Electronic Supplementary Information for Dalton Transactions
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Supporting Information

Probing the Mechanism of Hypoxia Selectivity of Copper *bis*(thiosemicarbazone) complexes: DFT Calculation of Redox Potentials and Absolute Acidities in Solution

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Table S1 Selected geometric parameters of the *in vacuo* optimised structures of Cu(II) *bis*(thiosemicarbazone) complexes **1 – 6**. The experimental values from X-ray crystal structures are given in parentheses. The numbering is given in Figure S1.

Parameter	**1**[a]	**2**[a]	**3**	**4**[a]	**5**	**6**[a]
Cu-N1 / Å	2.016 (1.9797(19))	2.007 (1.963(2))	1.998	2.014 (1.9767(19))	2.008	1.999 (1.9602(15))
Cu-N2 / Å	2.016 (1.9727(19))	2.012 (1.968(2))	2.008	2.012 (1.9701(17))	2.014	2.009 (1.9619(14))
Cu-S1 / Å	2.295 (2.2506(6))	2.292 (2.2340(8))	2.294	2.289 (2.2435(6))	2.288	2.291 (2.2464(5))
Cu-S2 / Å	2.295 (2.2710(6))	2.298 (2.2431(8))	2.287	2.289 (2.2812(6))	2.293	2.283 (2.2363(5))
C1-C2 / Å	1.454 (1.453(3))	1.463 (1.470(4))	1.481	1.453 (1.452(3))	1.462	1.480 (1.479(2))
C1-N1 / Å	1.301 (1.300(3))	1.306 (1.298(3))	1.304	1.302 (1.307(3))	1.306	1.305 (1.298(2))
C1-X1 / Å	1.088	1.499	1.500	1.088	1.499	1.500
C2-N2 / Å	1.301 (1.296(3))	1.299 (1.299(3))	1.305	1.301 (1.301(3))	1.299	1.305 (1.296(2))
C2-X2 / Å	1.088	1.089	1.501	1.088	1.089	1.501
N1-N3 / Å	1.341 (1.353(3))	1.348 (1.370(3))	1.350	1.340 (1.363(2))	1.349	1.350 (1.365(2))
N2-N4 / Å	1.341 (1.370(3))	1.342 (1.365(3))	1.351	1.343 (1.364(3))	1.343	1.352 (1.369(2))
C3-N3 / Å	1.333 (1.335(3))	1.330 (1.336(3))	1.331	1.335 (1.337(3))	1.332	1.332 (1.325(2))
C4-N4 / Å	1.333 (1.326(3))	1.333 (1.329(3))	1.328	1.334 (1.349(3))	1.335	1.330 (1.324(2))
C3-S1 / Å	1.761 (1.751(2))	1.763 (1.753(3))	1.760	1.770 (1.756(2))	1.769	1.767 (1.7614(19))
C4-S2 / Å	1.761 (1.759(2))	1.760 (1.756(3))	1.762	1.769 (1.755(2))	1.768	1.769 (1.7578(19))
N1-Cu-N2 / °	80.54 (80.75(8))	80.32 (81.20(9))	80.05	80.73 (81.02(7))	80.31	80.04 (80.63(6))
N1-Cu-S1 / °	83.89 (84.30(6))	84.27 (84.88(7))	84.52	83.86 (84.58(5))	84.28	84.51 (85.18(4))
N2-Cu-S2 / °	83.89 (83.93(6))	83.90 (84.89(7))	84.80	83.99 (83.93(6))	83.92	84.80 (85.12(5))
S1-Cu-S2 / °	111.69 (110.10(2))	111.51 (109.53(3))	110.64	111.55 (110.24(2))	111.49	110.65 (109.241(18))
N1-C1-C2-N2 / °	-0.04	0.016	0.026	-0.024	-0.053	0.01
C3-N3-N1-C1 / °	-179.96	-179.93	-179.97	179.73	-179.99	-179.99

[a] Reference 3

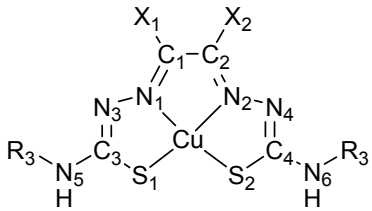

Fig. S1. Numbering scheme for the geometric parameters of Cu(II) *bis*(thiosemicarbazone) complexes

Hammett Analysis

Figure S3 shows a plot of the calculated one-electron reduction potentials for complexes **1 – 15** using the water solvation model verses the DMSO model. For simplicity, only complexes with a single substituents in the R_1 position have been included in the Hammett analysis. The data in Table S2 is plotted in Figures S5 and S6.

Table S2 Calculated one-electron reduction potentials in water and DMSO for copper bis(thiosemicarbazone) complexes with only one substituents at the R_1 position and the corresponding values of the Hammett $\sigma_{m/p}$ substituents constants.

	Complex	E_{calc}(SCE) / V in H_2O	E_{calc}(SCE) / V in DMSO	σ_m [a]	σ_p [a]
1	GTS	-0.218	-0.355	0.00	0.00
2	PTS	-0.330	-0.486	-0.07	-0.17
4	GTSM	-0.288	-0.456	0.00	0.00
5	PTSM	-0.391	-0.562	-0.07	-0.17
7	Amine	-0.355	-0.519	-0.16	-0.66
8	Chloro	-0.038	-0.168	0.37	0.23
9	Fluoro	-0.061	-0.178	0.34	0.06
10	Nitrile	0.037	-0.052	0.56	0.66
11	Hydroxo	-0.212	-0.331	0.12	-0.37
12	Thiol	-0.202	-0.340	0.25	0.15
13	Trifluoromethyl	-0.064	-0.166	0.43	0.54

[a] Reference 82

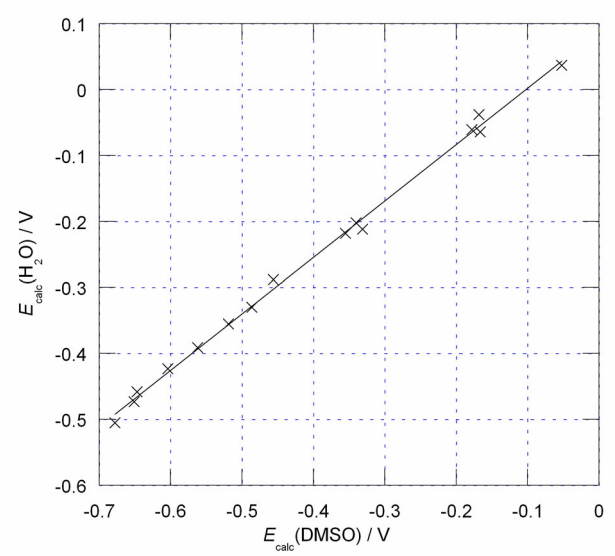

Fig. S2 Correlation between the calculated one-electron reduction potentials in water and DMSO.

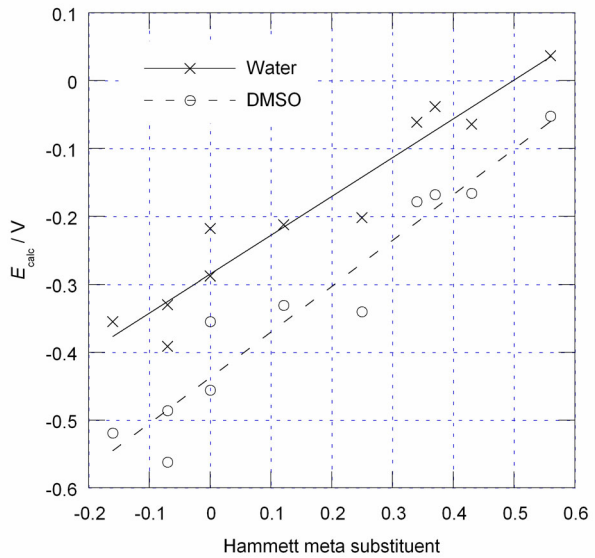

Fig. S3 Hammett plot of E_{calc} (Water/DMSO) / V *verses* the σ_m substituents constant.

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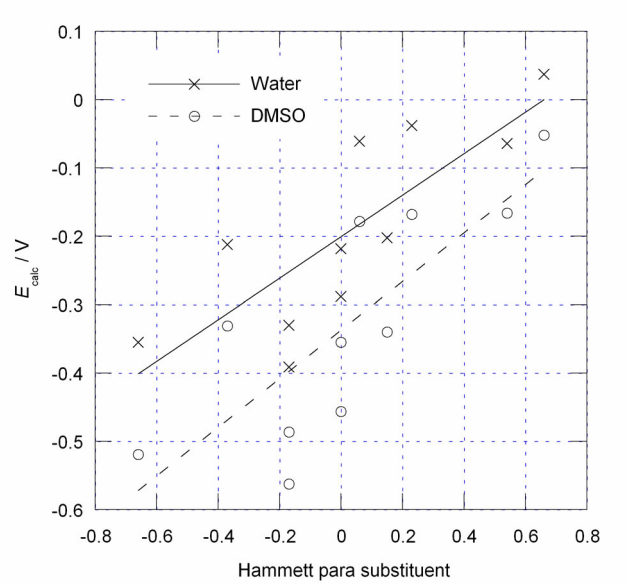

Fig. S4 Hammett plot of E_{calc} (Water/DMSO) / V verses the σ_p substituents constant.

Cartesian Coordinates

Geometry optimised Cartesian coordinates using Gaussian 03 Revision C.02 and the uB3LYP/6-31++G(d,p) model chemistry in the format: Atomic Number, X, Y, Z.

Optimised Cartesian coordinates for the Cu(II)A complexes (**1 – 15**) *in vacuo*.

Cu(II)GTS *in vacuo* (**1**)

29	-0.000002000	-0.281885000	0.000135000
16	-1.899139000	-1.570380000	-0.000562000
6	-2.984196000	-0.183264000	0.000249000
7	-2.635735000	1.103579000	0.000654000
7	-1.302999000	1.256156000	0.000623000
6	-0.726785000	2.422587000	0.000124000
6	0.726785000	2.422583000	-0.000078000
7	1.302995000	1.256151000	-0.000612000
7	2.635737000	1.103577000	-0.000332000
6	2.984199000	-0.183260000	-0.000247000
16	1.899140000	-1.570379000	0.000684000
7	4.312029000	-0.434433000	-0.002160000
1	4.961498000	0.338537000	0.004371000
1	4.653721000	-1.381365000	0.006210000
1	1.306758000	3.343212000	0.000243000
1	-1.306755000	3.343218000	-0.000233000
7	-4.312019000	-0.434431000	-0.001058000
1	-4.961511000	0.338537000	0.001723000
1	-4.653734000	-1.381383000	0.001727000

Cu(II)PTS *in vacuo* (**2**)

29	0.148859000	-0.486493000	0.001438000
16	2.188934000	-1.545320000	0.001292000
6	3.100790000	-0.039610000	-0.000562000
7	2.602439000	1.197186000	-0.001074000
7	1.260492000	1.190836000	-0.000178000
6	0.552614000	2.279928000	-0.000491000
6	-0.902362000	2.126883000	0.000023000
7	-1.313978000	0.887825000	0.000409000
7	-2.625714000	0.575255000	0.000713000
6	-2.820767000	-0.740495000	-0.000342000
16	-1.579602000	-1.992068000	-0.002117000
7	-4.110198000	-1.151237000	-0.000193000
1	-4.848666000	-0.463184000	0.000365000
1	-4.334401000	-2.132508000	-0.000592000
6	-1.830846000	3.303195000	-0.000138000
1	-1.275095000	4.243718000	-0.003216000
1	-2.486721000	3.271538000	-0.876957000
1	-2.482579000	3.275097000	0.879937000
1	1.024645000	3.260826000	-0.001491000
7	4.449381000	-0.130317000	-0.002362000
1	5.001928000	0.714628000	-0.000304000
1	4.901134000	-1.029877000	0.001597000

Cu(II)ATS *in vacuo* (**3**)

29	-0.007921000	-0.688022000	-0.000172000
16	-1.892242000	-1.983834000	0.000189000
6	-2.975839000	-0.594501000	0.000244000
7	-2.631502000	0.688231000	-0.000528000
7	-1.291112000	0.856606000	-0.000089000
6	-0.733795000	2.036574000	-0.000057000
6	0.746666000	2.023174000	-0.000373000
7	1.285261000	0.835224000	-0.000095000
7	2.624499000	0.668994000	0.000509000
6	2.965695000	-0.617185000	0.000154000
16	1.874801000	-1.998826000	-0.000395000
7	4.293858000	-0.878283000	0.000130000
1	4.948980000	-0.110515000	0.001655000
1	4.627756000	-1.827821000	0.001407000
6	1.581820000	3.269488000	-0.000333000
1	0.971564000	4.172662000	-0.016717000
1	2.226458000	3.290275000	0.885463000
1	2.250417000	3.273218000	-0.868116000
6	-1.517638000	3.316474000	0.000270000
1	-1.287027000	3.917957000	-0.886927000
1	-2.583992000	3.093633000	0.007524000
1	-1.275673000	3.924546000	0.879801000
7	-4.305435000	-0.853096000	0.003742000
1	-4.959494000	-0.084684000	-0.009352000
1	-4.640658000	-1.801976000	-0.011563000

Cu(II)GTSM *in vacuo* (**4**)

29	-0.000171000	-0.359319000	0.001672000
16	-1.895883000	-1.644408000	-0.048413000
6	-2.988605000	-0.252236000	-0.006361000
7	-2.635506000	1.034873000	0.004530000
7	-1.301228000	1.181259000	0.003116000
6	-0.727643000	2.349405000	-0.000177000
6	0.725606000	2.349568000	0.001110000
7	1.299628000	1.181642000	-0.000667000
7	2.634626000	1.037039000	-0.002956000
6	2.988740000	-0.249093000	0.001677000
16	1.897006000	-1.641862000	0.053671000
7	4.311667000	-0.518538000	-0.042655000
6	5.355862000	0.496022000	-0.014366000
1	5.148638000	1.255843000	-0.770029000
1	5.415014000	0.987909000	0.962883000
1	6.305474000	0.008346000	-0.236004000
1	4.571914000	-1.489934000	0.041445000
1	1.307201000	3.269197000	-0.001917000
1	-1.309296000	3.269010000	-0.002895000
7	-4.311250000	-0.520301000	0.014591000
6	-5.352390000	0.498627000	0.018989000
1	-5.339829000	1.083016000	-0.907182000
1	-6.317672000	-0.001311000	0.116610000
1	-5.214919000	1.185897000	0.858313000
1	-4.574515000	-1.493001000	-0.030801000

Cu(II)PTSM *in vacuo* (**5**)

29	0.110383000	-0.543825000	-0.001205000
16	2.072685000	-1.730640000	-0.000674000
6	3.089788000	-0.284989000	-0.000090000
7	2.669602000	0.982015000	0.000046000
7	1.328954000	1.059129000	-0.000787000
6	0.692213000	2.191681000	-0.000013000
6	-0.768990000	2.133164000	-0.000059000
7	-1.260922000	0.923355000	0.000207000
7	-2.591225000	0.700487000	0.000080000
6	-2.874698000	-0.600718000	0.000563000
16	-1.708783000	-1.931784000	0.000998000
7	-4.182357000	-0.941747000	0.000807000
6	-5.275359000	0.019597000	0.000449000
1	-5.234178000	0.659473000	-0.886820000
1	-6.216793000	-0.532883000	0.001926000
1	-5.232655000	0.661567000	0.886110000
1	-4.391565000	-1.928217000	0.000438000
6	-1.620640000	3.366234000	-0.000221000
1	-1.006745000	4.269942000	0.000213000
1	-2.275033000	3.377658000	-0.878838000
1	-2.275901000	3.377320000	0.877743000
1	1.226824000	3.140077000	0.001014000
7	4.425250000	-0.481380000	0.000155000
6	5.410069000	0.591899000	0.002008000
1	5.298754000	1.223556000	0.888738000
1	6.404601000	0.142081000	0.002735000
1	5.300691000	1.224743000	-0.884100000
1	4.739042000	-1.439833000	0.001215000

Cu(II)ATSM *in vacuo* (**6**)

29	-0.006583000	-0.713445000	0.000154000
16	-1.886216000	-2.009710000	-0.000641000
6	-2.979943000	-0.619692000	-0.000129000
7	-2.633926000	0.664101000	0.000124000
7	-1.292470000	0.830349000	0.000035000
6	-0.735813000	2.010919000	-0.000076000
6	0.743851000	1.999251000	-0.000160000
7	1.284668000	0.812008000	0.000069000
7	2.625232000	0.652322000	0.000158000
6	2.972374000	-0.633738000	0.000110000
16	1.875508000	-2.019431000	-0.000041000
7	4.295934000	-0.908110000	0.000171000

