Electronic Supplementary Information for Dalton Transactions

Supporting Information for

Can an Ancillary Ligand Lead to a Thermodynamically Stable End-on 1:1 Cu-O_2 Adduct Supported by a β-Diketiminate Ligand?

David E. Heppner, Benjamin F. Gherman, William B. Tolman, Christopher J. Cramer*

Department of Chemistry and Supercomputer Institute,

University of Minnesota,

207 Pleasant St. SE

Minneapolis, MN 55455

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Table S1. Singlet-triplet free energy differences ($^1A - ^3A$, kcal/mol) for all L^1CuXO_2 complexes.

	$^1A - ^3A$		$^1A - ^3A$
η^1 $L^1Cu(\mathbf{1})O_2$	-5.6	η^1 $L^1Cu(\mathbf{12})O_2$	-11.0
η^2 $L^1Cu(\mathbf{1})O_2$	n/a *	η^2 $L^1Cu(\mathbf{12})O_2$	n/a **
η^1 $L^1Cu(\mathbf{2})O_2$	-9.1	η^1 $L^1Cu(\mathbf{13})O_2$	-8.7
η^2 $L^1Cu(\mathbf{2})O_2$	n/a *	η^2 $L^1Cu(\mathbf{13})O_2$	-0.7
η^1 $L^1Cu(\mathbf{3})O_2$	-4.9	η^1 $L^1Cu(\mathbf{14})O_2$	-9.0
η^2 $L^1Cu(\mathbf{3})O_2$	n/a *	η^2 $L^1Cu(\mathbf{14})O_2$	0.9
η^1 $L^1Cu(\mathbf{4})O_2$	-4.8	η^1 $L^1Cu(\mathbf{15})O_2$	-11.6
η^2 $L^1Cu(\mathbf{4})O_2$	n/a *	η^2 $L^1Cu(\mathbf{15})O_2$	n/a **
η^1 $L^1Cu(\mathbf{5})O_2$	-4.1	η^1 $L^1Cu(\mathbf{16})O_2$	-10.0
η^2 $L^1Cu(\mathbf{5})O_2$	-6.4	η^2 $L^1Cu(\mathbf{16})O_2$	n/a **
η^1 $L^1Cu(\mathbf{6})O_2$	-3.6	η^1 $L^1Cu(\mathbf{17})O_2$	-10.0
η^2 $L^1Cu(\mathbf{6})O_2$	-5.6	η^2 $L^1Cu(\mathbf{17})O_2$	n/a **
η^1 $L^1Cu(\mathbf{7})O_2$	-4.9	η^1 $L^1Cu(\mathbf{18})O_2$	-4.4
η^2 $L^1Cu(\mathbf{7})O_2$	1.2	η^2 $L^1Cu(\mathbf{18})O_2$	-2.3
η^1 $L^1Cu(\mathbf{8})O_2$	-0.8	η^1 $L^1Cu(\mathbf{19})O_2$	-15.6
η^2 $L^1Cu(\mathbf{8})O_2$	n/a *	η^2 $L^1Cu(\mathbf{19})O_2$	-1.1
η^1 $L^1Cu(\mathbf{9})O_2$	-12.1	η^1 $L^1Cu(\mathbf{20})O_2$	-4.9
η^2 $L^1Cu(\mathbf{9})O_2$	n/a *	η^2 $L^1Cu(\mathbf{20})O_2$	-0.2
η^1 $L^1Cu(\mathbf{10})O_2$	-7.2	η^1 $L^1Cu(\mathbf{21})O_2$	-10.8
η^2 $L^1Cu(\mathbf{10})O_2$	n/a *	η^2 $L^1Cu(\mathbf{21})O_2$	n/a *
η^1 $L^1Cu(\mathbf{11})O_2$	-3.7	η^1 $L^1Cu(\mathbf{22})O_2$	-4.1
η^2 $L^1Cu(\mathbf{11})O_2$	-2.9	η^2 $L^1Cu(\mathbf{22})O_2$	n/a *

* No stable η^2 $LCuXO_2$ geometries (singlet or triplet) could be obtained in these cases.

** No stable triplet η^2 $LCuXO_2$ geometries could be obtained in these cases.

Atomic Coordinates for Computed Structures.

1. L^1CuX, X = THF

Cu	0.40609	-0.12351	0.48585
N	1.72372	1.31699	0.72389
N	-1.29421	0.87073	0.49141
C	2.30027	3.68877	1.00968
C	1.28595	2.57172	0.82298
C	-0.07368	2.95730	0.77118
C	-1.25645	2.19584	0.62322
C	-2.56458	2.97088	0.61666
C	3.10393	0.97855	0.80093
C	3.68234	0.66309	2.05628
C	4.99863	0.19156	2.09199
C	5.74418	0.03273	0.92614
C	5.17003	0.35222	-0.30191
C	3.85648	0.82756	-0.39046
C	2.86978	0.76975	3.34344
C	3.63906	1.44674	4.48900
C	2.35231	-0.61470	3.77829
C	3.24165	1.12643	-1.75526
C	2.90196	-0.17683	-2.50450
C	4.12753	2.03688	-2.62136
C	-2.51209	0.14994	0.34455
C	-3.16157	-0.37187	1.49124
C	-4.27363	-1.20183	1.31631
C	-4.75105	-1.51626	0.04620
C	-4.11111	-0.99247	-1.07466
C	-2.99442	-0.15763	-0.95219
C	-2.62457	-0.08997	2.89127
C	-1.78652	-1.27774	3.40476
C	-3.72682	0.27401	3.89942
C	-2.28264	0.35953	-2.19927
C	-3.24639	0.98097	-3.22593
C	-1.43475	-0.75304	-2.85004
H	1.81811	4.66755	1.01496
H	3.05115	3.67260	0.21280
H	2.84401	3.56604	1.95321
H	-0.23858	4.02375	0.86451
H	-2.39367	4.04320	0.72482
H	-3.21813	2.63932	1.43074
H	-3.11482	2.79818	-0.31443
H	5.44829	-0.06019	3.04843
H	6.76542	-0.33417	0.97494
H	5.75222	0.22762	-1.21084
H	1.99134	1.38349	3.12858
H	2.98203	1.58915	5.35378
H	4.02203	2.42676	4.18802
H	4.49088	0.84548	4.82379
H	1.73993	-0.53661	4.68384
H	3.18382	-1.29671	3.98851
H	1.73574	-1.06207	2.99270
H	2.29899	1.65211	-1.58196
H	2.43468	0.04077	-3.47182
H	2.20505	-0.79113	-1.92624
H	3.80437	-0.77061	-2.69134
H	3.61097	2.29514	-3.55227
H	5.06991	1.55036	-2.89430
H	4.37274	2.96765	-2.10059
H	-4.77431	-1.61270	2.18860
H	-5.61678	-2.16213	-0.06899
H	-4.48483	-1.23890	-2.06453

H	-1.94961	0.76666	2.81649
H	-1.36793	-1.06254	4.39403
H	-0.95389	-1.48794	2.72639
H	-2.39745	-2.18375	3.48541
H	-3.28145	0.57100	4.85481
H	-4.39446	-0.57017	4.10180
H	-4.34141	1.10494	3.53761
H	-1.59003	1.14367	-1.87949
H	-2.68227	1.42467	-4.05347
H	-3.86030	1.76758	-2.77309
H	-3.92505	0.23562	-3.65722
H	-0.89268	-0.37037	-3.72258
H	-2.06741	-1.58482	-3.18407
H	-0.69698	-1.14851	-2.14347
C	1.96117	-2.83984	0.40364
O	0.71214	-2.15148	0.18019
C	-0.31372	-3.16698	0.17530
C	1.84355	-4.13742	-0.41302
C	0.31174	-4.33921	-0.59313
H	2.06810	-3.04403	1.47670
H	2.76210	-2.17099	0.08787
H	-1.19824	-2.73289	-0.28934
H	-0.55069	-3.43900	1.21159
H	2.31653	-4.97459	0.10620
H	2.33368	-4.02789	-1.38333
H	0.04100	-4.29037	-1.65056
H	-0.03431	-5.30008	-0.20405

2. L^1CuXO_2 η^1 singlet, X = THF

Cu	-0.47998	-0.13310	0.82100
N	-0.56116	0.12972	-1.14084
N	-0.20271	-2.08194	0.91146
C	-1.11024	-0.75551	-3.36836
C	-0.84446	-0.93892	-1.88386
C	-0.91011	-2.26706	-1.39987
C	-0.55033	-2.81101	-0.14623
C	-0.56427	-4.32457	-0.03293
C	-0.30851	1.41307	-1.72603
C	-1.33990	2.37375	-1.86979
C	-1.01699	3.62592	-2.40746
C	0.27987	3.94563	-2.79089
C	1.28697	2.99945	-2.63632
C	1.02306	1.73224	-2.10464
C	-2.78426	2.10488	-1.46186
C	-3.73586	2.13170	-2.67274
C	-3.26521	3.10788	-0.39769
C	2.18155	0.74802	-1.95400
C	3.25857	1.28790	-0.99456
C	2.80457	0.38845	-3.31635
C	0.31238	-2.66300	2.11053
C	-0.53852	-2.80498	3.23702
C	0.00534	-3.29958	4.42868
C	1.35187	-3.63539	4.53021
C	2.18151	-3.47232	3.42409
C	1.68884	-2.99168	2.20521
C	-2.01232	-2.41063	3.20051
C	-2.32267	-1.28723	4.20882
C	-2.93380	-3.62176	3.43819
C	2.65439	-2.79663	1.03925
C	3.39617	-4.09380	0.66839
C	3.65979	-1.66918	1.33982
C	0.86230	2.48847	1.88585
O	1.02411	1.05545	1.97804
C	1.24831	0.78712	3.37805

C	1.92015	3.06350	2.83968
C	2.18625	1.90954	3.84557
H	-1.26279	-1.71564	-3.86299
H	-0.27840	-0.23910	-3.85474
H	-1.99870	-0.13706	-3.52522
H	-1.20223	-2.99991	-2.14136
H	-0.94843	-4.78581	-0.94413
H	-1.18517	-4.63964	0.81181
H	0.44156	-4.71336	0.15355
H	-1.80253	4.36621	-2.52345
H	0.50425	4.92445	-3.20427
H	2.30184	3.24738	-2.93319
H	-2.83118	1.11126	-1.01143
H	-4.75902	1.90509	-2.35361
H	-3.45144	1.40172	-3.43690
H	-3.74712	3.11923	-3.14944
H	-4.26376	2.83251	-0.04812
H	-3.31645	4.12539	-0.80140
H	-2.59648	3.10497	0.46410
H	1.78735	-0.17366	-1.51824
H	4.09028	0.57937	-0.91538
H	2.85072	1.43840	0.00856
H	3.66663	2.24163	-1.34682
H	3.58652	-0.36843	-3.18945
H	3.26111	1.26361	-3.79188
H	2.05830	-0.01213	-4.00989
H	-0.64072	-3.41703	5.29441
H	1.75361	-4.01574	5.46509
H	3.23568	-3.72187	3.50726
H	-2.23649	-2.01477	2.20656
H	-3.37139	-0.98613	4.12647
H	-1.71184	-0.40196	4.01206
H	-2.13891	-1.60909	5.24117
H	-3.98342	-3.32204	3.34329
H	-2.79502	-4.04283	4.44249
H	-2.74344	-4.42271	2.71383
H	2.07117	-2.48592	0.16846
H	4.02011	-3.93533	-0.21747
H	2.70164	-4.91037	0.45001
H	4.05333	-4.42828	1.47791
H	4.34342	-1.52747	0.49584
H	4.26482	-1.90309	2.22278
H	3.14388	-0.72190	1.51879
H	-0.15565	2.75119	2.19727
H	0.99610	2.76258	0.83860
H	1.66328	-0.21736	3.45790
H	0.28700	0.82316	3.90627
H	1.56062	3.97233	3.32848
H	2.83292	3.31710	2.29558
H	3.22815	1.58609	3.79457
H	1.97683	2.19694	4.87921
O	-3.02293	0.43991	1.47082
O	-1.86802	1.00521	1.53313

3. L^1CuXO_2 η^1 triplet, X = THF

Cu	-.4633119138	-.0803750419	.8114780982
N	-.5053993723	.1443929458	-1.1687234015
N	-.2241600312	-2.0615068395	.9563827126
C	-1.0393338739	-.7823972764	-3.3857799993
C	-.8000621546	-.9351467372	-1.8926918213
C	-.8956043037	-2.2493647708	-1.3761845406
C	-.5553588538	-2.7863676778	-.1099389810
C	-.5323281660	-4.3031466486	-.0205834408

C	-.2375196317	1.4072728492	-1.7855093383
C	-1.2541256749	2.3878104196	-1.9043754295
C	-.9309067038	3.6335518414	-2.4544444286
C	.3604549841	3.9321647233	-2.8761818780
C	1.3579416123	2.9725990971	-2.7356549611
C	1.0892534814	1.7115606560	-2.1908262127
C	-2.6803312049	2.1431655121	-1.4233245775
C	-3.7049843305	2.2403321176	-2.5689099653
C	-3.0565404171	3.1175662191	-.2901379832
C	2.2405685950	.7206773278	-2.0308760643
C	3.3072617804	1.2658272799	-1.0631137733
C	2.8775625446	.3469523390	-3.3813070004
C	.2915316119	-2.6620395126	2.1462432374
C	-.5493531421	-2.8386423263	3.2736167332
C	.0042616247	-3.3369694056	4.4582015664
C	1.3560567084	-3.6507909417	4.5547960224
C	2.1772728089	-3.4634374459	3.4471985925
C	1.6739168232	-2.9729468077	2.2366693771
C	-2.0357111631	-2.5022644550	3.2323605134
C	-2.4142567093	-1.4652284815	4.3058379266
C	-2.9089769876	-3.7629230867	3.3710573356
C	2.6387705229	-2.7477050189	1.0745392724
C	3.4126796469	-4.0237896296	.6968826969
C	3.6188245258	-1.6007540082	1.3874432591
C	.7784362222	2.6340919254	1.8510378188
O	.8043753539	1.1994500149	2.0055861771
C	1.1318767156	.9524263228	3.3881061038
C	1.9436393047	3.1473658366	2.7174719928
C	2.2267368593	1.9805644825	3.7053516512
H	-1.2527923034	-1.7441867904	-3.8547359386
H	-.1689002344	-.3394752726	-3.8795666227
H	-1.8810755490	-.1076610166	-3.5733076164
H	-1.1832366816	-2.9938792986	-2.1084091811
H	-1.1316568388	-4.7495061495	-.8166248537
H	-.9052166956	-4.6517282399	.9455357034
H	.4929361070	-4.6771856785	-.1228214614
H	-1.7090339948	4.3858375280	-2.5505190554
H	.5888719525	4.9043611521	-3.3033644682
H	2.3708367097	3.2063056355	-3.0523972131
H	-2.7274879594	1.1292241826	-1.0180173500
H	-4.7110791533	2.0104534702	-2.2020048643
H	-3.4737458263	1.5428454535	-3.3798973698
H	-3.7301698862	3.2481188831	-2.9979279587
H	-4.0493244773	2.8806786128	.1065887797
H	-3.0738983795	4.1536528446	-.6459085085
H	-2.3427334978	3.0572649631	.5359866996
H	1.8367059500	-.1936636887	-1.5896958802
H	4.1289064115	.5508256252	-.9500660963
H	2.8784161926	1.4441527001	-.0730796468
H	3.7329689164	2.2075866539	-1.4253750579
H	3.6670622173	-.3993054068	-3.2394725462
H	3.3283655061	1.2186271157	-3.8675956407
H	2.1392931636	-.0716710619	-4.0716215746
H	-.6388262352	-3.4798306886	5.3221924935
H	1.7664057531	-4.0352038859	5.4840803493
H	3.2355265611	-3.6979315226	3.5232869776
H	-2.2486629145	-2.0608593397	2.2566658550
H	-3.4650706237	-1.1762480988	4.2022977973
H	-1.8085391103	-.5594831609	4.2117991470
H	-2.2729609555	-1.8614695588	5.3173141369
H	-3.9706375945	-3.5023519914	3.3032109142
H	-2.7462644045	-4.2567097257	4.3356221397
H	-2.6892647255	-4.4906798267	2.5839280615
H	2.0528580781	-2.4439165526	.2037281511

H	4.0284034175	-3.8472522134	-.1916044333
H	2.7368613103	-4.8569086880	.4809818209
H	4.0824649280	-4.3434351503	1.5022589776
H	4.3102057523	-1.4448393495	.5527323248
H	4.2161841147	-1.8220787825	2.2784865984
H	3.0836485178	-.6631938936	1.5593697082
H	-.1882901798	3.0139726590	2.2076387480
H	.8766336277	2.8474477384	.7856821782
H	1.4441079677	-.0892190422	3.4708383834
H	.2370385017	1.1111353216	4.0054044462
H	1.6730491623	4.0725917916	3.2318817645
H	2.8220838982	3.3554819539	2.1025396580
H	3.2143900812	1.5513538306	3.5191563885
H	2.1916615050	2.2951215815	4.7511850967
O	-3.2680772717	.2227559807	1.4295668825
O	-2.1461847741	.6880295506	1.7314163743

4. L^1CuX, X = MeCN

Cu	-0.08477	0.18592	-0.11876
N	1.45949	1.39542	-0.33168
N	-1.55584	1.50332	-0.26162
N	-0.18415	-1.72360	0.17370
C	-0.24831	-2.86839	0.35167
C	-0.33045	-4.30426	0.57719
C	2.48844	3.59975	-0.69169
C	1.27481	2.70123	-0.52058
C	0.01177	3.33143	-0.57149
C	-1.28924	2.79500	-0.44638
C	-2.44147	3.78151	-0.53763
C	2.76320	0.81834	-0.29436
C	3.40871	0.62064	0.95056
C	4.63412	-0.05445	0.97443
C	5.22228	-0.52981	-0.19438
C	4.57721	-0.33446	-1.41341
C	3.35056	0.33374	-1.48920
C	2.76642	1.07802	2.25703
C	3.72465	1.89627	3.13931
C	2.19749	-0.12350	3.03694
C	2.63180	0.47021	-2.82836
C	1.92623	-0.84912	-3.19969
C	3.55275	0.93324	-3.96878
C	-2.89049	1.02255	-0.11627
C	-3.46653	0.92602	1.17457
C	-4.72858	0.33718	1.30686
C	-5.42053	-0.15127	0.20132
C	-4.84427	-0.05491	-1.06255
C	-3.58422	0.52503	-1.24633
C	-2.70682	1.38813	2.41478
C	-2.11637	0.18175	3.17121
C	-3.55872	2.25629	3.35577
C	-2.96159	0.56554	-2.63890
C	-3.89675	1.18526	-3.69116
C	-2.50224	-0.83925	-3.07555
H	-1.31173	-4.67764	0.27093
H	-0.18421	-4.52037	1.63925
H	0.44393	-4.81913	0.00161
H	2.19475	4.64071	-0.83406
H	3.08850	3.28606	-1.55220
H	3.14431	3.53884	0.18302
H	0.04666	4.40271	-0.72703
H	-2.08175	4.79749	-0.70650
H	-3.03754	3.77184	0.38077
H	-3.12157	3.51170	-1.35227

H	5.13383	-0.21542	1.92592
H	6.17491	-1.05058	-0.15611
H	5.03345	-0.71443	-2.32312
H	1.92215	1.72297	1.99945
H	3.19988	2.27108	4.02492
H	4.13100	2.75598	2.59696
H	4.57056	1.29536	3.49045
H	1.69746	0.20900	3.95391
H	2.99322	-0.82224	3.31987
H	1.46848	-0.67041	2.43102
H	1.85189	1.22700	-2.70758
H	1.36555	-0.74219	-4.13550
H	1.22507	-1.15073	-2.41573
H	2.65477	-1.65781	-3.33056
H	2.96731	1.11563	-4.87643
H	4.30996	0.18158	-4.21694
H	4.07555	1.85961	-3.71012
H	-5.17487	0.25239	2.29395
H	-6.40030	-0.60414	0.32433
H	-5.38100	-0.44339	-1.92394
H	-1.86417	1.99725	2.07688
H	-1.52933	0.51289	4.03566
H	-1.46116	-0.40385	2.51924
H	-2.91071	-0.48053	3.53455
H	-2.94436	2.63841	4.17830
H	-4.38391	1.69022	3.80134
H	-3.99030	3.11312	2.82858
H	-2.06799	1.19255	-2.58055
H	-3.38354	1.26709	-4.65556
H	-4.22274	2.18730	-3.39448
H	-4.79429	0.57730	-3.84855
H	-2.01677	-0.80222	-4.05753
H	-3.35166	-1.52867	-3.14426
H	-1.78769	-1.25498	-2.35852

5. L^1CuXO_2 η^1 singlet, X = MeCN

C	0.67615	-2.76549	-0.78365
C	1.51519	-3.94156	-0.59001
C	3.27243	0.96759	1.37558
C	4.56842	0.45342	1.23572
C	5.06777	0.06380	-0.00001
C	4.26487	0.16739	-1.13459
C	2.96186	0.66250	-1.05884
C	2.79543	1.39474	2.76242
C	3.57301	2.63001	3.26477
C	2.90666	0.26030	3.80168
C	2.10747	0.77419	-2.32143
C	2.32745	-0.38219	-3.31155
C	2.33184	2.12174	-3.03974
C	-3.06886	0.64512	-0.32151
C	-3.82247	-0.00925	0.68555
C	-4.97564	-0.71046	0.31406
C	-5.38110	-0.78469	-1.01401
C	-4.62288	-0.15723	-1.99788
C	-3.46370	0.55900	-1.68315
C	-3.41222	0.02005	2.15574
C	-3.09209	-1.39558	2.67607
C	-4.47450	0.70449	3.03671
C	-2.63599	1.15980	-2.81851
C	-3.46222	2.08085	-3.73673
C	-1.95411	0.04790	-3.64188
C	1.86796	3.93937	0.21300
C	0.79194	2.86423	0.21616

C	-0.53671	3.33852	0.17564
C	-1.75530	2.63990	0.04573
C	-3.00518	3.48883	-0.10607
C	2.47220	1.09590	0.20791
H	2.27709	-3.99507	-1.37250
H	0.90610	-4.84893	-0.62440
H	2.00298	-3.86728	0.38383
H	1.56410	4.78316	-0.41122
H	2.82545	3.55702	-0.14207
H	2.01502	4.31869	1.22989
H	-0.62807	4.41838	0.18238
H	-2.83724	4.49320	0.28743
H	-3.85154	3.03677	0.41698
H	-3.28951	3.58460	-1.15897
H	5.19525	0.35768	2.11748
H	6.07828	-0.32778	-0.08263
H	4.66105	-0.14804	-2.09481
H	1.73804	1.66345	2.68220
H	3.17063	2.96892	4.22594
H	3.52617	3.46730	2.56330
H	4.63128	2.38818	3.41644
H	2.44323	0.57159	4.74489
H	3.95497	0.02324	4.01945
H	2.41400	-0.64802	3.45033
H	1.06018	0.73667	-2.00695
H	1.59089	-0.32270	-4.11989
H	2.21103	-1.35307	-2.82401
H	3.31910	-0.34774	-3.77705
H	1.69550	2.19249	-3.92926
H	3.37453	2.22144	-3.36362
H	2.09932	2.97391	-2.39630
H	-5.56321	-1.20843	1.08045
H	-6.27935	-1.33373	-1.28326
H	-4.93250	-0.23353	-3.03685
H	-2.49673	0.61419	2.23453
H	-2.74752	-1.35446	3.71542
H	-2.30577	-1.86852	2.07985
H	-3.97605	-2.04249	2.64252
H	-4.13432	0.75637	4.07705
H	-5.42203	0.15427	3.02533
H	-4.67905	1.72500	2.69643
H	-1.83925	1.76245	-2.37633
H	-2.81120	2.56802	-4.47116
H	-3.97948	2.86451	-3.17362
H	-4.22230	1.52315	-4.29506
H	-1.32534	0.48335	-4.42786
H	-2.69809	-0.59263	-4.12940
H	-1.32823	-0.58562	-3.00747
N	-0.00179	-1.83738	-0.94469
N	1.13878	1.58127	0.27107
N	-1.85647	1.31223	0.03203
O	0.39948	-0.83912	1.86797
O	1.38501	-1.65008	1.74296
Cu	-0.30406	0.28218	0.56365

6. L^1CuXO_2 η^1 triplet, X = MeCN

C	-1.19661	-2.57679	-0.97697
C	-2.03963	-3.73392	-1.23886
C	3.21230	1.56989	1.61959
C	4.57761	1.27833	1.72706
C	5.34270	0.94024	0.61673
C	4.73969	0.88689	-0.63609
C	3.37980	1.16948	-0.80264

C	2.43029	1.88484	2.89714
C	3.01212	3.09067	3.66227
C	2.35608	0.66229	3.83672
C	2.76330	1.08339	-2.19744
C	2.77265	-0.36609	-2.72390
C	3.44779	2.03485	-3.19694
C	-2.97900	0.37863	-0.34962
C	-3.57024	-0.34060	0.72303
C	-4.63206	-1.21067	0.45127
C	-5.11646	-1.38313	-0.84227
C	-4.52710	-0.68103	-1.89125
C	-3.45915	0.19655	-1.67614
C	-3.07302	-0.18430	2.15878
C	-2.37944	-1.46555	2.66557
C	-4.20282	0.23474	3.11803
C	-2.82065	0.90295	-2.87203
C	-3.83869	1.74409	-3.66666
C	-2.11443	-0.09608	-3.81147
C	1.63617	4.15907	0.20230
C	0.69056	2.96824	0.15598
C	-0.68408	3.28832	0.09362
C	-1.83535	2.47298	0.01357
C	-3.17648	3.18671	0.07303
C	2.60892	1.52516	0.33325
H	-1.91954	-4.07560	-2.27072
H	-3.08540	-3.45310	-1.07915
H	-1.77355	-4.55198	-0.56429
H	1.12369	5.07170	-0.10643
H	2.49970	4.00169	-0.44934
H	2.02414	4.31399	1.21336
H	-0.89387	4.34994	0.13506
H	-3.05008	4.25110	0.27738
H	-3.80769	2.75356	0.85604
H	-3.72562	3.07778	-0.86797
H	5.05026	1.31360	2.70551
H	6.40029	0.71623	0.72771
H	5.33599	0.61648	-1.50346
H	1.40547	2.13416	2.61086
H	2.37876	3.34107	4.52101
H	3.08877	3.98051	3.02977
H	4.01515	2.87681	4.04860
H	1.74771	0.89254	4.71934
H	3.35263	0.36738	4.18581
H	1.90991	-0.19775	3.33258
H	1.71966	1.39911	-2.11726
H	2.26039	-0.43021	-3.69157
H	2.27418	-1.04431	-2.02484
H	3.79709	-0.72950	-2.86555
H	2.95260	1.98788	-4.17369
H	4.50108	1.77534	-3.35020
H	3.41002	3.07285	-2.84963
H	-5.09165	-1.76003	1.26946
H	-5.95131	-2.05325	-1.03112
H	-4.90466	-0.81888	-2.90160
H	-2.32137	0.60900	2.15890
H	-2.04546	-1.33930	3.70189
H	-1.49948	-1.70651	2.06127
H	-3.05756	-2.32733	2.63858
H	-3.80530	0.42203	4.12157
H	-4.96725	-0.54522	3.20884
H	-4.70095	1.14728	2.77507
H	-2.05325	1.57964	-2.48852
H	-3.33240	2.29732	-4.46550
H	-4.35512	2.47001	-3.03081

H	-4.60333	1.11595	-4.13749
H	-1.65912	0.43133	-4.65785
H	-2.82250	-0.82631	-4.22115
H	-1.32416	-0.64388	-3.29126
N	-0.53590	-1.64677	-0.77336
N	1.20099	1.73541	0.17910
N	-1.80725	1.15192	-0.12652
O	1.40138	-1.34010	1.26895
O	2.24255	-1.97878	0.63429
Cu	0.00022	0.21778	-0.04985

7. L^1CuX, X = 2,3-dihydrofuran

C	3.12743	0.84179	1.36324
C	4.44015	0.35815	1.35904
C	5.16771	0.24572	0.17623
C	4.57588	0.61764	-1.02809
C	3.26414	1.10457	-1.07840
C	2.33601	0.90010	2.66634
C	3.12043	1.55547	3.81483
C	1.84372	-0.50309	3.07212
C	2.63931	1.45056	-2.42752
C	2.42213	0.18885	-3.28515
C	3.46457	2.49223	-3.20375
C	-3.10390	0.42929	-0.29201
C	-3.79171	-0.05600	0.84706
C	-4.90696	-0.87971	0.65965
C	-5.34940	-1.22130	-0.61610
C	-4.67189	-0.73170	-1.73051
C	-3.55090	0.09479	-1.59554
C	-3.29375	0.26139	2.25407
C	-2.47277	-0.91230	2.82316
C	-4.42373	0.65393	3.21987
C	-2.79340	0.57120	-2.83207
C	-3.71803	1.08567	-3.94740
C	-1.86471	-0.53706	-3.36587
C	1.74254	3.94899	0.30233
C	0.72330	2.83126	0.15326
C	-0.63550	3.22248	0.08563
C	-1.82590	2.47144	-0.05792
C	1.38043	-2.43644	-0.45128
C	-0.86715	-2.92659	-0.30367
C	1.27686	-3.60774	-1.06977
C	-0.17934	-4.01244	-1.15951
C	-3.12168	3.26208	-0.13817
C	2.53435	1.22117	0.13203
H	-1.69663	-2.42255	-0.79892
H	2.23437	-1.81510	-0.21962
H	-0.53646	-4.00662	-2.19684
H	1.25857	4.92470	0.36311
H	2.43965	3.95970	-0.54151
H	2.34664	3.80241	1.20400
H	-0.79119	4.29293	0.14045
H	-2.94018	4.33471	-0.05702
H	-3.81069	2.96347	0.65894
H	-3.63754	3.06788	-1.08446
H	4.90011	0.06045	2.29723
H	6.18644	-0.13079	0.19292
H	5.14107	0.52214	-1.95159
H	1.44778	1.51037	2.48235
H	2.48153	1.65888	4.69860
H	3.47861	2.55162	3.53621
H	3.99061	0.95910	4.10988
H	1.24052	-0.45370	3.98581

H	2.68736	-1.17720	3.26073
H	1.22711	-0.94793	2.28507
H	1.65405	1.88195	-2.23297
H	1.92942	0.44526	-4.22990
H	1.79631	-0.54280	-2.76521
H	3.37413	-0.29756	-3.52616
H	2.95432	2.76937	-4.13274
H	4.45294	2.10407	-3.47338
H	3.61667	3.40330	-2.61667
H	-5.43793	-1.26298	1.52638
H	-6.21841	-1.86097	-0.74140
H	-5.02052	-0.99889	-2.72411
H	-2.61536	1.11562	2.17611
H	-2.09395	-0.67420	3.82363
H	-1.61272	-1.13626	2.18423
H	-3.08538	-1.81822	2.89984
H	-4.00560	0.97491	4.17996
H	-5.09986	-0.18331	3.42418
H	-5.02427	1.47655	2.81865
H	-2.15280	1.40247	-2.52554
H	-3.12428	1.51607	-4.76094
H	-4.39881	1.85910	-3.57780
H	-4.32738	0.28450	-4.37959
H	-1.29726	-0.18694	-4.23553
H	-2.44121	-1.41866	-3.67006
H	-1.14531	-0.84638	-2.60100
H	-1.19713	-3.30144	0.66856
H	2.10361	-4.17804	-1.46928
H	-0.36276	-5.01488	-0.75805
N	1.15508	1.57190	0.10150
N	-1.88253	1.14067	-0.12513
O	0.16221	-1.90928	-0.03374
Cu	-0.19653	0.15983	-0.01022

8. L^1CuXO_2 η^1 singlet, X = 2,3-dihydrofuran

C	-1.15587	2.36375	-2.60743
C	-0.87397	3.60057	-3.19952
C	0.40809	3.93736	-3.61986
C	1.44256	3.02239	-3.45465
C	1.22233	1.77082	-2.86916
C	-2.59513	2.07677	-2.17890
C	-3.55804	2.02983	-3.38506
C	-3.10407	3.11259	-1.15873
C	2.39873	0.80474	-2.72457
C	3.50818	1.38410	-1.82762
C	2.97594	0.40085	-4.09628
C	0.54620	-2.69702	1.41501
C	-0.34143	-2.86132	2.51063
C	0.15187	-3.43868	3.68596
C	1.48081	-3.83560	3.79797
C	2.34501	-3.65439	2.72080
C	1.90468	-3.09261	1.51722
C	-1.80161	-2.41784	2.44564
C	-2.12249	-1.34236	3.50034
C	-2.76891	-3.61140	2.57404
C	2.89655	-2.89826	0.36992
C	3.58529	-4.21453	-0.04133
C	3.95262	-1.83105	0.71661
C	1.08602	2.59936	1.20595
C	1.96841	0.94377	2.50580
C	2.12780	3.22728	2.14792
C	2.43876	2.06144	3.05320
C	-0.87472	-0.73451	-4.03593

C	-0.59757	-0.90401	-2.55090
C	-0.66759	-2.22627	-2.06723
C	-0.30495	-2.77180	-0.82052
C	-0.35287	-4.28727	-0.71731
C	-0.09112	1.43707	-2.44285
H	-1.03323	-1.69908	-4.52092
H	-0.04623	-0.22484	-4.53504
H	-1.76268	-0.11758	-4.19529
H	-0.97013	-2.95710	-2.80676
H	-0.76148	-4.73289	-1.62548
H	-0.96831	-4.59575	0.13381
H	0.64493	-4.70195	-0.55031
H	-1.68265	4.31271	-3.33835
H	0.59908	4.90440	-4.07646
H	2.44398	3.28469	-3.78527
H	-2.61725	1.10152	-1.68640
H	-4.57302	1.78940	-3.04988
H	-3.26498	1.27932	-4.12510
H	-3.60021	2.99631	-3.90020
H	-4.09538	2.82511	-0.79499
H	-3.18513	4.10963	-1.60661
H	-2.43613	3.16835	-0.29762
H	2.02951	-0.10389	-2.24138
H	4.34648	0.68277	-1.75371
H	3.13770	1.56900	-0.81564
H	3.89887	2.32648	-2.22699
H	3.77285	-0.34075	-3.97335
H	3.40216	1.26276	-4.62211
H	2.21079	-0.03530	-4.74626
H	-0.52062	-3.57593	4.52810
H	1.84339	-4.28138	4.71988
H	3.38464	-3.95621	2.81631
H	-1.97911	-1.96643	1.46711
H	-3.15738	-1.00424	3.38834
H	-1.47573	-0.46871	3.38029
H	-1.99699	-1.72512	4.51984
H	-3.80501	-3.27397	2.46152
H	-2.68225	-4.09909	3.55246
H	-2.57822	-4.37153	1.80839
H	2.34049	-2.53033	-0.49674
H	4.22874	-4.05173	-0.91279
H	2.85973	-4.99171	-0.29988
H	4.21578	-4.60923	0.76286
H	4.65033	-1.69558	-0.11749
H	4.53690	-2.12084	1.59696
H	3.48465	-0.86497	0.92227
H	0.06033	2.79739	1.53637
H	1.18444	2.88845	0.15854
H	2.00180	-0.08895	2.83691
H	1.72712	4.10801	2.65838
H	3.02047	3.55369	1.59733
H	2.98055	2.12715	3.99157
N	-0.29598	0.16580	-1.81534
N	0.06920	-2.05249	0.23561
O	1.31256	1.16052	1.28905
O	-2.69118	0.53542	0.83676
O	-1.52938	1.08138	0.87074
Cu	-0.16732	-0.08343	0.16180

9. L^1CuXO_2 η^1 triplet, X = 2,3-dihydrofuran

C	-1.19661	-2.57679	-0.97697
C	-2.03963	-3.73392	-1.23886
C	3.21230	1.56989	1.61959
C	4.57761	1.27833	1.72706
C	5.34270	0.94024	0.61673
C	4.73969	0.88689	-0.63609
C	3.37980	1.16948	-0.80264
C	2.43029	1.88484	2.89714
C	3.01212	3.09067	3.66227
C	2.35608	0.66229	3.83672
C	2.76330	1.08339	-2.19744
C	2.77265	-0.36609	-2.72390
C	3.44779	2.03485	-3.19694
C	-2.97900	0.37863	-0.34962
C	-3.57024	-0.34060	0.72303
C	-4.63206	-1.21067	0.45127
C	-5.11646	-1.38313	-0.84227
C	-4.52710	-0.68103	-1.89125
C	-3.45915	0.19655	-1.67614
C	-3.07302	-0.18430	2.15878
C	-2.37944	-1.46555	2.66557
C	-4.20282	0.23474	3.11803
C	-2.82065	0.90295	-2.87203
C	-3.83869	1.74409	-3.66666
C	-2.11443	-0.09608	-3.81147
C	1.63617	4.15907	0.20230
C	0.69056	2.96824	0.15598
C	-0.68408	3.28832	0.09362
C	-1.83535	2.47298	0.01357
C	-3.17648	3.18671	0.07303
C	2.60892	1.52516	0.33325
H	-1.91954	-4.07560	-2.27072
H	-3.08540	-3.45310	-1.07915
H	-1.77355	-4.55198	-0.56429
H	1.12369	5.07170	-0.10643
H	2.49970	4.00169	-0.44934
H	2.02414	4.31399	1.21336
H	-0.89387	4.34994	0.13506
H	-3.05008	4.25110	0.27738
H	-3.80769	2.75356	0.85604
H	-3.72562	3.07778	-0.86797
H	5.05026	1.31360	2.70551
H	6.40029	0.71623	0.72771
H	5.33599	0.61648	-1.50346
H	1.40547	2.13416	2.61086
H	2.37876	3.34107	4.52101
H	3.08877	3.98051	3.02977
H	4.01515	2.87681	4.04860
H	1.74771	0.89254	4.71934
H	3.35263	0.36738	4.18581
H	1.90991	-0.19775	3.33258
H	1.71966	1.39911	-2.11726
H	2.26039	-0.43021	-3.69157
H	2.27418	-1.04431	-2.02484
H	3.79709	-0.72950	-2.86555
H	2.95260	1.98788	-4.17369
H	4.50108	1.77534	-3.35020
H	3.41002	3.07285	-2.84963
H	-5.09165	-1.76003	1.26946
H	-5.95131	-2.05325	-1.03112
H	-4.90466	-0.81888	-2.90160
H	-2.32137	0.60900	2.15890
H	-2.04546	-1.33930	3.70189

H	-1.49948	-1.70651	2.06127
H	-3.05756	-2.32733	2.63858
H	-3.80530	0.42203	4.12157
H	-4.96725	-0.54522	3.20884
H	-4.70095	1.14728	2.77507
H	-2.05325	1.57964	-2.48852
H	-3.33240	2.29732	-4.46550
H	-4.35512	2.47001	-3.03081
H	-4.60333	1.11595	-4.13749
H	-1.65912	0.43133	-4.65785
H	-2.82250	-0.82631	-4.22115
H	-1.32416	-0.64388	-3.29126
N	-0.53590	-1.64677	-0.77336
N	1.20099	1.73541	0.17910
N	-1.80725	1.15192	-0.12652
O	1.40138	-1.34010	1.26895
O	2.24255	-1.97878	0.63429
Cu	0.00022	0.21778	-0.04985

10. L^1CuX, X = furan

C	3.15617	0.85411	1.40064
C	4.48278	0.40789	1.41348
C	5.21801	0.28778	0.23656
C	4.62343	0.61635	-0.97932
C	3.29998	1.06562	-1.04571
C	2.35727	0.92901	2.69872
C	3.11570	1.64350	3.82969
C	1.90505	-0.47405	3.14825
C	2.66016	1.36299	-2.39902
C	2.32413	0.05837	-3.14700
C	3.52153	2.28635	-3.27698
C	-3.10672	0.33582	-0.32139
C	-3.76756	-0.19041	0.81589
C	-4.89585	-0.99614	0.62619
C	-5.37528	-1.28308	-0.64969
C	-4.71675	-0.76276	-1.76108
C	-3.58264	0.04583	-1.62448
C	-3.23722	0.06540	2.22391
C	-2.50844	-1.17817	2.76961
C	-4.33125	0.52866	3.20076
C	-2.85108	0.54578	-2.86710
C	-3.78689	1.24441	-3.86856
C	-2.08202	-0.60229	-3.54967
C	1.72567	3.88978	0.30631
C	0.72140	2.75838	0.15863
C	-0.64225	3.13158	0.09166
C	-1.82926	2.37492	-0.05625
C	1.38525	-2.58894	-0.33250
C	-0.80742	-2.91105	-0.50616
C	1.21139	-3.80808	-0.90118
C	-0.20722	-4.01656	-1.01361
C	-3.12914	3.16180	-0.09764
C	2.56063	1.18308	0.15766
H	2.23788	-1.99414	-0.04693
H	1.22975	4.86026	0.35178
H	2.42988	3.89838	-0.53202
H	2.32399	3.76119	1.21447
H	-0.80847	4.19978	0.15706
H	-2.95199	4.23117	0.02461
H	-3.80970	2.82815	0.69258
H	-3.65188	3.00328	-1.04646
H	4.94785	0.14925	2.36068
H	6.24678	-0.05952	0.26682

H	5.19745	0.51679	-1.89640
H	1.45191	1.50648	2.49301
H	2.46751	1.76009	4.70493
H	3.45010	2.63864	3.51974
H	3.99859	1.08062	4.15138
H	1.29826	-0.41433	4.05884
H	2.76746	-1.11710	3.35844
H	1.30233	-0.96162	2.37550
H	1.71372	1.87620	-2.21061
H	1.82016	0.27297	-4.09602
H	1.66460	-0.57880	-2.54993
H	3.23195	-0.51466	-3.36816
H	2.98527	2.54287	-4.19702
H	4.46322	1.81008	-3.57048
H	3.76817	3.21773	-2.75730
H	-5.40675	-1.40737	1.49241
H	-6.25447	-1.90818	-0.77678
H	-5.08712	-0.99375	-2.75614
H	-2.49678	0.86674	2.15423
H	-2.09809	-0.98311	3.76681
H	-1.67926	-1.46810	2.11610
H	-3.19036	-2.03287	2.84613
H	-3.88968	0.78807	4.16905
H	-5.07698	-0.25306	3.38120
H	-4.85823	1.40977	2.82114
H	-2.10922	1.27903	-2.54073
H	-3.20967	1.65857	-4.70233
H	-4.33802	2.06455	-3.39751
H	-4.52159	0.55112	-4.29208
H	-1.51835	-0.23314	-4.41377
H	-2.76700	-1.38210	-3.90171
H	-1.37405	-1.06810	-2.85723
H	-1.82769	-2.59176	-0.36661
H	1.99656	-4.48455	-1.20423
H	-0.70975	-4.88224	-1.41854
N	1.17367	1.50441	0.10627
N	-1.88207	1.04503	-0.15363
O	0.15453	-2.01950	-0.07739
Cu	-0.17634	0.11243	-0.06003

11. L^1CuXO_2 η^1 singlet, X = furan

C	3.6565476229	1.5350805397	-1.8050844533
C	2.0960336770	3.2905873742	1.8643002602
C	2.2176279770	1.1050076896	2.3337738526
C	-.8462120856	-.6628416773	-4.0353341918
C	-.5992747962	-.8917194069	-2.5492280674
C	-.7000192358	-2.2390088788	-2.1415783576
C	-.3690013397	-2.8248878004	-.9106020833
C	-.3626150148	-4.3421342606	-.8683168727
C	-.0851673469	1.4258701054	-2.3302732953
C	-1.1446022986	2.3267460920	-2.6167814496
C	-.8354868388	3.5477873945	-3.2306074606
C	.4700183576	3.8893805639	-3.5624399600
C	1.5029334334	3.0051374810	-3.2684932886
C	1.2570048510	1.7754211795	-2.6475907482
C	-2.6090985484	2.0250875786	-2.3059654598
C	-3.4757522949	2.0126203119	-3.5845487478
C	-3.1866738015	3.0344050636	-1.2945825046
C	2.4233806180	.8226087811	-2.3919524580
C	2.6926706980	2.3132209016	2.7335098195
C	2.8164228721	.0651320942	-3.6791583503
C	.5014795187	-2.7565850970	1.3315955618
C	-.3125930943	-2.8900048521	2.4863998751

