

Complex A

charge = 2

multiplicity = 3

Cu	-0.92255	1.65310	-1.01340
Cu	-1.84870	-0.67343	0.71603
N	0.85267	2.24207	-1.51557
N	-1.88863	2.66052	-2.46622
N	-0.81005	-2.12825	1.50607
N	-3.63538	-1.65309	0.73904
O	-0.17586	0.09504	-0.05588
O	-2.46667	0.82245	-0.31040
H	-3.34884	1.08643	-0.43591
C	0.94508	-0.54242	-0.31621
C	1.96637	0.08135	-1.06000
C	3.17477	-0.58153	-1.31684
H	3.83967	-0.14548	-1.80030
C	3.40015	-1.87405	-0.86824
C	2.42730	-2.46067	-0.10005
H	2.57755	-3.31518	0.23466
C	1.22443	-1.82516	0.19863
C	4.69231	-2.54084	-1.16924
H	5.22701	-1.96791	-1.72243
H	4.52671	-3.36602	-1.62946
H	5.15850	-2.72074	-0.34875
C	1.89071	1.46969	-1.53649
H	2.67088	1.83143	-1.89095
C	1.02903	3.63040	-1.98044
H	1.94945	3.76728	-2.25354
H	0.83516	4.24244	-1.25408
C	0.10671	3.91198	-3.14260
H	0.34580	4.78018	-3.50171
H	0.29548	3.25692	-3.83293
C	-1.29290	3.91002	-2.92412
H	-1.72785	4.16423	-3.75274
H	-1.49651	4.59833	-2.26981
C	-2.00726	1.66327	-3.57842
H	-2.39617	0.85373	-3.24255
H	-1.13531	1.47751	-3.93520
H	-2.56574	2.02306	-4.27223
C	-3.30963	2.95383	-2.07689
H	-3.73071	2.14625	-1.77357
H	-3.78488	3.29798	-2.83695
H	-3.31981	3.60498	-1.37146
C	0.33819	-2.50955	1.13534
H	0.64877	-3.30931	1.49561
C	-1.43066	-2.88499	2.61710
H	-1.53434	-2.29642	3.38181
H	-0.83916	-3.60849	2.87743
C	-2.79721	-3.46575	2.24753
H	-2.69809	-4.01521	1.45377
H	-3.09526	-4.04259	2.96808
C	-3.85803	-2.42743	1.98837
H	-4.72174	-2.86544	1.93491
H	-3.88586	-1.81148	2.73797
C	-4.74444	-0.69494	0.64490
H	-4.64460	-0.16698	-0.15118
H	-4.73697	-0.12006	1.41310

H	-5.57622	-1.17206	0.60888
C	-3.70447	-2.54866	-0.47891
H	-2.98847	-3.18808	-0.44753
H	-3.62121	-2.01484	-1.27384
H	-4.54555	-3.01014	-0.48937

Complex B

charge = 0

multiplicity = 3

V	0.9334200000000000	1.1672600000000002	0.3724200000000000
O	5.9007100000000001	1.5694999999999999	1.2853699999999999
O	2.3981699999999999	0.7875000000000000	1.5834500000000000
O	2.4564200000000000	1.7787599999999999	-0.7994000000000001
O	-0.0700000000000000	-0.3304200000000000	1.1580100000000000
O	0.1807500000000000	2.5089899999999998	0.7650800000000000
C	4.8966200000000004	0.4736000000000000	3.1461299999999999
C	4.7420900000000001	1.1025000000000000	1.8228200000000001
C	3.5778300000000001	1.2236600000000000	1.1227799999999999
C	3.5815399999999999	1.7754600000000000	-0.1752400000000000
C	4.8102200000000002	2.2600699999999998	-0.6946200000000000
C	5.8962800000000000	2.1400199999999998	0.0532900000000000
C	-0.0326800000000000	-0.7500500000000000	2.5183499999999999
H	4.7816000000000001	0.9582200000000000	3.7124900000000007
H	4.1244100000000001	-0.0881100000000000	3.4053700000000000
H	5.6113400000000002	-0.0881100000000000	3.2879399999999999
H	4.8976400000000000	2.5772800000000000	-1.5626800000000001
H	6.7948100000000000	2.3900399999999999	-0.1716200000000000
H	-0.7043600000000000	-1.1895100000000001	2.7821099999999999
H	0.2144800000000000	0.0220300000000000	3.2427800000000002
H	0.6674500000000000	-1.3437100000000000	2.6285500000000002
V	-0.9334200000000000	-1.1672600000000002	-0.3724200000000000
O	-2.3981699999999999	-0.7875000000000000	-1.5834500000000000
C	-3.5778300000000001	-1.2236600000000000	-1.1227799999999999
C	-4.7420900000000001	-1.1025000000000000	-1.8228200000000001
O	-5.9007100000000001	-1.5694999999999999	-1.2853699999999999
C	-5.8962800000000000	-2.1400199999999998	-0.0532900000000000
C	-4.8102200000000002	-2.2600699999999998	0.6946200000000000
C	-3.5815399999999999	-1.7754600000000000	0.1752400000000000
O	-2.4564200000000000	-1.7787599999999999	0.7994000000000001
O	0.0700000000000000	0.3304200000000000	-1.1580100000000000
C	0.0326800000000000	0.7500500000000000	-2.5183499999999999
H	0.7043600000000000	1.1895100000000001	-2.7821099999999999
H	-0.2144800000000000	-0.0220300000000000	-3.2427800000000002
H	-0.6674500000000000	1.3437100000000000	-2.6285500000000002
O	-0.1807500000000000	-2.5089899999999998	-0.7650800000000000
H	-4.8976400000000000	-2.5772800000000000	1.5626800000000001
H	-6.7948100000000000	-2.3900399999999999	0.1716200000000000
C	-4.8966200000000004	-0.4736000000000000	-3.1461299999999999
H	-4.7816000000000001	-0.9582200000000000	-3.7124900000000007
H	-4.1244100000000001	0.0881100000000000	-3.4053700000000000
H	-5.6113400000000002	0.0881100000000000	-3.2879399999999999

