

Supporting information:

Table 5S: Additional results for hyperfine coupling tensors for Cu in various copper complexes.^a

Complex		A ^{FC}	A ^{dip}
[Cu(NH ₃) ₄] ²⁺	ref. 10:	-340	-478,239,239
	this work:	-329	-471,235,235
[Cu(dtc) ₂]	ref. 10:	-257	-322,153,163
	this work:	-290	-306,151,155
[Cu(KTS)]	ref. 10:	-292	-387,192,195
	this work:	-313	-398,198,201
[Cu(en) ₂] ²⁺	ref. 10:	-347	-458,228,229
	this work:	-358	-452,225,227
[Cu(gly) ₂]	ref. 10:	-315	-472,203,270
	this work:	-317	-467,197,270
[Cu(iz) ₄] ²⁺	ref. 10:	-291	-483,238,245
	this work:	-297	-476,237,240
[Cu(mnt) ₂] ²⁻	ref. 10:	-252	-323,163,160
	this work:	-270	-313,155,158
[Cu(sac) ₂]	ref. 10:	-275	-486,240,246
	this work:	-302	-478,240,237

^a (15s11p6d)/[9s7p4d] basis set for Cu, BII basis sets for the main group elements. Hybrid B3LYP functional, Gaussian98 calculations.

Table 6S: Cartesian coordinates of Cu complexes (optimized structures)

[Cu(acac) ₂]			
Cu	0.000000000000000	0.000000000000000	0.000000000000000
O	2.54575944224205	-2.67540160941653	0.000000000000000
O	2.54661683436842	2.67482361240178	0.000000000000000
O	-2.54575944224205	2.67540160941654	0.000000000000000
O	-2.54661683436842	-2.67482361240178	0.000000000000000
C	4.94631560687305	-2.35034045881625	0.000000000000000
C	4.94723206202789	2.34984855458364	0.000000000000000
C	-4.94631560687305	2.35034045881625	0.000000000000000
C	-4.94723206202789	-2.34984855458364	0.000000000000000
C	6.19087653473744	-0.00035705917405	0.000000000000000
C	-6.19087653473744	0.00035705917405	0.000000000000000
H	8.24852899892277	-0.00113096001075	0.000000000000000
H	-8.24852899892277	0.00113096001075	0.000000000000000
C	6.48532555239411	-4.76359675005665	0.000000000000000
C	6.48682976665986	4.76272477918974	0.000000000000000
C	-6.48532555239411	4.76359675005665	0.000000000000000
C	-6.48682976665986	-4.76272477918974	0.000000000000000
H	8.52457609776143	-4.39564901769127	0.000000000000000
H	5.99033309702350	-5.89581725547260	1.67091178687337
H	5.99033309702350	-5.89581725547260	-1.67091178687337
H	8.52591485753616	4.39403564771671	0.000000000000000
H	5.99235647869361	5.89514834031532	-1.67092169008253
H	5.99235647869361	5.89514834031532	1.67092169008253
H	-8.52591485753616	-4.39403564771671	0.000000000000000
H	-5.99235647869362	-5.89514834031532	-1.67092169008253
H	-5.99235647869362	-5.89514834031532	1.67092169008253
H	-8.52457609776143	4.39564901769127	0.000000000000000
H	-5.99033309702350	5.89581725547260	1.67091178687337
H	-5.99033309702350	5.89581725547260	-1.67091178687337

[Cu(NH₃)₄]²⁺

Cu	-0.00002379986480	0.00102252098790	0.00000000000000
N	-0.70246026977860	-3.85248744609011	0.00000000000000
N	-0.70159212336093	3.85329779358795	0.00000000000000
N	0.70204243120526	-0.00208375960060	3.85328318520520
N	0.70204243120526	-0.00208375960060	-3.85328318520520
H	0.91124615895717	-4.93640846710190	0.00000000000000
H	-1.73629854399372	-4.41881810977087	1.54465736275673
H	-1.73629854399372	-4.41881810977087	-1.54465736275673
H	-1.73483219536164	4.42019669703624	-1.54482453784611
H	-1.73483219536164	4.42019669703624	1.54482453784611
H	0.91284383623506	4.93623696120439	0.00000000000000
H	-0.91176399026610	-0.03088501331090	4.93670834670587
H	1.75866493448169	-1.53421594224749	4.41180288135553
H	1.71270934493664	1.55490503549821	4.42744553347994
H	1.71270934493664	1.55490503549821	-4.42744553347994
H	1.75866493448169	-1.53421594224749	-4.41180288135553
H	-0.91176399026610	-0.03088501331090	-4.93670834670587