C	.2542432717	-3.4428102584	3.6385633437
C	1.5878627597	-3.8392661595	3.6680027112
C	2.3810826615	-3.6868006861	2.5325168969
C	1.8655963479	-3.1476771052	1.3500453780
C	-1.7791877220	-2.4620064389	2.4845974469
C	-2.0860557117	-1.4325289207	3.5880143427
C	-2.7255540990	-3.6738988341	2.5739957944
C	2.7843973899	-2.9612323958	.1415129000
C	3.4999573498	-4.2648533968	-.2654883780
C	3.8158425030	-1.8412701855	.3826451964
C	1.3036975138	2.6043169486	1.0006496757
H	2.3645492696	.0924623429	2.6709514425
H	2.2411223212	4.3602284282	1.8818274610
H	-.7139023228	-4.7163431623	.0960646430
H	.6655777645	2.8872927233	.1803450458
H	-.6706256752	-1.5797598234	-4.6010942674
H	-.2197031716	.1301044532	-4.4448585328
H	-1.8880730539	-.3667722657	-4.1934261740
H	-.9728072360	-2.9348391887	-2.9254596782
H	-.9952221649	-4.7464074167	-1.6612082215
H	3.3814359013	2.4942017103	3.5448256049
H	.6491446811	-4.7302559215	-1.0198420921
H	-1.6407686687	4.2389152475	-3.4643855454
H	.6815863712	4.8365522677	-4.0516909491
H	2.5213949960	3.2708617510	-3.5353803387
H	-2.6627957166	1.0322575153	-1.8505810576
H	-4.5021358322	1.7122853463	-3.3474801317
H	-3.0896523177	1.3240279941	-4.3424602080
H	-3.5234311557	3.0059236431	-4.0453534777
H	-4.2165434226	2.7664160366	-1.0367545654
H	-3.1978341939	4.0468521119	-1.7151363071
H	-2.6041014839	3.0474846193	-.3713263852
H	2.0860714118	.0818681987	-1.6613091892
H	4.4107224226	.7968699946	-1.5119735715
H	3.3985794943	2.1277927066	-.9231072987
H	4.1283495302	2.2039506362	-2.5337126881
H	3.6568178154	-.6117553317	-3.4867020695
H	3.1259188547	.7655802230	-4.4639960152
H	1.9900208519	-.5328116323	-4.0736422219
H	-.3611732134	-3.5650792455	4.5259672030
H	2.0104084404	-4.2648704030	4.5737112463
H	3.4239486917	-3.9901886441	2.5673326362
H	-1.9842169636	-1.9719615609	1.5291301866
H	-3.1221903906	-1.0893144293	3.5027883665
H	-1.4395367965	-.5537635119	3.4980346040
H	-1.9482008105	-1.8539743136	4.5901343012
H	-3.7697343703	-3.3465472996	2.5169445053
H	-2.5953932773	-4.2167416807	3.5169236872
H	-2.5502179178	-4.3805675508	1.7556646368
H	2.1707666352	-2.6449104245	-.7059160384
H	4.0549170080	-4.1161802002	-1.1985213000
H	2.7941604509	-5.0869874226	-.4202903514
H	4.2198151300	-4.5885724909	.4939618041
H	4.4542711661	-1.7134570058	-.4993383580
H	4.4667145628	-2.0757225872	1.2328943460
H	3.3282604917	-.8833819220	.5845223094
N	-.0470928174	-2.1312412995	.1802978922
N	-.3268059139	.1369219684	-1.7457059665
O	1.3682813452	1.2637598486	1.2706811406
O	-2.7197128351	.8490212187	1.0886822719
O	-1.4676889463	1.1437527693	1.0327929887
Cu	-.4625252733	-.2462637520	.3071272615

12. L^1CuXO_2 η^1 triplet, X = furan

C	3.30423	0.55552	1.26086
C	4.65283	0.19935	1.14018
C	5.28544	0.15394	-0.09843
C	4.56607	0.47457	-1.24544
C	3.22035	0.85424	-1.18179
C	2.65486	0.58856	2.64354
C	3.10306	1.82674	3.44832
C	2.92117	-0.69575	3.45264
C	2.47932	1.19318	-2.47587
C	2.31399	-0.04558	-3.37821
C	3.16399	2.33455	-3.25407
C	-3.08214	0.02989	-0.45590
C	-3.81168	-0.63450	0.56561
C	-4.94549	-1.37565	0.21185
C	-5.35144	-1.48914	-1.11463
C	-4.61584	-0.85449	-2.11131
C	-3.48238	-0.08965	-1.81241
C	-3.39831	-0.55160	2.03482
C	-3.23721	-1.94479	2.67479
C	-4.38258	0.30617	2.85402
C	-2.69666	0.55371	-2.95474
C	-3.57890	1.46617	-3.82910
C	-2.00201	-0.51118	-3.82716
C	1.70450	3.60202	0.22102
C	0.72530	2.43674	0.20256
C	-0.64455	2.79796	0.18427
C	-1.82776	2.04739	-0.01467
C	1.20585	-3.04503	-1.13796
C	-0.99662	-3.20529	-1.25757
C	0.92445	-4.35584	-1.34631
C	-0.50669	-4.45973	-1.42331
C	-3.10785	2.86084	-0.13549
C	2.58535	0.89639	0.08602
H	2.11545	-2.47981	-1.01051
H	1.25512	4.47945	0.69080
H	1.97789	3.87991	-0.80405
H	2.62844	3.35134	0.74500
H	-0.81419	3.86556	0.26596
H	-3.00748	3.81808	0.38047
H	-3.96467	2.32365	0.27689
H	-3.33279	3.07309	-1.18685
H	5.21773	-0.04876	2.03479
H	6.33165	-0.13133	-0.16875
H	5.06029	0.43318	-2.21251
H	1.57420	0.66456	2.49482
H	2.61295	1.84821	4.42863
H	2.85662	2.75874	2.93099
H	4.18616	1.81553	3.61654
H	2.34657	-0.67979	4.38548
H	3.97791	-0.79421	3.72497
H	2.63360	-1.59215	2.89604
H	1.47512	1.53126	-2.20763
H	1.77158	0.21422	-4.29444
H	1.75358	-0.83702	-2.87299
H	3.28616	-0.45682	-3.67213
H	2.56192	2.62019	-4.12400
H	4.15169	2.03642	-3.62338
H	3.30206	3.22365	-2.63052
H	-5.51563	-1.87512	0.99081
H	-6.23126	-2.07323	-1.37064
H	-4.92671	-0.95724	-3.14778
H	-2.42300	-0.05942	2.07414
H	-2.84697	-1.85207	3.69456

H	-2.54360	-2.57129	2.10637
H	-4.19319	-2.47683	2.73748
H	-4.04649	0.39202	3.89378
H	-5.38396	-0.13936	2.86263
H	-4.47137	1.31746	2.44468
H	-1.91025	1.17238	-2.51536
H	-2.96929	1.98285	-4.57885
H	-4.09643	2.22371	-3.23228
H	-4.34285	0.89372	-4.36723
H	-1.42984	-0.03636	-4.63252
H	-2.73250	-1.18418	-4.29045
H	-1.31074	-1.12124	-3.23913
H	-1.98555	-2.77469	-1.24474
H	1.64405	-5.15711	-1.43587
H	-1.08875	-5.35597	-1.58422
N	1.18881	1.18792	0.16083
N	-1.87983	0.71945	-0.12112
O	-0.02736	-1.36252	1.92403
O	0.37255	-2.54130	1.89710
O	0.04077	-2.31828	-1.08677
Cu	-0.18099	-0.22510	0.19292

13. L^1CuX, X = oxetane

C	-0.59225	-3.20632	-0.45532
C	0.68272	-4.05977	-0.62360
C	3.12767	0.67589	1.38165
C	4.44759	0.21117	1.39373
C	5.19586	0.12071	0.22331
C	4.62079	0.50279	-0.98617
C	3.30516	0.97353	-1.05195
C	2.33058	0.73571	2.68185
C	3.06284	1.51715	3.78734
C	1.95266	-0.67744	3.16729
C	2.69013	1.32573	-2.40487
C	2.29975	0.04814	-3.17626
C	3.59553	2.22423	-3.26562
C	-3.12826	0.30178	-0.29001
C	-3.78317	-0.20099	0.86233
C	-4.92086	-0.99813	0.69641
C	-5.41725	-1.30004	-0.56864
C	-4.77070	-0.79803	-1.69486
C	-3.63082	0.00447	-1.58343
C	-3.23146	0.06117	2.26098
C	-2.52327	-1.19272	2.81296
C	-4.30399	0.56179	3.24356
C	-2.90515	0.48198	-2.83996
C	-3.85260	1.04721	-3.91226
C	-2.03113	-0.64654	-3.42479
C	1.76276	3.77310	0.28823
C	0.73845	2.65731	0.14050
C	-0.61793	3.05891	0.07179
C	-1.81841	2.32142	-0.06337
C	-3.10750	3.12848	-0.09904
C	2.54619	1.05407	0.14531
H	2.06937	-2.76316	0.60324
H	0.80152	-4.85432	0.11596
H	2.02275	-2.32638	-1.12900
H	-1.27162	-3.48739	0.35459
H	-1.16321	-3.01682	-1.36897
H	0.84602	-4.46561	-1.62399
H	1.28281	4.75082	0.35641
H	2.45328	3.78584	-0.56209
H	2.37449	3.62199	1.18395

H	-0.76374	4.13068	0.13244
H	-2.91274	4.19828	-0.00748
H	-3.77718	2.82543	0.71309
H	-3.65204	2.95353	-1.03320
H	4.89861	-0.08464	2.33791
H	6.21947	-0.24309	0.25298
H	5.20624	0.42971	-1.89900
H	1.39660	1.26280	2.46908
H	2.42621	1.61066	4.67430
H	3.32845	2.52573	3.45434
H	3.98693	1.01770	4.09948
H	1.36481	-0.62923	4.09128
H	2.84695	-1.27873	3.37037
H	1.35347	-1.20075	2.41521
H	1.76583	1.87762	-2.21512
H	1.83274	0.29545	-4.13702
H	1.58542	-0.54994	-2.60041
H	3.18023	-0.57316	-3.38051
H	3.06824	2.53380	-4.17488
H	4.50940	1.70880	-3.58140
H	3.89528	3.12800	-2.72520
H	-5.42492	-1.39521	1.57388
H	-6.30122	-1.92290	-0.67677
H	-5.15743	-1.04050	-2.68129
H	-2.47335	0.84419	2.17320
H	-2.09560	-0.99587	3.80309
H	-1.70862	-1.50499	2.15059
H	-3.22326	-2.03138	2.90917
H	-3.84695	0.82372	4.20439
H	-5.06754	-0.19836	3.44278
H	-4.81396	1.45100	2.85865
H	-2.22670	1.28643	-2.54366
H	-3.27609	1.46417	-4.74568
H	-4.48586	1.84373	-3.50796
H	-4.51235	0.27772	-4.32832
H	-1.47526	-0.29875	-4.30366
H	-2.64516	-1.50221	-3.73024
H	-1.30294	-0.99645	-2.68495
N	1.16493	1.39527	0.09078
N	-1.89145	0.99344	-0.15544
O	0.20290	-2.03598	-0.08245
C	1.45659	-2.76394	-0.30232
Cu	-0.21942	0.00243	-0.06939

14. L^1CuXO_2 η^1 singlet, X = oxetane

C	-1.15919	2.31417	-2.69266
C	-0.87665	3.52730	-3.33247
C	0.40516	3.84033	-3.76951
C	1.43713	2.93018	-3.56506
C	1.21410	1.70545	-2.92615
C	-2.59698	2.02779	-2.26334
C	-3.56691	1.98794	-3.46530
C	-3.08871	3.05220	-1.22440
C	2.37926	0.72989	-2.77521
C	3.55006	1.35470	-1.99262
C	2.86730	0.21229	-4.14426
C	0.46370	-2.70227	1.37753
C	-0.41100	-2.88806	2.47619
C	0.10618	-3.44776	3.64987
C	1.44686	-3.80887	3.74738
C	2.29655	-3.61260	2.66037
C	1.82959	-3.06414	1.46156
C	-1.88881	-2.50884	2.39358
C	-2.26170	-1.43401	3.42942
C	-2.80728	-3.74013	2.53212
C	2.79169	-2.85092	0.29333
C	3.53704	-4.13961	-0.10689
C	3.79049	-1.71557	0.58985
C	1.35701	2.45355	1.20803
C	1.40206	2.50092	2.74549
C	1.49588	0.96445	2.68099
C	-0.93981	-0.75031	-4.07024
C	-0.65250	-0.92219	-2.58336
C	-0.72954	-2.25138	-2.11304
C	-0.37105	-2.79667	-0.86525
C	-0.35191	-4.31509	-0.78822
C	-0.09871	1.39613	-2.48308
H	-1.06659	-1.71826	-4.55777
H	-0.13390	-0.21038	-4.57324
H	-1.84999	-0.16654	-4.22522
H	-1.02894	-2.97800	-2.85770
H	-0.81770	-4.75606	-1.67123
H	-0.87488	-4.67359	0.10149
H	0.67441	-4.68919	-0.72172
H	-1.68297	4.23685	-3.49854
H	0.59746	4.78371	-4.27362
H	2.43596	3.16867	-3.92160
H	-2.61444	1.04933	-1.77680
H	-4.57393	1.71452	-3.13198
H	-3.26190	1.26339	-4.22628
H	-3.63610	2.96423	-3.95833
H	-4.09495	2.79086	-0.88215
H	-3.12738	4.06201	-1.65018
H	-2.43090	3.06475	-0.35278
H	2.02278	-0.13113	-2.20396
H	4.37190	0.63654	-1.89734
H	3.24082	1.64368	-0.98428
H	3.94579	2.24409	-2.49597
H	3.67574	-0.51550	-4.01151
H	3.25352	1.02666	-4.76740
H	2.06623	-0.28033	-4.70394
H	-0.55461	-3.60656	4.49841
H	1.82952	-4.24513	4.66597
H	3.34307	-3.89509	2.74292
H	-2.06594	-2.06966	1.40884
H	-3.31601	-1.15823	3.32616
H	-1.67150	-0.52478	3.28012
H	-2.10003	-1.78480	4.45522

H	-3.85652	-3.44850	2.41339
H	-2.70227	-4.21505	3.51416
H	-2.58613	-4.49889	1.77447
H	2.19937	-2.53470	-0.56999
H	4.14854	-3.96126	-0.99874
H	2.84663	-4.95801	-0.33488
H	4.20834	-4.48588	0.68686
H	4.46455	-1.56682	-0.26170
H	4.40769	-1.94827	1.46545
H	3.26787	-0.77266	0.77447
H	0.43366	2.80262	0.74175
H	2.22223	2.87206	0.68577
H	0.49007	2.88021	3.20912
H	2.26790	3.00665	3.17563
H	2.43931	0.52080	3.01298
H	0.65637	0.41047	3.10770
N	-0.32119	0.13439	-1.83870
N	-0.02664	-2.06991	0.19908
O	1.42593	0.98479	1.21609
O	-2.63569	0.75122	0.88243
O	-1.43214	1.21063	0.87395
Cu	-0.22198	-0.09833	0.19845

15. L^1CuXO_2 η^1 triplet, X = oxetane

O	-0.09183	-1.07314	2.00052
O	-0.26342	-0.49356	3.08932
C	-0.89166	-2.98404	-0.52288
C	2.92915	-0.43780	3.40412
C	2.47433	1.41638	-2.41752
C	2.21258	0.10617	-3.18760
C	3.15371	2.45430	-3.32894
C	-3.05755	0.33102	-0.30078
C	-3.87188	-0.15985	0.75309
C	-5.03340	-0.87181	0.42987
C	-5.39083	-1.12254	-0.89028
C	-4.57757	-0.65288	-1.91722
C	-3.41369	0.07763	-1.65241
C	0.23122	-4.03750	-0.47850
C	-3.52162	0.05817	2.22420
C	-3.41550	-1.27672	2.98800
C	-4.53143	0.98565	2.92895
C	-2.56028	0.56594	-2.82249
C	-3.37048	1.41189	-3.82335
C	-1.86939	-0.60717	-3.54525
C	1.76486	3.89335	0.33601
C	0.78104	2.73422	0.28870
C	-0.58822	3.08932	0.26447
C	-1.77233	2.33338	0.07352
C	3.39831	0.91972	1.31148
C	-3.04683	3.14736	-0.09452
C	2.65021	1.21643	0.14450
C	4.75266	0.59468	1.17404
C	5.36400	0.53651	-0.07453
C	4.61535	0.80776	-1.21562
C	3.26252	1.15367	-1.13460
C	2.76525	0.92532	2.70179
C	1.19319	-2.83465	-0.44759
C	3.32463	2.05182	3.59182
H	1.64686	-2.63306	0.52755
H	0.24626	-4.68868	0.39732
H	1.95005	-2.76565	-1.23293
H	-1.43837	-2.85191	0.41528
H	-1.59233	-3.01746	-1.36040

H	0.30636	-4.64246	-1.38442
H	1.25638	4.83544	0.54644
H	2.28582	3.99345	-0.62267
H	2.53496	3.73139	1.09436
H	-0.76120	4.15641	0.33215
H	-2.89479	4.18694	0.19969
H	-3.86966	2.73159	0.49131
H	-3.36955	3.13429	-1.14140
H	5.33706	0.37607	2.06414
H	6.41547	0.27557	-0.15882
H	5.09195	0.75025	-2.19106
H	1.69398	1.10503	2.57676
H	2.82740	2.05123	4.56846
H	3.17341	3.03768	3.14127
H	4.39949	1.92797	3.76589
H	2.37927	-0.45021	4.35145
H	3.98054	-0.65224	3.62656
H	2.54550	-1.25433	2.78512
H	1.49901	1.81895	-2.13217
H	1.63198	0.29937	-4.09753
H	1.64654	-0.60188	-2.57448
H	3.15198	-0.37435	-3.48510
H	2.51338	2.68195	-4.18864
H	4.11112	2.09289	-3.72053
H	3.34757	3.39102	-2.79619
H	-5.66775	-1.24039	1.23206
H	-6.29548	-1.68011	-1.11750
H	-4.85445	-0.85380	-2.94914
H	-2.54212	0.54119	2.26420
H	-3.06370	-1.10543	4.01112
H	-2.71279	-1.96084	2.50328
H	-4.38513	-1.78345	3.05117
H	-4.24125	1.14547	3.97374
H	-5.53906	0.55408	2.92623
H	-4.59008	1.96576	2.44623
H	-1.77063	1.20160	-2.41443
H	-2.71202	1.82054	-4.59820
H	-3.87156	2.25101	-3.33032
H	-4.14170	0.81878	-4.32761
H	-1.25860	-0.24137	-4.37895
H	-2.60417	-1.31039	-3.95424
H	-1.21087	-1.15401	-2.86432
N	1.25149	1.48738	0.23403
N	-1.82990	1.00494	-0.00990
O	0.08786	-1.90665	-0.70323
Cu	-0.08303	0.05254	0.18393

16. L^1CuXO_2 η^2 singlet, X = oxetane

C	-1.08651	2.38970	-2.70805
C	3.64681	1.48783	-1.91800
C	2.89659	0.09754	-3.89121
C	0.43195	-2.56277	1.45278
C	-0.39962	-2.88270	2.56212
C	0.20251	-3.39873	3.71653
C	1.57483	-3.60631	3.79810
C	2.37695	-3.30796	2.70490
C	1.83600	-2.79089	1.52260
C	-1.91995	-2.73074	2.53762
C	-2.42565	-1.76868	3.62794
C	-0.76018	3.59562	-3.34081
C	-2.63409	-4.09508	2.67456
C	2.77838	-2.50674	0.35305
C	3.54355	-3.77017	-0.08985

C	3.77389	-1.38004	0.68744
C	1.52989	2.52426	1.23262
C	2.46819	2.30234	2.43676
C	1.71967	0.96391	2.61127
C	-0.83857	-0.73100	-4.05283
C	-0.61993	-0.88357	-2.55795
C	-0.75874	-2.19453	-2.05758
C	0.54062	3.88934	-3.72499
C	-0.44374	-2.71146	-0.78693
C	-0.44799	-4.22396	-0.66605
C	-0.04789	1.44734	-2.46474
C	1.55246	2.97029	-3.46962
C	1.29120	1.75238	-2.83315
C	-2.54809	2.14956	-2.33689
C	-3.45865	2.10398	-3.58531
C	-3.07463	3.23128	-1.37494
C	2.44604	0.78828	-2.58822
H	-0.80907	-1.70008	-4.55200
H	-0.09829	-0.07114	-4.51015
H	-1.81895	-0.28405	-4.23702
H	-1.05068	-2.93387	-2.79202
H	-0.94027	-4.67845	-1.52708
H	-0.95511	-4.54746	0.24504
H	0.57291	-4.61236	-0.61525
H	-1.54861	4.31675	-3.53888
H	0.76571	4.82860	-4.22272
H	2.56863	3.20166	-3.77684
H	-2.61266	1.19247	-1.81510
H	-4.48450	1.85083	-3.29598
H	-3.12897	1.36841	-4.32355
H	-3.48663	3.07715	-4.08951
H	-4.08855	2.97887	-1.04817
H	-3.12017	4.21188	-1.86304
H	-2.44392	3.31772	-0.48831
H	2.09168	0.01292	-1.90473
H	4.44180	0.76253	-1.71571
H	3.36336	1.95294	-0.96845
H	4.07704	2.26722	-2.55668
H	3.70820	-0.61059	-3.68877
H	3.26552	0.83316	-4.61469
H	2.08182	-0.45604	-4.36722
H	-0.42174	-3.65123	4.56865
H	2.01658	-4.00756	4.70620
H	3.44777	-3.48744	2.76607
H	-2.19947	-2.29954	1.57309
H	-3.50749	-1.62346	3.53419
H	-1.94962	-0.78881	3.54526
H	-2.23091	-2.16757	4.62926
H	-3.71937	-3.95940	2.60499
H	-2.42005	-4.56878	3.64024
H	-2.33537	-4.79806	1.89110
H	2.17614	-2.16199	-0.49019
H	4.14239	-3.56061	-0.98334
H	2.86997	-4.59923	-0.32580
H	4.22653	-4.11674	0.69380
H	4.46448	-1.21897	-0.14740
H	4.37726	-1.62121	1.56990
H	3.25060	-0.43872	0.87835
H	0.75211	3.28033	1.37933
H	1.99688	2.66450	0.25227
H	2.36307	3.01568	3.25653
H	3.52414	2.20073	2.17703
H	2.31186	0.04602	2.56866
H	1.03808	0.92059	3.46733

N	-0.32307	0.19179	-1.82457
N	-0.11088	-1.96603	0.26626
O	0.98031	1.18405	1.37641
O	-1.71011	0.40070	1.56795
O	-1.69844	1.34639	0.62708
Cu	-0.45325	-0.04910	0.13167

17. L^1CuXO_2 η^2 triplet, X = oxetane

C	0.30806	-1.35615	4.12159
C	1.49644	1.06030	-2.08233
C	-2.70904	-3.04361	-4.16468
C	-1.84713	-4.33475	-2.16752
C	-2.82689	1.19503	0.25204
C	-3.40147	1.42955	1.65929
C	-3.11752	2.42956	-0.62627
C	2.72265	0.72313	-0.03817
C	3.83660	-0.14400	0.10614
C	4.83490	0.19204	1.02865
C	4.74636	1.34083	1.80811
C	3.64116	2.17499	1.67365
C	2.58658	2.00174	-2.56976
C	2.61626	1.89387	0.76299
C	3.98903	-1.40618	-0.73922
C	4.35142	-2.64294	0.10245
C	5.02213	-1.19848	-1.86377
C	1.41476	2.84054	0.70422
C	1.82777	4.29889	0.42054
C	0.58647	2.77585	2.00527
C	-0.77501	-1.15422	3.04571
C	1.29202	-0.86940	3.03774
C	-2.50029	-0.84395	-1.28354
C	-1.99296	0.68533	-3.65359
C	-0.91563	0.40805	-2.61471
C	0.33936	0.99869	-2.88064
C	-2.95549	-2.06865	-1.83198
C	-4.24850	-2.50272	-1.51040
C	-5.07390	-1.76689	-0.66878
C	-4.60547	-0.58002	-0.11242
C	-3.32137	-0.10226	-0.39095
C	-2.09282	-2.92778	-2.75412
H	0.45053	-2.38069	4.46777
H	1.87052	0.02953	3.25476
H	0.21722	-0.68849	4.98033
H	-1.57128	-0.44047	3.28175
H	-1.87321	1.68691	-4.07351
H	-2.99857	0.58917	-3.24374
H	-1.90005	-0.03029	-4.47819
H	0.38611	1.57304	-3.79842
H	2.56178	2.07345	-3.65905
H	3.57890	1.67255	-2.25581
H	2.43509	3.01057	-2.17109
H	-4.61280	-3.43707	-1.92864
H	-6.07555	-2.11963	-0.43719
H	-5.25021	-0.01972	0.55732
H	-1.12021	-2.43500	-2.85108
H	-2.03923	-3.59807	-4.83152
H	-2.89651	-2.06103	-4.61068
H	-3.66505	-3.58119	-4.13854
H	-1.18212	-4.90835	-2.82316
H	-2.78366	-4.89848	-2.07624
H	-1.38636	-4.27910	-1.17860
H	-1.73918	1.10925	0.34990
H	-2.86306	2.24774	2.15133

H	-3.31689	0.53953	2.28800
H	-4.45837	1.71465	1.62757
H	-2.77189	3.34267	-0.12652
H	-4.19396	2.53116	-0.80656
H	-2.61798	2.37325	-1.59503
H	5.69841	-0.45837	1.13672
H	5.53216	1.58370	2.51881
H	3.56999	3.06580	2.29322
H	3.02326	-1.60334	-1.21285
H	4.34392	-3.54073	-0.52578
H	3.63585	-2.79794	0.91369
H	5.35168	-2.56205	0.54327
H	5.10507	-2.09883	-2.48332
H	6.01435	-0.98144	-1.45108
H	4.74137	-0.36560	-2.51622
H	0.76197	2.51647	-0.11101
H	0.93774	4.92455	0.28480
H	2.44374	4.38699	-0.47987
H	2.40048	4.72697	1.25121
H	-0.29211	3.42949	1.93094
H	1.17738	3.11563	2.86523
H	0.24515	1.75578	2.19981
H	-1.21060	-2.07179	2.63758
H	1.94890	-1.63914	2.62823
N	-1.18042	-0.36162	-1.56181
N	1.66783	0.38228	-0.94627
O	0.19626	-0.57832	2.12220
O	1.08914	-2.80189	0.41915
O	-0.19299	-2.76983	0.22697
Cu	0.34150	-0.96697	-0.44312

18. L^1CuX, X = methyloxirane

C	1.20676	-4.50552	-0.55277
C	-1.11342	-3.34261	-0.26959
C	3.16876	0.64287	1.50215
C	4.52122	0.29454	1.57509
C	5.30253	0.18140	0.42757
C	4.72639	0.40542	-0.82009
C	3.37778	0.75702	-0.94456
C	2.30343	0.66528	2.75746
C	2.99482	1.30554	3.97132
C	1.82210	-0.76111	3.09334
C	2.73953	0.90149	-2.32198
C	2.35973	-0.48634	-2.87482
C	3.61108	1.66691	-3.32977
C	-3.00303	-0.18893	-0.26734
C	-3.61059	-0.75625	0.88079
C	-4.66305	-1.66267	0.70857
C	-5.12211	-2.01062	-0.55862
C	-4.52903	-1.43722	-1.68213
C	-3.47579	-0.52366	-1.56375
C	-3.11397	-0.43112	2.28683
C	-2.38746	-1.63448	2.91735
C	-4.24566	0.06306	3.20473
C	-2.80375	0.04348	-2.81146
C	-3.79700	0.41314	-3.92431
C	-1.73169	-0.92838	-3.34142
C	1.67510	3.55752	0.26575
C	0.70750	2.39124	0.14514
C	-0.66658	2.72232	0.06122
C	-1.82586	1.91988	-0.06027
C	-3.15780	2.65094	-0.10429
C	2.59824	0.89024	0.22976

H	0.27874	-3.04970	-1.93132
H	2.22377	-4.10899	-0.63566
H	1.11961	-5.36539	-1.22609
H	1.05058	-4.84726	0.47344
H	-1.95058	-2.88460	-0.78754
H	-1.36588	-4.03231	0.53205
H	1.14739	4.51193	0.28938
H	2.37667	3.56815	-0.57524
H	2.28029	3.46994	1.17385
H	-0.86757	3.78587	0.10007
H	-3.02373	3.73144	-0.03668
H	-3.80182	2.32799	0.72064
H	-3.69896	2.42490	-1.02909
H	4.97055	0.10134	2.54479
H	6.35204	-0.08811	0.50505
H	5.33508	0.29893	-1.71326
H	1.41344	1.26032	2.53396
H	2.28932	1.39056	4.80487
H	3.36700	2.30828	3.73784
H	3.84213	0.70852	4.32562
H	1.15281	-0.75284	3.96143
H	2.67293	-1.41207	3.32584
H	1.28122	-1.20619	2.25193
H	1.80943	1.46272	-2.19760
H	1.84864	-0.39955	-3.84058
H	1.69133	-1.00720	-2.18132
H	3.25154	-1.10829	-3.01403
H	3.05708	1.83090	-4.26037
H	4.52200	1.11649	-3.58859
H	3.91159	2.64340	-2.93692
H	-5.12876	-2.10718	1.58409
H	-5.93838	-2.71830	-0.67178
H	-4.89188	-1.70797	-2.66944
H	-2.38198	0.37612	2.19742
H	-2.01459	-1.38106	3.91615
H	-1.53238	-1.94033	2.30790
H	-3.05866	-2.49528	3.01918
H	-3.84368	0.36197	4.17882
H	-4.99398	-0.71677	3.38351
H	-4.76273	0.92522	2.77156
H	-2.28166	0.95790	-2.51763
H	-3.27593	0.93035	-4.73677
H	-4.58744	1.07256	-3.55225
H	-4.27660	-0.47042	-4.35910
H	-1.23096	-0.51746	-4.22523
H	-2.17647	-1.89132	-3.61908
H	-0.96719	-1.10860	-2.57913
N	1.20092	1.15209	0.12531
N	-1.82256	0.58987	-0.13014
O	-0.03636	-2.42787	0.07607
C	0.19725	-3.45574	-0.92462
Cu	-0.06579	-0.30308	-0.01331

19. L^1CuXO_2 η^1 singlet, X = methyloxirane

C	2.11975	1.86786	1.97664
C	1.51106	1.52564	3.31042
C	1.39606	2.61756	0.94053
C	-1.14362	2.30023	-2.48912
C	-0.82264	3.56480	-2.99696
C	0.47054	3.87499	-3.40512
C	1.47298	2.91579	-3.29545
C	1.21231	1.63731	-2.78834
C	-2.58170	2.00833	-2.07014

C	-3.50725	1.88517	-3.29714
C	-3.13207	3.06471	-1.09339
C	2.35683	0.62649	-2.69739
C	3.58530	1.19350	-1.96192
C	2.77315	0.11030	-4.09031
C	0.38529	-2.75462	1.29611
C	-0.47743	-2.94245	2.40820
C	0.05381	-3.48278	3.58422
C	1.40114	-3.81099	3.68803
C	2.24537	-3.59405	2.60345
C	1.76897	-3.06753	1.39880
C	-1.96176	-2.58923	2.35219
C	-2.37539	-1.63950	3.49200
C	-2.84176	-3.85369	2.35148
C	2.76340	-2.81271	0.26603
C	3.58043	-4.06715	-0.10116
C	3.70831	-1.64688	0.62073
C	-0.80525	-0.82152	-4.18835
C	-0.59219	-1.03109	-2.69580
C	-0.64741	-2.37196	-2.26253
C	-0.35474	-2.91092	-0.99590
C	-0.26226	-4.42425	-0.90941
C	-0.12113	1.32147	-2.40600
H	1.85489	0.54225	3.64929
H	1.80876	2.26509	4.06313
H	1.94177	3.20878	0.20701
H	0.36647	2.91435	1.12425
H	3.21018	1.91863	1.95613
H	0.42096	1.50930	3.24290
H	-0.37983	-1.64949	-4.76021
H	-0.37740	0.11563	-4.54344
H	-1.88106	-0.79467	-4.39727
H	-0.85288	-3.09795	-3.03985
H	-0.78872	-4.88943	-1.74483
H	-0.68115	-4.79497	0.02909
H	0.78223	-4.75026	-0.94704
H	-1.60202	4.31705	-3.07759
H	0.69801	4.86048	-3.80251
H	2.48245	3.16492	-3.61002
H	-2.58851	1.04529	-1.55072
H	-4.52531	1.62606	-2.98560
H	-3.15926	1.11554	-3.99270
H	-3.55678	2.83117	-3.84864
H	-4.12840	2.77128	-0.74651
H	-3.22449	4.04843	-1.56749
H	-2.49364	3.16798	-0.21312
H	1.99701	-0.22621	-2.11552
H	4.35718	0.42158	-1.87148
H	3.31672	1.52001	-0.95543
H	4.03422	2.03711	-2.49747
H	3.57201	-0.63462	-3.99942
H	3.15095	0.92812	-4.71491
H	1.94017	-0.35603	-4.62306
H	-0.60094	-3.64707	4.43542
H	1.79412	-4.22738	4.61161
H	3.30093	-3.83559	2.69518
H	-2.14595	-2.06369	1.41087
H	-3.41159	-1.31375	3.35494
H	-1.74557	-0.74643	3.51089
H	-2.30473	-2.12328	4.47266
H	-3.90206	-3.58429	2.29191
H	-2.69476	-4.43937	3.26637
H	-2.61139	-4.50338	1.50087
H	2.20095	-2.51434	-0.62223

H	4.20062	-3.87068	-0.98286
H	2.93799	-4.92476	-0.32525
H	4.25448	-4.36491	0.70954
H	4.41545	-1.46409	-0.19673
H	4.29236	-1.87261	1.52061
H	3.14718	-0.72579	0.79634
N	-0.41045	0.01567	-1.89377
N	-0.13233	-2.18099	0.09507
O	1.58071	1.18921	0.81713
O	-2.58946	1.01960	1.35482
O	-1.31576	0.98722	1.20950
Cu	-0.54081	-0.27327	0.06723

20. L^1CuXO_2 η^1 triplet, X = methyloxirane

C	1.99004	1.33319	2.32900
C	1.15321	0.79999	3.45914
C	1.52034	2.38191	1.41211
C	-1.27985	2.26940	-2.68228
C	-1.06857	3.51257	-3.29058
C	0.17761	3.87743	-3.78958
C	1.24362	2.99064	-3.67838
C	1.08664	1.73039	-3.09183
C	-2.66151	1.94424	-2.11526
C	-3.71333	1.73371	-3.22268
C	-3.14527	3.03306	-1.13618
C	2.29803	0.80269	-2.99123
C	3.38048	1.38996	-2.06430
C	2.89946	0.47415	-4.37163
C	0.41981	-2.70595	1.39873
C	-0.48320	-2.81715	2.48901
C	-0.01550	-3.34400	3.69814
C	1.31039	-3.73550	3.85568
C	2.19235	-3.60490	2.78695
C	1.77399	-3.09961	1.55001
C	-1.94769	-2.39713	2.36972
C	-2.38722	-1.45753	3.50857
C	-2.88508	-3.61991	2.30306
C	2.79222	-2.96396	0.41867
C	3.53241	-4.28650	0.13680
C	3.80104	-1.83393	0.70492
C	-0.89663	-0.87993	-4.16153
C	-0.64486	-1.00164	-2.66631
C	-0.70792	-2.31484	-2.14170
C	-0.37693	-2.83841	-0.87197
C	-0.39974	-4.35431	-0.75725
C	-0.19408	1.36068	-2.60305
H	1.31743	-0.27361	3.59084
H	1.43108	1.30370	4.39157
H	2.23016	3.03439	0.90793
H	0.51279	2.77397	1.52918
H	3.06860	1.22989	2.44955
H	0.09098	0.97208	3.27326
H	-1.27106	-1.81729	-4.57581
H	0.02891	-0.61997	-4.68567
H	-1.61286	-0.08542	-4.38261
H	-0.99605	-3.06630	-2.86656
H	-1.00366	-4.79747	-1.55111
H	-0.78953	-4.68040	0.20942
H	0.61509	-4.75717	-0.84318
H	-1.89798	4.21035	-3.36963
H	0.31849	4.84867	-4.25619
H	2.22021	3.28107	-4.05756
H	-2.57736	1.00980	-1.55412

H	-4.68910	1.49687	-2.78341
H	-3.44425	0.91310	-3.89426
H	-3.83312	2.63632	-3.83288
H	-4.06922	2.71571	-0.64073
H	-3.35501	3.97562	-1.65429
H	-2.40094	3.23343	-0.36128
H	1.96370	-0.13685	-2.54370
H	4.24130	0.71384	-2.00250
H	2.99228	1.53109	-1.05250
H	3.74286	2.35581	-2.43504
H	3.71218	-0.25401	-4.26968
H	3.31595	1.36556	-4.85379
H	2.15289	0.05068	-5.05095
H	-0.70338	-3.44639	4.53308
H	1.65443	-4.13808	4.80468
H	3.22973	-3.90359	2.91489
H	-2.05743	-1.84562	1.43231
H	-3.40552	-1.09724	3.32823
H	-1.73388	-0.58345	3.58310
H	-2.38528	-1.96237	4.48120
H	-3.92774	-3.29922	2.19631
H	-2.81191	-4.22315	3.21541
H	-2.64743	-4.26881	1.45495
H	2.24964	-2.68583	-0.48882
H	4.17801	-4.18277	-0.74248
H	2.83595	-5.11000	-0.05040
H	4.17013	-4.58125	0.97769
H	4.52648	-1.74783	-0.11225
H	4.36049	-2.02630	1.62784
H	3.29257	-0.87122	0.80547
N	-0.35150	0.09071	-1.96251
N	-0.01942	-2.10349	0.18072
O	1.57544	1.00147	0.97119
O	-2.49397	0.77387	1.04843
O	-1.30118	1.17028	0.96289
Cu	-0.07352	-0.13084	-0.00563

21. L^1CuXO_2 η^2 singlet, X = methyloxirane

C	1.95584	2.45341	1.20470
C	2.06453	0.90000	3.29192
C	2.66664	1.47688	2.03783
C	-1.43150	2.07921	-2.74141
C	-1.32836	3.36255	-3.29112
C	-0.09740	3.90758	-3.63540
C	1.06601	3.17300	-3.42351
C	1.02713	1.89049	-2.86699
C	-2.81651	1.53434	-2.39538
C	-3.72047	1.44609	-3.64246
C	-3.50484	2.36919	-1.29677
C	2.32398	1.10737	-2.65217
C	3.49955	1.98825	-2.19612
C	2.73268	0.31871	-3.91322
C	0.24629	-2.52709	1.45044
C	-0.72448	-2.54254	2.48563
C	-0.33102	-2.97646	3.75537
C	0.97723	-3.37508	4.01221
C	1.91671	-3.35848	2.98665
C	1.57900	-2.94346	1.69267
C	-2.18136	-2.15475	2.23543
C	-2.76238	-1.23825	3.32706
C	-3.06359	-3.40806	2.06133
C	2.65469	-2.95625	0.60646
C	3.29978	-4.34850	0.45509

C	3.73686	-1.88845	0.86000
C	-0.76969	-0.92622	-4.19159
C	-0.51834	-1.05976	-2.69899
C	-0.57668	-2.36887	-2.18874
C	-0.35247	-2.81956	-0.87672
C	-0.36158	-4.32573	-0.68111
C	-0.24031	1.33933	-2.54215
H	0.97529	0.91150	3.22395
H	2.39049	-0.13372	3.44496
H	2.38220	1.48742	4.16124
H	0.93997	2.74057	1.45954
H	3.75795	1.49482	2.00198
H	2.51702	3.17553	0.61344
H	-0.38633	-1.80045	-4.72299
H	-0.31670	-0.02682	-4.60737
H	-1.84809	-0.87278	-4.37622
H	-0.78084	-3.14329	-2.91826
H	-1.07581	-4.78755	-1.36679
H	-0.61788	-4.60248	0.34220
H	0.62658	-4.74322	-0.90130
H	-2.23241	3.94333	-3.45257
H	-0.04236	4.90445	-4.06461
H	2.02335	3.60844	-3.69151
H	-2.69109	0.52139	-2.00289
H	-4.67378	0.96868	-3.38968
H	-3.25474	0.86863	-4.44722
H	-3.94746	2.44101	-4.04227
H	-4.48586	1.94292	-1.05667
H	-3.66580	3.40301	-1.62336
H	-2.90096	2.38216	-0.38711
H	2.13744	0.38419	-1.85355
H	4.35146	1.35683	-1.92244
H	3.23412	2.58874	-1.32425
H	3.84075	2.66487	-2.98793
H	3.66890	-0.22362	-3.73753
H	2.89094	0.99570	-4.76064
H	1.97556	-0.41294	-4.20505
H	-1.06189	-3.00133	4.55792
H	1.26216	-3.70125	5.00880
H	2.93560	-3.67436	3.19345
H	-2.21767	-1.59400	1.29859
H	-3.76312	-0.90252	3.03426
H	-2.13915	-0.35248	3.46816
H	-2.86293	-1.75155	4.29003
H	-4.10123	-3.12020	1.85738
H	-3.05797	-4.02182	2.96951
H	-2.72087	-4.03537	1.23259
H	2.18060	-2.70644	-0.34609
H	3.97961	-4.36072	-0.40396
H	2.55022	-5.13212	0.30631
H	3.88699	-4.61973	1.33922
H	4.50872	-1.93733	0.08310
H	4.23009	-2.04575	1.82627
H	3.30893	-0.88399	0.84941
N	-0.29417	0.02713	-1.96332
N	-0.11964	-2.02110	0.16213
O	2.08492	1.08307	0.76795
O	-0.84316	0.63524	1.61496
O	-0.91718	1.52745	0.60263
Cu	-0.28206	-0.11389	-0.03702

22. L^1CuXO_2 η^2 triplet, X = methyloxirane

C	1.50633	0.98422	-2.04989
C	2.59154	1.92659	-2.54750
C	-2.47422	-0.91632	-1.21485

C	-2.97532	-2.12693	-1.75553
C	-4.26675	-2.53541	-1.39807
C	-5.04920	-1.78576	-0.52700
C	-4.53843	-0.61094	0.01673
C	-3.25249	-0.15945	-0.29873
C	-2.16743	-2.99043	-2.72148
C	-2.81051	-3.02015	-4.12314
C	-1.98011	-4.42716	-2.19461
C	-2.72777	1.13562	0.32148
C	-3.09200	1.27743	1.81054
C	-3.21665	2.37776	-0.45283
C	2.71347	0.67520	0.01052
C	3.82622	-0.18185	0.21386
C	4.79255	0.17994	1.15903
C	4.67969	1.35018	1.90207
C	3.58186	2.18054	1.70376
C	2.58503	1.87123	0.77068
C	4.02909	-1.45303	-0.60530
C	4.38926	-2.67033	0.26594
C	5.09454	-1.23788	-1.69960
C	1.39643	2.82801	0.64221
C	1.83792	4.27388	0.33297
C	0.52092	2.80936	1.91185
C	-0.65757	-1.56380	2.93137
C	0.76740	-1.25185	3.09209
C	1.28076	-0.33972	4.17501
C	-2.01639	0.68918	-3.54884
C	-0.91136	0.34737	-2.55972
C	0.34488	0.92835	-2.84063
H	0.50481	0.36074	4.49783
H	1.60080	-0.92901	5.04205
H	-1.38004	-1.11100	3.60839
H	-1.91869	1.72222	-3.89183
H	-3.01033	0.54659	-3.12497
H	-1.93237	0.04250	-4.42991
H	0.38307	1.51213	-3.75347
H	2.60915	1.92811	-3.64039
H	3.57803	1.64570	-2.17580
H	2.39451	2.95393	-2.22414
H	-4.66481	-3.45718	-1.81323
H	-6.05124	-2.11660	-0.26730
H	-5.15132	-0.03447	0.70332
H	-1.17462	-2.54085	-2.81809
H	-2.18356	-3.58455	-4.82260
H	-2.94995	-2.01373	-4.52884
H	-3.79404	-3.50309	-4.09630
H	-1.34647	-5.00172	-2.88000
H	-2.93851	-4.95295	-2.11561
H	-1.50839	-4.43180	-1.20960
H	-1.63639	1.10775	0.25403
H	-2.56587	2.13419	2.24450
H	-2.81102	0.38619	2.37735
H	-4.16417	1.44808	1.95946
H	-2.82648	3.29471	0.00437
H	-4.31137	2.43772	-0.44026
H	-2.89537	2.36280	-1.49770
H	5.65409	-0.46389	1.31064
H	5.44228	1.61450	2.62983
H	3.49267	3.09129	2.29017
H	3.08510	-1.67679	-1.10920
H	4.41249	-3.57824	-0.34622
H	3.65610	-2.82280	1.06242
H	5.37644	-2.56536	0.72986
H	5.21637	-2.14411	-2.30389

H	6.06794	-0.99446	-1.25793
H	4.82046	-0.41918	-2.37249
H	0.76821	2.48938	-0.18503
H	0.96313	4.90400	0.13672
H	2.49639	4.32819	-0.53933
H	2.37572	4.72008	1.17695
H	-0.33423	3.48616	1.79462
H	1.08843	3.14580	2.78783
H	0.14339	1.80461	2.11282
H	-0.96476	-2.49717	2.46591
H	1.47694	-1.98358	2.70725
H	2.14070	0.23523	3.81730
N	-1.15212	-0.46358	-1.53378
N	1.68488	0.30406	-0.91432
O	-0.00918	-0.62981	2.03781
O	1.16886	-2.94832	0.36265
O	-0.10450	-2.95284	0.09627
Cu	0.40257	-1.11364	-0.47111

