Electronic Supplementary Material (ESI) for Dalton Transactions

Supporting Information

Non-Innocent Ligand Behaviour of a Bimetallic Cu Complex Employing a Bridging Catecholate

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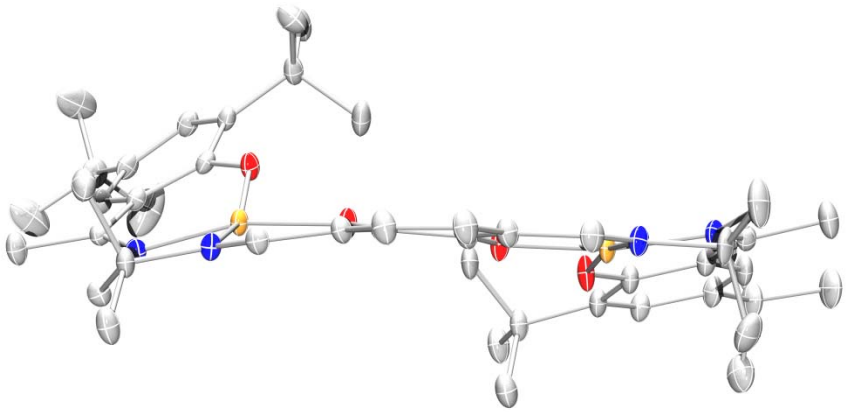

Figure S1. Side-view of the solid state structure for **1**.

Magnetism

For **1**, assuming that the intermolecular interaction between the dimers via the hydrogen bond of the CH-O cannot be approximated as 0 ($J' < 0$), the data was modeled using the alternating chain model established by Hatfield *et al.*.

$$\chi_M = \frac{N\beta^2 g^2}{kT} \frac{[A + Bx + Cx^2]}{[1 + Dx + Ex^2 + Fx^3]}$$

$$x = \frac{|J|}{kT}$$

A = 0.25
B = -0.068475+0.13194α
C = 0.0042563-0.031670α+0.12278α^2-0.29943α^3+0.21814α^4
D = 0.035255+0.65210α
E = -0.00089418-0.10209α+0.87155α^2-0.18472α^3
F = 0.045230-0.0081910α+0.83234α^2-2.6181α^3+1.92813α^4

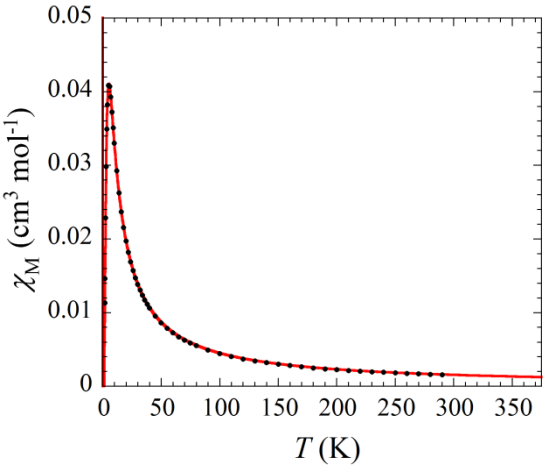

Figure S2. Fitting of the dc susceptibility of **1** between 1.8 and 300 K using the alternating Cu(II) chain model established by Hatfield and co-workers.

This resulted in the fitting parameters of J = -5.92(8) cm^{-1}, α = 0.278(7) and g = 2.223(2). Since J' = αJ, J' approximates -1.64(4) cm^{-1}. Thus taking into account intermolecular interactions does not the change the fitting outcome.

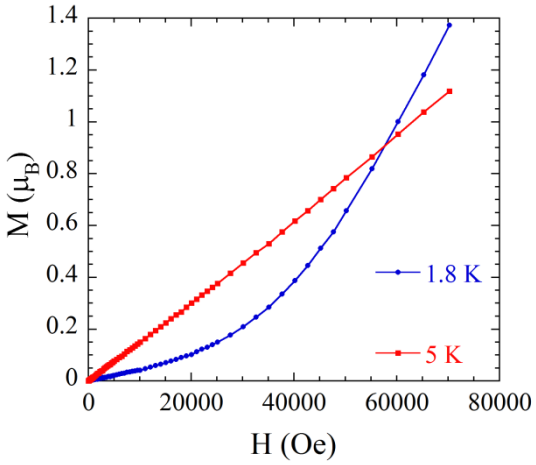

Figure S3. Field dependence of the magnetization of **1** measured between 0 and 70 000 Oe at 1.8 and 5 K.

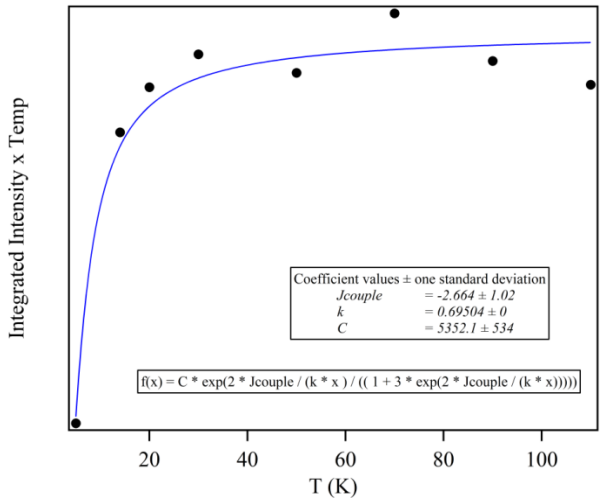

Figure S4. IT as a function of T for **1** and best fit using the parameters shown in the legend.

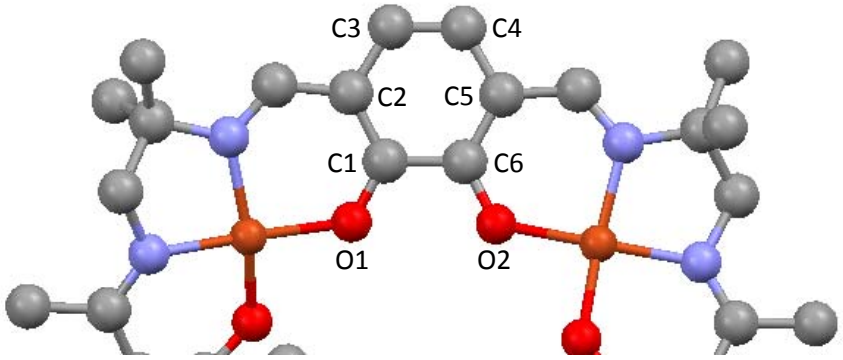

Figure S5. Atom labeling for Table S1.