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6	5.339520000	0.106308000	0.000269000
1	5.266004000	0.744586000	0.886659000
1	6.307333000	-0.398679000	0.000553000
1	5.266416000	0.744375000	-0.886315000
1	4.554022000	-1.882910000	0.000144000
6	1.578584000	3.245745000	-0.000450000
1	0.968716000	4.149420000	-0.003172000
1	2.234044000	3.258854000	0.877607000
1	2.237689000	3.255785000	-0.875765000
6	-1.521236000	3.290088000	-0.000147000
1	-1.287297000	3.894725000	-0.884353000
1	-2.587130000	3.064917000	0.001322000
1	-1.285033000	3.896247000	0.882388000
7	-4.304084000	-0.895863000	-0.000155000
6	-5.348844000	0.116968000	0.000788000
1	-5.276680000	0.756196000	-0.885103000
1	-6.316072000	-0.389210000	-0.000251000
1	-5.277433000	0.754051000	0.888317000
1	-4.560776000	-1.870919000	0.000351000

Cu(II)AGTS *in vacuo* (**7**)

6	0.853487000	2.130105000	-0.005335000
6	-0.606839000	2.292981000	-0.006487000
7	-1.289380000	1.191369000	0.006956000
7	-2.626241000	1.165967000	0.002575000
6	-3.095679000	-0.087928000	0.004842000
7	-4.441335000	-0.200136000	0.005843000
7	1.279936000	0.895997000	-0.012099000
7	2.622064000	0.631875000	0.006930000
6	2.858532000	-0.663347000	0.000879000
7	4.163444000	-1.063265000	-0.028902000
16	1.636946000	-1.946385000	-0.010642000
29	-0.129102000	-0.487177000	-0.003230000
16	-2.157751000	-1.571554000	0.007343000
1	-5.007275000	0.635909000	-0.008692000
1	-4.878046000	-1.107152000	-0.008951000
1	-1.084549000	3.271215000	-0.025597000
1	4.872593000	-0.366163000	0.148346000
1	4.378201000	-2.022577000	0.192307000
7	1.682185000	3.212296000	-0.045008000
1	2.665856000	3.018628000	0.090775000
1	1.338326000	4.115720000	0.240790000

Cu(II)CGTS *in vacuo* (**8**)

6	1.070574000	1.767651000	-0.000379000
6	-0.333617000	2.167768000	-0.000417000
7	-1.194784000	1.196447000	0.000264000
7	-2.518842000	1.405615000	-0.000015000
6	-3.198990000	0.257084000	0.000170000
7	-4.544013000	0.372392000	-0.000045000
7	1.335447000	0.500785000	-0.000818000
7	2.569720000	-0.022163000	-0.000217000
6	2.541126000	-1.354825000	-0.000198000
7	3.745142000	-1.966840000	-0.000267000
16	1.112053000	-2.384677000	-0.000071000
29	-0.352115000	-0.630179000	-0.000098000
16	-2.523369000	-1.368001000	0.000285000
1	-4.960959000	1.292076000	0.000108000
1	-5.129384000	-0.446832000	0.000151000
1	-0.629201000	3.213262000	-0.001059000
1	4.584248000	-1.405103000	0.002204000
1	3.809731000	-2.971459000	0.003206000
17	2.287924000	3.012139000	0.000439000

Cu(II)FGTS *in vacuo* (**9**)

6	0.826373000	2.126344000	-0.000052000
6	-0.619633000	2.289013000	0.000233000
7	-1.292543000	1.177846000	0.000106000
7	-2.628420000	1.138400000	0.000530000
6	-3.084096000	-0.119453000	-0.000060000
7	-4.426633000	-0.251156000	-0.000827000
7	1.327757000	0.940979000	-0.000358000
7	2.648984000	0.667263000	-0.000083000
6	2.868040000	-0.643145000	-0.000230000
7	4.163832000	-1.029248000	-0.004374000
16	1.649359000	-1.922176000	0.001040000
29	-0.117862000	-0.474044000	0.000026000
16	-2.122526000	-1.590644000	-0.000824000
1	-5.004774000	0.576863000	0.003688000
1	-4.852115000	-1.163760000	0.003929000
1	-1.085244000	3.270903000	0.000538000
1	4.887519000	-0.325381000	0.008737000
1	4.409129000	-2.005204000	0.013570000
9	1.571023000	3.241535000	0.000114000

Cu(II)NGTS *in vacuo* (**10**)

6	1.079828000	1.871615000	-0.000144000
6	-0.339047000	2.225165000	0.000053000
7	-1.176373000	1.233955000	0.000177000
7	-2.507545000	1.414743000	0.000372000
6	-3.163223000	0.255762000	-0.000046000
7	-4.510712000	0.337078000	-0.000717000
7	1.353051000	0.583884000	-0.000409000
7	2.586280000	0.105122000	-0.000326000
6	2.601004000	-1.242493000	-0.000045000
7	3.828897000	-1.791812000	-0.001314000
16	1.212330000	-2.305755000	0.000863000
29	-0.306416000	-0.575553000	0.000005000
16	-2.451180000	-1.358269000	-0.000589000
1	-4.951032000	1.245819000	0.002842000
1	-5.075822000	-0.496251000	0.003186000
1	-0.668518000	3.261318000	0.000066000
1	4.639059000	-1.187488000	0.001135000
1	3.944980000	-2.792582000	0.002598000
6	2.090196000	2.883517000	0.000057000
7	2.884467000	3.734631000	0.000273000

Cu(II)HYGTS *in vacuo* (**11**)

6	0.832243000	2.121223000	-0.000701000
6	-0.618437000	2.304215000	-0.001043000
7	-1.298253000	1.198076000	0.000704000
7	-2.633326000	1.164491000	-0.000555000
6	-3.096665000	-0.091584000	0.000739000
7	-4.440487000	-0.211654000	0.001435000
7	1.272122000	0.900314000	-0.002872000
7	2.616443000	0.663444000	0.003767000
6	2.871343000	-0.633367000	-0.001399000
7	4.176360000	-1.011208000	-0.030953000
16	1.663137000	-1.925422000	-0.002648000
29	-0.134219000	-0.486373000	-0.000354000
16	-2.151127000	-1.573123000	0.002629000
1	-5.011065000	0.621533000	-0.005461000
1	-4.873255000	-1.120784000	-0.005057000
1	-1.077112000	3.289346000	-0.002943000
1	4.888707000	-0.307297000	0.096824000
1	4.415333000	-1.977423000	0.122373000
8	1.628713000	3.198275000	0.002304000
1	2.546967000	2.862779000	0.000162000

Cu(II)THGTS *in vacuo* (**12**)

6	1.070881000	1.775067000	-0.000200000
6	-0.337521000	2.177143000	-0.000102000
7	-1.201996000	1.209685000	0.000207000
7	-2.525111000	1.422713000	0.000278000
6	-3.209068000	0.275865000	-0.000074000
7	-4.553853000	0.397300000	-0.000245000
7	1.296492000	0.491847000	-0.000468000
7	2.546008000	-0.024961000	0.000441000
6	2.533394000	-1.352670000	0.000105000
7	3.738914000	-1.969330000	-0.004589000
16	1.104671000	-2.385818000	0.000248000
29	-0.365141000	-0.628672000	-0.000062000
16	-2.542000000	-1.352066000	-0.000363000
1	-4.966684000	1.318777000	0.002741000
1	-5.142209000	-0.419729000	0.003076000
1	-0.640315000	3.221933000	-0.000348000
1	4.582566000	-1.416071000	0.012994000
1	3.796828000	-2.973945000	0.016149000
16	2.324212000	3.016433000	0.000142000
1	3.319492000	2.100534000	-0.001004000

Cu(II)TFGTS *in vacuo* (**13**)

6	1.258701000	-1.120293000	-0.000389000
6	0.054345000	-1.941166000	-0.000312000
7	-1.076374000	-1.299735000	-0.000619000
7	-2.259709000	-1.933809000	0.000678000
6	-3.279774000	-1.076774000	0.001086000
7	-4.513500000	-1.625748000	0.002123000
7	1.073930000	0.175096000	-0.000263000
7	2.062656000	1.063271000	0.000186000
6	1.603658000	2.325815000	0.000574000
7	2.557604000	3.275965000	0.000197000
16	-0.071623000	2.839148000	0.001143000
29	-0.888825000	0.694836000	-0.001695000
16	-3.176923000	0.682862000	-0.000301000
1	-4.607114000	-2.631168000	0.000427000
1	-5.334642000	-1.043107000	-0.000222000
1	0.094177000	-3.026123000	0.000441000
1	3.529199000	2.998411000	0.001439000
1	2.310583000	4.252515000	0.002608000
6	2.635321000	-1.750336000	0.000088000
9	2.535836000	-3.105694000	0.000698000
9	3.355394000	-1.406693000	-1.089835000
9	3.354849000	-1.405579000	1.090092000

Cu(II)DAGTS *in vacuo* (**14**)

6	0.741044000	2.020517000	0.012900000
7	1.286379000	0.843406000	-0.075022000
29	-0.000827000	-0.686495000	-0.001305000
16	1.909808000	-1.960440000	-0.020491000
6	2.996541000	-0.568513000	-0.019423000
7	4.331867000	-0.833258000	-0.028793000
6	-0.740033000	2.020519000	-0.013788000
7	-1.439397000	3.203130000	-0.055563000
7	-1.285263000	0.843143000	0.070309000
7	-2.640640000	0.706010000	0.023442000
6	-2.996370000	-0.567945000	0.019730000
16	-1.909890000	-1.960455000	0.022775000
7	2.641467000	0.705752000	-0.025495000
7	-4.331737000	-0.832265000	0.030875000
1	4.973649000	-0.065999000	0.109136000
1	4.647683000	-1.769510000	0.166705000
1	-4.973174000	-0.065412000	-0.110834000
1	-4.647614000	-1.768929000	-0.162528000

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1	-2.438698000	3.067654000	-0.166977000
1	-1.047993000	3.939338000	-0.629527000
7	1.439844000	3.203055000	0.059270000
1	2.439179000	3.067870000	0.170501000
1	1.047530000	3.937401000	0.635148000

Cu(II)MAGTS *in vacuo* (**15**)

29	-0.017801000	-0.690053000	-0.004670000
16	-1.942160000	-1.940763000	-0.000524000
6	-3.004666000	-0.525853000	0.006508000
7	-2.619361000	0.733892000	-0.003902000
7	-1.255278000	0.841189000	-0.006325000
6	-0.693394000	2.018686000	-0.001983000
6	0.789453000	2.033266000	-0.001571000
7	1.319542000	0.844799000	0.007037000
7	2.650775000	0.647170000	0.010603000
6	2.963137000	-0.649170000	0.005269000
16	1.852987000	-2.011888000	-0.004866000
7	4.286347000	-0.931389000	0.008773000
1	4.954417000	-0.174843000	0.011332000
1	4.604232000	-1.886496000	0.001973000
6	1.569465000	3.313583000	-0.009769000
1	1.250359000	3.963011000	-0.833241000
1	1.433153000	3.867129000	0.928859000
1	2.630939000	3.093223000	-0.122278000
7	-4.347629000	-0.768570000	0.059821000
1	-4.970105000	0.005689000	-0.123550000
1	-4.674823000	-1.696688000	-0.157334000
7	-1.410689000	3.179147000	-0.049966000
1	-2.407725000	3.074165000	0.090366000
1	-0.987356000	4.042012000	0.252532000

Optimised Cartesian coordinates for the reduced Cu(I)A$^-$ complexes (**1 – 15**) *in vacuo*.

Cu(I)GTS$^-$ *in vacuo* (**1**)

29	-0.001750000	-0.443052000	-0.004846000
16	2.045449000	-1.473477000	0.473282000
6	3.037241000	-0.124914000	-0.038259000
7	2.631669000	1.104638000	-0.283106000
7	1.276445000	1.211721000	-0.337255000
6	0.721892000	2.366845000	-0.061918000
6	-0.712571000	2.369158000	0.058307000
7	-1.270184000	1.214832000	0.330271000
7	-2.626522000	1.112872000	0.294359000
6	-3.039888000	-0.108564000	0.030247000
16	-2.053288000	-1.461639000	-0.484505000
7	-4.418551000	-0.312455000	0.101762000
1	-4.892207000	0.317033000	0.739678000
1	-4.678272000	-1.284992000	0.194211000
1	-1.312809000	3.265911000	-0.105161000
1	1.324865000	3.261214000	0.105621000
7	4.401697000	-0.356146000	-0.205018000
1	4.954364000	0.492527000	-0.236043000
1	4.778297000	-1.084708000	0.384438000

Cu(I)PTS$^-$ *in vacuo* (**2**)

29	-0.156540000	-0.652429000	0.011018000
16	-2.298638000	-1.472695000	-0.451500000
6	-3.146145000	-0.021051000	0.036193000
7	-2.617621000	1.164876000	0.259585000
7	-1.257345000	1.135878000	0.311622000
6	-0.592447000	2.219084000	0.003305000
6	0.846278000	2.098422000	-0.102969000
7	1.270138000	0.877093000	-0.338641000
7	2.610038000	0.630559000	-0.316286000
6	2.896831000	-0.624991000	-0.042599000
16	1.785684000	-1.864624000	0.500221000
7	4.246224000	-0.972332000	-0.132684000
1	4.771078000	-0.401902000	-0.786085000
1	4.399750000	-1.967630000	-0.221586000
6	1.758594000	3.280274000	0.087693000
1	1.195271000	4.217687000	0.024959000
1	2.248781000	3.240785000	1.069266000
1	2.556369000	3.281452000	-0.662325000
1	-1.106633000	3.161927000	-0.196763000
7	-4.527072000	-0.109005000	0.206674000
1	-4.990667000	0.791888000	0.221176000
1	-4.976202000	-0.806588000	-0.369333000

Cu(I)ATS$^-$ *in vacuo* (**3**)

29	-0.002448000	-0.847891000	-0.003259000
16	2.044256000	-1.884891000	0.444886000
6	3.025848000	-0.532386000	-0.069412000
7	2.619820000	0.699715000	-0.297444000
7	1.260352000	0.819483000	-0.339643000
6	0.732632000	1.985917000	-0.043227000
6	-0.725874000	1.987039000	0.037358000
7	-1.254435000	0.822476000	0.339129000
7	-2.615390000	0.706994000	0.316777000
6	-3.029245000	-0.515186000	0.061806000
16	-2.051689000	-1.869182000	-0.462296000
7	-4.407889000	-0.721558000	0.158647000
1	-4.867363000	-0.090948000	0.806173000
1	-4.659991000	-1.694678000	0.267480000
6	-1.572002000	3.197625000	-0.264995000
1	-0.964966000	4.071526000	-0.513618000
1	-2.234376000	2.981005000	-1.111249000
1	-2.227178000	3.443603000	0.579878000
6	1.578004000	3.196819000	0.259226000
1	2.180137000	3.014367000	1.157951000
1	2.289616000	3.392183000	-0.551782000
1	0.970286000	4.089020000	0.428602000
7	4.388115000	-0.763739000	-0.262654000
1	4.941035000	0.084945000	-0.291286000
1	4.772550000	-1.499602000	0.312678000

Cu(I)GTSM$^-$ *in vacuo* (**4**)

29	-0.008383000	-0.515936000	-0.028237000
16	1.995792000	-1.556004000	0.577301000
6	3.032823000	-0.225320000	0.082102000
7	2.648454000	1.003542000	-0.200610000
7	1.296420000	1.117665000	-0.321784000
6	0.739581000	2.280087000	-0.079212000
6	-0.697747000	2.295733000	-0.027760000
7	-1.278103000	1.148219000	0.230195000
7	-2.632384000	1.059510000	0.124363000
6	-3.044472000	-0.160494000	-0.153888000
16	-2.035391000	-1.526826000	-0.607640000
7	-4.415141000	-0.375852000	-0.148350000
6	-5.307757000	0.499200000	0.592920000
1	-5.229119000	1.519268000	0.207910000
1	-6.335656000	0.147800000	0.455399000
1	-5.079914000	0.533128000	1.669900000
1	-4.651908000	-1.357605000	-0.173412000
1	-1.282493000	3.194578000	-0.231280000
1	1.342976000	3.168956000	0.114007000
7	4.390108000	-0.491108000	0.001164000
6	5.362481000	0.575056000	-0.155708000
1	5.347999000	1.294114000	0.678412000
1	6.359751000	0.129014000	-0.229875000
1	5.156265000	1.134957000	-1.071771000
1	4.673856000	-1.296203000	0.539426000

Cu(I)PTSM$^-$ *in vacuo* (**5**)