23. L^1CuX, X = oxirane

C	-0.22453	-4.20007	-0.27547
C	3.12863	0.03354	1.44364
C	4.46577	-0.37584	1.48744
C	5.22221	-0.50321	0.32507
C	4.63568	-0.22643	-0.90758
C	3.30202	0.18454	-1.00334
C	2.30003	0.09575	2.72248
C	3.02510	0.79404	3.88415
C	1.84215	-1.31764	3.13368
C	2.66295	0.40736	-2.37053
C	2.30740	-0.94253	-3.02573
C	3.52770	1.26004	-3.31378
C	-3.11657	-0.52355	-0.27711
C	-3.78163	-1.00863	0.87485
C	-4.94190	-1.77304	0.71141
C	-5.44698	-2.06115	-0.55401
C	-4.77986	-1.58852	-1.68143
C	-3.61537	-0.82121	-1.56970
C	-3.20664	-0.76912	2.26693
C	-2.43145	-2.01200	2.74769
C	-4.26520	-0.35257	3.30102
C	-2.86231	-0.38194	-2.82144
C	-3.77556	0.21488	-3.90505
C	-2.03682	-1.55506	-3.38832
C	1.71582	3.02072	0.31658
C	0.71016	1.89025	0.16360
C	-0.65192	2.26778	0.09439
C	-1.83647	1.50655	-0.04154
C	-3.13947	2.28991	-0.07753
C	2.54405	0.32158	0.18560
H	1.85012	-3.99951	-1.04979
H	-0.77765	-4.49078	0.61397
H	-0.64314	-4.52049	-1.22610
H	1.70989	-3.97317	0.79090
H	1.22257	3.99367	0.32863
H	2.44391	3.00901	-0.50089
H	2.28804	2.90966	1.24386
H	-0.81796	3.33611	0.15820
H	-2.96059	3.36250	0.00957
H	-3.80338	1.98034	0.73601
H	-3.68243	2.10221	-1.00985
H	4.92295	-0.60144	2.44684
H	6.26022	-0.81893	0.37892

H	5.22495	-0.33605	-1.81385
H	1.39789	0.67259	2.50239
H	2.35146	0.89964	4.74138
H	3.36805	1.79321	3.59711
H	3.89841	0.22756	4.22520
H	1.19593	-1.27900	4.01810
H	2.70303	-1.95395	3.37031
H	1.27883	-1.79435	2.32455
H	1.72317	0.94243	-2.21021
H	1.79718	-0.79015	-3.98372
H	1.64599	-1.52791	-2.37878
H	3.21034	-1.53507	-3.21393
H	2.98260	1.47002	-4.24048
H	4.45727	0.75140	-3.59151
H	3.79657	2.21683	-2.85480
H	-5.45806	-2.15195	1.58894
H	-6.35141	-2.65324	-0.66109
H	-5.16985	-1.82411	-2.66778
H	-2.48396	0.04766	2.18739
H	-1.96533	-1.82963	3.72286
H	-1.63968	-2.27513	2.03821
H	-3.09981	-2.87529	2.84664
H	-3.78429	-0.09269	4.25024
H	-4.97793	-1.15808	3.50815
H	-4.83602	0.51742	2.96080
H	-2.15345	0.39474	-2.52352
H	-3.17490	0.59863	-4.73684
H	-4.37613	1.04118	-3.51161
H	-4.46441	-0.52973	-4.31852
H	-1.44873	-1.23703	-4.25687
H	-2.69216	-2.37517	-3.70385
H	-1.34493	-1.94508	-2.63473
N	1.15774	0.63557	0.10701
N	-1.88335	0.17655	-0.13818
O	0.24483	-2.83894	-0.26554
C	1.21396	-3.89940	-0.17396
Cu	-0.18208	-0.78472	-0.07780

24. L^1CuXO_2 η^1 singlet, X = oxirane

C	-1.14364	2.33269	-2.73900
C	3.58213	1.58560	-1.86624
C	2.98912	0.25872	-3.93465
C	0.52121	-2.64196	1.38903
C	-0.32720	-2.81988	2.51183
C	0.20699	-3.40433	3.66540
C	1.54034	-3.79703	3.72644
C	2.36457	-3.61043	2.62059
C	1.88281	-3.04010	1.43805
C	-1.80258	-2.42366	2.47250
C	-2.15953	-1.40955	3.57372
C	-0.87217	3.52631	-3.41917
C	-2.72592	-3.65643	2.54874
C	2.83667	-2.84674	0.25875
C	3.53735	-4.15683	-0.15494
C	3.88276	-1.75593	0.56255
C	1.60384	2.31131	1.54710
C	1.51375	1.33093	2.63257
C	-0.87089	-0.70468	-4.04731
C	-0.60793	-0.86480	-2.55616
C	-0.71625	-2.18826	-2.07761
C	0.41278	3.85569	-3.83592
C	-0.37012	-2.72813	-0.82788
C	-0.39545	-4.24497	-0.73612

C	-0.06669	1.44988	-2.47352
C	1.46494	2.98930	-3.55847
C	1.25676	1.78828	-2.87238
C	-2.58264	2.04400	-2.31175
C	-3.56008	2.01649	-3.50592
C	-3.06882	3.07401	-1.27330
C	2.45034	0.86545	-2.62196
H	-0.87903	-1.67624	-4.54433
H	-0.11757	-0.07371	-4.52320
H	-1.83828	-0.22687	-4.22132
H	-1.02507	-2.91519	-2.81842
H	-0.97952	-4.67040	-1.55411
H	-0.81619	-4.58217	0.21345
H	0.61731	-4.65475	-0.79888
H	-1.69083	4.20689	-3.63587
H	0.59334	4.78117	-4.37611
H	2.46782	3.24398	-3.89108
H	-2.60203	1.06235	-1.82914
H	-4.56190	1.72996	-3.16731
H	-3.25745	1.31106	-4.28508
H	-3.64313	3.00256	-3.97687
H	-4.06776	2.80709	-0.91308
H	-3.12575	4.07723	-1.71166
H	-2.39678	3.10571	-0.41418
H	2.10770	0.04137	-1.99130
H	4.40494	0.89234	-1.66150
H	3.22742	1.97836	-0.90897
H	3.99195	2.42124	-2.44472
H	3.82702	-0.41790	-3.73034
H	3.34981	1.03736	-4.61663
H	2.22144	-0.31411	-4.46359
H	-0.43574	-3.56102	4.52741
H	1.93557	-4.25221	4.63053
H	3.40566	-3.91901	2.67472
H	-1.99285	-1.93064	1.51631
H	-3.20617	-1.10253	3.47973
H	-1.54608	-0.50725	3.49009
H	-2.01824	-1.82820	4.57629
H	-3.77588	-3.35199	2.47531
H	-2.59908	-4.19602	3.49432
H	-2.52732	-4.36244	1.73596
H	2.25069	-2.50121	-0.59680
H	4.13695	-3.99810	-1.05828
H	2.82090	-4.95720	-0.36551
H	4.21390	-4.52039	0.62630
H	4.54435	-1.60900	-0.29939
H	4.50956	-2.03660	1.41697
H	3.40073	-0.80142	0.79092
H	0.70878	2.84347	1.23575
H	2.55242	2.79301	1.32353
H	2.39219	1.08028	3.22137
H	0.55202	1.16049	3.10962
N	-0.27280	0.19131	-1.81557
N	-0.00100	-2.00037	0.22548
O	1.58844	0.88821	1.25312
O	-2.45765	0.96658	1.06688
O	-1.24325	1.39117	0.91700
Cu	-0.18530	-0.02379	0.23481

25. L^1CuXO_2 η^1 triplet, X = oxirane

C	-5.05498	-1.69698	0.40399
C	-5.42105	-1.89193	-0.92399
C	-4.61730	-1.37609	-1.93573

C	-3.45534	-0.65178	-1.64841
C	-3.52743	-0.82310	2.22095
C	-3.43722	-2.17686	2.95128
C	-4.50929	0.11087	2.95707
C	-2.60272	-0.12384	-2.80232
C	-3.41520	0.74468	-3.78193
C	-1.90568	-1.27422	-3.55654
C	1.71076	3.09884	0.30257
C	0.72422	1.94153	0.31139
C	-0.64205	2.30500	0.30530
C	-1.82361	1.54944	0.12187
C	3.35247	0.20073	1.35409
C	-3.10001	2.36450	-0.02669
C	2.58798	0.42895	0.18281
C	4.71616	-0.08215	1.21796
C	5.31996	-0.16745	-0.03242
C	-0.92148	-3.82788	-0.63031
C	4.55238	0.02575	-1.17729
C	3.18839	0.32617	-1.09762
C	2.72941	0.23266	2.74799
C	0.51043	-3.95439	-0.33615
C	3.21172	1.43925	3.57720
C	2.99998	-1.07636	3.51488
C	2.38086	0.50429	-2.38248
C	2.23653	-0.83309	-3.13678
C	2.96804	1.58874	-3.30485
C	-3.09445	-0.45118	-0.29030
C	-3.89490	-0.99240	0.74758
H	0.84358	-3.93949	0.69801
H	1.16966	-4.44379	-1.04911
H	-1.63039	-3.71851	0.18632
H	-1.32323	-4.22341	-1.55987
H	1.22046	4.03641	0.56949
H	2.14335	3.21472	-0.69761
H	2.54464	2.92693	0.98575
H	-0.81178	3.37264	0.37529
H	-2.97015	3.37260	0.37111
H	-3.94411	1.89040	0.47783
H	-3.37283	2.45374	-1.08423
H	5.31519	-0.24491	2.11020
H	6.38021	-0.39070	-0.11492
H	5.02205	-0.05646	-2.15432
H	1.64714	0.32397	2.62446
H	2.73588	1.44084	4.56457
H	2.97243	2.39018	3.09160
H	4.29652	1.40828	3.73063
H	2.45086	-1.08451	4.46261
H	4.06429	-1.19536	3.74686
H	2.68440	-1.94898	2.93619
H	1.37474	0.82605	-2.10045
H	1.64607	-0.69865	-4.05063
H	1.73208	-1.58216	-2.51897
H	3.21536	-1.23289	-3.42675
H	2.31803	1.74362	-4.17337
H	3.95824	1.31090	-3.68292
H	3.07015	2.54720	-2.78548
H	-5.68271	-2.10114	1.19369
H	-6.32515	-2.44279	-1.16901
H	-4.90029	-1.53490	-2.97344
H	-2.53739	-0.36150	2.26213
H	-3.06870	-2.03550	3.97266
H	-2.75111	-2.86087	2.44236
H	-4.41352	-2.66958	3.01694
H	-4.21166	0.23262	4.00483

H	-5.52761	-0.29447	2.94415
H	-4.54232	1.10565	2.50271
H	-1.81638	0.50509	-2.37668
H	-2.75813	1.17650	-4.54532
H	-3.92181	1.56785	-3.26849
H	-4.18235	0.16063	-4.30292
H	-1.29202	-0.88308	-4.37643
H	-2.63767	-1.96560	-3.99018
H	-1.25118	-1.84325	-2.89014
N	1.18556	0.69168	0.27249
N	-1.87293	0.22082	0.02330
O	-0.04016	-1.96695	1.95896
O	-0.21514	-1.47605	3.09226
O	-0.03305	-2.69909	-0.80892
Cu	-0.14587	-0.75811	0.23733

26. L^1CuXO_2 η^2 singlet, X = oxirane

C	-1.22987	2.30020	-2.78227
C	-1.94294	-2.46567	2.51429
C	-2.36334	-1.58056	3.70345
C	-0.96179	3.53273	-3.39204
C	-2.76019	-3.77250	2.50390
C	2.69470	-2.64363	0.22008
C	3.48826	-3.91950	-0.12670
C	3.65825	-1.46762	0.46499
C	2.18470	1.95907	1.69982
C	1.86388	0.93872	2.70741
C	3.60332	1.79898	-1.94370
C	-0.73990	-0.77671	-4.18414
C	-0.56180	-0.93349	-2.68169
C	-0.65633	-2.25569	-2.20024
C	0.33147	3.92335	-3.71363
C	-0.40918	-2.75789	-0.90998
C	-0.35310	-4.26899	-0.77693
C	-0.14146	1.43590	-2.50734
C	1.39658	3.08559	-3.40111
C	1.19174	1.84632	-2.78613
C	-2.67781	1.95738	-2.44166
C	2.84253	0.09031	-3.62436
C	-3.54778	1.80936	-3.70664
C	-3.30123	3.00889	-1.50158
C	2.39950	0.97510	-2.44015
C	0.36612	-2.54951	1.36601
C	-0.44460	-2.75056	2.51089
C	0.15413	-3.24465	3.67648
C	1.51425	-3.52365	3.73641
C	2.30317	-3.32156	2.60929
C	1.75829	-2.84309	1.41318
H	-0.45540	-1.69354	-4.70441
H	-0.16364	0.05745	-4.58483
H	-1.79395	-0.58295	-4.40703
H	-0.85637	-3.00348	-2.95737
H	-0.83880	-4.74893	-1.62819
H	-0.82991	-4.60463	0.14642
H	0.68517	-4.61346	-0.74500
H	-1.78909	4.19945	-3.61796
H	0.51188	4.88038	-4.19589
H	2.40772	3.40248	-3.63697
H	-2.67839	1.00443	-1.90652
H	-4.56577	1.50886	-3.43502
H	-3.15038	1.06393	-4.40137
H	-3.61812	2.75815	-4.25107
H	-4.30010	2.68604	-1.18821

H	-3.40907	3.97911	-2.00005
H	-2.69437	3.14551	-0.60502
H	2.09194	0.30902	-1.62868
H	4.35653	1.13762	-1.50288
H	3.30953	2.53532	-1.18988
H	4.09440	2.33950	-2.76070
H	3.72581	-0.49997	-3.35371
H	3.10496	0.70607	-4.49266
H	2.06021	-0.60770	-3.93071
H	-0.46132	-3.41286	4.55528
H	1.95745	-3.89960	4.65470
H	3.36605	-3.54338	2.65648
H	-2.17906	-1.90968	1.60476
H	-3.41725	-1.30020	3.60508
H	-1.77410	-0.66131	3.73749
H	-2.25074	-2.10114	4.66138
H	-3.83313	-3.55090	2.48620
H	-2.55748	-4.37284	3.39844
H	-2.53214	-4.39130	1.63019
H	2.09228	-2.38279	-0.65312
H	4.06204	-3.76967	-1.04806
H	2.83065	-4.78173	-0.27622
H	4.20202	-4.18447	0.66087
H	4.32500	-1.33009	-0.39392
H	4.28621	-1.64626	1.34575
H	3.09569	-0.54357	0.61675
H	1.77970	2.96458	1.80190
H	3.10584	1.88054	1.12493
H	2.54472	0.10561	2.87152
H	1.22322	1.19865	3.54788
N	-0.35531	0.14136	-1.92059
N	-0.19164	-2.00072	0.16455
O	1.20362	0.94516	1.43545
O	-1.54121	0.51796	1.55523
O	-1.51494	1.42214	0.56790
Cu	-0.56612	-0.10273	0.00888

27. L^1CuXO_2 η^2 triplet, X = oxirane

C	4.81162	0.10934	1.76408
C	4.74532	1.26169	2.54028
C	3.68239	2.14139	2.36921
C	2.62600	1.98401	-1.90454
C	2.67137	1.89842	1.43231
C	3.96941	-1.44388	-0.04221
C	4.36155	-2.68903	0.77309
C	4.97817	-1.21303	-1.18595
C	1.53519	2.91644	1.31031
C	2.05697	4.33066	0.98062
C	1.52720	1.05839	-1.40555
C	0.67085	2.95783	2.58653
C	-0.48920	-1.22429	3.80726
C	0.89449	-0.73855	3.79312
C	-2.46145	-0.86245	-0.63937
C	-1.96166	0.70604	-2.98162
C	-0.88012	0.40992	-1.95264
C	0.37469	1.00135	-2.21001
C	-2.91271	-2.08094	-1.20206
C	-4.20031	-2.52892	-0.88043
C	-5.02631	-1.80630	-0.02653
C	-2.69113	-3.04937	-3.53993
C	-4.56462	-0.61988	0.53647
C	-3.28383	-0.13138	0.25858
C	-2.04713	-2.91358	-2.14515

C	-1.73948	-4.30663	-1.56009
C	-2.81031	1.17334	0.89919
C	-3.16628	1.26925	2.39349
C	-3.35560	2.40700	0.14943
C	2.74438	0.71345	0.64938
C	3.82608	-0.19055	0.81724
H	1.19597	0.06364	4.46363
H	-1.20823	-0.78062	4.49368
H	-1.83034	1.70647	-3.40074
H	-2.96425	0.62400	-2.56143
H	-1.89057	-0.00982	-3.80877
H	0.42805	1.57810	-3.12633
H	2.68345	1.93808	-2.99513
H	3.59996	1.72822	-1.48563
H	2.40854	3.02284	-1.63449
H	-4.56031	-3.46015	-1.30916
H	-6.02469	-2.16761	0.20510
H	-5.21184	-0.06412	1.20872
H	-1.09344	-2.39140	-2.26778
H	-2.01997	-3.58186	-4.22320
H	-2.91817	-2.07326	-3.97970
H	-3.62898	-3.61443	-3.49231
H	-1.07596	-4.86364	-2.23164
H	-2.65410	-4.89752	-1.43575
H	-1.25288	-4.22916	-0.58483
H	-1.71928	1.19381	0.82479
H	-2.67720	2.14213	2.83913
H	-2.83431	0.38175	2.93817
H	-4.24399	1.38340	2.55616
H	-2.99887	3.33161	0.61834
H	-4.45166	2.42271	0.16932
H	-3.04105	2.42167	-0.89760
H	5.64882	-0.57050	1.89246
H	5.51958	1.47468	3.27243
H	3.63383	3.04053	2.97792
H	2.99651	-1.64256	-0.50048
H	4.33358	-3.57900	0.13516
H	3.67559	-2.85379	1.60766
H	5.37712	-2.61177	1.17750
H	5.05304	-2.10331	-1.82081
H	5.97726	-0.99741	-0.78973
H	4.68218	-0.37182	-1.82015
H	0.88195	2.60448	0.49156
H	1.21867	5.01100	0.79269
H	2.70225	4.33623	0.09680
H	2.63582	4.74959	1.81128
H	-0.14244	3.68464	2.47204
H	1.26339	3.26142	3.45795
H	0.23309	1.97773	2.78749
H	-0.70765	-2.23601	3.47449
H	1.68738	-1.39714	3.44792
N	-1.14074	-0.38145	-0.91527
N	1.68643	0.39291	-0.26033
O	-0.03432	-0.33778	2.76650
O	1.08953	-2.69349	1.25481
O	-0.18062	-2.73845	0.97780
Cu	0.36055	-0.95593	0.24613

28. L^1CuX, X = triphenylphosphine

C	-2.41758	-3.38909	0.33244
C	-3.90579	-4.94811	-0.76702
C	-2.98629	-5.08253	-1.80506
C	1.72760	3.64882	0.19720

C	0.72299	2.53058	-0.03664
C	-0.59391	2.94808	-0.31821
C	-1.79791	2.21679	-0.40441
C	-3.06630	3.05271	-0.51155
C	2.44027	0.95749	0.52913
C	2.64289	0.73635	1.91663
C	3.90905	0.34283	2.36344
C	4.97141	0.17104	1.48046
C	4.77023	0.40931	0.12407
C	3.52461	0.81132	-0.37463
C	1.51517	0.90214	2.93313
C	1.83104	2.01212	3.95464
C	1.19900	-0.41875	3.65991
C	3.37744	1.05137	-1.87513
C	3.65895	-0.22860	-2.68111
C	4.28970	2.18613	-2.37729
C	-3.18300	0.27569	-0.29699
C	-3.77339	0.02480	0.96555
C	-4.98538	-0.67541	1.01875
C	-5.62008	-1.10965	-0.13940
C	-5.05480	-0.81918	-1.37896
C	-3.84879	-0.11890	-1.48580
C	-3.12609	0.50018	2.26363
C	-2.51934	-0.66691	3.06326
C	-4.10449	1.30233	3.14052
C	-3.26591	0.22708	-2.85385
C	-4.31560	0.35279	-3.96659
C	-2.17776	-0.77633	-3.26014
C	-1.77657	-4.38477	-1.76974
C	3.10537	-3.40626	2.03773
C	2.65040	-4.52201	2.74344
C	1.39313	-5.05298	2.45814
C	2.30365	-2.82037	1.05830
C	0.59339	-4.47882	1.46492
C	1.58749	-2.86407	-4.44062
C	2.25528	-4.08920	-4.42882
C	2.30418	-4.83895	-3.25162
C	0.97083	-2.39079	-3.28063
C	1.68217	-4.37003	-2.09514
C	1.00542	-3.13906	-2.09632
C	1.04180	-3.35585	0.75723
C	-1.47578	-3.53289	-0.69578
C	-3.61597	-4.10041	0.30476
H	2.07236	-0.79852	4.20320
H	0.88626	-1.19606	2.95656
H	2.33945	1.34452	-2.06080
H	0.39270	-0.27161	4.38653
H	3.03628	-1.05741	-2.34529
H	4.70582	-0.53787	-2.58432
H	-4.33067	-3.97113	1.11007
H	5.34711	1.91452	-2.27977
H	4.13682	3.11659	-1.82281
H	-5.43975	-0.87853	1.98469
H	-6.55754	-1.65559	-0.08099
H	-5.57015	-1.13579	-2.27938
H	-2.30376	1.16890	1.99653
H	-2.09577	-0.31169	4.00880
H	-1.71257	-1.14851	2.50299
H	-3.27545	-1.42505	3.29889
H	-3.58067	1.72206	4.00584
H	-4.91896	0.67690	3.52181
H	-4.55538	2.12981	2.58298
H	-2.77392	1.20120	-2.76119
H	-3.84786	0.74529	-4.87503

H	-5.13080	1.02641	-3.68435
H	-4.75422	-0.61651	-4.22479
H	-1.73316	-0.50410	-4.22455
H	-2.58463	-1.78843	-3.34322
H	-1.38984	-0.78705	-2.50703
H	-1.07238	-4.50964	-2.58288
H	2.70036	1.75436	4.57112
H	2.04521	2.96557	3.46075
H	0.98022	2.16463	4.62784
H	0.61783	1.20270	2.38474
H	5.60015	0.28688	-0.56698
H	5.94797	-0.13495	1.84589
H	4.06418	0.16736	3.42490
H	-3.67871	2.74389	-1.36340
H	1.55119	-2.26861	-5.34751
H	-3.68957	2.93031	0.38009
H	-2.82943	4.11158	-0.62051
H	-0.71639	4.02060	-0.39556
H	2.15207	3.58877	1.20419
H	2.56654	3.57916	-0.49970
H	4.07633	-2.97380	2.25543
H	1.72216	-4.96598	-1.18978
H	2.82471	-5.79223	-3.23179
H	2.73808	-4.45698	-5.32956
H	0.46995	-1.42944	-3.29740
H	-0.37693	-4.90782	1.24543
H	1.03105	-5.92022	3.00253
H	3.27160	-4.97231	3.51346
H	2.66170	-1.94092	0.53264
H	1.26070	4.62740	0.07842
H	-3.20468	-5.73316	-2.64799
H	-4.84515	-5.49303	-0.79625
H	3.45846	-0.06723	-3.74684
H	4.09652	2.38801	-3.43749
H	-2.22017	-2.71567	1.15877
N	-1.89120	0.88802	-0.36063
N	1.12080	1.26081	0.06554
P	0.08639	-2.54379	-0.60134
Cu	-0.18346	-0.23533	-0.26075

29. L^1CuXO_2 η^1 singlet, X = triphenylphosphine

O	0.90053	-1.36764	2.55544
O	0.16844	-0.40229	2.16877
C	-2.42138	-3.93703	-2.02253
C	-1.26308	-3.15889	-1.99141
C	3.87687	-2.52693	1.25381
C	3.80139	-3.91858	1.21907
C	2.71311	-4.54379	0.60263
C	2.86766	-1.75851	0.67294
C	1.70514	-3.78063	0.01580
C	1.13451	0.43671	-4.39539
C	1.88508	-0.50835	-5.09723
C	2.24561	-1.70845	-4.47976
C	0.74161	0.18064	-3.08152
C	1.85329	-1.96707	-3.16595
C	1.08846	-1.02732	-2.45837
C	1.78368	-2.37981	0.03059
C	-0.98202	-2.35910	-0.87367
C	-3.03080	-3.12571	0.17133
C	-2.75768	0.02745	-3.47298
C	-3.18805	2.62532	3.05724
C	-3.30568	-3.92150	-0.94217
C	1.83359	1.12521	4.57553

C	-3.96484	2.22342	-3.31175
C	-2.76249	0.21286	3.66666
C	4.31413	0.58661	-1.93120
C	1.82451	3.61051	4.15016
C	-2.99381	1.26648	-2.59038
C	-2.65539	1.26819	2.55439
C	-5.25985	-0.13732	0.13307
C	3.71644	1.86230	-1.30664
C	1.83334	2.21732	3.49077
C	5.36593	1.66785	2.13361
C	-4.71686	0.21225	-1.09695
C	-4.57412	0.19438	1.29881
C	5.15657	1.68290	0.75881
C	4.28322	1.83985	2.99200
C	-3.49477	0.89030	-1.19702
C	2.79353	2.09684	1.09869
C	-2.79621	1.21080	-0.00631
C	4.34246	3.08877	-2.00000
C	1.06221	3.56117	0.37163
C	-1.43337	3.17619	-0.13167
C	-1.87666	-2.34531	0.20676
C	-0.24530	3.92840	-0.00524
C	2.98923	2.04846	2.50451
C	-3.34677	0.86219	1.25628
C	2.03153	4.72340	0.54103
C	-2.66995	4.01673	-0.42400
C	3.88262	1.88889	0.21323
H	-1.66891	-1.71254	1.06262
H	-0.38228	4.99259	-0.15447
H	-3.69582	-0.50668	-3.65828
H	-3.05171	3.41434	2.31284
H	-3.72320	-3.09370	1.00616
H	2.15114	-2.89457	-2.68708
H	2.53117	4.69193	1.51083
H	-2.77166	4.16321	-1.50513
H	0.16800	0.92150	-2.53261
H	2.83756	-2.44263	-5.01838
H	2.19410	-0.30812	-6.11901
H	0.85922	1.37606	-4.86571
H	0.85676	-4.27299	-0.44846
H	2.92271	-0.67685	0.72582
H	2.82195	4.68554	-0.21193
H	1.51423	5.67904	0.44567
H	-3.58667	3.54704	-0.06702
H	-2.57844	5.00461	0.03221
H	2.64723	-5.62770	0.58167
H	4.58143	-4.51772	1.67970
H	4.70710	-2.02944	1.74526
H	-0.58944	-3.16579	-2.84223
H	4.44499	1.81035	4.06536
H	6.36405	1.51446	2.53414
H	5.99909	1.53141	0.08993
H	-5.00500	-0.06501	2.26071
H	-6.21263	-0.65664	0.18465
H	-5.25466	-0.04043	-2.00644
H	-2.63451	-4.54879	-2.89443
H	-4.21103	-4.52094	-0.97257
H	-2.06629	-0.67572	-3.00789
H	-4.25801	2.56166	3.28677
H	0.90731	2.10960	2.92127
H	2.75368	3.79063	4.70305
H	2.64330	1.86664	-1.51747
H	3.94632	-0.31829	-1.44387
H	-1.59356	1.39957	2.32967

H	-2.13744	0.50590	4.51635
H	-2.03649	1.78378	-2.47371
H	-3.53741	2.55340	-4.26528
H	1.70802	4.41464	3.41899
H	0.99332	3.68686	4.86019
H	2.67794	1.23852	5.26508
H	5.40737	0.58133	-1.86020
H	4.05300	0.52957	-2.99248
H	5.41713	3.14798	-1.79486
H	-2.42145	-0.76819	3.32469
H	-3.78733	0.10861	4.04009
H	-2.66319	2.92966	3.96970
H	-4.19213	3.10914	-2.71365
H	-4.91421	1.72416	-3.53332
H	-2.34573	0.32087	-4.44507
H	1.87543	0.12775	4.13369
H	0.91774	1.19694	5.17312
H	3.89031	4.02898	-1.67604
H	4.21283	3.01572	-3.08567
N	1.47118	2.30976	0.58620
N	-1.51120	1.85139	-0.01548
P	0.51420	-1.30305	-0.73284
Cu	0.20091	0.71592	0.37610

30. L^1CuXO_2 η^1 triplet, X = triphenylphosphine

O	.3438304940	-1.2900950400	2.6616690080
O	-.1140789174	-.2182098944	2.2484623418
C	-2.1519923235	-4.2492539872	-1.9165286233
C	-1.0484746890	-3.3959994373	-1.9047247885
C	3.9521999120	-2.3583793227	1.2611538030
C	3.8180481613	-3.7317680549	1.4717824607
C	2.6753497265	-4.3930604844	1.0200457119
C	2.9479990712	-1.6512490135	.6021866411
C	1.6714947289	-3.6897147153	.3522590976
C	1.2815290249	-.1150525421	-4.6421691226
C	2.0597111350	-1.1458350714	-5.1694862034
C	2.4322842545	-2.2179302215	-4.3562210281
C	.8685709162	-.1604715101	-3.3099188443
C	2.0135687738	-2.2683258549	-3.0267385416
C	1.2126510747	-1.2457074773	-2.4924172802
C	1.8019045997	-2.3114612122	.1292202363
C	-.9140275434	-2.4188609474	-.9048110921
C	-3.0194456797	-3.1622044880	.0553260280
C	-2.7318244475	.0853224289	-3.4860897342
C	-3.6338844903	2.5833779551	3.1929995172
C	-3.1368693748	-4.1385454023	-.9337773911
C	2.2529960614	.8004447039	4.4421859457
C	-3.4748208030	2.4893470784	-3.2964670563
C	-3.1096486396	.1512407245	3.5893499524
C	4.2548727719	.8481156462	-2.2081104762
C	2.0523961215	3.3022737355	4.2397656876
C	-2.7889135814	1.3194375747	-2.5642007431
C	-2.9812067298	1.3203041712	2.5937557556
C	-5.4249255332	.1179529657	-.0819531329
C	3.6005088780	2.0380558644	-1.4778513059
C	2.0928838042	1.9738393680	3.4569497017
C	5.5309264197	1.7554040020	1.8052757630
C	-4.7434495770	.4188878523	-1.2550325099
C	-4.8264921787	.4032011189	1.1414535903
C	5.2121660078	1.8444914002	.4548401510
C	4.5082300139	1.7953562450	2.7483452425
C	-3.4711791056	1.0028888403	-1.2360783502
C	2.8593538915	2.1032425948	.9898886631

C	-2.8732711652	1.3077345019	.0110215778
C	4.0469983003	3.3561565242	-2.1395964368
C	1.0552916257	3.5855823663	.5298577565
C	-1.4766484635	3.2394759361	.1030667393
C	-1.9191628956	-2.3057776203	.0662607865
C	-.2773852519	3.9704219882	.2747847409
C	3.1704757363	1.9590598444	2.3714912290
C	-3.5586333588	.9914157427	1.2175812792
C	2.0282207010	4.7433758346	.7299309987
C	-2.7117936000	4.1165763558	-.0854504568
C	3.8893002347	2.0017204333	.0215216806
H	-1.8507614922	-1.5348378508	.8256496949
H	-.4235634566	5.0439786867	.2473335681
H	-3.7352113606	-.2216441272	-3.8003199963
H	-3.4914820716	3.4575993876	2.5524373027
H	-3.7900072979	-3.0520756443	.8121629804
H	2.3171001862	-3.1019364504	-2.4009417865
H	2.6519686240	4.6026910799	1.6139716504
H	-2.7503601610	4.4819661201	-1.1189249590
H	.2747471051	.6516501786	-2.9023986673
H	3.0514640831	-3.0164473040	-4.7557189738
H	2.3840125586	-1.1095279309	-6.2057292878
H	1.0004094222	.7298219234	-5.2645882359
H	.7874387295	-4.2173888367	.0102653494
H	3.0547808610	-.5787528465	.4661240193
H	2.7131595141	4.8226662214	-.1204906426
H	1.4952400491	5.6907115587	.8253888388
H	-3.6412665081	3.5829137491	.1100033121
H	-2.6626436435	4.9929884722	.5656539576
H	2.5603777351	-5.4605241476	1.1878374430
H	4.5962941436	-4.2827087194	1.9926158253
H	4.8308577352	-1.8288926295	1.6179000510
H	-.2961168014	-3.4921750231	-2.6799873879
H	4.7524820974	1.6983176994	3.8025259315
H	6.5648456334	1.6418003823	2.1199530815
H	6.0071957802	1.7871820355	-.2833773187
H	-5.3584851379	.1717801644	2.0602969370
H	-6.4129711482	-.3330405826	-.1200146563
H	-5.2090423456	.1957051982	-2.2111666788
H	-2.2414067184	-4.9998329147	-2.6972692697
H	-3.9957442387	-4.8039109757	-.9455327309
H	-2.2650992426	-.7709039779	-2.9932966541
H	-4.7124407085	2.4396421299	3.3279304420
H	1.1281663934	1.8600744548	2.9571858161
H	3.0196249253	3.5105900491	4.7122058126
H	2.5158125794	1.9574826343	-1.6008085910
H	3.9996496454	-.1065786787	-1.7409734730
H	-1.9179851119	1.5313018267	2.4613944893
H	-2.5681089773	.3822122641	4.5133300869
H	-1.7651951925	1.6349282729	-2.3375717113
H	-2.9306402243	2.7421858798	-4.2137830554
H	1.8023183564	4.1497630318	3.5969429110
H	1.2971095272	3.2535747986	5.0325648284
H	3.1267290483	.9299506087	5.0910557982
H	5.3468958164	.9333122545	-2.2151608461
H	3.9231807792	.8130359003	-3.2498616556
H	5.1268622001	3.5068914974	-2.0260941161
H	-2.6975709226	-.7780142892	3.1861308309
H	-4.1529618762	-.0392575035	3.8654679685
H	-3.2009211214	2.8119675177	4.1738890564
H	-3.5227047445	3.3874130710	-2.6738503541
H	-4.5002553552	2.2270415941	-3.5804680182
H	-2.1624351713	.3077413244	-4.3952902257
H	2.3605494722	-.1532046545	3.9195203159

H	1.3747717595	.7324130376	5.0940249780
H	3.5421437713	4.2273941439	-1.7121442048
H	3.8256725800	3.3366506115	-3.2130779879
N	1.5035159480	2.3269399845	.5832142738
N	-1.5740571826	1.9137606146	.0666440670
P	.5497202365	-1.2963570465	-.7695246647
Cu	.1700924976	.8370918518	.2531716268

31. L^1CuX, X = trimethylphosphine

C	-1.44148	-3.68565	-0.65672
C	0.75819	-3.65818	1.18108
C	1.25158	-3.37021	-1.60375
C	3.14850	0.46744	1.41949
C	4.47278	0.01478	1.41228
C	5.19100	-0.11110	0.22618
C	4.59017	0.24664	-0.97757
C	3.26879	0.70364	-1.02464
C	2.40220	0.61574	2.74435
C	3.19013	1.44784	3.77290
C	2.01575	-0.75375	3.33143
C	2.65602	1.11256	-2.36383
C	2.40375	-0.10447	-3.27241
C	3.50527	2.16829	-3.09644
C	-3.05988	-0.09874	-0.38363
C	-3.76166	-0.64097	0.72428
C	-4.87257	-1.45883	0.48685
C	-5.30466	-1.73454	-0.80757
C	-4.62477	-1.17952	-1.88867
C	-3.50675	-0.35796	-1.70499
C	-3.31397	-0.36858	2.15906
C	-2.70578	-1.62602	2.80830
C	-4.44978	0.19549	3.03216
C	-2.77734	0.21856	-2.91773
C	-3.72211	0.95589	-3.88323
C	-1.98088	-0.86927	-3.66432
C	1.69429	3.45384	0.42179
C	0.69088	2.32510	0.23142
C	-0.66605	2.70781	0.16220
C	-1.82961	1.93408	-0.03378
C	-3.14384	2.69948	-0.08639
C	2.52756	0.77853	0.18338
H	-2.17707	-3.50979	0.13172
H	0.78569	-4.73487	0.98171
H	-1.24234	-4.76034	-0.73404
H	0.12519	-3.47650	2.05339
H	-1.87647	-3.33069	-1.59364
H	2.24948	-2.95106	-1.45304
H	1.76849	-3.31214	1.41389
H	0.89955	-3.06494	-2.59268
H	1.31213	-4.46300	-1.57233
H	1.19497	4.42173	0.49487
H	2.40207	3.49215	-0.41280
H	2.28953	3.30202	1.32820
H	-0.84153	3.77237	0.25975
H	-2.98868	3.76886	0.06745
H	-3.83932	2.33590	0.67698
H	-3.64005	2.55756	-1.05258
H	4.95368	-0.24014	2.35328
H	6.21730	-0.46830	0.24179
H	5.16138	0.17359	-1.89990
H	1.46943	1.14776	2.53816
H	2.58126	1.62476	4.66664
H	3.47992	2.42109	3.36338

H	4.10521	0.94037	4.09770
H	1.47907	-0.63668	4.28043
H	2.90288	-1.37021	3.52044
H	1.36554	-1.29607	2.64015
H	1.68169	1.56249	-2.15609
H	1.96018	0.20505	-4.22618
H	1.71682	-0.80653	-2.79302
H	3.33579	-0.63850	-3.49304
H	2.98994	2.51201	-4.00037
H	4.47726	1.76910	-3.40714
H	3.69423	3.04127	-2.46326
H	-5.41011	-1.88536	1.33027
H	-6.16971	-2.37118	-0.97311
H	-4.96979	-1.39104	-2.89773
H	-2.52280	0.38478	2.11797
H	-2.37055	-1.41457	3.83039
H	-1.83992	-1.97467	2.23692
H	-3.43350	-2.44455	2.85588
H	-4.07247	0.45723	4.02716
H	-5.25927	-0.53024	3.16909
H	-4.88560	1.09701	2.58940
H	-2.05175	0.94795	-2.54802
H	-3.14841	1.43746	-4.68291
H	-4.29696	1.73121	-3.36637
H	-4.43677	0.27556	-4.35957
H	-1.45037	-0.44574	-4.52530
H	-2.64040	-1.66403	-4.03334
H	-1.23577	-1.32385	-3.00378
N	1.13143	1.07063	0.13669
N	-1.84181	0.60882	-0.17154
P	0.10767	-2.73732	-0.29107
Cu	-0.14430	-0.46140	-0.11978

32. L^1CuXO_2 η^1 singlet, X = trimethylphosphine

C	-3.29934	-1.41250	2.64321
C	-4.21628	-1.06225	-2.35474
C	-4.85675	-1.15876	-0.03874
C	4.85766	0.28806	-0.48226
C	4.66521	0.57530	1.89436
C	-3.06279	-0.33680	-2.03587
C	2.71559	0.89263	0.49162
C	-2.83179	0.00322	-0.67563
C	2.98654	1.97310	-2.71524
C	0.87633	2.42716	0.26553
C	-1.62806	2.03122	-0.21627
C	3.51461	-0.47409	-2.99085
C	-0.46960	2.79722	0.05014
C	0.55425	-2.96017	-2.35396
C	3.30157	0.87800	1.78475
C	-3.72252	-0.42771	0.33691
C	1.83349	3.59162	0.46742
C	-2.91720	2.83497	-0.33973
C	3.49987	0.57570	-0.65363
C	1.89554	-3.27063	0.17725
C	-0.94544	-3.76028	-0.01719
C	-2.05927	-0.89954	-4.32982
C	3.03819	2.39671	3.81783
C	-4.61055	0.73938	2.41384
C	2.53638	-0.06159	4.01597
C	-2.30994	1.49985	-3.64420
C	-2.07058	0.06524	-3.12887
C	-3.48164	-0.12465	1.81536
C	-5.11318	-1.46916	-1.36934

C	2.89295	0.58118	-2.05724
C	2.51429	1.15372	3.06632
C	5.44414	0.28985	0.78001
H	1.86742	-3.13265	1.26143
H	2.76238	-2.73380	-0.21786
H	1.99360	-4.33777	-0.04837
H	-0.36517	-2.71746	-2.89096
H	0.77984	-4.02249	-2.49877
H	1.36624	-2.36473	-2.77888
H	-0.69607	-4.78316	-0.31883
H	-1.90930	-3.47657	-0.44901
H	-1.01683	-3.70573	1.07173
H	-0.64729	3.86619	0.09132
H	-2.95489	-0.78833	-4.95151
H	-4.76461	1.66109	1.84383
H	2.01295	3.75799	1.53324
H	-2.71978	3.82956	-0.74751
H	2.80370	3.40158	0.00437
H	1.41629	4.51024	0.05048
H	-3.65931	2.33630	-0.96395
H	-3.36021	2.96955	0.65423
H	5.12382	0.56003	2.87925
H	6.50030	0.06053	0.89343
H	5.46856	0.05817	-1.34982
H	-5.55027	-1.49170	0.72878
H	-6.00284	-2.03175	-1.63957
H	-4.41631	-1.32022	-3.39002
H	-2.00625	-1.94842	-4.02116
H	-5.56378	0.19872	2.42915
H	1.47181	1.32976	2.78927
H	4.05775	2.23859	4.18856
H	1.82858	0.34706	-1.94767
H	3.54851	-1.46457	-2.52524
H	-2.54951	0.44209	1.89274
H	-3.13802	-1.16512	3.69838
H	-1.07429	0.04844	-2.67022
H	-1.60052	1.74207	-4.44379
H	3.05675	3.29228	3.18953
H	2.40503	2.60822	4.68695
H	3.55518	-0.27617	4.35914
H	4.53822	-0.21458	-3.28269
H	2.93134	-0.54913	-3.91557
H	4.03245	2.28888	-2.80494
H	-2.43410	-1.98675	2.30575
H	-4.18654	-2.05380	2.58570
H	-4.37304	1.01541	3.44730
H	-2.18704	2.24465	-2.85633
H	-3.32257	1.59940	-4.05187
H	-1.19685	-0.68962	-4.97174
H	2.13349	-0.95661	3.54078
H	1.92845	0.14523	4.90437
H	2.45470	2.73158	-2.13640
H	2.55225	1.95496	-3.72171
N	1.32673	1.17322	0.29239
N	-1.63834	0.70763	-0.32506
O	0.25646	-2.06757	2.59578
O	0.09768	-0.87458	2.16258
P	0.35368	-2.56755	-0.55667
Cu	0.00873	-0.34506	0.20703

33. L^1CuXO_2 η^1 triplet, X = trimethylphosphine

C	-3.77045	0.73529	3.07792
C	2.67154	1.01358	0.81470

C	-2.85208	-0.02993	-0.32398
C	1.49697	0.68168	4.24820
C	3.57323	1.69158	-2.30347
C	0.88840	2.48258	0.15750
C	-1.61502	2.00900	-0.17540
C	-0.45447	2.81062	-0.10596
C	2.92896	1.19399	2.19974
C	-3.47039	-0.48129	0.86979
C	1.80229	3.69645	0.30977
C	3.43683	0.35721	-1.54166
C	-2.91893	2.79737	-0.08571
C	3.69350	0.52324	-0.04450
C	0.51848	-2.17567	-3.09669
C	-3.37606	1.46883	-3.39309
C	1.68028	-3.56525	-0.89140
C	-1.17158	-3.42590	-1.11014
C	-2.92802	-0.91841	-4.02320
C	-2.58748	-1.49947	3.02357
C	4.32396	-0.70784	-2.20724
C	2.33047	3.02972	3.85503
C	1.87466	1.72199	3.17530
C	-2.80048	0.12561	-2.89684
C	-2.87050	-0.20001	2.24550
C	-5.26600	-1.47200	-0.44313
C	5.20694	0.40363	1.85672
C	-4.64453	-1.04496	-1.61318
C	-4.67266	-1.19355	0.78285
C	4.94729	0.23211	0.49892
C	4.20206	0.87846	2.69041
C	-3.43990	-0.33195	-1.58449
H	1.62760	-3.87257	0.15468
H	2.65189	-3.09648	-1.06432
H	1.47546	-1.69450	-3.31615
H	-1.27290	-3.74489	-0.06895
H	-2.06481	-2.85645	-1.37729
H	1.59190	-4.45175	-1.52842
H	-1.09648	-4.31340	-1.74749
H	0.49043	-3.15095	-3.59406
H	-0.27915	-1.54851	-3.49825
H	-0.64845	3.87794	-0.14566
H	-3.95794	-1.00158	-4.38707
H	-3.97230	1.67330	2.55242
H	2.85303	3.42373	0.40385
H	-2.85472	3.71095	-0.68395
H	1.68643	4.34855	-0.56230
H	1.51945	4.28569	1.18749
H	-3.78808	2.22562	-0.40928
H	-3.08798	3.10678	0.95193
H	4.40748	1.01009	3.74962
H	6.18859	0.16932	2.25905
H	5.73929	-0.13277	-0.14741
H	-5.15551	-1.53122	1.69644
H	-6.20355	-2.01936	-0.48919
H	-5.10872	-1.26866	-2.56929
H	-2.61347	-1.91550	-3.70040
H	-4.73641	0.26564	3.29727
H	0.96748	1.94157	2.60763
H	3.18533	2.85795	4.51846
H	2.39299	0.03617	-1.64658
H	4.31822	-1.65277	-1.65423
H	-1.91355	0.30623	2.09064
H	-2.09024	-1.27640	3.97439
H	-1.73477	0.28070	-2.69288
H	-2.91080	1.75817	-4.34272

H	2.62774	3.78687	3.12445
H	1.52056	3.44606	4.46498
H	2.36201	0.40665	4.86204
H	5.36653	-0.38030	-2.28758
H	3.97587	-0.90580	-3.22747
H	4.58766	2.09437	-2.20169
H	-1.93944	-2.17361	2.45625
H	-3.51179	-2.04117	3.25414
H	-3.29541	0.97833	4.03527
H	-3.20737	2.27718	-2.67979
H	-4.45661	1.38706	-3.56068
H	-2.31214	-0.62697	-4.88164
H	1.10535	-0.23176	3.79548
H	0.72999	1.08707	4.91857
H	2.87168	2.44108	-1.93227
H	3.37457	1.54680	-3.37224
N	-1.61521	0.68200	-0.27029
N	1.37045	1.24446	0.28375
O	0.96619	-1.69321	1.91458
O	0.60070	-2.84295	2.15474
P	0.32899	-2.35538	-1.26308
Cu	0.20461	-0.32274	-0.15069