Table S1 Experimental and calculated semiquinone metrical parameters in Å.

Bond/Distance	**1 (Å) Experimental**	**1 (Å) (bs) Calculated**	**$[1^{\bullet}]^{+}$ (Å) S=1/2, Cu aligned**	**$[1^{\bullet}]^{+}$ (Å) S=1/2, Cu opposed**	**$[1^{\bullet}]^{+}$ (Å) S=3/2**
O(1)-C(1)	1.295	1.286	1.270	1.270	1.270
C(1)-C(2)	1.414	1.425	1.438	1.438	1.438
C(2)-C(3)	1.422	1.438	1.408	1.408	1.408
C(3)-C(4)	1.346	1.358	1.388	1.388	1.388
C(4)-C(5)	1.426	1.438	1.408	1.408	1.408
C(5)-C(6)	1.414	1.425	1.438	1.438	1.438
C(1)-C(6)	1.479	1.483	1.491	1.491	1.491
C(6)-O(2)	1.295	1.286	1.270	1.270	1.270

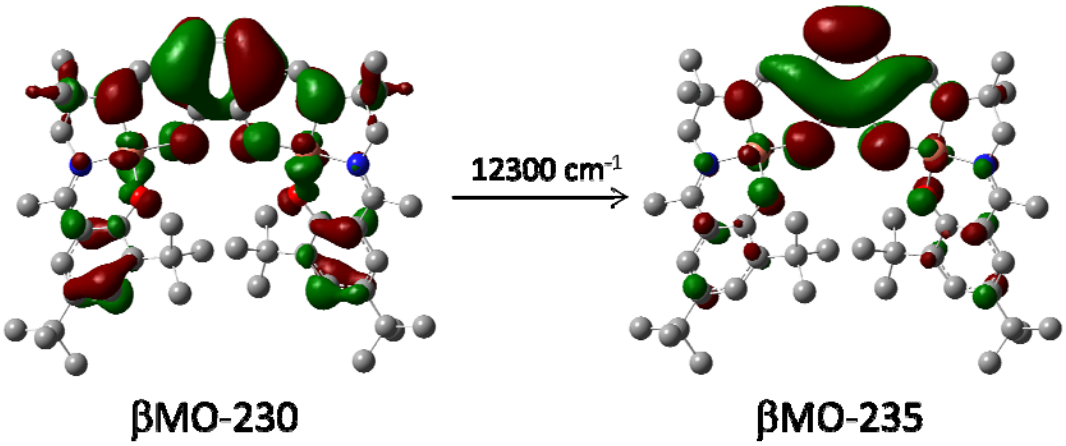

Figure S6. TD-DFT predicted transition for $[1^{\bullet}]^{+}$ (S = 3/2) at 12300 cm^{-1}.

Computed Metrical Parameters

1) Compound 1, triplet (S = 1):

Cu	-3.18525869	1.60681479	-0.22054834
Cu	3.16132911	1.61094429	0.23463031
O	-3.10741467	0.04497926	0.79910312
O	-1.32494160	1.95946850	-0.10848699
O	3.06450185	0.02344085	-0.74293158
O	1.29972767	1.96179716	0.13080775
N	-3.62445822	3.42993967	-0.65035570
N	-4.87720838	1.11653622	-1.01582830
N	3.60087678	3.44309909	0.62687891
N	4.86595696	1.14100076	1.01406326
C	-0.67834416	5.59341971	-0.16526192
C	-1.40948587	4.35978817	-0.26509717
C	-0.74800528	3.10919386	-0.09486363
C	0.72348880	3.11099246	0.08606187
C	1.38606729	4.36517872	0.22207144
C	0.65591690	5.59632786	0.09008106
C	-2.80127801	4.43629817	-0.57263190
C	2.77814492	4.44790191	0.52588178
C	5.02543901	3.60535212	0.98524126
C	5.40699724	2.29692263	1.73119516
C	5.41568913	-0.04928802	1.04953752
C	4.95761678	-1.14336991	0.20509257
C	3.82176013	-1.02940533	-0.67703315
C	3.49629645	-2.14829104	-1.53550190
C	4.27985695	-3.28348882	-1.45934501
C	5.39381093	-3.43143914	-0.59415671
C	5.70048217	-2.35883376	0.21297126
C	6.19213414	-4.74666878	-0.60078822
C	2.29862131	-2.06187636	-2.50706492
C	-5.04876989	3.58164525	-1.01346479
C	-5.42368733	2.26286198	-1.74460515
C	-5.41083224	-0.08112656	-1.05185110
C	-4.94415356	-1.16723857	-0.20140859
C	-5.65130297	-2.40344432	-0.23503539
C	-5.33649490	-3.47101884	0.57559764
C	-4.25445062	-3.29447725	1.47517776
C	-3.50675619	-2.13753031	1.57877010
C	-3.83517880	-1.02688362	0.71085383
C	-6.09286699	-4.81051493	0.55008897
C	-2.34394517	-2.01910975	2.58846480
C	-2.16694089	-3.30796762	3.41830601
C	-2.62130150	-0.86817885	3.58753400
C	-1.00742604	-1.76183034	1.84848717
C	2.12964380	-3.35562703	-3.33081625
C	0.98108950	-1.84102645	-1.72259674
C	2.51015297	-0.90420046	-3.51425751
H	-0.18583514	-1.71116980	2.57481093
H	-1.02846310	-0.82798728	1.28600139
H	-0.78759889	-2.58203397	1.15422587
H	-1.79651496	-0.79221852	4.30752201
H	-3.54327625	-1.05700914	4.15197789
H	-2.71711368	0.08788337	3.07155760

