

Supplementary Material

Mechanistic Investigation of the Hydrolysis of DNA Dinucleotide Analogues Mediated by Mononuclear/Dinuclear Facial Copper(II) Complexes Bearing Single Guanidine Pendant: Cooperation Between the Metal Centers and the Guanidine Pendant

Xuepeng Zhang^[a], Xueping Liu^[a], David Lee Phillips^[b] and Cunyuan Zhao^[a]*

[a] MOE Key Laboratory of Bioinorganic and Synthetic Chemistry, School of Chemistry and Chemical Engineering, Sun Yat-Sen University, Guangzhou 510275, P. R. China.

[b] Department of Chemistry, The University of Hong Kong, Pokfulam Road, Hong Kong, P. R. China.

Cartesian coordinates of optimized structures.

**[Cu₂(L¹)₂(μ-OH)]³⁺ Triplet
E : -1840.34083519 a.u.**

Cu	0.	2.02911	0.19598
O	0.	0.	0.74764
H	0.	0.	1.7181
N	0.40997	3.96325	-0.54827
N	1.57195	2.51929	1.54211
N	-1.17804	3.27121	1.7509
N	-1.00362	1.87393	-1.57587
N	-2.85069	1.29191	-2.92154
N	-2.42544	0.12916	-0.96518
C	1.67627	4.49238	0.04962
H	1.42185	5.26285	0.7793
H	2.28289	4.98549	-0.71817
C	2.47749	3.36907	0.70843
H	2.91659	2.71731	-0.05399
H	3.29806	3.78861	1.30426
C	1.08414	3.18446	2.79617
H	1.34615	4.24344	2.74669
H	1.61578	2.78284	3.66476
C	-0.42788	3.01843	3.00278
H	-0.65732	1.9923	3.31409
H	-0.7396	3.67932	3.82356
C	-1.15437	4.68765	1.28768
H	-0.45926	5.25988	1.90759
H	-2.13265	5.15988	1.42559
C	-0.78021	4.79305	-0.1996
H	-1.61825	4.43823	-0.80076
H	-0.60033	5.8432	-0.46815
C	0.55245	3.71624	-2.01165
H	1.48129	3.15414	-2.14917
H	0.65033	4.66535	-2.55559
C	-0.62913	2.9092	-2.55066
H	-1.4742	3.58403	-2.74778
H	-0.33676	2.46938	-3.51405
C	-2.06775	1.14289	-1.82906
H	2.08237	1.67698	1.80198
H	-2.14433	2.98527	1.89372
H	-3.42082	0.008	-0.81077
H	-3.57761	0.62336	-3.14067
H	-2.69314	2.01844	-3.60434
H	-1.84571	0.08864	-0.12837
Cu	0.	-2.02911	0.19598
N	-0.40997	-3.96325	-0.54827
N	-1.57195	-2.51929	1.54211
N	1.17804	-3.27121	1.7509
N	1.00362	-1.87393	-1.57587
N	2.85069	-1.29191	-2.92154
N	2.42544	-0.12916	-0.96518
C	-1.67627	-4.49238	0.04962

H	-1.42185	-5.26285	0.7793
H	-2.28289	-4.98549	-0.71817
C	-2.47749	-3.36907	0.70843
H	-2.91659	-2.71731	-0.05399
H	-3.29806	-3.78861	1.30426
C	-1.08414	-3.18446	2.79617
H	-1.34615	-4.24344	2.74669
H	-1.61578	-2.78284	3.66476
C	0.42788	-3.01843	3.00278
H	0.65732	-1.9923	3.31409
H	0.7396	-3.67932	3.82356
C	1.15437	-4.68765	1.28768
H	0.45926	-5.25988	1.90759
H	2.13265	-5.15988	1.42559
C	0.78021	-4.79305	-0.1996
H	1.61825	-4.43823	-0.80076
H	0.60033	-5.8432	-0.46815
C	-0.55245	-3.71624	-2.01165
H	-1.48129	-3.15414	-2.14917
H	-0.65033	-4.66535	-2.55559
C	0.62913	-2.9092	-2.55066
H	1.4742	-3.58403	-2.74778
H	0.33676	-2.46938	-3.51405
C	2.06775	-1.14289	-1.82906
H	-2.08237	-1.67698	1.80198
H	2.14433	-2.98527	1.89372
H	3.42082	-0.008	-0.81077
H	3.57761	-0.62336	-3.14067
H	2.69314	-2.01844	-3.60434
H	1.84571	-0.08864	-0.12837

**[Cu₂(L¹)₂(μ-OH)]³⁺ Open-shell singlet
E : -1840.34215898 a.u.**

Cu	0.	2.02525	0.19595
O	0.	0.	0.73878
H	0.	0.	1.70976
N	0.40871	3.95997	-0.54329
N	1.56527	2.51129	1.5472
N	-1.18498	3.26347	1.74926
N	-0.99881	1.8699	-1.57892
N	-2.83998	1.2899	-2.93371
N	-2.42394	0.12455	-0.97714
C	1.67262	4.48871	0.05962
H	1.41576	5.25743	0.79032
H	2.28161	4.98407	-0.7049
C	2.47263	3.36437	0.71809
H	2.91487	2.71486	-0.04441
H	3.2908	3.78273	1.31809
C	1.07365	3.17393	2.80139
H	1.33674	4.23278	2.75502
H	1.60248	2.76971	3.67051
C	-0.43924	3.00905	3.00311
H	-0.67045	1.9828	3.31297

H	-0.7527	3.66938	3.82369
C	-1.16126	4.68097	1.28849
H	-0.46829	5.25254	1.91153
H	-2.1403	5.15215	1.42485
C	-0.78302	4.78887	-0.19742
H	-1.61902	4.434	-0.80156
H	-0.60344	5.83954	-0.46434
C	0.55656	3.71589	-2.00638
H	1.48706	3.15593	-2.1419
H	0.65428	4.66588	-2.54892
C	-0.62144	2.90714	-2.55078
H	-1.4669	3.58081	-2.75034
H	-0.3245	2.46892	-3.51351
C	-2.06183	1.13951	-1.83788
H	2.07687	1.66969	1.80709
H	-2.15149	2.97618	1.88775
H	-3.42013	0.00262	-0.82886
H	-3.5667	0.62232	-3.15627
H	-2.67832	2.01614	-3.61579
H	-1.85009	0.08508	-0.13683
Cu	0.	-2.02525	0.19595
N	-0.40871	-3.95997	-0.54329
N	-1.56527	-2.51129	1.5472
N	1.18498	-3.26347	1.74926
N	0.99881	-1.8699	-1.57892
N	2.83998	-1.2899	-2.93371
N	2.42394	-0.12455	-0.97714
C	-1.67262	-4.48871	0.05962
H	-1.41576	-5.25743	0.79032
H	-2.28161	-4.98407	-0.7049
C	-2.47263	-3.36437	0.71809
H	-2.91487	-2.71486	-0.04441
H	-3.2908	-3.78273	1.31809
C	-1.07365	-3.17393	2.80139
H	-1.33674	-4.23278	2.75502
H	-1.60248	-2.76971	3.67051
C	0.43924	-3.00905	3.00311
H	0.67045	-1.9828	3.31297
H	0.7527	-3.66938	3.82369
C	1.16126	-4.68097	1.28849
H	0.46829	-5.25254	1.91153
H	2.1403	-5.15215	1.42485
C	0.78302	-4.78887	-0.19742
H	1.61902	-4.434	-0.80156
H	0.60344	-5.83954	-0.46434
C	-0.55656	-3.71589	-2.00638
H	-1.48706	-3.15593	-2.1419
H	-0.65428	-4.66588	-2.54892
C	0.62144	-2.90714	-2.55078
H	1.4669	-3.58081	-2.75034
H	0.3245	-2.46892	-3.51351
C	2.06183	-1.13951	-1.83788
H	-2.07687	-1.66969	1.80709

H	2.15149	-2.97618	1.88775
H	3.42013	-0.00262	-0.82886
H	3.5667	-0.62232	-3.15627
H	2.67832	-2.01614	-3.61579
H	1.85009	-0.08508	-0.13683

**[Cu₂(L¹)₂(OH)₂]²⁺ Triplet
E : -1916.34166747 a.u.**

O	0.9418	0.99161	-1.23907
Cu	-2.47232	0.09016	0.16493
O	-0.72944	0.48635	0.90619
N	-4.31569	-0.36626	-0.79423
N	-2.02164	0.98094	-1.7327
N	-3.55305	2.09563	0.43138
N	-2.90302	-1.61018	1.25754
N	-2.77759	-2.99885	3.16266
N	-1.01224	-1.59486	2.61027
C	-4.20918	-0.05157	-2.25258
H	-4.76209	0.86838	-2.45171
H	-4.69391	-0.83357	-2.84896
C	-2.746	0.11255	-2.68701
H	-2.24022	-0.85947	-2.68876
H	-2.71405	0.50126	-3.71518
C	-2.4081	2.41595	-1.76829
H	-3.2853	2.52964	-2.41201
H	-1.6133	3.01015	-2.23303
C	-2.69754	2.99267	-0.37011
H	-1.75821	3.0977	0.18003
H	-3.13516	3.99488	-0.49194
C	-4.95208	1.94219	-0.0261
H	-5.0691	2.42876	-0.99876
H	-5.65235	2.44863	0.64822
C	-5.34799	0.45796	-0.10594
H	-5.45299	0.06692	0.90914
H	-6.32345	0.35055	-0.60307
C	-4.50772	-1.82334	-0.56581
H	-3.82658	-2.34426	-1.24609
H	-5.53346	-2.12601	-0.82142
C	-4.17018	-2.22635	0.87142
H	-4.11838	-3.3252	0.89216
C	-2.26653	-2.05769	2.32015
H	-1.00387	0.89284	-1.8462
H	-3.52483	2.38711	1.40481
H	-0.76792	-1.56124	3.59347
H	-2.18002	-3.47345	3.82507
H	-3.69599	-3.39154	3.02544
H	-0.73918	-0.7614	2.04408
H	-4.98261	-1.93245	1.55368
Cu	2.57183	0.25596	-0.48877
N	4.50898	-0.51552	-0.11786
N	2.74939	-0.94621	-2.23052
N	2.00256	-1.80548	0.39362
N	3.15412	1.6865	0.89899

N	3.05356	3.40264	2.50829	C	-2.4081	2.41595	-1.76829
N	1.09677	2.5934	1.58108	H	-3.2853	2.52964	-2.41201
C	5.01838	-1.22833	-1.32947	H	-1.6133	3.01015	-2.23303
H	4.97056	-2.30353	-1.14658	C	-2.69754	2.99267	-0.37011
H	6.07573	-0.99235	-1.49794	H	-1.75821	3.0977	0.18003
C	4.18911	-0.86612	-2.56782	H	-3.13516	3.99488	-0.49194
H	4.39274	0.16366	-2.88021	C	-4.95208	1.94219	-0.0261
H	4.46094	-1.52396	-3.40493	H	-5.0691	2.42876	-0.99876
C	2.21365	-2.31943	-2.04391	H	-5.65235	2.44863	0.64822
H	3.05604	-3.0159	-2.01108	C	-5.34799	0.45796	-0.10594
H	1.60951	-2.61545	-2.90869	H	-5.45299	0.06692	0.90914
C	1.36481	-2.45537	-0.76675	H	-6.32345	0.35055	-0.60307
H	0.40057	-1.95741	-0.90684	C	-4.50772	-1.82334	-0.56581
H	1.16614	-3.52491	-0.59819	H	-3.82658	-2.34426	-1.24609
C	3.24411	-2.43759	0.89361	H	-5.53346	-2.12601	-0.82142
H	3.54927	-3.23334	0.20727	C	-4.17018	-2.22635	0.87142
H	3.07976	-2.92565	1.86137	H	-4.11838	-3.3252	0.89216
C	4.37598	-1.40629	1.06603	C	-2.26653	-2.05769	2.32015
H	4.1469	-0.77257	1.92564	H	-1.00387	0.89284	-1.8462
H	5.32615	-1.91959	1.27518	H	-3.52483	2.38711	1.40481
C	5.2972	0.71266	0.14893	H	-0.76792	-1.56124	3.59347
H	5.40973	1.22715	-0.81107	H	-2.18002	-3.47345	3.82507
H	6.30542	0.46267	0.50999	H	-3.69599	-3.39154	3.02544
C	4.60206	1.64454	1.14342	H	-0.73918	-0.7614	2.04408
H	5.07594	2.62937	1.01176	H	-4.98261	-1.93245	1.55368
C	2.45663	2.53252	1.6351	Cu	2.57183	0.25596	-0.48877
H	2.18466	-0.42217	-2.89599	N	4.50898	-0.51552	-0.11786
H	1.31257	-1.72063	1.13698	N	2.74939	-0.94621	-2.23052
H	0.6442	3.20425	2.24888	N	2.00256	-1.80548	0.39362
H	2.49577	4.10856	2.96978	N	3.15412	1.6865	0.89899
H	4.02751	3.64477	2.40238	N	3.05356	3.40264	2.50829
H	0.52337	1.76982	1.34515	N	1.09677	2.5934	1.58108
H	4.80793	1.33014	2.17667	C	5.01838	-1.22833	-1.32947
H	0.99635	1.9555	-1.13509	H	4.97056	-2.30353	-1.14658
H	-0.1442	0.5163	0.11209	H	6.07573	-0.99235	-1.49794

**[Cu₂(L¹)₂(OH)₂]²⁺ Open-shell singlet
E : -1916.34165760 a.u.**

O	0.9418	0.99161	-1.23907	C	4.18911	-0.86612	-2.56782
Cu	-2.47232	0.09016	0.16493	H	4.39274	0.16366	-2.88021
O	-0.72944	0.48635	0.90619	H	4.46094	-1.52396	-3.40493
N	-4.31569	-0.36626	-0.79423	C	2.21365	-2.31943	-2.04391
N	-2.02164	0.98094	-1.7327	H	3.05604	-3.0159	-2.01108
N	-3.55305	2.09563	0.43138	H	1.60951	-2.61545	-2.90869
N	-2.90302	-1.61018	1.25754	C	1.36481	-2.45537	-0.76675
N	-2.77759	-2.99885	3.16266	H	0.40057	-1.95741	-0.90684
N	-1.01224	-1.59486	2.61027	H	1.16614	-3.52491	-0.59819
C	-4.20918	-0.05157	-2.25258	C	3.24411	-2.43759	0.89361
H	-4.76209	0.86838	-2.45171	H	3.54927	-3.23334	0.20727
H	-4.69391	-0.83357	-2.84896	H	3.07976	-2.92565	1.86137
C	-2.746	0.11255	-2.68701	C	4.37598	-1.40629	1.06603
H	-2.24022	-0.85947	-2.68876	H	4.1469	-0.77257	1.92564
H	-2.71405	0.50126	-3.71518	H	5.32615	-1.91959	1.27518
				C	5.2972	0.71266	0.14893
				H	5.40973	1.22715	-0.81107
				H	6.30542	0.46267	0.50999

C	4.60206	1.64454	1.14342
H	5.07594	2.62937	1.01176
C	2.45663	2.53252	1.6351
H	2.18466	-0.42217	-2.89599
H	1.31257	-1.72063	1.13698
H	0.6442	3.20425	2.24888
H	2.49577	4.10856	2.96978
H	4.02751	3.64477	2.40238
H	0.52337	1.76982	1.34515
H	4.80793	1.33014	2.17667
H	0.99635	1.9555	-1.13509
H	-0.1442	0.5163	0.11209

[Cu₂(L¹)₂(μ-OH)(OH)]²⁺

E : -1916.26798746 a.u.

