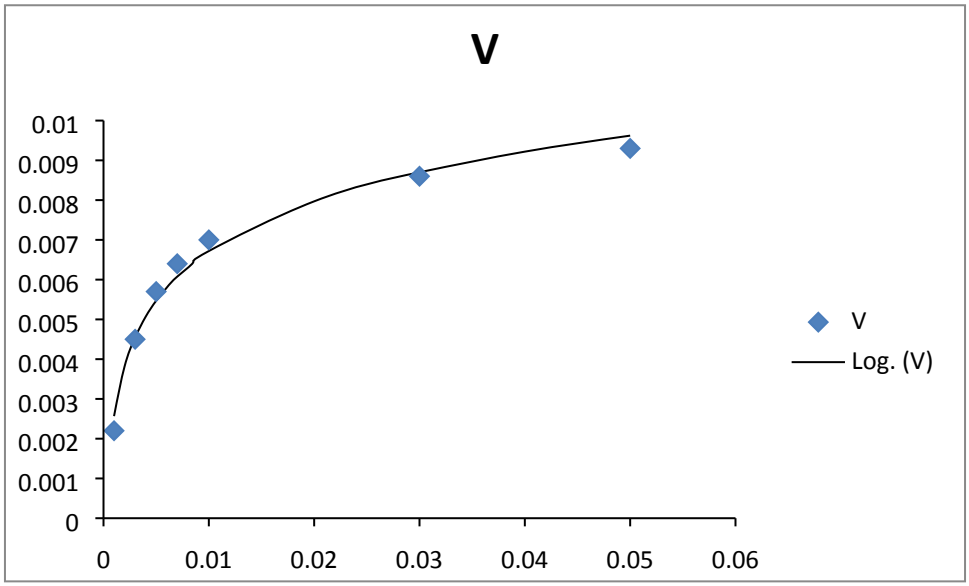

Fig. S33. Plot of rate vs concentration for complex **3.**

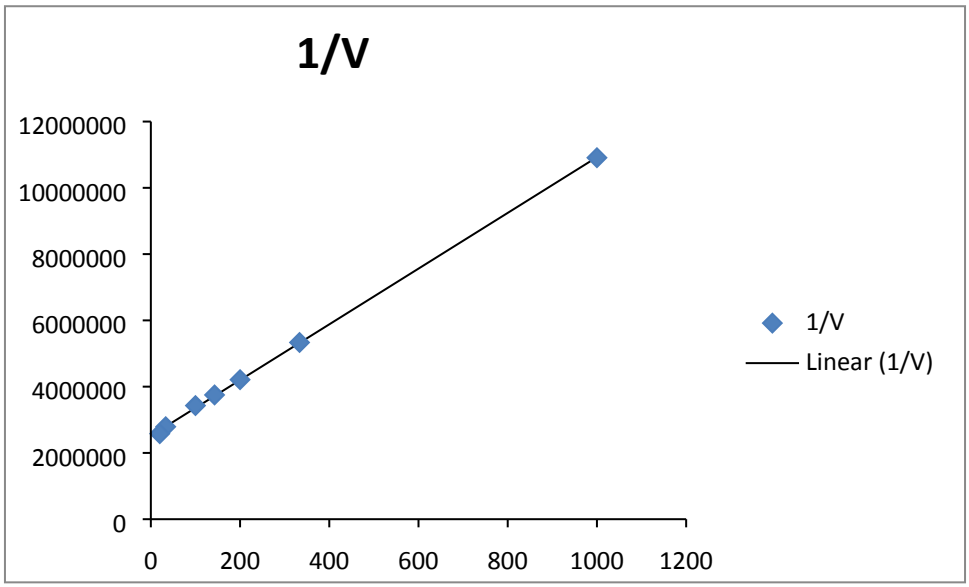

Fig. S34. Linewear-Burk plot of phenoxazinone synthase activity for complex **3.**

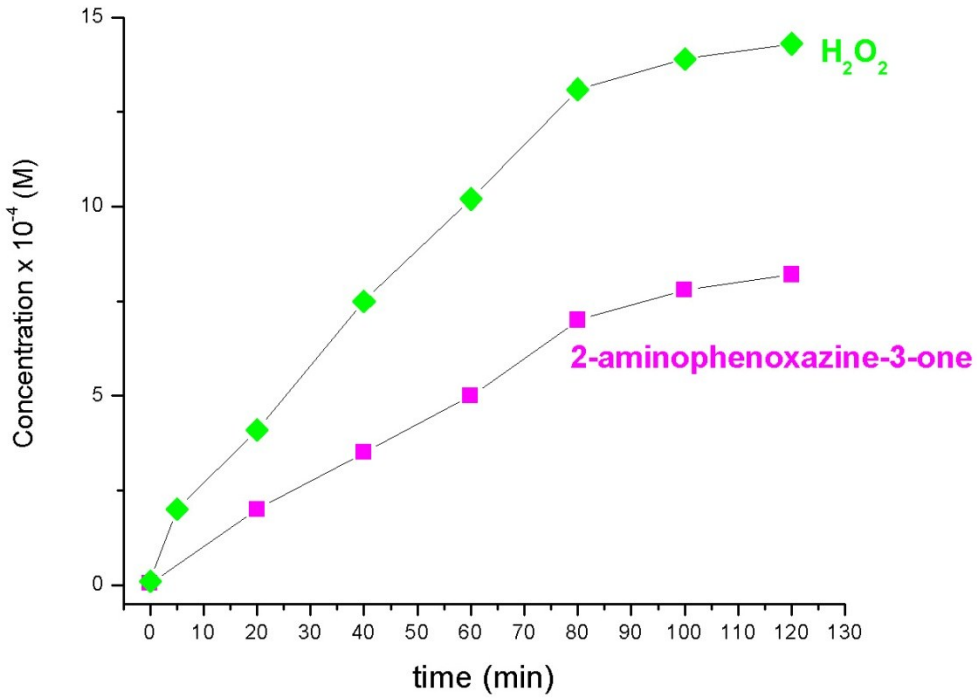

Fig.S35 Course of 2-aminophenoxazine-3-one and H_2O_2 formation during the catalytic reaction for compounds **1**.

Coordinates and energies of metal complexes

Structure **1**- LS

E(S12g/TZ2P)= -18007.6
E(BP86-D3/DZP)= -17590.99

Mn	0.00000000	0.00000000	1.28984460
O	1.00478222	0.91305659	-0.11141889
N	1.21378253	-1.52140015	1.22386360
N	-1.13194395	-0.93996290	2.64476196
N	0.55785778	2.98574040	-1.64081337
H	0.67454016	2.58710593	-0.68692976
N	1.69239659	4.36626802	0.82614282
C	1.44033464	0.25516600	-1.15248963
C	1.43570928	0.88424677	-2.43811586
C	1.84611119	0.17251135	-3.58472130
H	1.78158051	0.68649123	-4.54250204
C	2.32700432	-1.12857670	-3.50775548
C	2.81582754	-1.91220661	-4.72588505
C	2.38194787	-1.71431051	-2.23407270
H	2.78478121	-2.72298791	-2.13026530
C	1.90308417	-1.09249251	-1.07589975
C	1.90910175	-1.82859912	0.16039718
H	2.53743418	-2.72857976	0.18316865
C	1.34895722	-2.46774216	2.34963577
H	2.40356736	-2.76071213	2.45866752
H	0.77093703	-3.36655317	2.08779519
C	0.85598438	-1.93467398	3.68954869
H	1.03865538	-2.72212582	4.43523225
H	1.45652894	-1.07017496	4.00895520
C	-0.60585321	-1.60791234	3.70433570
C	-1.42057563	-2.02440046	4.75870238
H	-0.96018712	-2.52587773	5.61029950
C	-2.79392102	-1.82768456	4.70679903
H	-3.43387279	-2.14835785	5.52856564
C	-3.33608873	-1.24711404	3.55848993
H	-4.41031706	-1.11378749	3.43736981
C	-2.48204108	-0.82024716	2.55945026
H	-2.86323574	-0.33815702	1.66283173
C	0.92688214	2.19984247	-2.61611904
H	0.81952031	2.58697667	-3.63073672
C	-0.07131693	4.28531841	-1.82059355
H	-1.08836848	4.22760068	-1.40116076
H	-0.14896101	4.48672876	-2.89539034
C	0.70648945	5.40590216	-1.12822417
H	1.72866657	5.43069490	-1.53505260

H	0.21163319	6.35217042	-1.38627551
C	0.77786344	5.24524754	0.36563648
C	-0.05075775	5.98133832	1.21802649
H	-0.79323497	6.66578165	0.80475952
C	0.10586342	5.84839116	2.59663863
H	-0.51752167	6.42214841	3.28307606
C	1.07733399	4.97448887	3.07736104
H	1.24799057	4.85024659	4.14645162
C	1.83021964	4.24926626	2.15715649
H	2.59330656	3.54812566	2.49597009
C	4.31856280	-2.20459057	-4.55642404
H	4.51112777	-2.81594611	-3.66149920
H	4.88467803	-1.26453290	-4.46116248
H	4.69459469	-2.75630257	-5.43237890
C	2.04667279	-3.24131619	-4.83205819
H	2.19294976	-3.86958816	-3.94167399
H	2.40344672	-3.81241414	-5.70360079
H	0.96902129	-3.05819239	-4.96410293
C	2.60696806	-1.12752063	-6.02495270
H	2.95548240	-1.73295301	-6.87500079
H	3.17712084	-0.18597253	-6.02727027
H	1.54220964	-0.89855926	-6.18990816
O	-1.00478222	-0.91305659	-0.11141889
N	-1.21378253	1.52140015	1.22386360
N	1.13194395	0.93996290	2.64476196
N	-0.55785778	-2.98574040	-1.64081337
H	-0.67454016	-2.58710593	-0.68692976
N	-1.69239659	-4.36626802	0.82614282
C	-1.44033464	-0.25516600	-1.15248963
C	-1.43570928	-0.88424677	-2.43811586
C	-1.84611119	-0.17251135	-3.58472130
H	-1.78158051	-0.68649123	-4.54250204
C	-2.32700432	1.12857670	-3.50775548
C	-2.81582754	1.91220661	-4.72588505
C	-2.38194787	1.71431051	-2.23407270
H	-2.78478121	2.72298791	-2.13026530
C	-1.90308417	1.09249251	-1.07589975
C	-1.90910175	1.82859912	0.16039718
H	-2.53743418	2.72857976	0.18316865
C	-1.34895722	2.46774216	2.34963577
H	-2.40356736	2.76071213	2.45866752
H	-0.77093703	3.36655317	2.08779519
C	-0.85598438	1.93467398	3.68954869
H	-1.03865538	2.72212582	4.43523225
H	-1.45652894	1.07017496	4.00895520
C	0.60585321	1.60791234	3.70433570