Complex C

charge = 4

multiplicity = 7

Cr	-7.8166099469999999	-1.2755229749999999	1.8796748040000000
O	-6.2813869999999996	-2.2487979999999999	1.7707380000000001
N	-8.5281767459999998	-2.4518628850000002	3.4947717379999998
H	-8.7850417460000010	-3.2676398849999999	3.1864967380000002
H	-9.2389967459999998	-2.0367048849999998	3.8812217379999998
H	-7.8642057459999997	-2.5536328849999999	4.1098467379999999
N	-8.7944608399999993	-2.4925835150000002	0.4751922410000000
H	-9.5311288399999992	-2.0612725150000002	0.1610172410000000
H	-9.0464788400000007	-3.2712065149999998	0.8704922410000000
H	-8.2306508399999991	-2.6718935149999998	-0.2151077590000000
N	-7.2262542639999996	-0.0239168150000000	0.3014596130000000
H	-7.0889372640000001	0.8177061850000000	0.6171096130000000
H	-7.8789162639999999	-0.0077628150000000	-0.3327903870000000
H	-6.4556612639999997	-0.3389198150000000	-0.0643403870000000
N	-6.8417865910000000	0.0209453490000000	3.2694176979999998
H	-6.5946145910000009	-0.4539826510000001	4.0039676980000003
H	-7.4136735910000002	0.6848743490000000	3.5157426979999999
H	-6.1035035910000000	0.3844103490000000	2.8800176980000001
N	-9.5749393979999997	-0.0944361650000000	2.0731702560000000
H	-10.2938373980000009	-0.5661331650000000	1.7752202560000001
H	-9.4860863979999994	0.6648018350000000	1.5819952559999999
H	-9.6993323980000010	0.1236428350000000	2.9478452559999999
Cr	-4.7359931839999998	-3.2060225980000001	1.6634066370000002
N	-5.5702553100000003	-4.5140840530000004	0.2481391950000000
H	-4.9131974180000002	-5.0282483449999997	-0.1129508030000000
H	-5.9733827389999998	-4.0311609590000002	-0.4088684580000000
H	-6.1864732870000001	-5.0464549859999996	0.6523835059999999
N	-5.3352115360000001	-4.4726064579999996	3.2556828990000000
H	-4.6101315109999996	-4.9141999969999999	3.5813311180000005
H	-5.9461776449999997	-5.0756075359999997	2.9523030129999999
H	-5.7074200939999997	-3.9717318940000004	3.9175926849999998
N	-3.7875218970000000	-1.9326763140000001	3.0922129420000002
H	-3.0396712950000002	-1.5673549490000001	2.7236288100000001
H	-3.5584009380000006	-2.4183946500000002	3.8253047670000000
H	-4.3603768120000002	-1.2695636960000001	3.3338612429999999
N	-4.0070156250000002	-1.9914581000000000	0.1144631920000000
H	-3.7468712160000002	-2.5128893990000001	-0.5837560110000000
H	-3.2950755830000000	-1.5104300939999999	0.4138577600000000
H	-4.6626025450000004	-1.4233240229999999	-0.1588061040000000
N	-2.9110590130000000	-4.2876000779999996	1.5086990840000001
H	-3.0788208440000000	-5.1777368250000002	1.5947333319999999
H	-2.3438003809999999	-4.0214336590000004	2.1661025390000002
H	-2.5315525260000000	-4.1282518179999999	0.6979462100000000

Complex D

charge = -2

multiplicity = 11

Fe	1.6757400000000000	0.0373000000000000	-0.4676800000000000
O	0.0000000000000000	0.1859900000000000	-0.0000000000000000
Cl	1.9311700000000001	0.3356600000000000	-2.6481499999999998
Cl	2.4651500000000000	-1.9685400000000000	0.0102600000000000
Cl	2.8645400000000008	1.5320700000000000	0.6399899999999999