H	-1.33661641	-3.17031037	4.12010682
H	-1.92393555	-4.17428170	2.79147634
H	-3.05876397	-3.54923956	4.00956398
H	1.66198415	-0.85498627	-4.20890295
H	3.42002041	-1.06546725	-4.10620045
H	2.59190364	0.05502318	-3.00186947
H	0.13447654	-1.81232989	-2.42074375
H	0.99614305	-0.90651365	-1.16102902
H	0.80695805	-2.66690111	-1.02201510
H	1.27138844	-3.24222934	-4.00266034
H	1.93395724	-4.22832732	-2.69633423
H	3.00658055	-3.57143427	-3.95336639
H	4.98485502	2.33643583	2.74616072
H	6.49769156	2.26272641	1.82061495
H	4.03080069	-4.12103103	-2.09988795
H	-6.48472777	-2.50294309	-0.91513200
H	-5.00217100	2.29345635	-2.76011062
H	-6.51430841	2.22277946	-1.83319845
H	-4.00092191	-4.12701559	2.12039470
H	-3.18111433	5.44351851	-0.76888400
H	6.55742323	-2.43539963	0.86647731
H	3.15922186	5.45921640	0.69720608
H	1.19863860	6.53386315	0.18709004
C	6.57681721	-0.31576043	1.99855815
H	6.42655505	-1.26197905	2.52273028
H	7.52887148	-0.38652840	1.45910251
H	6.67281991	0.46094011	2.75629983
C	-6.56133544	-0.36739692	-2.00774072
H	-6.37489841	-1.29491283	-2.55404377
H	-7.50885350	-0.48838326	-1.46979768
H	-6.68857754	0.42194568	-2.74724738
C	5.30600810	4.79596032	1.91467097
H	6.33944660	4.74930789	2.27587579
H	5.19083306	5.75527001	1.40016500
H	4.63927280	4.78641653	2.78394351
C	5.84777320	3.73445021	-0.31248647
H	5.69568639	2.86423995	-0.95827763
H	5.54425984	4.62820332	-0.86814570
H	6.91752057	3.81709220	-0.08686800
C	-5.33384325	4.76017973	-1.95662728
H	-4.66633775	4.74405444	-2.82521657
H	-6.36667367	4.70452146	-2.31821170
H	-5.22369540	5.72565682	-1.45265893
C	-5.87347963	3.72234566	0.28165347
H	-5.57411406	4.62364209	0.82726561
H	-6.94318694	3.79812830	0.05348587
H	-5.71915091	2.86032391	0.93785074
C	6.78228673	-4.99181144	-2.01024424
H	6.00085799	-5.04598919	-2.77546966
H	7.46793947	-4.18427165	-2.29199278
H	7.33941888	-5.93692798	-2.03613862
C	-7.23343029	-4.82027964	-0.48503398
H	-7.98700652	-4.05366161	-0.26926236
H	-6.86023406	-4.65784267	-1.50297580
H	-7.73949022	-5.79240370	-0.47071422
C	-5.11314934	-5.95321733	0.18938845

H	-4.29155137	-6.02968767	0.90947251
H	-5.63523641	-6.91845219	0.17755748
H	-4.67269159	-5.79142165	-0.80110637
C	-6.70854181	-5.08941786	1.94222557
H	-7.23770429	-6.05080312	1.94428398
H	-5.94402192	-5.12981347	2.72523054
H	-7.42426489	-4.30578341	2.21661118
C	5.25798985	-5.92351932	-0.22898005
H	5.80971859	-6.87208621	-0.24180246
H	4.83808015	-5.78658857	0.77411337
H	4.42121251	-6.01756618	-0.92905518
C	7.35745943	-4.73013591	0.40626817
H	7.00460309	-4.58707084	1.43431464
H	7.89220257	-5.68621274	0.37102905
H	8.08160320	-3.93910387	0.17843835
H	-1.22034971	6.52848073	-0.28697711

2) Compound 1, broken symmetry (S = 0):

Cu	3.17322033	-1.60601378	-0.23418534
Cu	-3.17302972	-1.60578979	0.23476095
O	3.08629593	-0.03078391	0.76385529
O	1.31248530	-1.95778648	-0.12218355
O	-3.08576765	-0.03038161	-0.76291262
O	-1.31223740	-1.95768949	0.12372698
N	3.61123489	-3.43380100	-0.64744055
N	4.87099489	-1.12655703	-1.02305051
N	-3.61121769	-3.43370186	0.64731066
N	-4.87121661	-1.12658888	1.02300395
C	0.66656770	-5.59221277	-0.13045913
C	1.39704507	-4.35964841	-0.24753513
C	0.73573566	-3.10713845	-0.09213729
C	-0.73567973	-3.10709907	0.09243853
C	-1.39722537	-4.35964591	0.24657197
C	-0.66698162	-5.59222616	0.12825468
C	2.78818566	-4.43926804	-0.55664691
C	-2.78838124	-4.43926631	0.55558822
C	-5.03470135	-3.59123550	1.01131351
C	-5.41197568	-2.27701640	1.74923393
C	-5.41529654	0.06640116	1.05677986
C	-4.95686983	1.15516920	0.20557978
C	-3.83275239	1.02933117	-0.68990646
C	-3.50887213	2.14276283	-1.55611822
C	-4.28034540	3.28560102	-1.47201692
C	-5.38098061	3.44614104	-0.59214895
C	-5.68775286	2.37785802	0.22061444
C	-6.16573031	4.76949265	-0.58993119
C	-2.32545535	2.04248273	-2.54365976
C	5.03465760	-3.59119099	-1.01172284
C	5.41172258	-2.27684241	-1.74952835
C	5.41470666	0.06659226	-1.05723185
C	4.95649137	1.15525997	-0.20580532
C	5.68703726	2.37814470	-0.22129877
C	5.38050049	3.44633837	0.59166907
C	4.28048772	3.28548494	1.47225963
C	3.50939907	2.14242582	1.55687827