O	1.21222	0.87425	-1.69182
Cu	-2.06869	-0.05579	-0.0141
O	-0.07007	-0.5491	0.37731
N	-3.90979	-0.12424	-1.18952
N	-1.46234	1.25497	-1.50459
N	-3.12901	1.88083	0.72345
N	-2.82824	-1.77283	0.80933
N	-3.34683	-3.2102	2.61485
N	-1.41238	-1.94102	2.64819
C	-3.62427	0.51451	-2.50394
H	-4.12985	1.48239	-2.53392
H	-4.05013	-0.07692	-3.32463
C	-2.11391	0.70051	-2.71511
H	-1.63769	-0.2652	-2.92003
H	-1.94319	1.33924	-3.59394
C	-1.78464	2.67616	-1.22213
H	-2.58831	3.00308	-1.88921
H	-0.91478	3.29974	-1.45657
C	-2.17893	2.91172	0.24389
H	-1.29532	2.8432	0.88367
H	-2.58806	3.92931	0.33719
C	-4.47668	1.94648	0.10951
H	-4.46129	2.67236	-0.70822
H	-5.22072	2.31603	0.82473
C	-4.94881	0.57384	-0.40191
H	-5.19253	-0.05269	0.45862
H	-5.87329	0.69712	-0.98732
C	-4.11617	-1.58563	-1.28955
H	-3.34375	-1.97451	-1.96142
H	-5.09307	-1.82462	-1.7381
C	-3.99564	-2.27809	0.07305
H	-3.91378	-3.35961	-0.11036
C	-2.56218	-2.29429	1.98387
H	-0.42214	1.11683	-1.56509
H	-3.20754	1.95732	1.73438
H	-1.43407	-1.92995	3.66061
H	-2.97325	-3.76325	3.37461
H	-4.17764	-3.57457	2.17368

H	-0.86965	-1.2064	2.19825
H	-4.9183	-2.11987	0.65041
Cu	1.87152	-0.21055	-0.221
N	3.99186	0.27842	-0.45034
N	2.60663	-1.96105	-1.81037
N	2.66239	-1.68977	1.04001
N	2.21982	1.91094	0.9521
N	1.93676	3.66308	2.5402
N	0.41555	1.90925	2.40901
C	4.64789	-0.5221	-1.5218
H	5.29773	-1.26161	-1.04642
H	5.31036	0.12218	-2.11255
C	3.69281	-1.23738	-2.49386
H	3.22464	-0.50331	-3.15652
H	4.30917	-1.89454	-3.12693
C	2.99066	-3.12747	-0.99523
H	4.0813	-3.21455	-0.96428
H	2.63285	-4.0642	-1.43891
C	2.41991	-3.02869	0.43023
H	1.3363	-3.18252	0.40832
H	2.84983	-3.82223	1.05777
C	4.11037	-1.44095	1.34454
H	4.70037	-2.21545	0.85034
H	4.29522	-1.55076	2.41844
C	4.53987	-0.04601	0.89332
H	4.14811	0.68318	1.59912
H	5.63777	0.03096	0.90099
C	4.00784	1.7351	-0.74884
H	3.44496	1.86316	-1.67548
H	5.0419	2.07435	-0.91128
C	3.36917	2.58704	0.3642
H	3.09083	3.54911	-0.09221
C	1.58559	2.49153	1.9167
H	1.90112	-2.22458	-2.49232
H	2.12405	-1.62979	1.90233
H	0.32216	1.91154	3.42017
H	1.22961	4.18659	3.03953
H	2.68768	4.22135	2.16061
H	0.24522	1.00082	1.98479
H	4.1323	2.81102	1.12722
H	1.357	0.38165	-2.51603
H	-0.15938	-1.50504	0.21202

[Cu(L³H)(OH)(H₂O)]²⁺

E: -1113.75556652 a.u.

O	0.32699	1.60758	-1.04805
O	-1.36137	2.97855	0.4296
Cu	-1.1921	0.88516	-0.0856
N	-0.49875	-1.15678	0.23178
N	-2.65939	-0.11613	-1.46278
N	-2.60093	0.37092	1.31913
N	3.69631	-0.01039	-0.5306
N	4.88091	1.44878	0.8365

N	3.03645	2.19754	-0.38624
C	-1.26472	-2.05337	-0.68454
H	-2.03891	-2.56692	-0.11093
H	-0.61167	-2.84062	-1.07581
C	-1.89645	-1.31697	-1.8793
H	-1.11579	-0.9748	-2.5665
H	-2.52306	-2.0352	-2.42605
C	-3.89863	-0.38569	-0.68111
H	-3.96643	-1.45684	-0.47032
H	-4.79016	-0.13536	-1.26497
C	-3.92149	0.42616	0.62266
H	-4.11618	1.48061	0.40296
H	-4.72594	0.07102	1.27891
C	-2.27746	-0.94172	1.96423
H	-2.98199	-1.68977	1.59442
H	-2.42958	-0.8809	3.0465
C	-0.83167	-1.35522	1.66936
H	-0.14031	-0.73268	2.24832
H	-0.67761	-2.39699	1.9823
C	0.96496	-1.16105	-0.04281
H	1.36816	-0.27044	0.44062
H	1.0552	-0.99442	-1.12017
C	3.88083	1.22084	-0.0321
H	-2.88928	0.42412	-2.29425
H	-2.58082	1.10729	2.02538
H	3.29158	3.16671	-0.24328
H	4.94659	2.32573	1.33764
H	5.69856	0.85244	0.8584
H	2.06791	1.98802	-0.70164
H	0.14791	1.7244	-1.99509
C	1.7774	-2.39735	0.37791
H	1.25889	-3.31899	0.08611
H	1.87935	-2.43068	1.46982
C	3.17916	-2.43608	-0.2731
H	3.07928	-2.50858	-1.36591
H	3.67764	-3.36071	0.03717
C	4.14433	-1.2868	0.06394
H	4.21409	-1.14592	1.14827
H	5.14237	-1.54007	-0.31207
H	3.14161	-0.05895	-1.37594
H	-0.60434	3.17966	-0.16339
H	-2.05111	3.64609	0.27393

BNP

E : -1515.25559363 a.u.

O	5.60686	-1.90979	1.27135
N	5.05495	-1.96006	0.16221
C	3.95904	-1.05024	-0.10817
O	5.39812	-2.75342	-0.72801
C	3.55796	-0.13655	0.87478
C	3.31713	-1.09535	-1.35378
C	2.51145	0.73911	0.62374
H	4.07589	-0.11812	1.82616

C	2.27247	-0.22343	-1.60417
H	3.6432	-1.81013	-2.09937
C	1.85502	0.70102	-0.62365
H	2.20347	1.47203	1.35948
H	1.75182	-0.23236	-2.55603
O	0.82652	1.49991	-0.97646
P	-0.0003	2.63373	-0.00046
O	0.95202	3.2938	0.93776
O	-0.95222	3.29331	-0.9395
O	-0.82785	1.50186	0.97647
C	-1.85567	0.702	0.62381
C	-2.51137	0.73896	-0.62397
C	-2.27315	-0.22195	1.60477
C	-3.55735	-0.13736	-0.87499
H	-2.20315	1.47156	-1.35996
C	-3.31746	-1.09431	1.3545
H	-1.75279	-0.23012	2.55681
C	-3.9587	-1.05033	0.10849
H	-4.07468	-0.11991	-1.82671
H	-3.64365	-1.80869	2.10041
N	-5.05431	-1.96061	-0.16168
O	-5.39921	-2.75172	0.72983
O	-5.60378	-1.91334	-1.27215

OH⁻

E : -75.97878999 a.u.

O	0.	0.	0.10831
H	0.	0.	-0.86646

H₂O

E : -76.47252534 a.u.

O	0.	0.	0.11724
H	0.	0.77158	-0.46895
H	0.	-0.77158	-0.46895

L¹-2OH-³RC

E : -3431.61626639 a.u.

O	-2.58578	1.33296	-1.26569
O	7.27031	5.3486	-0.70875
N	7.3097	4.45362	-1.55787
C	6.29322	3.40003	-1.49051
O	8.14776	4.38985	-2.4603
C	5.33653	3.4424	-0.47581
C	6.30303	2.37831	-2.44345
C	4.36599	2.44858	-0.40915
H	5.36232	4.24668	0.24918
C	5.33162	1.38866	-2.37623
H	7.06004	2.3725	-3.21802
C	4.36295	1.42269	-1.36384
H	3.61531	2.47046	0.36998
H	5.30622	0.58056	-3.09956
O	3.46686	0.38087	-1.36112
P	1.96864	0.34779	-0.64754

O	1.30761	1.69036	-0.74319	H	-1.8923	-1.94679	1.59891
O	1.34272	-0.934	-1.10499	H	0.15975	-5.43834	-0.30576
O	2.3731	0.21292	0.98633	Cu	-2.77657	2.16674	0.47915
C	2.84637	-0.90772	1.5995	N	-3.41926	4.29907	0.88582
C	3.54268	-1.92922	0.93118	N	-0.92142	3.02593	0.28212
C	2.63414	-0.99161	2.986	N	-2.27843	2.35666	2.63018
C	3.99032	-3.03641	1.64366	N	-4.82407	1.90986	0.53744
H	3.73144	-1.85072	-0.13202	N	-6.86617	0.88133	1.11937
C	3.07998	-2.09523	3.69997	N	-4.8863	-0.32797	1.18629
H	2.12166	-0.17575	3.48519	C	-2.27478	5.13281	0.45571
C	3.74211	-3.11972	3.0165	H	-1.80689	5.55495	1.35007
H	4.53538	-3.83256	1.1503	H	-2.61153	5.99066	-0.14291
H	2.92617	-2.17489	4.76946	C	-1.23309	4.33031	-0.35238
N	4.16494	-4.31187	3.75102	H	-1.61555	4.09922	-1.35105
O	3.90085	-4.37142	4.95629	H	-0.32468	4.93609	-0.47834
O	4.74045	-5.20527	3.12304	C	-0.17394	3.09623	1.56427
Cu	-1.51065	-2.32195	-1.06078	H	-0.16466	4.12739	1.93
O	-2.4257	-1.10118	0.16561	H	0.86249	2.79841	1.3851
N	-0.58191	-3.60387	-2.48267	C	-0.80561	2.15927	2.59797
N	-1.76828	-1.07377	-2.75454	H	-0.62442	1.11986	2.30533
N	-3.40464	-3.34336	-2.05756	H	-0.34732	2.32309	3.58457
N	-0.48794	-3.50322	0.27158	C	-2.70171	3.6647	3.19426
N	0.04198	-4.42468	2.37941	H	-1.81546	4.29322	3.31284
N	-1.54649	-2.73126	2.17836	H	-3.12097	3.53692	4.1991
C	-0.36259	-2.84791	-3.75404	C	-3.74554	4.38369	2.3144
H	-1.06525	-3.22468	-4.50189	H	-4.71353	3.90498	2.46936
H	0.64246	-3.04888	-4.14383	H	-3.8451	5.42624	2.65815
C	-0.54725	-1.33747	-3.55226	C	-4.57787	4.3191	-0.02074
H	0.2925	-0.93538	-2.98227	H	-4.18771	4.2244	-1.03967
H	-0.58481	-0.83918	-4.5324	H	-5.13661	5.26866	0.03121
C	-3.04498	-1.31915	-3.46774	C	-5.54892	3.15488	0.26297
H	-2.82708	-1.81822	-4.41714	H	-6.20701	3.05787	-0.61489
H	-3.52131	-0.36643	-3.7287	C	-5.50606	0.84817	0.90921
C	-4.0441	-2.16146	-2.65283	H	-0.34968	2.46044	-0.36445
H	-4.42375	-1.56425	-1.81841	H	-2.71525	1.59614	3.14604
H	-4.89423	-2.4165	-3.30724	H	-5.46203	-1.1154	1.45184
C	-2.92289	-4.38327	-2.9832	H	-7.38225	0.0136	1.16165
H	-3.00616	-4.01825	-4.01138	H	-7.40098	1.67418	0.79943
H	-3.54217	-5.28802	-2.93465	H	-3.95495	-0.58503	0.78096
C	-1.47042	-4.77873	-2.66267	H	-6.19487	3.4271	1.11172
H	-1.46373	-5.34025	-1.7256	H	-3.50124	1.25501	-1.57844
H	-1.07894	-5.44328	-3.44906	H	-2.30743	-0.23606	-0.28673
C	0.70065	-3.95368	-1.81801				
H	1.30943	-3.04736	-1.8213				
H	1.22353	-4.74429	-2.37793	L¹-2OH-³TS			
C	0.4849	-4.38769	-0.36417	E : -3431.59989318 a.u.			
H	1.47149	-4.33011	0.12027	O	-1.44958	-0.00386	-0.91281
C	-0.62942	-3.53763	1.57482	O	-3.51274	6.92981	1.07539
H	-1.76598	-0.11513	-2.38007	N	-3.51112	6.4316	-0.05279
H	-3.99705	-3.73765	-1.33349	C	-2.59025	5.31919	-0.30996
H	-1.46776	-2.58113	3.17419	O	-4.24545	6.79683	-0.97474
H	0.05189	-4.27197	3.37863	C	-1.74573	4.88139	0.71373
H	0.86908	-4.88044	2.02318	C	-2.58784	4.71786	-1.57091
				C	-0.90089	3.79919	0.48763

H	-1.75123	5.39574	1.6673	C	3.70296	-0.57009	1.81668
C	-1.74844	3.63192	-1.79387	H	3.63216	0.50359	1.99207
H	-3.23594	5.10007	-2.35022	C	1.6016	-0.7781	2.93579
C	-0.92159	3.16303	-0.76284	H	0.85254	-2.96582	-1.81683
H	-0.21596	3.44316	1.24774	H	2.64386	-5.09847	1.54204
H	-1.71169	3.14273	-2.76181	H	0.13245	-1.24358	4.27809
O	-0.11099	2.09728	-1.05564	H	0.85412	0.80546	3.93349
P	0.04587	0.75655	-0.09596	H	1.75335	1.19388	2.55159
O	-0.59783	0.81721	1.27005	H	0.89697	-2.56945	3.56903
O	1.06813	-0.18169	-0.67252	H	4.46678	-0.94817	2.51147
O	1.68438	1.95859	0.93799	Cu	-2.95694	-1.05271	-0.09541
C	2.7422	2.53123	0.40849	N	-5.12732	-0.77109	-0.47474
C	3.02425	2.50829	-0.98984	N	-3.26522	0.43983	1.25944
C	3.68182	3.19904	1.24931	N	-3.78093	-2.28109	1.56005
C	4.17476	3.08697	-1.49896	N	-3.14671	-2.26068	-1.72111
H	2.31859	2.0291	-1.6571	N	-2.86334	-4.20469	-3.027
C	4.83242	3.77523	0.74146	N	-1.35161	-3.71722	-1.34614
H	3.46774	3.25736	2.31354	C	-5.50779	0.50535	0.18076
C	5.08742	3.70988	-0.63624	H	-6.12057	0.27004	1.05592
H	4.38537	3.0671	-2.56216	H	-6.13921	1.1151	-0.47868
H	5.54146	4.27754	1.38923	C	-4.26584	1.31326	0.60534
N	6.30382	4.28169	-1.17119	H	-3.7742	1.75311	-0.2679
O	7.08882	4.83463	-0.3877	H	-4.56586	2.1428	1.2606
O	6.51216	4.18516	-2.39041	C	-3.6025	-0.05053	2.61572
Cu	1.92891	-2.51759	0.46955	H	-4.66237	0.13329	2.81338
O	0.05938	-2.98182	0.81953	H	-3.03959	0.5135	3.36791
N	3.94702	-2.15394	-0.09428	C	-3.27725	-1.54384	2.74754
N	1.81728	-3.17523	-1.56836	H	-2.19215	-1.68174	2.77498
N	2.86239	-4.70687	0.63129	H	-3.69808	-1.93742	3.68464
N	2.451	-1.30048	2.08362	C	-5.26251	-2.35027	1.46685
N	1.62217	0.52006	3.3381	H	-5.68921	-1.68956	2.22615
N	0.6107	-1.60287	3.46066	H	-5.61921	-3.35882	1.70513
C	4.10403	-2.25657	-1.57396	C	-5.79566	-1.96395	0.06969
H	4.65284	-3.17313	-1.80601	H	-5.61145	-2.79519	-0.61277
H	4.71523	-1.42713	-1.94871	H	-6.88719	-1.83058	0.12918
C	2.74102	-2.25472	-2.2734	C	-5.07354	-0.70781	-1.94821
H	2.29118	-1.26155	-2.21713	H	-4.5514	0.21835	-2.2095
H	2.86789	-2.52846	-3.33156	H	-6.078	-0.65753	-2.39834
C	2.10139	-4.61781	-1.73965	C	-4.31641	-1.91135	-2.54022
H	3.07505	-4.72523	-2.22655	H	-4.02585	-1.64607	-3.56799
H	1.37575	-5.07877	-2.42236	C	-2.47387	-3.34973	-2.01992
C	2.09425	-5.39841	-0.41028	H	-2.31196	0.85867	1.27408
H	1.06959	-5.47398	-0.03132	H	-3.37942	-3.21609	1.54895
H	2.45756	-6.41964	-0.6132	H	-1.13267	-4.70608	-1.36722
C	4.31811	-4.58709	0.43008	H	-2.16908	-4.83228	-3.41063
H	4.57458	-4.94079	-0.57337	H	-3.54729	-3.89355	-3.70102
H	4.87524	-5.22884	1.12421	H	-0.9808	-3.24449	-0.47365
C	4.78742	-3.13573	0.63564	H	-5.00494	-2.76603	-2.61406
H	4.71768	-2.89601	1.69825	H	-1.15834	-0.3986	-1.75028
H	5.84372	-3.03624	0.34121	H	-0.21567	-2.35925	1.51236
C	4.14977	-0.75473	0.37108				
H	3.54103	-0.11748	-0.2729				
H	5.20413	-0.46107	0.25875				

L¹-2OH-³PC
E : -3431.61885440 a.u.