C	1.42057563	2.02440046	4.75870238
H	0.96018712	2.52587773	5.61029950
C	2.79392102	1.82768456	4.70679903
H	3.43387279	2.14835785	5.52856564
C	3.33608873	1.24711404	3.55848993
H	4.41031706	1.11378749	3.43736981
C	2.48204108	0.82024716	2.55945026
H	2.86323574	0.33815702	1.66283173
C	-0.92688214	-2.19984247	-2.61611904
H	-0.81952031	-2.58697667	-3.63073672
C	0.07131693	-4.28531841	-1.82059355
H	1.08836848	-4.22760068	-1.40116076
H	0.14896101	-4.48672876	-2.89539034
C	-0.70648945	-5.40590216	-1.12822417
H	-1.72866657	-5.43069490	-1.53505260
H	-0.21163319	-6.35217042	-1.38627551
C	-0.77786344	-5.24524754	0.36563648
C	0.05075775	-5.98133832	1.21802649
H	0.79323497	-6.66578165	0.80475952
C	-0.10586342	-5.84839116	2.59663863
H	0.51752167	-6.42214841	3.28307606
C	-1.07733399	-4.97448887	3.07736104
H	-1.24799057	-4.85024659	4.14645162
C	-1.83021964	-4.24926626	2.15715649
H	-2.59330656	-3.54812566	2.49597009
C	-4.31856280	2.20459057	-4.55642404
H	-4.51112777	2.81594611	-3.66149920
H	-4.88467803	1.26453290	-4.46116248
H	-4.69459469	2.75630257	-5.43237890
C	-2.04667279	3.24131619	-4.83205819
H	-2.19294976	3.86958816	-3.94167399
H	-2.40344672	3.81241414	-5.70360079
H	-0.96902129	3.05819239	-4.96410293
C	-2.60696806	1.12752063	-6.02495270
H	-2.95548240	1.73295301	-6.87500079
H	-3.17712084	0.18597253	-6.02727027
H	-1.54220964	0.89855926	-6.18990816

Structure **1**-IS

E(S12g/TZ2P)=-18006.3
E(BP86-D3/DZP)= -17579.32

MN	0.000000	0.000000	1.327528
O	1.120210	0.954068	-0.125692
N	1.307943	-1.444715	1.235745

N	-1.131634	-1.140757	2.699830
N	0.547381	3.008868	-1.649648
H	0.680540	2.599425	-0.701709
N	1.611038	4.490180	0.962874
C	1.453354	0.293202	-1.192738
C	1.374570	0.900634	-2.486245
C	1.737123	0.173747	-3.641765
H	1.640358	0.677740	-4.602071
C	2.223744	-1.125355	-3.565889
C	2.697224	-1.908808	-4.791207
C	2.323046	-1.704563	-2.289890
H	2.721823	-2.715731	-2.195965
C	1.902371	-1.064111	-1.118324
C	1.926303	-1.780453	0.126064
H	2.490932	-2.721725	0.127009
C	1.481917	-2.387975	2.363472
H	2.553826	-2.605696	2.477210
H	0.966483	-3.320354	2.089898
C	0.952457	-1.907205	3.711402
H	1.233523	-2.667318	4.454546
H	1.465574	-0.982191	4.020564
C	-0.534130	-1.712277	3.768598
C	-1.283805	-2.113774	4.874969
H	-0.777082	-2.557122	5.732507
C	-2.665429	-1.963265	4.862186
H	-3.261377	-2.271031	5.721365
C	-3.277350	-1.437518	3.722712
H	-4.359534	-1.334839	3.653097
C	-2.478358	-1.039082	2.665015
H	-2.896564	-0.610295	1.755759
C	0.882036	2.221366	-2.641388
H	0.757465	2.619172	-3.649776
C	-0.068946	4.315628	-1.824045
H	-1.103807	4.259575	-1.450460
H	-0.102170	4.539538	-2.896983
C	0.687632	5.416824	-1.081430
H	1.734822	5.418366	-1.417749
H	0.232744	6.374489	-1.371049
C	0.651335	5.263511	0.414269
C	-0.322261	5.910454	1.183097
H	-1.096003	6.507572	0.697623
C	-0.269431	5.807493	2.571304
H	-1.007216	6.315473	3.193112
C	0.748814	5.050520	3.146295
H	0.843121	4.956201	4.228039
C	1.647877	4.402271	2.303448

H	2.452036	3.792887	2.717518
C	4.215230	-2.141386	-4.663830
H	4.455263	-2.736300	-3.769262
H	4.746359	-1.179093	-4.591393
H	4.588040	-2.685605	-5.545959
C	1.980393	-3.268360	-4.862450
H	2.165762	-3.877691	-3.966380
H	2.343971	-3.838403	-5.731859
H	0.894683	-3.130941	-4.979225
C	2.420015	-1.147811	-6.091596
H	2.753000	-1.755090	-6.946600
H	2.963947	-0.191692	-6.127634
H	1.343889	-0.949162	-6.219226
O	-1.120210	-0.954068	-0.125692
N	-1.307943	1.444715	1.235745
N	1.131634	1.140757	2.699830
N	-0.547381	-3.008868	-1.649648
H	-0.680540	-2.599425	-0.701709
N	-1.611038	-4.490180	0.962874
C	-1.453354	-0.293202	-1.192738
C	-1.374570	-0.900634	-2.486245
C	-1.737123	-0.173747	-3.641765
H	-1.640358	-0.677740	-4.602071
C	-2.223744	1.125355	-3.565889
C	-2.697224	1.908808	-4.791207
C	-2.323046	1.704563	-2.289890
H	-2.721823	2.715731	-2.195965
C	-1.902371	1.064111	-1.118324
C	-1.926303	1.780453	0.126064
H	-2.490932	2.721725	0.127009
C	-1.481917	2.387975	2.363472
H	-2.553826	2.605696	2.477210
H	-0.966483	3.320354	2.089898
C	-0.952457	1.907205	3.711402
H	-1.233523	2.667318	4.454546
H	-1.465574	0.982191	4.020564
C	0.534130	1.712277	3.768598
C	1.283805	2.113774	4.874969
H	0.777082	2.557122	5.732507
C	2.665429	1.963265	4.862186
H	3.261377	2.271031	5.721365
C	3.277350	1.437518	3.722712
H	4.359534	1.334839	3.653097
C	2.478358	1.039082	2.665015
H	2.896564	0.610295	1.755759
C	-0.882036	-2.221366	-2.641388

H	-0.757465	-2.619172	-3.649776
C	0.068946	-4.315628	-1.824045
H	1.103807	-4.259575	-1.450460
H	0.102170	-4.539538	-2.896983
C	-0.687632	-5.416824	-1.081430
H	-1.734822	-5.418366	-1.417749
H	-0.232744	-6.374489	-1.371049
C	-0.651335	-5.263511	0.414269
C	0.322261	-5.910454	1.183097
H	1.096003	-6.507572	0.697623
C	0.269431	-5.807493	2.571304
H	1.007216	-6.315473	3.193112
C	-0.748814	-5.050520	3.146295
H	-0.843121	-4.956201	4.228039
C	-1.647877	-4.402271	2.303448
H	-2.452036	-3.792887	2.717518
C	-4.215230	2.141386	-4.663830
H	-4.455263	2.736300	-3.769262
H	-4.746359	1.179093	-4.591393
H	-4.588040	2.685605	-5.545959
C	-1.980393	3.268360	-4.862450
H	-2.165762	3.877691	-3.966380
H	-2.343971	3.838403	-5.731859
H	-0.894683	3.130941	-4.979225
C	-2.420015	1.147811	-6.091596
H	-2.753000	1.755090	-6.946600
H	-2.963947	0.191692	-6.127634
H	-1.343889	0.949162	-6.219226

Structure **1**-HS

E(S12g/TZ2P)=-18016.9
E(BP86-D3/DZP)= -17582.18

MN	0.000000	0.000000	1.300843
O	1.258927	0.858200	-0.127573
N	1.506145	-1.582787	1.218223
N	-1.007317	-1.238553	2.781126
N	0.647302	2.901873	-1.661894
H	0.780432	2.490709	-0.713110
N	1.724748	4.442851	1.020919
C	1.549141	0.180440	-1.196042
C	1.431861	0.777174	-2.495324
C	1.733693	0.039418	-3.657632
H	1.604558	0.541165	-4.615841
C	2.186091	-1.271510	-3.601945
C	2.578685	-2.072453	-4.843340

C	2.328502	-1.841185	-2.325955
H	2.698331	-2.864470	-2.242282
C	1.983709	-1.186632	-1.141662
C	2.024326	-1.947520	0.086561
H	2.498534	-2.939115	0.004660
C	1.576799	-2.574491	2.306799
H	2.612690	-2.935591	2.399601
H	0.942512	-3.430648	2.034032
C	1.131274	-2.036275	3.666727
H	1.447675	-2.759257	4.432008
H	1.668099	-1.099800	3.892208
C	-0.348580	-1.813322	3.811000
C	-1.031048	-2.199903	4.966464
H	-0.478493	-2.652694	5.790099
C	-2.406957	-2.017677	5.048025
H	-2.949205	-2.313991	5.946254
C	-3.085028	-1.477241	3.955332
H	-4.166335	-1.345927	3.963021
C	-2.348304	-1.099767	2.844409
H	-2.816060	-0.655327	1.966161
C	0.967851	2.107969	-2.651903
H	0.855087	2.507651	-3.660912
C	0.110420	4.243189	-1.842632
H	-0.925773	4.252570	-1.467817
H	0.090228	4.459689	-2.916883
C	0.933771	5.302523	-1.109772
H	1.988742	5.201558	-1.403041
H	0.575192	6.283084	-1.454177
C	0.822161	5.219415	0.387922
C	-0.163615	5.938949	1.072558
H	-0.886888	6.539680	0.518402
C	-0.188249	5.901094	2.464690
H	-0.938538	6.463280	3.021673
C	0.769698	5.136723	3.126970
H	0.803543	5.087619	4.215414
C	1.689386	4.421724	2.364838
H	2.450270	3.810285	2.850830
C	4.096118	-2.332077	-4.791418
H	4.370641	-2.924172	-3.904789
H	4.647455	-1.379232	-4.754669
H	4.413536	-2.890368	-5.686278
C	1.834333	-3.418622	-4.866471
H	2.048397	-4.023769	-3.973933
H	2.148920	-4.003464	-5.745050
H	0.747151	-3.263623	-4.939064
C	2.244922	-1.315855	-6.133366