C	3.83297946	1.02910976	0.69040679
C	6.16486092	4.76991770	0.58892124
C	2.32669999	2.04177290	2.54523639
C	2.15784614	3.33103323	3.37605997
C	2.56363833	0.88275629	3.54518102
C	0.99985198	1.81161457	1.77928589
C	-2.15636183	3.33184690	-3.37427670
C	-0.99908554	1.81265638	-1.77677928
C	-2.56135903	0.88346865	-3.54384460
H	0.16378630	1.77332533	2.48962728
H	1.01476858	0.87910441	1.21437406
H	0.80825024	2.63804131	1.08399776
H	1.72523062	0.82190609	4.25065677
H	3.47945350	1.05143843	4.12579324
H	2.64888364	-0.07367931	3.02812542
H	1.31108945	3.20704408	4.06054048
H	1.94414694	4.20400536	2.74779015
H	3.04207347	3.55316545	3.98595635
H	-1.72248658	0.82297452	-4.24879815
H	-3.47686918	1.05187805	-4.12501664
H	-2.64660170	-0.07304110	-3.02692675
H	-0.16250665	1.77459425	-2.48652703
H	-1.01415930	0.88012703	-1.21190586
H	-0.80819170	2.63912365	-1.08134422
H	-1.30903694	3.20815730	-4.05810653
H	-1.94341909	4.20484374	-2.74578591
H	-3.04018193	3.55374722	-3.98484863
H	-4.98706823	-2.31044136	2.76326943
H	-6.50237737	-2.24057331	1.84148916
H	-4.03181595	4.11939165	-2.11762007
H	6.53351379	2.46495480	-0.88695973
H	4.98668268	-2.31018525	-2.76351411
H	6.50211283	-2.24026916	-1.84192801
H	4.03214068	4.11921372	2.11801275
H	3.16798476	-5.44857057	-0.74199841
H	-6.53466570	2.46444973	0.88574875
H	-3.16840479	-5.44865645	0.74001255
H	-1.20921428	-6.52857720	0.23847069
C	-6.57002194	0.34256099	2.01075889
H	-6.40593487	1.28433795	2.53902110
H	-7.52238821	0.42854910	1.47425855
H	-6.67422027	-0.43613930	2.76523369
C	6.56882314	0.34293528	-2.01189131
H	6.40441369	1.28476404	-2.53994992
H	7.52152332	0.42885688	-1.47596683
H	6.67254786	-0.43569141	-2.76651489
C	-5.31472095	-4.77493346	1.94970268
H	-6.34702696	-4.72384710	2.31351089
H	-5.20282111	-5.73788828	1.44131638
H	-4.64553611	-4.76081147	2.81703279
C	-5.86121600	-3.72824057	-0.28300845
H	-5.70992380	-2.86289498	-0.93550287
H	-5.56062713	-4.62637356	-0.83315087
H	-6.93033931	-3.80772195	-0.05341164
C	5.31467454	-4.77475843	-1.95026739
H	4.64542069	-4.76061298	-2.81754566

H	6.34694198	-4.72354067	-2.31416124
H	5.20290600	-5.73777313	-1.44196358
C	5.86136152	-3.72829597	0.28247222
H	5.56090087	-4.62651783	0.83253901
H	6.93045763	-3.80767488	0.05271480
H	5.71010425	-2.86304456	0.93509837
C	-6.76891231	5.02081571	-1.99278852
H	-5.99534301	5.06786532	-2.76645708
H	-7.46529655	4.21999407	-2.26731780
H	-7.31720481	5.97124322	-2.01230544
C	7.31823697	4.76582200	-0.43188081
H	8.05328174	3.98218362	-0.21351110
H	6.95456504	4.61985320	-1.45573861
H	7.84356996	5.72730786	-0.40238564
C	5.21406995	5.93677780	0.22814836
H	4.38501834	6.02288790	0.93845498
H	5.75619421	6.89094301	0.23354810
H	4.78320584	5.79485786	-0.76959557
C	6.76881129	5.02150543	1.99140252
H	7.31688990	5.97206488	2.01050637
H	5.99568550	5.06845126	2.76552066
H	7.46554754	4.22087550	2.26559653
C	-5.21550324	5.93665911	-0.22865174
H	-5.75791404	6.89065890	-0.23443532
H	-4.78519915	5.79492782	0.76936062
H	-4.38605212	6.02298125	-0.93846161
C	-7.31972095	4.76511027	0.43017582
H	-6.95663973	4.61915194	1.45424534
H	-7.84522597	5.72649287	0.40041386
H	-8.05447101	3.98133753	0.21130541
H	1.20863258	-6.52854926	-0.24161959

3) Compound 1, singlet (S = 0):

Cu	-3.17683001	1.57609612	-0.34361564
Cu	3.17563697	1.57711569	0.34312066
O	-3.10194306	0.06459193	0.75387682
O	-1.30680076	1.91300272	-0.28110026
O	3.10056210	0.06435952	-0.75254126
O	1.30561592	1.91345794	0.27815999
N	-3.56062370	3.37255975	-0.88786530
N	-4.89005351	1.08540994	-1.07585514
N	3.55853026	3.37367175	0.88741632
N	4.88880400	1.08710707	1.07599783
C	-0.66246284	5.54158638	-0.15299832
C	-1.38232755	4.30862291	-0.32361567
C	-0.73309609	3.05011137	-0.16256470
C	0.73108809	3.05037014	0.16178049
C	1.37941378	4.30905020	0.32503728
C	0.65863467	5.54180191	0.15668637
C	-2.76334201	4.38078187	-0.67088954
C	2.76038519	4.38160472	0.67224133
C	4.98581277	3.54668863	1.22835086
C	5.40962714	2.19949815	1.87235615
C	5.43053843	-0.10551868	1.05989855
C	4.97752273	-1.15703041	0.15934701