O	-1.67071	1.13081	-1.80067	H	0.12949	-6.613	-0.50804
O	2.55188	6.97537	0.11519	H	0.75532	-6.67379	1.12288
N	1.87538	6.70999	-0.88152	C	1.61242	-5.08156	-0.0407
C	1.62812	5.29479	-1.18538	H	2.01562	-4.63899	0.87166
O	1.38286	7.55571	-1.63123	H	2.40923	-5.68958	-0.49719
C	2.13912	4.31713	-0.32781	C	2.23739	-2.87666	-0.98426
C	0.88381	4.96575	-2.32043	H	1.86682	-2.14806	-1.70782
C	1.88553	2.97717	-0.60213	H	3.20743	-3.26407	-1.33107
H	2.72205	4.61302	0.53578	C	2.39895	-2.19319	0.38358
C	0.63604	3.62413	-2.59283	H	2.79261	-1.18414	0.2122
H	0.51212	5.75175	-2.9666	C	1.05569	-1.65153	2.28659
C	1.12712	2.63725	-1.72961	H	-2.22284	-3.15589	-1.82947
H	2.25524	2.19304	0.04939	H	-0.82111	-5.17897	1.78764
H	0.06352	3.32665	-3.46524	H	-0.11948	-1.74354	3.96155
O	0.89219	1.31372	-2.03564	H	1.92711	-0.54994	3.73476
P	-0.27322	0.44344	-1.22881	H	2.93102	-0.80841	2.41543
O	-0.22883	0.76307	0.24523	H	-0.95237	-1.9693	2.44436
O	-0.16703	-0.96899	-1.748	H	3.14548	-2.72509	0.99281
O	4.22053	0.324	1.42835	Cu	-3.70249	0.79888	0.55176
C	5.44778	0.31798	1.11969	N	-5.03337	2.60482	0.41255
C	5.88897	0.74734	-0.19329	N	-2.35548	2.16393	1.34565
C	6.46147	-0.13492	2.05201	N	-4.49651	0.82634	2.66846
C	7.21461	0.68409	-0.55014	N	-4.86898	0.0425	-0.90514
H	5.13413	1.10638	-0.88457	N	-6.14391	-1.65221	-1.9605
C	7.78573	-0.18477	1.68924	N	-4.16603	-2.1947	-0.88146
H	6.13682	-0.4347	3.0429	C	-4.1785	3.76937	0.7121
C	8.15139	0.21201	0.38892	H	-4.43155	4.13342	1.71291
H	7.55678	0.98426	-1.53243	H	-4.38866	4.60482	0.02803
H	8.55313	-0.52593	2.37281	C	-2.67333	3.4267	0.64244
N	9.55896	0.11922	-0.00504	H	-2.36431	3.28831	-0.39818
O	10.36897	-0.2535	0.84675	H	-2.10025	4.27591	1.04707
O	9.84905	0.42075	-1.16809	C	-2.42894	2.22783	2.82151
Cu	-0.40701	-2.95007	-0.02281	H	-2.87237	3.18519	3.1177
O	-1.91922	-1.9924	0.79286	H	-1.42287	2.20711	3.2578
N	1.22538	-3.96657	-0.93926	C	-3.24241	1.06231	3.41637
N	-1.47924	-3.83059	-1.64729	H	-2.6539	0.14118	3.33949
N	-0.73901	-5.18696	0.77571	H	-3.4218	1.26302	4.48539
N	1.11419	-2.1634	1.08483	C	-5.52137	1.89113	2.77182
N	2.14748	-1.16775	2.96273	H	-5.0842	2.75145	3.28879
N	-0.14232	-1.60335	2.95855	H	-6.36643	1.56412	3.392
C	0.83437	-4.43475	-2.29838	C	-6.0837	2.3285	1.39905
H	0.75393	-5.52506	-2.27857	H	-6.70311	1.51553	1.00794
H	1.62079	-4.19761	-3.02529	H	-6.75106	3.19529	1.55441
C	-0.49275	-3.80893	-2.75508	C	-5.41888	2.47994	-0.9985
H	-0.34273	-2.76002	-3.01315	H	-4.54745	2.77741	-1.59142
H	-0.86276	-4.34568	-3.64163	H	-6.24739	3.15899	-1.26867
C	-2.05089	-5.16311	-1.34058	C	-5.81908	1.04669	-1.40046
H	-1.48465	-5.91893	-1.89368	H	-5.87899	1.03578	-2.50101
H	-3.08315	-5.23598	-1.70668	C	-5.05609	-1.206	-1.23778
C	-2.03534	-5.50042	0.16257	H	-1.44028	1.80773	1.03256
H	-2.78123	-4.89224	0.68604	H	-4.88705	-0.07127	2.94252
H	-2.32675	-6.55798	0.27759	H	-4.60846	-3.08077	-0.65902
C	0.42185	-5.98282	0.33812	H	-6.03181	-2.50526	-2.49316

H	-6.74811	-0.97089	-2.39743
H	-3.39267	-1.96585	-0.21386
H	-6.83206	0.83168	-1.0252
H	-2.01108	0.61894	-2.55219
H	-1.59995	-1.07333	0.72372

L¹-2OH-¹RC

E : -3431.54938949 a.u.

O	-2.57706	-0.17443	1.94392
O	8.41542	-3.47391	-2.39572
N	7.98559	-3.67566	-1.25742
C	6.72682	-3.02654	-0.87524
O	8.54192	-4.38944	-0.41983
C	6.06454	-2.22469	-1.80453
C	6.21769	-3.23024	0.40962
C	4.86332	-1.61499	-1.4531
H	6.48949	-2.08713	-2.79138
C	5.0216	-2.61964	0.76111
H	6.75869	-3.85402	1.11054
C	4.34394	-1.81787	-0.16761
H	4.3272	-1.00571	-2.1695
H	4.59844	-2.74991	1.75159
O	3.1612	-1.27085	0.28282
P	2.17596	-0.19799	-0.50315
O	1.95395	-0.62161	-1.93017
O	1.03254	0.04157	0.44841
O	3.13516	1.15243	-0.61998
C	3.64082	1.91458	0.4066
C	3.36135	1.69115	1.76254
C	4.47734	2.96973	0.01404
C	3.91523	2.53586	2.72044
H	2.71221	0.87728	2.05957
C	5.02775	3.81358	0.96923
H	4.68919	3.10721	-1.04116
C	4.73531	3.58956	2.31703
H	3.71665	2.38702	3.77492
H	5.67689	4.63388	0.68824
N	5.2971	4.48765	3.33144
O	6.01142	5.4157	2.94616
O	5.01818	4.26792	4.51293
Cu	-2.28199	1.66378	-1.25719
O	-2.95292	-0.20509	-0.88357
N	-1.10748	3.47473	-1.18024
N	-2.7713	2.23206	0.70692
N	-3.93924	3.29108	-1.7096
N	-1.04007	1.2377	-2.86894
N	0.12923	-0.44806	-4.03904
N	-2.21391	-0.52773	-3.81034
C	-1.06512	3.96393	0.22353
H	-1.71329	4.83919	0.31093
H	-0.05373	4.30194	0.48359
C	-1.51923	2.86289	1.1863
H	-0.76048	2.07469	1.23586

H	-1.63682	3.27905	2.19795
C	-3.97348	3.08783	0.79423
H	-3.67299	4.10005	1.08544
H	-4.63177	2.7212	1.59089
C	-4.79062	3.13781	-0.51217
H	-5.33611	2.19697	-0.62653
H	-5.53158	3.94848	-0.41889
C	-3.24889	4.59246	-1.85242
H	-3.41395	5.18608	-0.94789
H	-3.67435	5.17833	-2.6765
C	-1.74192	4.42094	-2.11987
H	-1.60674	4.02226	-3.12817
H	-1.24713	5.40536	-2.08504
C	0.21473	2.97154	-1.6182
H	0.59965	2.35541	-0.8019
H	0.91957	3.80407	-1.77283
C	0.14041	2.12233	-2.88705
H	1.08538	1.57883	-2.95725
C	-1.00331	0.13144	-3.56107
H	-2.88775	1.31438	1.19659
H	-4.49899	3.1035	-2.53643
H	-2.1761	-1.26144	-4.50992
H	0.04206	-1.2963	-4.58365
H	0.94222	-0.43865	-3.40162
H	-2.98578	0.10949	-3.97909
H	0.06984	2.75926	-3.77984
Cu	-2.73121	-1.59237	0.65148
N	-3.10867	-3.30581	2.14225
N	-0.58015	-2.28436	1.11013
N	-2.57271	-3.20723	-0.64599
N	-5.12537	-1.55719	1.29404
N	-7.44545	-1.03553	1.10271
N	-5.90022	-0.22946	-0.44052
C	-1.81965	-3.76305	2.70411
H	-1.56889	-4.72933	2.25531
H	-1.91781	-3.94905	3.78207
C	-0.64699	-2.78036	2.48618
H	-0.77285	-1.9109	3.13739
H	0.27795	-3.29158	2.79793
C	-0.18199	-3.2512	0.07411
H	-0.14441	-4.25901	0.49992
H	0.82564	-3.03645	-0.30075
C	-1.1538	-3.20027	-1.11336
H	-1.00037	-2.26749	-1.6614
H	-0.96565	-4.03895	-1.79993
C	-2.9824	-4.50943	-0.02657
H	-2.0794	-5.09945	0.14375
H	-3.59875	-5.08158	-0.72951
C	-3.7567	-4.31038	1.27921
H	-4.75528	-3.95136	1.03434
H	-3.86579	-5.28398	1.78657
C	-3.99543	-2.70612	3.16056
H	-3.44514	-1.86207	3.58393

H	-4.21025	-3.42778	3.96614
C	-5.32855	-2.19701	2.58283
H	-5.75046	-1.50309	3.32782
C	-6.12055	-0.98366	0.70715
H	0.0042	-1.44254	1.03212
H	-3.1794	-3.01692	-1.44126
H	-6.56723	-0.37793	-1.19084
H	-8.03591	-0.25355	0.84835
H	-7.65286	-1.42538	2.01163
H	-4.91636	-0.24785	-0.73321
H	-6.03711	-3.03891	2.50559
H	-1.62025	-0.05664	2.07313
H	-2.78333	-0.66476	-1.72797

L¹-2OH-¹TS

E : -3431.52312259 a.u.

O	1.22623	0.61064	0.598
O	0.98263	7.93033	-1.22629
N	0.93908	7.50564	-0.0683
C	0.52153	6.11709	0.13733
O	1.23378	8.17311	0.92699
C	0.17845	5.33585	-0.96853
C	0.479	5.60255	1.43595
C	-0.19626	4.00941	-0.78418
H	0.19926	5.77511	-1.95865
C	0.11119	4.27671	1.62029
H	0.73485	6.23815	2.27489
C	-0.21381	3.47345	0.51455
H	-0.48234	3.38937	-1.62371
H	0.06356	3.84412	2.61436
O	-0.57183	2.188	0.79685
P	-0.40722	0.85514	-0.21086
O	0.17604	1.02266	-1.60652
O	-1.06211	-0.37755	0.39422
O	-2.17195	1.50134	-1.01121
C	-3.3489	1.59688	-0.44738
C	-3.59213	1.4239	0.95074
C	-4.47356	1.87289	-1.2851
C	-4.87817	1.482	1.45774
H	-2.75416	1.24903	1.61245
C	-5.75593	1.93207	-0.77588
H	-4.28781	2.03677	-2.34226
C	-5.9599	1.72052	0.59695
H	-5.06788	1.35062	2.51677
H	-6.60744	2.13514	-1.41459
N	-7.30867	1.74027	1.13385
O	-8.24275	1.97519	0.35739
O	-7.45912	1.51036	2.34187
Cu	-0.64138	-2.65383	-0.31315
O	1.35225	-2.26876	-0.26536
N	-2.74975	-3.03431	-0.38785
N	-0.93553	-3.22122	1.74275
N	-0.73547	-5.1377	-0.41418

N	-1.08291	-2.15341	-2.30092
N	-0.23109	-0.62978	-3.87734
N	0.84225	-2.69856	-3.46979
C	-3.29068	-3.11958	0.9999
H	-3.56598	-4.15773	1.20347
H	-4.2122	-2.53208	1.08458
C	-2.26574	-2.62172	2.02349
H	-2.14545	-1.5409	1.93606
H	-2.61075	-2.86366	3.03997
C	-0.83414	-4.66905	2.03566
H	-1.83669	-5.05538	2.23927
H	-0.25463	-4.82896	2.9522
C	-0.18949	-5.48837	0.90246
H	0.88585	-5.28285	0.86039
H	-0.31096	-6.55609	1.15099
C	-2.15529	-5.47603	-0.64425
H	-2.59268	-5.85509	0.285
H	-2.25611	-6.29217	-1.37095
C	-2.95646	-4.27536	-1.17107
H	-2.64489	-4.0587	-2.19427
H	-4.02818	-4.53069	-1.19349
C	-3.25132	-1.83641	-1.10274
H	-3.24527	-1.02203	-0.38015
H	-4.29171	-2.00413	-1.4197
C	-2.37142	-1.43021	-2.30565
H	-2.25498	-0.34462	-2.25259
C	-0.1972	-1.80646	-3.19715
H	-0.20771	-2.7238	2.25466
H	-0.15209	-5.54396	-1.13904
H	1.37389	-2.51371	-4.31337
H	0.46219	-0.4615	-4.59568
H	-0.41972	0.18664	-3.27725
H	0.55098	-3.66861	-3.41594
H	-2.87276	-1.66208	-3.25539
Cu	2.69369	-0.60923	-0.06081
N	4.52845	0.74117	0.72419
N	3.00483	0.91583	-1.73002
N	4.30448	-1.48618	-1.09366
N	3.0343	-0.96651	2.4101
N	3.33997	-2.38672	4.29859
N	2.0636	-3.07175	2.46789
C	4.73465	1.86404	-0.21085
H	5.60602	1.64783	-0.83701
H	4.98315	2.78399	0.33653
C	3.50857	2.13679	-1.1035
H	2.6901	2.53822	-0.50229
H	3.78646	2.90771	-1.84032
C	3.81932	0.30835	-2.77907
H	4.7903	0.81311	-2.82469
H	3.37311	0.43412	-3.77647
C	4.0229	-1.20203	-2.5295
H	3.10426	-1.74131	-2.77575
H	4.82773	-1.58853	-3.17312

C	5.64988	-1.00729	-0.64266
H	6.05833	-0.3655	-1.42653
H	6.33665	-1.85707	-0.55209
C	5.60224	-0.25987	0.6961
H	5.41133	-0.98633	1.48725
H	6.59775	0.17985	0.886
C	4.13972	1.20993	2.06384
H	3.24602	1.82612	1.92605
H	4.92122	1.85023	2.50842
C	3.83104	0.07239	3.0476
H	3.30938	0.52316	3.9077
C	2.83615	-2.07004	3.05188
H	2.0021	1.00126	-1.94018
H	4.24475	-2.49171	-0.94531
H	2.3867	-4.01275	2.67198
H	2.86358	-3.1054	4.8291
H	3.68984	-1.63118	4.8716
H	1.91445	-2.91358	1.46143
H	4.77849	-0.33412	3.4376
H	1.05801	0.29786	1.50305
H	1.61759	-2.65456	-1.11982

L¹-2OH-¹PC

E : -3431.58215253 a.u.