34. L^1CuX, X = thiophene

C	3.21713	0.75204	1.29215
C	4.53519	0.29363	1.18477
C	5.16331	0.17288	-0.05210
C	4.46539	0.51570	-1.20708
C	3.14576	0.97770	-1.15386
C	2.56326	0.84861	2.66761
C	3.33760	1.78725	3.61054
C	2.39209	-0.54069	3.31042
C	2.40889	1.29405	-2.45337
C	2.16324	0.01788	-3.28083
C	3.14096	2.35188	-3.29902
C	-3.08347	0.27871	-0.34925
C	-3.83821	-0.27628	0.71364
C	-4.93623	-1.08888	0.40910
C	-5.29629	-1.35879	-0.90860
C	-4.54846	-0.80817	-1.94598
C	-3.44115	0.00950	-1.69481
C	-3.46810	-0.02562	2.17281
C	-3.00247	-1.31978	2.86643
C	-4.62135	0.62327	2.95913
C	-2.62590	0.54977	-2.86752
C	-3.48346	1.36906	-3.84907
C	-1.89440	-0.58559	-3.60874
C	1.72183	3.82362	0.27036
C	0.70147	2.69935	0.20773
C	-0.65824	3.08610	0.16637
C	-1.83952	2.32692	-0.00219
C	1.54686	-2.82907	-0.42595
C	-0.92812	-3.20706	-0.63404
C	1.21904	-3.71241	-1.40851
C	-0.19729	-3.92872	-1.52774
C	-3.13389	3.11236	-0.13180
C	2.51591	1.09875	0.11090
H	1.23618	4.79528	0.37039
H	2.33985	3.83885	-0.63314
H	2.40506	3.68420	1.11384
H	-0.81954	4.15557	0.22104
H	-2.96809	4.17918	0.02460
H	-3.87719	2.76283	0.59139

H	-3.57456	2.97419	-1.12443
H	5.07909	0.02608	2.08690
H	6.18742	-0.18360	-0.11533
H	4.95301	0.41699	-2.17332
H	1.56386	1.26917	2.52679
H	2.81270	1.88857	4.56670
H	3.44858	2.78627	3.17739
H	4.34217	1.40540	3.82295
H	1.89120	-0.45904	4.28148
H	3.35977	-1.02821	3.47264
H	1.78900	-1.19916	2.67746
H	1.42935	1.70036	-2.18933
H	1.58996	0.24974	-4.18551
H	1.60481	-0.72606	-2.70522
H	3.10852	-0.44109	-3.59220
H	2.55175	2.60491	-4.18721
H	4.11610	1.99022	-3.64295
H	3.31156	3.27325	-2.73320
H	-5.51946	-1.51842	1.21939
H	-6.15273	-1.99086	-1.12519
H	-4.82596	-1.02196	-2.97480
H	-2.62578	0.67142	2.18236
H	-2.70816	-1.11975	3.90274
H	-2.14065	-1.75672	2.35227
H	-3.79823	-2.07270	2.88327
H	-4.30664	0.85009	3.98361
H	-5.49133	-0.03976	3.01925
H	-4.94890	1.55672	2.49074
H	-1.86003	1.21502	-2.46101
H	-2.85572	1.79812	-4.63770
H	-4.00035	2.19119	-3.34401
H	-4.24482	0.74931	-4.33511
H	-1.27289	-0.18131	-4.41566
H	-2.60527	-1.29041	-4.05496
H	-1.24715	-1.14902	-2.93028
H	2.51901	-2.46846	-0.12064
H	-1.99975	-3.15903	-0.50045
H	1.95528	-4.19715	-2.03926
H	-0.64349	-4.59405	-2.25793
N	1.13211	1.43806	0.18328
N	-1.88333	0.99614	-0.06562
S	0.11556	-2.26472	0.40625
Cu	-0.20521	0.00192	0.14841

35. L^1CuXO_2 η^1 singlet, X = thiophene

C	-1.24551	2.38853	-2.63610
C	3.62467	1.69015	-2.12138
C	2.70699	0.30627	-4.01620
C	0.55585	-2.60854	1.41395
C	-0.25017	-2.67227	2.57987
C	0.27485	-3.29522	3.71736
C	1.55993	-3.83129	3.71944
C	2.34320	-3.75468	2.57037
C	1.86616	-3.15407	1.40000
C	-1.67911	-2.12990	2.58886
C	-1.96929	-1.24288	3.81244
C	-1.02738	3.62223	-3.26336
C	-2.71537	-3.26571	2.48177
C	2.76500	-3.10383	0.16211
C	3.26449	-4.50137	-0.25998
C	3.96616	-2.16095	0.36951
C	1.56051	2.77965	1.34605
C	1.63451	0.86207	2.95983

C	1.11033	3.10674	2.59131
C	1.15514	2.01138	3.51472
C	-0.97883	-0.67549	-3.99377
C	-0.65374	-0.78964	-2.50768
C	0.24225	4.02095	-3.66883
C	-0.77044	-2.10733	-2.01238
C	-0.39897	-2.65132	-0.77231
C	-0.48864	-4.16731	-0.67454
C	-0.13022	1.54134	-2.41941
C	1.32897	3.17778	-3.45003
C	1.16964	1.93415	-2.82847
C	-2.67302	1.99514	-2.24741
C	-3.57386	1.81081	-3.48792
C	-3.30999	3.01059	-1.27857
C	2.36867	0.99717	-2.67762
H	-0.35211	-1.37329	-4.55877
H	-0.83450	0.32579	-4.39380
H	-2.01864	-0.97489	-4.16395
H	-1.12675	-2.82836	-2.74038
H	-1.25622	-4.54367	-1.35406
H	-0.71809	-4.49972	0.33953
H	0.46077	-4.63071	-0.96123
H	-1.87325	4.27868	-3.44670
H	0.38339	4.97956	-4.16081
H	2.31553	3.48491	-3.78321
H	-2.62658	1.03752	-1.72286
H	-4.57071	1.46667	-3.18941
H	-3.16321	1.08107	-4.19069
H	-3.70049	2.75477	-4.03003
H	-4.29542	2.65641	-0.95796
H	-3.44882	3.98753	-1.75587
H	-2.69224	3.14104	-0.38857
H	2.08461	0.21280	-1.96930
H	4.40665	0.94906	-1.92473
H	3.42487	2.21995	-1.18494
H	4.03899	2.41430	-2.83082
H	3.53231	-0.40374	-3.88801
H	3.01248	1.04385	-4.76690
H	1.85132	-0.24207	-4.41895
H	-0.33679	-3.36836	4.61240
H	1.94802	-4.31407	4.61198
H	3.34506	-4.17625	2.58011
H	-1.80164	-1.49761	1.70630
H	-2.96780	-0.80218	3.72323
H	-1.25039	-0.42018	3.88294
H	-1.93726	-1.80974	4.75028
H	-3.73021	-2.85441	2.44529
H	-2.65674	-3.94085	3.34283
H	-2.56687	-3.86484	1.57764
H	2.17697	-2.69967	-0.66591
H	3.81854	-4.43952	-1.20363
H	2.43962	-5.20622	-0.40014
H	3.93965	-4.93217	0.48776
H	4.58164	-2.11841	-0.53656
H	4.60646	-2.50547	1.18914
H	3.64287	-1.14279	0.60311
H	1.61299	3.39161	0.45524
H	1.76975	-0.11410	3.40630
H	0.74793	4.09654	2.84779
H	0.83705	2.08344	4.54922
N	-0.27975	0.26346	-1.78742
N	0.03750	-1.93823	0.26673
S	2.04370	1.11164	1.28408
O	-2.42033	0.96686	1.12407

O	-1.25932	1.45754	0.86714
Cu	-0.13642	0.04171	0.26534

36. L^1CuXO_2 η^1 triplet, X = thiophene

C	-0.99758	2.41129	-2.43756
C	3.71987	1.43071	-2.05864
C	2.93426	0.27124	-4.16311
C	0.52984	-2.82210	1.54673
C	-0.33104	-2.98817	2.66176
C	0.17134	-3.61136	3.81044
C	1.48870	-4.05536	3.87994
C	2.33129	-3.86869	2.78739
C	1.87977	-3.25488	1.61262
C	-1.77224	-2.47968	2.65503
C	-1.99734	-1.41693	3.74893
C	-0.74159	3.64665	-3.04770
C	-2.79936	-3.61989	2.79981
C	2.85562	-3.03401	0.45885
C	3.39514	-4.36524	-0.10315
C	4.02092	-2.10915	0.87617
C	1.18608	2.94662	1.11020
C	1.41600	1.44046	3.10057
C	0.82244	3.54771	2.27518
C	0.95504	2.68633	3.41398
C	-0.99495	-0.67531	-3.87620
C	-0.61971	-0.85897	-2.41250
C	0.50948	3.95683	-3.57242
C	-0.78671	-2.16771	-1.89823
C	-0.43396	-2.77194	-0.66760
C	-0.62181	-4.27882	-0.59229
C	0.05101	1.45164	-2.36726
C	1.53768	3.02267	-3.47687
C	1.33846	1.77266	-2.87659
C	-2.39133	2.15576	-1.86113
C	-3.49436	2.18645	-2.94383
C	-2.72705	3.17106	-0.74587
C	2.51209	0.80044	-2.77888
H	-1.32589	-1.61342	-4.32392
H	-0.14816	-0.29341	-4.45411
H	-1.79829	0.05987	-3.98192
H	-1.20589	-2.86279	-2.61552
H	-1.21877	-4.64425	-1.42946
H	-1.10954	-4.56926	0.34228
H	0.34692	-4.79025	-0.61493
H	-1.54178	4.38182	-3.11027
H	0.68342	4.92052	-4.04590
H	2.51908	3.26923	-3.87590
H	-2.38838	1.15408	-1.41954
H	-4.46993	1.94229	-2.50662
H	-3.30077	1.46583	-3.74600
H	-3.58037	3.17979	-3.40417
H	-3.68878	2.92591	-0.28017
H	-2.80505	4.19053	-1.14562
H	-1.96067	3.17644	0.03766
H	2.18007	-0.05339	-2.18062
H	4.51663	0.68911	-1.92820
H	3.44903	1.80798	-1.06784
H	4.14109	2.26831	-2.62724
H	3.75662	-0.44744	-4.06740
H	3.27773	1.08635	-4.81091
H	2.10678	-0.23139	-4.67333
H	-0.48358	-3.74781	4.66797
H	1.85882	-4.53650	4.78243

H	3.36491	-4.20214	2.84882
H	-1.94948	-2.00509	1.68596
H	-3.01178	-1.00671	3.68418
H	-1.29257	-0.58554	3.64849
H	-1.87407	-1.84326	4.75128
H	-3.82134	-3.22473	2.74028
H	-2.69875	-4.13396	3.76362
H	-2.68415	-4.36981	2.01026
H	2.31048	-2.52661	-0.34459
H	4.04248	-4.17872	-0.96770
H	2.58165	-5.02736	-0.42490
H	3.98805	-4.91128	0.64309
H	4.68511	-1.91420	0.02562
H	4.62733	-2.56149	1.67357
H	3.65609	-1.14197	1.23998
H	1.18457	3.34272	0.10630
H	1.61801	0.59875	3.74829
H	0.46965	4.57389	2.33123
H	0.71655	2.99259	4.42501
N	-0.15769	0.18771	-1.72433
N	0.06802	-2.12931	0.38660
S	1.72534	1.30471	1.39041
O	-2.81359	0.40088	1.10695
O	-1.67768	0.76622	1.38802
Cu	0.23042	-0.19254	0.18414

37. L^1CuX, X = pyridine

Cu	-0.24104	1.35244	-0.22064
N	1.05638	2.86086	-0.28322
N	-1.94047	2.38362	-0.21815
C	1.63443	5.25190	-0.34050
C	0.62048	4.11936	-0.30036
C	-0.74113	4.49679	-0.28338
C	-1.91749	3.71536	-0.24870
C	-3.23405	4.47637	-0.24853
C	2.44372	2.54193	-0.30447
C	3.14076	2.34969	0.91560
C	4.46543	1.90064	0.87207
C	5.10599	1.64555	-0.33837
C	4.41614	1.84485	-1.53194
C	3.09053	2.29376	-1.54211
C	2.45400	2.57449	2.25995
C	3.28633	3.44289	3.21853
C	2.08492	1.23257	2.92172
C	2.35543	2.46737	-2.86881
C	2.00173	1.10230	-3.48999
C	3.13651	3.33493	-3.87081
C	-3.16101	1.65102	-0.19184
C	-3.72488	1.26582	1.05135
C	-4.84712	0.42971	1.05268
C	-5.41648	-0.02243	-0.13561
C	-4.86037	0.36694	-1.35180
C	-3.73845	1.20159	-1.40670
C	-3.09843	1.70681	2.37147
C	-2.30636	0.55356	3.01790
C	-4.12768	2.28027	3.36001
C	-3.13131	1.57419	-2.75673
C	-4.17103	2.13381	-3.74282
C	-2.38228	0.37778	-3.37489
C	1.33513	-1.16236	-0.22649
N	0.08473	-0.65577	-0.19331
C	-0.95145	-1.51832	-0.13889
C	-0.77835	-2.89899	-0.11592

C	1.59076	-2.52982	-0.20716
C	0.51562	-3.41668	-0.15067
H	1.14248	6.22508	-0.37562
H	2.28873	5.16083	-1.21356
H	2.28482	5.22410	0.54032
H	-0.91177	5.56616	-0.30248
H	-3.07026	5.55464	-0.27715
H	-3.82313	4.23807	0.64340
H	-3.84760	4.19526	-1.11082
H	5.00484	1.74555	1.80249
H	6.13547	1.29894	-0.35126
H	4.91681	1.64673	-2.47589
H	1.51733	3.10316	2.06499
H	2.71477	3.65737	4.12806
H	3.56107	4.39703	2.75751
H	4.21174	2.94353	3.52541
H	1.56247	1.39730	3.87090
H	2.98064	0.63532	3.12823
H	1.42815	0.64487	2.27324
H	1.41198	2.97680	-2.65607
H	1.44970	1.23309	-4.42763
H	1.37695	0.51459	-2.81078
H	2.90499	0.52101	-3.70854
H	2.53678	3.50798	-4.77105
H	4.06944	2.85556	-4.18668
H	3.39262	4.30893	-3.44178
H	-5.28217	0.12537	2.00073
H	-6.28906	-0.66918	-0.11382
H	-5.30523	0.01359	-2.27811
H	-2.38138	2.50005	2.14486
H	-1.83202	0.88129	3.94989
H	-1.51921	0.19621	2.34723
H	-2.96275	-0.29262	3.25203
H	-3.62154	2.67079	4.24951
H	-4.83979	1.51959	3.69802
H	-4.70207	3.09667	2.91062
H	-2.39074	2.35793	-2.57772
H	-3.67923	2.47122	-4.66168
H	-4.71044	2.98482	-3.31492
H	-4.91268	1.37954	-4.02733
H	-1.91928	0.65890	-4.32756
H	-3.06335	-0.45986	-3.56472
H	-1.59070	0.02547	-2.70670
H	2.14117	-0.43752	-0.27072
H	-1.94063	-1.07365	-0.11417
H	-1.64676	-3.54701	-0.07193
H	2.61551	-2.88355	-0.23602
H	0.68334	-4.48914	-0.13426

38. L^1CuXO_2 η^1 singlet, X = pyridine

Cu	-0.44257	0.07037	0.45367
O	0.33082	-2.57648	1.32489
O	-0.59926	-1.69547	1.30430
N	0.25748	0.95507	2.10587
N	-1.77001	1.46417	-0.08710
C	0.07922	2.65146	3.90671
C	-0.38110	2.00824	2.60621
C	-1.49895	2.63679	2.01329
C	-2.12232	2.42093	0.77116
C	-3.23864	3.38494	0.40589
C	1.40695	0.37890	2.72708
C	1.30227	-0.48771	3.84536
C	2.47898	-1.04252	4.36550

C	3.72269	-0.77481	3.80695
C	3.81252	0.06390	2.69802
C	2.67305	0.64651	2.13692
C	-0.02707	-0.83749	4.51031
C	-0.10290	-0.29606	5.95280
C	-0.28345	-2.35738	4.52326
C	2.79880	1.60183	0.95233
C	3.94685	1.25210	-0.00807
C	2.94392	3.06177	1.42837
C	-2.33473	1.39842	-1.39517
C	-3.33872	0.43466	-1.66649
C	-3.79722	0.29599	-2.98193
C	-3.28535	1.07718	-4.01435
C	-2.30246	2.02427	-3.73585
C	-1.81313	2.20834	-2.43767
C	-3.92481	-0.44695	-0.56709
C	-3.61689	-1.93729	-0.80520
C	-5.43926	-0.22034	-0.40435
C	-0.70674	3.23189	-2.18842
C	-1.06457	4.62536	-2.73560
C	0.64028	2.75658	-2.76731
C	1.64910	-1.57882	-0.97914
N	0.51977	-0.89703	-1.24262
C	0.00364	-0.97150	-2.48332
C	2.30831	-2.34125	-1.94068
C	0.59552	-1.71712	-3.49909
C	1.77146	-2.41405	-3.22447
H	0.08624	3.73955	3.80016
H	1.07199	2.31876	4.20707
H	-0.62238	2.40866	4.71093
H	-1.90456	3.46025	2.58968
H	-3.60091	3.91218	1.29008
H	-4.07587	2.86235	-0.06321
H	-2.88569	4.13286	-0.31226
H	2.41189	-1.70548	5.22299
H	4.61939	-1.21927	4.22924
H	4.78624	0.26952	2.26548
H	-0.82531	-0.37636	3.92272
H	-1.08947	-0.50178	6.38266
H	0.07349	0.78091	6.00683
H	0.64212	-0.78335	6.59161
H	-1.30122	-2.56029	4.87528
H	0.40513	-2.86665	5.20762
H	-0.15835	-2.78656	3.52914
H	1.86376	1.54071	0.38518
H	3.88372	1.87831	-0.90405
H	3.91000	0.20577	-0.32523
H	4.92879	1.43282	0.44240
H	3.01268	3.74087	0.57100
H	3.85163	3.18257	2.03035
H	2.09258	3.37511	2.03706
H	-4.56762	-0.43882	-3.19911
H	-3.65219	0.95183	-5.02901
H	-1.90301	2.63029	-4.54429
H	-3.44703	-0.16188	0.37369
H	-4.03489	-2.54516	0.00438
H	-2.53900	-2.11989	-0.83398
H	-4.05117	-2.29114	-1.74720
H	-5.82537	-0.81535	0.43023
H	-5.98993	-0.51455	-1.30465
H	-5.66799	0.83142	-0.20408
H	-0.57371	3.32512	-1.10787
H	-0.29388	5.35190	-2.45683
H	-2.02280	4.97925	-2.34244

H	-1.13560	4.62681	-3.82855
H	1.42547	3.49372	-2.56474
H	0.57972	2.62124	-3.85315
H	0.94632	1.80462	-2.32578
H	2.02440	-1.51634	0.03571
H	-0.91097	-0.41781	-2.65803
H	3.21809	-2.86882	-1.67586
H	0.13549	-1.74484	-4.48080
H	2.25801	-3.00444	-3.99511

39. L^1CuXO_2 η^1 triplet, X = pyridine

Cu	-.4453654278	.0275785623	.4573310107
O	-1.2539054443	-2.9235156174	1.1058593322
O	-1.5258919098	-1.7454627279	1.3779154199
N	.2522233119	.9561363058	2.1060983909
N	-1.8252027677	1.4081938888	-.0749224344
C	.0891730185	2.6945991641	3.8739157524
C	-.3967699163	2.0020800050	2.6062982213
C	-1.5588891535	2.5757737789	2.0376311255
C	-2.1737426076	2.3640473523	.7872676383
C	-3.2708414015	3.3482442803	.4117037008
C	1.4912983311	.4975926866	2.6451996888
C	1.5187598210	-.4656662997	3.6851012410
C	2.7594744459	-.9317811657	4.1371521902
C	3.9532727995	-.4790125365	3.5839344877
C	3.9153174679	.4507176040	2.5480475790
C	2.7031782230	.9456149437	2.0558818585
C	.2411310942	-.9972107625	4.3277472588
C	.0958452095	-.5179280289	5.7851349080
C	.1605095658	-2.5336971848	4.2645731462
C	2.7041442711	1.9710449688	.9255325896
C	3.6687367146	1.6016460502	-.2144091929
C	3.0139960014	3.3851381674	1.4530375531
C	-2.3305748675	1.3966304424	-1.4076638367
C	-3.3727517516	.5031977037	-1.7651259777
C	-3.7838753995	.4423070920	-3.1018980160
C	-3.1896617272	1.2309767874	-4.0830749364
C	-2.1610202975	2.0988628534	-3.7264889332
C	-1.7146419666	2.2010963037	-2.4043378840
C	-4.0531875677	-.3865175518	-.7294408739
C	-3.9424108178	-1.8781912250	-1.0950963050
C	-5.5273879879	.0077381018	-.5201829634
C	-.5537530620	3.1405441012	-2.0836233340
C	-.8338139639	4.5906211092	-2.5194664297
C	.7595111803	2.6397318227	-2.7148668503
C	1.6336812309	-1.8844284602	-.4608531410
N	.5587361388	-1.1841735749	-.8735135179
C	.1871938146	-1.2799834658	-2.1653393373
C	2.3712994834	-2.6975695443	-1.3165848391
C	.8713150513	-2.0722179252	-3.0831136107
C	1.9840151637	-2.7938583979	-2.6529855137
H	.1776270863	3.7720856633	3.7061129588
H	1.0508173857	2.3141204894	4.2164905678
H	-.6429724038	2.5544880316	4.6767575930
H	-1.9826847719	3.3868566353	2.6196688053
H	-3.6142739541	3.9040619662	1.2859300916
H	-4.1250087773	2.8389930453	-.0416981732
H	-2.9061031722	4.0711100044	-.3257128523
H	2.7879703685	-1.6618172128	4.9414399490
H	4.9052326950	-.8476115716	3.9552390471
H	4.8472783754	.8017529347	2.1145758878
H	-.6026602018	-.5994173900	3.7576750964
H	-.8487869097	-.8710810300	6.2133441503

H	.1127448304	.5730958312	5.8545615457
H	.9099122424	-.9027352207	6.4097289157
H	-.8033972675	-2.8796400066	4.6531826354
H	.9457178227	-3.0029288772	4.8674432344
H	.2605814500	-2.8983363388	3.2390818285
H	1.6932963139	1.9914244968	.5077959335
H	3.5521970040	2.3012206761	-1.0484541209
H	3.4745890460	.5925618784	-.5909962591
H	4.7163358634	1.6459414441	.1020754256
H	2.9779060376	4.1188435155	.6396954910
H	4.0142617919	3.4255296137	1.8993820962
H	2.2957671733	3.6928918135	2.2178909231
H	-4.5871503678	-.2357231724	-3.3774415255
H	-3.5240206451	1.1700850060	-5.1147399482
H	-1.6894331602	2.7091358768	-4.4923747631
H	-3.5319419160	-.2396155103	.2199192558
H	-4.3677056247	-2.5000485208	-.3002612233
H	-2.8996951472	-2.1782805982	-1.2330995384
H	-4.4832139044	-2.1071481834	-2.0200416535
H	-5.9862961577	-.6177402547	.2534036077
H	-6.1081443565	-.1187478134	-1.4408775769
H	-5.6234126127	1.0525305764	-.2090596548
H	-.4126939759	3.1397144459	-1.0001160671
H	-.0170905202	5.2484916129	-2.2027511763
H	-1.7624521700	4.9721202922	-2.0840552542
H	-.9214237434	4.6753987359	-3.6081480387
H	1.5899817493	3.3055495504	-2.4543898455
H	.6883919777	2.6070066667	-3.8079027009
H	1.0100641591	1.6344233145	-2.3640297627
H	1.9045261806	-1.7735386631	.5840605991
H	-.6813264995	-.6988297180	-2.4574575531
H	3.2315564249	-3.2371435357	-.9357993394
H	.5328005435	-2.1136515869	-4.1126108612
H	2.5395240563	-3.4185120007	-3.3457676223

40. L^1CuXO_2 η^2 singlet, X = pyridine

Cu	.4878874631	-.5656532197	-.7745956039
O	1.3135606528	-2.3894141837	-.4657295302
O	-.0051475859	-2.3856645950	-.6194450849
N	-1.0637821548	.0425064493	-1.8718766659
N	1.7711968901	.8064675239	-1.3462542428
N	.1696780274	-.5429619963	1.5055455751
C	-1.9809696370	1.1151896706	-3.8980500586
C	-.8510782742	.8297828255	-2.9218895830
C	.3889451090	1.4160140604	-3.2465597395
C	1.5754478682	1.4529658545	-2.4981511146
C	2.6682743519	2.3568357336	-3.0436225482
C	-2.3851194214	-.4303201907	-1.5630372437
C	-2.8973724445	-1.6225783008	-2.1316862583
C	-4.1914597328	-2.0268969860	-1.7758439581
C	-4.9745268023	-1.2884999362	-.8976998365
C	-4.4664497778	-.1142915097	-.3499978406
C	-3.1773587202	.3317785744	-.6594123040
C	-2.1221404928	-2.4792879650	-3.1290052910
C	-2.8381033444	-2.5258888555	-4.4963405928
C	-1.9138010235	-3.9181647125	-2.6207018512
C	-2.6731571892	1.6367322426	-.0434535936
C	-2.9980953286	1.7582260111	1.4562747937
C	-3.2237875369	2.8675116957	-.7922795726
C	2.8049260421	1.2184365056	-.4496700394
C	3.9005773631	.3536247541	-.2095577462
C	4.8559841632	.7329548971	.7405147338
C	4.7447832374	1.9278774945	1.4442139208

C	3.6667408627	2.7737896057	1.1979796347
C	2.6800888186	2.4453515160	.2610448810
C	4.0835057276	-.9387623342	-.9972460615
C	4.4239264700	-2.1385382166	-.0967666616
C	5.1448174340	-.7677688136	-2.1010516369
C	1.4994759667	3.4021373187	.0753191828
C	1.9534299989	4.8500703995	-.1946060697
C	.5485197533	3.3750016623	1.2876531488
C	-.8845644565	-1.2390420791	1.9656544024
C	1.0263092906	-.0322908738	2.4063714942
C	-1.1230567445	-1.4465441702	3.3233157016
C	.8698198913	-.1975749949	3.7809282530
C	-.2252840717	-.9207262684	4.2511162812
H	-1.7746341590	2.0205216717	-4.4714371597
H	-2.9432418707	1.2192742381	-3.3959476434
H	-2.0745506450	.2851324078	-4.6055734396
H	.4066882220	1.9749848883	-4.1737829220
H	2.5694784730	2.4524572152	-4.1267486013
H	3.6622191143	1.9738199033	-2.8066610468
H	2.5935657695	3.3612357720	-2.6151992868
H	-4.5920868768	-2.9409657533	-2.2039241167
H	-5.9768010404	-1.6224423989	-.6441469524
H	-5.0803455180	.4656213213	.3320460424
H	-1.1375427328	-2.0257236171	-3.2700413770
H	-2.2245648387	-3.0610995260	-5.2288882671
H	-3.0470552241	-1.5281579637	-4.8930629608
H	-3.7959645920	-3.0521639905	-4.4206040238
H	-1.3179636904	-4.4878365785	-3.3421990875
H	-2.8711114184	-4.4380153348	-2.5014459708
H	-1.3901291118	-3.9243599429	-1.6645304081
H	-1.5851682855	1.6463638015	-.1491462998
H	-2.5071875795	2.6439229860	1.8727110539
H	-2.6555457065	.8851161823	2.0172598541
H	-4.0726909200	1.8737187232	1.6343727847
H	-2.8436619466	3.7911480933	-.3413814521
H	-4.3184120028	2.8952949578	-.7443952565
H	-2.9350362231	2.8697009623	-1.8462382232
H	5.7035851830	.0810866330	.9273680704
H	5.4970122165	2.2018845550	2.1784243094
H	3.5816393426	3.7042183191	1.7517624571
H	3.1348092154	-1.1681237748	-1.4856174455
H	4.4238827859	-3.0577524847	-.6911618250
H	3.6807933197	-2.2565676563	.6957537203
H	5.4143711034	-2.0430436699	.3621362076
H	5.2559272556	-1.6984684273	-2.6680376438
H	6.1220783314	-.5146912253	-1.6743674630
H	4.8726104345	.0242040484	-2.8056468812
H	.9228144330	3.0759265147	-.7927333589
H	1.0902703286	5.4720931539	-.4546125534
H	2.6740760354	4.9083792512	-1.0159933249
H	2.4229629182	5.2979679545	.6875557898
H	-.2871058911	4.0662814604	1.1298911325
H	1.0662895083	3.6807398859	2.2037525777
H	.1360038450	2.3773252094	1.4505992695
H	-1.5449203810	-1.6515680692	1.2115959391
H	1.8695580724	.5196182353	2.0064414913
H	-1.9923553534	-2.0157363787	3.6356281004
H	1.5978170342	.2319243456	4.4609543509
H	-.3778041213	-1.0662994622	5.3164502972

41. L^1CuXO_2 η^2 triplet, X = pyridine

Cu	.4014453688	-.4725916857	-.7260920453
O	1.2174896454	-2.6278375402	-.4809793851

O	-.0540263141	-2.4376301373	-.5277417445
N	-1.1076062839	.0387511562	-1.9685953764
N	1.7137073823	.8902269393	-1.3275739286
N	.2565607211	-.5081175850	1.5615215640
C	-1.9098193573	.9990462777	-4.1031934859
C	-.8395327011	.7620215483	-3.0490922049
C	.4173356848	1.3444241649	-3.3309870850
C	1.5580477036	1.4726532343	-2.5192156352
C	2.6474027236	2.3865335693	-3.0565095416
C	-2.4230399471	-.4291928732	-1.6573875203
C	-2.9329380083	-1.6362659654	-2.1972910273
C	-4.2010102968	-2.0685541899	-1.7865221398
C	-4.9551974660	-1.3498131379	-.8672623148
C	-4.4423835254	-.1686299879	-.3363908138
C	-3.1827743997	.3099228302	-.7100624183
C	-2.1738575361	-2.4755219917	-3.2224570813
C	-2.9105874046	-2.5094258317	-4.5778211748
C	-1.9314831848	-3.9176793316	-2.7322526441
C	-2.6576531030	1.6236926715	-.1361672649
C	-3.0939007866	1.8807502440	1.3148207741
C	-3.0641797901	2.8213851163	-1.0190407075
C	2.7677879464	1.2755802685	-.4452838596
C	3.8736923580	.4074240258	-.2503716872
C	4.8491329865	.7622117026	.6887195782
C	4.7485811540	1.9340195311	1.4335553619
C	3.6578931053	2.7761400869	1.2389495552
C	2.6567133324	2.4738565503	.3079313112
C	4.0363554174	-.8798342882	-1.0528697017
C	4.3566917989	-2.0925284481	-.1617066559
C	5.1042582666	-.7215193272	-2.1517935400
C	1.4676795848	3.4226153383	.1673600267
C	1.9090862232	4.8649408445	-.1471834833
C	.5799942482	3.4066073438	1.4271242462
C	-.8768879687	-1.0217695775	2.0772646231
C	1.2590246789	-.2051750810	2.4056162386
C	-1.0573433275	-1.2398932783	3.4412126713
C	1.1643036506	-.3963833139	3.7836857803
C	-.0159194513	-.9198672939	4.3127876568
H	-1.7788378058	1.9786150292	-4.5701310705
H	-2.9181920103	.9293104998	-3.6907771302
H	-1.8190607119	.2444290427	-4.8934432750
H	.4733055659	1.8617700865	-4.2815442561
H	2.6159216168	2.4129292620	-4.1477065036
H	3.6402876270	2.0667678022	-2.7361857905
H	2.5028065299	3.4112983949	-2.6974459528
H	-4.6009460465	-2.9908125292	-2.1979558835
H	-5.9354945620	-1.7058721539	-.5638511190
H	-5.0337000463	.3897745836	.3818725508
H	-1.1943810550	-2.0105869287	-3.3746542207
H	-2.3110683114	-3.0413216983	-5.3248174582
H	-3.1217535653	-1.5069543429	-4.9600295714
H	-3.8690151395	-3.0339333234	-4.4876537426
H	-1.3284641934	-4.4666440828	-3.4640958611
H	-2.8765781864	-4.4612445183	-2.6119217365
H	-1.4039740766	-3.9278182130	-1.7762750757
H	-1.5647441804	1.5677552695	-.1507476481
H	-2.5623303512	2.7504181763	1.7134013234
H	-2.8779127962	1.0273944133	1.9638243059
H	-4.1645041929	2.0972907889	1.3890127365
H	-2.6743645891	3.7564718707	-.6014818412
H	-4.1548457705	2.9053288191	-1.0765179727
H	-2.6803391565	2.7242835638	-2.0365633997
H	5.7032543012	.1083690580	.8370456946
H	5.5153718436	2.1899092160	2.1591964462

H	3.5770855306	3.6866453846	1.8263298797
H	3.0837741172	-1.0805443963	-1.5480761410
H	4.3619673827	-3.0078919116	-.7623187442
H	3.6077802284	-2.2152051522	.6246570631
H	5.3409414718	-2.0044504402	.3115621686
H	5.1921083197	-1.6446937359	-2.7352085829
H	6.0869604479	-.5021551908	-1.7188797478
H	4.8551809539	.0900213893	-2.8421158759
H	.8513535074	3.0733875762	-.6646035996
H	1.0349135703	5.4954002903	-.3411449400
H	2.5621388799	4.9097643239	-1.0244576198
H	2.4547930325	5.3101441315	.6921989501
H	-.2730378292	4.0825986060	1.2997452400
H	1.1377352923	3.7371217300	2.3110889573
H	.1918130993	2.4049187861	1.6286764197
H	-1.6611097254	-1.2648414935	1.3670784156
H	2.1600703632	.1977794814	1.9541599319
H	-1.9942042354	-1.6537837918	3.8012657524
H	2.0036566057	-.1372291554	4.4206116235
H	-.1202819071	-1.0783398460	5.3819735817

42. L^1CuX, X = 4-pyridinecarboxylate

C	-2.81313	2.61805	-0.38545
C	1.95250	-0.27370	1.80779
C	1.71855	-1.36012	2.69095
C	2.81427	-2.01806	3.25824
C	4.12125	-1.62839	2.97632
C	4.34318	-0.56632	2.10448
C	3.28104	0.12334	1.50869
C	0.30201	-1.85582	2.97255
C	0.01869	-2.04622	4.47359
C	0.01096	-3.15120	2.18863
C	3.56621	1.25663	0.52578
C	4.21545	0.72504	-0.76671
C	4.42376	2.37364	1.14821
C	-1.97861	0.63446	-2.19314
C	-3.02091	-0.32469	-2.28372
C	-3.64231	-0.53346	-3.51967
C	-3.26013	0.17582	-4.65441
C	-2.23287	1.11131	-4.56013
C	-1.58085	1.35919	-3.34770
C	-3.44747	-1.15426	-1.07495
C	-3.06473	-2.63662	-1.25184
C	-4.95075	-1.01278	-0.77091
C	-0.42059	2.35053	-3.29502
C	-0.76415	3.70989	-3.92990
C	0.84337	1.74543	-3.93772
C	2.10282	-2.68577	-1.30309
C	0.55132	-2.24672	-2.95853
C	2.63516	-3.74119	-2.03036
C	1.03312	-3.28950	-3.73749
C	2.10056	-4.06771	-3.27992
C	0.64061	1.88575	3.04753
C	0.19568	1.35236	1.69139
C	-0.92930	1.98613	1.11721
C	-1.60736	1.73313	-0.09606
H	0.09194	2.79010	3.31789
H	1.71178	2.10966	3.05067
H	0.47765	1.13824	3.83235
H	-1.34779	2.79076	1.71055
H	-2.97823	3.34087	0.41620
H	-3.72022	2.01538	-0.50222
H	-2.68172	3.16413	-1.32531

H	2.64171	-2.85777	3.92711
H	4.95950	-2.15515	3.42470
H	5.36380	-0.27036	1.87393
H	-0.39149	-1.09714	2.60038
H	-1.03171	-2.31807	4.63088
H	0.21885	-1.13069	5.04093
H	0.63001	-2.84530	4.90853
H	-1.02281	-3.48074	2.34894
H	0.67679	-3.96327	2.50322
H	0.15488	-2.99664	1.11514
H	2.60321	1.69337	0.24877
H	4.37596	1.53932	-1.48355
H	3.58000	-0.02609	-1.24462
H	5.18789	0.26148	-0.56369
H	4.55120	3.19924	0.43798
H	5.42429	2.01618	1.41813
H	3.96066	2.77785	2.05467
H	-4.43561	-1.27339	-3.59618
H	-3.75109	-0.00582	-5.60695
H	-1.92445	1.65422	-5.45035
H	-2.89605	-0.77772	-0.20925
H	-3.33549	-3.21614	-0.36100
H	-1.98905	-2.74839	-1.41480
H	-3.58093	-3.08251	-2.10996
H	-5.21163	-1.56476	0.13984
H	-5.56854	-1.41118	-1.58420
H	-5.23501	0.03470	-0.62323
H	-0.18931	2.52909	-2.24159
H	0.06446	4.41437	-3.79200
H	-1.65972	4.14999	-3.47761
H	-0.94406	3.62688	-5.00789
H	1.69176	2.43570	-3.85530
H	0.68375	1.53217	-5.00121
H	1.11909	0.80776	-3.44589
H	2.50023	-2.41284	-0.32951
H	-0.27731	-1.62845	-3.29230
H	3.46515	-4.33551	-1.66124
H	0.60554	-3.53083	-4.70603
C	2.66801	-5.24768	-4.12507
N	1.06850	-1.93199	-1.74665
N	0.85845	0.34093	1.13842
N	-1.26082	0.79759	-0.97492
O	2.07260	-5.43490	-5.21168
O	3.63672	-5.83885	-3.59114
Cu	0.30520	-0.42899	-0.64398

43. L^1CuXO_2 η^1 singlet, X = 4-pyridinecarboxylate

O	4.84702	-5.06745	-3.96226
C	0.39692	-3.73734	3.59486
C	3.34198	0.35325	0.04899
C	4.32127	-0.14282	-1.02965
C	3.72442	1.77327	0.51634
C	-1.81220	0.09589	-2.29746
C	-2.75303	-0.90212	-2.65827
C	-3.20018	-0.95561	-3.98277
C	-2.73448	-0.06300	-4.94304
C	-1.80474	0.90847	-4.58182
C	-1.32990	1.01288	-3.26993
O	3.89686	-4.00293	-5.74870
C	1.97039	-0.92500	1.81088
C	-3.27847	-1.91368	-1.64099
C	-2.90430	-3.35821	-2.02578
C	-4.79953	-1.77858	-1.43293

C	-0.27937	2.07278	-2.93130
C	-0.71844	3.49035	-3.34622
C	1.09003	1.73588	-3.55466
C	2.02329	-3.32593	-1.40344
C	1.16137	-2.12554	-3.18305
C	2.94811	-3.95528	-2.22675
C	2.05176	-2.72491	-4.06473
C	1.90027	-1.79675	2.92971
C	2.98331	-3.65372	-3.59145
C	0.65106	1.34584	2.96773
C	0.15376	0.64456	1.70586
C	-1.00982	1.23092	1.14712
C	-1.64411	1.01520	-0.08935
C	3.09636	-2.29239	3.46373
C	4.33366	-1.95990	2.92377
C	4.39222	-1.11868	1.81730
C	3.23007	-0.59666	1.23943
C	0.58127	-2.20709	3.58466
C	0.46623	-1.65914	5.02281
C	-2.82396	1.92588	-0.39930
H	0.76994	2.41663	2.77149
H	1.60112	0.94881	3.32292
H	-0.08763	1.24673	3.77046
H	-1.43845	2.02730	1.74667
H	-3.17195	2.43438	0.50238
H	-3.65352	1.35455	-0.82481
H	-2.55302	2.68799	-1.13669
H	3.05317	-2.95619	4.32350
H	5.24652	-2.35931	3.35823
H	5.35792	-0.86249	1.39129
H	-0.23235	-1.78949	2.98701
H	-0.51146	-1.91123	5.45070
H	0.58177	-0.57246	5.06321
H	1.23205	-2.09656	5.67461
H	-0.57815	-3.99326	4.02742
H	1.16336	-4.22873	4.20680
H	0.43725	-4.15020	2.58469
H	2.35148	0.41640	-0.41052
H	4.27532	0.51174	-1.90721
H	4.08189	-1.15871	-1.35480
H	5.35967	-0.13846	-0.67826
H	3.76544	2.46424	-0.33422
H	4.71019	1.77470	0.99769
H	3.00198	2.16801	1.23810
H	-3.91988	-1.71917	-4.26750
H	-3.08629	-0.12886	-5.96925
H	-1.43122	1.59441	-5.33814
H	-2.79564	-1.70114	-0.68405
H	-3.26027	-4.05996	-1.26284
H	-1.82085	-3.47948	-2.10359
H	-3.35214	-3.64879	-2.98376
H	-5.14201	-2.47295	-0.65662
H	-5.35502	-2.00797	-2.35007
H	-5.07583	-0.76460	-1.12303
H	-0.14289	2.07612	-1.84731
H	0.01012	4.23178	-2.99802
H	-1.69470	3.75385	-2.92560
H	-0.79095	3.59095	-4.43499
H	1.83311	2.49581	-3.28381
H	1.03159	1.70076	-4.64863
H	1.45964	0.76626	-3.21046
H	1.96575	-3.55428	-0.34233
H	0.42657	-1.40153	-3.52309
H	3.66447	-4.67432	-1.84265

H	2.05293	-2.49622	-5.12551
N	1.14523	-2.40755	-1.86077
N	0.78963	-0.39992	1.19789
N	-1.26499	0.10375	-0.98399
C	4.02720	-4.31923	-4.54322
O	-0.21074	-4.11131	0.36208
O	-0.62609	-2.92136	0.55889
Cu	0.04093	-1.35497	-0.48120

44. L^1CuXO_2 η^1 triplet, X = 4-pyridinecarboxylate

O	4.36520	-5.61011	-4.18061
C	0.63065	-3.89731	3.29031
C	3.45040	0.77348	0.39396
C	4.40990	0.34706	-0.73282
C	3.87074	2.13502	0.98230
C	-1.75507	0.10239	-2.28539
C	-2.74534	-0.86207	-2.61003
C	-3.25059	-0.90001	-3.91494
C	-2.79340	-0.02970	-4.89889
C	-1.80809	0.90019	-4.58007
C	-1.27929	0.98928	-3.28827
O	2.93282	-4.96152	-5.83724
C	2.05501	-0.76467	1.90953
C	-3.26564	-1.86253	-1.58154
C	-3.02498	-3.31656	-2.03271
C	-4.75848	-1.64380	-1.26504
C	-0.17275	2.00174	-2.99345
C	-0.53860	3.42960	-3.43748
C	1.16517	1.56309	-3.62170
C	2.42975	-3.05758	-1.48168
C	0.99919	-2.37081	-3.16558
C	3.08933	-3.92233	-2.34342
C	1.61455	-3.21526	-4.08032
C	1.97465	-1.76698	2.91171
C	2.68705	-4.01667	-3.67919
C	0.53058	1.34697	3.09892
C	0.13817	0.67988	1.78208
C	-1.03622	1.20725	1.19451
C	-1.62440	0.98972	-0.07019
C	3.15916	-2.22862	3.49725
C	4.40370	-1.74361	3.10776
C	4.47636	-0.78424	2.10224
C	3.32404	-0.28516	1.48694
C	0.63927	-2.35720	3.36333
C	0.25616	-1.89740	4.78489
C	-2.84300	1.85116	-0.38033
H	0.80616	2.39201	2.91564
H	1.36994	0.85360	3.58799
H	-0.32085	1.35787	3.78756
H	-1.53023	1.96221	1.79721
H	-3.21373	2.34740	0.51878
H	-3.65026	1.25381	-0.81095
H	-2.59806	2.62122	-1.12003
H	3.10378	-2.99028	4.27106
H	5.31025	-2.12115	3.57359
H	5.44863	-0.41580	1.78456
H	-0.12850	-1.99189	2.67657
H	-0.71833	-2.30950	5.07368
H	0.19542	-0.80786	4.85850
H	0.99317	-2.24060	5.52071
H	-0.37060	-4.28259	3.51694
H	1.32292	-4.34072	4.01543
H	0.91111	-4.25605	2.29730
H	2.45939	0.89921	-0.05102
H	4.40975	1.09577	-1.53342

H	4.11147	-0.61019	-1.16911
H	5.44268	0.24768	-0.37852
H	3.90983	2.90150	0.19898
H	4.86465	2.07638	1.44267
H	3.16822	2.47214	1.75149
H	-4.01368	-1.63299	-4.16578
H	-3.19318	-0.08241	-5.90827
H	-1.43737	1.56867	-5.35320
H	-2.70274	-1.70470	-0.65900
H	-3.32158	-4.01789	-1.24437
H	-1.97067	-3.49428	-2.26105
H	-3.60689	-3.56208	-2.92880
H	-5.09895	-2.35791	-0.50555
H	-5.38062	-1.78620	-2.15673
H	-4.95012	-0.63533	-0.88456
H	-0.02681	2.02349	-1.91050
H	0.23562	4.13755	-3.11951
H	-1.49098	3.75534	-3.00524
H	-0.62541	3.51074	-4.52694
H	1.96183	2.27519	-3.37426
H	1.09148	1.50831	-4.71406
H	1.46848	0.57725	-3.25863
H	2.72302	-2.96210	-0.43950
H	0.16007	-1.74238	-3.44939
H	3.92295	-4.53768	-2.01984
H	1.28989	-3.28201	-5.11400
N	1.39246	-2.27980	-1.87271
N	0.87843	-0.28890	1.25860
N	-1.16982	0.13853	-0.98690
C	3.40827	-4.97452	-4.67900
O	-0.44095	-4.03373	0.05333
O	-0.71466	-2.87265	0.36810
Cu	0.43079	-1.07799	-0.56291