C	3.84168629	-1.00163587	-0.71557507
C	3.50062343	-2.08967770	-1.60785860
C	4.27988687	-3.23027464	-1.57892322
C	5.39860930	-3.41490632	-0.72779312
C	5.71348993	-2.37516356	0.11873011
C	6.19222711	-4.73165712	-0.78941583
C	2.29775353	-1.96132147	-2.56814888
C	-4.98792203	3.54496557	-1.22895650
C	-5.41124875	2.19738682	-1.87255851
C	-5.43175813	-0.10720131	-1.05875012
C	-4.97781264	-1.15839203	-0.15823665
C	-5.71302182	-2.37696217	-0.11731812
C	-5.39673062	-3.41683834	0.72853468
C	-4.27724616	-3.23191093	1.57857935
C	-3.49876969	-2.09076573	1.60734810
C	-3.84156472	-1.00242501	0.71610960
C	-6.18930081	-4.73421071	0.79020847
C	-2.29510874	-1.96203281	2.56660976
C	-2.10497150	-3.22926188	3.42644207
C	-2.51280634	-0.77796841	3.54103460
C	-0.98632143	-1.74960061	1.76543064
C	2.10978088	-3.22792675	-3.42935480
C	0.98796603	-1.75100255	-1.76804546
C	2.51518536	-0.77608737	-3.54122038
H	-0.13462083	-1.69199177	2.45550231
H	-1.01479410	-0.83126815	1.17834550
H	-0.80872515	-2.59290628	1.08691533
H	-1.65822067	-0.69556510	4.22453104
H	-3.41421821	-0.93416334	4.14707488
H	-2.61423253	0.16433305	3.00127167
H	-1.24084856	-3.08775933	4.08528554
H	-1.90790321	-4.11870681	2.81607087
H	-2.97310397	-3.43429770	4.06467417
H	1.66110101	-0.69375588	-4.22534836
H	3.41725616	-0.93087812	-4.14663586
H	2.61527865	0.16576104	-3.00041996
H	0.13685923	-1.69399455	-2.45889742
H	1.01480457	-0.83303860	-1.18030879
H	0.81076450	-2.59497069	-1.09024203
H	1.24636879	-3.08657706	-4.08916038
H	1.91270120	-4.11809096	-2.82003681
H	2.97890092	-3.43166154	-4.06666113
H	4.99907782	2.15305191	2.89149375
H	6.50209648	2.18219327	1.94635547
H	4.02235131	-4.04252073	-2.24808782
H	-6.57141214	-2.48281654	-0.76483203
H	-5.00052999	2.15070771	-2.89161657
H	-6.50369618	2.17972999	-1.94672313
H	-4.01846606	-4.04434309	2.24702914
H	-3.16428197	5.39479785	-0.76732626
H	6.57128842	-2.48079702	0.76706810
H	3.16060454	5.39574465	0.77016965
H	1.19645754	6.47782841	0.28701836
C	6.57743190	-0.42433006	2.01115877
H	6.41370705	-1.39165732	2.49129237
H	7.53436937	-0.47869778	1.47854368

H	6.67149755	0.31843453	2.80236825
C	-6.57937229	-0.42636575	-2.00904548
H	-6.41636352	-1.39404658	-2.48867192
H	-7.53600669	-0.47995274	-1.47579334
H	-6.67361722	0.31590956	-2.80070567
C	5.22725453	4.67409333	2.24459670
H	6.26528792	4.64733526	2.59508900
H	5.06188762	5.66290233	1.80539736
H	4.56762886	4.56668301	3.11226118
C	5.79633083	3.79682407	-0.05859591
H	5.66755475	2.97128146	-0.76556382
H	5.46307193	4.71922603	-0.54646680
H	6.86442134	3.89637478	0.16834453
C	-5.22934768	4.67194744	-2.24567347
H	-4.56968400	4.56411767	-3.11325416
H	-6.26737578	4.64514532	-2.59619078
H	-5.06386001	5.66090844	-1.80685850
C	-5.79879034	3.79527078	0.05773495
H	-5.46597060	4.71793245	0.54542124
H	-6.86686137	3.89441919	-0.16947226
H	-5.66989265	2.96997380	0.76497085
C	6.77137806	-4.92488971	-2.21144594
H	5.98431464	-4.94856101	-2.97243230
H	7.45706446	-4.10891290	-2.46761074
H	7.32594698	-5.86959378	-2.27685566
C	-7.36360778	-4.75931369	-0.20612715
H	-8.08845367	-3.96257329	-0.00161691
H	-7.02067172	-4.65431481	-1.24211239
H	-7.89467346	-5.71501099	-0.12970269
C	-5.25373126	-5.92032526	0.45353605
H	-4.41075632	-5.98650125	1.14949479
H	-5.80191338	-6.86961199	0.50506127
H	-4.84263192	-5.81826797	-0.55733967
C	-6.76630500	-4.92925461	2.21285590
H	-7.31981884	-5.87458191	2.27813256
H	-5.97822291	-4.95286903	2.97278054
H	-7.45248638	-4.11422384	2.47069903
C	5.25723494	-5.91885907	-0.45507229
H	5.80633069	-6.86760773	-0.50672659
H	4.84474399	-5.81809652	0.55537088
H	4.41518797	-5.98524388	-1.15213842
C	7.36507260	-4.75672452	0.20863787
H	7.02046333	-4.65260428	1.24415367
H	7.89682467	-5.71205284	0.13236411
H	8.08980714	-3.95945113	0.00579817
H	-1.20099084	6.47745100	-0.28157553

4) Compound $[1]^{+}$, quartet (S = 3/2):

Cu	-3.20277789	1.57778110	-0.27049265
Cu	3.19535695	1.57694898	0.27640637
O	-3.06907881	-0.00462685	0.66782042
O	-1.32464345	1.95657047	-0.08976220
O	3.05343804	-0.01518461	-0.64422678
O	1.31703779	1.95595159	0.09635536