[Cu(dtc)₂]

Cu	0.00072641319019	-0.00654501602877	0.00129947923872
S	-2.76147133830996	0.01828369845989	3.48986420066381
C	0.00451967199764	-0.02473833200841	5.26020357445880
S	2.76881843503154	0.00442523323251	3.48570868056969
N	-0.00016556039114	-0.08774901260382	7.80613241463760
C	2.33475185255683	0.04157365628931	9.27716731095320
C	-2.34962303391911	0.03259456765335	9.25665761899494
H	2.23759906814390	-1.32366982088718	10.84024589911420
H	3.94413320149254	-0.41632840450934	8.05848426885322
H	2.60299901081971	1.95136459173366	10.06432193038713
H	-2.16697475985444	-1.16722094787422	10.94111361957340
H	-2.75270027353637	1.98628534325556	9.85686855809579
H	-3.92007295320782	-0.64570132963943	8.09011344936828
S	-2.76426614517353	-0.02182975775394	-3.48444431562665
C	-0.00030671458159	0.02134004873155	-5.25967052364472
S	2.76441963799624	-0.01344276301159	-3.48558610811751
N	-0.00154177805934	0.08781390687087	-7.80543691103452
C	2.33423480648669	-0.00747072375682	-9.27718239164035
C	-2.33940519386013	-0.01196388469503	-9.27372571315968
H	2.23569916609365	1.39003401260965	-10.81208139366874
H	3.94372944276001	0.42554569275627	-8.05017683319881
H	2.60144682956157	-1.89988497076240	-10.10502800225892
H	-2.23356912426175	1.36693987074411	-10.82463892210185
H	-2.61876451950982	-1.91231744841597	-10.07928742154262
H	-3.94557206899309	0.44456640389300	-8.05060983117984

[Cu(KTS)]

Cu	-1.21127994072293	-0.01128731014074	0.00011306341591
N	1.26098552742836	-0.01318110919424	2.78933875428067
N	3.76301664730344	-0.00346600043032	3.22714352722009
C	5.41479663498937	-0.00703725219126	1.37552292089797
C	5.41449231079960	0.00153392412692	-1.37621403022022
N	3.76285201517350	-0.00189969801919	-3.22787850895694
N	1.26061355128596	-0.01437441225488	-2.78968452175337
H	7.34769262178240	0.00729114789610	-2.11645353699803
H	7.34818226841745	-0.00608963938562	2.11496760297077
C	-0.29184095455010	0.00449805644804	4.80665958161507
S	-3.45177403899989	0.00132493529247	3.89628992102525
N	0.57164032871568	0.03999562016724	7.19125149000570
H	-0.62974224832983	-0.01556346197179	8.67665728055420
H	2.47889820941294	-0.00373578319987	7.44694302995429
C	-0.29240422195084	0.00626246862542	-4.80673696647369
S	-3.45224632011431	0.00152775565906	-3.89579354819172
N	0.57139159985548	0.02862467862349	-7.19109304944428
H	-0.63202956489347	0.04685170421143	-8.67573183234120
H	2.47892211830295	0.03330713892982	-7.44732577514768

[Cu(en)₂]²⁺

Cu	-0.00007612401996	-0.00001397406785	0.00004281809207
N	-2.60593170811838	0.02794365946600	2.91495093144261
C	-1.28029905294645	-0.64670359350207	5.33556806472921
C	1.28020879769084	0.64697968115329	5.33534634346184
N	2.60601521537867	-0.02842213494189	2.91453189371261
H	-4.11625468271288	-1.15776435824088	2.63566561304269
H	-3.36018474642477	1.81455740121857	3.06020869329512
H	4.11594257108609	1.15793605353680	2.63597926447328