H	2.518712	-1.935889	-6.999951
H	2.804138	-0.370770	-6.207938
H	1.167132	-1.097889	-6.204109
O	-1.258927	-0.858200	-0.127573
N	-1.506145	1.582787	1.218223
N	1.007317	1.238553	2.781126
N	-0.647302	-2.901873	-1.661894
H	-0.780432	-2.490709	-0.713110
N	-1.724748	-4.442851	1.020919
C	-1.549141	-0.180440	-1.196042
C	-1.431861	-0.777174	-2.495324
C	-1.733693	-0.039418	-3.657632
H	-1.604558	-0.541165	-4.615841
C	-2.186091	1.271510	-3.601945
C	-2.578685	2.072453	-4.843340
C	-2.328502	1.841185	-2.325955
H	-2.698331	2.864470	-2.242282
C	-1.983709	1.186632	-1.141662
C	-2.024326	1.947520	0.086561
H	-2.498534	2.939115	0.004660
C	-1.576799	2.574491	2.306799
H	-2.612690	2.935591	2.399601
H	-0.942512	3.430648	2.034032
C	-1.131274	2.036275	3.666727
H	-1.447675	2.759257	4.432008
H	-1.668099	1.099800	3.892208
C	0.348580	1.813322	3.811000
C	1.031048	2.199903	4.966464
H	0.478493	2.652694	5.790099
C	2.406957	2.017677	5.048025
H	2.949205	2.313991	5.946254
C	3.085028	1.477241	3.955332
H	4.166335	1.345927	3.963021
C	2.348304	1.099767	2.844409
H	2.816060	0.655327	1.966161
C	-0.967851	-2.107969	-2.651903
H	-0.855087	-2.507651	-3.660912
C	-0.110420	-4.243189	-1.842632
H	0.925773	-4.252570	-1.467817
H	-0.090228	-4.459689	-2.916883
C	-0.933771	-5.302523	-1.109772
H	-1.988742	-5.201558	-1.403041
H	-0.575192	-6.283084	-1.454177
C	-0.822161	-5.219415	0.387922
C	0.163615	-5.938949	1.072558
H	0.886888	-6.539680	0.518402

C	0.188249	-5.901094	2.464690
H	0.938538	-6.463280	3.021673
C	-0.769698	-5.136723	3.126970
H	-0.803543	-5.087619	4.215414
C	-1.689386	-4.421724	2.364838
H	-2.450270	-3.810285	2.850830
C	-4.096118	2.332077	-4.791418
H	-4.370641	2.924172	-3.904789
H	-4.647455	1.379232	-4.754669
H	-4.413536	2.890368	-5.686278
C	-1.834333	3.418622	-4.866471
H	-2.048397	4.023769	-3.973933
H	-2.148920	4.003464	-5.745050
H	-0.747151	3.263623	-4.939064
C	-2.244922	1.315855	-6.133366
H	-2.518712	1.935889	-6.999951
H	-2.804138	0.370770	-6.207938
H	-1.167132	1.097889	-6.204109

Structure **2** - LS

E(S12g/TZ2P)= -11123.31
E(BP86-D3/DZP)= -10882.07

Mn	1.52510000	-0.45490000	-0.07070000
O	-0.23930000	0.12230000	-0.40900000
N	0.97090000	-2.24270000	0.30350000
O	2.01740000	1.55820000	-0.36450000
N	-1.65150000	1.89650000	-2.03930000
O	1.77420000	-0.69560000	-2.14150000
C	-1.36430000	-0.52430000	-0.32170000
C	-1.44730000	-1.88160000	0.11470000
N	3.45990000	-0.83400000	0.18340000
N	0.14560000	3.17550000	0.45860000
C	-2.58150000	0.14020000	-0.66900000
C	-0.28110000	-2.66390000	0.35830000
H	-0.44570000	-3.71950000	0.60200000
C	-3.80060000	-0.48690000	-0.44310000
H	-4.70740000	0.07070000	-0.68500000
C	-2.71810000	-2.48600000	0.27920000
H	-2.73400000	-3.52080000	0.62140000
C	-2.57370000	1.48350000	-1.25280000
H	-3.44090000	2.12310000	-0.98970000
C	-3.90280000	-1.80830000	0.03760000
C	-5.28460000	-2.43050000	0.23460000

C	3.13840000	-3.18720000	-0.43490000
H	3.72590000	-4.11400000	-0.37580000
H	2.71610000	-3.15640000	-1.45420000
C	-0.74420000	3.92600000	-0.21690000
C	4.04680000	-2.02530000	-0.15790000
C	1.99460000	-3.26830000	0.56870000
H	1.54170000	-4.26810000	0.52110000
H	2.38880000	-3.11410000	1.58730000
C	5.42950000	-2.17900000	-0.16210000
H	5.84790000	-3.13900000	-0.46630000
C	-1.82020000	4.52880000	0.44080000
H	-2.53220000	5.12920000	-0.12680000
C	-6.01410000	-2.48740000	-1.12150000
H	-6.14540000	-1.48220000	-1.55000000
H	-7.01230000	-2.93710000	-0.99550000
H	-5.44240000	-3.09700000	-1.83960000
C	-5.19850000	-3.85180000	0.80080000
H	-4.69480000	-3.86430000	1.78010000
H	-4.65840000	-4.52690000	0.11880000
H	-6.21460000	-4.25280000	0.93690000
C	5.65890000	0.04160000	0.68500000
H	6.25050000	0.87820000	1.05650000
C	6.26160000	-1.13850000	0.24440000
H	7.34470000	-1.25560000	0.24640000
C	4.28290000	0.15900000	0.64170000
H	3.78170000	1.07610000	0.94250000
C	0.01250000	3.02890000	1.78800000
H	0.78190000	2.42790000	2.27140000
C	-1.97510000	4.35110000	1.81100000
H	-2.81540000	4.80740000	2.33480000
C	-1.03450000	3.58950000	2.50470000
H	-1.10970000	3.43510000	3.58060000
C	-6.09920000	-1.56400000	1.21370000
H	-5.58590000	-1.49740000	2.18620000
H	-7.09530000	-2.00790000	1.37110000
H	-6.24160000	-0.54330000	0.82850000
C	-1.70680000	3.28750000	-2.44230000
H	-2.68320000	3.76430000	-2.22180000
H	-1.52090000	3.36240000	-3.52470000
C	-0.58370000	4.04350000	-1.70400000
H	0.38740000	3.62690000	-1.99940000
H	-0.61100000	5.10250000	-2.00420000
H	1.22840000	2.20590000	-0.12550000
H	2.35700000	-1.45860000	-2.34860000
C	0.09520000	-0.18290000	2.66800000
H	-0.00560000	0.09150000	-2.80070000

H	0.86130000	-0.95990000	-3.99970000
C	2.62040000	2.00620000	-1.58980000
H	1.94400000	1.84820000	-2.44200000
H	2.87870000	3.07200000	-1.50100000
H	3.53320000	1.41920000	-1.75080000
C	0.56260000	-0.83330000	-2.95170000
O	1.36010000	0.07390000	1.98540000
H	-0.02820000	-1.69200000	-2.60340000
H	0.15460000	0.22120000	3.68670000
H	-0.11940000	-1.25830000	2.68320000
H	-0.66980000	0.34250000	2.08920000
H	2.05820000	-0.42170000	2.47290000

Structure **2** - IS

E(S12g/TZ2P)= -11140.09
E(BP86-D3/DZP)= -10887.73

Mn	-1.48100000	0.46580000	-0.18860000
O	0.26170000	-0.09700000	-0.37480000
N	-0.93980000	2.25790000	0.20910000
O	-1.98890000	-1.46480000	-0.53850000
N	1.67570000	-1.95430000	-1.89210000
O	-1.56120000	0.82310000	-2.58130000
C	1.40640000	0.52790000	-0.27390000
C	1.48690000	1.88810000	0.14120000
N	-3.48350000	0.85510000	0.09030000
N	-0.29770000	-3.14570000	0.43700000
C	2.61120000	-0.17380000	-0.55690000
C	0.32070000	2.66890000	0.34720000
H	0.47410000	3.71220000	0.64200000
C	3.83690000	0.43930000	-0.31440000
H	4.74070000	-0.13720000	-0.51810000
C	2.76470000	2.47330000	0.33710000
H	2.78940000	3.51280000	0.66280000
C	2.59460000	-1.53180000	-1.10770000
H	3.45640000	-2.17060000	-0.82660000
C	3.94220000	1.77130000	0.13830000
C	5.32690000	2.37940000	0.35980000
C	-3.13760000	3.20470000	-0.46150000
H	-3.70260000	4.14470000	-0.40780000
H	-2.75540000	3.11860000	-1.49180000
C	0.57240000	-3.97720000	-0.16720000
C	-4.05330000	2.06820000	-0.13830000
C	-1.95970000	3.27670000	0.50240000
H	-1.50460000	4.27400000	0.42880000

H	-2.32010000	3.13790000	1.53600000
C	-5.42580000	2.25770000	-0.00590000
H	-5.84420000	3.24340000	-0.20790000
C	1.52610000	-4.67690000	0.57670000
H	2.22510000	-5.33970000	0.06490000
C	6.09100000	2.40140000	-0.97790000
H	6.21990000	1.38670000	-1.38410000
H	7.09140000	2.84100000	-0.83490000
H	5.54560000	3.00440000	-1.72160000
C	5.24610000	3.81190000	0.89780000
H	4.71860000	3.84900000	1.86390000
H	4.73250000	4.48170000	0.19080000
H	6.26400000	4.20160000	1.05200000
C	-5.64940000	-0.02730000	0.66390000
H	-6.23640000	-0.88130000	0.99910000
C	-6.24280000	1.20210000	0.38890000
H	-7.31850000	1.34210000	0.49390000
C	-4.28140000	-0.16470000	0.50330000
H	-3.77720000	-1.10950000	0.68850000
C	-0.26830000	-3.01130000	1.77500000
H	-1.01210000	-2.33410000	2.19300000
C	1.57600000	-4.51780000	1.95690000
H	2.32030000	-5.05280000	2.54720000
C	0.65410000	-3.67150000	2.57290000
H	0.64860000	-3.52600000	3.65250000
C	6.10420000	1.52170000	1.37590000
H	5.56440000	1.47960000	2.33550000
H	7.10090000	1.95710000	1.55210000
H	6.24500000	0.49230000	1.01380000
C	1.73310000	-3.34550000	-2.29330000
H	2.67610000	-3.84560000	-1.99300000
H	1.63800000	-3.41010000	-3.38850000
C	0.53470000	-4.08080000	-1.66200000
H	-0.39720000	-3.64270000	-2.03940000
H	0.56660000	-5.13830000	-1.96580000
H	-1.24330000	-2.16610000	-0.21700000
H	-1.93390000	1.71690000	-2.73550000
C	-0.24300000	0.21490000	2.78180000
H	0.21730000	-0.15590000	-2.87940000
H	-0.25530000	0.95870000	-4.22570000
C	-2.48230000	-1.87240000	-1.82940000
H	-1.71300000	-1.73420000	-2.60080000
H	-2.79040000	-2.92690000	-1.77820000
H	-3.34930000	-1.24690000	-2.07410000
C	-0.21710000	0.81840000	-3.13550000
O	-1.50140000	-0.13810000	2.15420000