29	0.105381000	-0.707864000	-0.038963000
16	2.159440000	-1.662849000	0.537163000
6	3.128428000	-0.268635000	0.082325000
7	2.684540000	0.948040000	-0.162947000
7	1.327571000	1.001493000	-0.279776000
6	0.718740000	2.122931000	0.011752000
6	-0.726606000	2.093687000	0.050028000
7	-1.237961000	0.899826000	0.257410000
7	-2.588831000	0.742081000	0.162836000
6	-2.942192000	-0.490567000	-0.141665000
16	-1.875769000	-1.795208000	-0.640841000
7	-4.300608000	-0.774960000	-0.123544000
6	-5.228239000	0.038968000	0.643299000
1	-5.216745000	1.066348000	0.269695000
1	-6.236372000	-0.370003000	0.518977000
1	-4.984065000	0.074174000	1.716704000
1	-4.487516000	-1.766843000	-0.165585000
6	-1.552833000	3.331111000	-0.177161000
1	-0.934584000	4.230791000	-0.085283000
1	-1.999494000	3.324490000	-1.180300000
1	-2.382098000	3.382757000	0.536101000
1	1.283215000	3.027718000	0.248459000
7	4.497217000	-0.465025000	-0.007547000
6	5.416602000	0.651095000	-0.131269000
1	5.371889000	1.340731000	0.726464000
1	6.433813000	0.256198000	-0.223216000
1	5.179813000	1.230677000	-1.027464000
1	4.820483000	-1.271789000	0.505332000

Cu(I)ATSM$^-$ *in vacuo*

29	-0.006583000	-0.713445000	0.000154000
16	-1.886216000	-2.009710000	-0.000641000
6	-2.979943000	-0.619692000	-0.000129000
7	-2.633926000	0.664101000	0.000124000
7	-1.292470000	0.830349000	0.000035000
6	-0.735813000	2.010919000	-0.000076000
6	0.743851000	1.999251000	-0.000160000
7	1.284668000	0.812008000	0.000069000
7	2.625232000	0.652322000	0.000158000
6	2.972374000	-0.633738000	0.000110000
16	1.875508000	-2.019431000	-0.000041000
7	4.295934000	-0.908110000	0.000171000
6	5.339520000	0.106308000	0.000269000
1	5.266004000	0.744586000	0.886659000
1	6.307333000	-0.398679000	0.000553000
1	5.266416000	0.744375000	-0.886315000
1	4.554022000	-1.882910000	0.000144000
6	1.578584000	3.245745000	-0.000450000
1	0.968716000	4.149420000	-0.003172000
1	2.234044000	3.258854000	0.877607000
1	2.237689000	3.255785000	-0.875765000
6	-1.521236000	3.290088000	-0.000147000
1	-1.287297000	3.894725000	-0.884353000
1	-2.587130000	3.064917000	0.001322000
1	-1.285033000	3.896247000	0.882388000
7	-4.304084000	-0.895863000	-0.000155000
6	-5.348844000	0.116968000	0.000788000
1	-5.276680000	0.756196000	-0.885103000

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1	-6.316072000	-0.389210000	-0.000251000
1	-5.277433000	0.754051000	0.888317000
1	-4.560776000	-1.870919000	0.000351000

Cu(I)AGTS$^-$ *in vacuo* (**7**)

29	-0.013497000	-0.875722000	-0.029599000
16	1.990445000	-1.928790000	0.540554000
6	3.019153000	-0.589753000	0.057207000
7	2.635616000	0.645190000	-0.198286000
7	1.279473000	0.774555000	-0.307592000
6	0.748953000	1.946321000	-0.035158000
6	-0.710602000	1.962812000	-0.028238000
7	-1.266808000	0.803560000	0.246205000
7	-2.626227000	0.704111000	0.150677000
6	-3.039911000	-0.514850000	-0.127355000
16	-2.041114000	-1.880798000	-0.598272000
7	-4.411768000	-0.730798000	-0.101989000
6	-5.293600000	0.145314000	0.650328000
1	-5.229453000	1.162928000	0.255864000
1	-6.322126000	-0.212991000	0.536497000
1	-5.044511000	0.189884000	1.722326000
1	-4.646277000	-1.713435000	-0.115850000
6	-1.526118000	3.183071000	-0.373779000
1	-0.896400000	4.051646000	-0.581736000
1	-2.139483000	2.978414000	-1.259421000
1	-2.226769000	3.432078000	0.432710000
6	1.591459000	3.147871000	0.310186000
1	2.173296000	2.943886000	1.217446000
1	2.322203000	3.357623000	-0.480308000
1	0.983164000	4.039063000	0.483293000
7	4.375696000	-0.856215000	-0.048817000
6	5.349838000	0.210583000	-0.183708000
1	5.347591000	0.904085000	0.672421000
1	6.344910000	-0.236002000	-0.281640000
1	5.136707000	0.799125000	-1.080085000
1	4.662368000	-1.678008000	0.462055000

Cu(I)CGTS$^-$ *in vacuo* (**8**)

6	1.025459000	1.762996000	-0.147884000
6	-0.381746000	2.107250000	-0.059659000
7	-1.197809000	1.127414000	0.196473000
7	-2.530779000	1.373732000	0.195857000
6	-3.254557000	0.279227000	0.023624000
7	-4.626594000	0.461363000	0.121906000
7	1.360873000	0.541627000	-0.335576000
7	2.625977000	0.082052000	-0.301720000
6	2.685311000	-1.219691000	-0.058626000
7	3.940818000	-1.783507000	-0.221481000
16	1.389416000	-2.275526000	0.445981000
29	-0.417242000	-0.890818000	0.015319000
16	-2.683647000	-1.317688000	-0.392955000
1	-4.908314000	1.263925000	0.672143000
1	-5.154037000	-0.386643000	0.272009000
1	-0.724341000	3.128512000	-0.220896000
1	4.697338000	-1.111382000	-0.260248000
1	4.116990000	-2.614060000	0.324080000
17	2.195641000	3.108666000	0.105134000

Cu(I)FGTS$^-$ *in vacuo* (**9**)

6	0.817527000	2.099582000	-0.094784000
6	-0.619357000	2.244322000	0.006307000
7	-1.277975000	1.145258000	0.232892000
7	-2.628565000	1.167148000	0.228860000
6	-3.155727000	-0.033336000	0.029990000
7	-4.537689000	-0.089131000	0.133787000
7	1.336117000	0.950397000	-0.315245000
7	2.676448000	0.726504000	-0.282683000
6	2.959680000	-0.541539000	-0.043103000
7	4.298768000	-0.882416000	-0.192274000
16	1.860704000	-1.816448000	0.437866000
29	-0.145188000	-0.726197000	-0.003425000
16	-2.321136000	-1.495148000	-0.427081000
1	-4.949400000	0.638018000	0.706530000
1	-4.914144000	-1.018102000	0.256077000
1	-1.103014000	3.211226000	-0.133822000
1	4.924726000	-0.085905000	-0.205079000
1	4.603922000	-1.664036000	0.369196000
9	1.548090000	3.247283000	0.100670000

Cu(I)NGTS$^-$ *in vacuo* (**10**)

6	0.998882000	1.870261000	-0.140465000
6	-0.411227000	2.170993000	-0.035548000
7	-1.187625000	1.166506000	0.277411000
7	-2.538182000	1.343695000	0.233863000
6	-3.194588000	0.224751000	0.017825000
7	-4.582358000	0.310590000	0.079286000
7	1.296562000	0.590231000	-0.362911000
7	2.571507000	0.184364000	-0.292176000
6	2.691195000	-1.117490000	-0.060174000
7	3.950682000	-1.646534000	-0.280172000
16	1.429842000	-2.176450000	0.504930000
29	-0.312253000	-0.705619000	0.021167000
16	-2.506016000	-1.325676000	-0.429008000
1	-4.926003000	1.061236000	0.666548000
1	-5.045323000	-0.578756000	0.204422000
1	-0.807763000	3.165625000	-0.236650000
1	4.684198000	-0.956124000	-0.381352000
1	4.187283000	-2.461414000	0.265829000
6	1.979438000	2.894863000	0.036884000
7	2.746494000	3.766312000	0.164911000

Cu(I)HYGTS$^-$ *in vacuo* (**11**)

6	0.794873000	2.080510000	-0.094424000
6	-0.641964000	2.266425000	0.005298000
7	-1.308666000	1.179072000	0.257687000
7	-2.658453000	1.193536000	0.241040000
6	-3.173713000	-0.011968000	0.047117000
7	-4.557584000	-0.080265000	0.138204000
7	1.234623000	0.887092000	-0.361494000
7	2.603429000	0.729015000	-0.296311000
6	2.954959000	-0.512324000	-0.032498000
7	4.316607000	-0.790351000	-0.128602000
16	1.896613000	-1.835347000	0.405822000
29	-0.143686000	-0.725464000	-0.028856000
16	-2.326259000	-1.473800000	-0.393972000
1	-4.977281000	0.644607000	0.708418000
1	-4.922845000	-1.012622000	0.269830000
1	-1.111803000	3.235589000	-0.166807000
1	4.908244000	0.032054000	-0.109301000
1	4.627408000	-1.553144000	0.455966000
8	1.623111000	3.140111000	0.121260000
1	2.517994000	2.754880000	0.012437000

Cu(I)THGTS$^-$ *in vacuo* (**12**)

6	0.990191000	1.773798000	-0.144000000
6	-0.418012000	2.119247000	-0.060820000
7	-1.225999000	1.144866000	0.247706000
7	-2.564437000	1.369153000	0.222966000
6	-3.264438000	0.266791000	0.028407000
7	-4.645049000	0.413635000	0.115324000
7	1.269742000	0.520771000	-0.361245000
7	2.558804000	0.088731000	-0.322939000
6	2.662547000	-1.201208000	-0.057764000
7	3.932121000	-1.744410000	-0.219358000
16	1.387317000	-2.274267000	0.463415000
29	-0.399256000	-0.836138000	0.009454000
16	-2.650002000	-1.309874000	-0.411479000
1	-4.945747000	1.187018000	0.696998000
1	-5.144495000	-0.453751000	0.253038000
1	-0.777462000	3.125529000	-0.279177000
1	4.675666000	-1.057863000	-0.260519000
1	4.123176000	-2.552094000	0.355644000
16	2.219869000	3.053100000	0.118828000
1	3.234342000	2.194841000	-0.144518000

Cu(I)TFGTS$^-$ *in vacuo* (**13**)

6	-1.155109000	-1.177562000	-0.171860000
6	0.083928000	-1.904199000	-0.054998000
7	1.137255000	-1.193899000	0.266681000
7	2.359853000	-1.793542000	0.223076000
6	3.341659000	-0.944436000	0.012633000
7	4.629341000	-1.470838000	0.083929000
7	-1.038284000	0.124433000	-0.381282000
7	-2.118961000	0.923354000	-0.321569000
6	-1.817371000	2.189075000	-0.069040000
7	-2.842972000	3.097135000	-0.281793000
16	-0.289112000	2.791835000	0.511738000
29	0.907003000	0.858578000	0.016225000
16	3.187690000	0.743524000	-0.436986000
1	4.710145000	-2.285992000	0.680310000
1	5.350179000	-0.774240000	0.211675000
1	0.159787000	-2.970866000	-0.254762000
1	-3.757608000	2.674556000	-0.382284000
1	-2.809213000	3.931840000	0.284489000
6	-2.474698000	-1.870629000	0.016437000
9	-2.308826000	-3.226824000	0.118695000
9	-3.133437000	-1.489197000	1.146070000
9	-3.345257000	-1.683958000	-1.012354000

Cu(I)DAGTS$^-$ *in vacuo* (**14**)

6	0.753129000	1.972066000	-0.042067000
7	1.293692000	0.838829000	-0.370125000
29	-0.015957000	-0.936968000	-0.007771000
16	2.102815000	-1.859038000	0.372212000
6	3.079512000	-0.471321000	-0.053055000
7	4.464904000	-0.650797000	-0.066823000
6	-0.715898000	1.979375000	0.010064000
7	-1.415884000	3.129614000	-0.309606000
7	-1.263903000	0.838290000	0.308680000
7	-2.637478000	0.777761000	0.274718000
6	-3.083984000	-0.443355000	0.073464000
16	-2.149439000	-1.865418000	-0.338341000
7	2.664545000	0.751161000	-0.311246000
7	-4.463265000	-0.610852000	0.217291000
1	4.951870000	0.000591000	-0.672551000
1	4.741392000	-1.616886000	-0.178273000
1	-4.981642000	0.258257000	0.156758000
1	-4.843610000	-1.366057000	-0.335935000
1	-2.379992000	3.141776000	-0.005128000
1	-0.907802000	4.000021000	-0.326014000
7	1.467236000	3.153058000	0.227282000
1	2.462868000	2.940221000	0.220438000
1	1.200171000	3.595428000	1.102504000

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Cu(I)MAGTS$^-$ *in vacuo* (**15**)

29	-0.025407000	-0.920257000	0.015645000
16	-2.144067000	-1.866382000	-0.394003000
6	-3.069054000	-0.446930000	0.050057000
7	-2.612602000	0.766728000	0.267389000
7	-1.238060000	0.823602000	0.287099000
6	-0.688701000	1.974925000	0.021544000
6	0.780847000	2.003716000	-0.043829000
7	1.317759000	0.844500000	-0.299891000
7	2.669229000	0.703073000	-0.294788000
6	3.051934000	-0.539036000	-0.058144000
16	2.056648000	-1.887054000	0.434516000
7	4.424183000	-0.763597000	-0.154642000
1	4.903334000	-0.119487000	-0.773884000
1	4.669482000	-1.736923000	-0.272887000
6	1.546946000	3.278641000	0.200090000
1	1.344131000	4.022270000	-0.584225000
1	1.281212000	3.733715000	1.164410000
1	2.616150000	3.060930000	0.196921000
7	-4.447790000	-0.610584000	0.206350000
1	-4.963148000	0.261453000	0.165253000
1	-4.837123000	-1.354368000	-0.356047000
7	-1.430568000	3.124017000	-0.255145000
1	-2.392536000	3.031671000	0.055656000
1	-0.992894000	4.001082000	-0.010017000

Optimised Cartesian coordinates for the Cu(II)A complexes (**1 – 15**) in solution phase using the water solvation model.

Cu(II)GTS in water

29	-0.000004954	-0.274685363	0.000169168
16	-1.890289826	-1.567391388	-0.051113300
6	-3.000295177	-0.185126144	0.003208665
7	-2.639047126	1.101480809	0.025416844
7	-1.303028092	1.255633512	0.009050618
6	-0.727122931	2.422622950	0.007917489
6	0.727085079	2.422630539	-0.007649279
7	1.303010471	1.255657897	-0.009139640
7	2.639056572	1.101515089	-0.024812737
6	3.000272476	-0.185079858	-0.003340299
16	1.890341844	-1.567313615	0.051399362
7	4.316110176	-0.447443675	-0.024668318
1	4.987253854	0.321087816	-0.039180124
1	4.664070306	-1.402867768	0.006445591
1	1.301258143	3.349043987	-0.018253698
1	-1.301311844	3.349022614	0.018736502
7	-4.316183409	-0.447291076	0.018550537
1	-4.987046449	0.320959390	0.050576844
1	-4.663979515	-1.403243304	0.010591430

Cu(II)PTS in water

29	-0.146225000	-0.479613000	0.001062000
16	-2.178971000	-1.547222000	0.011018000
6	-3.117464000	-0.042276000	-0.002469000
7	-2.607112000	1.192292000	-0.005974000
7	-1.260472000	1.186798000	-0.002303000
6	-0.554839000	2.276992000	0.000034000
6	0.902062000	2.128094000	0.002554000
7	1.315998000	0.889226000	0.003066000
7	2.630814000	0.575056000	0.002764000
6	2.838832000	-0.741001000	-0.001742000
16	1.574570000	-1.988572000	-0.004427000
7	4.115774000	-1.160587000	-0.006103000
1	4.874382000	-0.478829000	0.000457000
1	4.345787000	-2.151011000	-0.003762000
6	1.815212000	3.314789000	0.002855000
1	1.243714000	4.246114000	0.008051000
1	2.470963000	3.293482000	0.881396000
1	2.463603000	3.299323000	-0.881378000
1	-1.022612000	3.262008000	-0.000591000
7	-4.455407000	-0.146941000	-0.009650000
1	-5.031633000	0.695034000	-0.016490000
1	-4.913268000	-1.055138000	-0.003913000

Cu(II)ATS in water

29	-0.008126000	-0.679186000	-0.000200000
16	-1.884278000	-1.982863000	0.000206000
6	-2.992659000	-0.595073000	-0.000087000
7	-2.636190000	0.685654000	-0.000686000
7	-1.291122000	0.855967000	-0.000355000
6	-0.734629000	2.036279000	0.000014000
6	0.748900000	2.023273000	-0.000565000
7	1.286585000	0.834711000	0.000175000
7	2.629665000	0.664459000	0.000886000
6	2.981335000	-0.620419000	0.000423000
16	1.864024000	-1.999339000	-0.000597000
7	4.297399000	-0.895448000	0.000722000
1	4.975861000	-0.134166000	0.002103000
1	4.635673000	-1.854055000	0.000538000
6	1.574472000	3.274195000	-0.001337000
1	0.958422000	4.173074000	-0.019266000
1	2.215456000	3.302908000	0.888089000
1	2.241146000	3.284096000	-0.871736000
6	-1.505125000	3.321873000	0.001204000
1	-1.262150000	3.920157000	-0.885740000
1	-2.575877000	3.120734000	0.008285000
1	-1.250871000	3.925226000	0.881417000
7	-4.311008000	-0.865623000	0.002398000
1	-4.986747000	-0.102243000	-0.005827000
1	-4.652265000	-1.822918000	-0.005671000