H	3.36086852589667	-1.81478969573494	3.05908676281264
H	-2.40672198243673	-0.07793827215106	6.98655401002656
H	-1.07506269409082	-2.71296053708328	5.39186971512996
H	1.07688920694722	2.71346766628630	5.38976619110988
H	2.40837199871143	0.07891126846805	6.98531371373234
N	2.60545945035451	0.02824323835685	-2.91433058374068
C	1.28055104914976	-0.64644575699988	-5.33579146717887
C	-1.28040172494196	0.64614223168467	-5.33638433547831
N	-2.60544835408952	-0.02778769515148	-2.91435693333527
H	-3.36038983526542	-1.81426477557173	-3.05891001367039
H	-4.11554134157764	1.15827789584974	-2.63493993315942
H	3.35961078207515	1.81491707639549	-3.05917579233654
H	4.11622414569052	-1.15707081829943	-2.63525487175411
H	-2.40962046367247	0.07621710194433	-6.98488855188661
H	-1.07769483362806	2.71264363071007	-5.39342735713725
H	1.07717812749272	-2.71289459882349	-5.39145294004780
H	2.40916541475742	-0.07771852918161	-6.98511421265171

[Cu(gly)₂]

Cu	-0.00092307162624	-0.00059927263382	0.00000000000000
O	-1.85025353859802	-3.14124784476819	0.00000000000000
C	-0.51698528329734	-5.23149279121389	0.00000000000000
O	-1.39955407777922	-7.37123776816095	0.00000000000000
C	2.39923912407016	-4.90330910877327	0.00000000000000
N	3.16766829276817	-2.19641930447406	0.00000000000000
H	4.21765051724069	-1.71418774017971	1.54857339130468
H	4.21765051724069	-1.71418774017971	-1.54857339130468
H	3.15184576666342	-5.87698024310456	-1.67028382144283
H	3.15184576666342	-5.87698024310456	1.67028382144283
O	1.84928906230063	3.14005468007488	0.00000000000000
C	0.51837174483989	5.23219180443186	0.00000000000000
O	1.40244141779432	7.37114934762160	0.00000000000000
C	-2.39762382545935	4.90403304516214	0.00000000000000
N	-3.16828286452409	2.19861786959237	0.00000000000000
H	-4.21899928638546	1.71801342970239	1.54856712194632
H	-4.21899928638546	1.71801342970239	-1.54856712194632
H	-3.15027832230323	5.87846050252462	-1.66993538909029
H	-3.15027832230323	5.87846050252462	1.66993538909029

[Cu(iz)₄]²⁺

Cu	0.10232004489049	-0.02930219702609	-0.00851769178197
N	-2.65645504268406	-0.98709612479293	-2.48588549588866
C	-4.18595426246421	0.66013629336349	-3.83547781729705
C	-5.97811568503481	-0.71079335070368	-5.11381287067476
N	-5.51856749193082	-3.20706526771093	-4.51826060965400
C	-3.51498490350075	-3.32368793621895	-2.92952718018635
N	2.77538824611568	-0.89377153327744	2.54387904331492
C	2.80009019174194	-0.38058226108334	5.11680527331906
C	4.87999719540226	-1.50117527350056	6.17934074501226
N	6.11477666851638	-2.70530139243163	4.22111377384486
C	4.81941925038717	-2.30776785282650	2.05658060095205
N	2.61719947245316	0.86016558615739	-2.71248164945551
C	4.69078494217660	2.43457736595909	-2.34719175874375
C	5.85882350541808	2.82729418539327	-4.62607901004824
N	4.47926423613514	1.46502632996129	-6.37267591899018
C	2.54133453010172	0.30542362456229	-5.17871758692762
N	-2.48303950375782	0.97231139523016	2.61884920981630
C	-4.03538738286729	-0.62293988392283	4.00285408538985
C	-5.61090472689588	0.81118404749866	5.48122607370510
N	-4.99558243904950	3.29285488244386	4.97266322822866
C	-3.10859259252362	3.34069095438643	3.24410155751595
H	-3.90687738324744	2.68907790042184	-3.80440701974041
H	-7.49894616682426	-0.13878929141291	-6.36117251255988
H	-6.52309048007407	-4.71871926009769	-5.15918765021624
H	-2.75675645104143	-5.07086060142316	-2.17119419555425
H	1.34195748835566	0.73432813006835	6.01814976434486
H	5.56838752256154	-1.54759627162099	8.10795503888539
H	7.73525232543028	-3.73201518711841	4.37814639933078
H	5.38741410365855	-3.03370187335178	0.22770084344823
H	5.18363605210207	3.18018069824264	-0.50537490497957
H	7.50178557231519	3.93614022306426	-5.14322999933787
H	4.85456971679868	1.35311679029897	-8.25722204088215
H	-3.91371218962066	-2.66264131198886	3.86632449168858
H	-7.07336162873684	0.29125692230621	6.81788589707662
H	1.15857940671156	-0.88061661086512	-6.11240237055448
H	-5.81936783752856	4.84074090973927	5.76637265038674
H	-2.26543363884244	5.06247077242294	2.51808751185080