H	0.39530000	1.60580000	-2.66980000
H	-0.22810000	-0.11580000	3.83040000
H	-0.06340000	1.29740000	2.71770000
H	0.53470000	-0.30670000	2.21190000
H	-2.20890000	0.38200000	2.59630000

Structure **2** - HS

E(S12g/TZ2P)= -11148.56
E(BP86-D3/DZP)= -10887.55

Mn	1.52690000	-0.20390000	-0.00500000
O	-0.40580000	0.29800000	0.02030000
N	0.85240000	-2.15720000	0.67200000
O	2.13760000	1.83630000	-0.47010000
N	-1.66470000	2.00200000	-1.84100000
O	1.56530000	-0.71030000	-2.21830000
C	-1.46890000	-0.41990000	-0.10930000
C	-1.53820000	-1.79830000	0.28560000
N	3.63470000	-0.89820000	0.16530000
N	0.27030000	3.37400000	0.53860000
C	-2.66880000	0.15800000	-0.64740000
C	-0.37970000	-2.56590000	0.66200000
H	-0.58870000	-3.61100000	0.94690000
C	-3.86620000	-0.54610000	-0.59610000
H	-4.76270000	-0.04240000	-0.96430000
C	-2.77870000	-2.47560000	0.27300000
H	-2.77730000	-3.51550000	0.60070000
C	-2.66800000	1.50600000	-1.22040000
H	-3.61270000	2.07580000	-1.10310000
C	-3.96070000	-1.87100000	-0.13020000
C	-5.31870000	-2.57070000	-0.11030000
C	2.97170000	-3.26160000	0.00300000
H	3.46920000	-4.23100000	0.14340000
H	2.49250000	-3.30210000	-0.99050000
C	-0.74430000	4.01530000	-0.06920000
C	4.02490000	-2.18680000	0.01880000
C	1.87780000	-3.11920000	1.07030000
H	1.43450000	-4.11000000	1.26450000
H	2.33810000	-2.76090000	2.00650000
C	5.37640000	-2.51550000	-0.10490000
H	5.66560000	-3.56000000	-0.22130000
C	-1.85820000	4.44960000	0.65420000
H	-2.66970000	4.96460000	0.13850000
C	-5.87920000	-2.63960000	-1.54330000
H	-6.01860000	-1.63520000	-1.97110000

H	-6.85760000	-3.14660000	-1.54290000
H	-5.19290000	-3.20120000	-2.19720000
C	-5.21970000	-3.99610000	0.44370000
H	-4.83790000	-4.00070000	1.47670000
H	-4.56310000	-4.62610000	-0.17650000
H	-6.22010000	-4.45550000	0.45020000
C	5.93200000	-0.19130000	0.09800000
H	6.65050000	0.62620000	0.14320000
C	6.34000000	-1.51270000	-0.07200000
H	7.39710000	-1.76130000	-0.16740000
C	4.57530000	0.06970000	0.21250000
H	4.19710000	1.08400000	0.34070000
C	0.21440000	3.16260000	1.86510000
H	1.06890000	2.63870000	2.29140000
C	-1.92530000	4.21020000	2.02200000
H	-2.79360000	4.53320000	2.59720000
C	-0.86280000	3.55550000	2.64540000
H	-0.87050000	3.35160000	3.71570000
C	-6.28690000	-1.76690000	0.77850000
H	-5.89560000	-1.69440000	1.80600000
H	-7.27040000	-2.26290000	0.81140000
H	-6.43590000	-0.74670000	0.39370000
C	-1.76650000	3.38230000	-2.27120000
H	-2.76100000	3.82570000	-2.06220000
H	-1.58610000	3.44040000	-3.35650000
C	-0.66910000	4.19470000	-1.55740000
H	0.31640000	3.86580000	-1.90860000
H	-0.78690000	5.25870000	-1.81730000
H	1.39300000	2.49840000	-0.15140000
H	2.03430000	-1.54520000	-2.43650000
C	0.63400000	0.02710000	3.04450000
H	-0.23610000	0.19830000	-2.58950000
H	0.35640000	-0.86100000	-3.93090000
C	2.48470000	2.16090000	-1.83090000
H	1.63670000	1.97320000	-2.50590000
H	2.79990000	3.21290000	-1.90110000
H	3.31720000	1.51040000	-2.12700000
C	0.24900000	-0.75350000	-2.84300000
O	1.77040000	0.40410000	2.22030000
H	-0.34360000	-1.58340000	-2.42990000
H	0.68840000	0.53280000	4.01870000
H	0.59220000	-1.06290000	3.17600000
H	-0.25290000	0.35560000	2.49100000
H	2.58190000	0.02670000	2.62770000

Structure **3** - LS

E(S12g/TZ2P)= -15580.81
E(BP86-D3/DZP)= -15243.00

Mn	-0.19250000	-0.53750000	0.18000000
O	1.41960000	-0.01950000	-0.69040000
N	-0.17150000	0.89850000	1.41130000
O	0.03690000	-2.29420000	-1.08860000
N	3.38890000	-1.15740000	-2.20510000
O	-1.17340000	0.23070000	-1.31640000
C	2.27980000	0.87040000	-0.30440000
C	1.99220000	1.84030000	0.71440000
N	-1.71600000	-1.44130000	1.09110000
N	2.17620000	-3.87140000	-0.53590000
C	3.61250000	0.84810000	-0.83400000
C	0.79660000	1.80230000	1.48460000
H	0.68100000	2.59980000	2.22820000
C	4.53240000	1.82760000	-0.45050000
H	5.53930000	1.76190000	-0.86780000
C	2.95100000	2.83520000	1.01580000
H	2.67050000	3.57960000	1.76160000
C	4.10920000	-0.24830000	-1.65650000
H	5.21570000	-0.26690000	-1.75060000
C	4.21540000	2.86490000	0.44240000
C	5.26430000	3.92840000	0.76830000
C	-2.59390000	0.68360000	1.94110000
H	-3.33160000	0.99430000	2.69540000
H	-2.79230000	1.26770000	1.02780000
C	3.34490000	-3.95960000	-1.20340000
C	-2.75770000	-0.78000000	1.68520000
C	-1.20370000	1.02370000	2.45400000
H	-1.20730000	2.05160000	2.84790000
H	-0.94190000	0.34730000	3.28800000
C	-3.91500000	-1.44690000	2.07870000
H	-4.73390000	-0.86170000	2.49910000
C	4.50240000	-4.43390000	-0.57820000
H	5.44060000	-4.46740000	-1.13470000
C	5.66400000	4.66030000	-0.52710000
H	6.09380000	3.96510000	-1.26420000
H	6.41730000	5.43530000	-0.31020000
H	4.78380000	5.14270000	-0.98180000
C	4.74070000	4.96510000	1.76840000
H	4.47480000	4.49970000	2.73040000
H	3.85610000	5.49090000	1.37630000
H	5.52330000	5.71510000	1.96140000
C	-2.90810000	-3.51800000	1.45100000

H	-2.90800000	-4.60420000	1.35480000
C	-4.02170000	-2.82880000	1.94630000
H	-4.92820000	-3.35590000	2.24410000
C	-1.79990000	-2.80460000	1.03850000
H	-0.96030000	-3.30600000	0.57020000
C	2.11780000	-4.32890000	0.72710000
H	1.15300000	-4.23320000	1.22370000
C	4.44140000	-4.87620000	0.73900000
H	5.33540000	-5.25050000	1.23900000
C	3.21410000	-4.84930000	1.40040000
H	3.11220000	-5.20560000	2.42530000
C	6.50950000	3.25470000	1.37530000
H	6.24170000	2.71360000	2.29700000
H	7.27030000	4.01340000	1.62130000
H	6.96250000	2.53690000	0.67480000
C	4.08700000	-2.22310000	-2.90060000
H	5.15470000	-2.30560000	-2.61120000
H	4.05030000	-2.02510000	-3.98630000
C	3.36530000	-3.55230000	-2.64890000
H	2.33160000	-3.46950000	-3.00620000
H	3.86480000	-4.34170000	-3.23330000
H	0.90360000	-2.79620000	-0.90550000
C	2.44120000	-1.42380000	1.72340000
C	0.01110000	-2.05250000	-2.50980000
H	0.82150000	-1.35900000	-2.77400000
H	0.12830000	-3.00930000	-3.04350000
H	-0.96020000	-1.60700000	-2.73570000
O	1.01830000	-1.68710000	1.56160000
H	2.85950000	-2.13700000	2.44650000
H	2.60520000	-0.38960000	2.05450000
H	2.88910000	-1.57510000	0.73530000
H	0.59240000	-1.56320000	2.43900000
C	-2.45090000	0.59990000	-1.28490000
C	-3.48200000	-0.36260000	-1.16950000
C	-2.85940000	1.96040000	-1.41360000
C	-4.78370000	0.00170000	-0.83400000
C	-4.17780000	2.29700000	-1.09480000
C	-5.14040000	1.34510000	-0.72090000
H	-5.49530000	-0.79890000	-0.62640000
H	-4.46720000	3.34490000	-1.10670000
C	-6.49570000	1.79390000	-0.17920000
C	-1.86610000	3.00980000	-1.92360000
C	-0.68880000	3.17660000	-0.95590000
C	-1.32220000	2.53250000	-3.28690000
C	-2.52980000	4.37800000	-2.12530000
H	-1.04790000	3.39640000	0.06210000

H	-0.10260000	2.25480000	-0.92230000
H	-0.03610000	4.00130000	-1.28880000
H	-2.14460000	2.42240000	-4.01300000
H	-0.60230000	3.26880000	-3.68200000
H	-0.81270000	1.56510000	-3.16690000
H	-1.78980000	5.07550000	-2.54860000
H	-3.38120000	4.32150000	-2.82240000
H	-2.88280000	4.80330000	-1.17220000
O	-3.12540000	-1.68420000	-1.33440000
C	-7.41390000	0.60600000	0.13000000
C	-7.20640000	2.70770000	-1.19340000
C	-6.25470000	2.56950000	1.13160000
H	-5.72400000	1.93160000	1.85670000
H	-7.21380000	2.88760000	1.57340000
H	-5.63980000	3.46490000	0.95410000
H	-7.37870000	2.16880000	-2.13890000
H	-6.61170000	3.60670000	-1.41290000
H	-8.18020000	3.03520000	-0.79380000
H	-7.62730000	0.01470000	-0.77430000
H	-8.37190000	0.97540000	0.52800000
H	-6.96820000	-0.05870000	0.88660000
H	-3.85260000	-2.23960000	-0.97460000