O	-0.24579	-2.06296	-1.69635
O	-7.06168	-3.9937	-1.47321
N	-6.91682	-2.98565	-2.16824
C	-5.64358	-2.26314	-2.06733
O	-7.76331	-2.55068	-2.95096
C	-4.66025	-2.73634	-1.20021
C	-5.44173	-1.12246	-2.84642
C	-3.44113	-2.06857	-1.11484
H	-4.8572	-3.6164	-0.60032
C	-4.22439	-0.45837	-2.76345
H	-6.22986	-0.77402	-3.50247
C	-3.2219	-0.93306	-1.9068
H	-2.67362	-2.41738	-0.43604
H	-4.03121	0.4276	-3.35928
O	-2.0445	-0.21775	-1.91827
P	-0.64601	-0.57571	-1.09725
O	-0.91381	-0.76312	0.37101
O	0.33776	0.4524	-1.60608
O	-2.64071	2.85381	3.17275
C	-3.6957	2.28403	2.73612
C	-3.65999	1.0027	2.06675
C	-4.98658	2.91679	2.88502
C	-4.81055	0.42626	1.5763
H	-2.70472	0.49979	1.94535
C	-6.13062	2.3336	2.39173
H	-5.01841	3.87317	3.39695
C	-6.04086	1.09134	1.7328
H	-4.78571	-0.5279	1.06434
H	-7.09978	2.80698	2.4949

N	-7.24594	0.48377	1.1935
O	-8.31094	1.10161	1.31033
O	-7.14194	-0.61941	0.64044
Cu	1.87849	1.93972	-0.50373
O	2.86516	0.33312	0.31769
N	0.79299	3.668	-1.32561
N	2.82389	2.06266	-2.39674
N	3.57113	4.01996	-0.2987
N	0.69845	2.46499	1.0566
N	0.03872	2.49792	3.31856
N	2.29091	2.20081	2.71659
C	0.96716	3.67186	-2.80228
H	1.5274	4.56828	-3.08355
H	-0.00583	3.74838	-3.30266
C	1.6897	2.40767	-3.29755
H	1.00662	1.55952	-3.27336
H	2.03702	2.56387	-4.32986
C	3.99495	2.9631	-2.54116
H	3.69755	3.8095	-3.16661
H	4.79517	2.45016	-3.08799
C	4.58367	3.49032	-1.22407
H	5.09685	2.68033	-0.69329
H	5.34998	4.23753	-1.49514
C	2.77118	5.16415	-0.78356
H	3.05661	5.41	-1.8119
H	2.98931	6.06584	-0.19741
C	1.25715	4.91675	-0.68396
H	0.98257	4.8581	0.37082
H	0.72652	5.78234	-1.11526
C	-0.57912	3.30115	-0.89406
H	-0.88868	2.46844	-1.52428
H	-1.26843	4.1426	-1.06561
C	-0.63222	2.86454	0.59172
H	-1.34268	2.03592	0.67703
C	0.9518	2.40731	2.33437
H	3.11213	1.10018	-2.56685
H	4.03995	4.27847	0.56524
H	2.48293	2.37012	3.69867
H	0.3307	2.69483	4.26632
H	-0.99114	2.53764	3.15054
H	2.93152	2.7161	2.11972
H	-1.018	3.67212	1.22959
Cu	2.97692	-1.74366	0.6046
N	3.02507	-3.97617	0.8588
N	1.18993	-2.01067	1.76452
N	3.9013	-1.97125	2.75322
N	4.21828	-2.26171	-1.01048
N	6.07862	-1.91894	-2.44058
N	4.99207	-0.11389	-1.45771
C	1.74393	-4.42008	1.46013
H	1.9189	-4.67233	2.50882
H	1.39007	-5.34397	0.98235
C	0.67141	-3.33432	1.34248

H	0.34375	-3.22718	0.3063	C	-3.69453	-0.75127	-2.79559
H	-0.20981	-3.62598	1.93356	C	-5.18858	-2.01444	-0.79466
C	1.43014	-1.88786	3.21909	H	-4.16305	-0.72368	0.58759
H	1.27384	-2.86345	3.69237	C	-4.60236	-1.74232	-3.14523
H	0.69204	-1.21282	3.66842	H	-3.11474	-0.23249	-3.55198
C	2.8369	-1.36103	3.57379	C	-5.33287	-2.37745	-2.13594
H	2.87577	-0.28361	3.38617	H	-5.79178	-2.5063	-0.04075
H	2.99844	-1.51505	4.65326	H	-4.75546	-2.02715	-4.17932
C	4.17265	-3.40316	3.01082	N	-6.26276	-3.45112	-2.49182
H	3.41522	-3.79105	3.69865	O	-6.34284	-3.7737	-3.68085
H	5.13574	-3.53806	3.51885	O	-6.90227	-3.98697	-1.58271
C	4.19821	-4.23339	1.71456	Cu	0.76649	-2.57549	0.85027
H	5.09257	-3.96217	1.1477	O	2.02851	-1.64722	-0.32877
H	4.28459	-5.30353	1.96966	N	-0.49901	-3.60451	2.22525
C	3.16889	-4.43606	-0.53348	N	1.3069	-1.49113	2.58305
H	2.21423	-4.23773	-1.03094	N	2.30668	-4.09876	1.86869
H	3.3523	-5.52243	-0.58492	N	-0.47517	-3.45543	-0.52833
C	4.28302	-3.69749	-1.28103	N	-1.19078	-4.12802	-2.67527
H	4.1553	-3.91536	-2.35321	N	0.79867	-2.94506	-2.39024
C	5.06637	-1.48244	-1.61788	C	-0.54856	-2.84228	3.50978
H	0.50052	-1.32071	1.43189	H	-0.00089	-3.40948	4.26735
H	4.75535	-1.43127	2.85948	H	-1.5829	-2.77071	3.86717
H	5.89128	0.3552	-1.42941	C	0.04491	-1.43336	3.35673
H	6.44887	-1.2698	-3.12256	H	-0.63945	-0.80265	2.78718
H	6.08718	-2.8835	-2.73902	H	0.19621	-0.99032	4.35235
H	4.34078	0.1717	-0.70531	C	2.45745	-2.07323	3.31312
H	5.26316	-4.10507	-0.98804	H	2.09277	-2.51006	4.24816
H	-0.00974	-2.00385	-2.63701	H	3.16186	-1.28417	3.60426
H	2.86252	0.62161	1.24847	C	3.21968	-3.13932	2.50361
L¹-2OH-^{os}RC				H	3.77002	-2.65335	1.69243
E : -3431.61156460 a.u.				H	3.95187	-3.6197	3.17429
O	2.75358	0.66588	1.15045	C	1.53877	-4.98436	2.7595
O	-5.22079	7.18162	0.44132	H	1.68549	-4.66731	3.79668
N	-5.24537	6.47579	1.45357	H	1.89583	-6.02114	2.70951
C	-4.63149	5.14743	1.37798	C	0.04417	-4.97486	2.39413
O	-5.74974	6.81817	2.52591	H	-0.08088	-5.49357	1.4411
C	-4.06145	4.72843	0.17505	H	-0.53233	-5.52942	3.1513
C	-4.62685	4.33113	2.51197	C	-1.80684	-3.59511	1.52021
C	-3.46629	3.47351	0.0998	H	-2.15204	-2.55964	1.52429
H	-4.09119	5.38403	-0.68671	H	-2.53826	-4.22537	2.04891
C	-4.03123	3.07948	2.43504	C	-1.66863	-4.05342	0.0636
H	-5.08029	4.68323	3.43042	H	-2.59048	-3.73008	-0.44324
C	-3.44793	2.65029	1.23454	C	-0.31788	-3.48666	-1.82935
H	-3.0184	3.13691	-0.82644	H	1.55859	-0.56104	2.22301
H	-4.00616	2.4194	3.29564	H	2.78953	-4.62482	1.14717
O	-2.90752	1.38773	1.25078	H	0.78978	-2.75475	-3.38235
P	-1.74048	0.79322	0.22192	H	-1.13249	-3.94618	-3.66777
O	-0.74359	1.86369	-0.10576	H	-2.12146	-4.34184	-2.34757
O	-1.38155	-0.54962	0.78291	H	1.32952	-2.29646	-1.77841
O	-2.60825	0.59117	-1.20197	H	-1.63443	-5.15206	-0.00571
C	-3.51671	-0.39579	-1.44824	Cu	3.38179	1.39372	-0.53518
C	-4.27883	-1.02097	-0.4473	N	4.68705	3.24484	-0.67396
				N	1.86042	2.7743	-0.48697

N	3.25949	1.82463	-2.69507	H	-1.70931	3.14083	-2.76327
N	5.24553	0.51748	-0.35824	O	-0.11083	2.09491	-1.05547
N	6.93212	-1.0822	-0.77621	P	0.04575	0.75528	-0.09417
N	4.69824	-1.63077	-1.07211	O	-0.59862	0.81726	1.2714
C	3.79324	4.36487	-0.30593	O	1.06831	-0.18334	-0.6696
H	3.60195	4.95684	-1.20612	O	1.68347	1.95795	0.9393
H	4.28212	5.0456	0.40484	C	2.7422	2.52922	0.41018
C	2.45652	3.88108	0.29859	C	3.02424	2.50686	-0.98816
H	2.61294	3.48623	1.30655	C	3.68272	3.1952	1.25146
H	1.76546	4.73254	0.37586	C	4.17556	3.08433	-1.49686
C	1.34783	3.1341	-1.83321	H	2.31791	2.02917	-1.65577
H	1.70185	4.13263	-2.10624	C	4.83409	3.7702	0.74404
H	0.25572	3.16243	-1.8028	H	3.46861	3.25327	2.3157
C	1.80431	2.09322	-2.8592	C	5.08905	3.7054	-0.6337
H	1.27656	1.15167	-2.67662	H	4.38614	3.06497	-2.56009
H	1.56244	2.43053	-3.87761	H	5.54376	4.27117	1.39216
C	4.12711	2.96529	-3.094	N	6.30625	4.27593	-1.16823
H	3.49261	3.83974	-3.25786	O	7.09232	4.8266	-0.38424
H	4.61857	2.76145	-4.05244	O	6.51414	4.18058	-2.38762
C	5.21025	3.28856	-2.04441	Cu	1.92869	-2.51597	0.4676
H	6.0016	2.54211	-2.12711	O	0.06038	-2.98478	0.819
H	5.6629	4.26374	-2.2882	N	3.9476	-2.15355	-0.09433
C	5.66403	2.86	0.35617	N	1.81764	-3.17027	-1.57155
H	5.12808	2.83706	1.31098	N	2.86048	-4.70645	0.62629
H	6.48387	3.59143	0.45484	N	2.45115	-1.30183	2.08406
C	6.27092	1.46912	0.08207	N	1.62153	0.51815	3.33882
H	6.76151	1.13772	1.01074	N	0.61042	-1.60506	3.46015
C	5.61189	-0.69932	-0.70233	C	4.10545	-2.25414	-1.57408
H	1.07738	2.34866	0.02943	H	4.65333	-3.17099	-1.80712
H	3.51359	0.99364	-3.22487	H	4.71787	-1.42486	-1.94722
H	5.03146	-2.53118	-1.3881	C	2.7429	-2.24965	-2.27442
H	7.16498	-2.06545	-0.76315	H	2.29414	-1.25609	-2.21681
H	7.65143	-0.47295	-0.41804	H	2.8702	-2.52175	-3.33296
H	3.6919	-1.60008	-0.77428	C	2.10047	-4.61287	-1.74483
H	7.06569	1.57024	-0.6734	H	3.07423	-4.72048	-2.23152
H	3.56074	0.27759	1.52431	H	1.3747	-5.07215	-2.42854
H	2.06818	-0.75916	0.08853	C	2.09207	-5.39549	-0.41663
L¹-2OH-^{0s}TS				H	1.06723	-5.47033	-0.0381
E: -3431.59981104 a.u.				H	2.45429	-6.41683	-0.62104
O	-1.44907	-0.00636	-0.91062	C	4.31638	-4.58778	0.4264
O	-3.50642	6.93471	1.06912	H	4.57331	-4.94016	-0.5774
N	-3.50649	6.43396	-0.05796	H	4.87244	-5.23108	1.11997
C	-2.5869	5.32014	-0.31362	C	4.78675	-3.13713	0.63459
O	-4.24141	6.79787	-0.97995	H	4.71647	-2.89905	1.69754
C	-1.74349	4.88216	0.7109	H	5.84332	-3.03794	0.34101
C	-2.5845	4.71776	-1.57407	C	4.1512	-0.75514	0.37307
C	-0.89979	3.79878	0.48619	H	3.54336	-0.11656	-0.27045
H	-1.74894	5.39729	1.66406	H	5.20584	-0.46207	0.26167
C	-1.74618	3.63073	-1.7957	C	3.70379	-0.57209	1.8187
H	-3.23168	5.10011	-2.35407	H	3.63394	0.50141	1.99575
C	-0.92043	3.16171	-0.76381	C	1.60136	-0.77985	2.93604
H	-0.21576	3.44256	1.24702	H	0.8533	-2.95937	-1.82029
				H	2.6406	-5.09856	1.53647

H	0.13096	-1.24577	4.27688	C	-1.62189	0.69293	-2.61476
H	0.85344	0.80321	3.93431	C	-2.62544	2.91837	-2.58749
H	1.75284	1.19232	2.55267	C	-0.36361	1.25611	-2.77112
H	0.89723	-2.5714	3.56922	H	-1.7408	-0.38143	-2.56163
H	4.46698	-0.95193	2.51322	C	-1.36646	3.47942	-2.7461
Cu	-2.95935	-1.05201	-0.09441	H	-3.51185	3.53877	-2.52392
N	-5.12944	-0.7702	-0.47249	C	-0.22644	2.65536	-2.8184
N	-3.26616	0.44141	1.2597	H	0.51949	0.63381	-2.85717
N	-3.78314	-2.27939	1.56293	H	-1.23935	4.55445	-2.82354
N	-3.14941	-2.26013	-1.71967	O	0.97098	3.27495	-2.96561
N	-2.8646	-4.2029	-3.027	P	2.41004	2.69016	-2.29781
N	-1.35196	-3.71472	-1.34726	O	2.79526	1.39651	-2.95485
C	-5.50925	0.50682	0.18234	O	2.25043	2.7562	-0.78921
H	-6.12151	0.27224	1.05805	O	-5.5382	-1.93312	1.13159
H	-6.14099	1.11618	-0.47715	C	-6.69477	-1.9518	0.62815
C	-4.26687	1.3147	0.60554	C	-6.95843	-1.36203	-0.6764
H	-3.7756	1.75372	-0.26834	C	-7.80616	-2.56229	1.34081
H	-4.56623	2.14487	1.2603	C	-8.2259	-1.39041	-1.21231
C	-3.60295	-0.04786	2.61653	H	-6.12699	-0.90254	-1.20359
H	-4.66259	0.13672	2.81468	C	-9.06461	-2.58508	0.79064
H	-3.03927	0.51643	3.36793	H	-7.60082	-2.99804	2.3129
C	-3.27849	-1.54128	2.74943	C	-9.26164	-1.99969	-0.47796
H	-2.19343	-1.67972	2.77642	H	-8.44523	-0.95587	-2.18005
H	-3.69904	-1.93371	3.68714	H	-9.90617	-3.03737	1.30115
C	-5.26473	-2.34794	1.47032	N	-10.61616	-2.02837	-1.06002
H	-5.69091	-1.6864	2.2292	O	-11.5041	-2.57332	-0.40283
H	-5.6219	-3.35611	1.7095	O	-10.77126	-1.50569	-2.16357
C	-5.79805	-1.96248	0.07299	Cu	-0.09748	1.08218	1.63099
H	-5.61429	-2.79425	-0.60894	O	1.30617	0.18781	0.64698
H	-6.88951	-1.82862	0.13259	N	-1.58819	2.08557	2.79957
C	-5.07664	-0.70785	-1.94607	N	0.68214	3.0476	1.4644
H	-4.55446	0.21804	-2.20827	N	1.00985	1.23163	3.6596
H	-6.08139	-0.65758	-2.39552	N	-1.64804	-0.22899	1.25503
C	-4.32007	-1.9118	-2.53782	N	-2.61345	-2.27997	0.55864
H	-4.0307	-1.64726	-3.56613	N	-0.49849	-1.65185	-0.16528
C	-2.47529	-3.34817	-2.01966	C	-1.41051	3.56076	2.66385
H	-2.3128	0.85995	1.27378	H	-0.95969	3.9455	3.58199
H	-3.3821	-3.2146	1.55244	H	-2.38495	4.05607	2.56855
H	-1.13156	-4.70322	-1.36997	C	-0.52177	3.89927	1.4616
H	-2.16995	-4.82939	-3.41171	H	-1.05408	3.70499	0.52424
H	-3.54963	-3.89218	-3.70012	H	-0.27419	4.97163	1.48021
H	-0.98101	-3.24308	-0.47422	C	1.66822	3.36215	2.52424
H	-5.00845	-2.76673	-2.61026	H	1.2336	4.09352	3.21487
H	-1.15816	-0.40102	-1.74823	H	2.54795	3.8394	2.07776
H	-0.21538	-2.36427	1.51339	C	2.13246	2.11334	3.29643
L¹-2OH-^{os}PC				H	2.79523	1.51997	2.66124
E : -3431.62280513 a.u.				H	2.70911	2.44286	4.17563
O	3.39199	3.87081	-2.82856	C	0.06461	1.73641	4.66942
O	-4.13636	-0.30898	-2.27772	H	0.30171	2.78084	4.89623
N	-4.04701	0.92993	-2.2812	H	0.15872	1.19488	5.61966
C	-2.74201	1.52459	-2.50721	C	-1.39567	1.6048	4.19146
O	-5.01173	1.67717	-2.07897	H	-1.67821	0.54901	4.20997
				H	-2.06706	2.13747	4.88331