[Cu(mnt)₂]²⁻

Cu	0.00055207192220	0.00107892957767	0.00004450530385
S	-3.02260776471236	-0.13081136975987	2.90906976469021
C	-1.31148785382727	-0.04620775455165	5.72963565697447
C	1.30963148666107	0.04688052616693	5.73056475608732
S	3.02547809883419	0.12372595416044	2.91307547591761
C	2.75330348566140	0.08502843456632	7.98651688440651
N	3.99297988810930	0.11713537456961	9.81416813348330
C	-2.75722442446863	-0.08415204459255	7.98382707222982
N	-3.99814112616145	-0.11590293865562	9.81070822267826
S	3.02345144152084	-0.14460210376768	-2.90859379466311
C	1.31373148667562	-0.04659872465476	-5.72932835447517
C	-1.30857832588414	0.04295766697717	-5.73123875545280
S	-3.02159138050829	0.15273598353479	-2.91069069561287
C	2.75471542088553	-0.07167286000019	-7.98750343057116
N	3.98984416907132	-0.09062642855789	-9.81835437051486
C	-2.75508201514422	0.06798039853295	-7.98493531854920
N	-3.99716653668596	0.08705965592062	-9.81116188282721

[Cu(sac)₂]

Cu	1.12185836121188	-0.00017459972927	0.00010704824927
O	-1.55883260118223	-0.37535779203089	2.50880300152707
C	-1.41532595910698	-0.23813287953167	4.95003712798506
C	-3.67081220219182	-0.59129335944968	6.40068327651835
C	-3.64670394377434	-0.47985809393836	9.00776287272601
C	-1.39057837477725	0.00156978592003	10.36365274525655
C	0.82128013931978	0.36143241988405	9.03267271826997
C	0.88559381418397	0.25499395853227	6.34627197089624
H	-5.40790991738927	-0.95794210619452	5.35421220513756
H	-5.41002810108017	-0.76464690060519	10.04348855851781
H	-1.40832022615060	0.08859161103773	12.42165145852428
H	2.58769037240192	0.74042859858644	10.03687741854423
C	3.23820049329879	0.65935838161555	5.11086317874004
N	3.62782088322065	0.61616170356240	2.66559365294909
H	4.85759345836337	1.04239895062749	6.36052505375320
H	5.46605118147618	0.96875135733740	2.18852437559961
O	-1.55968365830784	0.37136511535412	-2.50865076456535
C	-1.41542529665887	0.23775241696576	-4.95011188605730
C	-3.67077163917332	0.59235735421709	-6.40069381166086
C	-3.64635748000025	0.48165525238116	-9.00780869276808
C	-1.39046917926810	-0.00039030650924	-10.36390619188414
C	0.82121957909434	-0.36053656423578	-9.03275156597980
C	0.88551035954413	-0.25520856027810	-6.34627764447722
H	-5.4077778092343	0.95876239549664	-5.35405253374830
H	-5.40961785682183	0.76631889437486	-10.04370634966363
H	-1.40845803798689	-0.08574827656105	-12.42195334345748
H	2.58776838831841	-0.73883922576140	-10.03700699626520
C	3.23844380316260	-0.65836033026245	-5.11101168084055
N	3.62724740861294	-0.61613850924648	-2.66571560700850
H	4.85817092494125	-1.04024015191906	-6.36058877010733
H	5.46567794501785	-0.96740191594832	-2.18808168183130