Cu(II)GTSM in water

29	-0.000015000	-0.347108000	0.000240000
16	1.889166000	-1.639394000	0.001014000
6	3.007635000	-0.252465000	0.000044000
7	2.641830000	1.033604000	0.000030000
7	1.303746000	1.181671000	0.000471000
6	0.726678000	2.348335000	0.000247000
6	-0.726815000	2.348333000	0.000178000
7	-1.303875000	1.181649000	-0.000157000
7	-2.641935000	1.033558000	-0.000043000
6	-3.007612000	-0.252564000	-0.000451000
16	-1.889121000	-1.639467000	-0.000581000
7	-4.319475000	-0.528543000	-0.000927000
6	-5.370920000	0.484866000	0.000405000
1	-5.302094000	1.119678000	0.890923000
1	-5.301458000	1.122560000	-0.887977000
1	-6.332963000	-0.031826000	-0.000788000
1	-4.603239000	-1.512872000	-0.000602000
1	-1.300104000	3.275423000	0.000301000
1	1.299955000	3.275437000	-0.000012000
7	4.319512000	-0.528455000	-0.000556000
6	5.371127000	0.484807000	-0.001027000
1	5.303042000	1.120569000	0.888870000
1	6.333070000	-0.032061000	-0.002323000
1	5.301157000	1.121560000	-0.890052000
1	4.603189000	-1.512809000	-0.000316000

Cu(II)PTSM in water

29	-0.108250000	-0.534679000	0.000912000
16	-2.064123000	-1.728972000	-0.000149000
6	-3.106714000	-0.284630000	-0.001181000
7	-2.673242000	0.979877000	-0.001386000
7	-1.327714000	1.056655000	-0.000320000
6	-0.692289000	2.189937000	-0.000618000
6	0.770280000	2.134728000	0.000179000
7	1.264009000	0.924620000	0.000278000
7	2.597129000	0.700480000	0.000733000
6	2.892751000	-0.599466000	0.000371000
16	1.702294000	-1.928355000	0.000324000
7	4.189735000	-0.948702000	-0.000306000
6	5.291656000	0.008245000	-0.000427000
1	5.256297000	0.647239000	0.889198000
1	6.226228000	-0.556802000	-0.002504000
1	5.253759000	0.649629000	-0.888183000
1	4.419131000	-1.946118000	0.000244000
6	1.607536000	3.375983000	0.000762000
1	0.979849000	4.270439000	-0.000048000
1	2.259761000	3.396934000	0.882036000
1	2.261581000	3.396558000	-0.879152000
1	-1.222504000	3.142868000	-0.001718000
7	-4.431934000	-0.491035000	-0.000700000
6	-5.428941000	0.575681000	-0.001173000
1	-5.327384000	1.206996000	-0.891083000
1	-6.416644000	0.109850000	-0.000548000
1	-5.326869000	1.208201000	0.887813000
1	-4.766241000	-1.458987000	-0.000882000

Cu(II)ATSM in water

29	0.006372000	-0.704495000	-0.000414000
16	1.879688000	-2.008813000	0.000499000
6	2.997335000	-0.618884000	0.000684000
7	2.638279000	0.661915000	0.000573000
7	1.292558000	0.828793000	0.000302000
6	0.736877000	2.010397000	0.000266000
6	-0.744971000	1.999980000	-0.000072000
7	-1.285777000	0.811951000	-0.000479000
7	-2.629833000	0.650523000	-0.000446000
6	-2.989160000	-0.632814000	-0.000095000
16	-1.867691000	-2.018326000	-0.001227000
7	-4.302620000	-0.916112000	-0.000358000
6	-5.355336000	0.094409000	0.001178000
1	-5.287880000	0.733004000	-0.886900000
1	-6.317000000	-0.423274000	0.001412000
1	-5.286551000	0.731564000	0.890190000
1	-4.581767000	-1.900721000	-0.000676000
6	-1.570606000	3.250747000	0.000107000
1	-0.954961000	4.150191000	0.003248000
1	-2.223699000	3.269944000	-0.880632000
1	-2.228053000	3.266538000	0.877608000
6	1.512386000	3.293285000	0.000554000
1	1.267399000	3.895113000	0.884523000
1	2.581564000	3.084136000	0.000016000
1	1.266624000	3.896007000	-0.882583000
7	4.311910000	-0.902845000	0.000761000
6	5.364385000	0.107599000	-0.000048000
1	5.296748000	0.746377000	0.887965000
1	6.326227000	-0.409827000	0.000465000
1	5.296871000	0.744925000	-0.889132000
1	4.590649000	-1.887274000	0.000208000

Cu(II)AGTS in water

6	0.851715000	2.139374000	-0.001152000

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6	-0.615601000	2.289191000	-0.001864000
7	-1.289543000	1.184392000	-0.000155000
7	-2.632457000	1.153311000	-0.000875000
6	-3.109918000	-0.098452000	0.000414000
7	-4.444133000	-0.230458000	0.001591000
7	1.279690000	0.898403000	-0.009227000
7	2.628337000	0.628676000	0.001960000
6	2.878051000	-0.661742000	-0.001116000
7	4.176699000	-1.072306000	-0.053990000
16	1.636095000	-1.943923000	0.002592000
29	-0.125701000	-0.476292000	-0.001069000
16	-2.139103000	-1.578827000	0.001573000
1	-5.037218000	0.599955000	-0.002764000
1	-4.883405000	-1.147933000	0.000194000
1	-1.090681000	3.271017000	-0.003139000
1	4.900055000	-0.376811000	0.128173000
1	4.396825000	-2.031663000	0.200958000
7	1.637616000	3.231498000	0.018043000
1	2.649396000	3.129726000	-0.015906000
1	1.239535000	4.167354000	-0.022260000

Cu(II)CGTS in water

6	1.063496000	1.766567000	-0.000192000
6	-0.340515000	2.167555000	-0.000396000
7	-1.198620000	1.193235000	-0.000583000
7	-2.525960000	1.399999000	-0.001144000
6	-3.215972000	0.253117000	0.000145000
7	-4.551959000	0.351573000	-0.000015000
7	1.336354000	0.502009000	-0.000530000
7	2.574849000	-0.017306000	-0.000015000
6	2.560462000	-1.355543000	0.000147000
7	3.751301000	-1.970681000	0.001448000
16	1.112517000	-2.377155000	-0.001169000
29	-0.349549000	-0.623499000	-0.000377000
16	-2.511484000	-1.373278000	0.001419000
1	-4.993649000	1.271868000	-0.000962000
1	-5.144004000	-0.476272000	0.004050000
1	-0.634585000	3.217732000	-0.000626000
1	4.609163000	-1.417598000	0.002719000
1	3.821684000	-2.985787000	-0.001121000
17	2.279717000	3.016262000	0.000618000

Cu(II)FGTS in water

6	-0.820216000	2.120926000	-0.000557000
6	0.624192000	2.289977000	-0.000441000
7	1.295420000	1.177309000	0.000133000
7	2.633431000	1.136510000	0.000615000
6	3.100973000	-0.121065000	0.000693000
7	4.431265000	-0.265480000	0.001541000
7	-1.325655000	0.938126000	-0.000407000
7	-2.651508000	0.669744000	0.000122000
6	-2.886329000	-0.643072000	0.000544000
7	-4.170503000	-1.034196000	0.003799000
16	-1.647888000	-1.916899000	-0.001379000
29	0.120287000	-0.466264000	-0.000467000
16	2.112646000	-1.590241000	-0.000283000
1	5.032370000	0.559931000	0.002694000
1	4.863688000	-1.187014000	0.000132000
1	1.085101000	3.278623000	-0.000598000
1	-4.914257000	-0.335713000	0.000698000
1	-4.423073000	-2.019387000	-0.000553000
9	-1.574126000	3.233862000	-0.000476000

Cu(II)NGTS in water

6	-1.073706000	1.872487000	-0.000289000
6	0.344344000	2.226204000	-0.000146000
7	1.180006000	1.233541000	0.000024000
7	2.515053000	1.414866000	0.000167000
6	3.181828000	0.258164000	0.000421000
7	4.520609000	0.324484000	0.002081000
7	-1.356656000	0.585069000	-0.000104000
7	-2.588240000	0.111699000	0.000059000
6	-2.615388000	-1.245204000	0.000346000
7	-3.827715000	-1.796014000	0.002810000
16	-1.205665000	-2.296925000	-0.001256000
29	0.304465000	-0.568692000	-0.000411000
16	2.444236000	-1.356808000	-0.000010000
1	4.984612000	1.233580000	0.000617000
1	5.092450000	-0.517307000	-0.004070000
1	0.670345000	3.266151000	-0.000020000
1	-4.658407000	-1.199706000	0.001103000
1	-3.951120000	-2.808121000	0.001509000
6	-2.087964000	2.878845000	-0.000312000
7	-2.911514000	3.702672000	-0.000337000

Cu(II)HYGTS in water

6	0.837845000	2.130863000	0.000146000
6	-0.618411000	2.294276000	-0.000190000
7	-1.293722000	1.187477000	-0.000477000
7	-2.634580000	1.153738000	-0.000805000
6	-3.109657000	-0.099201000	-0.000477000
7	-4.442486000	-0.235337000	-0.000033000
7	1.289164000	0.912805000	-0.000808000
7	2.630618000	0.654548000	-0.000445000
6	2.882958000	-0.644938000	-0.000460000
7	4.172581000	-1.039779000	-0.004109000
16	1.646395000	-1.928196000	0.000401000
29	-0.128077000	-0.473947000	-0.000048000
16	-2.133983000	-1.577448000	0.000611000
1	-5.038134000	0.593496000	-0.001107000
1	-4.879589000	-1.154116000	0.002222000
1	-1.080776000	3.282425000	-0.000207000
1	4.917350000	-0.344227000	0.009420000
1	4.420791000	-2.024754000	0.012935000
8	1.578499000	3.242795000	0.001610000
1	2.540560000	3.019402000	0.001684000

Cu(II)THGTS in water

6	1.071316000	1.773272000	-0.000821000
6	-0.338616000	2.172875000	-0.001407000
7	-1.201810000	1.204323000	-0.000757000
7	-2.528599000	1.417619000	-0.000859000
6	-3.224475000	0.274430000	0.000495000
7	-4.560410000	0.381195000	-0.000198000
7	1.301019000	0.490097000	-0.000926000
7	2.551725000	-0.026995000	0.001158000
6	2.550877000	-1.358044000	0.000792000
7	3.743924000	-1.977500000	0.001547000
16	1.101066000	-2.384187000	-0.003198000
29	-0.361368000	-0.623635000	-0.000473000
16	-2.531135000	-1.356736000	0.002442000
1	-4.996638000	1.303920000	0.000081000
1	-5.156857000	-0.443250000	0.005574000
1	-0.638832000	3.221089000	-0.002174000
1	4.603006000	-1.427762000	0.010236000
1	3.810310000	-2.992099000	0.005862000
16	2.306727000	3.032922000	0.000769000
1	3.336625000	2.155173000	-0.000191000

Cu(II)TFGTS in water

6	1.252744000	-1.123624000	-0.000026000
6	0.046512000	-1.940701000	-0.000177000
7	-1.081942000	-1.295460000	-0.000499000
7	-2.269506000	-1.928930000	-0.000313000
6	-3.298077000	-1.076290000	-0.000084000
7	-4.528812000	-1.607171000	0.001695000
7	1.077607000	0.174164000	-0.000075000
7	2.070065000	1.057261000	-0.000699000
6	1.623126000	2.331124000	-0.000116000
7	2.563658000	3.277706000	-0.001593000
16	-0.067396000	2.832506000	0.002945000
29	-0.882941000	0.692859000	-0.000612000
16	-3.169172000	0.693263000	-0.001099000
1	-4.645181000	-2.621161000	0.001466000
1	-5.358938000	-1.018554000	-0.003464000
1	0.084784000	-3.028172000	0.000417000
1	3.550841000	3.013637000	-0.005309000
1	2.320342000	4.267018000	-0.004359000
6	2.623700000	-1.758811000	0.000286000
9	2.532085000	-3.111938000	0.001104000
9	3.352398000	-1.414201000	-1.089346000
9	3.352518000	-1.412877000	1.089415000

Cu(II)DAGTS in water

6	0.747388000	2.033011000	0.016837000
7	1.279632000	0.842505000	-0.067589000
29	-0.000030000	-0.671832000	-0.000205000
16	1.896942000	-1.963988000	-0.018296000
6	3.009050000	-0.572570000	-0.017293000
7	4.337925000	-0.852832000	-0.042373000
6	-0.747441000	2.033073000	-0.016949000
7	-1.443297000	3.192254000	-0.075452000
7	-1.279689000	0.842551000	0.067130000
7	-2.643118000	0.694594000	0.022310000
6	-3.009054000	-0.572630000	0.017333000
16	-1.896843000	-1.964015000	0.018400000
7	2.643068000	0.694611000	-0.022521000
7	-4.337870000	-0.852864000	0.042743000
1	4.996368000	-0.089703000	0.111909000
1	4.655366000	-1.792815000	0.178505000
1	-4.996571000	-0.089814000	-0.110745000
1	-4.655729000	-1.793108000	-0.176261000
1	-2.452722000	3.119674000	-0.199935000
1	-1.011820000	4.031104000	-0.461183000
7	1.443355000	3.192056000	0.075856000
1	2.452762000	3.119375000	0.200395000
1	1.011915000	4.031038000	0.461306000

Cu(II)MAGTS in water

29	0.018385000	-0.676990000	0.001538000
16	1.935946000	-1.940966000	0.001085000
6	3.020121000	-0.525299000	0.001822000
7	2.623088000	0.728469000	-0.001905000
7	1.252777000	0.843915000	0.012715000
6	0.693359000	2.030381000	-0.002784000
6	-0.797370000	2.033472000	0.001578000
7	-1.317871000	0.841616000	-0.005608000
7	-2.653999000	0.635432000	-0.002276000
6	-2.974490000	-0.658667000	-0.002961000
16	-1.834529000	-2.016617000	-0.002979000
7	-4.285107000	-0.957758000	-0.003224000
1	-4.977301000	-0.208809000	-0.003180000
1	-4.605390000	-1.922600000	-0.001170000
6	-1.577086000	3.310298000	0.015749000

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1	-1.313625000	3.916610000	0.891974000
1	-1.360351000	3.909202000	-0.878824000
1	-2.645627000	3.098320000	0.042731000
7	4.357592000	-0.780210000	0.050761000
1	4.995248000	-0.004619000	-0.127594000
1	4.689510000	-1.708453000	-0.198202000
7	1.385470000	3.186903000	-0.001456000
1	2.400967000	3.152729000	-0.056428000
1	0.939871000	4.091981000	-0.107085000

Optimised Cartesian coordinates for the reduced Cu(I)A$^-$ complexes (**1 – 15**) in solution phase using the water solvation model.