45. L^1CuXO_2 η^2 singlet, X = 4-pyridinecarboxylate

O	-2.44471	-1.99651	4.67757
C	-3.06785	-2.72816	-5.53904
C	-2.33252	-4.29246	-3.69372
C	-2.71604	1.22156	-0.92423
C	-3.10832	1.33820	0.55954
C	-3.15828	2.50097	-1.66729
C	2.65535	0.83338	-1.51194
C	3.87119	0.11326	-1.40952
C	4.84613	0.56920	-0.51504
C	4.64539	1.70625	0.25971
C	3.44786	2.40689	0.15092
O	-0.54616	-0.84871	5.23221
C	2.49533	1.93138	-4.11559
C	2.43452	1.99152	-0.71918
C	4.15634	-1.12138	-2.25939
C	4.47478	-2.35363	-1.39156
C	5.29366	-0.86389	-3.26847
C	1.14121	2.80506	-0.79426
C	1.37015	4.17655	-1.46482
C	0.49253	3.00303	0.59007
C	-1.25776	-2.00259	0.64612
C	0.59399	-0.76425	1.20217
C	-1.66550	-2.06535	1.97515
C	-2.54759	-0.80253	-2.53628
C	0.26224	-0.79039	2.55198
C	-0.90755	-1.43347	2.96574
C	-2.17383	0.82741	-4.84366
C	-1.02516	0.40584	-3.93019

C	0.22058	0.97144	-4.29172
C	-3.13382	-1.95252	-3.12466
C	-4.45255	-2.28559	-2.78472
C	-5.18485	-1.52522	-1.88233
C	-4.59495	-0.41363	-1.29153
C	-3.28219	-0.03248	-1.59036
C	-2.40624	-2.82249	-4.14717
C	1.40101	1.04263	-3.54407
H	-2.20285	1.91764	-4.93338
H	-3.14513	0.48000	-4.49668
H	-1.99986	0.42942	-5.84949
H	0.21448	1.53828	-5.21578
H	2.10872	2.56465	-4.91645
H	3.29445	1.30515	-4.52765
H	2.94876	2.56520	-3.35159
H	-4.91272	-3.15663	-3.24311
H	-6.20747	-1.79841	-1.63467
H	-5.16511	0.17181	-0.57700
H	-1.37798	-2.46202	-4.22443
H	-2.50916	-3.32023	-6.27343
H	-3.11489	-1.69786	-5.90271
H	-4.09422	-3.11418	-5.51529
H	-1.75255	-4.88056	-4.41409
H	-3.32878	-4.74510	-3.62399
H	-1.84687	-4.37641	-2.71904
H	-1.62611	1.15512	-0.97939
H	-2.57670	2.17650	1.02028
H	-2.85859	0.43492	1.11797
H	-4.18021	1.53282	0.68578
H	-2.75054	3.39155	-1.17439
H	-4.25156	2.59127	-1.66503
H	-2.82554	2.51413	-2.70749
H	5.78115	0.02197	-0.42929
H	5.41493	2.04327	0.94898
H	3.29144	3.29207	0.76131
H	3.25280	-1.35174	-2.82783
H	4.60895	-3.23611	-2.02743
H	3.65701	-2.56504	-0.69943
H	5.39565	-2.21478	-0.81307
H	5.43507	-1.73845	-3.91428
H	6.24526	-0.66823	-2.76016
H	5.08086	-0.00234	-3.90992
H	0.43280	2.25075	-1.41500
H	0.42539	4.72887	-1.53184
H	1.77297	4.08065	-2.47812
H	2.07051	4.78812	-0.88389
H	-0.44558	3.56042	0.48746
H	1.13721	3.57812	1.26391
H	0.26975	2.04887	1.07335
H	-1.83041	-2.48870	-0.13957
H	1.49456	-0.25925	0.86090
H	-2.57239	-2.58209	2.27485
H	0.87770	-0.31310	3.30832
N	-1.21063	-0.40361	-2.89764
N	1.62351	0.39167	-2.39625
N	-0.15582	-1.34110	0.23969
C	-1.34747	-1.42964	4.46178
O	1.52289	-2.81396	-2.04862
O	0.22030	-3.05527	-2.19068
Cu	0.49189	-1.17682	-1.99882

46. L^1CuX, X = 4-methoxypyridine

C	3.22057	-5.30381	-3.85928

C	-2.60188	3.34938	-0.24123
C	-0.02768	-2.66891	2.19222
C	3.64305	1.69023	0.60750
C	4.11730	1.19791	-0.77530
C	4.65457	2.68285	1.20715
C	-1.93219	1.26917	-2.04592
C	-3.04428	0.38739	-2.08674
C	-3.67139	0.14509	-3.31425
C	-3.22968	0.75014	-4.48783
C	-2.13949	1.61529	-4.44002
C	-1.47717	1.89225	-3.23842
C	2.01727	0.15376	1.87560
C	-3.53302	-0.33187	-0.83157
C	-3.19724	-1.83603	-0.88802
C	-5.03508	-0.11870	-0.57259
C	-0.25699	2.81149	-3.24036
C	-0.53546	4.16668	-3.91530
C	0.95783	2.11821	-3.88980
C	1.95196	-2.16892	-1.31125
C	0.30624	-1.64302	-2.83782
C	2.41830	-3.21965	-2.09499
C	0.69901	-2.66385	-3.68427
C	1.77641	-0.97571	2.70093
C	1.78138	-3.47610	-3.31584
C	0.84926	2.39779	3.16040
C	0.33321	1.88593	1.82427
C	-0.75362	2.58587	1.25255
C	-1.46074	2.38466	0.04299
C	2.86717	-1.71908	3.16443
C	4.17540	-1.37309	2.83528
C	4.40479	-0.26403	2.02595
C	3.34921	0.51319	1.53613
C	0.35496	-1.42680	3.02542
C	0.13797	-1.68774	4.52589
H	3.30657	-6.00435	-4.69050
H	4.15214	-4.73393	-3.76478
H	3.03528	-5.86048	-2.93330
H	0.29480	3.27618	3.49503
H	1.90996	2.66342	3.08928
H	0.77436	1.62318	3.93166
H	-1.11033	3.41989	1.84499
H	-2.66903	4.12821	0.52047
H	-3.55849	2.81593	-0.27506
H	-2.47629	3.82540	-1.21892
H	2.68907	-2.58980	3.79060
H	5.00892	-1.96443	3.20521
H	5.42618	0.00197	1.76484
H	-0.32172	-0.62161	2.72750
H	-0.91413	-1.92303	4.72213
H	0.40718	-0.81392	5.12820
H	0.73285	-2.53471	4.88616
H	-1.06016	-2.97469	2.39735
H	0.62639	-3.51807	2.42506
H	0.05512	-2.46339	1.12003
H	2.70379	2.22693	0.45097
H	4.29217	2.04267	-1.45188
H	3.36762	0.54771	-1.23728
H	5.05331	0.63200	-0.69660
H	4.77471	3.54988	0.54766
H	5.64474	2.23136	1.33581
H	4.32641	3.04606	2.18647
H	-4.51955	-0.53438	-3.35269
H	-3.73047	0.54882	-5.43116
H	-1.79173	2.08264	-5.35770

H	-2.98883	0.08785	0.01889
H	-3.52324	-2.34255	0.02795
H	-2.11924	-1.99372	-0.99378
H	-3.69454	-2.32293	-1.73543
H	-5.32683	-0.57840	0.37826
H	-5.65429	-0.56950	-1.35638
H	-5.28654	0.94581	-0.52427
H	0.00680	3.01095	-2.19854
H	0.33517	4.82554	-3.82126
H	-1.39220	4.67265	-3.45834
H	-0.74704	4.05716	-4.98486
H	1.83876	2.77014	-3.86266
H	0.75777	1.86718	-4.93823
H	1.20883	1.19247	-3.36303
H	2.42852	-1.94293	-0.36238
H	-0.52656	-0.99946	-3.09984
H	3.25939	-3.80710	-1.74859
H	0.18702	-2.84262	-4.62301
N	0.91715	-1.37934	-1.65705
N	0.92523	0.83112	1.26926
N	-1.19651	1.42176	-0.83702
O	2.12187	-4.45306	-4.18208
Cu	0.28057	0.14513	-0.45534

47. L^1CuXO_2 η^1 singlet, X = 4-methoxypyridine

C	3.52261	-4.79555	-4.29233
H	3.85811	-5.22867	-5.23478
H	3.06917	-5.57815	-3.67345
H	4.37995	-4.36222	-3.76431
C	-2.58032	3.27488	-0.18779
C	0.29147	-2.65121	3.84539
C	3.34091	1.07570	-0.02883
C	4.18346	0.47393	-1.16820
C	3.89641	2.45667	0.37673
C	-1.90664	1.22773	-2.03582
C	-2.96971	0.32425	-2.29353
C	-3.47458	0.23841	-3.59605
C	-2.95226	1.00908	-4.63027
C	-1.90685	1.89141	-4.36824
C	-1.36843	2.02366	-3.08340
C	1.98918	-0.03519	1.85673
C	-3.57479	-0.54399	-1.19158
C	-3.39312	-2.04708	-1.48064
C	-5.06034	-0.20883	-0.95486
C	-0.19440	2.97717	-2.85423
C	-0.47485	4.39589	-3.38486
C	1.10990	2.42482	-3.46439
C	1.57084	-2.42256	-1.38994
C	0.45597	-1.32251	-3.07837
C	2.24149	-3.24370	-2.28920
C	1.06881	-2.09540	-4.05002
C	1.91256	-0.88574	2.99162
C	1.98983	-3.07779	-3.65695
C	0.98807	2.40048	3.02785
C	0.34138	1.73274	1.82023
C	-0.77834	2.42811	1.30114
C	-1.50786	2.24053	0.11226
C	3.08948	-1.49901	3.43999
C	4.30926	-1.30186	2.80224
C	4.37091	-0.48072	1.68054
C	3.22755	0.15421	1.18379
C	0.61466	-1.14624	3.75518
C	0.66181	-0.53917	5.17333

H	1.19128	3.45259	2.80433
H	1.91895	1.91930	3.32528
H	0.30048	2.38009	3.87987
H	-1.07169	3.29501	1.88293
H	-2.82613	3.85208	0.70543
H	-3.48956	2.79499	-0.55946
H	-2.24846	3.97349	-0.96223
H	3.04509	-2.14537	4.31219
H	5.20723	-1.78603	3.17712
H	5.32474	-0.32511	1.18456
H	-0.19958	-0.67401	3.20072
H	-0.29798	-0.68621	5.68171
H	0.87578	0.53288	5.16081
H	1.43411	-1.02249	5.78289
H	-0.68250	-2.79380	4.32792
H	1.03371	-3.18467	4.45138
H	0.25134	-3.11193	2.85641
H	2.32925	1.23012	-0.41567
H	4.13360	1.11845	-2.05295
H	3.82319	-0.51940	-1.45324
H	5.24090	0.38142	-0.89594
H	3.93760	3.12917	-0.48817
H	4.91148	2.36637	0.78132
H	3.27504	2.93005	1.14284
H	-4.29177	-0.44792	-3.80229
H	-3.35704	0.92398	-5.63509
H	-1.49826	2.48792	-5.17977
H	-3.03695	-0.32529	-0.26541
H	-3.81649	-2.64493	-0.66596
H	-2.33556	-2.31110	-1.56743
H	-3.89867	-2.34242	-2.40773
H	-5.45455	-0.79520	-0.11728
H	-5.67177	-0.43774	-1.83531
H	-5.20144	0.85156	-0.71990
H	-0.02952	3.05672	-1.77708
H	0.33981	5.07330	-3.10565
H	-1.40644	4.80354	-2.97933
H	-0.55492	4.41564	-4.47724
H	1.94328	3.11244	-3.27867
H	1.01831	2.29705	-4.54939
H	1.37310	1.45487	-3.03260
H	1.73312	-2.54384	-0.32393
H	-0.26064	-0.55599	-3.35269
H	2.93597	-3.98422	-1.91372
H	0.84989	-1.95253	-5.10191
N	0.69856	-1.47046	-1.75850
N	0.82814	0.60532	1.31835
N	-1.29874	1.24349	-0.74802
O	2.56917	-3.79359	-4.64466
O	-0.34025	-3.03205	0.63650
O	-0.74134	-1.83612	0.85328
Cu	-0.14172	-0.28918	-0.20368

48. L^1CuXO_2 η^1 triplet, X = 4-methoxypyridine

C	3.30962	-5.35496	-3.86591
H	3.49507	-5.97770	-4.74146
H	2.98945	-5.98622	-3.02881
H	4.23084	-4.82657	-3.59527
C	-2.60116	3.24454	-0.20193
C	0.61666	-3.00840	3.25460
C	3.39016	1.63571	0.25973
C	4.09475	1.14512	-1.02021
C	4.06589	2.91072	0.79974

C	-1.90323	1.24907	-2.07151
C	-3.03695	0.42951	-2.31638
C	-3.58307	0.39772	-3.60506
C	-3.03364	1.13602	-4.64836
C	-1.91246	1.92431	-4.40648
C	-1.33334	2.00151	-3.13483
C	2.07695	0.09788	1.85176
C	-3.67534	-0.41474	-1.21610
C	-3.73031	-1.90688	-1.59790
C	-5.08483	0.09063	-0.84851
C	-0.08364	2.85800	-2.93421
C	-0.28718	4.31338	-3.39525
C	1.13672	2.23292	-3.63968
C	1.84445	-2.37239	-1.24978
C	0.40735	-1.66921	-2.91045
C	2.37195	-3.37586	-2.05535
C	0.86726	-2.63772	-3.78453
C	2.04543	-0.94852	2.81159
C	1.87362	-3.51680	-3.35717
C	0.83886	2.35754	3.13308
C	0.28142	1.71445	1.86795
C	-0.85358	2.36576	1.32971
C	-1.53527	2.20252	0.10366
C	3.25777	-1.49680	3.24687
C	4.47954	-1.05113	2.75114
C	4.49948	-0.04272	1.79229
C	3.31806	0.54159	1.32315
C	0.73315	-1.47757	3.38540
C	0.54375	-1.05710	4.85701
H	1.21457	3.36274	2.91160
H	1.64991	1.77883	3.57457
H	0.04343	2.47119	3.87685
H	-1.21227	3.19258	1.93343
H	-2.87363	3.80522	0.69405
H	-3.50016	2.78456	-0.61844
H	-2.23660	3.95735	-0.94981
H	3.24265	-2.28799	3.99219
H	5.40840	-1.48800	3.10812
H	5.45337	0.30143	1.40004
H	-0.07999	-1.03394	2.80534
H	-0.41940	-1.41511	5.23883
H	0.56842	0.03011	4.97331
H	1.33163	-1.47830	5.49230
H	-0.37478	-3.34287	3.57989
H	1.35601	-3.52765	3.87513
H	0.75616	-3.33755	2.22105
H	2.36426	1.89478	-0.01436
H	4.08380	1.92639	-1.78881
H	3.59571	0.26245	-1.43301
H	5.14188	0.88117	-0.83255
H	4.05685	3.70397	0.04326
H	5.11092	2.72428	1.07309
H	3.55259	3.28663	1.69028
H	-4.45723	-0.22036	-3.79372
H	-3.47315	1.09539	-5.64146
H	-1.47546	2.49262	-5.22391
H	-3.04715	-0.32297	-0.32650
H	-4.10583	-2.50356	-0.75902
H	-2.74087	-2.28996	-1.86446
H	-4.39721	-2.08250	-2.44974
H	-5.50825	-0.50900	-0.03444
H	-5.76797	0.02135	-1.70298
H	-5.06840	1.13466	-0.52076
H	0.13772	2.87780	-1.86411

H	0.59575	4.91750	-3.15764
H	-1.15144	4.77279	-2.90487
H	-0.44810	4.38072	-4.47713
H	2.03567	2.83588	-3.46629
H	0.98067	2.16959	-4.72307
H	1.33357	1.22233	-3.26881
H	2.20956	-2.23749	-0.23647
H	-0.37066	-0.97474	-3.21164
H	3.14613	-4.02204	-1.66108
H	0.46299	-2.72776	-4.78633
N	0.88029	-1.52463	-1.65190
N	0.86691	0.64737	1.33413
N	-1.27553	1.24921	-0.79033
O	2.28290	-4.44226	-4.25037
O	-1.06113	-2.97936	0.31861
O	-1.16750	-1.78768	0.62991
Cu	0.09995	-0.15317	-0.32453

49. L^1CuXO_2 η^2 singlet, X = 4-methoxypyridine

C	-0.05436	-1.08162	6.45386
H	-0.50035	-1.39044	7.40003
H	0.05069	0.01007	6.44242
H	0.93521	-1.54253	6.35020
C	1.57544	0.86861	-2.71514
C	-2.56984	-3.20848	-4.59544
C	-2.02241	-4.49497	-2.49248
C	-2.78044	1.30345	-0.53630
C	-3.25711	1.59594	0.89851
C	-3.15668	2.47784	-1.46285
C	2.66539	0.72997	-0.56504
C	3.79856	-0.08109	-0.30263
C	4.73768	0.36759	0.63400
C	4.57832	1.57334	1.30829
C	3.45581	2.35559	1.05528
C	2.76576	1.62499	-3.28431
C	2.48134	1.95712	0.13238
C	4.04909	-1.40499	-1.01995
C	4.27823	-2.56260	-0.02908
C	5.23483	-1.29413	-1.99955
C	1.27654	2.87108	-0.10447
C	1.69271	4.19096	-0.78634
C	0.50494	3.17400	1.19425
C	-1.28808	-1.44835	1.84394
C	0.66520	-0.36654	2.34588
C	-1.54599	-1.71520	3.17992
C	-2.47411	-0.86973	-1.87948
C	0.50414	-0.57955	3.71491
C	-0.63797	-1.26202	4.14690
C	-1.87806	0.50244	-4.34369
C	-0.82997	0.24521	-3.27182
C	0.45045	0.77269	-3.55097
C	-2.94549	-2.12959	-2.32784
C	-4.26339	-2.49112	-2.01834
C	-5.09148	-1.65807	-1.27409
C	-4.60312	-0.44276	-0.80282
C	-3.29411	-0.03043	-1.07892
C	-2.08213	-3.09621	-3.13670
H	-1.83243	1.54307	-4.67594
H	-2.88856	0.28052	-4.00331
H	-1.66414	-0.12530	-5.21580
H	0.54696	1.25294	-4.51765
H	2.44654	2.35931	-4.02651
H	3.43482	0.91237	-3.78244

H	3.34765	2.12690	-2.51153
H	-4.64404	-3.44694	-2.36652
H	-6.11105	-1.96012	-1.04990
H	-5.24746	0.19352	-0.20434
H	-1.06210	-2.70477	-3.14488
H	-1.90682	-3.86518	-5.16998
H	-2.59792	-2.23589	-5.09500
H	-3.57932	-3.63334	-4.64246
H	-1.32813	-5.13321	-3.05016
H	-3.00036	-4.98975	-2.50174
H	-1.67122	-4.43863	-1.46054
H	-1.68870	1.23753	-0.50746
H	-2.73672	2.47625	1.29064
H	-3.05374	0.75779	1.57082
H	-4.33054	1.81204	0.94104
H	-2.76859	3.42273	-1.06484
H	-4.24556	2.57197	-1.54822
H	-2.75300	2.34930	-2.47047
H	5.61444	-0.24175	0.83420
H	5.32356	1.90147	2.02794
H	3.33188	3.29630	1.58506
H	3.15499	-1.64876	-1.59741
H	4.36481	-3.50967	-0.57236
H	3.44310	-2.65289	0.66912
H	5.20059	-2.42899	0.54838
H	5.37154	-2.23693	-2.54113
H	6.17002	-1.07613	-1.47034
H	5.07956	-0.49970	-2.73664
H	0.58785	2.35331	-0.77630
H	0.81191	4.80959	-0.99219
H	2.20845	4.01699	-1.73474
H	2.36468	4.77224	-0.14473
H	-0.36382	3.80577	0.97704
H	1.12465	3.71233	1.92028
H	0.14616	2.25853	1.67111
H	-1.97225	-1.79262	1.07532
H	1.54188	0.16351	1.98759
H	-2.43576	-2.25314	3.48797
H	1.25339	-0.21002	4.40383
N	-1.13684	-0.44039	-2.17665
N	1.66673	0.31286	-1.50468
N	-0.20609	-0.76987	1.41193
O	-0.94646	-1.52948	5.43812
O	1.23522	-2.61499	-0.39867
O	-0.05583	-2.84721	-0.66327
Cu	0.33747	-1.03844	-1.04005

50. L^1CuXO_2 η^2 triplet, X = 4-methoxypyridine

C	0.57565	-0.89766	6.44693
H	0.17769	-1.10907	7.43968
H	0.81292	0.16982	6.36897
H	1.48570	-1.48717	6.28658
C	1.55730	0.87640	-2.65169
C	-2.40771	-3.12804	-4.75998
C	-1.99562	-4.53312	-2.70790
C	-3.01796	1.29327	-0.74551
C	-3.37395	1.52501	0.73439
C	-3.62385	2.41272	-1.61659
C	2.65182	0.80516	-0.52203
C	3.74594	-0.06070	-0.25942
C	4.71943	0.34347	0.66335
C	4.63262	1.56281	1.32721
C	3.55168	2.40230	1.07284

C	2.75894	1.62772	-3.20644
C	2.55198	2.05070	0.15913
C	3.89669	-1.41393	-0.95070
C	3.97079	-2.56926	0.06640
C	5.12529	-1.44415	-1.88197
C	1.37593	3.00635	-0.05417
C	1.83327	4.39971	-0.52910
C	0.51504	3.13769	1.21854
C	-1.09003	-1.34257	1.98137
C	1.02576	-0.48826	2.25994
C	-1.26694	-1.48824	3.34587
C	-2.54133	-0.90272	-2.00278
C	0.94815	-0.60113	3.64557
C	-0.22787	-1.10875	4.20882
C	-1.82055	0.48903	-4.42649
C	-0.83327	0.21456	-3.29844
C	0.46026	0.74551	-3.51948
C	-2.95361	-2.17890	-2.46734
C	-4.26509	-2.59309	-2.19963
C	-5.15079	-1.79413	-1.48395
C	-4.73051	-0.55306	-1.01360
C	-3.43256	-0.08789	-1.25259
C	-2.02744	-3.09668	-3.26499
H	-1.93182	1.56963	-4.56593
H	-2.80447	0.06065	-4.24055
H	-1.43342	0.08543	-5.36780
H	0.59517	1.19607	-4.49626
H	2.58113	1.95626	-4.23169
H	3.64745	0.98791	-3.19586
H	2.99993	2.50436	-2.59947
H	-4.59586	-3.56317	-2.55975
H	-6.16387	-2.13735	-1.29197
H	-5.42446	0.06912	-0.45490
H	-1.01594	-2.69029	-3.18297
H	-1.70904	-3.76094	-5.31927
H	-2.39231	-2.13216	-5.20983
H	-3.41398	-3.54002	-4.89905
H	-1.23225	-5.12025	-3.23090
H	-2.95345	-5.04645	-2.85078
H	-1.75734	-4.53922	-1.64245
H	-1.92966	1.36001	-0.83413
H	-2.97648	2.48941	1.07023
H	-2.95145	0.74759	1.37714
H	-4.45689	1.54484	0.90052
H	-3.27739	3.39673	-1.27961
H	-4.71859	2.40495	-1.55894
H	-3.34651	2.29918	-2.66828
H	5.56393	-0.31151	0.86173
H	5.40149	1.85777	2.03651
H	3.48094	3.35237	1.59669
H	3.00472	-1.57225	-1.56297
H	4.01473	-3.53207	-0.45385
H	3.09065	-2.58390	0.71420
H	4.86315	-2.49364	0.69863
H	5.18462	-2.40401	-2.40724
H	6.05638	-1.31684	-1.31723
H	5.08639	-0.65078	-2.63515
H	0.73787	2.58365	-0.83379
H	0.96542	5.03549	-0.73734
H	2.43247	4.34297	-1.44299
H	2.43753	4.90798	0.23078
H	-0.33401	3.80782	1.03971
H	1.09364	3.55294	2.05206
H	0.11854	2.16864	1.53410

H	-1.87200	-1.64275	1.29180
H	1.92545	-0.09671	1.80096
H	-2.18696	-1.89047	3.75435
H	1.79355	-0.29411	4.24817
N	-1.20199	-0.44499	-2.20872
N	1.60475	0.39941	-1.40289
N	0.03527	-0.84172	1.42424
O	-0.45257	-1.26900	5.53023
O	0.81723	-3.28925	-0.39675
O	-0.35064	-2.82036	-0.57973
Cu	0.14701	-0.83175	-0.76745

51. L^1CuX, X = N,N-dimethyl-4-pyridinamine

C	3.09007	-5.14015	-3.06064
C	1.64161	-4.33681	-4.90576
C	-2.81521	3.70598	0.17654
C	1.95063	0.72533	2.28411
C	1.73980	-0.41232	3.10895
C	2.85036	-1.10133	3.60850
C	4.14953	-0.69454	3.31650
C	4.34865	0.42001	2.50614
C	3.27241	1.14375	1.98022
C	0.33273	-0.92312	3.41254
C	0.08675	-1.13667	4.91667
C	0.02976	-2.21206	2.62179
C	3.53614	2.33073	1.05646
C	4.10605	1.85988	-0.29702
C	4.45316	3.38787	1.69755
C	-1.96840	1.75198	-1.69222
C	-3.00653	0.79112	-1.80766
C	-3.58546	0.56847	-3.06232
C	-3.16752	1.26809	-4.19114
C	-2.14970	2.21115	-4.07074
C	-1.53829	2.47240	-2.83964
C	-3.46821	-0.02861	-0.60453
C	-3.01919	-1.49885	-0.72772
C	-4.98866	0.05911	-0.37872
C	-0.39015	3.47691	-2.76117
C	-0.72276	4.82094	-3.43355
C	0.90487	2.87997	-3.34832
C	1.96435	-1.64302	-0.86217
C	0.51403	-1.03004	-2.52949
C	2.41849	-2.73180	-1.58539
C	0.91019	-2.08734	-3.32959
C	1.89666	-2.99614	-2.87487
C	0.64142	2.86601	3.59626
C	0.18377	2.36694	2.23377
C	-0.93745	3.01887	1.66972
C	-1.61487	2.81127	0.44597
H	3.56850	-5.70957	-3.86024
H	2.47038	-5.82898	-2.46691
H	3.88021	-4.75320	-2.41673
H	1.65583	-3.46038	-5.56053
H	2.17433	-5.13991	-5.41758
H	0.59656	-4.65069	-4.76777
H	0.04269	3.71430	3.93276
H	1.69250	3.17213	3.56621
H	0.56941	2.07149	4.34707
H	-1.35130	3.81083	2.28241
H	-2.96126	4.43278	0.97755
H	-3.72874	3.10880	0.07972
H	-2.69571	4.24663	-0.76779
H	2.69476	-1.97578	4.23573
H	4.99901	-1.24200	3.71644
H	5.36324	0.73378	2.27335
H	-0.37307	-0.16377	3.06722
H	-0.95708	-1.41854	5.09580
H	0.29358	-0.22675	5.48944
H	0.71472	-1.93584	5.32648
H	-0.99167	-2.55919	2.81783
H	0.71807	-3.01950	2.89940
H	0.12546	-2.04190	1.54474
H	2.57381	2.80787	0.85211
H	4.25776	2.70990	-0.97275
H	3.42236	1.15857	-0.78610
H	5.07183	1.35656	-0.16896

H	4.56024	4.25409	1.03472
H	5.45863	2.99572	1.88741
H	4.05028	3.74116	2.65247
H	-4.37762	-0.17030	-3.15757
H	-3.63074	1.08070	-5.15632
H	-1.82058	2.75409	-4.95324
H	-2.97758	0.38464	0.28096
H	-3.32647	-2.07518	0.15302
H	-1.93040	-1.57043	-0.81465
H	-3.46032	-1.97653	-1.61071
H	-5.27071	-0.47188	0.53758
H	-5.55152	-0.39172	-1.20402
H	-5.31990	1.09825	-0.28222
H	-0.19914	3.67665	-1.70371
H	0.08827	5.53899	-3.26739
H	-1.64423	5.25412	-3.03080
H	-0.85005	4.71972	-4.51728
H	1.73608	3.58945	-3.26052
H	0.78183	2.63589	-4.41046
H	1.18853	1.96361	-2.82113
H	2.37077	-1.44099	0.12377
H	-0.25202	-0.34485	-2.87828
H	3.17658	-3.35926	-1.13545
H	0.43481	-2.20453	-4.29441
N	2.31587	-4.05383	-3.64566
N	1.01541	-0.78497	-1.29880
N	0.84184	1.36278	1.65943
N	-1.27186	1.89964	-0.46081
Cu	0.28027	0.70194	-0.12595

52. L^1CuXO_2 η^1 singlet, X = N,N-dimethyl-4-pyridinamine

C	4.45279	-4.63257	-3.92538
C	3.31441	-3.46305	-5.82993
H	2.34134	-3.87656	-6.13125
H	3.35350	-2.41395	-6.14267
H	4.09573	-3.99871	-6.37048
H	5.05741	-4.98826	-4.76059
H	3.91307	-5.49032	-3.49947
H	5.13597	-4.24409	-3.16253
C	-2.83494	2.73593	-0.23787
C	0.44657	-2.98542	3.78488
C	3.25891	1.26467	0.30248
C	4.23600	0.81887	-0.80022
C	3.61736	2.68127	0.79698
C	-1.77509	0.87149	-2.09721
C	-2.69883	-0.13779	-2.47305
C	-3.10146	-0.21394	-3.81114
C	-2.60931	0.66628	-4.77003
C	-1.69548	1.64802	-4.39443
C	-1.26435	1.77554	-3.06921
C	1.93779	-0.08997	2.04468
C	-3.26313	-1.13170	-1.45898
C	-2.88156	-2.58421	-1.80562
C	-4.79015	-0.98771	-1.30919
C	-0.22993	2.84776	-2.71930
C	-0.66549	4.25588	-3.16970
C	1.15678	2.50791	-3.30286
C	2.02861	-2.42280	-1.25349
C	0.98880	-1.34114	-2.98865
C	2.85225	-3.12582	-2.11253
C	1.76160	-2.00017	-3.92913
C	1.89512	-0.99703	3.13602
C	2.74841	-2.92619	-3.51041

C	0.55091	2.14371	3.23044
C	0.08922	1.46460	1.94739
C	-1.06266	2.04507	1.36110
C	-1.66903	1.82459	0.11018
C	3.10779	-1.48339	3.64147
C	4.33220	-1.10751	3.09972
C	4.36274	-0.23078	2.01922
C	3.18380	0.28180	1.46846
C	0.59243	-1.45060	3.79332
C	0.47696	-0.92449	5.23940
H	0.58524	3.22779	3.08584
H	1.53270	1.80076	3.55556
H	-0.16507	1.94839	4.03581
H	-1.50448	2.84456	1.94558
H	-3.23143	3.21889	0.65715
H	-3.63780	2.17304	-0.72077
H	-2.52819	3.52013	-0.93715
H	3.08774	-2.17230	4.48163
H	5.25773	-1.49603	3.51646
H	5.31970	0.06434	1.59771
H	-0.23589	-1.04490	3.20751
H	-0.49089	-1.20571	5.67020
H	0.56760	0.16365	5.29475
H	1.25794	-1.35317	5.87822
H	-0.52624	-3.26892	4.20326
H	1.21658	-3.46411	4.40236
H	0.50998	-3.38862	2.77216
H	2.26173	1.31489	-0.14449
H	4.16586	1.49621	-1.65885
H	4.01270	-0.19406	-1.14926
H	5.27813	0.83549	-0.46078
H	3.63094	3.39280	-0.03709
H	4.60876	2.69332	1.26536
H	2.89671	3.04299	1.53659
H	-3.81318	-0.98048	-4.10631
H	-2.93417	0.58804	-5.80418
H	-1.30638	2.32913	-5.14719
H	-2.81576	-0.90417	-0.48822
H	-3.27623	-3.27216	-1.04964
H	-1.79616	-2.71459	-1.83341
H	-3.29027	-2.88661	-2.77717
H	-5.16350	-1.66605	-0.53369
H	-5.31253	-1.23173	-2.24148
H	-5.07212	0.03255	-1.02822
H	-0.12027	2.86874	-1.63248
H	0.04506	5.00798	-2.80885
H	-1.65671	4.51698	-2.78562
H	-0.70357	4.34079	-4.26140
H	1.88833	3.27725	-3.02900
H	1.12456	2.45381	-4.39748
H	1.52413	1.54748	-2.92941
H	2.09474	-2.59424	-0.18388
H	0.22882	-0.63527	-3.30815
H	3.55887	-3.82812	-1.69041
H	1.58375	-1.79697	-4.97700
N	1.10641	-1.52874	-1.65998
N	0.74479	0.42564	1.44796
N	-1.27204	0.90042	-0.76506
N	3.55410	-3.58943	-4.39963
O	-0.02940	-3.29916	0.53536
O	-0.51975	-2.14635	0.79457
Cu	0.01007	-0.51857	-0.17595

53. L^1CuXO_2 η^1 triplet, X = N,N-dimethyl-4-pyridinamine

C	4.27374	-5.06620	-3.73771
C	2.69579	-4.41562	-5.57596
H	1.71313	-4.90534	-5.52006
H	2.58679	-3.48936	-6.14930
H	3.37106	-5.06777	-6.13109
H	4.72190	-5.61467	-4.56706
H	3.85724	-5.79509	-3.02769
H	5.07598	-4.51675	-3.23462
C	-2.93215	2.59751	-0.20976
C	0.87104	-3.27879	3.27119
C	3.22677	1.81819	0.67898
C	4.12902	1.49638	-0.52819
C	3.64034	3.15288	1.32900
C	-1.76031	0.89982	-2.12634
C	-2.71893	-0.06827	-2.52628
C	-3.15494	-0.07727	-3.85706
C	-2.65929	0.82551	-4.79259
C	-1.70092	1.75608	-4.39994
C	-1.23744	1.81502	-3.08150
C	1.99673	0.05330	2.09271
C	-3.27614	-1.10093	-1.54771
C	-3.01722	-2.54234	-2.02972
C	-4.77919	-0.89246	-1.27743
C	-0.15370	2.82881	-2.71307
C	-0.54766	4.27508	-3.06581
C	1.19373	2.46213	-3.36763
C	2.39312	-2.20327	-1.25308
C	0.95609	-1.59493	-2.93733
C	3.05320	-3.10390	-2.06938
C	1.54972	-2.47184	-3.82817
C	2.02322	-1.02355	3.01774
C	2.64156	-3.27200	-3.41364
C	0.33310	2.02341	3.36305
C	-0.00907	1.39450	2.01617
C	-1.18271	1.90668	1.41376
C	-1.72844	1.72777	0.12484
C	3.25518	-1.41797	3.55379
C	4.44361	-0.79356	3.18904
C	4.41142	0.24337	2.26124
C	3.20830	0.67968	1.69682
C	0.75263	-1.75268	3.45049
C	0.37133	-1.42256	4.90773
H	0.51568	3.09681	3.24106
H	1.21382	1.57623	3.82293
H	-0.51210	1.91927	4.05159
H	-1.71305	2.62614	2.02858
H	-3.32263	3.09245	0.68133
H	-3.73299	2.00712	-0.66324
H	-2.66209	3.37013	-0.93788
H	3.28227	-2.23206	4.27361
H	5.38731	-1.11475	3.62214
H	5.34023	0.72768	1.96990
H	-0.05935	-1.40672	2.80574
H	-0.56275	-1.92493	5.18481
H	0.23224	-0.34825	5.05651
H	1.14875	-1.75738	5.60445
H	-0.08724	-3.76263	3.49142
H	1.61768	-3.70993	3.94791
H	1.15192	-3.54401	2.24841
H	2.20793	1.93647	0.30096
H	4.07932	2.30193	-1.26981
H	3.81837	0.56863	-1.01910
H	5.17873	1.38454	-0.23334

H	3.59405	3.97002	0.59972
H	4.66578	3.10883	1.71417
H	2.98294	3.40877	2.16598
H	-3.89793	-0.80860	-4.16530
H	-3.01346	0.80190	-5.81986
H	-1.30230	2.45208	-5.13406
H	-2.74778	-0.97033	-0.59997
H	-3.34375	-3.26464	-1.27316
H	-1.95418	-2.71660	-2.22028
H	-3.56412	-2.76243	-2.95379
H	-5.14344	-1.62311	-0.54597
H	-5.37050	-1.01494	-2.19232
H	-4.98413	0.10717	-0.88180
H	-0.01010	2.78180	-1.63091
H	0.21598	4.97601	-2.71016
H	-1.50120	4.55628	-2.60734
H	-0.64605	4.42042	-4.14756
H	1.97476	3.17269	-3.07207
H	1.12213	2.48078	-4.46153
H	1.51925	1.46106	-3.06904
H	2.70158	-2.08124	-0.21908
H	0.11551	-0.98537	-3.25315
H	3.86748	-3.68017	-1.64947
H	1.14840	-2.53657	-4.83106
N	1.35008	-1.44631	-1.65467
N	0.77469	0.46463	1.48082
N	-1.24338	0.89856	-0.79909
N	3.26482	-4.15183	-4.26013
O	-0.43425	-3.32151	0.15550
O	-0.75148	-2.17728	0.50926
Cu	0.29366	-0.32202	-0.29278

54. L^1CuXO_2 η^2 singlet, X = N,N-dimethyl-4-pyridinamine

C	-2.01046	-2.57505	5.06417
C	-0.13055	-1.07649	5.70562
H	0.95807	-1.12907	5.61729
H	-0.43128	-0.02001	5.64962
H	-0.39629	-1.45742	6.69284
H	-1.98142	-2.79817	6.13158
H	-2.10165	-3.52818	4.53579
H	-2.91089	-1.97747	4.85550
C	1.52830	0.89204	-3.33528
C	-2.82805	-2.78645	-5.45567
C	-2.10503	-4.38516	-3.64612
C	-2.70318	1.06599	-0.77508
C	-3.05900	1.14617	0.72029
C	-3.17759	2.34500	-1.49438
C	2.73793	0.72685	-1.27677
C	3.92239	-0.04136	-1.15918
C	4.92112	0.40324	-0.28435
C	4.77783	1.57414	0.45237
C	3.61323	2.32655	0.32623
C	2.69739	1.65655	-3.93598
C	2.57637	1.92660	-0.52356
C	4.15140	-1.31853	-1.96298
C	4.35162	-2.54150	-1.04687
C	5.34366	-1.17555	-2.93149
C	1.32598	2.80737	-0.62933
C	1.63639	4.16531	-1.29400
C	0.65207	3.04866	0.73651
C	-0.97195	-1.96191	0.99952
C	0.82764	-0.68762	1.59010
C	-1.29402	-2.21872	2.32265

C	-2.47334	-0.90342	-2.41775
C	0.59273	-0.88127	2.94282
C	-0.50062	-1.67487	3.35982
C	-2.02532	0.73650	-4.72449
C	-0.91091	0.33421	-3.76711
C	0.36132	0.84725	-4.10621
C	-2.98861	-2.07954	-3.02438
C	-4.28759	-2.48423	-2.68907
C	-5.06023	-1.77544	-1.77599
C	-4.53348	-0.64262	-1.16434
C	-3.24225	-0.19162	-1.45788
C	-2.20602	-2.90109	-4.04769
H	-2.05847	1.82628	-4.81902
H	-3.00490	0.38046	-4.40916
H	-1.81257	0.33628	-5.72131
H	0.40358	1.37813	-5.04978
H	2.40714	2.15517	-4.86221
H	3.51307	0.96106	-4.16106
H	3.10054	2.39994	-3.24626
H	-4.70108	-3.37212	-3.15877
H	-6.06822	-2.10574	-1.53933
H	-5.13813	-0.09626	-0.44654
H	-1.18870	-2.50523	-4.08571
H	-2.22413	-3.33722	-6.18557
H	-2.90083	-1.74920	-5.79321
H	-3.83865	-3.21082	-5.47607
H	-1.47778	-4.92374	-4.36523
H	-3.08691	-4.87260	-3.63898
H	-1.65429	-4.49439	-2.65823
H	-1.61215	1.02930	-0.84975
H	-2.53352	1.98922	1.18233
H	-2.77189	0.23610	1.25307
H	-4.13096	1.30959	0.88040
H	-2.75784	3.23714	-1.01502
H	-4.27021	2.42853	-1.46029
H	-2.87627	2.35616	-2.54472
H	5.83502	-0.17690	-0.18971
H	5.57217	1.90298	1.11704
H	3.50762	3.24553	0.89712
H	3.25605	-1.50226	-2.56173
H	4.48412	-3.44584	-1.65110
H	3.48242	-2.69656	-0.40414
H	5.24150	-2.42991	-0.41596
H	5.43684	-2.07423	-3.55146
H	6.28892	-1.04832	-2.39133
H	5.22923	-0.31593	-3.59991
H	0.60329	2.28640	-1.26185
H	0.72172	4.76173	-1.38785
H	2.05937	4.04873	-2.29530
H	2.35043	4.74482	-0.69752
H	-0.25309	3.65276	0.60626
H	1.30980	3.59164	1.42500
H	0.36223	2.11136	1.21768
H	-1.57523	-2.38755	0.20485
H	1.67932	-0.09557	1.27273
H	-2.16555	-2.82456	2.53412
H	1.26018	-0.41209	3.65390
N	-1.15281	-0.43620	-2.71704
N	1.67630	0.31008	-2.13843
N	0.06513	-1.19830	0.60722
N	-0.77694	-1.89948	4.68981
O	1.35113	-2.87946	-1.65959
O	0.02527	-2.98958	-1.68692
Cu	0.42371	-1.13366	-1.67273

55. L^1CuXO_2 η^2 triplet, X = N,N-dimethyl-4-pyridinamine

C	-1.46301	-2.04332	5.45548
C	0.84370	-1.07678	5.74654
H	1.80377	-1.55258	5.51505
H	0.97488	0.01157	5.67007
H	0.59601	-1.31619	6.78103
H	-1.35458	-2.09621	6.53914
H	-1.71398	-3.04789	5.09479
H	-2.30608	-1.37674	5.22840
C	1.45768	1.02190	-3.24704
C	-2.43304	-2.81012	-5.76186
C	-1.73930	-4.38134	-3.91741
C	-3.11188	0.93321	-1.05891
C	-3.61575	0.98416	0.39490
C	-3.61812	2.16700	-1.83413
C	2.67390	0.71007	-1.20739
C	3.76480	-0.19141	-1.11856
C	4.80557	0.09551	-0.22654
C	4.78950	1.23574	0.57062
C	3.71214	2.11326	0.48387
C	2.63966	1.80815	-3.79659
C	2.64478	1.87502	-0.38995
C	3.83893	-1.45748	-1.96758
C	3.94998	-2.72243	-1.09530
C	5.00402	-1.39952	-2.97622
C	1.47877	2.86605	-0.42544
C	1.92913	4.27864	-0.84861
C	0.74184	2.92724	0.92813
C	-0.98818	-1.61239	1.26839
C	1.10270	-0.71613	1.53782
C	-1.14274	-1.80129	2.63045
C	-2.55580	-0.97673	-2.68586
C	1.04777	-0.86792	2.91262
C	-0.10767	-1.41617	3.51695
C	-1.97666	0.72987	-4.94214
C	-0.95065	0.38866	-3.86689
C	0.31786	0.98254	-4.06888
C	-2.90001	-2.18414	-3.34631
C	-4.17227	-2.72674	-3.12179
C	-5.08187	-2.12173	-2.26126
C	-4.72427	-0.95255	-1.59568
C	-3.46932	-0.36557	-1.78324
C	-1.94705	-2.90219	-4.30086
H	-2.05016	1.81704	-5.04899
H	-2.96666	0.33088	-4.72428
H	-1.64972	0.33728	-5.91066
H	0.40324	1.54228	-4.99335
H	2.36693	2.34956	-4.70397
H	3.46315	1.12685	-4.03832
H	3.02973	2.52128	-3.06740
H	-4.45218	-3.64432	-3.63192
H	-6.06435	-2.55981	-2.10643
H	-5.43652	-0.48583	-0.92104
H	-0.97519	-2.40493	-4.23505
H	-1.70694	-3.27733	-6.43691
H	-2.57706	-1.77569	-6.08436
H	-3.38813	-3.33243	-5.89034
H	-0.98447	-4.83571	-4.56951
H	-2.66200	-4.96154	-4.03443
H	-1.40269	-4.47984	-2.88440
H	-2.01930	0.99614	-1.02878
H	-3.21583	1.87193	0.89770