Structure **3** - IS

E(S12g/TZ2P)= -15594.91
E(BP86-D3/DZP)= -15246.16

Mn	-0.17670000	-0.47440000	0.05310000
O	1.46630000	0.02940000	-0.67620000
N	-0.13150000	0.97150000	1.32210000
O	0.10480000	-2.24000000	-1.05450000
N	3.41700000	-1.14320000	-2.21500000
O	-1.28000000	0.25270000	-1.60420000
C	2.36660000	0.88550000	-0.27700000
C	2.08420000	1.86300000	0.72690000
N	-1.74330000	-1.38620000	1.03470000
N	2.18640000	-3.84940000	-0.50940000
C	3.69830000	0.80860000	-0.78030000
C	0.87320000	1.83570000	1.46200000
H	0.76280000	2.60020000	2.23830000
C	4.64280000	1.76570000	-0.39020000
H	5.65080000	1.67220000	-0.79780000
C	3.06580000	2.83510000	1.04110000
H	2.79180000	3.59650000	1.77130000
C	4.16500000	-0.29700000	-1.60790000

H	5.27100000	-0.37750000	-1.66050000
C	4.33790000	2.82130000	0.48540000
C	5.40540000	3.86930000	0.80190000
C	-2.58130000	0.77570000	1.78810000
H	-3.33710000	1.14870000	2.49300000
H	-2.74720000	1.28800000	0.82580000
C	3.35070000	-3.93520000	-1.18670000
C	-2.75750000	-0.69590000	1.61930000
C	-1.20370000	1.13890000	2.31640000
H	-1.22500000	2.18970000	2.64210000
H	-0.96860000	0.51830000	3.20030000
C	-3.90730000	-1.34170000	2.07210000
H	-4.70900000	-0.74280000	2.50360000
C	4.51350000	-4.40420000	-0.56900000
H	5.44730000	-4.43620000	-1.13270000
C	5.82460000	4.57250000	-0.50350000
H	6.24500000	3.85730000	-1.22660000
H	6.59050000	5.33720000	-0.29490000
H	4.95580000	5.06390000	-0.97040000
C	4.89640000	4.93130000	1.78240000
H	4.61100000	4.48590000	2.74810000
H	4.02790000	5.47160000	1.37440000
H	5.69390000	5.66650000	1.97150000
C	-2.95460000	-3.43360000	1.41860000
H	-2.97910000	-4.51940000	1.32770000
C	-4.02620000	-2.72210000	1.96320000
H	-4.92500000	-3.23440000	2.30710000
C	-1.84980000	-2.73880000	0.96250000
H	-1.02810000	-3.24830000	0.47170000
C	2.13560000	-4.31640000	0.75140000
H	1.17400000	-4.22810000	1.25260000
C	4.46370000	-4.84530000	0.74920000
H	5.36370000	-5.21260000	1.24380000
C	3.24000000	-4.82960000	1.41660000
H	3.14530000	-5.18980000	2.44070000
C	6.63490000	3.18200000	1.42470000
H	6.35350000	2.66040000	2.35350000
H	7.40780000	3.93100000	1.66220000
H	7.07810000	2.44610000	0.73700000
C	4.08800000	-2.22410000	-2.91350000
H	5.16020000	-2.31500000	-2.64370000
H	4.03110000	-2.03360000	-3.99930000
C	3.35880000	-3.54360000	-2.63660000
H	2.32380000	-3.46390000	-2.98840000
H	3.84990000	-4.34310000	-3.21450000
H	0.95640000	-2.77910000	-0.84530000

C	2.50070000	-1.44850000	1.89890000
C	0.05060000	-2.11950000	-2.49540000
H	0.87800000	-1.47800000	-2.82920000
H	0.12740000	-3.12300000	-2.94060000
H	-0.91050000	-1.65680000	-2.72950000
O	1.11390000	-1.84480000	1.80040000
H	3.03130000	-2.06030000	2.64610000
H	2.59100000	-0.38090000	2.14750000
H	2.93980000	-1.61480000	0.90660000
H	0.64740000	-1.48820000	2.58640000
C	-2.54130000	0.61180000	-1.48830000
C	-3.55230000	-0.36960000	-1.30490000
C	-2.98360000	1.97260000	-1.52210000
C	-4.83990000	-0.04130000	-0.89750000
C	-4.29190000	2.27240000	-1.12550000
C	-5.22420000	1.29430000	-0.74510000
H	-5.52370000	-0.85970000	-0.66510000
H	-4.59560000	3.31570000	-1.07730000
C	-6.57240000	1.70120000	-0.15290000
C	-2.00910000	3.07010000	-1.96310000
C	-0.83630000	3.18730000	-0.97650000
C	-1.45090000	2.70660000	-3.35370000
C	-2.69190000	4.44040000	-2.06560000
H	-1.20490000	3.34710000	0.04950000
H	-0.24000000	2.26980000	-0.98760000
H	-0.18940000	4.03670000	-1.25530000
H	-2.26690000	2.65210000	-4.09350000
H	-0.73060000	3.47400000	-3.68400000
H	-0.94070000	1.73400000	-3.30350000
H	-1.96500000	5.17690000	-2.44360000
H	-3.54730000	4.41900000	-2.76000000
H	-3.04530000	4.79380000	-1.08370000
O	-3.15700000	-1.68650000	-1.47600000
C	-7.44640000	0.48530000	0.17680000
C	-7.34250000	2.59940000	-1.13800000
C	-6.31970000	2.47700000	1.15530000
H	-5.75660000	1.84930000	1.86450000
H	-7.27490000	2.76970000	1.62290000
H	-5.73110000	3.38800000	0.96850000
H	-7.53010000	2.06000000	-2.08050000
H	-6.77810000	3.51430000	-1.37260000
H	-8.31170000	2.89940000	-0.70630000
H	-7.67170000	-0.10640000	-0.72450000
H	-8.40130000	0.82400000	0.60850000
H	-6.95740000	-0.17180000	0.91310000
H	-3.86760000	-2.26120000	-1.11490000

Structure **3** - HS

E(S12g/TZ2P)= -15609.04
E(BP86-D3/DZP)= -15252.56

Mn	-0.25420000	-0.35670000	-0.33880000
O	1.63490000	0.13210000	-0.94150000
N	0.06680000	1.16880000	1.24300000
O	0.03690000	-2.36110000	-1.32720000
N	3.63430000	-1.28660000	-2.19910000
O	-1.28130000	0.47430000	-1.90610000
C	2.54000000	0.90920000	-0.47670000
C	2.28160000	1.93350000	0.50240000
N	-1.94090000	-1.14500000	0.95040000
N	2.07990000	-3.97000000	-0.46990000
C	3.91770000	0.74360000	-0.87180000
C	1.07100000	1.98760000	1.28370000
H	1.06370000	2.78730000	2.04550000
C	4.87720000	1.67110000	-0.46660000
H	5.90330000	1.50940000	-0.80510000
C	3.29180000	2.85800000	0.84110000
H	3.02650000	3.64040000	1.55330000
C	4.38000000	-0.43570000	-1.59320000
H	5.48120000	-0.57620000	-1.55440000
C	4.58880000	2.77920000	0.34330000
C	5.68910000	3.78830000	0.67120000
C	-2.36880000	1.08510000	1.84420000
H	-3.04950000	1.55910000	2.56500000
H	-2.53360000	1.58380000	0.87440000
C	3.32900000	-3.98130000	-0.97830000
C	-2.75210000	-0.35600000	1.69050000
C	-0.93050000	1.33010000	2.30820000
H	-0.86370000	2.34090000	2.74770000
H	-0.68510000	0.61020000	3.10970000
C	-3.91940000	-0.85970000	2.26850000
H	-4.54370000	-0.20720000	2.87750000
C	4.43700000	-4.27850000	-0.17870000
H	5.43870000	-4.25640000	-0.61080000
C	6.19290000	4.42460000	-0.63880000
H	6.60680000	3.66470000	-1.31920000
H	6.98620000	5.15920000	-0.42460000
H	5.36860000	4.93940000	-1.15820000
C	5.18480000	4.90410000	1.59230000
H	4.84360000	4.50520000	2.56050000
H	4.35650000	5.46370000	1.13000000

H	6.00320000	5.61360000	1.78920000
C	-3.44570000	-2.99020000	1.27760000
H	-3.68590000	-4.03530000	1.08220000
C	-4.27970000	-2.18420000	2.05120000
H	-5.19780000	-2.58520000	2.48220000
C	-2.28200000	-2.43570000	0.76180000
H	-1.59520000	-3.01090000	0.14180000
C	1.90130000	-4.33210000	0.81360000
H	0.87510000	-4.30360000	1.17610000
C	4.24680000	-4.62370000	1.15530000
H	5.10050000	-4.85960000	1.79180000
C	2.94760000	-4.67840000	1.65780000
H	2.74930000	-4.96350000	2.69090000
C	6.86150000	3.07240000	1.36850000
H	6.52040000	2.59390000	2.30060000
H	7.65420000	3.79730000	1.61500000
H	7.30340000	2.29730000	0.72450000
C	4.29730000	-2.44740000	-2.76630000
H	5.34400000	-2.56130000	-2.41680000
H	4.32430000	-2.33880000	-3.86440000
C	3.48770000	-3.70920000	-2.44800000
H	2.49110000	-3.62370000	-2.89690000
H	3.99080000	-4.57370000	-2.91260000
H	0.82990000	-2.91500000	-1.01530000
C	2.25300000	-1.38160000	1.74310000
C	0.20440000	-2.15520000	-2.74790000
H	1.14820000	-1.61870000	-2.92750000
H	0.20100000	-3.12070000	-3.27950000
H	-0.64520000	-1.54380000	-3.07060000
O	0.88660000	-1.72970000	1.43440000
H	2.64630000	-2.01300000	2.55510000
H	2.34100000	-0.31940000	2.01590000
H	2.82620000	-1.56290000	0.82430000
H	0.33510000	-1.51190000	2.21630000
C	-2.56440000	0.70850000	-1.65470000
C	-3.47190000	-0.37790000	-1.54740000
C	-3.10920000	2.01550000	-1.47340000
C	-4.75240000	-0.22820000	-1.02980000
C	-4.41270000	2.13710000	-0.97660000
C	-5.23280000	1.03870000	-0.68290000
H	-5.34960000	-1.12800000	-0.87180000
H	-4.80270000	3.13280000	-0.77970000
C	-6.59340000	1.25700000	-0.02140000
C	-2.26840000	3.25000000	-1.82400000
C	-1.02600000	3.35880000	-0.92420000
C	-1.80600000	3.12740000	-3.28940000