Cu(I)GTS$^-$ in water

29	-0.000695082	-0.448702094	-0.000459910
16	2.039365973	-1.464775378	0.472841126
6	3.060000188	-0.118014375	-0.039692913
7	2.638790274	1.114196763	-0.276239931
7	1.277865185	1.219082906	-0.324656935
6	0.722870256	2.371384051	-0.045565913
6	-0.716467857	2.373589196	0.056818095
7	-1.275481014	1.219703160	0.321022115
7	-2.635933130	1.119161287	0.276459112
6	-3.061650284	-0.111096763	0.033591093
16	-2.042124341	-1.465473966	-0.464801946
7	-4.411999412	-0.324404645	0.096305098
1	-4.974586388	0.340760463	0.629766139
1	-4.748120529	-1.284647687	0.065403095
1	-1.305224813	3.278710325	-0.105745918
1	1.315027388	3.271956060	0.129721100
7	4.397866262	-0.364227527	-0.211629926
1	5.002341391	0.449930475	-0.339063936
1	4.808583220	-1.140115627	0.304911114

Cu(I)PTS$^-$ in water

29	-0.155988709	-0.659890777	0.005389457
16	-2.291878143	-1.465536483	-0.457629652
6	-3.165780603	-0.014349919	0.038627008
7	-2.620936189	1.170094725	0.259856897
7	-1.253971922	1.138177060	0.302548797
6	-0.591935951	2.218599466	-0.013709138
6	0.853884769	2.105334209	-0.103925472
7	1.279979904	0.884244906	-0.331294383
7	2.623420866	0.633781134	-0.303016242
6	2.917294906	-0.629961109	-0.045644059
16	1.771877616	-1.867096553	0.484849460
7	4.239903170	-0.986588469	-0.120082080
1	4.854230272	-0.392213291	-0.679424593
1	4.463723990	-1.979557890	-0.107739714
6	1.741071833	3.303858055	0.086907396
1	1.157237241	4.227629296	0.032150935
1	2.233522281	3.271068778	1.067919049
1	2.533338706	3.333306928	-0.668623969
1	-1.099302080	3.163336587	-0.223310104
7	-4.522505645	-0.120621132	0.218139767
1	-5.038785082	0.754733971	0.325222653
1	-5.008725364	-0.853845097	-0.294609158

Cu(I)ATS$^-$ in water

29	-0.001575792	-0.856983441	0.001014838
16	2.037743754	-1.875161553	0.455775057
6	3.047633062	-0.528569301	-0.074224425
7	2.630393052	0.703199611	-0.306758332
7	1.264549979	0.827152349	-0.331980984
6	0.736540434	1.988243488	-0.026203458
6	-0.730774471	1.991589422	0.025906465
7	-1.263914147	0.830402090	0.322691659
7	-2.629685198	0.710739720	0.301576468
6	-3.051094336	-0.519886156	0.067215463
16	-2.041684098	-1.874730041	-0.446533765
7	-4.403352666	-0.740105337	0.157288370
1	-4.950075506	-0.075587154	0.707325013
1	-4.726262333	-1.705141639	0.162644158
6	-1.544559665	3.220909135	-0.281590416
1	-0.921040908	4.048614998	-0.624659716
1	-2.278641722	2.991585454	-1.062090204
1	-2.113313276	3.552144031	0.597038124
6	1.556856749	3.210269132	0.292751325
1	2.266833787	2.979093940	1.095131470
1	2.153410264	3.526210345	-0.572697839
1	0.934738026	4.048116381	0.612669179
7	4.383672903	-0.782985184	-0.278575318
1	4.987556221	0.032327007	-0.398710912
1	4.796280712	-1.560735238	0.233236973

Cu(I)GTSM$^-$ in water

29	-0.000445581	-0.529578667	0.003155318
16	-2.013043602	-1.542531382	-0.575194868
6	-3.065416777	-0.194419533	-0.097038838
7	-2.649726982	1.037831988	0.164699200
7	-1.290925713	1.134411689	0.272695703
6	-0.720297566	2.287502191	0.025045038
6	0.720752436	2.287979615	-0.017222372
7	1.291733741	1.135717735	-0.267495649
7	2.650322094	1.039008783	-0.160397904
6	3.065927095	-0.193905907	0.096390638
16	2.015048850	-1.540653771	0.579661584
7	4.399836336	-0.448416133	0.009550757
6	5.388018983	0.562749344	-0.339767474
1	5.419226630	1.378641346	0.396021771
1	6.368227549	0.080238419	-0.377174664
1	5.168372319	0.998554670	-1.320710529
1	4.738594555	-1.322624854	0.420940347
1	1.303385605	3.190443353	0.179280671
1	-1.303464854	3.190127059	-0.169034588
7	-4.399936531	-0.446337646	-0.023501221
6	-5.391759261	0.563287893	0.319794537
1	-5.388104869	1.398177205	-0.394276846
1	-6.376425404	0.088792379	0.307563365
1	-5.206568084	0.971439590	1.320217807
1	-4.734875529	-1.329721809	-0.417864382

Cu(I)PTSM$^-$ in water

29	-0.113670000	-0.720022000	0.010695000
16	-2.176253000	-1.646698000	-0.537190000
6	-3.159465000	-0.238917000	-0.088454000
7	-2.685090000	0.976579000	0.141527000
7	-1.320726000	1.013230000	0.245047000
6	-0.701952000	2.125098000	-0.054682000
6	0.748563000	2.088957000	-0.085675000
7	1.250842000	0.891356000	-0.289194000
7	2.604597000	0.720848000	-0.197213000
6	2.957518000	-0.526090000	0.075563000
16	1.850534000	-1.818328000	0.588636000
7	4.278119000	-0.852704000	-0.021343000
6	5.318665000	0.112910000	-0.344677000
1	5.375097000	0.921381000	0.397849000
1	6.275613000	-0.415189000	-0.371133000
1	5.137369000	0.567847000	-1.324666000
1	4.570304000	-1.731487000	0.413632000
6	1.563367000	3.333071000	0.134626000
1	0.937859000	4.225590000	0.036196000
1	2.004638000	3.337063000	1.140410000
1	2.393356000	3.391423000	-0.577131000
1	-1.250449000	3.039049000	-0.295282000
7	-4.506292000	-0.428315000	0.005173000
6	-5.445280000	0.647606000	0.290711000
1	-5.430402000	1.425654000	-0.485899000
1	-6.448975000	0.217472000	0.344122000
1	-5.211497000	1.122243000	1.249925000
1	-4.883633000	-1.282774000	-0.413762000

Cu(I)ATSM$^-$ in water

29	0.000067438	-0.895195431	0.000385455
16	2.016517269	-1.908766812	0.541906502
6	3.056058765	-0.555012757	0.049430992
7	2.643589637	0.676564178	-0.197953188
7	1.278682203	0.791191998	-0.278065648
6	0.733511736	1.951159138	0.002955669
6	-0.733785410	1.950847780	-0.002802291
7	-1.278462954	0.790780880	0.279070907
7	-2.643590283	0.675634376	0.200034615
6	-3.055901112	-0.555684849	-0.048506166
16	-2.016295898	-1.909281516	-0.541223038
7	-4.392395750	-0.818058163	0.064511123
6	-5.382931473	0.216789955	0.327120508
1	-5.392316114	0.987442334	-0.456967773
1	-6.366618268	-0.258245647	0.374130166
1	-5.182814397	0.712432415	1.283062383
1	-4.726355400	-1.679833266	-0.374310611
6	-1.533956720	3.179663484	-0.346987436
1	-0.899388425	3.991286533	-0.709014629
1	-2.269493395	2.936013800	-1.121289262
1	-2.102556055	3.541096381	0.519965658
6	1.533466522	3.179984223	0.347297834
1	2.253337873	2.942292234	1.138266861
1	2.120081998	3.527747510	-0.513059873
1	0.896619563	3.998819530	0.688298673
7	4.392221693	-0.817628000	-0.065188789
6	5.382808334	0.215983775	-0.332173892
1	5.394749906	0.988125099	0.450413047
1	6.366035538	-0.259837199	-0.380701291
1	5.180582232	0.709973942	-1.288538611
1	4.726701529	-1.679654256	0.372757201

Cu(I)AGTS$^-$ in water

6	0.821248000	2.108382000	-0.085453000
6	-0.637651000	2.242976000	-0.014520000
7	-1.295096000	1.159659000	0.262044000
7	-2.654978000	1.175762000	0.230214000
6	-3.183504000	-0.029380000	0.040252000
7	-4.543521000	-0.114617000	0.114406000
7	1.254966000	0.899770000	-0.351313000
7	2.623731000	0.694510000	-0.317204000
6	2.958872000	-0.547602000	-0.046314000
7	4.290523000	-0.888035000	-0.189481000
16	1.852420000	-1.841237000	0.445877000
29	-0.133721000	-0.707505000	-0.013237000
16	-2.294757000	-1.489529000	-0.391743000
1	-5.050524000	0.639796000	0.580200000
1	-4.977595000	-1.034869000	0.108506000
1	-1.126887000	3.199586000	-0.217254000
1	4.941805000	-0.102338000	-0.250296000

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1	4.622245000	-1.665918000	0.378669000
7	1.614746000	3.195056000	0.185664000
1	2.578968000	3.154820000	-0.143323000
1	1.180920000	4.117846000	0.157116000

Cu(I)CGTS$^-$ in water

6	1.020249000	1.771675000	-0.138355000
6	-0.391188000	2.113999000	-0.068159000
7	-1.205923000	1.132486000	0.184991000
7	-2.542796000	1.374928000	0.165800000
6	-3.275151000	0.270988000	0.029298000
7	-4.617375000	0.411596000	0.205628000
7	1.360414000	0.548001000	-0.317366000
7	2.634349000	0.101769000	-0.279115000
6	2.714019000	-1.211231000	-0.056684000
7	3.943563000	-1.771579000	-0.211621000
16	1.390376000	-2.267682000	0.428132000
29	-0.412892000	-0.893008000	0.020084000
16	-2.663654000	-1.333274000	-0.365321000
1	-4.996023000	1.354888000	0.306673000
1	-5.243422000	-0.307314000	-0.150968000
1	-0.729031000	3.138603000	-0.238521000
1	4.740477000	-1.152396000	-0.369774000
1	4.133953000	-2.680806000	0.204460000
17	2.178069000	3.112150000	0.107405000

Cu(I)FGTS$^-$ in water

6	0.811902000	2.102002000	-0.086253000
6	-0.626412000	2.258317000	0.000004000
7	-1.288849000	1.158211000	0.206807000
7	-2.640019000	1.181302000	0.188030000
6	-3.179160000	-0.032238000	0.035634000
7	-4.523100000	-0.114145000	0.206633000
7	1.335523000	0.955413000	-0.304184000
7	2.682670000	0.746302000	-0.264403000
6	2.989028000	-0.527235000	-0.040788000
7	4.303216000	-0.868842000	-0.179799000
16	1.862887000	-1.808349000	0.412750000
29	-0.147584000	-0.744443000	-0.001096000
16	-2.310759000	-1.505141000	-0.381770000
1	-5.053596000	0.747861000	0.343220000
1	-5.025855000	-0.932931000	-0.128866000
1	-1.095287000	3.236552000	-0.132869000
1	4.980088000	-0.111202000	-0.287739000
1	4.637153000	-1.716625000	0.274030000
9	1.549459000	3.240920000	0.116129000

Cu(I)NGTS$^-$ in water

6	0.992836000	1.877269000	-0.139098000
6	-0.420579000	2.178494000	-0.053543000
7	-1.196630000	1.175473000	0.260880000
7	-2.550487000	1.351903000	0.206188000
6	-3.219401000	0.224867000	0.018873000
7	-4.581842000	0.293925000	0.081123000
7	1.306752000	0.598211000	-0.343392000
7	2.582825000	0.204040000	-0.262097000
6	2.716706000	-1.115544000	-0.061814000
7	3.947537000	-1.637338000	-0.275188000
16	1.430024000	-2.169870000	0.492892000
29	-0.313385000	-0.708618000	0.032115000
16	-2.498383000	-1.332566000	-0.405606000
1	-5.001362000	1.093290000	0.558298000
1	-5.114320000	-0.573274000	0.078057000
1	-0.809043000	3.175116000	-0.269170000
1	4.711078000	-1.012818000	-0.539722000
1	4.187602000	-2.552559000	0.100391000
6	1.973837000	2.896862000	0.041760000
7	2.770065000	3.740565000	0.176365000

Cu(I)HYGTS$^-$ in water

6	0.807241000	2.096028000	-0.086464000
6	-0.638841000	2.257687000	0.001178000
7	-1.299853000	1.167895000	0.253449000
7	-2.655889000	1.183813000	0.225548000
6	-3.183939000	-0.026370000	0.049012000
7	-4.531669000	-0.131288000	0.224634000
7	1.258686000	0.906867000	-0.353873000
7	2.624805000	0.720909000	-0.309602000
6	2.968777000	-0.524056000	-0.040126000
7	4.299263000	-0.845578000	-0.164614000
16	1.864900000	-1.821588000	0.435781000
29	-0.139037000	-0.717981000	-0.018605000
16	-2.300282000	-1.483857000	-0.397245000
1	-5.066364000	0.731576000	0.338938000
1	-5.020698000	-0.924331000	-0.185408000
1	-1.111533000	3.228370000	-0.171293000
1	4.950622000	-0.061775000	-0.241849000
1	4.638755000	-1.641414000	0.372579000
8	1.563379000	3.196429000	0.141411000
1	2.513546000	2.966678000	0.008329000

Cu(I)THGTS$^-$ in water

6	1.000019924	1.776295257	-0.147050805
6	-0.414304578	2.118536451	-0.079764825
7	-1.224435560	1.144455409	0.220098133
7	-2.565939289	1.372254504	0.188628316
6	-3.282168699	0.263865014	0.032350223
7	-4.636106612	0.395710304	0.122256232
7	1.280855746	0.523448931	-0.370510906
7	2.574111157	0.090494609	-0.328986416
6	2.687791828	-1.202192696	-0.061961529
7	3.928241245	-1.759069400	-0.222315773
16	1.380420937	-2.262045765	0.468605321
29	-0.394224392	-0.841988357	0.008476651
16	-2.638513192	-1.326799533	-0.374501824
1	-5.015098283	1.232151129	0.568951280
1	-5.213144456	-0.442159889	0.127427604
1	-0.766185293	3.130119602	-0.293193709
1	4.710767928	-1.116915358	-0.361771287
1	4.138935463	-2.613210645	0.290521362
16	2.187749195	3.077742040	0.144883532
1	3.257603233	2.295244954	-0.127176074

Cu(I)TFGTS$^-$ in water

6	-1.159657000	-1.179113000	-0.166446000
6	0.084128000	-1.905686000	-0.069479000
7	1.138169000	-1.199899000	0.255980000
7	2.363484000	-1.802184000	0.199171000
6	3.359673000	-0.951671000	0.011993000
7	4.629127000	-1.455795000	0.077231000
7	-1.054187000	0.124567000	-0.359714000
7	-2.136621000	0.922349000	-0.300141000
6	-1.836550000	2.203818000	-0.073598000
7	-2.826970000	3.108973000	-0.293752000
16	-0.285952000	2.786719000	0.511710000
29	0.905484000	0.862794000	0.027718000
16	3.177083000	0.752797000	-0.418381000
1	4.767738000	-2.337629000	0.572125000
1	5.407736000	-0.801140000	0.079267000
1	0.153282000	-2.970985000	-0.287428000
1	-3.755696000	2.759843000	-0.533589000
1	-2.772272000	4.026015000	0.143726000
6	-2.472465000	-1.887171000	0.019362000
9	-2.300609000	-3.235335000	0.109553000
9	-3.125666000	-1.510405000	1.155774000
9	-3.347025000	-1.687205000	-1.004618000

Cu(I)DAGTS$^-$ in water

6	0.746575000	1.987450000	-0.022973000
7	1.276486000	0.843819000	-0.355881000
29	-0.004719000	-0.929826000	-0.002634000
16	2.096623000	-1.862037000	0.361953000
6	3.093153000	-0.463425000	-0.064216000
7	4.459987000	-0.649466000	-0.064440000
6	-0.737796000	1.989110000	0.020613000
7	-1.425554000	3.113892000	-0.337243000
7	-1.267806000	0.842889000	0.353571000
7	-2.650174000	0.757575000	0.311751000
6	-3.092556000	-0.457935000	0.073960000
16	-2.107294000	-1.861263000	-0.363126000
7	2.658040000	0.752796000	-0.318688000
7	-4.451644000	-0.668905000	0.209656000
1	5.009738000	0.038567000	-0.582914000
1	4.790533000	-1.610102000	-0.132300000
1	-5.028067000	0.174977000	0.233076000
1	-4.846812000	-1.434790000	-0.333491000
1	-2.411664000	3.171920000	-0.089153000
1	-0.932778000	3.991610000	-0.482196000
7	1.430697000	3.153725000	0.231054000
1	2.441216000	3.047734000	0.324152000
1	1.018936000	3.802382000	0.905199000

Cu(I)MAGTS$^-$ in water

29	-0.025144000	-0.893402000	0.018850000
16	-2.109134000	-1.843181000	-0.417631000
6	-3.081697000	-0.442028000	0.061194000
7	-2.625312000	0.761243000	0.321184000
7	-1.240162000	0.837713000	0.361104000
6	-0.703527000	1.986122000	0.019413000
6	0.775066000	2.000947000	-0.033774000
7	1.291923000	0.835452000	-0.308604000
7	2.651155000	0.699748000	-0.291773000
6	3.054641000	-0.543952000	-0.074568000
16	2.032938000	-1.897724000	0.409873000
7	4.402567000	-0.772876000	-0.162687000
1	4.963219000	-0.093759000	-0.679932000
1	4.722609000	-1.738483000	-0.181932000
6	1.585158000	3.232774000	0.262635000
1	0.954694000	4.099688000	0.476117000
1	2.226773000	3.056177000	1.134565000
1	2.249761000	3.478712000	-0.574356000
7	-4.440928000	-0.649536000	0.213553000
1	-5.010396000	0.197519000	0.265331000
1	-4.847838000	-1.394780000	-0.348896000
7	-1.427488000	3.093086000	-0.337147000
1	-2.401365000	3.129550000	-0.041756000
1	-0.969247000	3.991540000	-0.450480000

Optimised Cartesian coordinates for the reduced Cu(II)A complexes (**1 – 15**) in solution phase using the DMSO solvation model.