C	-2.87693	1.63953	2.21155
H	-2.99358	2.17539	1.264
H	-3.71918	1.91889	2.86302
C	-2.89039	0.13789	1.93007
H	-3.77857	-0.066	1.31758
C	-1.60248	-1.3558	0.57055
H	1.15489	3.07611	0.54665
H	1.37347	0.30872	3.88579
H	-0.3217	-2.6219	-0.38814
H	-2.65387	-2.88999	-0.24861
H	-3.53831	-2.0234	0.89428
H	0.31758	-1.01705	-0.03879
H	-3.02242	-0.43367	2.86174
Cu	4.40301	-1.62006	-0.24941
N	6.65685	-1.8991	-0.39003
N	4.68104	-0.48715	-1.99246
N	4.5187	-3.34503	-1.73541
N	4.66884	-1.76576	1.74851
N	4.02723	-2.69159	3.83488
N	2.49474	-1.49253	2.5879
C	7.09962	-0.95387	-1.431
H	7.35814	-1.52589	-2.3267
H	8.02195	-0.43356	-1.13318
C	6.02724	0.10025	-1.78635
H	5.93237	0.82413	-0.96997
H	6.3664	0.65544	-2.67438
C	4.56571	-1.3242	-3.21326
H	5.55466	-1.45701	-3.66501
H	3.95274	-0.80147	-3.95535
C	3.93075	-2.69558	-2.92996
H	2.86327	-2.56227	-2.72323
H	4.01951	-3.3209	-3.83303
C	5.93056	-3.77636	-1.88628
H	6.31681	-3.38628	-2.83219
H	6.00063	-4.86897	-1.96153
C	6.83148	-3.31676	-0.72048
H	6.56902	-3.90087	0.16686
H	7.88038	-3.56458	-0.96548
C	7.02515	-1.52442	0.97835
H	6.98736	-0.43191	1.03731
H	8.05498	-1.8316	1.23478
C	6.06974	-2.09545	2.04082
H	6.3832	-1.67482	3.00877
C	3.78188	-1.98176	2.6801
H	4.01334	0.2861	-2.11588
H	3.94396	-4.1417	-1.47523
H	1.7675	-2.15979	2.82544
H	3.47088	-2.48416	4.65285
H	4.95611	-3.03773	4.02253
H	2.25841	-0.92825	1.75025
H	6.20498	-3.18672	2.10656
H	3.31902	4.67157	-2.28367
H	1.74308	0.8487	0.07476

L¹-OH-³RC

E : -3355.62238768 a.u.

O	3.58333	-0.86241	-2.15049
O	4.95693	-1.52614	3.51165
N	4.53019	-2.386	2.73581
C	3.15492	-2.23148	2.24273
O	5.18683	-3.34301	2.3273
C	2.29906	-1.34509	2.89914
C	2.76784	-2.9383	1.10491
C	1.01991	-1.14314	2.38664
H	2.63344	-0.83205	3.79317
C	1.49512	-2.71741	0.58468
H	3.46561	-3.60663	0.61582
C	0.64426	-1.81421	1.22022
H	0.32501	-0.46796	2.87347
H	1.17128	-3.2202	-0.3204
O	-0.62786	-1.6183	0.6695
P	-1.03178	-0.20066	-0.06636
O	0.13012	0.47785	-0.7076
O	-2.25927	-0.55349	-0.92049
O	-1.56942	0.58331	1.28603
C	-2.12738	1.8494	1.30482
C	-2.89148	2.16214	2.4353
C	-1.93808	2.78646	0.28179
C	-3.49802	3.40987	2.53642
H	-2.99456	1.4276	3.22758
C	-2.55114	4.03383	0.37964
H	-1.30702	2.55144	-0.56774
C	-3.33148	4.3264	1.49694
H	-4.09308	3.67876	3.40111
H	-2.42368	4.78253	-0.39325
N	-4.00385	5.63407	1.5766
O	-3.86712	6.4015	0.6227
O	-4.67047	5.87046	2.58265
Cu	-4.09717	-1.28553	-0.50833
N	-5.95742	-2.00183	0.16243
N	-3.35131	-2.88776	0.60578
N	-4.39498	-2.94193	-2.05785
N	-5.17294	0.38109	-0.92303
N	-5.78443	2.28352	-2.16827
N	-3.76579	1.2189	-2.56989
C	-5.74127	-3.03734	1.21995
H	-5.9604	-4.01766	0.79223
H	-6.44939	-2.89485	2.04438
C	-4.30103	-2.99502	1.74442
H	-4.14686	-2.11328	2.3756
H	-4.10134	-3.88102	2.36203
C	-3.20541	-4.12594	-0.21682
H	-3.98967	-4.82995	0.07424
H	-2.2532	-4.61454	0.01413
C	-3.27064	-3.84263	-1.72595
H	-2.35585	-3.33535	-2.04697
H	-3.32726	-4.80406	-2.25721

C	-5.75289	-3.49973	-1.85479	H	7.30918	-3.80879	-0.29055
H	-5.67546	-4.47043	-1.35655	H	7.85498	-2.45386	0.55303
H	-6.24923	-3.69426	-2.81207	H	4.54848	-2.20715	-1.80312
C	-6.64507	-2.54002	-1.04479	H	7.78442	-0.05943	0.28271
H	-6.91101	-1.69018	-1.67559	H	2.64339	-0.90269	-1.91465
H	-7.57875	-3.04476	-0.75807				
C	-6.59536	-0.77088	0.70508	L¹-OH-³TS			
H	-6.06159	-0.51939	1.62712	E : -3355.60170457 a.u.			
H	-7.64564	-0.9597	0.96791	O	1.67039	-1.24889	0.06904
C	-6.49094	0.3946	-0.28387	O	2.97622	5.38219	3.15639
H	-6.66331	1.32104	0.28378	N	3.06716	4.29166	3.71841
C	-4.91645	1.28912	-1.84972	C	2.27845	3.17485	3.16596
H	-2.42926	-2.60412	0.94215	O	3.77708	4.05537	4.69528
H	-4.28631	-2.61109	-3.01346	C	1.4515	3.40558	2.06658
H	-3.47656	2.02016	-3.11406	C	2.38762	1.91338	3.75221
H	-5.56678	2.96717	-2.87964	C	0.72896	2.3456	1.51984
H	-6.65176	2.41475	-1.67201	H	1.37185	4.40568	1.65641
H	-3.01744	0.64557	-2.17944	C	1.67083	0.85426	3.20208
H	-7.29355	0.32336	-1.03339	H	3.02337	1.77579	4.61883
Cu	4.526	0.37702	-1.02838	C	0.85257	1.06836	2.08465
N	5.57892	1.83035	0.11532	H	0.06914	2.5101	0.67697
N	2.89652	1.77397	-0.78899	H	1.72799	-0.13828	3.6387
N	5.07718	1.83357	-2.68234	O	0.14784	-0.02448	1.6187
N	5.89159	-0.91262	-0.17169	P	-0.0427	-0.40741	-0.00884
N	7.32133	-2.79791	-0.2328	O	0.41762	0.55422	-1.06622
N	5.30463	-2.7976	-1.39068	O	-0.80734	-1.73148	-0.07579
C	4.6275	2.86605	0.61446	O	-1.87177	0.51248	0.19387
H	4.7541	3.7718	0.01822	C	-2.29924	1.56881	-0.53385
H	4.87048	3.14391	1.64735	C	-2.82005	2.69688	0.13435
C	3.17288	2.38488	0.53071	C	-2.26968	1.57099	-1.9444
H	2.98399	1.61374	1.28544	C	-3.31447	3.78721	-0.57625
H	2.50136	3.22921	0.74835	H	-2.81719	2.71269	1.22074
C	2.86673	2.72721	-1.93112	C	-2.75731	2.65651	-2.66067
H	3.18433	3.71337	-1.57727	H	-1.84494	0.72135	-2.46463
H	1.8379	2.8459	-2.289	C	-3.28139	3.7533	-1.97061
C	3.74209	2.27937	-3.11769	H	-3.7149	4.65766	-0.0698
H	3.27921	1.41702	-3.60502	H	-2.73986	2.67069	-3.74412
H	3.78781	3.10568	-3.84374	N	-3.80276	4.89509	-2.73148
C	5.98996	2.85934	-2.14064	O	-3.75026	4.83342	-3.96211
H	5.4415	3.79754	-2.01199	O	-4.26337	5.84452	-2.09644
H	6.80739	3.08186	-2.83684	Cu	-3.01796	-1.31581	0.48315
C	6.60265	2.39648	-0.80573	N	-5.11646	-1.30506	1.16717
H	7.32921	1.60602	-1.00792	N	-2.64637	-0.99934	2.48131
H	7.14202	3.22591	-0.32391	N	-3.24711	-3.47625	1.26796
C	6.17881	1.05713	1.23548	N	-3.93864	-1.33089	-1.3101
H	5.36829	0.82027	1.93127	N	-4.15849	-1.73912	-3.62165
H	6.91857	1.66488	1.77664	N	-2.2511	-2.41344	-2.48517
C	6.80834	-0.25137	0.75492	C	-5.12664	-0.76795	2.552
H	6.999	-0.85636	1.65409	H	-5.35336	-1.58755	3.23893
C	6.1718	-2.13615	-0.58105	H	-5.92743	-0.02899	2.68288
H	2.00686	1.27169	-0.74573	C	-3.77497	-0.13081	2.91188
H	5.51616	1.30281	-3.42978	H	-3.65128	0.81776	2.383
H	5.6818	-3.5359	-1.97149	H	-3.73352	0.07863	3.98959

C	-6.28215	3.06407	-1.06246
H	-5.48019	3.68119	-1.46988
H	-7.09907	3.75087	-0.81224
C	-6.74893	2.05369	-2.11706
H	-7.65996	1.54623	-1.78182
H	-6.99516	2.59686	-3.0415
C	-4.46717	1.47738	-2.97411
H	-4.5072	2.56549	-3.08531
H	-4.39274	1.07364	-3.98977
C	-3.20615	1.06591	-2.19148
H	-3.02198	-0.003	-2.32594
H	-2.33768	1.60528	-2.5942
C	-3.3479	2.70799	-0.30094
H	-3.41405	3.3568	-1.1791
H	-2.40148	2.94623	0.19559
C	-4.50466	2.98485	0.66981
H	-4.28342	2.52572	1.63798
H	-4.62125	4.06595	0.83579
C	-6.8402	2.34285	1.22305
H	-7.79627	2.22173	0.70631
H	-6.87265	3.29064	1.77868
C	-6.65998	1.15359	2.16777
H	-7.56155	1.11695	2.79426
C	-6.9934	-1.20262	1.71839
H	-6.10808	0.22218	-2.81691
H	-2.52881	0.83687	-0.2858
H	-7.0204	-3.19333	1.26066
H	-8.26378	-2.20629	2.98964
H	-7.78144	-0.67386	3.55993
H	-6.28108	-2.17301	0.09107
H	-5.80801	1.30894	2.84509
Cu	3.50623	-1.06815	-0.20226
N	5.48727	-1.46643	-0.80025
N	3.31633	-0.33974	-2.11104
N	3.10669	-3.04293	-1.23746
N	4.30075	-1.28287	1.67095
N	4.27994	-1.34428	4.02569
N	2.30606	-1.64515	2.81505
C	5.73574	-0.81376	-2.1242
H	5.73866	-1.5883	-2.89361
H	6.73054	-0.35361	-2.14163
C	4.65174	0.23001	-2.41623
H	4.78151	1.11332	-1.78219
H	4.7195	0.56422	-3.46045
C	2.83997	-1.373	-3.07429
H	3.67373	-1.66301	-3.71962
H	2.07563	-0.93435	-3.72405
C	2.25478	-2.60102	-2.36591
H	1.27757	-2.35345	-1.94319
H	2.10127	-3.39916	-3.10676
C	4.42488	-3.59976	-1.62504
H	4.57466	-3.47081	-2.70135
H	4.46182	-4.67954	-1.44246

C	5.58164	-2.95119	-0.83851
H	5.54759	-3.30549	0.19384
H	6.54659	-3.2604	-1.26543
C	6.28999	-0.84476	0.2831
H	6.21516	0.23867	0.14829
H	7.35079	-1.11757	0.18978
C	5.76924	-1.22048	1.67584
H	6.14811	-0.45093	2.36347
C	3.67773	-1.43324	2.81463
H	2.59146	0.39682	-2.03396
H	2.5712	-3.72922	-0.70339
H	1.86991	-1.68306	3.73086
H	3.80766	-1.63164	4.87152
H	5.24548	-1.06782	4.12496
H	1.96896	-2.42099	2.23525
H	6.18623	-2.18169	2.0065
H	1.56984	-0.45787	1.39162

L¹-OH-¹TS

E : -3355.53791901 a.u.