N	-3.62007640	3.42339087	-0.68239525
N	-4.87185344	1.11090859	-1.08588826
N	3.61404341	3.42539797	0.67425806
N	4.86845570	1.11638708	1.08682399
C	-0.68067232	5.54668828	-0.15795058
C	-1.40936324	4.34754232	-0.27156436
C	-0.74341541	3.08608411	-0.09260989
C	0.73719834	3.08609420	0.08692180
C	1.40487368	4.34851028	0.25238310
C	0.67785855	5.54735547	0.12577899
C	-2.81322101	4.42935806	-0.59831487
C	2.80856705	4.43157658	0.57921584
C	5.04473947	3.57897802	1.04650562
C	5.40396770	2.27412125	1.80855960
C	5.43375932	-0.06888262	1.10726977
C	4.99290796	-1.15251606	0.24000671
C	3.84513202	-1.04904594	-0.62934767
C	3.53472724	-2.14469799	-1.51910777
C	4.35066091	-3.26017409	-1.48138518
C	5.47512542	-3.40287528	-0.63039129
C	5.76456421	-2.34473422	0.20775611
C	6.30885524	-4.69357998	-0.68288704
C	2.33099977	-2.06194142	-2.48264963
C	-5.05102669	3.57402889	-1.05424879
C	-5.40961841	2.26578405	-1.81079353
C	-5.43221529	-0.07678241	-1.10673684
C	-4.98898973	-1.15827708	-0.23789327
C	-5.74871974	-2.35843575	-0.21619105
C	-5.45741592	-3.41543560	0.62271151
C	-4.34424641	-3.26277932	1.48674706
C	-3.54008097	-2.13926160	1.53534183
C	-3.85083246	-1.04575258	0.64302245
C	-6.27739433	-4.71534076	0.66237690
C	-2.34790491	-2.04619873	2.51219292
C	-2.21200036	-3.31824484	3.37491392
C	-2.54412951	-0.85518438	3.48332953
C	-1.02129388	-1.87794502	1.72960904
C	2.19615530	-3.33523439	-3.34362433
C	1.01185800	-1.90461619	-1.68538164
C	2.50650774	-0.86947039	-3.45595763
H	-0.18001475	-1.85141142	2.43352056
H	-1.00886730	-0.95876623	1.14280322
H	-0.86189189	-2.72566631	1.05272849
H	-1.70418973	-0.80937295	4.18707983
H	-3.46355988	-0.97710925	4.06851728
H	-2.59527740	0.09453665	2.94872824
H	-1.35760761	-3.20198673	4.05030802
H	-2.02842956	-4.21323089	2.76914606
H	-3.09683404	-3.49657257	3.99704425

H	1.65921632	-0.83155582	-4.15134151
H	3.42115479	-0.98308710	-4.05023392
H	2.55402905	0.08080295	-2.92200632
H	0.16247537	-1.88568908	-2.37970981
H	0.99830373	-0.98518784	-1.09904239
H	0.86741119	-2.75332468	-1.00633512
H	1.33302136	-3.22656246	-4.00907609
H	2.02744860	-4.23159048	-2.73557021
H	3.07521151	-3.50603192	-3.97598589
H	4.96872363	2.31953323	2.81680532
H	6.49183912	2.23445340	1.91168661
H	4.12063897	-4.08456977	-2.14425620
H	-6.60628016	-2.44199581	-0.86692518
H	-4.97601288	2.30810530	-2.81986667
H	-6.49762731	2.22461811	-1.91200516
H	-4.11329611	-4.08599699	2.15073783
H	-3.18668350	5.43676383	-0.79870185
H	6.63047224	-2.42023020	0.84843050
H	3.18331225	5.44040446	0.76984927
H	1.19845775	6.49424333	0.24079217
C	6.59361213	-0.33236124	2.05423919
H	6.47091032	-1.30109085	2.54215962
H	7.55061680	-0.35143302	1.51934745
H	6.65843190	0.41776940	2.84137059
C	-6.58849991	-0.34665163	-2.05618308
H	-6.45183290	-1.30894225	-2.55342616
H	-7.54471245	-0.38516134	-1.52113591
H	-6.66484066	0.40968913	-2.83612931
C	5.32399907	4.78088112	1.95914146
H	6.35391569	4.72862907	2.32680655
H	5.22693770	5.73369164	1.42927981
H	4.65517114	4.79136049	2.82674895
C	5.86667139	3.68435362	-0.25347337
H	5.71020347	2.81126962	-0.89413612
H	5.58048625	4.57854393	-0.81685096
H	6.93447065	3.75505308	-0.02046482
C	-5.33280362	4.77205145	-1.97109878
H	-4.66535857	4.77988635	-2.83980597
H	-6.36321555	4.71732980	-2.33697389
H	-5.23588665	5.72693955	-1.44495451
C	-5.87170720	3.68369401	0.24622915
H	-5.58570145	4.58036926	0.80572625
H	-6.93981296	3.75242941	0.01405170
H	-5.71384082	2.81333328	0.89025745
C	6.89371807	-4.87261908	-2.10500575
H	6.10989988	-4.92968087	-2.86753423
H	7.55437126	-4.03798641	-2.36587453
H	7.47793372	-5.79861640	-2.16117941
C	-7.43836825	-4.70718674	-0.34975156

H	-8.15409392	-3.90215503	-0.14565117
H	-7.08129691	-4.60064520	-1.38083655
H	-7.98607988	-5.65356018	-0.28942643
C	-5.35708561	-5.91468904	0.32779656
H	-4.52678069	-6.00672075	1.03584327
H	-5.92665321	-6.85077862	0.36389927
H	-4.93101119	-5.81471979	-0.67694861
C	-6.87346260	-4.90671588	2.07820096
H	-7.44824757	-5.83911396	2.12500993
H	-6.09616969	-4.95875478	2.84775830
H	-7.54539012	-4.08031105	2.33649941
C	5.40500160	-5.90434569	-0.34463263
H	5.98423092	-6.83403958	-0.39070394
H	4.98791839	-5.81350538	0.66473679
H	4.56872795	-6.00214320	-1.04478298
C	7.47922555	-4.67645136	0.31826924
H	7.13084832	-4.57734769	1.35306768
H	8.03652598	-5.61660974	0.24931405
H	8.18413637	-3.86296314	0.11017198
H	-1.20007011	6.49296754	-0.28296917

5) Compound $[1]^{+}$, broken symmetry, Cu spins aligned (S = 1/2):

Cu	-3.20253813	1.55662448	-0.31520047
Cu	3.20221726	1.55643851	0.31556187
O	-3.04899081	-0.03310439	0.60205616
O	-1.31318014	1.93377373	-0.16909497
O	3.04796199	-0.03401705	-0.6003277
O	1.3128869	1.93373068	0.16960705
N	-3.6120851	3.40802509	-0.72801734
N	-4.87554492	1.10121234	-1.1194288
N	3.61198061	3.40801597	0.72743788
N	4.87555873	1.10138768	1.11933249
C	-0.67732367	5.52190088	-0.15887854
C	-1.40175841	4.32617556	-0.29954604
C	-0.73726782	3.0621559	-0.12048185
C	0.73711389	3.06214792	0.12017348
C	1.40177214	4.32619922	0.29837625
C	0.67750015	5.52192533	0.15689005
C	-2.80231808	4.41067191	-0.64673831
C	2.8023369	4.41071697	0.64552071
C	5.03932626	3.56367843	1.11439814
C	5.39867328	2.25071428	1.86221826
C	5.44106286	-0.08441616	1.13377719
C	5.01164651	-1.15756445	0.25005082
C	3.86190102	-1.05238415	-0.61499524
C	3.56882371	-2.13164892	-1.52895275
C	4.39933095	-3.23709183	-1.51277966
C	5.52573525	-3.38287638	-0.66470773
C	5.80082984	-2.33854722	0.19391877
C	6.3777329	-4.66032856	-0.74545333
C	2.36372473	-2.04626654	-2.49089431
C	-5.03942924	3.56353768	-1.11501942