H	-3.29908	0.10568	0.96492
H	-4.70832	1.04653	0.45305
H	-3.32740	3.09230	-1.32263
H	-4.71152	2.15506	-1.91304
H	-3.21067	2.20145	-2.84799
H	5.64830	-0.58779	-0.16022
H	5.61107	1.44095	1.25202
H	3.69812	3.00300	1.10886
H	2.90598	-1.52994	-2.53379
H	3.94634	-3.61935	-1.72410
H	3.10881	-2.80016	-0.40233
H	4.87910	-2.72973	-0.51322
H	4.99980	-2.28841	-3.61735
H	5.97313	-1.36473	-2.46466
H	4.94169	-0.51792	-3.62243
H	0.76099	2.51038	-1.16849
H	1.06626	4.95091	-0.91640
H	2.42490	4.27348	-1.82405
H	2.62794	4.71226	-0.12421
H	-0.10778	3.61776	0.87060
H	1.40101	3.28164	1.72934
H	0.35932	1.94469	1.21966
H	-1.77749	-1.91619	0.58813
H	1.98552	-0.28863	1.07856
H	-2.06285	-2.24231	2.99185
H	1.89886	-0.54948	3.50027
N	-1.26225	-0.39135	-2.84071
N	1.56424	0.42032	-2.05834
N	0.10457	-1.06269	0.70020
N	-0.21620	-1.56669	4.87376
O	0.77933	-3.36030	-1.47335
O	-0.38753	-2.85815	-1.44669
Cu	0.11091	-0.84291	-1.43415

56. L^1CuX, X = 4-oxypyridine

C	-2.82084	2.31938	-0.36204
C	1.92884	-0.55864	1.85587
C	1.68456	-1.61412	2.77509
C	2.77333	-2.26867	3.35901
C	4.08482	-1.90747	3.05866
C	4.31647	-0.88194	2.14648
C	3.26149	-0.19789	1.53265
C	0.26205	-2.08765	3.06815
C	-0.02749	-2.24430	4.57142
C	-0.04121	-3.39620	2.30985
C	3.55925	0.88779	0.50091
C	4.19769	0.29143	-0.76888
C	4.43313	2.01792	1.07605
C	-1.96307	0.32322	-2.14719
C	-3.00574	-0.63424	-2.23658
C	-3.61569	-0.85859	-3.47561
C	-3.22305	-0.16431	-4.61604
C	-2.19372	0.76954	-4.52395
C	-1.55231	1.03100	-3.30926
C	-3.43138	-1.45452	-1.02161
C	-2.98480	-2.92328	-1.16400
C	-4.94359	-1.36234	-0.74728
C	-0.38300	2.01254	-3.26166
C	-0.70146	3.36132	-3.93166
C	0.88482	1.38061	-3.87133
C	2.06354	-3.04911	-1.18863
C	0.60922	-2.56413	-2.91070
C	2.61772	-4.09578	-1.88130
C	1.09828	-3.58749	-3.68246
C	2.16874	-4.45690	-3.21772
C	0.65985	1.64162	3.06439
C	0.19504	1.08517	1.72387
C	-0.92902	1.71785	1.14603
C	-1.60868	1.44549	-0.06271
H	0.07946	2.52087	3.35248
H	1.71902	1.91729	3.02843
H	0.56293	0.88915	3.85473
H	-1.34315	2.53304	1.72827
H	-2.97494	3.06850	0.41766
H	-3.72800	1.71007	-0.44297
H	-2.70739	2.83267	-1.32231
H	2.59181	-3.08431	4.05500
H	4.91803	-2.43033	3.52145
H	5.33983	-0.61123	1.89649
H	-0.42281	-1.32948	2.67997
H	-1.08170	-2.50095	4.73007
H	0.18095	-1.31971	5.12115
H	0.57192	-3.04210	5.02525
H	-1.07899	-3.71098	2.47603
H	0.61537	-4.20776	2.64608
H	0.10728	-3.26772	1.23377
H	2.60143	1.32559	0.20670
H	4.36426	1.07283	-1.52068
H	3.55330	-0.47368	-1.21045
H	5.16704	-0.17138	-0.54820
H	4.57762	2.80936	0.33075
H	5.42637	1.65507	1.36599
H	3.97417	2.46959	1.96235
H	-4.40758	-1.60034	-3.55050
H	-3.70586	-0.35745	-5.57086
H	-1.87406	1.29907	-5.41839
H	-2.91202	-1.04136	-0.15242
H	-3.24954	-3.49888	-0.26835

H	-1.90237	-2.99072	-1.30515
H	-3.46682	-3.40179	-2.02486
H	-5.20003	-1.90212	0.17220
H	-5.53320	-1.80333	-1.55960
H	-5.26799	-0.32237	-0.63039
H	-0.16507	2.21237	-2.20965
H	0.13285	4.05974	-3.79541
H	-1.59951	3.82164	-3.50465
H	-0.86388	3.25699	-5.01077
H	1.73773	2.06629	-3.79168
H	0.73808	1.14675	-4.93255
H	1.14521	0.45161	-3.35594
H	2.42274	-2.80088	-0.19204
H	-0.19384	-1.93214	-3.28449
H	3.41719	-4.68064	-1.43342
H	0.68412	-3.76779	-4.67137
O	2.64522	-5.40028	-3.88539
N	1.05753	-2.25160	-1.65767
N	0.84297	0.06007	1.18248
N	-1.25718	0.50097	-0.92736
Cu	0.30435	-0.75312	-0.59929

57. L^1CuXO_2 η^1 singlet, X = 4-oxypyridine

C	-2.84772	2.06069	-0.32957
C	1.96829	-0.72006	1.89736
C	1.91928	-1.58942	3.01862
C	3.12364	-2.08662	3.53084
C	4.35126	-1.76001	2.96353
C	4.38807	-0.92642	1.84995
C	3.21490	-0.40424	1.29475
C	0.60763	-1.99580	3.68852
C	0.49661	-1.42067	5.11561
C	0.42922	-3.52558	3.72342
C	3.30169	0.51264	0.07645
C	4.11718	-0.10668	-1.07363
C	3.85809	1.89803	0.46240
C	-1.79848	0.24749	-2.20317
C	-2.75813	-0.73643	-2.55691
C	-3.22561	-0.77907	-3.87459
C	-2.76384	0.10974	-4.84037
C	-1.80925	1.06080	-4.49130
C	-1.31170	1.15182	-3.18678
C	-3.27394	-1.75601	-1.54347
C	-2.91371	-3.19612	-1.95705
C	-4.79065	-1.61652	-1.30922
C	-0.22770	2.18400	-2.87034
C	-0.64928	3.61782	-3.24514
C	1.10639	1.82584	-3.55543
C	1.76354	-3.37039	-1.36274
C	0.91522	-2.05805	-3.06760
C	2.48184	-4.14060	-2.24278
C	1.59311	-2.76929	-4.02313
C	2.46468	-3.88130	-3.67556
C	0.67421	1.59337	3.01954
C	0.15033	0.85555	1.79018
C	-1.01863	1.42277	1.22774
C	-1.64622	1.17896	-0.00949
H	0.85316	2.64513	2.77091
H	1.59997	1.16422	3.40160
H	-0.07413	1.57494	3.81934
H	-1.45056	2.22978	1.81054
H	-3.13916	2.65943	0.53620
H	-3.70191	1.44825	-0.63608

H	-2.63543	2.73889	-1.16129
H	3.09533	-2.74973	4.39195
H	5.27221	-2.16044	3.38053
H	5.34478	-0.67880	1.39754
H	-0.20897	-1.59278	3.08499
H	-0.47509	-1.67506	5.55594
H	0.59939	-0.33186	5.13210
H	1.27312	-1.83590	5.76966
H	-0.54661	-3.77741	4.15746
H	1.19514	-4.00596	4.34469
H	0.47107	-3.95151	2.71831
H	2.28288	0.66037	-0.29133
H	4.07720	0.54262	-1.95599
H	3.72298	-1.08568	-1.35810
H	5.17380	-0.22899	-0.80680
H	3.87281	2.56657	-0.40698
H	4.88456	1.82093	0.84186
H	3.25072	2.37045	1.24199
H	-3.95909	-1.53300	-4.15054
H	-3.13503	0.05406	-5.86074
H	-1.43290	1.74127	-5.25174
H	-2.77189	-1.56158	-0.59273
H	-3.25593	-3.90759	-1.19693
H	-1.83265	-3.31684	-2.05862
H	-3.38325	-3.46937	-2.91034
H	-5.12392	-2.32025	-0.53717
H	-5.36284	-1.83154	-2.22004
H	-5.05843	-0.60552	-0.98170
H	-0.05075	2.16300	-1.79241
H	0.11704	4.33580	-2.92976
H	-1.59305	3.90316	-2.76862
H	-0.77899	3.73242	-4.32756
H	1.88256	2.55501	-3.29223
H	1.00454	1.82668	-4.64720
H	1.45551	0.83460	-3.25493
H	1.78001	-3.59631	-0.29767
H	0.26156	-1.23830	-3.35008
H	3.08395	-4.96832	-1.87749
H	1.48618	-2.50909	-5.07284
O	3.11318	-4.54897	-4.50927
N	0.99857	-2.30637	-1.72686
N	0.77716	-0.20487	1.30524
N	-1.25288	0.26211	-0.88978
O	-0.31530	-3.96714	0.57833
O	-0.68690	-2.75147	0.71676
Cu	0.07770	-1.22462	-0.32254

58. L^1CuXO_2 η^1 triplet, X = 4-oxypyridine

C	-2.83710	2.06762	-0.24010
C	1.99585	-0.75751	1.93629
C	1.77887	-1.64660	3.02525
C	2.88770	-2.23597	3.64504
C	4.18414	-1.99554	3.20557
C	4.38701	-1.15768	2.11225
C	3.31781	-0.53661	1.46009
C	0.38135	-1.99306	3.54150
C	0.11179	-1.38518	4.93348
C	0.14562	-3.51636	3.59651
C	3.57589	0.39135	0.27523
C	4.67838	-0.11260	-0.67167
C	3.88598	1.82526	0.75001
C	-1.90961	0.24011	-2.15371
C	-2.89526	-0.75316	-2.38360

C	-3.49675	-0.83360	-3.64431
C	-3.13494	0.02310	-4.67894
C	-2.14862	0.98020	-4.45570
C	-1.52571	1.11072	-3.20972
C	-3.30272	-1.74114	-1.29404
C	-3.05800	-3.19834	-1.73290
C	-4.76766	-1.55104	-0.85616
C	-0.42210	2.15314	-3.02501
C	-0.86391	3.56391	-3.45726
C	0.86809	1.74194	-3.76146
C	2.29950	-2.92254	-1.58069
C	0.92351	-2.11729	-3.25037
C	2.93956	-3.77400	-2.44456
C	1.50230	-2.93181	-4.19011
C	2.58855	-3.84060	-3.85591
C	0.73395	1.57622	3.03883
C	0.24463	0.88117	1.76781
C	-0.91910	1.45947	1.21334
C	-1.60405	1.20330	0.00519
H	1.03112	2.60386	2.80072
H	1.58578	1.07115	3.49373
H	-0.07119	1.64024	3.77808
H	-1.34114	2.26044	1.81154
H	-3.08598	2.66051	0.64255
H	-3.70147	1.45044	-0.50232
H	-2.67832	2.75153	-1.08009
H	2.72697	-2.90673	4.48557
H	5.02932	-2.46672	3.70110
H	5.39821	-0.98528	1.75526
H	-0.34479	-1.57330	2.84027
H	-0.91080	-1.61010	5.26027
H	0.23676	-0.29963	4.93960
H	0.79695	-1.80215	5.68166
H	-0.89457	-3.72805	3.87239
H	0.78575	-3.99669	4.34602
H	0.34187	-3.98942	2.63292
H	2.64713	0.43236	-0.30387
H	4.72712	0.52851	-1.55873
H	4.47965	-1.13288	-1.01052
H	5.67033	-0.09097	-0.20348
H	4.02853	2.49543	-0.10651
H	4.80332	1.84680	1.35154
H	3.07454	2.22896	1.36229
H	-4.25855	-1.58982	-3.81942
H	-3.60883	-0.06040	-5.65384
H	-1.85143	1.63839	-5.26892
H	-2.66699	-1.54905	-0.42648
H	-3.26637	-3.88904	-0.90745
H	-2.02111	-3.34871	-2.04360
H	-3.70566	-3.47872	-2.57244
H	-5.02048	-2.24728	-0.04727
H	-5.46153	-1.74004	-1.68394
H	-4.95404	-0.53472	-0.49346
H	-0.18238	2.19479	-1.95982
H	-0.07978	4.29571	-3.22957
H	-1.77760	3.87883	-2.94170
H	-1.05788	3.61796	-4.53487
H	1.66159	2.47996	-3.59020
H	0.70260	1.67252	-4.84317
H	1.22857	0.76963	-3.41579
H	2.58108	-2.89431	-0.52959
H	0.10586	-1.45601	-3.52519
H	3.73333	-4.42238	-2.08238
H	1.14902	-2.91201	-5.21783

O	3.15154	-4.59133	-4.67906
N	1.29691	-2.06700	-1.93738
N	0.90267	-0.15161	1.25485
N	-1.23566	0.30766	-0.90451
O	-0.21328	-3.90812	0.25234
O	-0.63012	-2.74727	0.37655
Cu	0.40532	-0.94951	-0.55624

59. L^1CuXO_2 η^2 singlet, X = 4-oxypyridine

C	1.45179	0.96551	-2.47066
C	2.59814	1.74304	-3.10511
C	-2.55129	-0.85267	-1.51709
C	-3.06609	-2.05981	-2.06079
C	-4.35627	-2.46611	-1.69544
C	-5.12816	-1.72948	-0.80432
C	-4.59955	-0.57068	-0.24284
C	-3.31689	-0.12038	-0.56996
C	-2.25813	-2.93009	-3.02234
C	-2.90144	-2.98085	-4.42301
C	-2.06965	-4.35654	-2.47097
C	-2.76508	1.14718	0.07752
C	-3.00728	1.19854	1.59675
C	-3.32958	2.41073	-0.60159
C	2.71796	0.88150	-0.42781
C	3.84239	0.04603	-0.19417
C	4.85052	0.49512	0.66648
C	4.77639	1.73544	1.29181
C	3.66551	2.54487	1.07117
C	2.62426	2.14087	0.22989
C	3.97658	-1.33189	-0.83893
C	3.95165	-2.45491	0.21770
C	5.23925	-1.43908	-1.71591
C	1.39442	3.03864	0.08866
C	1.74098	4.43448	-0.46576
C	0.64465	3.16818	1.42927
C	-0.90235	-2.03513	1.60211
C	0.86018	-0.65816	2.22367
C	-1.24682	-2.26273	2.90887
C	0.58955	-0.82969	3.55672
C	-0.51550	-1.66015	4.01563
C	-2.09398	0.69834	-3.89478
C	-0.99963	0.32566	-2.89707
C	0.28708	0.85820	-3.22989
H	-2.14206	1.78564	-4.01784
H	-3.07606	0.33822	-3.58778
H	-1.86026	0.27411	-4.87803
H	0.32960	1.34223	-4.20015
H	2.33076	2.08871	-4.10563
H	3.48671	1.10541	-3.18060
H	2.88715	2.60955	-2.50451
H	-4.75894	-3.38403	-2.11729
H	-6.12716	-2.06409	-0.53510
H	-5.19225	-0.00751	0.47294
H	-1.26065	-2.49449	-3.11763
H	-2.28003	-3.56750	-5.11059
H	-3.02392	-1.98042	-4.85012
H	-3.89277	-3.45024	-4.39185
H	-1.46232	-4.95334	-3.16197
H	-3.02787	-4.87406	-2.33947
H	-1.55117	-4.32823	-1.51041
H	-1.68286	1.13893	-0.08017
H	-2.48697	2.06074	2.02957
H	-2.63466	0.29712	2.09082

H	-4.07098	1.30743	1.84154
H	-2.89786	3.31716	-0.15952
H	-4.41863	2.46497	-0.48091
H	-3.11328	2.42294	-1.67398
H	5.70988	-0.14500	0.85108
H	5.57146	2.06411	1.95647
H	3.59592	3.50428	1.57833
H	3.11631	-1.49021	-1.49339
H	3.98015	-3.43521	-0.27083
H	3.04095	-2.41239	0.82163
H	4.81144	-2.39030	0.89638
H	5.26972	-2.41309	-2.21808
H	6.15703	-1.34341	-1.12298
H	5.26017	-0.66168	-2.48757
H	0.71141	2.56329	-0.61853
H	0.82764	5.02322	-0.61176
H	2.25793	4.37554	-1.42930
H	2.38535	4.99465	0.22178
H	-0.26183	3.77270	1.30313
H	1.26688	3.65679	2.18876
H	0.34995	2.18980	1.81777
H	-1.45757	-2.49432	0.79008
H	1.69052	-0.03447	1.90359
H	-2.09187	-2.90515	3.14144
H	1.20397	-0.33320	4.30297
O	-0.80159	-1.83609	5.22001
N	-1.23919	-0.40952	-1.83840
N	1.65063	0.43604	-1.24973
N	0.13000	-1.22489	1.22275
O	1.02623	-2.53984	-2.11112
O	0.51223	-3.00250	-0.97175
Cu	0.60512	-1.15013	-0.70066

60. L^1CuX, X = 2,3-dihydro-1*H*-imidazol-2-ylidene

C	-4.48065	-5.58834	-0.56003
C	-4.02346	-3.35369	-0.35612
C	-3.13112	-5.45983	-0.48079
C	-1.00915	-0.61301	1.36954
C	0.30562	-1.09296	1.38831
C	1.05016	-1.22248	0.21921
C	0.47290	-0.86804	-0.99742
C	-0.83748	-0.38195	-1.07122
C	-1.80407	-0.54862	2.67131
C	-1.09183	0.27176	3.76149
C	-2.13508	-1.96478	3.18454
C	-1.44414	-0.05585	-2.43463
C	-1.71358	-1.34262	-3.23979
C	-0.58166	0.92568	-3.24873
C	-7.11509	-1.09359	-0.34156
C	-7.74233	-1.66007	0.80072
C	-8.82403	-2.52954	0.61861
C	-9.29592	-2.84854	-0.65274
C	-8.67646	-2.29009	-1.76839
C	-7.59152	-1.41500	-1.64149
C	-7.22813	-1.38184	2.21161
C	-6.57182	-2.63601	2.82291
C	-8.32658	-0.83552	3.14177
C	-6.91391	-0.86540	-2.89564
C	-7.89772	-0.13033	-3.82404
C	-6.17191	-1.97970	-3.66077
C	-2.35981	2.46572	0.35083
C	-3.38592	1.35875	0.16152
C	-4.74094	1.75630	0.10321

C	-5.91402	0.98464	-0.05688
C	-7.23334	1.74085	-0.07322
C	-1.59230	-0.25181	0.12572
H	-1.97130	-3.67412	-0.27677
H	-5.10028	-6.46488	-0.66198
H	-5.97392	-4.05607	-0.50971
H	-2.34945	-6.20236	-0.50080
H	-2.83367	3.44812	0.39033
H	-1.62931	2.46429	-0.46516
H	-1.79278	2.31736	1.27642
H	-4.90686	2.82257	0.19994
H	-7.08031	2.81629	0.03322
H	-7.88668	1.40167	0.73806
H	-7.77481	1.55789	-1.00773
H	0.75403	-1.37553	2.33781
H	2.07024	-1.59574	0.25582
H	1.05206	-0.97334	-1.91165
H	-2.75464	-0.05536	2.45169
H	-1.72636	0.35856	4.65062
H	-0.85813	1.28320	3.41366
H	-0.15126	-0.19497	4.07567
H	-2.73833	-1.91726	4.09861
H	-1.22248	-2.52767	3.41501
H	-2.70173	-2.52834	2.43623
H	-2.41177	0.42075	-2.25755
H	-2.18217	-1.10921	-4.20286
H	-2.38533	-2.01140	-2.69199
H	-0.78321	-1.88639	-3.44368
H	-1.09003	1.19859	-4.18032
H	0.38687	0.49119	-3.52103
H	-0.38542	1.84606	-2.68921
H	-9.30366	-2.96881	1.49005
H	-10.13847	-3.52433	-0.77272
H	-9.04186	-2.54134	-2.76123
H	-6.44937	-0.61877	2.13223
H	-6.17687	-2.41951	3.82228
H	-5.74075	-2.98568	2.20219
H	-7.29276	-3.45675	2.92001
H	-7.90468	-0.57288	4.11850
H	-9.11853	-1.57304	3.31481
H	-8.79581	0.06138	2.72464
H	-6.16127	-0.14222	-2.57068
H	-7.36380	0.31536	-4.67088
H	-8.42286	0.67223	-3.29605
H	-8.65539	-0.80727	-4.23490
H	-5.66013	-1.57288	-4.54056
H	-6.86556	-2.75547	-4.00727
H	-5.41933	-2.45651	-3.02505
N	-2.88357	-4.10050	-0.35788
N	-4.99343	-4.30228	-0.48264
N	-2.96954	0.09929	0.05908
N	-5.92162	-0.33767	-0.19189
Cu	-4.23674	-1.42840	-0.18834

61. L^1CuXO_2 η^1 singlet, X = 2,3-dihydro-1*H*-imidazol-2-ylidene

C	1.12627	-4.08517	-0.72399
C	0.78802	-1.89539	-0.28365
C	2.25451	-3.42128	-1.09949
C	3.18149	0.39797	1.46108
C	4.49511	-0.04672	1.27437
C	5.11383	0.01940	0.02879
C	4.42168	0.55746	-1.05524
C	3.10593	1.02448	-0.92282

C	2.53919	0.31387	2.84453
C	3.35633	1.07792	3.90402
C	2.30615	-1.14643	3.28043
C	2.38809	1.61122	-2.14187
C	2.02899	0.52994	-3.18160
C	3.20132	2.73823	-2.80732
C	-3.11756	0.24658	0.20142
C	-3.91136	0.01476	1.35496
C	-5.16942	-0.56828	1.18545
C	-5.63409	-0.94845	-0.07082
C	-4.82531	-0.76455	-1.18588
C	-3.56046	-0.17417	-1.07562
C	-3.43059	0.36142	2.76474
C	-3.52710	-0.85027	3.71297
C	-4.19184	1.55799	3.37211
C	-2.70432	-0.00475	-2.32865
C	-3.39210	0.86529	-3.39783
C	-2.30602	-1.37242	-2.91708
C	1.78546	3.59647	0.82186
C	0.72702	2.52277	0.62097
C	-0.60449	2.96089	0.57489
C	-1.78396	2.21452	0.37844
C	-3.04223	3.03775	0.14359
C	2.47542	0.92237	0.34878
H	2.68881	-1.33520	-0.94406
H	0.87984	-5.13411	-0.77034
H	-0.67622	-3.26573	0.22885
H	3.17692	-3.77391	-1.53216
H	1.32623	4.56180	1.04178
H	2.41296	3.71018	-0.06751
H	2.45331	3.33175	1.64760
H	-0.74451	4.03102	0.66114
H	-2.89587	4.07275	0.45767
H	-3.91472	2.62830	0.65146
H	-3.27376	3.04022	-0.92821
H	5.04174	-0.45670	2.11941
H	6.13331	-0.33505	-0.09597
H	4.91430	0.62337	-2.02191
H	1.55862	0.79338	2.77868
H	2.82721	1.07870	4.86321
H	3.52312	2.11976	3.61041
H	4.33754	0.61975	4.07147
H	1.84896	-1.17835	4.27582
H	3.24911	-1.70382	3.32837
H	1.63612	-1.66611	2.58929
H	1.44605	2.04349	-1.79684
H	1.52915	0.98198	-4.04560
H	1.35504	-0.22214	-2.76200
H	2.92577	0.01695	-3.55016
H	2.61325	3.21071	-3.60151
H	4.12279	2.36114	-3.26468
H	3.48362	3.51529	-2.08994
H	-5.79488	-0.74040	2.05701
H	-6.61698	-1.40011	-0.17589
H	-5.18133	-1.08139	-2.16283
H	-2.37391	0.63047	2.69133
H	-3.04629	-0.61578	4.67004
H	-3.03573	-1.72344	3.28175
H	-4.56893	-1.11323	3.93024
H	-3.83279	1.76141	4.38752
H	-5.26631	1.35002	3.43684
H	-4.06514	2.47404	2.78831
H	-1.78379	0.50739	-2.03406
H	-2.72764	1.01450	-4.25662

H	-3.65971	1.85121	-3.00402
H	-4.31067	0.39815	-3.77008
H	-1.63270	-1.24453	-3.77296
H	-3.18471	-1.92709	-3.26520
H	-1.79836	-1.98855	-2.16953
N	0.25493	-3.13372	-0.23686
N	2.01854	-2.08529	-0.82373
N	1.09868	1.25016	0.48580
N	-1.84295	0.88662	0.32149
O	-1.19670	-1.61308	1.55595
O	-1.92668	-2.58157	1.06770
Cu	-0.24374	-0.29893	0.40316

62. L^1CuXO_2 η^1 triplet, X = 2,3-dihydro-1*H*-imidazol-2-ylidene

C	1.09535	-4.09316	-0.77351
C	0.76080	-1.90523	-0.26545
C	2.18912	-3.40669	-1.20026
C	3.18799	0.35741	1.40900
C	4.48859	-0.11065	1.18897
C	5.08900	-0.02911	-0.06405
C	4.39014	0.55128	-1.12157
C	3.08892	1.04580	-0.95401
C	2.57167	0.24272	2.80124
C	3.37970	1.03516	3.84761
C	2.40857	-1.22591	3.23933
C	2.36508	1.67543	-2.14711
C	1.92706	0.61917	-3.18175
C	3.20874	2.77092	-2.82668
C	-3.12361	0.24644	0.17944
C	-3.93003	-0.01166	1.32065
C	-5.14555	-0.67920	1.13693
C	-5.56153	-1.10715	-0.12024
C	-4.75178	-0.87164	-1.22552
C	-3.53116	-0.19780	-1.10227
C	-3.51888	0.41269	2.73269
C	-3.68415	-0.72373	3.76246
C	-4.29764	1.65488	3.21500
C	-2.67974	0.03674	-2.34861
C	-3.41342	0.89351	-3.39830
C	-2.21137	-1.29360	-2.97013
C	1.77724	3.61400	0.84096
C	0.72324	2.53888	0.62273
C	-0.61068	2.97306	0.56405
C	-1.79373	2.23072	0.34858
C	-3.03418	3.06338	0.05756
C	2.47251	0.92890	0.32512
H	2.60442	-1.31632	-1.03937
H	0.85866	-5.14422	-0.81665
H	-0.62330	-3.32416	0.29509
H	3.08988	-3.74072	-1.68934
H	1.31608	4.57629	1.07025
H	2.41010	3.73953	-0.04348
H	2.44119	3.33992	1.66703
H	-0.75102	4.04413	0.64529
H	-2.95195	4.05672	0.50403
H	-3.95264	2.58996	0.40290
H	-3.12970	3.19575	-1.02750
H	5.03929	-0.55284	2.01528
H	6.09747	-0.40445	-0.21502
H	4.86645	0.62731	-2.09570
H	1.57198	0.68320	2.75241
H	2.88034	1.00017	4.82225
H	3.48746	2.08666	3.56156

H	4.38691	0.62283	3.97812
H	1.93936	-1.27919	4.22798
H	3.37702	-1.73597	3.30290
H	1.77793	-1.78104	2.53940
H	1.45345	2.14629	-1.77269
H	1.42229	1.09798	-4.02831
H	1.23166	-0.10391	-2.74559
H	2.78859	0.06879	-3.57971
H	2.61838	3.28060	-3.59591
H	4.09652	2.35803	-3.31844
H	3.54937	3.52378	-2.10867
H	-5.77569	-0.87635	1.99964
H	-6.50897	-1.62690	-0.23528
H	-5.07444	-1.21278	-2.20602
H	-2.45747	0.67216	2.69828
H	-3.23442	-0.42722	4.71710
H	-3.20191	-1.64420	3.42929
H	-4.74019	-0.94208	3.96002
H	-3.98885	1.92705	4.23097
H	-5.37564	1.45590	3.23759
H	-4.13313	2.52526	2.57468
H	-1.78648	0.58750	-2.04053
H	-2.75627	1.10664	-4.24937
H	-3.74243	1.84897	-2.97725
H	-4.30092	0.38182	-3.78762
H	-1.56033	-1.10982	-3.83303
H	-3.06043	-1.89347	-3.31677
H	-1.65279	-1.89318	-2.24525
N	0.24814	-3.15387	-0.21720
N	1.95731	-2.08003	-0.87842
N	1.10302	1.26933	0.47949
N	-1.85835	0.90349	0.32787
O	-1.21548	-1.51919	1.86792
O	-1.61443	-2.72426	1.71764
Cu	-0.24275	-0.29161	0.42229

63. L^1CuXO_2 η^2 singlet, X = 2,3-dihydro-1*H*-imidazol-2-ylidene

C	1.09028	-3.90935	-0.95186
C	3.98908	1.50611	2.98755
C	3.03310	-0.83009	2.73259
C	2.37144	1.73010	-2.85804
C	2.01432	0.67291	-3.92215
C	3.09978	2.91312	-3.52856
C	-2.82876	0.47196	-0.58079
C	-3.75070	0.17470	0.45390
C	-4.92988	-0.49941	0.11521
C	-5.19429	-0.89923	-1.19106
C	-4.26327	-0.63695	-2.19058
C	0.91618	-1.66516	-0.63237
C	-3.07129	0.03985	-1.91139
C	-3.50565	0.58393	1.90363
C	-3.73512	-0.58459	2.88066
C	-4.37648	1.79017	2.30967
C	-2.07914	0.29649	-3.04481
C	-2.64547	1.27160	-4.09583
C	-1.62773	-1.01668	-3.71235
C	2.05744	3.83182	0.12207
C	0.98455	2.76541	-0.02811
C	-0.33745	3.21456	-0.08898
C	2.08483	-3.31889	-1.66645
C	-1.53125	2.47963	-0.31325
C	-2.74433	3.34125	-0.64131
C	2.70252	1.09810	-0.35740

C	3.53036	0.59163	0.67872
C	4.80063	0.10203	0.35120
C	5.26882	0.11301	-0.95863
C	4.46590	0.63849	-1.96881
C	3.18483	1.14129	-1.69963
C	3.08674	0.58962	2.13784
H	2.59188	-1.24433	-1.79372
H	0.82004	-4.94731	-0.84343
H	-0.37014	-2.91712	0.32374
H	2.85268	-3.74194	-2.29420
H	1.62912	4.83364	0.06573
H	2.83389	3.73942	-0.63966
H	2.55489	3.72343	1.09218
H	-0.46821	4.28910	-0.04055
H	-2.61232	3.79096	-1.63212
H	-2.82547	4.16456	0.07466
H	-3.67677	2.77918	-0.64360
H	5.43513	-0.29236	1.14026
H	6.25781	-0.27220	-1.19174
H	4.84434	0.66936	-2.98771
H	2.07146	0.99141	2.17263
H	3.61210	1.56543	4.01417
H	4.02944	2.52306	2.58328
H	5.01741	1.12895	3.03132
H	2.73792	-0.78312	3.78627
H	4.00778	-1.33007	2.68174
H	2.29145	-1.44297	2.21543
H	1.43093	2.10592	-2.45020
H	1.43695	1.12978	-4.73352
H	1.40992	-0.13573	-3.50169
H	2.91230	0.23083	-4.37020
H	2.46310	3.36400	-4.29779
H	4.02644	2.58948	-4.01556
H	3.35977	3.69609	-2.81064
H	-5.65501	-0.71795	0.89388
H	-6.11979	-1.41729	-1.42799
H	-4.46684	-0.95845	-3.20907
H	-2.45542	0.87156	1.99105
H	-3.43412	-0.29053	3.89169
H	-3.14348	-1.45562	2.59246
H	-4.78965	-0.88127	2.92631
H	-4.16934	2.07823	3.34657
H	-5.44375	1.54898	2.23748
H	-4.19130	2.66265	1.67691
H	-1.19202	0.76212	-2.60681
H	-1.89838	1.48514	-4.86930
H	-2.94113	2.22196	-3.64126
H	-3.52821	0.85464	-4.59415
H	-0.86536	-0.81750	-4.47419
H	-2.46060	-1.52881	-4.20698
H	-1.20070	-1.70610	-2.97735
N	0.39997	-2.87822	-0.34044
N	1.95174	-1.95456	-1.45725
N	1.35861	1.47878	-0.07670
N	-1.61246	1.16192	-0.28716
O	-1.00689	-1.15489	1.23522
O	-0.32061	-0.72348	2.27864
Cu	0.03364	0.02744	0.14758

64. L^1CuX, X = methyl-2,3-dihydro-1*H*-imidazol-2-ylidene

C	-0.08255	-1.84372	-0.36819
C	0.31871	-4.07809	-0.56735
C	-1.02477	-3.90411	-0.66887
C	3.17552	1.10464	1.35102
C	4.52194	0.72229	1.35989
C	5.26358	0.64785	0.18382
C	4.65300	0.95828	-1.02850
C	3.30941	1.34498	-1.09186
C	2.38441	1.12966	2.65813
C	3.09301	1.91954	3.77292
C	2.05301	-0.30064	3.12855
C	2.66505	1.62718	-2.44700
C	2.44909	0.31911	-3.23427
C	3.45907	2.64446	-3.28527
C	-2.94814	0.38780	-0.32961
C	-3.57668	-0.20975	0.79889
C	-4.62633	-1.11326	0.59166
C	-5.06687	-1.43726	-0.68996
C	-4.45227	-0.84461	-1.79112
C	-3.39914	0.06488	-1.64007
C	-3.10696	0.08618	2.22266
C	-2.43149	-1.14396	2.86168
C	-4.24998	0.60420	3.11554
C	-2.73263	0.65891	-2.87965
C	-3.73917	1.38581	-3.79041
C	-1.95832	-0.41240	-3.67389
C	1.69376	4.07428	0.33989
C	0.70241	2.93238	0.16812
C	-0.66183	3.29164	0.13335
C	-1.81200	2.48664	-0.02083
C	-3.15192	3.20718	-0.02493
C	2.55853	1.41494	0.11015
C	2.30590	-2.57397	-0.26540
H	-1.82225	-4.61635	-0.80881
H	-2.14125	-2.08619	-0.57037
H	0.91926	-4.97319	-0.60630
H	2.46222	-1.51680	-0.05786
H	2.72145	-3.16947	0.55242
H	2.81529	-2.83732	-1.19666
H	1.18257	5.03511	0.42014
H	2.38792	4.12030	-0.50622
H	2.30637	3.93133	1.23627
H	-0.85684	4.35238	0.23500
H	-3.02818	4.28375	0.10625
H	-3.79811	2.83251	0.77627
H	-3.68576	3.03237	-0.96529
H	4.99893	0.47560	2.30519
H	6.30872	0.35071	0.21172
H	5.23260	0.89600	-1.94635
H	1.43233	1.62716	2.45622
H	2.44755	1.99425	4.65529
H	3.34082	2.93590	3.44961
H	4.02397	1.43724	4.09145
H	1.46393	-0.28040	4.05295
H	2.96652	-0.87472	3.32491
H	1.47091	-0.83365	2.36974
H	1.67708	2.05488	-2.25755
H	1.95733	0.51751	-4.19387
H	1.81846	-0.37517	-2.66909
H	3.40350	-0.17947	-3.44282
H	2.91721	2.88398	-4.20710
H	4.44254	2.25882	-3.57666
H	3.61955	3.57815	-2.73619

H	-5.10451	-1.57542	1.45206
H	-5.88272	-2.14154	-0.82862
H	-4.79372	-1.09855	-2.79156
H	-2.35003	0.87246	2.15932
H	-2.07547	-0.90870	3.87137
H	-1.57195	-1.47141	2.26880
H	-3.12900	-1.98645	2.94254
H	-3.86729	0.88160	4.10420
H	-5.02588	-0.15544	3.26529
H	-4.73097	1.48598	2.68002
H	-2.00149	1.39533	-2.53655
H	-3.21847	1.87040	-4.62402
H	-4.29218	2.15680	-3.24429
H	-4.47285	0.69447	-4.22033
H	-1.46733	0.03377	-4.54645
H	-2.62690	-1.20241	-4.03682
H	-1.18573	-0.87965	-3.05590
N	0.87305	-2.81797	-0.38383
N	-1.23840	-2.54471	-0.54488
N	1.16094	1.68566	0.06070
N	-1.77853	1.16627	-0.16022
Cu	-0.01176	0.10268	-0.16655

65. L^1CuXO_2 η^1 singlet, X = methyl-2,3-dihydro-1*H*-imidazol-2-ylidene

H	-1.08343	-3.94142	0.03096
H	-1.47247	-2.34099	-0.62265
H	-1.26274	-3.72252	-1.73623
C	1.47404	-3.89450	-1.18167
C	3.75616	1.55255	3.49006
C	3.06498	-0.84999	3.15311
C	2.97804	1.65692	-2.51427
C	2.66475	0.52372	-3.51188
C	3.79845	2.76495	-3.20384
C	-2.61726	0.63342	-0.16880
C	-3.37115	0.30691	0.99361
C	-4.60145	-0.33786	0.81813
C	-5.07565	-0.67861	-0.44513
C	-4.31593	-0.37434	-1.57177
C	1.05433	-1.73616	-0.62724
C	-3.08568	0.28132	-1.46030
C	-2.89621	0.64556	2.40898
C	-3.02517	-0.54962	3.37219
C	-3.64712	1.85580	3.00594
C	-2.29513	0.63247	-2.72117
C	-3.10612	1.52617	-3.67887
C	-1.78719	-0.62245	-3.45691
C	2.41440	3.79609	0.41282
C	1.31941	2.75142	0.24274
C	0.00427	3.24705	0.22014
C	2.67441	-3.26981	-1.07465
C	-1.21715	2.56714	0.03616
C	-2.43938	3.45409	-0.14769
C	3.01429	1.08899	0.00492
C	3.70281	0.59110	1.14638
C	5.01612	0.12768	0.99061
C	5.65641	0.14498	-0.24520
C	4.98124	0.64461	-1.35546
C	3.66949	1.12613	-1.25779
C	3.06211	0.56023	2.53377
H	3.07102	-1.23722	-0.55546
H	1.22759	-4.91499	-1.42810
C	-0.91945	-3.25904	-0.80747
H	3.68031	-3.63333	-1.20929

H	1.98960	4.77205	0.65539
H	3.00568	3.90196	-0.50234
H	3.11042	3.51190	1.20659
H	-0.08107	4.32204	0.32169
H	-2.26674	4.44918	0.26693
H	-3.33581	3.02774	0.30248
H	-2.64653	3.57147	-1.21834
H	5.54675	-0.25348	1.85868
H	6.67520	-0.22085	-0.34046
H	5.48313	0.66342	-2.31926
H	2.01941	0.87189	2.42799
H	3.23888	1.57324	4.45539
H	3.76122	2.57190	3.09161
H	4.79725	1.26533	3.67761
H	2.59584	-0.82381	4.14228
H	4.08509	-1.23216	3.28137
H	2.49487	-1.55641	2.54518
H	2.02254	2.09134	-2.21083
H	2.16632	0.92282	-4.40254
H	2.00664	-0.22798	-3.06649
H	3.58076	0.01955	-3.84206
H	3.23483	3.19089	-4.04115
H	4.74232	2.38144	-3.60723
H	4.04295	3.57903	-2.51413
H	-5.19661	-0.58388	1.69312
H	-6.03301	-1.18184	-0.55072
H	-4.68892	-0.64299	-2.55700
H	-1.83558	0.89774	2.35224
H	-2.52283	-0.31861	4.31782
H	-2.56220	-1.44660	2.95742
H	-4.07198	-0.77684	3.60663
H	-3.29457	2.05291	4.02513
H	-4.72615	1.66696	3.05834
H	-3.49655	2.76943	2.42541
H	-1.41394	1.19916	-2.40818
H	-2.48892	1.83514	-4.53026
H	-3.46673	2.42980	-3.17742
H	-3.98033	1.00023	-4.07890
H	-1.22953	-0.34122	-4.35796
H	-2.61393	-1.27252	-3.76590
H	-1.11707	-1.20582	-2.81963
N	0.50045	-2.94369	-0.90690
N	2.38647	-1.96144	-0.73650
N	1.64448	1.46503	0.10588
N	-1.34019	1.24796	-0.04716
O	-0.68014	-1.24879	1.39289
O	0.02556	-1.12624	2.46536
Cu	0.20399	-0.02885	0.01016

66. L^1CuXO_2 η^1 triplet, X = methyl-2,3-dihydro-1*H*-imidazol-2-ylidene

H	-1.97458	-2.35082	-0.07064
H	-1.95833	-3.79630	-1.10475
H	-1.57781	-3.93570	0.63323
C	0.81893	-4.04595	-0.93320
C	3.48722	1.42637	3.48745
C	2.84469	-0.97899	3.04725
C	2.35788	1.61586	-2.49239
C	2.02286	0.47110	-3.46997
C	3.07958	2.76286	-3.22262
C	-3.05742	0.49640	-0.07459
C	-3.93541	0.18513	1.00033
C	-5.13307	-0.48410	0.71339
C	-5.47279	-0.85144	-0.58472

C	-4.60053	-0.55317	-1.62799
C	0.53781	-1.83900	-0.45662
C	-3.39151	0.11275	-1.39940
C	-3.63564	0.56553	2.45055
C	-3.76297	-0.63477	3.40954
C	-4.54525	1.71092	2.94250
C	-2.47839	0.44998	-2.57860
C	-3.10566	1.53214	-3.48059
C	-2.09036	-0.79277	-3.40104
C	1.93748	3.78043	0.48641
C	0.86352	2.71038	0.36173
C	-0.46918	3.15412	0.39754
C	2.02652	-3.44656	-1.09348
C	-1.68373	2.45147	0.22879
C	-2.90916	3.35093	0.11066
C	2.58683	1.07623	0.01445
C	3.35047	0.56409	1.10041
C	4.65596	0.11838	0.86051
C	5.21468	0.14764	-0.41463
C	4.45831	0.63736	-1.47814
C	3.15237	1.10853	-1.29109
C	2.77931	0.46496	2.51262
H	2.53826	-1.39241	-0.81566
H	0.51893	-5.07443	-1.05724
C	-1.48078	-3.30315	-0.25383
H	2.98425	-3.84814	-1.38317
H	1.50291	4.76756	0.65487
H	2.55590	3.82491	-0.41751
H	2.61178	3.55128	1.31799
H	-0.58840	4.22735	0.50250
H	-3.00885	3.97503	1.00488
H	-3.83064	2.78597	-0.02399
H	-2.79157	4.03026	-0.74067
H	5.24277	-0.26574	1.69087
H	6.22922	-0.20505	-0.57844
H	4.89101	0.65642	-2.47523
H	1.72535	0.74973	2.46362
H	3.02620	1.37354	4.48028
H	3.43037	2.46466	3.14540
H	4.54817	1.17411	3.60141
H	2.35726	-1.04646	4.02519
H	3.88076	-1.31659	3.16813
H	2.33805	-1.67537	2.37302
H	1.41070	2.01115	-2.11793
H	1.44187	0.84709	-4.31984
H	1.43454	-0.30939	-2.97823
H	2.93337	0.00819	-3.86918
H	2.44736	3.16241	-4.02334
H	4.01748	2.42864	-3.68096
H	3.31946	3.58420	-2.53944
H	-5.81425	-0.71696	1.52717
H	-6.41122	-1.36256	-0.78215
H	-4.86810	-0.83437	-2.64298
H	-2.60256	0.91684	2.49247
H	-3.39542	-0.36184	4.40465
H	-3.18330	-1.49184	3.05989
H	-4.80570	-0.95247	3.52288
H	-4.29226	1.98499	3.97329
H	-5.59977	1.41084	2.92793
H	-4.44731	2.60612	2.32384
H	-1.55306	0.86258	-2.16698
H	-2.41999	1.81004	-4.28957
H	-3.34004	2.43684	-2.91037
H	-4.03662	1.17850	-3.93901

H	-1.39605	-0.51798	-4.20296
H	-2.96121	-1.26524	-3.86868
H	-1.59649	-1.54209	-2.77412
N	-0.07304	-3.05369	-0.54680
N	1.82538	-2.11167	-0.79765
N	1.22904	1.44026	0.20234
N	-1.79441	1.12950	0.14676
O	-0.90101	-1.20760	1.96216
O	-0.46610	-0.63580	2.98139
Cu	-0.17142	-0.05443	0.13345