Fe	-1.6757400000000000	0.0373000000000000	0.4676800000000000
Cl	-1.9311700000000001	0.3356600000000000	2.6481499999999998
Cl	-2.4651500000000000	-1.9685400000000000	-0.0102600000000000
Cl	-2.8645400000000000	1.5320700000000000	-0.6399899999999999

Metal Ligand coupling

charge = 0

multiplicity = 4

C	21.872209999999999	6.553289999999999	5.300589999999999
C	22.120039999999999	7.939470000000000	5.535599999999999
H	22.910350000000000	8.208899999999999	5.989449999999999
C	21.231380000000000	8.871330000000000	5.114110000000000
H	21.388760000000000	9.788899999999999	5.302290000000000
C	20.068280000000000	8.497849999999999	4.397999999999999
H	19.490259999999999	9.169500000000000	4.051440000000000
C	19.769649999999999	7.191440000000000	4.203000000000000
H	18.965689999999999	6.954740000000000	3.758520000000000
C	20.644970000000000	6.179039999999999	4.654300000000000
C	23.971270000000000	5.736089999999999	6.137609999999999
C	24.445150000000000	4.977599999999999	7.218169999999999
C	25.746800000000000	5.050449999999999	7.651580000000000
C	26.624710000000000	5.915759999999999	7.047019999999999
C	26.201689999999999	6.664259999999999	5.971569999999999
C	24.919489999999999	6.544069999999999	5.516020000000000
C	19.250830000000000	4.335000000000000	4.043770000000000
C	18.025220000000000	4.632399999999999	4.639820000000000
C	16.846990000000000	4.060649999999999	4.231959999999999
C	16.859159999999999	3.123100000000000	3.225480000000000
C	18.036670000000000	2.771139999999999	2.653270000000000
C	19.220590000000000	3.367480000000000	3.049220000000000
C	22.018390000000000	1.016699999999999	5.442789999999999
C	21.710149999999999	-0.359650000000000	5.677800000000000
H	20.876210000000000	-0.602490000000000	6.057570000000000
C	22.609449999999999	-1.311029999999999	5.360190000000000
H	22.406990000000000	-2.220909999999999	5.533050000000000
C	23.842539999999999	-0.982120000000000	4.779469999999999
H	24.442250000000000	-1.678360000000000	4.543599999999999
C	24.198519999999999	0.312000000000000	4.546160000000000
H	25.046970000000000	0.514880000000000	4.173199999999999
C	23.286349999999999	1.351599999999999	4.867180000000000
C	19.921749999999999	1.958550000000000	6.175080000000000
C	19.467189999999999	2.797270000000000	7.204539999999999
C	18.150050000000000	2.891020000000000	7.561320000000000
C	17.220099999999999	2.130230000000000	6.928659999999999
C	17.603970000000000	1.292580000000000	5.900900000000000
C	18.927060000000000	1.220350000000000	5.534749999999999
C	24.674959999999999	3.192569999999999	4.174050000000000
C	25.899869999999999	3.000150000000000	4.810979999999999
C	27.042359999999999	3.641060000000000	4.421840000000000
C	27.008700000000000	4.561700000000000	3.389819999999999
C	25.812860000000000	4.813760000000000	2.770779999999999
C	24.691829999999999	4.149639999999999	3.149700000000000
F	23.606739999999999	4.137649999999999	7.842320000000000
F	26.163850000000000	4.268290000000000	8.658899999999999
F	27.875669999999999	6.026420000000000	7.505969999999999

F	27.0716600000000014	7.4574800000000003	5.3278400000000001
F	24.59227000000000063	7.2089600000000003	4.3869300000000004
F	17.98842000000000014	5.4832599999999996	5.6854699999999996
F	15.70419000000000005	4.3812600000000002	4.8424800000000001
F	15.7178799999999992	2.5421299999999998	2.8431600000000001
F	18.0657999999999994	1.8050100000000000	1.7123699999999999
F	20.3580399999999990	2.9844700000000000	2.4616899999999999
F	20.35854000000000014	3.5860300000000009	7.8380599999999996
F	17.78179000000000009	3.7698499999999999	8.5098900000000004
F	15.92889000000000009	2.2224400000000002	7.2590399999999997
F	16.6851899999999986	0.6104800000000000	5.1958500000000001
F	19.2556699999999985	0.4778400000000000	4.4490900000000000
F	25.96039000000000003	2.1887799999999999	5.8915300000000004
F	28.19207000000000011	3.4140500000000000	5.0723900000000004
F	28.11848000000000017	5.1989200000000002	3.0108999999999999
F	25.74411999999999988	5.7551500000000004	1.8128400000000000
F	23.53288999999999983	4.4410499999999997	2.5247000000000002
N	22.65702999999999989	5.5239900000000004	5.6871700000000001
N	20.48725999999999991	4.8500300000000003	4.4686700000000004
N	21.25088999999999983	2.0848900000000001	5.7714699999999999
N	23.44547000000000003	2.6713900000000002	4.5810700000000004
Cu	21.96237999999999996	3.7843000000000000	5.1601800000000004