C	-5.39873387	2.25037743	-1.86252691
C	-5.44077547	-0.08472763	-1.13392586
C	-5.01134854	-1.15773704	-0.25002649
C	-5.7998416	-2.33923063	-0.19460625
C	-5.52479103	-3.38346481	0.66414063
C	-4.39919973	-3.23702982	1.51318123
C	-3.56940294	-2.13107597	1.53010852
C	-3.86232917	-1.0519613	0.61592461
C	-6.37602111	-4.66148259	0.74403842
C	-2.36519014	-2.04498353	2.49307655
C	-2.25115955	-3.29973839	3.38374624
C	-2.52406379	-0.82767447	3.43789207
C	-1.04244832	-1.92625682	1.69519464
C	2.24952774	-3.30115926	-3.38134709
C	1.0416082	-1.92811781	-1.69189972
C	2.52116246	-0.8289708	-3.435967
H	-0.19364818	-1.90644338	2.39023221
H	-1.01347123	-1.01983062	1.08942487
H	-0.9108272	-2.79107373	1.03408518
H	-1.6752865	-0.78340667	4.13113946
H	-3.43923753	-0.91544282	4.03575866
H	-2.56054817	0.10998361	2.88112083
H	-1.38942425	-3.18747546	4.0504711
H	-2.09199687	-4.21196975	2.79715415
H	-3.13523612	-3.44418583	4.01566055
H	1.67184217	-0.78529135	-4.12858728
H	3.43594382	-0.91624595	-4.03450656
H	2.55748296	0.10876904	-2.87932214
H	0.19220039	-1.90884862	-2.38620862
H	1.01267729	-1.02161864	-1.0862415
H	0.91100854	-2.79290895	-1.03055247
H	1.38714797	-3.18938057	-4.04731929
H	2.09132797	-4.21340946	-2.79452576
H	3.13311116	-3.44523502	-4.01403369
H	4.95587143	2.28141613	2.86787076
H	6.4859507	2.21409757	1.97366705
H	4.18033873	-4.05066251	-2.19266235
H	-6.66830497	-2.41359936	-0.83214177
H	-4.95598489	2.28089067	-2.86820798
H	-6.48601791	2.21368942	-1.97390927
H	-4.1802639	-4.0505031	2.19320151
H	-3.16901008	5.41827109	-0.85866441
H	6.66988927	-2.41237805	0.83071399
H	3.16916298	5.4183954	0.85683744
H	1.19299284	6.46977402	0.28630423
C	6.5912049	-0.35424979	2.09074327
H	6.4800064	-1.3381137	2.54981117
H	7.55639071	-0.33992514	1.57034923
H	6.62977668	0.37556042	2.89877875
C	-6.59062021	-0.35488125	-2.09115592
H	-6.47849316	-1.33832891	-2.55090937
H	-7.55583343	-0.34183104	-1.57079134
H	-6.62983929	0.37544002	-2.89868903
C	5.30613124	4.75530224	2.04365795
H	6.33357903	4.70286202	2.41806777
H	5.20884509	5.71430555	1.52507405

H	4.6312788	4.75190234	2.90666567
C	5.86906968	3.68892655	-0.17889076
H	5.72068584	2.8233049	-0.8314175
H	5.58308356	4.58919126	-0.73263573
H	6.93485012	3.76099878	0.06260301
C	-5.30631978	4.75493468	-2.04453838
H	-4.6315116	4.75137066	-2.90758053
H	-6.33378229	4.70236835	-2.41888846
H	-5.20904814	5.71405488	-1.52616738
C	-5.86915853	3.68905898	0.17825519
H	-5.58318257	4.58945884	0.73178481
H	-6.93494267	3.76104797	-0.06324591
H	-5.72075426	2.82359413	0.83098554
C	6.96614609	-4.7991376	-2.17051203
H	6.18355226	-4.85064328	-2.93474998
H	7.6142899	-3.94898505	-2.41201106
H	7.56413019	-5.71485706	-2.24718825
C	-7.54464244	-4.65041258	-0.2592446
H	-8.2392776	-3.82361132	-0.06979807
H	-7.19323144	-4.57756627	-1.29520638
H	-8.11427995	-5.58159244	-0.17145391
C	-5.48885196	-5.8917009	0.43367256
H	-4.65441133	-5.98566685	1.13659054
H	-6.08074899	-6.81221546	0.49952147
H	-5.06966841	-5.82884099	-0.57698294
C	-6.96516245	-4.80108196	2.16871909
H	-7.56260272	-5.7172084	2.24478407
H	-6.18297498	-4.85231139	2.93339462
H	-7.61399371	-3.95141935	2.41009659
C	5.49152346	-5.89119913	-0.43493121
H	6.083952	-6.81132179	-0.50147309
H	5.07294617	-5.8289428	0.57601286
H	4.65669472	-5.9854439	-1.13734665
C	7.54692897	-4.6487913	0.25715895
H	7.19607291	-4.57654389	1.29335077
H	8.11716344	-5.57954284	0.16871432
H	8.24086687	-3.82143636	0.06758057
H	-1.19269308	6.46972697	-0.28894879

6) Compound 1^{+}, broken symmetry, Cu spins opposed (S = 1/2):

Cu	-3.20044425	1.5799078	-0.27753287
Cu	3.20118859	1.55577313	0.30966119
O	-3.08242952	0.00364034	0.67164241
O	-1.32380681	1.95395117	-0.0654833
O	3.02580992	-0.0440983	-0.58694593
O	1.31103045	1.93926891	0.20062003
N	-3.6008333	3.42255399	-0.71871104
N	-4.85859809	1.11177693	-1.11314572
N	3.62843119	3.41041763	0.68631889
N	4.8870179	1.10349482	1.08893938
C	-0.65788965	5.53651739	-0.18180911
C	-1.39185537	4.34129999	-0.2856631
C	-0.73530654	3.0787097	-0.07617092
C	0.74257095	3.07137911	0.13507753
C	1.41696128	4.33399864	0.27621406