67. L^1CuXO_2 η^2 singlet, X = methyl-2,3-dihydro-1*H*-imidazol-2-ylidene

H	-1.93219	-2.26902	0.67216
H	-2.32081	-3.23807	-0.76585
H	-1.62299	-4.02068	0.68282
C	0.44900	-3.79353	-1.18550
C	3.95588	1.25838	3.37219
C	2.87569	-1.00368	2.99622
C	2.17482	1.59857	-2.49059
C	1.81326	0.50232	-3.51266
C	2.84280	2.78537	-3.21386
C	-3.00185	0.40405	-0.22010
C	-3.92997	0.06137	0.80043
C	-5.08864	-0.64263	0.44687
C	-5.34292	-1.01868	-0.86858
C	-4.42257	-0.69085	-1.85940
C	0.44138	-1.73522	-0.24992
C	-3.24673	0.00770	-1.56161
C	-3.71969	0.46368	2.25920
C	-3.82995	-0.73488	3.21995
C	-4.70796	1.57035	2.68109
C	-2.26941	0.33852	-2.68863
C	-2.84696	1.40267	-3.64242
C	-1.84531	-0.91627	-3.47653
C	1.92857	3.70431	0.47953
C	0.84959	2.63609	0.37829
C	-0.46807	3.08083	0.36307
C	1.64854	-3.22330	-1.46475
C	-1.68682	2.36982	0.11918
C	-2.88083	3.27501	-0.16097
C	2.58609	0.99614	-0.00333
C	3.44007	0.48342	1.01223
C	4.71136	0.01830	0.65794
C	5.15965	0.05820	-0.66033
C	4.32914	0.57931	-1.64971
C	3.04331	1.05314	-1.35281
C	3.00719	0.44084	2.47523
H	2.35791	-1.28106	-0.90896
H	0.04821	-4.76014	-1.44620
C	-1.62391	-3.11792	0.06688
H	2.49929	-3.59124	-2.01507
H	1.48798	4.68565	0.66406
H	2.52285	3.76453	-0.43672
H	2.62334	3.47382	1.29385
H	-0.58877	4.15485	0.45163
H	-3.00999	3.98549	0.66264
H	-3.80845	2.71847	-0.29207
H	-2.69833	3.86708	-1.06495
H	5.36419	-0.37708	1.43156
H	6.15131	-0.30674	-0.91372
H	4.68385	0.61849	-2.67647
H	2.01556	0.89269	2.54263
H	3.57241	1.28688	4.39788
H	4.05270	2.29084	3.01972
H	4.96154	0.82406	3.40812
H	2.54112	-0.99975	4.03882
H	3.83397	-1.53525	2.95152
H	2.14016	-1.57241	2.41951
H	1.23906	1.95694	-2.05475
H	1.18682	0.91571	-4.31092
H	1.25951	-0.31560	-3.04497
H	2.70994	0.08154	-3.98286
H	2.15953	3.20901	-3.95803
H	3.75247	2.47716	-3.74135
H	3.11921	3.58494	-2.52042

H	-5.80818	-0.89496	1.22102
H	-6.25229	-1.55795	-1.12053
H	-4.62315	-0.97793	-2.88885
H	-2.70489	0.85597	2.35652
H	-3.61508	-0.41254	4.24477
H	-3.10786	-1.51178	2.95793
H	-4.83439	-1.17457	3.21925
H	-4.51585	1.88096	3.71463
H	-5.74539	1.21851	2.62753
H	-4.62581	2.45537	2.04360
H	-1.36874	0.75663	-2.23076
H	-2.11336	1.67661	-4.40980
H	-3.12655	2.31138	-3.10124
H	-3.74262	1.03324	-4.15505
H	-1.11048	-0.65848	-4.24741
H	-2.69559	-1.38947	-3.98058
H	-1.39040	-1.66310	-2.81710
N	-0.27477	-2.86975	-0.44106
N	1.61432	-1.96999	-0.88220
N	1.24754	1.34857	0.31889
N	-1.78227	1.06139	0.10642
O	-0.68727	-1.03689	2.31788
O	-0.41385	0.19709	2.74316
Cu	0.01132	-0.10348	0.82778

68. L^1CuX, X = 2-pyridinamine

C	3.14389	2.54958	-3.58990
C	2.07164	-3.10900	-0.27067
C	-0.17731	-3.90225	0.01012
C	1.67595	4.34073	-0.09611
C	0.64510	3.22193	-0.05866
C	-0.71214	3.62044	-0.06298
C	-1.90139	2.86350	-0.03268
C	-3.19927	3.65672	-0.08304
C	2.44221	1.62817	-0.06002
C	3.13381	1.37725	1.15369
C	4.45140	0.90928	1.09495
C	5.09111	0.69003	-0.12219
C	4.40751	0.94215	-1.30881
C	3.08851	1.41092	-1.30694
C	2.45096	1.56065	2.50745
C	3.26602	2.44839	3.46475
C	2.13326	0.20016	3.16042
C	2.36230	1.62970	-2.63418
C	2.03461	0.28906	-3.32284
C	1.16257	-4.17116	-0.18314
C	-3.21507	0.85611	0.06567
C	-3.81818	0.53673	1.31269
C	-4.99263	-0.22502	1.31890
C	-5.57358	-0.67686	0.13716
C	-4.97408	-0.36666	-1.08102
C	-3.80290	0.39701	-1.14493
C	-3.19237	0.96605	2.63821
C	-2.69771	-0.25184	3.44431
C	-4.15161	1.82113	3.48672
C	-3.15682	0.68223	-2.49970
C	-4.14667	1.28151	-3.51505
C	-2.48688	-0.58399	-3.07076
C	1.57907	-1.82071	-0.16720
C	-0.60600	-2.55916	0.11068
H	1.50245	-5.19995	-0.26343
H	-2.60754	-2.97765	0.18486
H	-3.81578	3.46131	0.80032

H	3.13242	-3.27386	-0.41898
H	1.20008	5.32284	-0.10349
H	2.31248	4.25745	-0.98331
H	2.34176	4.28359	0.77177
H	-0.86413	4.69214	-0.10201
H	-3.00687	4.72935	-0.13924
H	-2.22871	-1.31003	0.24085
H	-3.79963	3.36732	-0.95219
H	4.98503	0.70656	2.02015
H	6.11427	0.32452	-0.14599
H	4.90703	0.76510	-2.25814
H	1.49554	2.06050	2.32686
H	2.70503	2.62761	4.38877
H	3.49393	3.41994	3.01418
H	4.21712	1.98235	3.74584
H	1.62103	0.34038	4.11960
H	3.04813	-0.37378	3.34942
H	1.48492	-0.40272	2.51717
H	1.40933	2.11688	-2.41237
H	1.49929	0.45834	-4.26460
H	1.40386	-0.33906	-2.68666
H	2.94684	-0.27392	-3.55340
H	2.55384	2.75294	-4.49057
H	4.08729	2.09589	-3.91398
H	3.38295	3.50889	-3.11948
H	-5.45657	-0.47489	2.26987
H	-6.48589	-1.26676	0.16475
H	-5.42545	-0.72482	-2.00291
H	-2.31768	1.57831	2.40395
H	-2.19273	0.07288	4.36133
H	-1.99407	-0.85433	2.86212
H	-3.53073	-0.90237	3.73602
H	-3.65105	2.16489	4.39879
H	-5.03798	1.25339	3.79218
H	-4.49742	2.70413	2.93983
H	-2.36479	1.41767	-2.33621
H	-3.62472	1.55278	-4.43953
H	-4.62788	2.18319	-3.12251
H	-4.93859	0.57343	-3.78389
H	-1.99707	-0.36742	-4.02704
H	-3.22194	-1.37934	-3.24337
H	-1.72684	-0.96885	-2.38332
H	2.24422	-0.96919	-0.23265
N	-1.91416	-2.26634	0.35334
H	-0.90719	-4.70139	0.09302
N	-1.96023	1.53076	0.02962
N	1.05785	1.95924	-0.02808
N	0.26764	-1.52608	0.01203
Cu	-0.28579	0.45928	0.05185

69. L^1CuXO_2 η^1 singlet, X = 2-pyridinamine

Cu	0.12626	-1.12031	-0.31406
O	0.70338	-3.36018	1.37077
O	-0.23394	-2.75485	0.71233
N	1.10281	-2.16854	-2.06663
N	0.91005	-0.20806	1.31223
N	-1.23574	0.25981	-0.84952
C	-2.75217	2.11936	-0.25183
C	1.85824	-0.91568	2.07963
C	1.49011	-1.58939	3.28956
C	2.48376	-2.29309	3.98518
C	3.78852	-2.35667	3.52346
C	4.13878	-1.71041	2.33642

C	3.19944	-1.00181	1.59171
C	0.09586	-1.51473	3.91598
C	0.13693	-0.76231	5.26653
C	-0.54452	-2.89901	4.14382
C	3.62471	-0.25030	0.33263
C	4.82208	-0.88642	-0.39258
C	3.93181	1.22914	0.64905
C	-1.90685	0.16454	-2.10622
C	-2.81990	-0.89580	-2.32945
C	-3.38559	-1.03422	-3.60175
C	-3.05962	-0.16671	-4.63948
C	-2.15532	0.86732	-4.41149
C	-1.56659	1.06008	-3.15673
C	-3.19985	-1.87888	-1.22414
C	-2.82775	-3.32805	-1.59267
C	-4.69306	-1.77126	-0.85890
C	-0.54290	2.18570	-2.97739
C	-1.08138	3.54981	-3.45093
C	0.78888	1.86684	-3.68829
C	2.09406	-3.09270	-1.98416
C	0.71516	-1.77598	-3.30077
C	2.74302	-3.57912	-3.14783
C	1.28546	-2.22069	-4.48071
C	2.33765	-3.14130	-4.39006
C	0.90940	1.68283	2.92065
C	0.31706	0.90750	1.74747
C	-0.81181	1.51647	1.17529
C	-1.55379	1.22095	0.00926
H	3.11931	-4.31159	-0.74290
H	1.86324	-3.44797	0.05730
H	1.24054	2.66472	2.56448
H	1.76231	1.17792	3.37051
H	0.15430	1.85949	3.69109
H	-1.15961	2.39067	1.71554
H	-3.11727	2.55165	0.68202
H	-3.56306	1.56386	-0.72720
H	-2.48790	2.94421	-0.92158
H	2.21960	-2.80120	4.90796
H	4.54038	-2.90477	4.08541
H	5.16604	-1.76130	1.99189
H	-0.55791	-0.96475	3.23486
H	-0.87961	-0.62393	5.65151
H	0.60679	0.22066	5.19188
H	0.69448	-1.33708	6.01441
H	-1.54961	-2.77320	4.56238
H	0.03404	-3.49190	4.86208
H	-0.61042	-3.46136	3.21431
H	2.77345	-0.26754	-0.35596
H	4.97128	-0.39644	-1.36075
H	4.65561	-1.95175	-0.56989
H	5.75496	-0.76905	0.17143
H	4.21587	1.76536	-0.26373
H	4.76407	1.30848	1.35849
H	3.06898	1.73970	1.08342
H	-4.09052	-1.84138	-3.78237
H	-3.50480	-0.29687	-5.62202
H	-1.89535	1.53623	-5.22756
H	-2.62816	-1.61502	-0.33049
H	-3.06158	-4.00261	-0.76221
H	-1.75903	-3.41908	-1.80651
H	-3.38243	-3.67608	-2.47175
H	-4.93180	-2.44362	-0.02731
H	-5.33498	-2.04642	-1.70370
H	-4.95977	-0.75301	-0.55662

H	-0.31699	2.27369	-1.91208
H	-0.37159	4.34576	-3.19953
H	-2.04181	3.79265	-2.98549
H	-1.22643	3.57531	-4.53649
H	1.50564	2.68348	-3.54241
H	0.64280	1.74036	-4.76729
H	1.24251	0.94987	-3.30255
N	2.48862	-3.52446	-0.75849
H	-0.09738	-1.06194	-3.32627
H	3.54665	-4.30181	-3.04049
H	0.92064	-1.85639	-5.43396
H	2.82700	-3.51674	-5.28480

70. L^1CuXO_2 η^1 triplet, X = 2-pyridinamine

Cu	0.23115	-1.07933	-0.30914
O	-0.89443	-3.89560	0.44388
O	-1.06408	-2.69049	0.65817
N	0.95319	-2.43235	-1.72105
N	0.87687	-0.20474	1.37491
N	-1.21881	0.24055	-0.86998
C	-2.71355	2.13469	-0.34361
C	2.05584	-0.66981	2.03505
C	1.96975	-1.67425	3.04229
C	3.15220	-2.13393	3.63564
C	4.39617	-1.63492	3.26242
C	4.47275	-0.66441	2.26784
C	3.32519	-0.17527	1.63424
C	0.63044	-2.23190	3.52066
C	0.28665	-1.72409	4.93613
C	0.58758	-3.77133	3.48723
C	3.46420	0.88371	0.54293
C	4.34969	0.38853	-0.61876
C	3.99276	2.21409	1.11052
C	-1.79063	0.20907	-2.17743
C	-2.87463	-0.65928	-2.47105
C	-3.35279	-0.72128	-3.78565
C	-2.78216	0.03330	-4.80523
C	-1.70834	0.86970	-4.51440
C	-1.19655	0.97802	-3.21665
C	-3.53238	-1.52245	-1.39600
C	-3.42634	-3.02554	-1.72274
C	-5.00759	-1.13613	-1.16850
C	0.01341	1.87722	-2.96201
C	-0.19653	3.31177	-3.48167
C	1.29509	1.26575	-3.56311
C	1.92997	-3.32777	-1.43610
C	0.35475	-2.49730	-2.93348
C	2.29485	-4.33311	-2.36158
C	0.66623	-3.44622	-3.89148
C	1.65744	-4.38733	-3.58426
C	0.66163	1.56706	3.10845
C	0.20736	0.85316	1.83893
C	-0.93939	1.41958	1.24146
C	-1.57188	1.18608	-0.00177
H	3.08563	-4.01193	0.11288
H	2.29439	-2.52681	0.42992
H	0.97129	2.59119	2.87150
H	1.49215	1.06755	3.60484
H	-0.17306	1.64110	3.81326
H	-1.36600	2.23876	1.80972
H	-2.98277	2.75485	0.51317
H	-3.59878	1.58168	-0.66724
H	-2.43884	2.79580	-1.17224
H	3.09394	-2.88924	4.41515
H	5.29958	-2.00375	3.74067

H	5.44506	-0.27923	1.97254
H	-0.14136	-1.86428	2.84063
H	-0.69864	-2.09083	5.24575
H	0.26866	-0.63110	4.98027
H	1.01899	-2.07602	5.67155
H	-0.41363	-4.12959	3.75218
H	1.29236	-4.21375	4.20086
H	0.82982	-4.15961	2.49405
H	2.46618	1.06782	0.13774
H	4.37146	1.12713	-1.42790
H	3.97348	-0.55392	-1.02774
H	5.38352	0.22206	-0.29483
H	4.02769	2.97966	0.32747
H	5.00708	2.10535	1.51157
H	3.35506	2.58515	1.91972
H	-4.18930	-1.37713	-4.01351
H	-3.16751	-0.03288	-5.81919
H	-1.25441	1.45013	-5.31375
H	-2.99232	-1.34905	-0.46115
H	-3.82548	-3.62769	-0.89862
H	-2.38846	-3.32954	-1.88703
H	-3.99548	-3.28297	-2.62320
H	-5.44242	-1.73927	-0.36298
H	-5.60726	-1.30460	-2.07029
H	-5.11533	-0.08285	-0.89220
H	0.16346	1.93793	-1.88176
H	0.65417	3.94491	-3.20521
H	-1.10167	3.76332	-3.06273
H	-0.28618	3.34353	-4.57332
H	2.16306	1.90186	-3.35296
H	1.21359	1.16078	-4.65137
H	1.49508	0.27471	-3.14442
N	2.59613	-3.21192	-0.25500
H	-0.42181	-1.76100	-3.10947
H	3.08161	-5.03527	-2.10496
H	0.14525	-3.45459	-4.84178
H	1.93180	-5.15464	-4.30295

71. L^1CuXO_2 η^2 singlet, X = 2-pyridinamine

Cu	-0.2574428600	-1.2443400354	0.0550900043
O	-0.2367029198	-3.0549589307	0.6617262531
O	-1.1503894595	-2.8815169288	-0.2998761965
N	1.3483155292	-2.3186254712	-1.7163385777
N	0.6251825276	-0.1677519857	1.4263440011
N	-1.3212801385	0.1621950349	-0.8005388473
C	-2.7609552658	2.1512600696	-0.5282387365
C	1.8749197664	-0.5870400328	1.9844172835
C	1.8985150908	-1.6094391723	2.9716851842
C	3.1408502373	-2.0184550456	3.4722816791
C	4.3296125838	-1.4555959607	3.0181208222
C	4.2922696630	-0.4638221093	2.0443172215
C	3.0811881127	-0.0105296267	1.5091624815
C	0.6245472192	-2.2444771834	3.5289389845
C	0.3072015122	-1.7193703055	4.9440677572
C	0.6867895425	-3.7838332936	3.5357054717
C	3.1078297456	1.0645632400	0.4232800968
C	3.7257397147	0.5254790314	-0.8819723243
C	3.8458488800	2.3368073555	0.8847028618
C	-1.8305393491	0.0276083011	-2.1361795474
C	-3.0244835840	-0.6896175708	-2.3969758485
C	-3.4958969621	-0.7334260177	-3.7155080566
C	-2.8164431620	-0.1101123694	-4.7550288291
C	-1.6204417616	0.5522567525	-4.4943035581

C	-1.0964358906	0.6237925466	-3.1991319490
C	-3.8099166066	-1.4280545068	-1.3151252718
C	-3.9332772999	-2.9303847918	-1.6413454676
C	-5.2140293967	-0.8248818045	-1.1034857816
C	0.2414299533	1.3277390716	-2.9594784483
C	0.0710679924	2.8505352519	-2.7833817622
C	1.2721151097	1.0485102060	-4.0707212817
C	2.3551360493	-3.1708490483	-1.4369382434
C	0.7657625566	-2.4223215804	-2.9248652941
C	2.8213138040	-4.1164547631	-2.3794604297
C	1.1533533171	-3.3194510604	-3.9100399438
C	2.2148164747	-4.1840935061	-3.6199139267
C	0.5981863792	1.7327518830	3.0021363442
C	0.0390865630	0.9608815023	1.8184760465
C	-1.0742357528	1.5412342389	1.1827858480
C	-1.6558470090	1.2183261847	-0.0576116914
H	3.5116690644	-3.8466513138	0.0986311416
H	2.4344528720	-2.6059329991	0.5181170413
H	1.3301260320	2.4735056560	2.6607343906
H	1.0991358807	1.0813165076	3.7190235431
H	-0.2044512215	2.2739363547	3.5092720325
H	-1.4771923267	2.4208917956	1.6688396712
H	-2.6970308861	3.1150694649	-0.0200754571
H	-3.7353637622	1.7094382560	-0.2936414650
H	-2.7339407521	2.3143999834	-1.6062253563
H	3.1744078025	-2.7909671906	4.2350719919
H	5.2816018759	-1.7920610455	3.4201167845
H	5.2236480298	-0.0362958738	1.6838905884
H	-0.2011192892	-1.9640290188	2.8727959590
H	-0.6192471713	-2.1700570727	5.3174957332
H	0.1783164513	-0.6327467905	4.9580227596
H	1.1086004262	-1.9701226740	5.6485538651
H	-0.2864487892	-4.1934365655	3.8253957580
H	1.4257643081	-4.1641551152	4.2504820611
H	0.9293726072	-4.1760755643	2.5454478496
H	2.0757055371	1.3465895308	0.1995987596
H	3.7388837845	1.3097874190	-1.6478812916
H	3.1565857456	-0.3230246503	-1.2688168841
H	4.7591517618	0.1961334467	-0.7248438773
H	3.7605840651	3.1213628115	0.1246515727
H	4.9140313923	2.1507859172	1.0428272609
H	3.4381241217	2.7282917704	1.8221771088
H	-4.4158989628	-1.2708173170	-3.9281985474
H	-3.2074615527	-0.1531115952	-5.7679959039
H	-1.0792361233	1.0141215388	-5.3140631615
H	-3.2538428336	-1.3449345750	-0.3782617994
H	-4.4112625431	-3.4574887102	-0.8085859757
H	-2.9536087784	-3.3824383762	-1.8075925625
H	-4.5474503935	-3.0974046104	-2.5341177280
H	-5.7316766946	-1.3438157423	-0.2888826801
H	-5.8313529812	-0.9269156558	-2.0037251251
H	-5.1749918932	0.2393802505	-0.8520936395
H	0.6508092916	0.9294158868	-2.0262409926
H	1.0462639475	3.3297880030	-2.6409037906
H	-0.5492564430	3.0980937191	-1.9184516730
H	-0.3932666189	3.2954564322	-3.6711286888
H	2.2496587957	1.4443734504	-3.7770623039
H	1.0012199495	1.5331966594	-5.0151608744
H	1.3878321777	-0.0220633379	-4.2598719992
N	2.9655904991	-3.0585103523	-0.2127677103
H	-0.0619740974	-1.7449891420	-3.1048722162
H	3.6431246652	-4.7767813077	-2.1174629268
H	0.6371865110	-3.3447645730	-4.8635423308
H	2.5592896329	-4.9067088314	-4.3549012259

72. L^1CuXO_2 η^2 triplet, X = 2-pyridinamine

Cu	-0.05908	-1.17150	-0.14277
O	-0.30294	-3.22755	0.59687
O	-1.16600	-3.01365	-0.31804
N	1.27674	-2.29268	-1.65673
N	0.67398	-0.16163	1.41731
N	-1.35329	0.18516	-0.84318
C	-2.81359	2.14810	-0.45805
C	1.88483	-0.59032	2.04286
C	1.86071	-1.62791	3.01460
C	3.07672	-2.06812	3.55370
C	4.29202	-1.52348	3.15136
C	4.30712	-0.51709	2.19107
C	3.12399	-0.03231	1.62302
C	0.55533	-2.25053	3.50571
C	0.15769	-1.70625	4.89323
C	0.61105	-3.78983	3.54327
C	3.20754	1.05426	0.55103
C	3.80794	0.50556	-0.75897
C	3.99986	2.28565	1.03049
C	-1.91182	0.05152	-2.15486
C	-3.08253	-0.71763	-2.38185
C	-3.57457	-0.81408	-3.68966
C	-2.93737	-0.19426	-4.75838
C	-1.76815	0.52613	-4.53333
C	-1.22898	0.65565	-3.24864
C	-3.82667	-1.44376	-1.26246
C	-4.00581	-2.94485	-1.57083
C	-5.20552	-0.81195	-0.98170
C	0.06696	1.44412	-3.04750
C	-0.19371	2.96330	-2.97932
C	1.12861	1.14827	-4.12462
C	2.28379	-3.14203	-1.35286
C	0.73974	-2.37547	-2.89346
C	2.77414	-4.08161	-2.29049
C	1.16051	-3.26451	-3.86820
C	2.20667	-4.13900	-3.54704
C	0.57007	1.71316	3.02377
C	0.04962	0.94500	1.81766
C	-1.05966	1.52279	1.16928
C	-1.67701	1.21399	-0.06179
H	3.42647	-3.80965	0.20563
H	2.38301	-2.51623	0.60087
H	1.34728	2.42084	2.71246
H	1.01439	1.05574	3.77240
H	-0.23308	2.28946	3.48794
H	-1.46875	2.39275	1.66916
H	-2.65153	3.14963	-0.05369
H	-3.75615	1.77518	-0.04160
H	-2.93993	2.21632	-1.53896
H	3.06868	-2.85298	4.30466
H	5.22241	-1.88348	3.58232
H	5.25864	-0.10216	1.86944
H	-0.22715	-1.96593	2.79810
H	-0.78585	-2.15520	5.22387
H	0.02502	-0.62067	4.88398
H	0.92229	-1.94377	5.64218
H	-0.38154	-4.19458	3.76705
H	1.29337	-4.15688	4.31872
H	0.92986	-4.20524	2.58396
H	2.18999	1.38233	0.32537
H	3.85643	1.29606	-1.51715

H	3.20491	-0.31297	-1.15944
H	4.82575	0.12974	-0.60360
H	3.95446	3.08181	0.27916
H	5.05774	2.05099	1.19303
H	3.60254	2.68374	1.96959
H	-4.47706	-1.39101	-3.87222
H	-3.34215	-0.28159	-5.76307
H	-1.26166	0.99378	-5.37262
H	-3.22226	-1.35977	-0.35516
H	-4.43489	-3.45878	-0.70350
H	-3.05482	-3.42603	-1.80773
H	-4.68744	-3.10314	-2.41453
H	-5.69272	-1.31602	-0.13921
H	-5.86582	-0.90748	-1.85155
H	-5.13115	0.25188	-0.74140
H	0.48371	1.13646	-2.08343
H	0.74607	3.50874	-2.83466
H	-0.86231	3.22704	-2.15613
H	-0.64939	3.32115	-3.91019
H	2.07875	1.61939	-3.85037
H	0.84330	1.54767	-5.10454
H	1.30797	0.07551	-4.24055
N	2.85700	-3.04475	-0.11840
H	-0.08077	-1.69567	-3.09427
H	3.58770	-4.74294	-2.00816
H	0.67998	-3.27809	-4.83977
H	2.57030	-4.85973	-4.27433

73. L^1CuX, X = pyrazole

N	-0.03074	-1.80861	-0.44075
C	0.49271	-4.00634	-0.54575
C	-0.88115	-3.87584	-0.66405
C	3.14870	1.02816	1.40192
C	4.48475	0.61492	1.43822
C	5.24062	0.49813	0.27560
C	4.65412	0.79209	-0.95170
C	3.32084	1.20588	-1.04406
C	2.33966	1.08978	2.69474
C	3.04465	1.88976	3.80466
C	1.98515	-0.32915	3.18420
C	2.70498	1.46017	-2.41731
C	2.52261	0.13742	-3.18953
C	3.51254	2.47139	-3.25110
C	-3.00789	0.41251	-0.32263
C	-3.62931	-0.16158	0.82109
C	-4.68737	-1.05875	0.63771
C	-5.14477	-1.39469	-0.63455
C	-4.54072	-0.82025	-1.75046
C	-3.47990	0.08497	-1.62385
C	-3.13241	0.14410	2.23197
C	-2.38081	-1.06368	2.82822
C	-4.26371	0.59755	3.17182
C	-2.82866	0.66780	-2.87692
C	-3.84382	1.38207	-3.78725
C	-2.05845	-0.41195	-3.66405
C	1.72802	4.02969	0.33017
C	0.72456	2.89940	0.15464
C	-0.63996	3.27729	0.09803
C	-1.81399	2.50537	-0.05033
C	-3.13319	3.26140	-0.06645
C	2.55995	1.33329	0.14680
H	-1.66656	-4.60436	-0.79534
H	-2.05162	-2.08349	-0.62251

H	1.05873	-4.92487	-0.56361
H	1.99222	-2.33281	-0.28924
H	1.23351	5.00213	0.35610
H	2.46083	4.03278	-0.48327
H	2.29509	3.90468	1.25907
H	-0.81235	4.34333	0.18412
H	-2.97971	4.33623	0.04353
H	-3.78781	2.92015	0.74302
H	-3.67421	3.08251	-1.00201
H	4.94147	0.37576	2.39546
H	6.27849	0.17960	0.32575
H	5.24329	0.69214	-1.86013
H	1.39718	1.59584	2.47029
H	2.39164	1.98276	4.67973
H	3.30439	2.89909	3.46890
H	3.96856	1.40432	4.13868
H	1.37187	-0.28798	4.09209
H	2.88950	-0.90477	3.41519
H	1.42282	-0.87735	2.42113
H	1.70908	1.88215	-2.25968
H	2.03903	0.31383	-4.15769
H	1.90111	-0.56412	-2.62369
H	3.48745	-0.34729	-3.38030
H	2.99860	2.68405	-4.19537
H	4.51029	2.09258	-3.50021
H	3.64253	3.41860	-2.71754
H	-5.16177	-1.50459	1.50847
H	-5.96815	-2.09354	-0.75528
H	-4.90067	-1.07987	-2.74314
H	-2.41374	0.96406	2.15628
H	-2.00482	-0.83160	3.83130
H	-1.52423	-1.34163	2.20592
H	-3.03820	-1.93750	2.91194
H	-3.85299	0.89300	4.14364
H	-4.99157	-0.20104	3.35488
H	-4.80808	1.45390	2.76059
H	-2.09678	1.41085	-2.55013
H	-3.32923	1.85885	-4.62892
H	-4.39386	2.15765	-3.24470
H	-4.57925	0.68557	-4.20576
H	-1.58572	0.01908	-4.55387
H	-2.72706	-1.21436	-3.99804
H	-1.26911	-0.86024	-3.05238
C	0.98115	-2.69506	-0.40629
N	-1.15214	-2.55172	-0.59569
N	1.17045	1.64729	0.07155
N	-1.82510	1.17959	-0.17425
Cu	-0.11283	0.18038	-0.18760

74. L^1CuXO_2 η^1 singlet, X = pyrazole

C	0.86117	-3.67832	-0.85496
C	3.98372	1.33011	3.41808
C	3.04546	-0.92774	2.73782
C	2.57850	2.20622	-2.49092
C	2.15442	1.14597	-3.52744
C	3.32006	3.35736	-3.19828
C	-2.67608	0.69826	-0.17546
C	-3.61470	0.51700	0.87679
C	-4.83439	-0.09777	0.57731
C	-5.12819	-0.54946	-0.70529
C	-4.18734	-0.40098	-1.71862
N	1.03040	-1.49032	-0.45142
C	-2.95253	0.21060	-1.48030

C	-3.35420	0.98978	2.30476
C	-3.59946	-0.13280	3.33336
C	-4.20802	2.22323	2.66757
C	-1.97194	0.37279	-2.63866
C	-2.51478	1.33795	-3.71270
C	-1.60848	-0.98394	-3.27283
C	2.19984	4.09999	0.50647
C	1.14652	3.01444	0.35967
C	-0.19266	3.44093	0.32465
C	2.03184	-3.24435	-1.45924
C	-1.36868	2.69975	0.07402
C	-2.58650	3.53397	-0.29832
C	2.88119	1.40127	-0.04097
C	3.66676	0.78026	0.96127
C	4.95907	0.35623	0.63387
C	5.47616	0.52880	-0.64606
C	4.69737	1.13896	-1.62571
C	3.39902	1.58551	-1.35521
C	3.14009	0.56842	2.37827
H	2.84639	-1.14953	-1.45186
H	0.40034	-4.65426	-0.80608
H	-0.54699	-2.52922	0.34743
H	2.73732	-3.83358	-2.02475
H	1.74330	5.04933	0.79190
H	2.75006	4.25262	-0.42588
H	2.93527	3.81939	1.26658
H	-0.33600	4.51236	0.39076
H	-2.54339	4.51523	0.17926
H	-3.52923	3.05143	-0.04564
H	-2.58481	3.69661	-1.38319
H	5.56950	-0.12075	1.39588
H	6.48058	0.18809	-0.88178
H	5.10431	1.26479	-2.62550
H	2.12802	0.98213	2.41807
H	3.54830	1.21949	4.41734
H	4.03465	2.39963	3.18793
H	5.01089	0.95063	3.46059
H	2.62851	-1.05210	3.74342
H	4.03224	-1.40447	2.72430
H	2.40145	-1.46491	2.03669
H	1.66064	2.61874	-2.06575
H	1.55030	1.60482	-4.31898
H	1.56179	0.35086	-3.06896
H	3.02805	0.68407	-4.00203
H	2.65793	3.84266	-3.92384
H	4.19686	2.99938	-3.74877
H	3.66365	4.12107	-2.49360
H	-5.56780	-0.22778	1.36781
H	-6.08564	-1.01959	-0.91361
H	-4.41980	-0.75711	-2.71872
H	-2.29975	1.26797	2.37177
H	-3.26961	0.19543	4.32543
H	-3.05217	-1.03663	3.06160
H	-4.66438	-0.38146	3.41222
H	-4.00622	2.52942	3.70005
H	-5.27787	1.99593	2.59317
H	-4.00571	3.08209	2.02170
H	-1.05265	0.80779	-2.23733
H	-1.77320	1.48859	-4.50555
H	-2.76089	2.31759	-3.29079
H	-3.42393	0.94355	-4.18092
H	-0.86023	-0.84826	-4.06181
H	-2.48296	-1.46189	-3.72876
H	-1.19787	-1.67304	-2.52982

N	0.28801	-2.60695	-0.27502
C	2.09360	-1.87086	-1.17445
N	1.52738	1.74168	0.24781
N	-1.44270	1.37193	0.06767
O	-0.69333	-0.80630	1.77007
O	-1.55489	-1.73554	1.45547
Cu	0.19664	0.29553	0.46552

75. L^1CuXO_2 η^1 triplet, X = pyrazole

C	0.92953	-3.62811	-1.08632
C	3.71513	1.43044	3.52198
C	2.86332	-0.86479	2.86219
C	2.77308	2.14612	-2.47461
C	2.36875	1.07627	-3.50986
C	3.59548	3.25604	-3.15784
C	-2.72398	0.75007	-0.14643
C	-3.56206	0.50998	0.97494
C	-4.76551	-0.17336	0.76797
C	-5.13899	-0.63100	-0.49200
C	-4.29788	-0.41157	-1.57704
N	1.04672	-1.46809	-0.53116
C	-3.08497	0.27019	-1.43025
C	-3.20651	0.98447	2.38481
C	-3.40822	-0.11327	3.44833
C	-4.01196	2.23892	2.78340
C	-2.20121	0.49247	-2.65639
C	-2.88445	1.41094	-3.68923
C	-1.77907	-0.83780	-3.31019
C	2.20909	4.09385	0.44088
C	1.14599	3.02028	0.26810
C	-0.18379	3.46805	0.21007
C	2.12055	-3.14058	-1.60019
C	-1.38067	2.74486	0.00224
C	-2.60066	3.60364	-0.29867
C	2.88676	1.38846	-0.00316
C	3.59067	0.78566	1.07042
C	4.89842	0.33877	0.84988
C	5.50894	0.46825	-0.39371
C	4.81146	1.06280	-1.44208
C	3.50370	1.53328	-1.27632
C	2.96150	0.61797	2.45177
H	2.90878	-1.04331	-1.40606
H	0.48520	-4.61221	-1.11374
H	-0.50508	-2.59671	0.15449
H	2.86449	-3.68526	-2.16088
H	1.76108	5.03477	0.76509
H	2.74564	4.27827	-0.49503
H	2.95478	3.78594	1.17934
H	-0.30919	4.54343	0.26071
H	-2.62348	4.48079	0.35366
H	-3.53749	3.05846	-0.19640
H	-2.53433	3.97002	-1.33007
H	5.44611	-0.12230	1.66768
H	6.52322	0.10970	-0.54597
H	5.29178	1.15912	-2.41214
H	1.94322	1.01363	2.39968
H	3.21201	1.34428	4.49147
H	3.76308	2.49257	3.26010
H	4.74326	1.07310	3.64971
H	2.36530	-0.96023	3.83336
H	3.85515	-1.32325	2.94983
H	2.28937	-1.44169	2.13187
H	1.84738	2.59850	-2.11089

H	1.85623	1.54096	-4.36015
H	1.69336	0.33264	-3.07783
H	3.24687	0.54799	-3.89970
H	2.99646	3.75033	-3.93058
H	4.49079	2.85682	-3.64696
H	3.92319	4.01910	-2.44470
H	-5.42106	-0.35634	1.61444
H	-6.07901	-1.15965	-0.62526
H	-4.58849	-0.77375	-2.55977
H	-2.14551	1.24832	2.38379
H	-3.01123	0.22677	4.41154
H	-2.89690	-1.03839	3.17659
H	-4.46973	-0.34014	3.60106
H	-3.73199	2.56829	3.79060
H	-5.08713	2.02487	2.79016
H	-3.84444	3.07481	2.09963
H	-1.28960	0.99580	-2.32174
H	-2.21486	1.60810	-4.53435
H	-3.16435	2.37246	-3.24736
H	-3.79643	0.95302	-4.08900
H	-1.09589	-0.65386	-4.14732
H	-2.64222	-1.38593	-3.70412
H	-1.26875	-1.48911	-2.59423
N	0.31375	-2.60183	-0.46944
C	2.14999	-1.78847	-1.22237
N	1.51710	1.74219	0.16723
N	-1.46909	1.42051	0.01425
O	-0.69715	-0.82709	1.76659
O	-1.22368	-1.99336	1.64593
Cu	0.15300	0.26935	0.23970

76. L^1CuXO_2 η^2 singlet, X = pyrazole

C	0.06656	-3.70515	-0.83862
C	3.76210	1.77737	3.26150
C	3.13874	-0.65387	2.92927
C	1.97262	2.14506	-2.50351
C	1.57960	1.07199	-3.53752
C	2.63123	3.34029	-3.22189
C	-2.95480	0.76095	-0.38723
C	-3.89233	0.49849	0.64786
C	-5.05752	-0.20592	0.32323
C	-5.29729	-0.65853	-0.97003
C	-4.35670	-0.42084	-1.96558
N	0.56050	-1.51402	-0.79691
C	-3.17243	0.27711	-1.70054
C	-3.69953	0.98024	2.08585
C	-3.86641	-0.15697	3.11145
C	-4.66007	2.13895	2.42666
C	-2.17894	0.51100	-2.83469
C	-2.71488	1.54544	-3.84526
C	-1.80711	-0.79914	-3.55460
C	1.83930	4.20855	0.42986
C	0.76560	3.14092	0.32342
C	-0.56216	3.58147	0.22036
C	1.11182	-3.51005	-1.72480
C	-1.71188	2.82274	-0.09555
C	-2.92592	3.63324	-0.51626
C	2.45739	1.45619	-0.04041
C	3.33123	0.90096	0.92756
C	4.59824	0.47261	0.51616
C	5.00736	0.57493	-0.80822
C	4.14266	1.12016	-1.75193
C	2.86516	1.56751	-1.40073

C	2.95789	0.78213	2.40153
H	2.13889	-1.56074	-2.17679
H	-0.47223	-4.59496	-0.54737
H	-0.86490	-2.23020	0.43689
H	1.60809	-4.25549	-2.32766
H	1.39315	5.19513	0.56555
H	2.46952	4.23433	-0.46207
H	2.49749	3.99670	1.27770
H	-0.70850	4.65394	0.25096
H	-3.04298	4.50069	0.13880
H	-3.84554	3.05067	-0.50889
H	-2.77151	4.01350	-1.53244
H	5.27739	0.05171	1.25183
H	5.99495	0.23213	-1.10469
H	4.46537	1.19780	-2.78675
H	1.90060	1.03479	2.50449
H	3.45518	1.70863	4.31100
H	3.61251	2.81186	2.93500
H	4.83672	1.56754	3.21293
H	2.76963	-0.72314	3.95816
H	4.19226	-0.95604	2.93613
H	2.57677	-1.36690	2.32241
H	1.04717	2.50455	-2.04849
H	0.93248	1.50464	-4.30971
H	1.04112	0.24681	-3.06757
H	2.46210	0.66013	-4.04081
H	1.93175	3.78139	-3.94070
H	3.52267	3.03314	-3.77938
H	2.93521	4.12747	-2.52539
H	-5.79087	-0.40080	1.10024
H	-6.21192	-1.19874	-1.19943
H	-4.54461	-0.78268	-2.97232
H	-2.67585	1.34968	2.18092
H	-3.63512	0.21205	4.11681
H	-3.18907	-0.98434	2.89165
H	-4.89269	-0.54062	3.13424
H	-4.48665	2.48954	3.45025
H	-5.70528	1.81606	2.35883
H	-4.53288	2.99192	1.75440
H	-1.26405	0.91575	-2.39372
H	-1.97311	1.74079	-4.62813
H	-2.95517	2.49788	-3.36270
H	-3.62687	1.18427	-4.33467
H	-1.03729	-0.60971	-4.31026
H	-2.66807	-1.23826	-4.07074
H	-1.41566	-1.54037	-2.85359
N	-0.23416	-2.49444	-0.32060
C	1.38205	-2.12869	-1.65578
N	1.13296	1.85707	0.32305
N	-1.75637	1.49611	-0.08904
O	-1.05755	-0.80119	1.68062
O	0.23509	-0.69069	2.07574
Cu	-0.23457	0.54121	0.67217

77. L^1CuXO_2 η^2 triplet, X = pyrazole

C	0.84671	-3.89319	-0.66369
C	-5.23447	-0.77742	-0.65690
C	-4.34163	-0.52114	-1.69212
C	-3.14276	0.16317	-1.46378
C	-3.47089	0.77761	2.35744
C	-3.67700	-0.35741	3.37687
C	-4.34256	1.98794	2.75714
C	-2.19540	0.42890	-2.63154

C	-2.82231	1.39536	-3.65625
C	-1.74483	-0.87272	-3.31974
C	3.80141	1.45760	3.40494
C	2.09091	3.92017	0.48858
C	1.01694	2.85056	0.36714
C	-0.30895	3.31320	0.33915
C	2.03885	-3.42562	-1.18703
C	-1.51168	2.60585	0.11683
C	-2.72234	3.48425	-0.16962
C	2.72827	1.21165	-0.00530
C	3.52223	0.64399	1.02395
C	4.81540	0.20719	0.71391
C	5.32868	0.31408	-0.57436
C	3.04864	-0.92760	2.97364
C	4.54509	0.87769	-1.57845
C	3.24835	1.33985	-1.32337
C	3.01608	0.52548	2.46089
C	2.42865	1.92200	-2.47943
C	1.94971	0.82228	-3.44870
C	3.19474	3.00994	-3.25937
C	-2.85350	0.61309	-0.14990
C	2.02336	-2.04056	-0.94782
C	-3.74556	0.33445	0.92010
C	-4.92906	-0.35344	0.63336
H	2.76556	-1.29788	-1.19438
H	0.42708	-4.88664	-0.60712
H	-0.65819	-2.78203	0.37999
H	2.81141	-4.00534	-1.66801
H	1.66306	4.85766	0.84894
H	2.56637	4.11595	-0.47645
H	2.88140	3.60610	1.17449
H	-0.42459	4.38734	0.42792
H	-2.74347	4.34101	0.50957
H	-3.66317	2.94159	-0.09008
H	-2.64751	3.88389	-1.18724
H	5.43099	-0.22334	1.49931
H	6.33340	-0.03553	-0.79594
H	4.94847	0.95779	-2.58431
H	1.97105	0.84837	2.47118
H	3.39667	1.40408	4.42169
H	3.74996	2.50100	3.07704
H	4.86037	1.17818	3.45241
H	2.63138	-0.98332	3.98497
H	4.06991	-1.32302	3.01572
H	2.45500	-1.58310	2.33151
H	1.53420	2.38664	-2.05802
H	1.35212	1.25828	-4.25789
H	1.33254	0.07882	-2.93707
H	2.79694	0.29970	-3.90706
H	2.54026	3.47430	-4.00551
H	4.05550	2.59426	-3.79440
H	3.56906	3.80127	-2.60293
H	-5.62450	-0.56489	1.44071
H	-6.16287	-1.30702	-0.85349
H	-4.58103	-0.85501	-2.69867
H	-2.42238	1.08335	2.41295
H	-3.34854	-0.02975	4.36967
H	-3.10563	-1.24613	3.10391
H	-4.73236	-0.64027	3.46350
H	-4.10558	2.31085	3.77738
H	-5.40690	1.72655	2.73014
H	-4.19500	2.84229	2.09296
H	-1.30000	0.90938	-2.22792
H	-2.11147	1.62429	-4.45863

H	-3.11895	2.33886	-3.18830
H	-3.71654	0.95990	-4.11705
H	-1.01740	-0.65424	-4.10970
H	-2.58564	-1.40045	-3.78427
H	-1.27288	-1.55613	-2.60663
N	0.89286	-1.67664	-0.32942
N	0.19006	-2.82197	-0.17163
N	1.37342	1.56510	0.26677
N	-1.61355	1.28220	0.09699
O	-1.07032	-1.15579	1.63490
O	-0.35063	-1.16701	2.70137
Cu	-0.01566	0.12761	0.43208

78. L^1CuX, X = 1-methylpyrazole

N	-0.03074	-1.80861	-0.44075
C	0.49271	-4.00634	-0.54575
C	-0.88115	-3.87584	-0.66405
C	3.14870	1.02816	1.40192
C	4.48475	0.61492	1.43822
C	5.24062	0.49813	0.27560
C	4.65412	0.79209	-0.95170
C	3.32084	1.20588	-1.04406
C	2.33966	1.08978	2.69474
C	3.04465	1.88976	3.80466
C	1.98515	-0.32915	3.18420
C	2.70498	1.46017	-2.41731
C	2.52261	0.13742	-3.18953
C	3.51254	2.47139	-3.25110
C	-3.00789	0.41251	-0.32263
C	-3.62931	-0.16158	0.82109
C	-4.68737	-1.05875	0.63771
C	-5.14477	-1.39469	-0.63455
C	-4.54072	-0.82025	-1.75046
C	-3.47990	0.08497	-1.62385
C	-3.13241	0.14410	2.23197
C	-2.38081	-1.06368	2.82822
C	-4.26371	0.59755	3.17182
C	-2.82866	0.66780	-2.87692
C	-3.84382	1.38207	-3.78725
C	-2.05845	-0.41195	-3.66405
C	1.72802	4.02969	0.33017
C	0.72456	2.89940	0.15464
C	-0.63996	3.27729	0.09803
C	-1.81399	2.50537	-0.05033
C	-3.13319	3.26140	-0.06645
C	2.55995	1.33329	0.14680
H	-1.66656	-4.60436	-0.79534
H	-2.05162	-2.08349	-0.62251
H	1.05873	-4.92487	-0.56361
H	1.99222	-2.33281	-0.28924
H	1.23351	5.00213	0.35610
H	2.46083	4.03278	-0.48327
H	2.29509	3.90468	1.25907
H	-0.81235	4.34333	0.18412
H	-2.97971	4.33623	0.04353
H	-3.78781	2.92015	0.74302
H	-3.67421	3.08251	-1.00201
H	4.94147	0.37576	2.39546
H	6.27849	0.17960	0.32575
H	5.24329	0.69214	-1.86013
H	1.39718	1.59584	2.47029
H	2.39164	1.98276	4.67973
H	3.30439	2.89909	3.46890