C	-3.06950000	4.55090000	-1.68210000
H	-1.31510000	3.42810000	0.13610000
H	-0.38190000	2.48200000	-1.05230000
H	-0.45280000	4.26490000	-1.18480000
H	-2.67700000	3.08410000	-3.96410000
H	-1.19090000	3.99940000	-3.56760000
H	-1.20870000	2.21320000	-3.41440000
H	-2.43820000	5.39790000	-1.99460000
H	-3.97030000	4.54630000	-2.31630000
H	-3.37520000	4.72890000	-0.63880000
O	-2.97480000	-1.61460000	-1.92560000
C	-7.28690000	-0.06810000	0.31570000
C	-7.50830000	2.06310000	-0.96230000
C	-6.39980000	2.04350000	1.28980000
H	-5.72390000	1.49710000	1.96460000
H	-7.36790000	2.18550000	1.79830000
H	-5.96120000	3.03510000	1.10370000
H	-7.65860000	1.51770000	-1.90800000
H	-7.06970000	3.04480000	-1.19730000
H	-8.49230000	2.23020000	-0.49280000
H	-7.50050000	-0.65570000	-0.59080000
H	-8.24490000	0.13360000	0.82020000
H	-6.66680000	-0.67940000	0.99010000
H	-3.64040000	-2.29130000	-1.67170000

Structure **4** - LS

E(S12g/TZ2P)= -15564.30
E(BP86-D3/DZP)= -15225.20

Mn	-0.13880000	0.48820000	-0.24040000
O	1.49560000	-0.14020000	0.51270000
N	-0.24740000	-0.89160000	-1.52460000
O	0.37460000	2.20750000	1.01540000
N	3.58100000	0.72690000	2.07170000
O	-1.07370000	-0.23740000	1.25180000
C	2.24490000	-1.12280000	0.12450000
C	1.83750000	-2.05390000	-0.89390000
N	-1.66490000	1.52520000	-1.04620000
N	2.72220000	3.53930000	0.47810000
C	3.56970000	-1.26130000	0.65300000
C	0.64720000	-1.87450000	-1.64480000
H	0.44520000	-2.63860000	-2.40560000
C	4.36570000	-2.35300000	0.27970000
H	5.36680000	-2.41780000	0.71050000
C	2.67330000	-3.15770000	-1.19340000

H	2.30580000	-3.86600000	-1.93670000
C	4.18700000	-0.24900000	1.49850000
H	5.28720000	-0.36960000	1.60160000
C	3.92390000	-3.34100000	-0.61490000
C	4.82630000	-4.53790000	-0.91880000
C	-2.64960000	-0.48370000	-2.02180000
H	-3.42210000	-0.74300000	-2.76030000
H	-2.86790000	-1.04050000	-1.09430000
C	3.89110000	3.51290000	1.14990000
C	-2.70660000	0.97940000	-1.74490000
C	-1.29280000	-0.91170000	-2.55770000
H	-1.37780000	-1.92810000	-2.97410000
H	-0.99210000	-0.24080000	-3.38550000
C	-3.76120000	1.75350000	-2.22090000
H	-4.57030000	1.25950000	-2.75930000
C	5.09300000	3.87630000	0.53370000
H	6.02710000	3.81950000	1.09550000
C	5.08480000	-5.31890000	0.38400000
H	5.58380000	-4.68840000	1.13560000
H	5.72970000	-6.19100000	0.18610000
H	4.13350000	-5.67510000	0.81110000
C	4.19680000	-5.49440000	-1.93760000
H	4.01580000	-4.99390000	-2.90170000
H	3.24170000	-5.90130000	-1.57000000
H	4.87890000	-6.33990000	-2.11720000
C	-2.71310000	3.69280000	-1.31010000
H	-2.66970000	4.76250000	-1.10120000
C	-3.78620000	3.12870000	-2.00330000
H	-4.61050000	3.74170000	-2.36960000
C	-1.70090000	2.87280000	-0.84090000
H	-0.88560000	3.26410000	-0.24080000
C	2.71550000	4.00070000	-0.78470000
H	1.74490000	3.99870000	-1.28070000
C	5.08190000	4.32210000	-0.78410000
H	6.01060000	4.60980000	-1.27840000
C	3.86180000	4.40910000	-1.45380000
H	3.80060000	4.77320000	-2.47940000
C	6.17120000	-4.04450000	-1.48550000
H	6.00870000	-3.47130000	-2.41250000
H	6.82590000	-4.90170000	-1.71310000
H	6.69870000	-3.39750000	-0.76880000
C	4.40100000	1.66890000	2.80940000
H	5.47520000	1.62150000	2.53360000
H	4.32360000	1.44570000	3.88850000
C	3.86270000	3.08900000	2.58980000
H	2.82560000	3.13220000	2.94570000

H	4.46200000	3.79390000	3.18770000
H	1.30130000	2.56210000	0.82090000
C	2.40190000	1.17170000	-1.98680000
C	0.33030000	1.94330000	2.43180000
H	1.02910000	1.12900000	2.66750000
H	0.60450000	2.85910000	2.98250000
H	-0.70820000	1.66260000	2.63380000
O	1.06520000	1.63920000	-1.65920000
H	2.85180000	1.83920000	-2.73510000
H	2.36740000	0.13730000	-2.35530000
H	2.97020000	1.21180000	-1.05110000
H	0.53450000	1.62620000	-2.48660000
C	-2.41710000	-0.32840000	1.25660000
C	-3.20780000	0.89060000	1.33160000
C	-3.07710000	-1.58560000	1.26330000
C	-4.57350000	0.76030000	0.93690000
C	-4.45020000	-1.63520000	0.97180000
C	-5.18930000	-0.46610000	0.70900000
H	-5.09380000	1.70470000	0.76800000
H	-4.94680000	-2.59940000	0.90190000
C	-6.59950000	-0.58590000	0.12740000
C	-2.30370000	-2.86960000	1.60080000
C	-1.26400000	-3.18970000	0.52140000
C	-1.56560000	-2.66570000	2.93950000
C	-3.22930000	-4.08500000	1.75280000
H	-1.73360000	-3.23090000	-0.47500000
H	-0.49930000	-2.40960000	0.50640000
H	-0.77960000	-4.16020000	0.72770000
H	-2.28710000	-2.46430000	3.74920000
H	-0.99140000	-3.57190000	3.19930000
H	-0.87500000	-1.81450000	2.84820000
H	-2.63000000	-4.95680000	2.06190000
H	-4.00560000	-3.91440000	2.51610000
H	-3.72500000	-4.34010000	0.80250000
O	-2.70180000	2.03270000	1.66660000
C	-7.25880000	0.78110000	-0.08620000
C	-7.50190000	-1.42150000	1.05280000
C	-6.49730000	-1.28220000	-1.24500000
H	-5.83480000	-0.70430000	-1.90840000
H	-7.49220000	-1.36370000	-1.71660000
H	-6.07170000	-2.29200000	-1.14340000
H	-7.58690000	-0.93930000	2.04040000
H	-7.09790000	-2.43420000	1.19950000
H	-8.51320000	-1.51720000	0.62210000
H	-7.36710000	1.32800000	0.86370000
H	-8.26270000	0.64550000	-0.52020000

H -6.66640000 1.40150000 -0.77700000

Structure **4** - IS

E(S12g/TZ2P)= -16468.11
E(BP86-D3/DZP)= -15227.64

Mn -0.27930000 -0.37030000 0.17400000
O 1.35290000 0.20390000 -0.51640000
N -0.22270000 0.98220000 1.59540000
O 0.42930000 -2.39590000 -0.76150000
N 3.30810000 -0.67140000 -2.31110000
O -1.22160000 0.01210000 -1.53380000
C 2.21290000 1.10080000 -0.10930000
C 1.90510000 2.02960000 0.94080000
N -1.87690000 -1.34550000 1.05390000
N 3.03310000 -3.33690000 -0.33210000
C 3.51900000 1.14260000 -0.67620000
C 0.71710000 1.92780000 1.70030000
H 0.56650000 2.69770000 2.46720000
C 4.42590000 2.13640000 -0.27610000
H 5.41690000 2.12560000 -0.73220000
C 2.84190000 3.04920000 1.25240000
H 2.54930000 3.76850000 2.01760000
C 4.01300000 0.15160000 -1.62310000
H 5.11980000 0.15280000 -1.71980000
C 4.09210000 3.13250000 0.65650000
C 5.10040000 4.23870000 0.97160000
C -2.65490000 0.72640000 2.06070000
H -3.42090000 1.06960000 2.77010000
H -2.81590000 1.25390000 1.10360000
C 4.06510000 -3.25000000 -1.19610000
C -2.82870000 -0.73100000 1.81150000
C -1.27850000 1.07210000 2.60770000
H -1.31080000 2.09830000 3.00810000
H -1.03570000 0.39730000 3.45090000
C -3.91320000 -1.42890000 2.32640000
H -4.63600000 -0.90240000 2.94810000
C 5.39210000 -3.32550000 -0.76130000
H 6.20370000 -3.22880000 -1.48440000
C 5.38770000 5.03960000 -0.31340000
H 5.81260000 4.39600000 -1.09870000
H 6.10800000 5.84840000 -0.10670000
H 4.45840000 5.48740000 -0.70110000
C 4.57960000 5.21030000 2.03660000
H 4.37890000 4.69430000 2.98870000