Cu(II)GTS in DMSO

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29	0.000001421	-0.276782870	0.000099699
16	1.893151098	-1.568909375	0.001059710
6	2.994043292	-0.183711376	-0.000190245
7	2.638480658	1.102550694	0.000026562
7	1.303324410	1.255647038	-0.000009099
6	0.727077851	2.422094922	0.000200889
6	-0.727069844	2.422100123	0.000101263
7	-1.303322029	1.255657161	-0.000030914
7	-2.638478086	1.102558928	-0.000121514
6	-2.994033682	-0.183704320	-0.000127107
16	-1.893165539	-1.568923150	-0.000868555
7	-4.314437188	-0.442699850	-0.000403212
1	-4.978302371	0.322794267	0.002899889
1	-4.660103133	-1.391907047	0.004026512
1	-1.301955678	3.346305617	0.000108141
1	1.301971987	3.346294832	0.000377446
7	4.314441612	-0.442712433	-0.001663917
1	4.978312706	0.322778643	0.000912267
1	4.660094899	-1.391929521	0.001231862

Cu(II)PTS in DMSO

29	0.147228155	-0.482188794	0.000435765
16	2.182186415	-1.546030217	-0.005732445
6	3.110285965	-0.040395720	-0.000025346
7	2.605095051	1.194558663	0.003141932
7	1.260204016	1.188727765	0.002477742
6	0.553356950	2.278307186	0.001297561
6	-0.902866564	2.127921865	-0.000658006
7	-1.315321959	0.888545191	-0.002469837
7	-2.628458120	0.574501032	-0.004060013
6	-2.830539635	-0.740795660	-0.000891319
16	-1.575061569	-1.990512864	0.005939602
7	-4.112487634	-1.157667738	-0.001255411
1	-4.862891369	-0.477347248	-0.008573647
1	-4.341102265	-2.141277442	-0.002930159
6	-1.822499082	3.310035565	-0.000211249
1	-1.259159134	4.245592799	-0.002049314
1	-2.476962225	3.285608902	-0.878484272
1	-2.473594197	3.287436622	0.880698604
1	1.022383648	3.261030344	0.001455167
7	4.452742038	-0.140182562	0.001563019
1	5.020561921	0.698939575	0.003641158
1	4.908309996	-1.041635106	-0.002561099

Cu(II)ATS in DMSO

29	-0.007913711	-0.682602958	-0.000069721
16	-1.886820884	-1.983346079	0.000186370
6	-2.985586622	-0.594366187	-0.000322494
7	-2.634210404	0.686357852	-0.001435324
7	-1.290973144	0.855766979	-0.000663882
6	-0.734295590	2.036199070	0.000005659
6	0.748083420	2.023185183	-0.000000065
7	1.286136204	0.834699136	0.001165571
7	2.627662688	0.666248407	0.002365956
6	2.974973824	-0.618210808	0.000397920
16	1.867882768	-1.998890333	-0.000973098
7	4.296216790	-0.888357741	-0.000017682
1	4.965358278	-0.128091952	0.001295683
1	4.633401283	-1.840144223	-0.000635188
6	1.576858205	3.272476030	-0.000922999
1	0.963364028	4.172661792	-0.022360910
1	2.216337133	3.300817324	0.888539069
1	2.246986180	3.277929619	-0.867545898
6	-1.510854313	3.318939194	0.001089513
1	-1.274429211	3.918887291	-0.885531522
1	-2.579206192	3.107159268	0.008469802
1	-1.262519161	3.924443557	0.880530490
7	-4.308784183	-0.860659921	0.001338684
1	-4.975764009	-0.098709798	-0.004693889
1	-4.648430060	-1.811402479	-0.004216550

Cu(II)GTSM in DMSO

29	0.000000518	-0.350709472	-0.000394975
16	1.890856072	-1.641130814	0.000551368
6	2.999883171	-0.252089936	0.000318504
7	2.640557748	1.033677074	-0.000092132
7	1.304311659	1.181532737	-0.000186295
6	0.726526353	2.347914738	-0.000345104
6	-0.726434159	2.347947404	-0.000575875
7	-1.304289699	1.181598493	-0.000848822
7	-2.640554133	1.033796186	-0.000943702
6	-2.999880816	-0.251982184	-0.000802341
16	-1.890862867	-1.641037054	-0.001124467
7	-4.316433223	-0.525578565	0.000610564
6	-5.364439904	0.489512465	0.002651418
1	-5.290987842	1.125014808	0.890548720
1	-5.292980178	1.126452948	-0.884357574
1	-6.328477235	-0.021150083	0.003296965
1	-4.589815641	-1.500647309	0.001485432
1	-1.301750569	3.271890659	-0.000553104
1	1.301894933	3.271825512	-0.000327356
7	4.316450993	-0.525588204	0.000372375
6	5.364335550	0.489638821	0.001065332
1	5.291890708	1.125191193	0.889006830
1	6.328434848	-0.020907536	0.000574894
1	5.291709100	1.126507225	-0.885902009
1	4.589930695	-1.500628777	0.000595526

Cu(II)PTSM in DMSO

29	-0.109703431	-0.538552190	0.000406915
16	-2.067708945	-1.728337558	-0.000080162
6	-3.099461295	-0.281212825	0.000227436
7	-2.671591501	0.983174482	-0.000291090
7	-1.328006423	1.058654801	-0.000012483
6	-0.690037481	2.190829805	-0.000252709
6	0.771738791	2.132305358	-0.000212094
7	1.262191997	0.921087126	-0.000110087
7	2.593176048	0.696676210	0.000044669
6	2.884495156	-0.602246742	-0.000395606
16	1.704073294	-1.933335278	-0.000862002
7	4.186917213	-0.944926725	-0.000173191
6	5.281101165	0.019294208	0.001201670
1	5.238246725	0.657799002	0.889152449
1	6.220545715	-0.535512210	0.000028957
1	5.237724591	0.660608611	-0.884662470
1	4.410927505	-1.932034053	0.000333776
6	1.619600423	3.366878213	-0.000520985
1	1.002588715	4.268037302	-0.001231719
1	2.273471268	3.380773170	0.878538153
1	2.274134142	3.379801828	-0.879093292
1	-1.220835409	3.141626832	-0.000663430
7	-4.429286468	-0.484289059	0.000075471
6	-5.422675860	0.583967356	0.000431411
1	-5.317934325	1.215623161	-0.887107867
1	-6.412029296	0.124269428	0.001076951
1	-5.316855545	1.215820227	0.887691909
1	-4.752785713	-1.443564557	-0.000397077

Cu(II)ATSM in DMSO

29	0.006424946	-0.710152825	-0.000317440
16	1.883479103	-2.011346488	-0.000262889
6	2.990177054	-0.619057470	0.000029892
7	2.634810258	0.661067482	0.000365639
7	1.291403867	0.827208442	0.000267817
6	0.736172116	2.009070163	0.000284815
6	-0.744621637	1.997988567	0.000306794
7	-1.284365000	0.809544457	0.000167902
7	-2.626304544	0.649243783	0.000189074
6	-2.982302886	-0.633274886	-0.000308685
16	-1.871947992	-2.021129155	-0.001002177
7	-4.301184674	-0.908664479	0.000164584
6	-5.344923741	0.109471872	0.000950887
1	-5.270481419	0.746838292	-0.885822077
1	-6.311435558	-0.396891540	0.001405344
1	-5.269473305	0.746475171	0.887899230
1	-4.574930721	-1.883114770	0.000190403
6	-1.575873808	3.245547628	0.000353332
1	-0.964360802	4.147529730	0.003228986
1	-2.230024768	3.260743852	-0.878638707
1	-2.234224002	3.257731310	0.876197269
6	1.518081070	3.288888213	0.000286935
1	1.279269569	3.892571888	0.883757211
1	2.585090330	3.069896226	-0.000616301
1	1.277851157	3.893425033	-0.882200737
7	4.309980108	-0.895760153	0.000124093
6	5.354402575	0.121260117	0.000432321
1	5.280386379	0.758683285	0.887293264
1	6.320601649	-0.385786079	0.000965801
1	5.281259040	0.758432439	-0.886697601
1	4.582606564	-1.870334615	-0.000486781

Cu(II)AGTS in DMSO

6	0.852736259	2.135708602	-0.001246927
6	-0.612165926	2.291470666	-0.001262696
7	-1.289388750	1.187883584	0.000297389
7	-2.629927857	1.158815576	-0.000460447
6	-3.103345615	-0.093341236	0.000451474
7	-4.442275415	-0.218503780	0.001045916
7	1.278247336	0.896254843	-0.009129715
7	2.624499684	0.628916905	0.000818905
6	2.869351802	-0.661763085	-0.001797066
7	4.171865878	-1.068412274	-0.052908945
16	1.635531584	-1.945643804	0.002286408
29	-0.127388556	-0.480003221	-0.000880578
16	-2.145722970	-1.575807613	0.001433307
1	-5.026011399	0.609769960	-0.001232002
1	-4.880314181	-1.128755313	-0.000231369
1	-1.087964304	3.271130030	-0.001985504
1	4.886953355	-0.374195415	0.131446550
1	4.390363566	-2.021993661	0.200583240
7	1.657010735	3.219385502	0.017610093
1	2.659360394	3.086417266	-0.013980479
1	1.285262427	4.158111005	-0.026360206

Cu(II)CGTS in DMSO

6	1.067120679	1.767235112	-0.000443945
6	-0.337193759	2.167270729	-0.000836115
7	-1.197154478	1.194554265	-0.000918723
7	-2.522661544	1.402274539	-0.001129657
6	-3.208295248	0.254660152	-0.000357905
7	-4.547740816	0.359654983	-0.000073645
7	1.336767735	0.501489034	-0.000817582
7	2.573567019	-0.019761065	-0.000525907
6	2.552174272	-1.355267010	0.000394884

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7	3.747739700	-1.970878171	0.000950834
16	1.111227502	-2.379784232	-0.000587131
29	-0.350378531	-0.626073001	-0.000384226
16	-2.515487567	-1.371419436	0.001463072
1	-4.981085431	1.275918522	-0.000329880
1	-5.137064817	-0.461258414	0.002488625
1	-0.631485097	3.214122940	-0.000982317
1	4.598070674	-1.419554627	0.000764209
1	3.816478618	-2.978858450	-0.000263335
17	2.281633261	3.015898630	0.001206556

Cu(II)FGTS in DMSO

6	-0.822546750	2.123637424	-0.000046443
6	0.622504695	2.290106886	-0.000036579
7	1.294627509	1.177848251	-0.000039843
7	2.630871756	1.136891255	-0.000018001
6	3.092939540	-0.121151777	0.000152450
7	4.427787643	-0.260783476	0.000114696
7	-1.326555048	0.939611960	-0.000201061
7	-2.650626043	0.668503904	-0.000317178
6	-2.877923886	-0.643211660	-0.000385977
7	-4.166530109	-1.033888284	0.001432867
16	-1.647035400	-1.918858915	-0.000278601
29	0.119517342	-0.468444599	-0.000086038
16	2.114770789	-1.590840221	0.000212557
1	5.020410746	0.561748474	0.000070297
1	4.858267122	-1.175212318	-0.000528943
1	1.084577649	3.274679756	0.000039041
1	-4.903423918	-0.338589443	-0.001324827
1	-4.416104536	-2.012535665	-0.001284686
9	-1.572263089	3.237379798	0.000186651

Cu(II)NGTS in DMSO

6	-1.077672341	1.872156647	-0.001365807
6	0.340610615	2.225064425	-0.001839031
7	1.177321936	1.233252865	-0.000952656
7	2.510379303	1.414666188	-0.000052669
6	3.172560560	0.257307328	0.001721881
7	4.514786060	0.330391461	0.005083564
7	-1.357423344	0.584098910	-0.000739234
7	-2.588761968	0.107771142	0.000310360
6	-2.607717584	-1.246175480	0.000354820
7	-3.825432800	-1.798186224	0.006080042
16	-1.206219295	-2.300493128	-0.002554886
29	0.305460652	-0.570776195	-0.001245871
16	2.446062190	-1.357775728	0.000068260
1	4.969928189	1.236082032	0.002793308
1	5.084532159	-0.504252602	-0.002761535
1	0.668565315	3.262511082	-0.001925284
1	-4.648042665	-1.203882639	0.004908359
1	-3.946317675	-2.802876217	0.005103770
6	-2.089095606	2.881988639	-0.000123853
7	-2.896101235	3.721602847	0.001029107

Cu(II)HYGTS in DMSO

6	0.835731513	2.124561404	-0.000108144
6	-0.617298898	2.299643089	-0.000217013
7	-1.295778380	1.193346757	-0.000036068
7	-2.633870027	1.160183420	-0.000125342
6	-3.104508069	-0.093812284	-0.000398973
7	-4.441572398	-0.223281745	0.001181517
7	1.280004188	0.904401564	0.000034894
7	2.622441507	0.658727629	0.000857048
6	2.878486893	-0.639092153	0.000058145
7	4.173655042	-1.024258227	-0.003492815
16	1.653466835	-1.927399725	-0.000163004
29	-0.132352750	-0.478981033	-0.000034194
16	-2.141787082	-1.574609953	-0.000571447
1	-5.027829970	0.603521329	0.001904910
1	-4.877998337	-1.134604621	0.002386668
1	-1.076547935	3.285710525	-0.000484392
1	4.907996623	-0.327454013	0.011430042
1	4.425469608	-2.001475014	0.014405077
8	1.608358751	3.216717454	-0.000203536
1	2.544765521	2.931530763	-0.000209909

Cu(II)THGTS in DMSO

6	1.070503762	1.774288484	-0.000011716
6	-0.338413349	2.175525169	-0.000703067
7	-1.202782659	1.207744141	-0.000753898
7	-2.528153658	1.420952845	-0.001255055
6	-3.218595514	0.276402040	-0.000370159
7	-4.558319906	0.388282884	-0.000928476
7	1.297002737	0.490398317	0.000396962
7	2.547358966	-0.024663926	0.001435146
6	2.543504656	-1.353537886	0.000738450
7	3.742358640	-1.970342019	-0.001110555
16	1.102465824	-2.383979104	-0.001693041
29	-0.363936659	-0.625132965	0.000056033
16	-2.536054226	-1.353847270	0.001917360
1	-4.987172276	1.306515810	-0.000703717
1	-5.150906792	-0.430104449	0.002649836
1	-0.639454502	3.221541132	-0.001197499
1	4.593232872	-1.421008615	0.003809863
1	3.809004223	-2.977949827	0.002124067
16	2.319910139	3.018754869	0.000307618
1	3.324065625	2.112333467	0.000771580

Cu(II)TFGTS in DMSO

6	1.257141609	-1.120533613	0.000987465
6	0.052247604	-1.939848524	0.000472149
7	-1.078257500	-1.297967300	-0.000034473
7	-2.263449609	-1.932768254	-0.000542555
6	-3.288774927	-1.079026686	-0.000832444
7	-4.520711644	-1.617376069	-0.000281096
7	1.077049145	0.176668883	0.001346144
7	2.066311552	1.062489309	0.000660015
6	1.611573021	2.330754986	-0.001486327
7	2.555390300	3.280801972	-0.008019406
16	-0.073869572	2.833744417	0.004587549
29	-0.885624620	0.692227629	0.000433166
16	-3.171689904	0.686992494	-0.000858503
1	-4.630464487	-2.624874442	-0.001476445
1	-5.346138785	-1.034635943	-0.003982550
1	0.092622849	-3.025474352	0.000335926
1	3.534580278	3.016549851	-0.013046160
1	2.311790602	4.262345948	-0.010651669
6	2.630303430	-1.753000123	0.000311011
9	2.534995734	-3.107233179	-0.017057062
9	3.362083545	-1.395764082	-1.080535671
9	3.349632396	-1.422927068	1.098479712

Cu(II)DAGTS in DMSO

6	-0.744556464	2.027220588	-0.016062461
7	-1.281035846	0.841864312	0.073273434
29	0.000000137	-0.678815007	-0.000004078
16	-1.903377713	-1.962166167	0.020743767
6	-3.004456394	-0.568511407	0.019000403
7	-4.337234922	-0.841575054	0.038220985
6	0.744631856	2.027268034	0.015968656
7	1.443600166	3.192948516	0.072244685
7	1.281058262	0.841886977	-0.073558149
7	2.641385010	0.699581647	-0.026113338
6	3.004428851	-0.568575876	-0.019050027
16	1.903343496	-1.962231494	-0.020603317
7	-2.641401976	0.699664490	0.025883110
7	4.337214405	-0.841567994	-0.038185446
1	-4.985327760	-0.078918678	-0.120193482
1	-4.653538552	-1.774874067	-0.184174996
1	4.985287379	-0.078819783	0.119849915
1	4.653655854	-1.774834045	0.184117866
1	2.446335177	3.094241089	0.191705708
1	1.029346552	3.995351324	0.532118051
7	-1.443546899	3.192856952	-0.072070963
1	-2.446272496	3.094340865	-0.190830202
1	-1.029497182	3.995484216	-0.531721459

Cu(II)MAGTS in DMSO

29	-0.018052965	-0.682574600	-0.002239036
16	-1.939880539	-1.940546938	-0.000612089
6	-3.014517721	-0.523200508	-0.001253107
7	-2.620806598	0.731154172	0.000092968
7	-1.252594431	0.841452740	-0.013283961
6	-0.692336994	2.024546640	0.000311546
6	0.795304737	2.033380603	-0.000720393
7	1.319222027	0.842549375	0.006692969
7	2.653179482	0.639620250	0.005724026
6	2.969991149	-0.654504980	0.003794333
16	1.840807308	-2.014924403	0.000826335
7	4.285626016	-0.947919186	0.003824153
1	4.968367058	-0.199771146	0.004078883
1	4.605579556	-1.905684894	-0.000091473
6	1.574339464	3.312074982	-0.010396713
1	1.293278711	3.935623119	-0.867538929
1	1.386353099	3.893829245	0.901184098
1	2.640518001	3.095395002	-0.067134628
7	-4.355700048	-0.772354150	-0.045140929
1	-4.983972035	0.001287454	0.138883310
1	-4.685311592	-1.694979753	0.202259600
7	-1.394158664	3.181052770	-0.019760869
1	-2.400555031	3.121581359	0.073827648
1	-0.955608343	4.072252150	0.158583112

Optimised Cartesian coordinates for the reduced Cu(I)A$^-$ complexes (**1 – 15**) in solution phase using the water solvation model.