H	3.96856	1.40432	4.13868
H	1.37187	-0.28798	4.09209
H	2.88950	-0.90477	3.41519
H	1.42282	-0.87735	2.42113
H	1.70908	1.88215	-2.25968
H	2.03903	0.31383	-4.15769
H	1.90111	-0.56412	-2.62369
H	3.48745	-0.34729	-3.38030
H	2.99860	2.68405	-4.19537
H	4.51029	2.09258	-3.50021
H	3.64253	3.41860	-2.71754
H	-5.16177	-1.50459	1.50847
H	-5.96815	-2.09354	-0.75528
H	-4.90067	-1.07987	-2.74314
H	-2.41374	0.96406	2.15628
H	-2.00482	-0.83160	3.83130
H	-1.52423	-1.34163	2.20592
H	-3.03820	-1.93750	2.91194
H	-3.85299	0.89300	4.14364
H	-4.99157	-0.20104	3.35488
H	-4.80808	1.45390	2.76059
H	-2.09678	1.41085	-2.55013
H	-3.32923	1.85885	-4.62892
H	-4.39386	2.15765	-3.24470
H	-4.57925	0.68557	-4.20576
H	-1.58572	0.01908	-4.55387
H	-2.72706	-1.21436	-3.99804
H	-1.26911	-0.86024	-3.05238
C	0.98115	-2.69506	-0.40629
N	-1.15214	-2.55172	-0.59569
N	1.17045	1.64729	0.07155
N	-1.82510	1.17959	-0.17425
Cu	-0.11283	0.18038	-0.18760

79. L^1CuXO_2 η^1 singlet, X = 1-methylpyrazole

H	-1.97947	-2.06421	-0.71175
H	-1.89690	-3.83879	-0.65520
H	-1.60999	-2.87921	0.82715
C	0.71339	-3.94469	-0.93898
C	3.67822	1.65540	3.48208
C	2.86564	-0.71207	3.08438
C	2.59071	1.73842	-2.52395
C	2.22771	0.56566	-3.45717
C	3.34558	2.83150	-3.30410
C	-2.85482	0.57179	-0.13817
C	-3.70987	0.23238	0.94419
C	-4.89976	-0.44908	0.65989
C	-5.25642	-0.79298	-0.64033
C	-4.41612	-0.44795	-1.69376
N	0.69210	-1.76271	-0.46922
C	-3.21155	0.22950	-1.47068
C	-3.41215	0.62128	2.39192
C	-3.43198	-0.59024	3.34325
C	-4.39980	1.69601	2.89444
C	-2.34557	0.62648	-2.66563
C	-3.04827	1.69543	-3.52786
C	-1.94025	-0.58239	-3.52878
C	2.07953	3.95095	0.37772
C	1.03151	2.85313	0.29675
C	-0.31278	3.27196	0.33806
C	2.01587	-3.49557	-1.06276
C	-1.51265	2.54382	0.17774
C	-2.75659	3.41892	0.06953

C	2.78236	1.23956	-0.00117
C	3.51792	0.75788	1.11219
C	4.82709	0.30884	0.90520
C	5.40686	0.31751	-0.36009
C	4.67504	0.78935	-1.44710
C	3.36560	1.25957	-1.29590
C	2.92095	0.72056	2.51827
H	2.74002	-1.39533	-0.73651
H	0.27875	-4.92446	-1.07236
C	-1.47345	-2.91527	-0.25621
H	2.88469	-4.07182	-1.33993
H	1.63626	4.89418	0.70183
H	2.54799	4.11243	-0.59860
H	2.87931	3.67972	1.07191
H	-0.45333	4.34210	0.44185
H	-2.80918	4.10574	0.91980
H	-3.67917	2.84310	0.02729
H	-2.69307	4.03281	-0.83583
H	5.40039	-0.05833	1.75240
H	6.42317	-0.04089	-0.49908
H	5.12917	0.79040	-2.43467
H	1.89125	1.08078	2.45005
H	3.19432	1.66225	4.46536
H	3.70252	2.68607	3.11258
H	4.71513	1.33033	3.62571
H	2.40634	-0.70775	4.07921
H	3.86801	-1.14429	3.18531
H	2.26895	-1.37202	2.44954
H	1.64993	2.17159	-2.17567
H	1.65422	0.92383	-4.32025
H	1.62432	-0.18453	-2.93834
H	3.12725	0.06861	-3.83854
H	2.72110	3.21910	-4.11680
H	4.26704	2.44723	-3.75548
H	3.62113	3.67258	-2.65969
H	-5.56523	-0.70905	1.47836
H	-6.18851	-1.31795	-0.83168
H	-4.70304	-0.70144	-2.71113
H	-2.40346	1.03808	2.42375
H	-3.17763	-0.26657	4.35906
H	-2.70550	-1.34901	3.04519
H	-4.42528	-1.05199	3.39117
H	-4.13929	2.00326	3.91361
H	-5.42582	1.31102	2.91763
H	-4.39613	2.58940	2.26394
H	-1.42570	1.06892	-2.27481
H	-2.39495	2.02422	-4.34412
H	-3.31731	2.57503	-2.93484
H	-3.96931	1.30434	-3.97543
H	-1.30432	-0.25901	-4.36021
H	-2.81142	-1.08868	-3.95955
H	-1.37645	-1.31830	-2.94671
N	-0.05614	-2.88991	-0.58861
C	1.94971	-2.12939	-0.75770
N	1.41190	1.58555	0.16772
N	-1.59742	1.22005	0.07850
O	-0.42509	-0.58565	2.12643
O	-0.46011	-1.83013	2.41319
Cu	0.06379	0.09560	0.32057

80. L^1CuXO_2 η^1 triplet, X = 1-methylpyrazole

H	-2.11526	-2.09231	-0.48917
H	-2.06192	-3.86407	-0.32954

H	-1.70898	-2.83084	1.08107
C	0.54536	-4.02085	-0.70619
C	3.73174	1.69139	3.43701
C	3.17031	-0.75093	3.08431
C	2.51630	1.68946	-2.52180
C	2.21078	0.50437	-3.45985
C	3.18626	2.83389	-3.30734
C	-2.88552	0.61882	-0.21420
C	-3.75049	0.20552	0.83291
C	-4.93864	-0.45601	0.49992
C	-5.27880	-0.72342	-0.82351
C	-4.41880	-0.32492	-1.84271
N	0.55140	-1.81706	-0.33939
C	-3.22111	0.34496	-1.56643
C	-3.43061	0.48552	2.30079
C	-3.50146	-0.78140	3.17426
C	-4.35455	1.57463	2.88399
C	-2.31102	0.76233	-2.72088
C	-3.00262	1.77157	-3.65751
C	-1.79698	-0.45591	-3.51230
C	2.09971	3.89822	0.43899
C	1.04996	2.79908	0.35560
C	-0.29181	3.23946	0.39656
C	1.84416	-3.58587	-0.89766
C	-1.50831	2.55420	0.18574
C	-2.72386	3.46209	0.03937
C	2.80400	1.20887	-0.00198
C	3.60026	0.75044	1.07990
C	4.92246	0.36489	0.82992
C	5.46214	0.40466	-0.45194
C	4.66966	0.83714	-1.51143
C	3.34552	1.24643	-1.31559
C	3.05186	0.67125	2.50269
H	2.58776	-1.47310	-0.69675
H	0.10213	-5.00303	-0.78062
C	-1.60958	-2.92649	-0.00240
H	2.69982	-4.18004	-1.17856
H	1.67586	4.81341	0.85670
H	2.48849	4.13196	-0.55794
H	2.95358	3.59331	1.04803
H	-0.40658	4.31113	0.51865
H	-2.72851	4.21811	0.83029
H	-3.66498	2.91428	0.07056
H	-2.67577	3.99754	-0.91590
H	5.54034	0.02570	1.65745
H	6.49065	0.09933	-0.62457
H	5.08896	0.86041	-2.51420
H	1.98914	0.92123	2.45742
H	3.30262	1.63623	4.44409
H	3.60565	2.71686	3.07588
H	4.80750	1.49898	3.52244
H	2.68910	-0.80404	4.06721
H	4.21681	-1.04959	3.21397
H	2.68994	-1.48867	2.43497
H	1.55804	2.06010	-2.14874
H	1.59174	0.83010	-4.30418
H	1.67281	-0.29101	-2.93544
H	3.13162	0.07327	-3.86969
H	2.52288	3.19070	-4.10339
H	4.11981	2.50951	-3.78063
H	3.42417	3.68425	-2.66045
H	-5.61257	-0.76521	1.29453
H	-6.20711	-1.23728	-1.05809
H	-4.68344	-0.53370	-2.87643

H	-2.40423	0.85877	2.34637
H	-3.18427	-0.55279	4.19763
H	-2.84992	-1.57340	2.79521
H	-4.51940	-1.18303	3.23062
H	-4.08537	1.79080	3.92420
H	-5.40173	1.25080	2.87049
H	-4.28822	2.50839	2.31923
H	-1.43796	1.25834	-2.28900
H	-2.31141	2.10921	-4.43815
H	-3.34821	2.65278	-3.10783
H	-3.87298	1.32906	-4.15545
H	-1.11904	-0.13781	-4.31225
H	-2.61848	-1.01422	-3.97600
H	-1.24562	-1.14394	-2.86330
N	-0.20518	-2.94399	-0.37925
C	1.79510	-2.20543	-0.65557
N	1.43125	1.53288	0.20640
N	-1.63107	1.23280	0.07910
O	-0.18769	-0.45870	2.40729
O	-0.17027	-1.63246	2.80068
Cu	-0.00668	0.08410	0.20029

81. L^1CuXO_2 η^2 singlet, X = 1-methylpyrazole

H	-1.67156	-3.07524	0.75530
H	-2.02592	-2.43244	-0.85978
H	-1.93818	-4.19361	-0.62097
C	0.69470	-4.30367	-0.80156
C	3.85088	1.64735	3.62438
C	3.35545	-0.82678	3.45694
C	2.37646	1.53958	-2.22698
C	2.00970	0.38611	-3.18127
C	3.06667	2.67270	-3.01393
C	-2.77264	0.49270	-0.02407
C	-3.63864	0.09831	1.03089
C	-4.82040	-0.57486	0.70163
C	-5.14847	-0.86668	-0.61926
C	-4.28934	-0.47846	-1.64131
N	0.60398	-2.06819	-0.63028
C	-3.09485	0.20302	-1.37289
C	-3.35227	0.42599	2.49669
C	-3.51902	-0.79213	3.42343
C	-4.23659	1.58968	2.99270
C	-2.20719	0.62676	-2.54264
C	-2.93266	1.62823	-3.46481
C	-1.70425	-0.58225	-3.35451
C	2.15374	3.76929	0.59659
C	1.06178	2.71518	0.57997
C	-0.25793	3.19636	0.54941
C	1.99015	-3.84052	-0.93184
C	-1.44911	2.48565	0.30357
C	-2.66531	3.34569	0.00276
C	2.75074	1.02639	0.28979
C	3.58554	0.57271	1.34266
C	4.88330	0.15203	1.02737
C	5.35686	0.16299	-0.27993
C	4.53003	0.61251	-1.30478
C	3.22710	1.05436	-1.05040
C	3.13940	0.55222	2.80347
H	2.65435	-1.69758	-0.85587
H	0.28492	-5.30317	-0.82099
C	-1.52221	-3.23175	-0.31434
H	2.88242	-4.42476	-1.09718
H	1.76200	4.71450	0.97648

H	2.53674	3.94650	-0.41320
H	2.99949	3.45865	1.21276
H	-0.36367	4.27317	0.59626
H	-2.65218	4.24300	0.62675
H	-3.60371	2.81501	0.15855
H	-2.63491	3.67497	-1.04203
H	5.53414	-0.19203	1.82602
H	6.36608	-0.17487	-0.49931
H	4.90287	0.62165	-2.32535
H	2.06744	0.75653	2.83140
H	3.49865	1.63376	4.66209
H	3.66420	2.64845	3.22235
H	4.93593	1.49233	3.63911
H	2.91935	-0.83593	4.46169
H	4.42034	-1.06649	3.55925
H	2.87720	-1.61811	2.87600
H	1.43984	1.93652	-1.82934
H	1.40630	0.76082	-4.01649
H	1.43757	-0.39048	-2.66940
H	2.90776	-0.07835	-3.60501
H	2.38575	3.07693	-3.77134
H	3.96075	2.31595	-3.53709
H	3.37562	3.49729	-2.36389
H	-5.49806	-0.87302	1.49634
H	-6.07215	-1.39068	-0.84999
H	-4.55140	-0.70228	-2.67191
H	-2.30925	0.74011	2.57005
H	-3.20531	-0.52947	4.43969
H	-2.90228	-1.62911	3.08985
H	-4.56126	-1.12620	3.48188
H	-4.00593	1.82362	4.03818
H	-5.29967	1.32876	2.93584
H	-4.08646	2.50070	2.40627
H	-1.32704	1.12694	-2.13011
H	-2.25579	1.98738	-4.24809
H	-3.30189	2.49741	-2.91189
H	-3.79333	1.16460	-3.96019
H	-1.07990	-0.24705	-4.18983
H	-2.53551	-1.15869	-3.77607
H	-1.10063	-1.25037	-2.73483
N	-0.10492	-3.22317	-0.62814
C	1.87541	-2.44401	-0.81398
N	1.39856	1.42456	0.55402
N	-1.54145	1.15953	0.28406
O	-0.71649	-1.23558	1.99295
O	0.60442	-1.12220	2.20372
Cu	-0.00419	0.11593	0.89422

82. L^1CuXO_2 η^2 triplet, X = 1-methylpyrazole

H	-1.62609	-3.17095	0.85874
H	-1.87755	-2.19947	-0.60621
H	-1.81078	-3.97098	-0.72918
C	0.82728	-4.09831	-0.75756
C	3.83482	1.51105	3.61833
C	3.32531	-0.93924	3.25189
C	2.43333	1.56606	-2.30865
C	2.12580	0.38284	-3.24856
C	3.06343	2.72410	-3.10652
C	-2.81595	0.49485	0.00952
C	-3.70154	0.11870	1.05327
C	-4.87564	-0.56540	0.71723
C	-5.18332	-0.88502	-0.60214
C	-4.30799	-0.51297	-1.61827

N	0.75023	-1.92059	-0.25555
C	-3.12032	0.17432	-1.34052
C	-3.43289	0.47503	2.51506
C	-3.65229	-0.71287	3.47157
C	-4.29208	1.67358	2.96872
C	-2.20997	0.58850	-2.49704
C	-2.89820	1.62512	-3.40756
C	-1.72825	-0.61524	-3.32840
C	2.15514	3.75312	0.62588
C	1.08002	2.67918	0.55481
C	-0.24570	3.14948	0.56305
C	2.12996	-3.63597	-0.78276
C	-1.45904	2.45937	0.34857
C	-2.66313	3.35792	0.10222
C	2.80377	1.06137	0.20209
C	3.63881	0.59881	1.25323
C	4.95761	0.23451	0.95414
C	5.45571	0.30366	-0.34254
C	4.62562	0.74063	-1.37095
C	3.30216	1.12567	-1.12863
C	3.14570	0.48588	2.69530
H	2.80831	-1.53471	-0.37977
H	0.41196	-5.07811	-0.94330
C	-1.40863	-3.09962	-0.20931
H	3.02289	-4.19631	-1.01297
H	1.72675	4.71142	0.92486
H	2.64287	3.88761	-0.34426
H	2.93966	3.48105	1.33647
H	-0.34944	4.22529	0.64534
H	-2.68570	4.16831	0.83676
H	-3.60884	2.81899	0.13994
H	-2.57582	3.82398	-0.88605
H	5.60605	-0.10904	1.75571
H	6.48333	0.01828	-0.55124
H	5.01359	0.78414	-2.38535
H	2.07521	0.70554	2.69618
H	3.44000	1.43486	4.63785
H	3.67613	2.53818	3.27481
H	4.91683	1.34145	3.66775
H	2.88749	-1.01276	4.25304
H	4.38385	-1.21141	3.33289
H	2.83023	-1.67869	2.61734
H	1.47892	1.91942	-1.91040
H	1.48733	0.70715	-4.07865
H	1.61050	-0.42288	-2.71952
H	3.04488	-0.03074	-3.67947
H	2.37532	3.06484	-3.88826
H	3.99260	2.41784	-3.59988
H	3.29705	3.58237	-2.46907
H	-5.56439	-0.85153	1.50717
H	-6.10267	-1.41488	-0.83673
H	-4.55395	-0.75321	-2.64954
H	-2.38255	0.76831	2.59126
H	-3.33205	-0.44038	4.48330
H	-3.07440	-1.58568	3.16004
H	-4.70849	-0.99972	3.53331
H	-4.07005	1.92934	4.01110
H	-5.36025	1.43598	2.90344
H	-4.11149	2.56372	2.36004
H	-1.32279	1.06078	-2.06679
H	-2.20861	1.97316	-4.18503
H	-3.23652	2.49679	-2.83953
H	-3.77400	1.19724	-3.90902
H	-1.06866	-0.28024	-4.13645

H	-2.56472	-1.15347	-3.78825
H	-1.16451	-1.32512	-2.71597
N	0.02560	-3.05468	-0.44229
C	2.02722	-2.27414	-0.46134
N	1.43680	1.39448	0.45962
N	-1.57498	1.13750	0.30820
O	-0.84574	-1.23785	2.07199
O	0.12606	-1.23417	2.89582
Cu	0.02796	-0.03456	0.63923

83. L^1CuX, X = tetrazole

C	2.9716867626	1.5510939131	3.7919050819
C	1.9707378363	-.6539204303	3.0374406041
C	2.5191846018	1.3875398339	-2.4493066479
C	2.1647615525	.0535111239	-3.1381115660
C	3.3493054128	2.2811476927	-3.3863958044
C	-3.1171937306	.1746408988	-.3950762125
C	-3.7736215213	-.3768122796	.7424483001
C	-4.8018470875	-1.3060872879	.5493064531
C	-5.1990283602	-1.7017607032	-.7263910681
C	-4.5711329364	-1.1437318353	-1.8383155963
N	-.0326541074	-4.1879695805	-.2699531868
C	-3.5404672274	-.2015451615	-1.7031918874
C	-3.3400421650	-.0162025432	2.1615928004
C	-2.6113284197	-1.1934622700	2.8411431265
C	-4.5171172958	.4666894795	3.0285160148
C	-2.8917092195	.3885004093	-2.9552773030
C	-3.9237728476	1.1050862067	-3.8471719289
C	-2.1253961383	-.6759509796	-3.7658429495
C	1.5723816734	3.8408380770	.3317304753
C	.5863624520	2.6982430836	.1485786188
C	-.7837444163	3.0553907470	.0773144531
C	-1.2887537699	-3.9698968281	-.6208426320
C	-1.9429934405	2.2712001769	-.0975859270
C	-3.2709594999	3.0109610115	-.1362993905
C	2.4564176123	1.1770073584	.1070330454
C	3.0733177986	.8426422041	1.3365423272
C	4.4223397393	.4711029896	1.3298983278
C	5.1567098433	.4257733088	.1490019700
C	4.5380914783	.7474590441	-1.0556095345
N	.5233382547	-2.9709860762	-.0930173357
C	3.1924656539	1.1248563705	-1.1037074168
C	2.2788054076	.8041498107	2.6393234375
H	-2.0326110666	-4.7186908742	-.8439235652
H	-2.3358690908	-2.0992270712	-.8848970922
H	1.0620554591	4.8036857864	.3868880215
H	2.2891164538	3.8722020511	-.4955589044
H	2.1590009865	3.7031038816	1.2462662794
H	-.9725502161	4.1180526846	.1695343968
H	-3.1350575475	4.0879783936	-.0249233786
H	-3.9342675622	2.6619383814	.6627113198
H	-3.7926331082	2.8240726052	-1.0814965205
H	4.9044585997	.2016282551	2.2657183472
H	6.2023776423	.1308770486	.1654216173
H	5.1101671814	.6946595022	-1.9778755076
H	1.3207683700	1.2997893167	2.4573530413
H	2.3274868643	1.5639426120	4.6781755339
H	3.1952200690	2.5884431290	3.5216286116
H	3.9138397662	1.0737630438	4.0827789090
H	1.3509736781	-.6891950477	3.9412242340
H	2.8938118002	-1.2093524102	3.2391329336
H	1.4407469769	-1.1795446056	2.2366816565
H	1.5774047519	1.9076294439	-2.2533792109

H	1.6246498942	.2279934025	-4.0763090221
H	1.5351026695	-.5665645025	-2.4912058428
H	3.0688848675	-.5214020498	-3.3691298842
H	2.7785375667	2.5122895519	-4.2928619941
H	4.2781501288	1.7954545025	-3.7050812867
H	3.6174355342	3.2278665092	-2.9058272603
H	-5.2934067331	-1.7398611573	1.4162930090
H	-5.9942636288	-2.4311163764	-.8531278210
H	-4.8888089615	-1.4415051460	-2.8345114170
H	-2.6232920495	.8056248622	2.0874385190
H	-2.2899968436	-.9175199822	3.8517359467
H	-1.7201326901	-1.4873272829	2.2781895452
H	-3.2643462594	-2.0701600954	2.9267394840
H	-4.1547047349	.8014460284	4.0065931724
H	-5.2485466780	-.3294249778	3.2073037184
H	-5.0451925465	1.3029654393	2.5591592674
H	-2.1618021056	1.1319581228	-2.6247493557
H	-3.4243134208	1.5988741837	-4.6878245977
H	-4.4770113350	1.8663149417	-3.2878691354
H	-4.6554845342	.4047347803	-4.2657243120
H	-1.6750804454	-.2299058051	-4.6596033891
H	-2.7897461438	-1.4826205242	-4.0986473286
H	-1.3153462316	-1.1211313350	-3.1792881884
N	-.3513184170	-2.0341101248	-.3218576518
N	-1.5057624533	-2.6484832549	-.6569080649
N	1.0544346784	1.4555386826	.0614021267
N	-1.9415806392	.9442959468	-.2291123986
Cu	-.1747265856	-.0238446150	-.1409479424

84. L^1CuXO_2 η^1 singlet, X = tetrazole

C	.5867919612	-3.7867015206	-.8171956685
C	-5.2270765722	-.8618318145	-.6653863800
C	-4.2732278305	-.6990465593	-1.6657346642
C	-3.0621408656	-.0488703262	-1.4158538739
C	-3.5686848806	.7865383876	2.3546716675
C	-3.7705161690	-.3283246862	3.4000043600
C	-4.4956741020	1.9759913140	2.6858097474
C	-2.0678165884	.1381248975	-2.5590285487
C	-2.5528154242	1.2183454520	-3.5489912270
C	-1.7813565802	-1.1770760506	-3.3071317479
C	3.8171672215	1.1512823432	3.4824279416
C	2.0156327445	3.9255591828	.4678531128
C	.9630397746	2.8347474287	.3963037979
C	-.3782204084	3.2593751297	.3710890161
N	1.5608279134	-3.3096562305	-1.5835541170
C	-1.5546012893	2.5161209241	.1386788213
C	-2.7775906983	3.3532376781	-.2066712202
C	2.6829629008	1.1856095229	.0266865304
C	3.4678559371	.5711841906	1.0349284477
C	4.7535243329	.1315574492	.7058301810
C	5.2602005194	.2775950087	-.5808755417
C	2.8528058418	-1.1059037528	2.8379042988
C	4.4777036063	.8716139596	-1.5658220840
C	3.1867777283	1.3337052165	-1.2964052037
C	2.9553012563	.3852829862	2.4610706559
C	2.3624570609	1.9146482233	-2.4483124238
C	1.9899955481	.8259236069	-3.4757322177
C	3.0819881590	3.0759339683	-3.1640460191
C	-2.8297427367	.4759104729	-.1133249527
N	1.6062084482	-1.9844177481	-1.3374271366
C	-3.7812412114	.2792777838	.9283788355
C	-4.9733063481	-.3824837606	.6150349154
H	.2763783190	-4.8187450916	-.7557601238

H	-.7374256056	-2.6700022876	.6265914290
H	1.5862294564	4.8469378645	.8657394939
H	2.4231722800	4.1436461942	-.5227170747
H	2.8518246961	3.6173885675	1.1005292064
H	-.5224649245	4.3324371564	.4166926060
H	-2.8514055082	4.2153488517	.4611546456
H	-3.7058827284	2.7877359164	-.1670647905
H	-2.6625702465	3.7424774857	-1.2251525892
H	5.3661530972	-.3377087045	1.4707745219
H	6.2581643925	-.0793139521	-.8194259501
H	4.8724857285	.9626680164	-2.5739490401
H	1.9473627489	.8081756421	2.5117099125
H	3.3962260633	1.0525342304	4.4891749619
H	3.8693358369	2.2180259585	3.2404443902
H	4.8429099368	.7671941824	3.5123649116
H	2.4443327806	-1.2184758717	3.8482434193
H	3.8343852071	-1.5920064874	2.8162805189
H	2.1970741076	-1.6452125044	2.1485192495
H	1.4263100800	2.3052953544	-2.0408923580
H	1.3390868982	1.2450988732	-4.2527802063
H	1.4815814144	-.0150752883	-3.0006193287
H	2.8836187669	.4284555151	-3.9701304956
H	2.4227499586	3.5227887899	-3.9167177707
H	3.9819236742	2.7309531830	-3.6847948748
H	3.3884861346	3.8669325581	-2.4724220670
H	-5.7162834171	-.5269447609	1.3935289874
H	-6.1645308504	-1.3662930474	-.8833927192
H	-4.4767115757	-1.0776133056	-2.6634388414
H	-2.5325543649	1.1233117505	2.4368113044
H	-3.4815867505	.0371586154	4.3916786424
H	-3.1673353873	-1.2037298785	3.1578054024
H	-4.8210979176	-.6354035367	3.4615352323
H	-4.3171304582	2.3188530514	3.7110185424
H	-5.5493289360	1.6829454447	2.6137177325
H	-4.3433187382	2.8281572493	2.0190920788
H	-1.1244479352	.4841587187	-2.1277852848
H	-1.8139484731	1.3728072079	-4.3433501333
H	-2.7193623665	2.1787832833	-3.0515569039
H	-3.4964463872	.9239864827	-4.0228504465
H	-.9896199597	-1.0249007473	-4.0478758496
H	-2.6643862943	-1.5429930077	-3.8428500523
H	-1.4558942609	-1.9652649145	-2.6223530257
N	.6957928457	-1.6637972712	-.4652309465
N	.0371231203	-2.7847749190	-.1223640426
N	1.3401994142	1.5592046801	.3346101710
N	-1.6205215425	1.1879446218	.1234876720
O	-.8092973914	-.9460685093	1.9243777001
O	-1.6098273363	-1.9508800932	1.6325882942
Cu	.0061189094	.1698175309	.6274350839

85. L^1CuXO_2 η^1 triplet, X = tetrazole

C	1.2269738870	-3.6047876902	-1.1927239478
C	-5.3631371083	-.8645349549	-.0213883537
C	-4.5862020699	-.7966245661	-1.1739809387
C	-3.3751443494	-.0997720019	-1.1920179538
C	-3.3142339238	1.1440858157	2.4964183658
C	-3.1570416383	.1129620783	3.6324993144
C	-4.3106537313	2.2430342095	2.9217629259
C	-2.5633310500	-.0388536758	-2.4834459034
C	-3.2203771929	.9054259677	-3.5099439367
C	-2.3262638704	-1.4315376972	-3.0962751032
C	2.8342048172	1.1688283110	3.5358045864
C	1.9939572136	3.8599281869	.5450562171

C	.9330525192	2.7961725857	.3123571784
C	-.3913760754	3.2706438761	.2284980331
N	1.6128434095	-2.9531009418	-2.2850409079
C	-1.6002661014	2.5749708612	.0367817851
C	-2.8279337007	3.4553110999	-.1461430167
C	2.6343094745	1.0905277534	.0907984514
C	3.1875249098	.3485242422	1.1699947450
C	4.4901432231	-.1429555128	1.0453552651
C	5.2338062768	.0647183379	-.1124361474
C	2.5568094714	-1.2972058728	3.0297939528
C	4.6792160721	.7832046558	-1.1655472688
C	3.3852571201	1.3115634191	-1.0946486142
C	2.4191474794	.1307630135	2.4725987212
C	2.8412834076	2.0739521181	-2.3040072438
C	2.6822595812	1.1590691260	-3.5353505621
C	3.7281416846	3.2844946282	-2.6626534975
C	-2.9559303740	.5666998829	-.0098289971
N	1.3095302250	-1.6628684461	-2.0670219198
C	-3.7300402909	.4868739999	1.1801306579
C	-4.9297987180	-.2318737966	1.1388619431
H	1.3183445628	-4.6663880452	-1.0228847468
H	.1904123854	-2.7756882995	.6530787819
H	1.6131665044	4.6208131233	1.2312076098
H	2.2503374025	4.3629200154	-.3923939611
H	2.9097832550	3.4343228767	.9572786497
H	-.4945909116	4.3479931679	.3015305504
H	-2.9207013821	4.1674384892	.6785974470
H	-3.7488987551	2.8793386426	-.2200852666
H	-2.7107876401	4.0395105351	-1.0657994345
H	4.9299636041	-.6996700942	1.8673466018
H	6.2409837584	-.3347989288	-.1936974437
H	5.2615184836	.9324772010	-2.0704302794
H	1.3567836286	.2935467774	2.2669591733
H	2.2593089686	1.0276962912	4.4580571724
H	2.6640191647	2.1918618860	3.1859813429
H	3.8979134557	1.0723209533	3.7821765849
H	1.8819723813	-1.4336539502	3.8808855448
H	3.5727594792	-1.5090064895	3.3808724463
H	2.2981317363	-2.0473974181	2.2768952621
H	1.8457442899	2.4498706447	-2.0528748414
H	2.2508740153	1.7231775916	-4.3707338594
H	2.0396780492	.3038014424	-3.3191751133
H	3.6527100627	.7712541019	-3.8658955919
H	3.2630194049	3.8731902060	-3.4611768896
H	4.7104996579	2.9632721969	-3.0259615616
H	3.8962949014	3.9444738566	-1.8063354202
H	-5.5344535444	-.3012280006	2.0387474837
H	-6.3009688511	-1.4132603052	-.0263593578
H	-4.9277003467	-1.2933309991	-2.0777370860
H	-2.3373747723	1.6129212516	2.3494304393
H	-2.8089955061	.6112524787	4.5449321526
H	-2.4355762676	-.6586864382	3.3597421605
H	-4.1109953130	-.3720812364	3.8686973920
H	-3.9588025169	2.7451354922	3.8299208583
H	-5.2958715660	1.8173751649	3.1425389833
H	-4.4461481134	3.0025277488	2.1471300241
H	-1.5826367650	.3805719953	-2.2404120712
H	-2.6115736091	.9713828204	-4.4186637807
H	-3.3370944088	1.9162770351	-3.1058729617
H	-4.2150652849	.5452710694	-3.7969384089
H	-1.6393017268	-1.3599565867	-3.9458730666
H	-3.2553915280	-1.8828277514	-3.4614104523
H	-1.8878252239	-2.1181793772	-2.3655658166
N	.7664215212	-1.5299717406	-.8904542514

N	.7041173161	-2.7396968477	-.3185906844
N	1.2761464271	1.5176123978	.1912683104
N	-1.7021970870	1.2496554846	-.0272197591
O	-.9873145038	-1.1434589785	1.5195129873
O	-.5976454382	-2.3588558038	1.8147531723
Cu	-.1090256740	.0951508396	.0810474157

86. L^1CuX, X = N-methyltetrazole

C	3.0179007772	1.0178837926	3.8552802592
C	1.9794981464	-1.1324357568	3.0053576059
C	2.9627280990	1.1915359676	-2.3810516584
C	3.0340607725	.0268312946	-3.3890457622
C	3.6831607148	2.4308614119	-2.9452692859
C	-2.9589363793	.1417445456	-.2899746957
C	-3.6357124307	-.2134912407	.9089200603
C	-4.7890836941	-1.0014190094	.8241333408
C	-5.2894198385	-1.4303326250	-.4032309965
C	-4.6320914918	-1.0629753901	-1.5740254514
C	-3.4728290201	-.2776830021	-1.5454428016
C	-3.1038483275	.2082867506	2.2786743374
C	-2.3749225900	-.9561972830	2.9786216614
C	-4.1990473225	.7880273940	3.1916529513
C	-2.7812012084	.0980141810	-2.8547183184
C	-3.7112702689	.8885847706	-3.7941311596
C	-2.2112433767	-1.1409071036	-3.5728016966
C	1.9403899560	3.4980166310	.5477212147
C	.9149552903	2.4250627400	.2160352200
C	-.4323634393	2.8579693004	.1180007702
C	.4988633819	-4.3286104433	-.9271716602
C	-1.6277362713	2.1395071779	-.0756507243
C	-2.9092291383	2.9587257372	-.1073287035
C	2.6942443836	.8068513083	.1543563934
C	3.2177420152	.3659676071	1.3949006581
C	4.5430051799	-.0786438706	1.4476774078
C	5.3498258772	-.0890536633	.3146098723
C	4.8253052649	.3387755347	-.9007506165
C	3.5030338085	.7818179209	-1.0111235057
C	2.3555334301	.3207008309	2.6536835114
H	-1.5740191803	-3.2921574370	1.1289962122
H	-2.1683215370	-2.4518365571	-.3256475797
H	-2.1216423936	-4.2332991944	-.2871102860
H	.2019058559	-5.3659907017	-.8934492931
C	-1.6215789197	-3.3207380936	.0393492251
H	1.4976713657	4.4950923100	.5207760977
H	2.7848901506	3.4676856552	-.1455597100
H	2.3535545467	3.3322862816	1.5493377976
H	-.5663805759	3.9268189292	.2313441405
H	-2.6956207515	4.0281451700	-.0703292280
H	-3.5622820640	2.7100487843	.7358142845
H	-3.4806549565	2.7494114590	-1.0178624024
H	4.9508105531	-.4267651833	2.3933276456
H	6.3775670993	-.4365886382	.3766236655
H	5.4524580651	.3167944848	-1.7886093638
H	1.4245847655	.8518998976	2.4367454056
H	2.3343490031	1.0373224225	4.7117426144
H	3.2904570313	2.0510056464	3.6163384581
H	3.9291405893	.5016976513	4.1771651405
H	1.3247618422	-1.1667768712	3.8842408554
H	2.8717001660	-1.7301833936	3.2245551726
H	1.4572917390	-1.6107726803	2.1700153002
H	1.9075640631	1.4495870613	-2.2542279341
H	2.5585120470	.3102294145	-4.3358211277
H	2.5341211673	-.8629333581	-2.9988829949
H	4.0718919581	-.2472044764	-3.6116531135
H	3.2479991974	2.7217189437	-3.9083397044

H	4.7483437793	2.2328777997	-3.1109845792
H	3.6073722463	3.2895053719	-2.2705813705
H	-5.3075709622	-1.2854565219	1.7361940871
H	-6.1879214992	-2.0401062373	-.4456310379
H	-5.0281876904	-1.3899467443	-2.5324310604
H	-2.3608712977	.9934421089	2.1197539559
H	-1.9990493994	-.6478057158	3.9610193347
H	-1.5163703042	-1.2899186675	2.3868669631
H	-3.0458222651	-1.8107674555	3.1297895395
H	-3.7549349058	1.1800876722	4.1132227061
H	-4.9369728949	.0323858555	3.4828457399
H	-4.7379463002	1.6056167207	2.7021725711
H	-1.9366175080	.7446787759	-2.6020236286
H	-3.1679366696	1.2095195213	-4.6898686218
H	-4.1099160278	1.7821519514	-3.3032327613
H	-4.5633902722	.2840731094	-4.1249645751
H	-1.6978834945	-.8523893479	-4.4968391852
H	-3.0031827440	-1.8507279722	-3.8396329940
H	-1.4865794347	-1.6640617051	-2.9403113560
N	.4333178009	-2.1715441708	-.7183692543
N	1.6521610542	-3.8573725726	-1.3668902419
N	1.5845218570	-2.5209324191	-1.2213516414
N	-.2783865948	-3.3098306380	-.5256259946
N	1.3158900539	1.1696534707	.0523967437
N	-1.7062140192	.8131896936	-.2277365972
Cu	-.0391236464	-.2304943631	-.3269840552

87. L^1CuXO_2 η^1 singlet, X = N-methyltetrazole

C	.6446771964	-3.9449435062	-.8513010441
C	-1.9555406314	-.4260083754	-3.5071108024
C	3.5370446346	1.8486676717	3.4387565693
C	1.8924751376	4.1384638960	.1062320306
C	.8402163700	3.0446564503	.1684761747
C	-.5037738311	3.4740008766	.1771913865
C	-1.6949170197	2.7263578834	.0803498471
C	-2.9591802480	3.5542028993	-.1063267979
C	2.5723219320	1.3726507824	-.0165742021
C	3.3328457780	.9095847776	1.0876770940
C	4.6410906531	.4713237158	.8614536956
C	-5.2245839808	-.9148182410	-.6018787623
C	5.1935565801	.4685069780	-.4144790083
C	2.7683608941	-.5441574426	3.0915749502
C	4.4324691849	.9079894438	-1.4928326076
C	3.1213371056	1.3629812104	-1.3252530107
C	2.7759810017	.8831569967	2.5094092794
C	2.3181135981	1.7742776666	-2.5583110931
C	2.0018837233	.5509480501	-3.4424719984
C	3.0259694814	2.8635366587	-3.3874073917
C	-2.9533896807	.6529758757	-.1061582931
C	-3.7657664732	.2280757311	.9807523839
C	-4.4221607224	-.4917156531	-1.6587183705
C	-4.8925729705	-.5557535684	.7004705654
C	-1.7619398972	-3.1902601216	-.5649513631
C	-3.2773452443	.2823132550	-1.4402680397
C	-3.4873087652	.6521228157	2.4215867992
C	-3.5876854044	-.5089907777	3.4277888346
C	-4.4321850299	1.7967029285	2.8479540280
C	-2.4482058812	.7462791968	-2.6379356773
C	-3.2301473231	1.7600400478	-3.4985333406
H	-2.0481797002	-2.9249067985	.4528136148
H	-2.2819165982	-2.5429730928	-1.2709512698
H	-2.0057643639	-4.2332378675	-.7725156115
H	.4661540513	-5.0086689230	-.8906495913

H	1.4963308140	5.0723045879	.5105353453
H	2.1993671526	4.3259965886	-.9279196071
H	2.7878584409	3.8576794712	.6653640450
H	-.6434081476	4.5491352695	.1756414953
H	-3.0694626386	4.2559654160	.7266897628
H	-3.8565752842	2.9397519443	-.1667353867
H	-2.8818257740	4.1503056649	-1.0215282073
H	5.2355906720	.1216046064	1.7011019975
H	6.2097267262	.1167113815	-.5698863627
H	4.8628767264	.8855262173	-2.4902876641
H	1.7386611375	1.2274554072	2.4698702307
H	3.0921097922	1.8479388312	4.4403879771
H	3.5115746500	2.8753922866	3.0587036567
H	4.5886231009	1.5585548489	3.5426553471
H	2.2934099937	-.5519478441	4.0789944062
H	3.7855129258	-.9339535600	3.2091144758
H	2.2182876874	-1.2338136025	2.4459669941
H	1.3617236165	2.1831603814	-2.2212528966
H	1.3795715894	.8447120948	-4.2963513795
H	1.4767535836	-.2203834622	-2.8749292750
H	2.9201926948	.1024765459	-3.8380677538
H	2.3811151298	3.1981503119	-4.2077740378
H	3.9541187692	2.4908012327	-3.8343787238
H	3.2834375376	3.7380560716	-2.7813676854
H	-5.5267457971	-.8806094217	1.5197783447
H	-6.1099988382	-1.5148929234	-.7941841287
H	-4.6945093447	-.7613525674	-2.6758445154
H	-2.4625096414	1.0300430482	2.4642085835
H	-3.3047777588	-.1551645022	4.4251932886
H	-2.9166355013	-1.3276838580	3.1590921818
H	-4.6098261655	-.8979452156	3.5037861716
H	-4.1957804952	2.1246991787	3.8663478343
H	-5.4768909872	1.4648135393	2.8376940208
H	-4.3531096446	2.6645881125	2.1880528298
H	-1.5612537835	1.2532972373	-2.2510253890
H	-2.5992625112	2.1434503944	-4.3082772509
H	-3.5745082204	2.6125119409	-2.9055395233
H	-4.1123505248	1.2971913438	-3.9554478152
H	-1.3601794879	-.0515796253	-4.3469938687
H	-2.7871625852	-1.0032212231	-3.9271271227
H	-1.3203930555	-1.1049606027	-2.9312412530
N	.2740369234	-1.8104883504	-.7050891366
N	1.8167225472	-3.3428930908	-.9286788452
N	-.3225630618	-3.0224532878	-.7160834520
N	1.5490814651	-2.0201728152	-.8381406830
N	1.2165342881	1.7691672896	.1963369350
N	-1.7610030234	1.3976399050	.1221464592
O	-.4959801000	-.6917777501	2.0910309267
O	-.9346992493	-1.8966660320	2.0852387869
Cu	-.1301989157	.4192022421	.6310944758

88. L^1CuXO_2 η^1 triplet, X = N-methyltetrazole

C	.7563356361	-3.9147060885	-.9491117294
C	-5.1700279445	-.9148637104	-.7384671100
C	-4.2941454857	-.5638587510	-1.7615063071
C	-3.1279396405	.1676480853	-1.5041173717
C	-3.4854765403	.6208536151	2.3337636901
C	-3.6813536294	-.5331270221	3.3346953642
C	-4.3765454386	1.8151767903	2.7331922710
C	-2.2106255650	.5435015099	-2.6687361796
C	-2.8991847716	1.5354017332	-3.6280394481
C	-1.7128685987	-.6891171501	-3.4480746482
C	3.7289039562	1.7084941272	3.4182331464

C	2.0815674847	3.9065833308	.3422050816
C	1.0245664640	2.8122551711	.3271843733
C	-.3102396155	3.2681020364	.3015199725
C	-1.5158431938	2.5646050760	.0991461534
C	-2.7260899578	3.4384512053	-.1983108731
C	2.7639932198	1.1888224726	.0338480983
C	3.5962591098	.7279014310	1.0832964315
C	4.9203755352	.3834424505	.7885833521
C	5.4222910279	.4669811662	-.5047051820
C	3.3607631944	-.7797205569	3.1150444555
C	4.5909244593	.8972825210	-1.5330019332
C	3.2624775648	1.2632305330	-1.2946759860
C	3.1044513911	.6191471230	2.5235775185
C	2.3966900214	1.6833561805	-2.4842674463
C	2.1386400776	.4936272073	-3.4304279194
C	3.0054237316	2.8577280753	-3.2763556339
C	-2.8507757954	.5601648537	-.1661108312
C	-3.7356378992	.2009303563	.8859830746
C	-4.8858394339	-.5315512396	.5691050683
H	-1.6148678398	-3.1234440776	.9401564362
H	-2.0731215615	-2.2650084126	-.5493772762
H	-1.8909748632	-4.0383661444	-.5764313469
H	.4974262151	-4.9498881374	-1.1119591718
C	-1.5145799158	-3.1097635995	-.1451962258
H	1.6815766303	4.8119600016	.8041783414
H	2.3909203190	4.1635889246	-.6760887042
H	2.9768101213	3.5950788326	.8831847257
H	-.4209271521	4.3463774431	.3299470195
H	-2.7743214361	4.2704509357	.5101873206
H	-3.6639992372	2.8853882646	-.1586339147
H	-2.6291938688	3.8740199342	-1.1991733040
H	5.5699182619	.0427161812	1.5901191669
H	6.4528419814	.1917572635	-.7123219549
H	4.9803474290	.9445220920	-2.5466524787
H	2.0228404044	.7769798972	2.5186807980
H	3.3480212761	1.6318277378	4.4432466602
H	3.5000697514	2.7137685965	3.0497714567
H	4.8199986227	1.6100300162	3.4589635981
H	2.9063123017	-.8609029988	4.1085063936
H	4.4313507572	-.9863285589	3.2238259180
H	2.9290971879	-1.5595674537	2.4819411604
H	1.4263376863	2.0102035665	-2.1014045930
H	1.4744544269	.7916717970	-4.2509086674
H	1.6825197155	-.3434108738	-2.8977353375
H	3.0729079144	.1322025158	-3.8747355176
H	2.3144757913	3.1867433170	-4.0609880434
H	3.9421467012	2.5707113795	-3.7668400524
H	3.2220130098	3.7183382249	-2.6360733548
H	-5.5738361732	-.8055083030	1.3637072383
H	-6.0709499108	-1.4810291546	-.9591981046
H	-4.5215137687	-.8585898798	-2.7828599450
H	-2.4429527869	.9415690269	2.4037070651
H	-3.3715259436	-.2140568158	4.3357576295
H	-3.0805931253	-1.4028764473	3.0601094924
H	-4.7301479462	-.8433891795	3.4047061672
H	-4.1630490214	2.1234136960	3.7628945261
H	-5.4379092376	1.5468015708	2.6771718973
H	-4.2174247672	2.6804923353	2.0845264552
H	-1.3312306004	1.0406160259	-2.2510279928
H	-2.2076901423	1.8519207708	-4.4171221825
H	-3.2441397251	2.4300141264	-3.1012945494
H	-3.7705124183	1.0800956466	-4.1128081545
H	-1.0307933959	-.3844795907	-4.2489889249
H	-2.5389995405	-1.2408297063	-3.9108772802

H	-1.1678058168	-1.3804237335	-2.7981622238
N	.5771077668	-1.8165941720	-.4402678350
N	1.9405100324	-3.3632518901	-1.1459226620
N	-.1073910912	-2.9816271661	-.5143471613
N	1.7940642553	-2.0621234040	-.8192885471
N	1.3963347927	1.5308200302	.3012440918
N	-1.6294831180	1.2401877007	.1212386064
O	-.8503487909	-1.0588960150	1.9729733950
O	.2342641614	-1.2687143423	2.6189203472
Cu	-.0139440136	.1611072215	.5624682354