C	0.6987373	5.53291248	0.11827624
C	-2.79014218	4.42540933	-0.63653261
C	2.82305346	4.41630343	0.59883673
C	5.0621833	3.56436798	1.04912907
C	5.42687859	2.25964115	1.80873294
C	5.44848786	-0.08408134	1.10686169
C	5.00072933	-1.16495612	0.24196982
C	3.83757919	-1.0646555	-0.60505647
C	3.52814395	-2.15155982	-1.50420551
C	4.35560102	-3.259372	-1.49054989
C	5.49435387	-3.40083769	-0.65847618
C	5.78569727	-2.34915519	0.18514651
C	6.34119882	-4.68184834	-0.74004606
C	2.30898331	-2.07164996	-2.44900207
C	-5.02560674	3.57610899	-1.11323506
C	-5.38055441	2.26069321	-1.85889272
C	-5.42332516	-0.07404438	-1.13104803
C	-4.99722595	-1.14873396	-0.24552075
C	-5.76372075	-2.34416911	-0.22065939
C	-5.48752606	-3.39453666	0.63197155
C	-4.38262977	-3.24004276	1.50636144
C	-3.57270407	-2.12062498	1.55327602
C	-3.86874358	-1.03375196	0.64779296
C	-6.31559188	-4.68902737	0.67549257
C	-2.3900153	-2.02498986	2.54115617
C	-2.26904317	-3.29048809	3.41558683
C	-2.59063045	-0.82498681	3.50029496
C	-1.05465748	-1.86927373	1.77074817
C	2.17851322	-3.33369693	-3.32706632
C	0.99937215	-1.94388024	-1.63132711
C	2.45467179	-0.86280725	-3.40662953
H	-0.22042404	-1.84478247	2.48292037
H	-1.0297311	-0.95294549	1.17989718
H	-0.89377861	-2.72108551	1.09943356
H	-1.7571216	-0.77674214	4.21139337
H	-3.51600675	-0.93810652	4.07784716
H	-2.63248484	0.1205212	2.95742775
H	-1.42161612	-3.17218687	4.09928277
H	-2.08247934	-4.19108505	2.819145
H	-3.16134755	-3.46005788	4.02945693
H	1.5957407	-0.82345865	-4.08767638
H	3.36078177	-0.95674817	-4.01721885
H	2.50058021	0.0794513	-2.85841117
H	0.1395128	-1.925018	-2.31282043
H	0.98365687	-1.03413968	-1.03006403
H	0.87573303	-2.80477442	-0.96351241
H	1.30636483	-3.2255501	-3.98087366
H	2.02742543	-4.24072138	-2.73032707
H	3.05212799	-3.48509896	-3.97175464
H	4.99928293	2.30562922	2.82039196
H	6.51553446	2.21923355	1.90444297
H	4.12400011	-4.07836468	-2.15970346
H	-6.61440684	-2.42946731	-0.88008947
H	-4.93353014	2.28883537	-2.86258079
H	-6.4672972	2.2234517	-1.97408694
H	-4.16323982	-4.05846838	2.1800617

H	-3.15491712	5.43177686	-0.85679392
H	6.66445674	-2.41904973	0.80903924
H	3.19908544	5.42533281	0.78640098
H	1.22408901	6.47900805	0.21767778
C	6.61360942	-0.34742656	2.04746714
H	6.50762945	-1.32639416	2.51806494
H	7.57024198	-0.34069528	1.51134991
H	6.66703219	0.39030314	2.8474787
C	-6.56667944	-0.34832824	-2.09465647
H	-6.4295239	-1.31784058	-2.57741954
H	-7.53119446	-0.37299867	-1.57381674
H	-6.62552057	0.39845678	-2.88527021
C	5.3483318	4.76675655	1.95869373
H	6.38117519	4.71474395	2.31807194
H	5.24693788	5.71944375	1.42932986
H	4.68661409	4.7775021	2.83176384
C	5.87282546	3.66859176	-0.25796797
H	5.71022496	2.79498607	-0.89625745
H	5.58249728	4.56274692	-0.8193238
H	6.94258071	3.73864843	-0.03395334
C	-5.28772518	4.76440156	-2.04824856
H	-4.60762146	4.75858146	-2.9070829
H	-6.31288566	4.71010785	-2.42860718
H	-5.19403911	5.72498408	-1.53203458
C	-5.86411774	3.70598687	0.174053
H	-5.58112994	4.60780904	0.72674596
H	-6.92825165	3.77795584	-0.07465162
H	-5.72086798	2.84271141	0.83095659
C	6.90796321	-4.83611321	-2.17219225
H	6.11391179	-4.89122084	-2.9242493
H	7.55575347	-3.9908024	-2.43103615
H	7.50119218	-5.75490027	-2.24948909
C	-7.4659875	-4.68374232	-0.3486512
H	-8.17871665	-3.87215621	-0.16053783
H	-7.09756704	-4.59038463	-1.37701877
H	-8.02041116	-5.62591046	-0.28427786
C	-5.39912356	-5.89693494	0.36199575
H	-4.57673677	-5.98737122	1.07944956
H	-5.97486174	-6.82907939	0.40103762
H	-4.96208054	-5.80925122	-0.63917494
C	-6.92717943	-4.86284897	2.08708387
H	-7.5089242	-5.7907543	2.13654947
H	-6.15799733	-4.9133177	2.8648644
H	-7.59586834	-4.02946252	2.33089306
C	5.45612843	-5.90701656	-0.40477213
H	6.04437748	-6.8298042	-0.47200975
H	5.05324134	-5.8341163	0.61182352
H	4.61037276	-6.00459372	-1.09350211
C	7.52532351	-4.66451004	0.24479306
H	7.19025853	-4.58104529	1.28536117
H	8.09149368	-5.5978039	0.15676201
H	8.21856004	-3.84104995	0.0366963
H	-1.16793229	6.48411234	-0.33238296