Cu(I)GTS$^-$ in DMSO

29	-0.000959000	-0.443632000	-0.002329000
16	2.036445000	-1.466322000	0.474404000
6	3.049168000	-0.121426000	-0.037566000
7	2.636196000	1.109473000	-0.280015000
7	1.277278000	1.216474000	-0.331539000
6	0.722555000	2.369583000	-0.051245000
6	-0.714545000	2.371915000	0.057154000
7	-1.273206000	1.218006000	0.325895000
7	-2.632216000	1.115724000	0.284032000
6	-3.050894000	-0.111661000	0.033390000
16	-2.041718000	-1.462475000	-0.473498000
7	-4.411955000	-0.324282000	0.096693000
1	-4.944918000	0.317002000	0.674683000

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1	-4.717958000	-1.288005000	0.114263000
1	-1.306923000	3.273310000	-0.105278000
1	1.318353000	3.266628000	0.122736000
7	4.396078000	-0.367055000	-0.208849000
1	4.987786000	0.452332000	-0.299311000
1	4.792896000	-1.124013000	0.332025000

Cu(I)PTS$^-$ in DMSO

29	-0.155095945	-0.654455375	0.010860255
16	-2.287876007	-1.465992153	-0.458422021
6	-3.156809361	-0.017415309	0.034689486
7	-2.620139105	1.165619679	0.266647487
7	-1.254764460	1.135418972	0.315297985
6	-0.592418455	2.216048594	-0.003816315
6	0.850346336	2.101726549	-0.103492398
7	1.274540052	0.880421712	-0.337502904
7	2.616839293	0.631034953	-0.317110971
6	2.906824256	-0.627197666	-0.048366808
16	1.773644015	-1.862716082	0.495107575
7	4.238661313	-0.985356449	-0.126688989
1	4.823515343	-0.406283725	-0.720059727
1	4.433372844	-1.977328725	-0.158417097
6	1.745824151	3.294802293	0.085159382
1	1.173068071	4.223902517	0.011796565
1	2.226070857	3.270368666	1.071681515
1	2.548740505	3.304701897	-0.658301435
1	-1.103669925	3.157708110	-0.212783871
7	-4.523497085	-0.121485961	0.204335238
1	-5.027077548	0.756461687	0.277538352
1	-4.992607466	-0.838349983	-0.333255562

Cu(I)ATS$^-$ in DMSO

29	-0.002635226	-0.854697120	-0.001925416
16	2.035085464	-1.871969413	0.462822497
6	3.037439441	-0.528618875	-0.075145842
7	2.627307054	0.698087277	-0.325223589
7	1.262386692	0.821796149	-0.347852353
6	0.737417884	1.982797476	-0.034935078
6	-0.727058837	1.987311950	0.031306974
7	-1.258968678	0.826076637	0.330919360
7	-2.624025023	0.709835430	0.316529110
6	-3.042034573	-0.514072613	0.065098656
16	-2.044512508	-1.870809012	-0.452155358
7	-4.405585365	-0.730710398	0.145810197
1	-4.924120172	-0.082718971	0.729769728
1	-4.698293553	-1.697093144	0.206048996
6	-1.546413960	3.215483624	-0.267855227
1	-0.928579376	4.043898553	-0.619287303
1	-2.290298163	2.982912467	-1.036950961
1	-2.107377299	3.546044882	0.615229259
6	1.564421137	3.200788933	0.284239476
1	2.284098179	2.960435621	1.074076349
1	2.153514861	3.521960745	-0.583619555
1	0.948191590	4.037493238	0.618278754
7	4.383786417	-0.783757814	-0.271931589
1	4.972378756	0.039206233	-0.352309972
1	4.780805146	-1.532902314	0.279915832

Cu(I)GTSM$^-$ in DMSO

29	-0.000290695	-0.527087753	0.000220593
16	-2.014312876	-1.542645821	-0.569646328
6	-3.055672486	-0.193745255	-0.088754390
7	-2.648117034	1.037621820	0.172774051
7	-1.291141353	1.134761470	0.278704291
6	-0.719183050	2.286557795	0.025970672
6	0.720138638	2.286122319	-0.024830390
7	1.291330941	1.134331931	-0.279329998
7	2.648302220	1.036512194	-0.174035922
6	3.055805611	-0.194668875	0.087331179
16	2.014516180	-1.542340756	0.571124685
7	4.396832451	-0.451629718	0.002376365
6	5.388245948	0.564081823	-0.309427086
1	5.405179196	1.368683309	0.438151341
1	6.370481897	0.087118756	-0.341662777
1	5.183363614	1.018458751	-1.283844565
1	4.714332837	-1.313893472	0.423886812
1	1.307018602	3.185060605	0.170064764
1	-1.305439103	3.186124494	-0.167863948
7	-4.396679767	-0.448721036	-0.010080696
6	-5.388924406	0.562650181	0.311851999
1	-5.389881529	1.384545292	-0.416419944
1	-6.373289076	0.089153071	0.315780734
1	-5.199622104	0.993344978	1.300521438
1	-4.713120476	-1.319390253	-0.414373280

Cu(I)PTSM$^-$ in DMSO

29	-0.115681433	-0.720298058	0.005012348
16	-2.183842004	-1.641180996	-0.531978449
6	-3.150980791	-0.233349016	-0.068357963
7	-2.680498512	0.978244699	0.167903622
7	-1.317212937	1.011647605	0.262362182
6	-0.696496099	2.121645553	-0.044788369
6	0.750881265	2.077179149	-0.095193634
7	1.244030290	0.877614231	-0.313749971
7	2.596376707	0.705315442	-0.228611973
6	2.946907485	-0.534877038	0.055679797
16	1.852740006	-1.826191544	0.576257763
7	4.278598579	-0.855883509	-0.044485964
6	5.305503370	0.146079544	-0.288595878
1	5.326222564	0.918922606	0.492123815
1	6.274910792	-0.356919129	-0.322390395
1	5.132729427	0.645773031	-1.245892804
1	4.559527366	-1.695295804	0.444993985
6	1.585127827	3.308513815	0.127366039
1	0.977010260	4.212051921	0.022714460
1	2.020600919	3.308213491	1.135002589
1	2.421459777	3.347401511	-0.577052608
1	-1.247334806	3.034791104	-0.278666282
7	-4.505725307	-0.424184432	0.036976541
6	-5.439469617	0.666796053	0.268409274
1	-5.415967692	1.414371145	-0.536783357
1	-6.446339932	0.248439862	0.338323653
1	-5.203811849	1.178825170	1.205660336
1	-4.864435694	-1.251177094	-0.421737157

Cu(I)ATSM$^-$ in DMSO

29	-0.000024035	-0.897837184	-0.002459839
16	2.025903466	-1.916323039	0.520603538
6	3.047056840	-0.557255785	0.027658470
7	2.632959545	0.667202974	-0.230633240
7	1.269772239	0.778750035	-0.306492875
6	0.732002136	1.941073982	-0.013854137
6	-0.731550144	1.941467944	0.011447037
7	-1.269611904	0.779318652	0.304354003
7	-2.632822288	0.667916078	0.230512939
6	-3.047459624	-0.556658445	-0.026860690
16	-2.026937828	-1.915264637	-0.521693037
7	-4.395408541	-0.805563616	0.086576157
6	-5.365289656	0.261139962	0.287326229
1	-5.345785400	1.000370277	-0.525716768
1	-6.360954537	-0.185606132	0.343721547
1	-5.161723080	0.791073457	1.221788140
1	-4.719692555	-1.634231422	-0.394505590
6	-1.552576986	3.159001594	-0.325340997
1	-0.928408203	4.006222302	-0.615623713
1	-2.233943024	2.927131914	-1.151302222
1	-2.185831859	3.457670006	0.518803769
6	1.553695535	3.157895280	0.323730463
1	2.226857680	2.928611266	1.157217408
1	2.195521004	3.449636286	-0.516258656
1	0.929575140	4.008525800	0.603911444
7	4.395330836	-0.805729359	-0.082403927
6	5.365930702	0.261374239	-0.277409718
1	5.342970706	0.999252289	0.536766524
1	6.361824451	-0.185284157	-0.330384009
1	5.166336696	0.792808994	-1.211875295
1	4.718107818	-1.634995692	0.398653408

Cu(I)AGTS$^-$ in DMSO

6	0.819158375	2.104085833	-0.087309145
6	-0.636373420	2.244099581	-0.015983093
7	-1.296145412	1.162973454	0.267261658
7	-2.653967845	1.178405400	0.234224815
6	-3.175952681	-0.025727468	0.040108030
7	-4.544280479	-0.109179867	0.116303537
7	1.253714244	0.896510388	-0.344276309
7	2.619987543	0.695567102	-0.307928146
6	2.950129232	-0.548441275	-0.044890901
7	4.289826318	-0.881061159	-0.180991471
16	1.853476457	-1.846963433	0.434669527
29	-0.135550523	-0.707892588	-0.012478228
16	-2.298592942	-1.484112229	-0.396700601
1	-5.032864271	0.627413359	0.612521179
1	-4.957012084	-1.030722592	0.141713536
1	-1.127637469	3.197130042	-0.225644841
1	4.928346690	-0.092817676	-0.215814144
1	4.610282831	-1.654183548	0.387230927
7	1.628807244	3.187398891	0.177803386
1	2.585629424	3.110577309	-0.145789017
1	1.218723436	4.110299407	0.111816521

Cu(I)CGTS$^-$ in DMSO

6	1.018051369	1.769020218	-0.144370598
6	-0.391648209	2.109365365	-0.064349871
7	-1.204843376	1.128889438	0.200684054
7	-2.541353153	1.367912700	0.180265149
6	-3.264333166	0.263350539	0.029935554
7	-4.614905998	0.401675337	0.214165288
7	1.353916814	0.544735653	-0.335467116
7	2.626403584	0.094371884	-0.303627422
6	2.698940037	-1.210843712	-0.062092080
7	3.933178098	-1.781796853	-0.233217229
16	1.388933690	-2.260629560	0.453472605
29	-0.407943644	-0.883107795	0.021050086
16	-2.657272097	-1.331064358	-0.381678396
1	-4.981136369	1.345237588	0.276445771
1	-5.223580847	-0.294337195	-0.193674705
1	-0.733856463	3.129082299	-0.238861772
1	4.718744116	-1.151641822	-0.352415506
1	4.122901583	-2.652411752	0.243712898
17	2.175757425	3.107378125	0.111251551

Cu(I)FGTS$^-$ in DMSO

6	0.811565163	2.100468006	-0.092285051

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6	-0.625421679	2.251993631	0.002685576
7	-1.284840842	1.152456659	0.227017893
7	-2.635481583	1.171768581	0.209381518
6	-3.166045361	-0.039391155	0.040226403
7	-4.516860313	-0.126957063	0.230601511
7	1.331930055	0.951625823	-0.314061004
7	2.676954511	0.736788364	-0.275608328
6	2.973908616	-0.533571685	-0.040276530
7	4.296225103	-0.878268622	-0.184601060
16	1.856907542	-1.808496507	0.428884253
29	-0.145242075	-0.730840941	-0.002783196
16	-2.306223572	-1.499606608	-0.408294440
1	-5.034815729	0.738827644	0.331041675
1	-5.009899190	-0.913438853	-0.168413922
1	-1.100957066	3.222719340	-0.139791973
1	4.959310120	-0.114389915	-0.260672182
1	4.620553050	-1.699238842	0.308028612
9	1.547484052	3.240074321	0.107763041

Cu(I)NGTS$^-$ in DMSO

6	0.996151670	1.874874020	-0.138454202
6	-0.415963298	2.174196124	-0.045889647
7	-1.191991979	1.171047894	0.270922838
7	-2.544584537	1.346332286	0.217233482
6	-3.205948538	0.221597817	0.016795062
7	-4.578596565	0.294502692	0.068614501
7	1.305320975	0.594970973	-0.349688758
7	2.580869718	0.195028165	-0.272254263
6	2.703976820	-1.118808247	-0.061125500
7	3.937649371	-1.654093529	-0.290551752
16	1.424643105	-2.167994003	0.504326180
29	-0.310843288	-0.703922282	0.030980926
16	-2.492831320	-1.331164140	-0.415125821
1	-4.977631845	1.065955875	0.592446115
1	-5.082789435	-0.580600567	0.116613975
1	-0.808777161	3.168107126	-0.258842052
1	4.699105587	-1.017373361	-0.495826283
1	4.178903480	-2.532055498	0.147576102
6	1.972737462	2.899892563	0.040870637
7	2.747180349	3.764458558	0.169895586

Cu(I)HYGTS$^-$ in DMSO

6	0.800472729	2.085199661	-0.092774101
6	-0.639851273	2.264293594	0.000117641
7	-1.305485380	1.176655051	0.255050077
7	-2.657938447	1.191557640	0.227001048
6	-3.179726710	-0.020590005	0.055795601
7	-4.533891904	-0.120298831	0.241786408
7	1.243524190	0.894328575	-0.368401766
7	2.612372524	0.726690519	-0.306734490
6	2.962766848	-0.514655936	-0.034686097
7	4.306085480	-0.814889571	-0.135093612
16	1.875544768	-1.825685211	0.415533524
29	-0.140973551	-0.721591785	-0.027401861
16	-2.309630045	-1.479267654	-0.385604429
1	-5.055118386	0.745947671	0.321039893
1	-5.015701322	-0.899594074	-0.184655030
1	-1.107847409	3.234313640	-0.173411401
1	4.937011099	-0.020942996	-0.175677240
1	4.635294298	-1.597933139	0.413935471
8	1.600840401	3.155848385	0.140003050
1	2.518601130	2.833041807	0.028560433

Cu(I)THGTS$^-$ in DMSO

6	0.994161122	1.773670977	-0.152482433
6	-0.416911506	2.119871402	-0.074963756
7	-1.226525996	1.146301148	0.229495055
7	-2.566923411	1.372250287	0.203693607
6	-3.275602821	0.264907447	0.034675845
7	-4.639053404	0.399957752	0.123096599
7	1.269266880	0.520800624	-0.385813721
7	2.562844798	0.090440431	-0.347939985
6	2.677102125	-1.194537438	-0.061985428
7	3.929694265	-1.747221830	-0.215745532
16	1.383175945	-2.257408866	0.475843297
29	-0.395159381	-0.838753898	0.004419050
16	-2.641137334	-1.319072815	-0.386067587
1	-4.997319758	1.208445083	0.619541265
1	-5.189935260	-0.445924698	0.173192486
1	-0.770747870	3.129898195	-0.285865916
1	4.697218234	-1.091385181	-0.318209345
1	4.134812675	-2.573518420	0.330175238
16	2.205805194	3.052533714	0.143777706
1	3.242477643	2.218342355	-0.102808357

Cu(I)TFGTS$^-$ in DMSO

6	-1.155791450	-1.179090002	-0.177413291
6	0.085960713	-1.905160347	-0.070291356
7	1.139446821	-1.197016315	0.253769638
7	2.364328293	-1.796549616	0.203487416
6	3.353692132	-0.943316905	0.013724625
7	4.630836879	-1.453699550	0.079098260
7	-1.045918621	0.122872934	-0.385005187
7	-2.130048401	0.919531790	-0.329047345
6	-1.833355556	2.190527190	-0.074173299
7	-2.834934817	3.101081535	-0.288571019
16	-0.293548047	2.777853616	0.520224504
29	0.904013444	0.861164375	0.020042065
16	3.179589812	0.755237679	-0.418145326
1	4.755011687	-2.307624654	0.612178050
1	5.386882628	-0.784594189	0.134528780
1	0.157599444	-2.971094203	-0.277316942
1	-3.760465990	2.730056178	-0.471865742
1	-2.795083627	3.978560297	0.211426528
6	-2.470709319	-1.879574987	0.022296606
9	-2.297759885	-3.228202304	0.140484416
9	-3.123547411	-1.481427211	1.149682088
9	-3.343331868	-1.703968945	-1.006213113