O	1.50673	-1.29137	-0.03834
O	2.89574	5.53856	3.0613
N	2.99442	4.46205	3.64845
C	2.24147	3.3184	3.10139
O	3.68252	4.26105	4.64847
C	1.44275	3.50768	1.97422
C	2.35423	2.07354	3.72155
C	0.7488	2.42406	1.43678
H	1.36245	4.49481	1.53399
C	1.6664	0.99071	3.18188
H	2.97143	1.96664	4.60569
C	0.8724	1.16475	2.04016
H	0.11236	2.55867	0.57167
H	1.73021	0.00946	3.64207
O	0.19813	0.04554	1.59105
P	-0.07433	-0.33986	-0.02434
O	0.36395	0.57285	-1.13307
O	-0.91783	-1.64514	-0.00303
O	-1.81533	0.66942	0.25236
C	-2.28736	1.66445	-0.50804
C	-2.83759	2.80452	0.12764
C	-2.31237	1.60421	-1.92331
C	-3.41893	3.82903	-0.61012
H	-2.78835	2.87242	1.21088
C	-2.88552	2.62692	-2.66409
H	-1.86028	0.75634	-2.42216
C	-3.44294	3.72771	-2.00294
H	-3.84339	4.70249	-0.12902
H	-2.91076	2.59241	-3.74701
N	-4.06179	4.79775	-2.79232
O	-4.06927	4.67071	-4.0193
O	-4.5409	5.7551	-2.18314
Cu	-2.94068	-1.45502	0.50136

H	-3.71667	4.65679	-0.06957	C	4.22562	1.82402	-0.31349
H	-2.74101	2.66993	-3.74376	H	4.03106	1.63688	0.74781
N	-3.80428	4.89419	-2.73126	H	4.21593	2.91232	-0.46031
O	-3.75147	4.83265	-3.96189	C	3.05001	1.52865	-2.5209
O	-4.26524	5.84352	-2.09627	H	3.95282	2.07847	-2.80033
Cu	-3.01801	-1.31577	0.48346	H	2.20496	2.20842	-2.66384
N	-5.11642	-1.3066	1.16772	C	2.85847	0.29973	-3.41691
N	-2.64615	-0.9996	2.48151	H	1.84512	-0.08691	-3.2789
N	-3.24585	-3.47668	1.26804	H	2.97406	0.60199	-4.46788
N	-3.93876	-1.33118	-1.30964	C	5.22901	-0.48052	-3.29663
N	-4.15874	-1.73923	-3.62112	H	5.32617	0.56679	-3.59442
N	-2.25124	-2.41356	-2.48497	H	5.60928	-1.06901	-4.13917
C	-5.12661	-0.7697	2.55262	C	6.11459	-0.77672	-2.0725
H	-5.35274	-1.5895	3.2395	H	6.20299	-1.85857	-1.96075
H	-5.92777	-0.03119	2.68378	H	7.12603	-0.37894	-2.23951
C	-3.77523	-0.13183	2.91235	C	6.07598	-0.91414	0.40409
H	-3.65216	0.81687	2.38357	H	5.64594	-0.39898	1.26909
H	-3.73374	0.0775	3.99009	H	7.16889	-0.81207	0.46733
C	-2.45458	-2.2473	3.27032	C	5.68182	-2.3984	0.43761
H	-3.32721	-2.39034	3.91319	H	5.80485	-2.75525	1.47028
H	-1.59296	-2.14354	3.93875	C	3.796	-3.76345	-0.16136
C	-2.2511	-3.46743	2.35998	H	2.21945	1.29694	-0.66704
H	-1.26787	-3.40941	1.88524	H	3.53254	-1.64024	-3.50951
H	-2.28731	-4.37983	2.97459	H	2.07766	-4.80937	-0.55893
C	-4.64613	-3.71816	1.68069	H	4.10215	-5.80736	-0.05726
H	-4.70578	-3.68967	2.77253	H	5.43746	-4.86652	0.45005
H	-4.97836	-4.72093	1.38807	H	1.93741	-3.10129	-0.64893
C	-5.61837	-2.69146	1.06381	H	6.37714	-2.97978	-0.18651
H	-5.74132	-2.92219	0.00437	H	1.78799	-1.6443	0.94895
H	-6.60634	-2.79441	1.5379				
C	-5.68596	-0.38165	0.1619				
H	-5.27554	0.6115	0.36845	L³-RC1			
H	-6.78097	-0.31207	0.249	E : -2552.56535424 a.u.			
C	-5.30817	-0.80354	-1.26895	O	-2.25306	-0.09259	-1.60143
H	-5.41577	0.08144	-1.91203	O	-0.39533	6.49275	0.17246
C	-3.47481	-1.80326	-2.44278	N	-0.45346	5.95078	-0.93365
H	-1.78378	-0.45337	2.46186	C	0.07303	4.58323	-1.04974
H	-2.96263	-4.14041	0.55199	O	-0.94004	6.46493	-1.94094
H	-1.78697	-2.44975	-3.38344	C	0.68236	3.99464	0.0599
H	-3.88025	-2.31734	-4.40219	C	-0.05946	3.90257	-2.2619
H	-5.10784	-1.39857	-3.6486	C	1.1375	2.68161	-0.02947
H	-1.63059	-2.23277	-1.6895	H	0.80548	4.56951	0.97032
H	-6.0223	-1.55757	-1.6331	C	0.39145	2.58903	-2.34763
Cu	3.49911	-0.83786	-0.76384	H	-0.50996	4.39996	-3.1126
N	5.54417	-0.24113	-0.81006	C	0.97009	1.97453	-1.22898
N	3.1459	1.15399	-1.08022	H	1.63293	2.21293	0.81325
N	3.7997	-0.78102	-3.03531	H	0.31609	2.03111	-3.27558
N	4.29997	-2.55333	-0.0279	O	1.38843	0.67486	-1.39113
N	4.46349	-4.8956	0.18811	P	1.2354	-0.52775	-0.26258
N	2.545	-3.92156	-0.68929	O	-0.05077	-0.29632	0.52205
C	5.59198	1.2513	-0.72121	O	1.49399	-1.80332	-1.00461
H	5.89053	1.64274	-1.69628	O	2.40183	-0.20008	0.83469
H	6.36389	1.56993	-0.01101	C	3.75691	-0.4779	0.69715
				C	4.40284	-0.52996	-0.54167

C	4.46	-0.65865	1.89146	C	-2.81327	-5.16564	-1.19076
C	5.7736	-0.77256	-0.58019	H	-2.05699	-5.37711	-0.42892
H	3.85078	-0.38941	-1.46313	H	-2.97036	-6.08566	-1.76452
C	5.82894	-0.89688	1.85421	H	-2.9309	-3.68569	-2.72189
H	3.92655	-0.6091	2.83473				
C	6.4685	-0.95306	0.61501	L³-RC2			
H	6.30519	-0.82031	-1.52273	E : -2552.55896771 a.u.			
H	6.40056	-1.04094	2.76275	O	-1.93417	0.18175	-2.48116
N	7.91628	-1.21028	0.56894	O	-0.24103	6.11341	2.04788
O	8.50407	-1.36217	1.64075	N	-0.30883	5.96923	0.82583
O	8.45386	-1.25965	-0.53814	C	0.10689	4.67117	0.26885
Cu	-1.98048	0.30885	0.25509	O	-0.71356	6.82492	0.03933
N	-3.45065	-1.2598	1.14629	C	0.59522	3.69005	1.13351
N	-3.72804	1.53834	0.37468	C	-0.00741	4.45205	-1.10602
N	-1.85443	0.84158	2.26879	C	0.96592	2.45158	0.6128
N	-2.27748	-4.12933	-2.08697	H	0.69134	3.90629	2.1908
N	-0.03395	-4.15387	-1.41768	C	0.35665	3.21241	-1.62329
N	-0.89695	-2.32588	-2.5545	H	-0.37942	5.24137	-1.7482
C	-4.77596	-0.61137	1.15477	C	0.83579	2.22086	-0.76191
H	-5.01629	-0.28999	2.17251	H	1.3608	1.67932	1.26331
H	-5.56923	-1.3165	0.87473	H	0.27197	2.99565	-2.68222
C	-4.8523	0.58622	0.18659	O	1.22421	1.03264	-1.34943
H	-4.77712	0.23594	-0.84588	P	0.9085	-0.4707	-0.81694
H	-5.82163	1.08817	0.31548	O	-0.40438	-0.55791	-0.05266
C	-3.73703	2.31716	1.64427	O	1.19197	-1.41177	-1.95257
H	-4.52311	1.9205	2.29285	O	2.02053	-0.71938	0.39224
H	-3.98842	3.36634	1.45647	C	3.4057	-0.60859	0.26806
C	-2.36802	2.2312	2.33824	C	4.0696	-0.55147	-0.96156
H	-1.64467	2.8654	1.81575	C	4.10953	-0.57903	1.47658
H	-2.44301	2.59253	3.37295	C	5.46035	-0.46071	-0.9726
C	-2.5293	-0.13321	3.17141	H	3.51821	-0.58664	-1.89337
H	-3.4509	0.32462	3.54047	C	5.49697	-0.49426	1.46428
H	-1.90764	-0.32759	4.05239	H	3.56249	-0.6175	2.41328
C	-2.83653	-1.46683	2.46822	C	6.15527	-0.43651	0.23523
H	-1.89943	-2.0091	2.30262	H	6.00624	-0.41348	-1.90716
H	-3.45812	-2.07781	3.14253	H	6.06865	-0.46807	2.38391
C	-3.34047	-2.40625	0.22241	N	7.62515	-0.35002	0.21555
H	-2.2702	-2.5801	0.08322	O	8.20938	-0.3372	1.29958
H	-3.72492	-2.05696	-0.7412	O	8.17947	-0.30007	-0.88237
C	-1.06634	-3.54286	-2.01722	Cu	-2.30129	-0.18987	-0.64687
H	-3.69974	2.16275	-0.42863	N	-3.3322	-1.05248	1.10635
H	-0.84754	0.8216	2.42376	N	-4.27097	0.19557	-1.26287
H	0.06168	-1.98402	-2.48749	N	-2.68845	1.74932	0.50191
H	0.77945	-3.5781	-1.18093	N	-0.54349	-5.32306	0.0818
H	0.01284	-5.15807	-1.32109	N	0.90778	-3.61095	0.67719
H	-1.58392	-1.56967	-2.33436	N	0.47493	-4.02128	-1.56589
H	-1.93445	0.63353	-2.16113	C	-4.8	-1.04505	0.79959
C	-4.02767	-3.72137	0.62968	H	-5.2657	-0.21714	1.33836
H	-5.04504	-3.52135	0.99023	H	-5.2795	-1.95411	1.18103
H	-3.48828	-4.17975	1.46919	C	-5.08249	-0.89735	-0.70526
C	-4.13501	-4.74149	-0.52353	H	-4.80392	-1.81054	-1.23972
H	-4.81386	-4.35655	-1.2987	H	-6.16023	-0.7387	-0.8588
H	-4.60913	-5.65264	-0.1403	C	-4.71545	1.57125	-0.93267

H	-5.48705	1.506	-0.15895	O	0.27017	1.47122	-0.5967
H	-5.18912	2.03718	-1.8037	C	1.11012	2.42623	-0.12729
C	-3.55473	2.46192	-0.4557	C	1.53653	2.47086	1.21609
H	-2.92258	2.71792	-1.3104	C	1.49306	3.45583	-1.01188
H	-3.97356	3.39422	-0.04697	C	2.32555	3.52561	1.65842
C	-3.26354	1.39759	1.81204	H	1.22636	1.68038	1.88978
H	-4.33868	1.60092	1.80385	C	2.27321	4.51999	-0.56551
H	-2.85073	2.02208	2.61433	H	1.20293	3.38688	-2.05669
C	-2.98498	-0.07233	2.18147	C	2.67921	4.5454	0.76907
H	-1.91347	-0.1906	2.36862	H	2.66093	3.57877	2.68756
H	-3.51943	-0.32005	3.11249	H	2.58112	5.313	-1.23657
C	-2.85646	-2.40351	1.52474	N	3.48858	5.6698	1.24973
H	-3.36799	-2.68507	2.46078	O	3.74912	6.57288	0.4511
H	-1.79012	-2.30039	1.74673	O	3.85623	5.65152	2.42645
C	0.27523	-4.30817	-0.27794	Cu	-1.54428	-1.69639	0.45398
H	-4.07914	0.08585	-2.25963	N	-3.73087	-1.10042	0.47468
H	-1.80913	2.24644	0.61164	N	-2.07676	-2.73411	2.13574
H	0.93353	-3.12115	-1.81488	N	-2.33461	-3.43626	-0.57209
H	1.42479	-2.76025	0.47136	N	-3.88214	3.61812	-1.17023
H	1.03255	-4.00662	1.59747	N	-1.99928	2.3947	-1.86456
H	-0.19565	-4.35753	-2.2457	N	-1.77588	4.12556	-0.35853
H	-1.12976	-0.24123	-2.82185	C	-4.29766	-1.67163	1.71825
C	-3.07206	-3.50955	0.48099	H	-4.84113	-2.59017	1.4831
H	-2.44452	-3.31324	-0.39851	H	-5.03411	-0.99525	2.17081
H	-4.10754	-3.48679	0.12617	C	-3.19218	-1.95993	2.74877
C	-2.83221	-4.93729	1.01583	H	-2.75774	-1.02143	3.10725
H	-3.25064	-5.65266	0.29533	H	-3.61499	-2.4894	3.61354
H	-3.3997	-5.08655	1.94401	C	-2.39797	-4.15737	1.80192
C	-1.37539	-5.34204	1.29929	H	-3.47396	-4.30293	1.93137
H	-0.9228	-4.67983	2.03957	H	-1.90555	-4.83272	2.50911
H	-1.34445	-6.35365	1.71423	C	-1.97464	-4.51714	0.3665
H	-0.873	-5.90831	-0.67764	H	-0.88733	-4.62337	0.31268

L³-1-TS1

E : -2552.50718582 a.u.

O	0.59773	-2.13346	-0.16081	H	-4.35637	-3.85056	-0.17073
O	6.62692	-4.18919	-1.64889	H	-4.01854	-3.6003	-1.86929
N	6.27667	-3.65766	-0.5942	C	-4.17691	-1.75669	-0.77163
C	5.13312	-2.73356	-0.64041	H	-3.69597	-1.2201	-1.59479
O	6.81336	-3.85083	0.49816	H	-5.2669	-1.6879	-0.91375
C	4.48542	-2.5166	-1.85878	C	-3.76414	0.38576	0.43915
C	4.72773	-2.10072	0.53526	H	-2.933	0.70121	-0.19582
C	3.39254	-1.65794	-1.89652	H	-3.51909	0.71749	1.45277
H	4.83814	-3.01979	-2.75071	C	-2.55758	3.36365	-1.14451
C	3.6366	-1.23678	0.49097	H	-1.26877	-2.69016	2.75576
H	5.26842	-2.28041	1.4565	H	-1.77829	-3.50158	-1.4213
C	2.9673	-1.03304	-0.72118	H	-0.76599	4.00059	-0.36604
H	2.85976	-1.46846	-2.82197	H	-1.107	1.96487	-1.53949
H	3.30807	-0.70887	1.38101	H	-2.54875	1.86844	-2.52711
O	1.93186	-0.1239	-0.79132	H	-2.16665	4.69135	0.38163
P	0.38939	-0.31475	-0.20355	H	1.20888	-2.38211	0.5526
O	-0.9107	-0.56226	-1.0751	C	-5.08426	1.05011	-0.03279
O	0.03732	-0.23424	1.30402	H	-5.23239	1.96854	0.54805
				H	-5.93504	0.40612	0.21938

C	-5.11588	1.39101	-1.54418
H	-6.08127	1.11244	-1.98264
H	-4.37591	0.78396	-2.07667
C	-4.92861	2.88136	-1.90425
H	-4.77081	2.98573	-2.98576
H	-5.85006	3.42085	-1.67138
H	-4.15807	4.52109	-0.80626

L³-1-IM

E : -2552.50991806 a.u.

O	0.69441	-2.30497	-0.33286
O	6.92938	-3.74959	-2.11043
N	6.56089	-3.37776	-0.99605
C	5.33917	-2.55929	-0.91749
O	7.13722	-3.64607	0.05899
C	4.64605	-2.26365	-2.09312
C	4.91059	-2.10354	0.32928
C	3.48499	-1.50181	-2.01621
H	5.01662	-2.63244	-3.04171
C	3.75065	-1.33528	0.40114
H	5.48535	-2.3417	1.21601
C	3.04256	-1.04809	-0.77099
H	2.91683	-1.25506	-2.9065
H	3.40207	-0.93999	1.35029
O	1.93585	-0.2209	-0.71879
P	0.42373	-0.6123	-0.15126
O	-0.95792	-0.70228	-0.9138
O	0.1003	-0.58381	1.38557
O	0.22688	1.3071	-0.38398
C	1.02466	2.25864	0.13235
C	1.37194	2.2882	1.50093
C	1.46911	3.30469	-0.70909
C	2.12086	3.33999	2.01039
H	1.03292	1.48114	2.14016
C	2.20899	4.36717	-0.19686
H	1.27285	3.24227	-1.77691
C	2.52259	4.37873	1.16289
H	2.39068	3.37859	3.05931
H	2.5603	5.16924	-0.83522
N	3.28784	5.49923	1.71118
O	3.59393	6.41774	0.94586
O	3.57744	5.46728	2.91023
Cu	-1.77341	-1.23371	0.87287
N	-3.856	-1.03066	0.30797
N	-2.54871	-1.79243	2.70376
N	-2.10516	-3.34083	0.3744
N	-3.66617	3.08481	-2.26452
N	-1.61369	1.93993	-2.28041
N	-1.85125	3.87296	-1.05498
C	-4.67625	-1.27865	1.52292
H	-5.06538	-2.29882	1.49029
H	-5.55283	-0.61952	1.55047
C	-3.84555	-1.07138	2.80186

H	-3.61219	-0.00963	2.93425
H	-4.42377	-1.39631	3.67785
C	-2.65438	-3.28453	2.79645
H	-3.71511	-3.54911	2.75845
H	-2.28268	-3.62595	3.76808
C	-1.88561	-4.00004	1.66863
H	-0.81037	-3.94773	1.86384
H	-2.17317	-5.06251	1.66983
C	-3.42689	-3.46034	-0.25523
H	-4.12162	-3.9184	0.45641
H	-3.40134	-4.12749	-1.12549
C	-3.96194	-2.08892	-0.73092
H	-3.35316	-1.75351	-1.57465
H	-4.99714	-2.21385	-1.08021
C	-3.9817	0.36532	-0.208
H	-3.03677	0.58658	-0.70613
H	-4.03001	1.00837	0.67669
C	-2.3773	2.95005	-1.88188
H	-1.90598	-1.44319	3.41324
H	-1.32991	-3.50635	-0.26581
H	-0.87283	3.81851	-0.77977
H	-0.81772	1.63835	-1.66396
H	-1.98665	1.23608	-2.90042
H	-2.42514	4.5674	-0.59884
H	1.49235	-2.61104	0.12855
C	-5.16788	0.67025	-1.16238
H	-5.64646	1.60696	-0.85276
H	-5.94027	-0.09993	-1.05787
C	-4.7458	0.77165	-2.64659
H	-5.55078	0.40813	-3.29606
H	-3.90015	0.09877	-2.83219
C	-4.42514	2.1939	-3.16409
H	-3.92209	2.13147	-4.13768
H	-5.3649	2.72445	-3.33578
H	-4.07532	3.997	-2.10965

L³-1-TS2

E : -2552.51298512 a.u.