H	3.65510000	5.71010000	1.70790000
H	5.33640000	5.98760000	2.22500000
C	-3.13240000	-3.39440000	1.21210000
H	-3.21880000	-4.44300000	0.92800000
C	-4.08730000	-2.77660000	2.00800000
H	-4.95050000	-3.32910000	2.38150000
C	-2.04100000	-2.65990000	0.75920000
H	-1.24940000	-3.10270000	0.16450000
C	3.30220000	-3.57560000	0.96390000
H	2.43210000	-3.64960000	1.61560000
C	5.66120000	-3.53600000	0.58710000
H	6.69040000	-3.59570000	0.94360000
C	4.59160000	-3.68340000	1.46910000
H	4.75200000	-3.86990000	2.53090000
C	6.41340000	3.61720000	1.48260000
H	6.22750000	3.02630000	2.39360000
H	7.14230000	4.40960000	1.71910000
H	6.86630000	2.95490000	0.73000000
C	4.05550000	-1.61860000	-3.11780000
H	5.15220000	-1.44700000	-3.07670000
H	3.73610000	-1.52930000	-4.16980000
C	3.74550000	-3.05000000	-2.64860000
H	2.68310000	-3.26490000	-2.80840000
H	4.33540000	-3.75400000	-3.25690000
H	1.39670000	-2.61260000	-0.58150000
C	2.20890000	-1.06250000	2.44220000
C	0.25420000	-2.39420000	-2.19500000
H	0.87170000	-1.59740000	-2.63470000
H	0.53800000	-3.37700000	-2.61050000
H	-0.81400000	-2.19420000	-2.35180000
O	1.04400000	-1.80420000	2.01920000
H	2.76570000	-1.60850000	3.22210000
H	1.93420000	-0.06200000	2.80420000
H	2.84280000	-0.94510000	1.55360000
H	0.34260000	-1.65690000	2.68860000
C	-2.54870000	0.16450000	-1.42370000
C	-3.37940000	-1.02880000	-1.40450000
C	-3.16200000	1.44480000	-1.36220000
C	-4.71680000	-0.86330000	-0.95360000
C	-4.50850000	1.52850000	-0.96910000
C	-5.27540000	0.38600000	-0.68200000
H	-5.26520000	-1.78970000	-0.77160000
H	-4.96740000	2.50720000	-0.85280000
C	-6.66610000	0.55780000	-0.06540000
C	-2.37190000	2.70860000	-1.74200000
C	-1.24310000	3.01250000	-0.74440000

C	-1.73920000	2.49810000	-3.13210000
C	-3.27560000	3.94820000	-1.81900000
H	-1.62880000	3.07310000	0.28490000
H	-0.47880000	2.22920000	-0.77760000
H	-0.76620000	3.97570000	-0.99700000
H	-2.52200000	2.31760000	-3.88770000
H	-1.16510000	3.39260000	-3.42930000
H	-1.06350000	1.63130000	-3.09460000
H	-2.68080000	4.80780000	-2.16830000
H	-4.11010000	3.80010000	-2.52300000
H	-3.69320000	4.20920000	-0.83340000
O	-2.89060000	-2.19760000	-1.70390000
C	-7.33130000	-0.78750000	0.24660000
C	-7.58190000	1.34580000	-1.02000000
C	-6.53190000	1.33720000	1.25840000
H	-5.86120000	0.79810000	1.94420000
H	-7.51740000	1.45420000	1.74180000
H	-6.10510000	2.33740000	1.09050000
H	-7.69360000	0.80550000	-1.97430000
H	-7.16730000	2.34190000	-1.23660000
H	-8.58280000	1.48050000	-0.57500000
H	-7.48780000	-1.38140000	-0.66750000
H	-8.31420000	-0.61650000	0.71470000
H	-6.71450000	-1.37820000	0.94190000

Structure **4** - HS

E(S12g/TZ2P)= -15564.64
E(BP86-D3/DZP)= -15208.03

Mn	-0.14210000	-0.12220000	-0.25760000
O	1.60400000	0.55710000	-1.02710000
N	0.00210000	1.51880000	1.15080000
O	0.14740000	-2.08930000	-1.27740000
N	3.53390000	-0.99340000	-2.33680000
O	-1.39780000	0.66730000	-1.85530000
C	2.58040000	1.18260000	-0.44790000
C	2.34900000	2.13810000	0.61380000
N	-1.88760000	-0.90310000	0.96130000
N	2.25850000	-3.62600000	-0.58560000
C	3.93930000	0.90140000	-0.80600000
C	1.10790000	2.24640000	1.29820000
H	1.10310000	3.00660000	2.09970000
C	4.99120000	1.69700000	-0.26530000
H	6.01000000	1.46870000	-0.58470000
C	3.44550000	2.94390000	1.06660000

H	3.22200000	3.70480000	1.81510000
C	4.30630000	-0.23000000	-1.62080000
H	5.39770000	-0.44610000	-1.59190000
C	4.75400000	2.74580000	0.63020000
C	5.92730000	3.61190000	1.09980000
C	-2.42320000	1.34100000	1.75810000
H	-3.14330000	1.81960000	2.43780000
H	-2.62140000	1.73580000	0.74960000
C	3.40830000	-3.81890000	-1.27100000
C	-2.69370000	-0.13290000	1.73050000
C	-1.01010000	1.75340000	2.17820000
H	-1.04510000	2.82710000	2.44380000
H	-0.74540000	1.20530000	3.10730000
C	-3.76560000	-0.68750000	2.43210000
H	-4.39130000	-0.04710000	3.05360000
C	4.53630000	-4.36880000	-0.65830000
H	5.45430000	-4.49270000	-1.23600000
C	6.58100000	4.29310000	-0.11800000
H	6.96600000	3.54920000	-0.83160000
H	7.42280000	4.93020000	0.20160000
H	5.84530000	4.92310000	-0.64410000
C	5.48770000	4.70670000	2.07870000
H	5.04430000	4.27660000	2.99030000
H	4.75120000	5.38370000	1.61800000
H	6.36190000	5.30710000	2.37640000
C	-3.21180000	-2.83210000	1.51140000
H	-3.39070000	-3.90000000	1.38330000
C	-4.03830000	-2.04810000	2.31800000
H	-4.88340000	-2.48910000	2.84790000
C	-2.14570000	-2.22410000	0.86500000
H	-1.47570000	-2.77550000	0.20640000
C	2.19710000	-4.04160000	0.69740000
H	1.25200000	-3.85280000	1.20580000
C	4.47620000	-4.76800000	0.67680000
H	5.34920000	-5.19900000	1.16800000
C	3.26830000	-4.61620000	1.36370000
H	3.16310000	-4.92870000	2.40300000
C	6.97650000	2.73060000	1.80440000
H	6.52740000	2.22810000	2.67600000
H	7.82430000	3.34580000	2.15000000
H	7.36940000	1.95790000	1.12690000
C	4.18900000	-2.10950000	-2.98350000
H	5.25040000	-2.23050000	-2.67200000
H	4.18370000	-1.95610000	-4.07860000
C	3.43810000	-3.42680000	-2.71720000
H	2.40880000	-3.33410000	-3.08340000

H	3.93090000	-4.22640000	-3.29390000
H	0.99430000	-2.60460000	-1.02380000
C	2.35950000	-1.12740000	1.68300000
C	0.20200000	-1.88360000	-2.70670000
H	1.09710000	-1.29140000	-2.95050000
H	0.22770000	-2.85340000	-3.23150000
H	-0.71550000	-1.34630000	-2.96830000
O	0.95540000	-1.43180000	1.49150000
H	2.79880000	-1.79360000	2.44250000
H	2.49820000	-0.07400000	1.96460000
H	2.84430000	-1.29980000	0.71380000
H	0.46960000	-1.08770000	2.27250000
C	-2.67450000	0.69870000	-1.69820000
C	-3.41880000	-0.58330000	-1.56610000
C	-3.41880000	1.92960000	-1.62020000
C	-4.72800000	-0.53440000	-0.98930000
C	-4.71420000	1.87210000	-1.13350000
C	-5.36580000	0.65920000	-0.74300000
H	-5.17530000	-1.49940000	-0.75050000
H	-5.26480000	2.80070000	-1.00210000
C	-6.73640000	0.74600000	-0.07730000
C	-2.74620000	3.25430000	-1.99580000
C	-1.64450000	3.60930000	-0.97880000
C	-2.11970000	3.12610000	-3.39870000
C	-3.75390000	4.41080000	-2.03520000
H	-2.08190000	3.78510000	0.01740000
H	-0.90620000	2.80240000	-0.89000000
H	-1.13390000	4.53490000	-1.29590000
H	-2.89400000	2.87410000	-4.14230000
H	-1.65530000	4.08230000	-3.69060000
H	-1.35290000	2.34030000	-3.40250000
H	-3.23870000	5.32770000	-2.36270000
H	-4.57390000	4.20810000	-2.74320000
H	-4.18770000	4.61090000	-1.04300000
O	-2.87410000	-1.67340000	-1.92560000
C	-7.24230000	-0.63120000	0.36670000
C	-7.75340000	1.35110000	-1.06300000
C	-6.63220000	1.64550000	1.17020000
H	-5.87950000	1.24420000	1.86530000
H	-7.60510000	1.68830000	1.68710000
H	-6.34070000	2.67340000	0.90770000
H	-7.83800000	0.71920000	-1.96190000
H	-7.45610000	2.36280000	-1.37920000
H	-8.74600000	1.42100000	-0.58830000
H	-7.37810000	-1.30760000	-0.49110000
H	-8.21620000	-0.52040000	0.86870000

H -6.54060000 -1.09940000 1.07410000

Structure **5** - LS

E(S12g/TZ2P)= -11185.35
E(BP86-D3/DZP)= -10946.10

Mn 1.60860000 0.44010000 -0.04040000
O -0.17750000 -0.19340000 0.28440000
N 1.02620000 2.17690000 -0.35420000
O 2.04510000 -1.66700000 0.24380000
N -1.50680000 -2.01670000 1.94990000
O 1.78610000 0.69410000 2.05220000
C -1.30210000 0.44830000 0.27550000
C -1.40120000 1.82430000 -0.13600000
N 3.47180000 0.78130000 -0.21240000
N 0.02010000 -3.18820000 -0.62100000
C -2.51000000 -0.21230000 0.67050000
C -0.23950000 2.60960000 -0.39310000
H -0.40620000 3.65840000 -0.66730000
C -3.74970000 0.40930000 0.47530000
H -4.64600000 -0.15220000 0.74740000
C -2.68210000 2.41010000 -0.27200000
H -2.71700000 3.44770000 -0.60750000
C -2.48880000 -1.53890000 1.26820000
H -3.41280000 -2.13700000 1.11460000
C -3.86550000 1.72180000 -0.00760000
C -5.25330000 2.34010000 -0.19060000
C 3.17170000 3.16210000 0.34670000
H 3.76530000 4.08490000 0.26330000
H 2.72280000 3.17560000 1.35850000
C -0.84860000 -3.98590000 0.02850000
C 4.08030000 1.98410000 0.13830000
C 2.03180000 3.20710000 -0.66350000
H 1.57590000 4.20940000 -0.64770000
H 2.43140000 3.02540000 -1.67700000
C 5.45730000 2.11770000 0.24050000
H 5.86170000 3.08150000 0.55770000
C -1.98060000 -4.49950000 -0.61120000
H -2.67030000 -5.13840000 -0.05740000
C -5.96980000 2.41540000 1.17160000
H -6.08790000 1.41570000 1.61650000
H -6.97290000 2.85790000 1.05350000
H -5.39240000 3.03860000 1.87370000
C -5.18480000 3.75510000 -0.77680000
H -4.69250000 3.75730000 -1.76200000