O	-0.71555	-2.44588	0.19703
O	-7.04765	-3.57984	2.16168
N	-6.72039	-3.2192	1.03066
C	-5.44477	-2.49517	0.88732
O	-7.38142	-3.4193	0.01139
C	-4.67369	-2.25539	2.02632
C	-5.05051	-2.06262	-0.37871
C	-3.47529	-1.56261	1.89307
H	-5.01818	-2.60619	2.99142
C	-3.84997	-1.36574	-0.50776
H	-5.68368	-2.25934	-1.23547
C	-3.07208	-1.12174	0.62952
H	-2.85296	-1.35108	2.75578
H	-3.52889	-0.98378	-1.47203
O	-1.94076	-0.32979	0.52628

P	-0.4161	-0.78411	0.05669
O	0.93622	-0.86152	0.86328
O	-0.03604	-0.66557	-1.46238
O	-0.19674	1.19626	0.36951
C	-0.9702	2.15001	-0.16549
C	-1.13933	2.2682	-1.56488
C	-1.58522	3.1062	0.67704
C	-1.85707	3.32719	-2.09966
H	-0.69552	1.51214	-2.20247
C	-2.29797	4.17598	0.1423
H	-1.5396	2.96397	1.75462
C	-2.41596	4.28504	-1.24435
H	-1.98318	3.43485	-3.17071
H	-2.77417	4.91148	0.77999
N	-3.13508	5.42274	-1.81445
O	-3.59307	6.26536	-1.03667
O	-3.23761	5.48369	-3.04323
Cu	1.88069	-1.03648	-0.95168
N	3.88028	-0.91221	-0.24601
N	2.77559	-1.29699	-2.81045
N	2.2116	-3.22547	-0.78029
N	3.38261	2.76395	2.84538
N	1.36548	1.58965	2.54935
N	1.64733	3.66254	1.59557
C	4.7982	-0.95393	-1.41871
H	5.20615	-1.96214	-1.51585
H	5.65711	-0.28866	-1.26869
C	4.06135	-0.5573	-2.70792
H	3.81874	0.51074	-2.6951
H	4.70771	-0.74115	-3.57722
C	2.92134	-2.7568	-3.11872
H	3.98284	-3.01106	-3.04526
H	2.62753	-2.94929	-4.15584
C	2.09418	-3.65614	-2.178
H	1.03384	-3.58076	-2.43697
H	2.40475	-4.69966	-2.34234
C	3.49471	-3.41202	-0.09077
H	4.24769	-3.74334	-0.81349
H	3.4368	-4.20417	0.66605
C	3.95476	-2.11986	0.62492
H	3.28333	-1.93349	1.46695
H	4.97102	-2.26912	1.01648
C	3.93848	0.39188	0.48712
H	2.9552	0.52144	0.94084
H	4.03582	1.16229	-0.28437
C	2.13224	2.65368	2.34369
H	2.17583	-0.85456	-3.50511
H	1.40928	-3.51948	-0.226
H	0.70771	3.60718	1.20745
H	0.6412	1.36068	1.82063
H	1.70933	0.81502	3.098
H	2.23812	4.41472	1.27179
H	-1.53395	-2.72649	-0.24454

C	5.04464	0.56024	1.56255
H	5.52935	1.53471	1.42741
H	5.83625	-0.18193	1.41001
C	4.50781	0.44783	3.00814
H	5.27377	0.01906	3.66503
H	3.67461	-0.26425	3.03341
C	4.09911	1.78019	3.68066
H	3.52547	1.57633	4.594
H	5.00447	2.30476	3.99593
H	3.77795	3.69517	2.83454

L³-1-PC

E : -2552.58897952 a.u.

O	0.57042	-1.48276	-3.59169
O	7.60358	-0.6728	-0.96362
N	6.68846	-1.4787	-0.79849
C	5.32163	-1.03241	-1.10304
O	6.83553	-2.6347	-0.39467
C	5.10875	0.28012	-1.53194
C	4.26826	-1.93156	-0.95199
C	3.81447	0.69328	-1.82023
H	5.94987	0.95457	-1.63749
C	2.96979	-1.51301	-1.23489
H	4.47185	-2.94018	-0.61297
C	2.74582	-0.20094	-1.67619
H	3.61245	1.70301	-2.16034
H	2.13565	-2.19019	-1.08873
O	1.50048	0.3022	-1.96817
P	0.13771	-0.53999	-2.34594
O	-0.84815	0.46759	-2.84523
O	-0.23044	-1.46082	-1.16853
O	-1.30443	0.69757	0.7726
C	-0.3287	1.42798	1.28934
C	-0.62456	2.7361	1.75506
C	1.00922	0.96912	1.40364
C	0.36226	3.5435	2.29586
H	-1.64762	3.092	1.6754
C	1.99937	1.77466	1.95153
H	1.26779	-0.00966	1.0092
C	1.67257	3.05878	2.39474
H	0.13808	4.54209	2.65232
H	3.02378	1.4294	2.02898
N	2.71235	3.90822	2.96151
O	3.85328	3.44355	3.05465
O	2.39777	5.04925	3.31648
Cu	-1.2832	-1.20944	0.57282
N	-3.49389	-1.46234	1.27735
N	-0.87157	-1.61935	2.65999
N	-1.44804	-3.28345	0.50697
N	-4.1417	2.36912	-2.55955
N	-1.88331	2.95246	-2.6859
N	-3.51097	4.59105	-2.41134
C	-3.37302	-1.64026	2.75312

H	-3.47096	-2.70182	2.99599
H	-4.20906	-1.14533	3.26307
C	-2.06884	-1.09381	3.35407
H	-2.03377	-0.00615	3.25501
H	-2.05396	-1.33877	4.42605
C	-0.59322	-3.06857	2.8314
H	-1.41702	-3.52749	3.38614
H	0.30824	-3.22457	3.43345
C	-0.41291	-3.75121	1.46424
H	0.55514	-3.47283	1.03626
H	-0.42774	-4.84386	1.57837
C	-2.81947	-3.81119	0.74035
H	-2.8499	-4.25639	1.73765
H	-3.04141	-4.62138	0.0366
C	-3.88983	-2.7157	0.59869
H	-4.02606	-2.49096	-0.46156
H	-4.8503	-3.10637	0.97453
C	-4.40661	-0.31571	0.99929
H	-3.90981	0.56378	1.42005
H	-5.34724	-0.46752	1.55379
C	-3.16012	3.28505	-2.56272
H	-0.06279	-1.05883	2.92359
H	-1.14077	-3.47291	-0.44614
H	-2.79461	5.3045	-2.41384
H	-1.19229	3.67831	-2.82318
H	-1.51517	1.97522	-2.68195
H	-4.43188	4.90087	-2.69153
H	1.05227	-2.28683	-3.33927
C	-4.77519	-0.02138	-0.46394
H	-5.37947	0.89604	-0.40975
H	-5.45402	-0.7912	-0.85477
C	-3.59727	0.18555	-1.42507
H	-3.16678	-0.77924	-1.71774
H	-2.79316	0.72934	-0.92274
C	-3.95851	0.91398	-2.72801
H	-3.17165	0.75869	-3.46829
H	-4.89289	0.53813	-3.15735
H	-5.05451	2.69423	-2.26946

L³-2-TS1

E : -2552.50713333 a.u.

O	0.24266	-1.91592	-0.26437
O	5.91306	-4.84417	-1.81429
N	5.61767	-4.31882	-0.74006
C	4.63532	-3.22408	-0.7611
O	6.08162	-4.65078	0.35226
C	4.05893	-2.85341	-1.97818
C	4.30651	-2.58787	0.43653
C	3.11357	-1.8339	-1.99271
H	4.35028	-3.36498	-2.88736
C	3.36493	-1.56219	0.41625
H	4.79256	-2.8895	1.35641
C	2.76337	-1.20272	-0.79598

H	2.63896	-1.5217	-2.91657
H	3.10489	-1.0266	1.32422
O	1.88268	-0.14426	-0.84376
P	0.35645	-0.06562	-0.1886
O	-1.01375	-0.0711	-1.01179
O	0.05985	-0.05231	1.33294
O	0.53867	1.69018	-0.46918
C	1.625	2.41452	-0.03952
C	2.044	2.39185	1.30075
C	2.26116	3.25234	-0.96711
C	3.09902	3.20321	1.70609
H	1.53269	1.7429	2.00296
C	3.30881	4.07266	-0.56307
H	1.93016	3.24288	-2.00076
C	3.71628	4.03733	0.77186
H	3.44152	3.20737	2.73394
H	3.81524	4.72694	-1.26226
N	4.81741	4.9059	1.20684
O	5.329	5.64967	0.36739
O	5.16591	4.84423	2.38807
Cu	-1.74059	-1.23804	0.48516
N	-3.93743	-0.63636	0.63954
N	-2.17823	-2.24609	2.20218
N	-2.65967	-3.01005	-0.46104
N	-3.78553	3.6598	-1.41075
N	-2.40803	1.97722	-2.28875
N	-1.60137	3.39397	-0.66663
C	-4.4129	-1.17702	1.93829
H	-4.97771	-2.0962	1.76527
H	-5.10918	-0.48405	2.42678
C	-3.23351	-1.44979	2.88592
H	-2.766	-0.50776	3.18965
H	-3.58955	-1.95754	3.79265
C	-2.53374	-3.67337	1.92841
H	-3.59631	-3.80613	2.14909
H	-1.98912	-4.33507	2.60972
C	-2.23162	-4.0696	0.47259
H	-1.1539	-4.1865	0.33186
H	-2.70618	-5.03922	0.26165
C	-4.10838	-2.81366	-0.63509
H	-4.64248	-3.3976	0.12036
H	-4.45018	-3.1932	-1.60572
C	-4.49352	-1.32315	-0.54696
H	-4.08136	-0.81412	-1.42327
H	-5.59014	-1.24161	-0.59641
C	-3.9957	0.85143	0.57487
H	-3.20121	1.15422	-0.10278
H	-3.70176	1.20446	1.56817
C	-2.60193	3.01281	-1.46422
H	-1.31571	-2.18801	2.74343
H	-2.1754	-3.11107	-1.34968
H	-0.74386	2.80872	-0.62999
H	-1.72514	1.24282	-2.02033

H	-3.07494	1.77712	-3.01902
H	-1.79367	3.97494	0.1384
H	0.8494	-2.30312	0.38835
C	-5.34037	1.51173	0.16591
H	-5.4258	2.46414	0.70467
H	-6.17417	0.89985	0.53161
C	-5.52828	1.77214	-1.35013
H	-6.59148	1.69462	-1.60733
H	-5.03321	0.98808	-1.9301
C	-5.09158	3.16017	-1.87513
H	-5.13211	3.16656	-2.97196
H	-5.80869	3.91384	-1.53967
H	-3.77971	4.56216	-0.95368

L³-2-IM

E : -2552.52995329 a.u.

O	-0.07024	0.37193	2.53053
O	-6.39571	-4.34115	-0.67945
N	-5.41645	-3.95467	-1.32221
C	-4.45999	-3.07563	-0.65205
O	-5.19122	-4.2652	-2.49696
C	-4.67884	-2.70407	0.67799
C	-3.34001	-2.62583	-1.35254
C	-3.75999	-1.87678	1.30619
H	-5.5572	-3.06544	1.19899
C	-2.42151	-1.7962	-0.72013
H	-3.20012	-2.93068	-2.38273
C	-2.6208	-1.41472	0.61978
H	-3.90544	-1.57069	2.33717
H	-1.53967	-1.46404	-1.25226
O	-1.80296	-0.5889	1.31553
P	-0.14267	-0.02592	0.9413
O	1.35893	0.58531	0.63734
O	0.25687	-1.45337	0.38856
O	-0.81242	1.21345	-0.02965
C	-2.08039	1.77189	0.08752
C	-2.95907	1.66228	-0.99257
C	-2.41147	2.53372	1.21358
C	-4.19081	2.31105	-0.94651
H	-2.68003	1.06472	-1.85343
C	-3.64294	3.17729	1.26842
H	-1.70701	2.61513	2.03482
C	-4.51581	3.05769	0.1852
H	-4.89527	2.24167	-1.76637
H	-3.93109	3.77184	2.12677
N	-5.81453	3.74926	0.23651
O	-6.08156	4.3874	1.25579
O	-6.55435	3.65028	-0.74264
Cu	2.17116	-1.12295	0.15006
N	4.17367	-0.53262	-0.48063
N	2.77118	-2.99027	-0.58574
N	3.30583	-1.85208	1.9776
N	3.13657	3.96339	-1.4543

N	2.26326	3.08098	0.53851
N	1.02309	2.99499	-1.39505
C	4.78875	-1.68232	-1.20195
H	5.49172	-2.18847	-0.53738
H	5.37792	-1.3376	-2.0601
C	3.71763	-2.67489	-1.6847
H	3.13131	-2.23378	-2.498
H	4.20415	-3.57758	-2.08001
C	3.33228	-3.85627	0.49483
H	4.40892	-3.95548	0.32787
H	2.91553	-4.86626	0.4226
C	3.0602	-3.30213	1.90583
H	2.00671	-3.45192	2.16134
H	3.66396	-3.8784	2.62361
C	4.69623	-1.38461	1.84708
H	5.33624	-2.22589	1.56396
H	5.08992	-1.01976	2.8039
C	4.81899	-0.23468	0.82453
H	4.30491	0.64065	1.23146
H	5.88218	0.02096	0.70189
C	3.98561	0.65961	-1.36471
H	3.1402	1.20451	-0.95277
H	3.65506	0.25952	-2.3287
C	2.1496	3.35643	-0.76257
H	1.92961	-3.41926	-0.96716
H	2.85697	-1.4587	2.80034
H	0.33632	2.41961	-0.88868
H	1.81977	2.18431	0.86098
H	3.02833	3.47343	1.06731
H	1.01701	2.92014	-2.40334
H	-0.89206	0.08051	2.9659
C	5.19258	1.608	-1.58946
H	5.14379	1.97849	-2.62153
H	6.12616	1.03434	-1.53505
C	5.29173	2.81588	-0.62638
H	6.34153	3.12186	-0.54075
H	4.99694	2.51443	0.38302
C	4.54376	4.10681	-1.03466
H	4.62185	4.84251	-0.22364
H	5.04433	4.55087	-1.89912
H	2.88167	4.37325	-2.34367

L³-2-TS2

E: -2552.53831922 a.u.

O	-0.49613	0.44329	2.41828
O	-5.76848	-5.29007	0.0089
N	-5.14033	-4.6128	-0.81374
C	-4.43719	-3.43363	-0.33994
O	-5.06894	-4.88973	-2.01938
C	-4.46363	-3.11126	1.02323
C	-3.72759	-2.64202	-1.25486
C	-3.75731	-2.00839	1.47372
H	-5.03019	-3.73338	1.70599

C	-3.03117	-1.53683	-0.80095
H	-3.73901	-2.90996	-2.3048
C	-3.01386	-1.19356	0.57817
H	-3.76954	-1.7393	2.52603
H	-2.46557	-0.92212	-1.49332
O	-2.34987	-0.14764	1.02337
P	-0.11313	0.33254	0.86936
O	1.44325	0.66445	0.87621
O	-0.07343	-1.02569	0.12258
O	-0.61367	1.66683	0.02591
C	-1.86248	2.29628	0.01063
C	-2.57994	2.29631	-1.18471
C	-2.28859	3.02217	1.12405
C	-3.76341	3.02418	-1.26798
H	-2.21888	1.72046	-2.0301
C	-3.47376	3.7463	1.04663
H	-1.70617	3.00493	2.0391
C	-4.19265	3.73863	-0.14964
H	-4.35217	3.04235	-2.17681
H	-3.84201	4.31628	1.89078
N	-5.43753	4.52075	-0.23825
O	-5.79629	5.1384	0.76479
O	-6.04186	4.51267	-1.31106
Cu	1.91912	-1.13557	0.06232
N	4.00706	-0.89209	-0.47754
N	2.10359	-2.93359	-0.96843
N	2.79419	-2.3498	1.74425
N	3.8962	3.80912	-0.93322
N	2.7946	2.99881	0.96984
N	1.62795	3.30505	-0.99278
C	4.37562	-2.01906	-1.38134
H	4.93389	-2.76479	-0.81188
H	5.04867	-1.67849	-2.17717
C	3.12776	-2.66429	-2.00915
H	2.67417	-1.98495	-2.73874
H	3.41655	-3.57912	-2.54491
C	2.43183	-4.05865	-0.04056
H	3.46553	-4.36329	-0.22803
H	1.80708	-4.92796	-0.26988
C	2.24423	-3.68624	1.44154
H	1.17662	-3.64475	1.67826
H	2.69186	-4.4817	2.05587
C	4.25964	-2.18847	1.68115
H	4.70589	-3.09629	1.26417
H	4.69304	-2.07548	2.68225
C	4.66613	-0.95036	0.85353
H	4.35071	-0.05388	1.39583
H	5.76236	-0.92471	0.76496
C	4.09111	0.43838	-1.15358
H	3.38391	1.07945	-0.63216
H	3.68752	0.28341	-2.15934
C	2.78125	3.37669	-0.31155
H	1.19719	-3.09759	-1.40462

H	2.42816	-2.02102	2.634
H	0.80768	2.87392	-0.55514
H	2.17534	2.20514	1.23348
H	3.60586	3.18978	1.53946
H	1.63616	3.32084	-2.00378
H	-1.45841	0.16592	2.43566
C	5.47803	1.12974	-1.24598
H	5.56998	1.59348	-2.23623
H	6.27139	0.37359	-1.20837
C	5.7537	2.19667	-0.16004
H	6.83578	2.28455	-0.0046
H	5.34977	1.86031	0.8008
C	5.28592	3.63987	-0.46221
H	5.46441	4.27393	0.41577
H	5.90036	4.05282	-1.26637
H	3.76603	4.32794	-1.79246

L³-2-PC

E : -2552.56328092 a.u.

O	0.82984	-0.56055	-1.45251
O	8.23995	-0.99306	-2.50369
N	7.98936	-1.54766	-1.43418
C	6.57356	-1.60825	-1.01895
O	8.81987	-2.05665	-0.68365
C	5.59515	-1.10093	-1.89803
C	6.26437	-2.17324	0.23459
C	4.27372	-1.15671	-1.52269
H	5.90467	-0.68025	-2.84716
C	4.94661	-2.23672	0.62234
H	7.06627	-2.54277	0.8623
C	3.89347	-1.73023	-0.24144
H	3.48468	-0.78051	-2.16628
H	4.6521	-2.6601	1.57675
O	2.68547	-1.78851	0.12505
P	-0.38708	0.28112	-0.8398
O	-1.40627	0.57721	-1.90873
O	-0.83644	-0.29192	0.50237
O	0.29018	1.79196	-0.51658
C	1.44593	1.98611	0.21972
C	1.68518	1.31129	1.42372
C	2.35871	2.92388	-0.27758
C	2.86216	1.56657	2.12266
H	0.95995	0.59518	1.79308
C	3.5294	3.18744	0.4253
H	2.14491	3.42736	-1.21477
C	3.76995	2.49634	1.61472
H	3.08021	1.05712	3.05341
H	4.2561	3.90385	0.06184
N	5.02034	2.74617	2.3466
O	5.78756	3.59829	1.89687
O	5.23132	2.08224	3.36383
Cu	-2.37629	-1.52901	0.65179
N	-4.6036	-0.75111	0.38124

N	-3.38944	-2.88436	1.99013	C	-0.04396	4.66683	-0.87532
N	-3.09507	-2.97986	-0.85351	C	0.43199	2.482	0.8274
N	-4.30063	3.90977	-0.70922	H	-0.26454	3.77882	2.41261
N	-2.97858	2.72076	-2.23142	C	0.45423	3.47761	-1.39768
N	-2.04291	3.56781	-0.29723	H	-0.22733	5.52604	-1.5093
C	-5.4061	-1.52662	1.34521	C	0.67965	2.38582	-0.55075
H	-5.93404	-2.32665	0.81929	H	0.64796	1.63826	1.47258
H	-6.1928	-0.91095	1.80193	H	0.67363	3.37638	-2.45473
C	-4.56176	-2.12631	2.48616	O	1.20815	1.25495	-1.11521
H	-4.17283	-1.32244	3.12002	P	0.68776	-0.28672	-0.8478
H	-5.21995	-2.75172	3.10985	O	-0.43228	-0.52313	0.22192
C	-3.71904	-4.14377	1.27239	O	1.09993	-1.2728	-1.9212
H	-4.80487	-4.20492	1.1494	O	1.92765	-0.60866	0.36023
H	-3.43264	-5.01633	1.87069	C	3.28099	-0.41632	0.20592
C	-3.02801	-4.24791	-0.10229	C	3.92336	-0.31244	-1.03768
H	-1.96597	-4.47454	0.0382	C	4.02826	-0.35901	1.39334
H	-3.47674	-5.09076	-0.65162	C	5.30534	-0.15308	-1.08388
C	-4.43227	-2.58903	-1.34971	H	3.35043	-0.36533	-1.95459
H	-5.18057	-3.26659	-0.92613	C	5.40824	-0.20861	1.34875
H	-4.49823	-2.71516	-2.43763	H	3.51034	-0.42578	2.34536
C	-4.79112	-1.12375	-1.03211	C	6.03403	-0.10756	0.10492
H	-4.12886	-0.47596	-1.61665	H	5.82362	-0.0707	-2.03168
H	-5.82571	-0.95522	-1.38017	H	6.00019	-0.16181	2.2546
C	-4.62889	0.70416	0.63522	N	7.49192	0.04837	0.04814
H	-3.77612	1.13248	0.10062	O	8.10852	0.07566	1.11567
H	-4.41713	0.83129	1.70261	O	8.01761	0.1408	-1.06312
C	-3.11665	3.39109	-1.09022	Cu	-2.16758	-0.3462	-0.64844
H	-2.78314	-3.09076	2.77965	N	-3.34018	-1.37448	0.85666
H	-2.42952	-3.00421	-1.62101	N	-3.98424	-0.23364	-1.6732
H	-1.1568	3.11562	-0.53653	N	-3.01819	1.49314	0.36258
H	-2.27033	1.94985	-2.27522	N	0.23156	-5.25841	0.48094
H	-3.73851	2.70587	-2.89609	N	1.13743	-3.20887	1.10038
H	-2.18224	3.74951	0.68783	N	1.23818	-3.87884	-1.11605
H	1.40318	-1.04094	-0.7969	C	-4.70932	-1.57578	0.28673
C	-5.93511	1.47405	0.28674	H	-5.38709	-0.84281	0.72935
H	-6.06444	2.28328	1.01828	H	-5.10546	-2.55731	0.57064
H	-6.7924	0.80828	0.44307	C	-4.73229	-1.44248	-1.24415
C	-6.01849	2.06879	-1.13943	H	-4.24284	-2.30283	-1.71022
H	-7.0518	2.01967	-1.50433	H	-5.77359	-1.42108	-1.59471
H	-5.43234	1.46022	-1.83491	C	-4.69289	1.06088	-1.41672
C	-5.61809	3.55251	-1.26631	H	-5.57203	0.84867	-0.80139
H	-5.67935	3.87284	-2.31469	H	-5.06848	1.47264	-2.35904
H	-6.33356	4.17034	-0.71719	C	-3.79548	2.10194	-0.72796
H	-4.27649	4.61737	0.01313	H	-3.07042	2.49816	-1.44498

L³-3-TS1

E : -2552.54937029 a.u.

O	-0.9401	0.28247	-2.02392	H	-3.58751	1.70681	2.4097
O	-1.20459	5.98188	2.23612	C	-3.34049	-0.37691	1.9747
N	-0.88909	5.97982	1.04332	H	-2.31508	-0.34467	2.35357
C	-0.3195	4.74293	0.49204	H	-3.99207	-0.72404	2.79133
O	-1.03468	6.93511	0.2802	C	-2.74052	-2.64755	1.36611
C	-0.07547	3.6685	1.35125	H	-3.37015	-3.0187	2.19141

H	-1.76493	-2.37978	1.7798
C	0.86547	-4.10226	0.1489
H	-3.76648	-0.30366	-2.66531
H	-2.24004	2.09605	0.61951
H	1.46498	-2.90486	-1.41353
H	1.49213	-2.26476	0.88012
H	1.11882	-3.48681	2.07041
H	0.80756	-4.43596	-1.84321
H	-0.82714	-0.24514	-2.83133
C	-2.57533	-3.75548	0.31639
H	-1.81546	-3.45623	-0.41713
H	-3.5103	-3.88254	-0.24058
C	-2.24267	-5.14133	0.91449
H	-2.40077	-5.89753	0.13424
H	-2.96355	-5.37994	1.70797
C	-0.83173	-5.35107	1.49631
H	-0.62079	-4.63541	2.2934
H	-0.76925	-6.34546	1.9476
H	0.18498	-5.95489	-0.25395

L³-3-IM

E : -2629.03510705 a.u.

O	0.85899	0.33378	1.84139
O	1.12165	6.0358	-2.24887
N	0.7628	6.0271	-1.06814
C	0.20645	4.77604	-0.53577
O	0.85538	6.9867	-0.30253
C	0.01618	3.69693	-1.4029
C	-0.11082	4.69172	0.82198
C	-0.47763	2.49767	-0.89558
H	0.23502	3.81375	-2.45792
C	-0.59528	3.48982	1.32792
H	0.03098	5.55458	1.46163
C	-0.76503	2.39304	0.47436
H	-0.65274	1.64879	-1.54665
H	-0.84512	3.38286	2.37771
O	-1.28128	1.24632	1.01646
P	-0.67694	-0.27766	0.78708
O	0.3955	-0.55349	-0.33087
O	-1.11596	-1.28736	1.84948
O	-1.9491	-0.64753	-0.40841
C	-3.29926	-0.46203	-0.25728
C	-3.94651	-0.35417	0.98456
C	-4.04911	-0.41344	-1.44498
C	-5.32882	-0.20128	1.02912
H	-3.37428	-0.39712	1.90205
C	-5.42966	-0.26985	-1.40274
H	-3.53079	-0.47988	-2.39698
C	-6.05768	-0.16514	-0.16022
H	-5.84842	-0.11597	1.97593
H	-6.02071	-0.22979	-2.30956
N	-7.51514	-0.01414	-0.10521
O	-8.13159	0.00607	-1.17333

O	-8.04259	0.08198	1.00521
Cu	2.13784	-0.26687	0.49632
N	3.3793	-1.20884	-0.99107
N	3.91044	-0.18253	1.60656
N	2.99761	1.6286	-0.39245
N	-0.10286	-5.16025	-0.81517
N	-1.13857	-3.14523	-1.34867
N	-1.1139	-3.87514	0.85039
C	4.72978	-1.41783	-0.37949
H	5.40811	-0.64874	-0.7545
H	5.15649	-2.37413	-0.70184
C	4.68584	-1.36469	1.1547
H	4.18199	-2.24827	1.55714
H	5.7108	-1.3541	1.55117
C	4.61051	1.1279	1.4325
H	5.5121	0.95265	0.83835
H	4.94899	1.504	2.40345
C	3.72498	2.18957	0.75792
H	2.96641	2.5404	1.46381
H	4.35856	3.04878	0.49036
C	3.79074	1.24008	-1.57253
H	4.85611	1.29541	-1.3287
H	3.64023	1.93733	-2.40578
C	3.4095	-0.16681	-2.06759
H	2.39971	-0.13309	-2.48719
H	4.09736	-0.47283	-2.87076
C	2.81599	-2.46678	-1.57581
H	3.46257	-2.77449	-2.41401
H	1.83768	-2.20007	-1.98428
C	-0.78044	-4.04504	-0.43587
H	3.64662	-0.30527	2.58286
H	2.22763	2.24114	-0.65154
H	-1.42087	-2.94003	1.17785
H	-1.48824	-2.20903	-1.07859
H	-1.13553	-3.39086	-2.32765
H	-0.59417	-4.39453	1.54698
H	0.91392	-0.17153	2.68258
C	2.67137	-3.63786	-0.59406
H	1.91123	-3.3969	0.16009
H	3.6099	-3.78588	-0.04896
C	2.35671	-4.98593	-1.28088
H	2.53961	-5.79131	-0.55729
H	3.0694	-5.15609	-2.09891
C	0.94044	-5.17604	-1.85458
H	0.70736	-4.40796	-2.59481
H	0.88161	-6.13813	-2.37179
H	-0.01164	-5.8757	-0.10275
O	0.72143	-1.66679	3.78604
H	-0.10545	-1.65793	3.2389
H	0.44758	-1.5924	4.71305

L³-3-TS2

E: -2552.55389301 a.u.

H	6.18044	-1.36035	2.74556
C	6.99822	0.22871	-0.14314
H	5.77092	0.45787	-1.89998
H	8.08791	-0.09544	1.69206
N	8.11912	0.9716	-0.75192
O	9.14502	1.09503	-0.084
O	7.95175	1.41829	-1.88652
Cu	-2.51501	-0.2925	-0.76963
N	-4.05016	-1.07598	0.75596
N	-4.25725	-0.50344	-2.11765
N	-3.51357	1.60292	-0.33158
N	-0.32022	-4.47545	0.75289
N	1.35657	-2.97406	1.3542
N	1.27142	-3.79384	-0.80877
C	-5.28564	-1.38744	-0.00487
H	-6.0078	-0.57916	0.13905
H	-5.77446	-2.28632	0.39435
C	-5.05055	-1.59433	-1.51348
H	-4.49312	-2.52067	-1.68071
H	-6.03386	-1.70819	-1.99776
C	-4.95512	0.80179	-2.21753
H	-5.92112	0.7271	-1.70758
H	-5.18484	1.04169	-3.26222
C	-4.13267	1.96153	-1.62435
H	-3.31249	2.21209	-2.30483
H	-4.78243	2.84715	-1.54645
C	-4.45273	1.42921	0.80018
H	-5.47766	1.44373	0.41777
H	-4.38558	2.27155	1.49981
C	-4.19055	0.13843	1.59581
H	-3.25182	0.25122	2.14836
H	-4.99553	0.01992	2.34257
C	-3.58908	-2.20914	1.58789
H	-4.35186	-2.46343	2.34665
H	-2.70302	-1.85997	2.12978
C	0.76313	-3.74075	0.43752
H	-3.94107	-0.7971	-3.03766
H	-2.81437	2.30434	-0.10178
H	1.72773	-2.92558	-1.14692
H	2.24201	-2.49052	1.15937
H	1.13499	-3.08962	2.33183
H	0.67984	-4.2059	-1.52035
H	0.98295	0.40535	-3.49181
C	-3.23693	-3.47106	0.78898
H	-2.55603	-3.19576	-0.02699
H	-4.14177	-3.88023	0.32545
C	-2.60801	-4.57772	1.66057
H	-2.72854	-5.55094	1.16513
H	-3.14657	-4.66469	2.61227
C	-1.11906	-4.37724	1.97999
H	-0.96251	-3.38317	2.4109
H	-0.78548	-5.12296	2.71176
H	-0.68605	-5.07549	0.02484