H	-4.63970000	4.44290000	-0.11180000
H	-6.20520000	4.14880000	-0.90550000
C	5.71780000	-0.10950000	-0.57740000
H	6.32140000	-0.95610000	-0.90980000
C	6.31820000	1.06150000	-0.08810000
H	7.39980000	1.16380000	-0.01000000
C	4.34310000	-0.20990000	-0.64150000
H	3.85920000	-1.12410000	-0.97860000
C	-0.20330000	-2.90070000	-1.91450000
H	0.54860000	-2.26910000	-2.38490000
C	-2.22140000	-4.17840000	-1.94290000
H	-3.10430000	-4.56420000	-2.45390000
C	-1.30990000	-3.36150000	-2.61370000
H	-1.45260000	-3.09150000	-3.65990000
C	-6.08370000	1.46310000	-1.14700000
H	-5.58140000	1.38340000	-2.12430000
H	-7.08330000	1.90290000	-1.29850000
H	-6.21640000	0.44700000	-0.74650000
C	-1.61180000	-3.40770000	2.33630000
H	-2.63270000	-3.82110000	2.19050000
H	-1.33970000	-3.52400000	3.39770000
C	-0.61220000	-4.22740000	1.48910000
H	0.41120000	-3.92420000	1.74280000
H	-0.72940000	-5.29590000	1.72900000
H	1.20940000	-2.21590000	0.00790000
H	2.34630000	1.48260000	2.21800000
C	0.33670000	0.32590000	-2.78920000
H	-0.00150000	-0.07730000	2.68750000
H	0.81970000	1.01710000	3.87990000
C	2.46900000	-2.07930000	1.55050000
H	1.68280000	-1.88300000	2.29500000
H	2.72560000	-3.15130000	1.54740000
H	3.35820000	-1.49000000	1.80730000
C	0.55920000	0.85490000	2.82490000
O	1.49900000	-0.13840000	-2.04070000
H	-0.03010000	1.69530000	2.43060000
H	0.35390000	-0.11830000	-3.79410000
H	0.32790000	1.42160000	-2.84250000
H	-0.53500000	-0.02150000	-2.22520000
H	2.29940000	0.22080000	-2.48910000

Structure **5** - IS

E(S12g/TZ2P)= -11206.69
E(BP86-D3/DZP)= -10955.48

Mn	-1.56820000	0.44830000	-0.04210000
O	0.18940000	-0.11780000	-0.36850000
N	-1.01950000	2.21410000	0.34750000
O	-2.01720000	-1.53820000	-0.39040000
N	1.57850000	-1.92350000	-2.01260000
O	-1.69040000	0.88240000	-2.55100000
C	1.32780000	0.51730000	-0.29390000
C	1.41320000	1.88120000	0.14260000
N	-3.46540000	0.78820000	0.19060000
N	-0.13530000	-3.17490000	0.45600000
C	2.52920000	-0.15160000	-0.65700000
C	0.25130000	2.65280000	0.39730000
H	0.40370000	3.70660000	0.65660000
C	3.76990000	0.46630000	-0.45520000
H	4.66760000	-0.09820000	-0.71250000
C	2.69820000	2.47090000	0.28460000
H	2.73010000	3.50510000	0.62890000
C	2.51140000	-1.48920000	-1.24630000
H	3.39780000	-2.11800000	-1.01590000
C	3.87750000	1.78660000	0.01830000
C	5.26320000	2.41330000	0.18610000
C	-3.18670000	3.16080000	-0.38350000
H	-3.77970000	4.08490000	-0.31870000
H	-2.74520000	3.14200000	-1.39730000
C	0.72610000	-3.97020000	-0.20500000
C	-4.08690000	1.98870000	-0.13490000
C	-2.04210000	3.22830000	0.62570000
H	-1.59200000	4.23170000	0.58590000
H	-2.44660000	3.07260000	1.64150000
C	-5.46440000	2.12140000	-0.14030000
H	-5.88850000	3.08620000	-0.42600000
C	1.79030000	-4.58960000	0.45710000
H	2.47890000	-5.22310000	-0.10360000
C	5.96400000	2.47860000	-1.18490000
H	6.08700000	1.47530000	-1.62010000
H	6.96380000	2.93160000	-1.08170000
H	5.37360000	3.08850000	-1.88790000
C	5.19170000	3.83350000	0.75850000
H	4.71030000	3.84310000	1.74900000
H	4.63450000	4.51040000	0.09220000
H	6.21080000	4.23500000	0.87160000
C	-5.66960000	-0.10940000	0.70240000
H	-6.24830000	-0.95250000	1.08310000
C	-6.30360000	1.06260000	0.24720000
H	-7.38780000	1.16510000	0.24400000
C	-4.29690000	-0.21140000	0.67460000

H	-3.79050000	-1.11800000	0.99610000
C	0.01970000	-2.99490000	1.77920000
H	-0.72100000	-2.35090000	2.25220000
C	1.96360000	-4.38320000	1.82100000
H	2.79370000	-4.85290000	2.34980000
C	1.05620000	-3.57070000	2.50070000
H	1.14900000	-3.38760000	3.57100000
C	6.10610000	1.54870000	1.14260000
H	5.61510000	1.47680000	2.12640000
H	7.10460000	1.99540000	1.27930000
H	6.24100000	0.52960000	0.75080000
C	1.66290000	-3.30940000	-2.42480000
H	2.65070000	-3.76740000	-2.20850000
H	1.47590000	-3.38330000	-3.50770000
C	0.56290000	-4.10330000	-1.68930000
H	-0.42080000	-3.71700000	-1.98390000
H	0.62470000	-5.16140000	-1.98780000
H	-1.22580000	-2.17270000	-0.15020000
H	-2.01840000	1.80560000	-2.51720000
C	-0.19830000	0.23290000	2.85940000
H	0.09950000	-0.06020000	-2.88640000
H	-0.34690000	1.16000000	-4.15140000
C	-2.49840000	-1.89380000	-1.69760000
H	-1.72770000	-1.70190000	-2.45750000
H	-2.79190000	-2.95500000	-1.70990000
H	-3.37220000	-1.26470000	-1.90680000
C	-0.33840000	0.92870000	-3.07430000
O	-1.46430000	-0.24870000	2.34700000
H	0.26370000	1.67290000	-2.53020000
H	-0.07290000	-0.04680000	3.91690000
H	-0.11400000	1.32150000	2.73460000
H	0.57720000	-0.24340000	2.24680000
H	-2.17400000	0.30590000	2.74020000

Structure **5** - HS

E(S12g/TZ2P)= -11203.88
E(BP86-D3/DZP)= -10947.05

Mn	-1.47880000	0.49950000	-0.65790000
O	0.31220000	0.25940000	-1.50240000
N	-0.93410000	2.51720000	-0.29470000
O	-2.04000000	-1.54670000	-1.26770000
N	1.53620000	-2.24440000	-1.67580000
O	-2.46880000	1.12260000	-2.66720000
C	1.41560000	0.68140000	-0.94800000

C	1.49520000	1.98500000	-0.32700000
N	-3.42910000	0.69180000	0.29230000
N	-0.95210000	-3.27100000	0.46920000
C	2.56420000	-0.16220000	-0.86800000
C	0.35580000	2.78820000	-0.05630000
H	0.58150000	3.73050000	0.46860000
C	3.78460000	0.34590000	-0.35610000
H	4.63990000	-0.33110000	-0.32690000
C	2.76460000	2.44680000	0.13640000
H	2.79670000	3.45250000	0.55640000
C	2.51100000	-1.58280000	-1.14590000
H	3.42000000	-2.12510000	-0.80780000
C	3.90970000	1.65880000	0.11440000
C	5.26930000	2.15640000	0.60950000
C	-3.32320000	3.12140000	0.11740000
H	-3.93480000	3.96990000	0.45650000
H	-3.55620000	2.95600000	-0.94640000
C	0.12510000	-4.04650000	0.22820000
C	-3.68680000	1.89650000	0.89950000
C	-1.84990000	3.51590000	0.25360000
H	-1.71160000	4.48130000	-0.26440000
H	-1.64590000	3.68730000	1.33080000
C	-4.21320000	1.97720000	2.18020000
H	-4.39190000	2.96010000	2.62030000
C	0.91670000	-4.52910000	1.27450000
H	1.79640000	-5.13420000	1.04960000
C	6.29460000	2.06520000	-0.53640000
H	6.41240000	1.02830000	-0.88540000
H	7.27980000	2.42750000	-0.19900000
H	5.96910000	2.68010000	-1.39140000
C	5.21510000	3.61110000	1.08930000
H	4.52280000	3.73030000	1.93740000
H	4.89840000	4.28940000	0.28140000
H	6.21640000	3.92480000	1.42360000
C	-4.33940000	-0.42300000	2.24350000
H	-4.61550000	-1.36250000	2.72430000
C	-4.52590000	0.80590000	2.89300000
H	-4.93080000	0.85580000	3.90330000
C	-3.81110000	-0.43990000	0.96830000
H	-3.65440000	-1.37190000	0.42780000
C	-1.29760000	-3.01550000	1.74410000
H	-2.16180000	-2.36970000	1.88410000
C	0.56420000	-4.24760000	2.59010000
H	1.17100000	-4.61940000	3.41650000
C	-0.58340000	-3.49440000	2.83270000
H	-0.90630000	-3.26040000	3.84690000

C	5.74120000	1.27820000	1.78380000
H	5.01020000	1.31880000	2.60720000
H	6.71570000	1.63250000	2.15860000
H	5.85450000	0.22770000	1.47720000
C	1.70080000	-3.68460000	-1.73080000
H	2.59050000	-4.03880000	-1.16770000
H	1.82880000	-3.99750000	-2.78240000
C	0.44280000	-4.38880000	-1.19770000
H	-0.41700000	-4.12730000	-1.82570000
H	0.59380000	-5.47770000	-1.27740000
H	-1.59940000	-2.24190000	-0.64730000
H	-3.26450000	1.65400000	-2.44330000
C	0.55070000	-0.48550000	1.84000000
H	-0.68060000	1.33860000	-3.62060000
H	-2.03980000	2.23380000	-4.40180000
C	-1.63820000	-1.87380000	-2.62290000
H	-0.54360000	-1.80960000	-2.69710000
H	-1.99520000	-2.88200000	-2.88490000
H	-2.11340000	-1.14060000	-3.28350000
C	-1.57040000	1.95300000	-3.44870000
O	-0.80810000	-0.13520000	1.46970000
H	-1.27640000	2.83990000	-2.87020000
H	0.56680000	-0.91240000	2.85340000
H	1.21580000	0.38750000	1.77130000
H	0.87270000	-1.24200000	1.11380000
H	-1.12550000	0.55840000	2.09020000