Cu(I)DAGTS$^-$ in DMSO

6	0.743147286	1.983393007	-0.024850128
7	1.278038274	0.841766182	-0.345382112
29	-0.004965655	-0.934682981	-0.001230199
16	2.102547202	-1.863526358	0.356646614
6	3.086879000	-0.461640161	-0.058477912
7	4.459991973	-0.641346919	-0.062728859
6	-0.735663646	1.983867901	0.025676300
7	-1.428099140	3.113793929	-0.323120434
7	-1.269452574	0.840515471	0.353046079
7	-2.649016561	0.761430799	0.309558139
6	-3.087491269	-0.454759242	0.073433109
16	-2.114369562	-1.859504294	-0.362935263
7	2.655869063	0.757270593	-0.306301804
7	-4.453473298	-0.657956221	0.208067308
1	4.991837667	0.040094157	-0.594994378
1	4.777842758	-1.597675816	-0.151805376
1	-5.015077867	0.188014159	0.211918824
1	-4.840362045	-1.413614395	-0.342649237
1	-2.410258190	3.153078270	-0.085156971
1	-0.939533742	3.985704444	-0.465727954
7	1.437113474	3.159459173	0.205282419
1	2.440167981	3.017561368	0.272920291
1	1.070518521	3.771434596	0.928155574

Cu(I)MAGTS$^-$ in DMSO

29	-0.027457135	-0.900233087	0.022714384
16	-2.121121959	-1.849764173	-0.397902186
6	-3.077350206	-0.438308284	0.055535589
7	-2.620846160	0.767461441	0.300465715
7	-1.239265457	0.832700391	0.345855571
6	-0.695744493	1.979707165	0.023465209
6	0.778978656	1.995668807	-0.028197372
7	1.297477494	0.834790117	-0.319012358
7	2.655706706	0.699540917	-0.313609519
6	3.050976901	-0.540549723	-0.080623005
16	2.038201566	-1.886211547	0.423993014
7	4.408277973	-0.773778971	-0.172704460
1	4.936680205	-0.120223790	-0.741946805
1	4.692846393	-1.742134156	-0.240902749
6	1.584778268	3.230717383	0.273019299
1	0.968582351	4.038986391	0.676084272
1	2.363523710	2.992446886	1.004381827
1	2.100504938	3.600015574	-0.622448533
7	-4.447127690	-0.626673670	0.195047812
1	-4.994517563	0.228984576	0.202001364
1	-4.843219046	-1.362806299	-0.375976366
7	-1.423577739	3.094279734	-0.332351252
1	-2.394682328	3.088133806	-0.041697163
1	-0.971086158	3.997316138	-0.320705098

Optimised Cartesian coordinates for the protonated Cu(II)AH$^+$ complexes *in vacuo*.

Cu(II)GTSH$^+$-X *in vacuo*

6	-0.667342105	2.429798837	0.000003886
6	0.776923844	2.444384338	-0.000198911
7	1.348380588	1.260929952	-0.000296890
7	2.649827721	1.094713208	-0.000471526
6	2.997018083	-0.218280193	-0.000419761
7	4.309889227	-0.452038945	0.000168835
7	-1.234381161	1.260772659	0.000528844
7	-2.576477833	1.037163749	0.000365542
6	-2.997780220	-0.259638795	0.000023980
7	-4.319346778	-0.470404223	0.000061300
16	-1.899197953	-1.577519915	-0.000586464
29	0.043361293	-0.284940568	0.000100864
16	1.898325928	-1.583021426	0.000409324
1	4.954615752	0.328713840	-0.000012942
1	4.674167389	-1.394019136	0.000552859
1	1.353177199	3.364330913	-0.000284797
1	-1.233263496	3.361855443	-0.000258414
1	-5.003212882	0.274944790	0.000909882
1	-4.664146550	-1.420800299	-0.000199708
1	-3.223022304	1.821372464	0.000254401

Cu(II)GTSH$^+$-Y *in vacuo*

6	-0.664673274	2.414787772	-0.013466622
6	0.780312013	2.435980543	-0.012290360
7	1.362336987	1.262561950	-0.006132063
7	2.669457826	1.090858591	-0.002221825
6	3.012996278	-0.211042190	0.015466323
7	4.322259470	-0.469736693	0.020112590

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7	-1.238798696	1.244472794	-0.002361387
7	-2.592006301	1.141468537	-0.001999247
6	-3.060425683	-0.063950878	0.005031365
7	-4.375254942	-0.322641787	0.123134477
16	-1.981743138	-1.565245442	-0.147141037
29	0.072078081	-0.263713882	-0.006643066
16	1.895672802	-1.575883275	0.029553612
1	4.981864316	0.298212634	0.008978376
1	4.669817536	-1.417599862	0.030976532
1	1.355636873	3.357213743	-0.011911664
1	-1.254026570	3.329085803	-0.019445274
1	-5.014242788	0.461477376	0.183424223
1	-4.754604924	-1.223369300	-0.129844385
1	-2.142799847	-1.982793576	1.129697873

Cu(II)GTSH^{+}-Z *in vacuo*

6	-0.643095304	2.424602809	-0.000362083
6	0.794907499	2.447461948	-0.000888713
7	1.368996942	1.261801904	-0.000737379
7	2.666340671	1.093436198	-0.000882518
6	3.012408568	-0.223799152	-0.000292271
7	4.326254832	-0.451538326	-0.000499769
7	-1.211725845	1.248869505	0.001544677
7	-2.568102613	1.106281600	0.001094264
6	-2.881614225	-0.152239138	-0.000132031
7	-4.373511530	-0.325300805	0.000206088
16	-1.939534039	-1.585586089	-0.001924757
29	0.054720891	-0.286735958	0.000884059
16	1.916368750	-1.585907258	0.000869306
1	4.967484094	0.332097080	-0.001020802
1	4.693563968	-1.392317868	0.000227051
1	1.374034588	3.365660000	-0.001420403
1	-1.233645192	3.339405818	-0.001662507
1	-4.814190610	0.604595024	-0.000854867
1	-4.678495429	-0.851137673	-0.828171534
1	-4.678419048	-0.850075439	0.829125614

Cu(II)PTSH^{+}-*syn in vacuo*

29	0.186233498	-0.484363893	0.001135400
16	2.175537631	-1.566342754	0.001116350
6	3.111501189	-0.083217967	-0.000359738
7	2.617227656	1.178531847	-0.000794059
7	1.301925620	1.194657270	-0.000243216
6	0.602852068	2.302702855	-0.000449226
6	-0.845485160	2.149972469	-0.000118546
7	-1.250684784	0.909053350	0.000491419
7	-2.560309388	0.524314454	0.000575270
6	-2.828201767	-0.811440616	-0.000345039
16	-1.586766096	-1.994623973	-0.001629178
7	-4.117700580	-1.173565535	-0.000333948
1	-4.882823677	-0.512310713	-0.000001079
1	-4.350747267	-2.157191611	-0.000827449
6	-1.760394745	3.338414812	-0.000526341
1	-1.190270306	4.268264473	-0.002813205
1	-2.403518138	3.340065432	-0.889310842
1	-2.400680796	3.342712837	0.890314749
1	1.079587423	3.278432433	-0.001110278
7	4.443332034	-0.169023898	-0.001115925
1	4.996943397	0.678430904	-0.001514128
1	4.909770309	-1.064472681	-0.000197309
1	-3.297540367	1.221727708	0.001474753

Cu(II)PTSH^{+}-*anti in vacuo*

29	0.109312179	-0.495333625	0.001078249
16	2.197897280	-1.545066336	0.001181476
6	3.126678013	-0.104772522	-0.000246010
7	2.550602680	1.132878541	-0.000696053
7	1.192376844	1.193399606	-0.000224722
6	0.489973068	2.283592212	-0.000466822
6	-0.958843759	2.139668912	-0.000118284
7	-1.356578502	0.883897883	0.000253717
7	-2.637882434	0.558817552	0.000356882
6	-2.826158878	-0.779194412	-0.000283259
16	-1.569960946	-2.007053696	-0.001575246
7	-4.101043038	-1.178868960	-0.000044891
1	-4.839981513	-0.487480022	0.000498770
1	-4.342045016	-2.159227208	-0.000377908
6	-1.896036410	3.306016104	-0.000379583
1	-1.351423066	4.252630973	-0.002483914
1	-2.549477998	3.271693424	-0.878848955
1	-2.546903270	3.274235427	0.880125627
1	0.943281942	3.275686606	-0.001093058
7	4.464352028	-0.149391319	-0.001243933
1	5.050758506	0.674720175	-0.000780544
1	4.924095862	-1.049766750	-0.000179663
1	3.098194773	1.989108131	-0.001672519

Cu(II)ATSH^{+} *in vacuo*

29	-0.038387085	-0.690148872	-0.000150227
16	-1.860089474	-2.014459643	0.000019216
6	-2.974852309	-0.655148126	0.000394348
7	-2.646782825	0.650169954	0.000190987
7	-1.334273871	0.846037605	0.000177382
6	-0.799224252	2.046486821	0.000081870
6	0.676333129	2.044164658	-0.000408651
7	1.219282919	0.859038808	0.000033110
7	2.564634243	0.631635924	0.000602595
6	2.990899947	-0.664273020	0.000267209
16	1.903456285	-1.986373126	-0.000725893
7	4.315536241	-0.865758422	0.000795596
1	4.994247270	-0.116096264	0.001211304
1	4.665879611	-1.813917754	0.000909194
6	1.484413030	3.308988704	-0.000752722
1	0.849615283	4.193288962	-0.012984917
1	2.115962380	3.367674715	0.894856143
1	2.134034026	3.356199221	-0.883921955
6	-1.604018963	3.311801408	0.000168744
1	-1.395515570	3.917342443	-0.889413862
1	-2.665327191	3.066527737	0.007279846
1	-1.384708617	3.924282899	0.882256290
7	-4.286232638	-0.921281768	0.000437107
1	-4.950063563	-0.158022584	-0.000289207
1	-4.625738685	-1.871682372	-0.000663061
1	3.214519526	1.411027269	0.002261429

Cu(II)GTSMH^{+} *in vacuo*

29	0.043171683	-0.355526223	0.002318274
16	1.893762695	-1.649816280	0.000136832
6	3.004330794	-0.281714097	-0.000778223
7	2.651971577	1.030354809	-0.000953147
7	1.349211386	1.191441777	-0.004413921
6	0.775549317	2.374481066	-0.001693614
6	-0.668100162	2.358656566	-0.001861764
7	-1.234502867	1.189280183	0.010933317
7	-2.577772100	0.968563612	-0.004330262
6	-3.001880000	-0.328808492	-0.002352536
16	-1.893151310	-1.648077800	-0.002762214
7	-4.319791620	-0.548357506	-0.002052626
6	-5.371885110	0.468750755	0.003459136
1	-5.315190012	1.093332252	0.902078402
1	-5.325255916	1.093624945	-0.895584662
1	-6.334587328	-0.041030989	0.008713231
1	-4.594443360	-1.522361399	-0.005024932
1	-1.234471090	3.290469882	-0.013442807
1	1.350468245	3.295260714	0.000468571
7	4.311239190	-0.538294978	0.000055473
6	5.370048495	0.476111694	0.000460876
1	5.295929971	1.105899365	0.889979188
1	6.328886713	-0.041783664	-0.000407543
1	5.295195896	1.107264594	-0.887984756
1	4.581902589	-1.513258751	0.001920329
1	-3.221065740	1.753368536	-0.004013944

Cu(II)PTSMH^{+}-*syn in vacuo*

29	-0.148760890	-0.539106170	-0.002284789
16	-2.060745311	-1.741347460	0.001749868
6	-3.100138377	-0.317344336	0.000749293
7	-2.682028411	0.972608791	-0.001105023
7	-1.369522156	1.066807194	0.002297786
6	-0.738968400	2.215925592	-0.003455850
6	0.714804071	2.153420858	-0.002985536
7	1.198403839	0.940608284	-0.016661100
7	2.531016776	0.642657273	0.001770132
6	2.884997943	-0.674160591	0.001749753
16	1.710860373	-1.934396332	0.007612108
7	4.190738826	-0.963499518	-0.000042249
6	5.293573862	-0.003132758	-0.007813725
1	5.278920029	0.626777600	0.889009830
1	6.228923225	-0.561632774	-0.010403405
1	5.270634140	0.621201384	-0.908351618
1	4.413627510	-1.950459449	0.004963103
6	1.553625710	3.397000506	0.014472227
1	0.926810760	4.289596195	0.019370369
1	2.188123265	3.430184820	0.908941947
1	2.200669687	3.448966993	-0.870002858
1	-1.274717438	3.160638323	-0.008135274
7	-4.419090477	-0.509846048	0.000227836
6	-5.424981115	0.556093432	-0.002159839
1	-5.319573187	1.180067027	-0.892750462
1	-6.409032089	0.087667681	-0.000378330
1	-5.318731266	1.184754813	0.884980436
1	-4.736966832	-1.470140865	-0.000322779
1	3.219426206	1.386189657	-0.009203286

Cu(II)ATSMH^{+} *in vacuo*

29	0.042058952	-0.711810584	-0.003611156
16	1.868223923	-2.022472016	0.002260351
6	2.985489343	-0.654011623	0.001826248
7	2.645108836	0.649401991	0.000546145
7	1.330440966	0.832847021	0.003909635
6	0.786206100	2.029840121	-0.004187698
6	-0.688001646	2.017981545	-0.000096071
7	-1.224344971	0.829820498	-0.019978439
7	-2.569406988	0.597972916	0.003049968
6	-2.991219332	-0.700555143	0.001486556
16	-1.886445877	-2.018169720	0.008945123
7	-4.311065567	-0.918765880	-0.002130576
6	-5.361881596	0.098020947	-0.010847420
1	-5.305267409	0.721182800	-0.910773239
1	-6.325183054	-0.410799886	-0.015641179
1	-5.316331924	0.725720093	0.886551167
1	-4.585620208	-1.892623286	0.003253189
6	-1.504292737	3.277578468	0.027774397
1	-0.875605151	4.165738159	0.060925710
1	-2.136397565	3.353039588	-0.866255272
1	-2.154774255	3.299357885	0.911331225

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6	1.582632550	3.300845910	-0.013938134
1	1.400072215	3.893702973	0.890099263
1	2.644457890	3.061661349	-0.057010520
1	1.331672182	3.923861742	-0.879869494
7	4.292599223	-0.931998856	0.001415384
6	5.360651047	0.068505402	-0.000303405
1	5.294687569	0.702621718	0.887397819
1	6.315016342	-0.458106976	0.001331328
1	5.295546635	0.698838053	-0.890810636
1	4.549040502	-1.909967795	0.000328919
1	-3.220295025	1.374370552	-0.013393996

Optimised Cartesian coordinates for the reduced, protonated Cu(I)AH complexes *in vacuo*.

Cu(I)GTSH-X *in vacuo*

6	-0.701600855	2.371811097	0.006344926
6	0.724248255	2.418645046	-0.099077082
7	1.306396258	1.242754936	-0.232983093
7	2.626301358	1.140220880	-0.197865090
6	3.042774341	-0.133662235	-0.054004079
7	4.369561434	-0.324973300	-0.270185096
7	-1.224000937	1.225903027	0.375819954
7	-2.582007047	1.033225061	0.250872944
6	-3.042085130	-0.208729015	-0.023577076
7	-4.402987237	-0.358300975	0.026186927
16	-2.013762097	-1.488077154	-0.458001110
29	0.048544099	-0.459854149	0.055702930
16	2.073914215	-1.490939304	0.437680959
1	4.946725508	0.477455741	-0.476521111
1	4.801343435	-1.190593384	0.008934926
1	1.288340333	3.348151096	-0.058519079
1	-1.316562869	3.241700187	-0.237866093
1	-4.936264261	0.190981086	0.688730979
1	-4.737429301	-1.300081035	-0.121727084
1	-3.209232067	1.832223148	0.265658946

Cu(I)GTSH-Y *in vacuo*

6	0.704852687	2.352902657	0.002199214
6	-0.728492331	2.400194096	0.128366564
7	-1.317926046	1.238663888	0.269589475
7	-2.644915178	1.131206896	0.242932998
6	-3.052922601	-0.132362838	0.053642070
7	-4.384825927	-0.339123842	0.222153542
7	1.250027239	1.200983494	-0.290520956
7	2.618674818	1.126934176	-0.302718522
6	3.103466077	-0.036345783	-0.040633852
7	4.419174187	-0.354956768	-0.298132026
16	2.076460468	-1.364070911	0.647508976
29	-0.086076137	-0.440058558	-0.110276795
16	-2.074174972	-1.497865287	-0.441505625
1	-4.974407849	0.459836328	0.406723113
1	-4.800526809	-1.196135860	-0.104403436
1	-1.282790799	3.335881524	0.070984582
1	1.321196711	3.240717087	0.142155579
1	4.959239200	0.421746809	-0.663323544
1	4.902164592	-0.894654802	0.408543655
1	2.591878330	-2.346997420	-0.123282105

Cu(I)GTSH-Z *in vacuo*

6	0.687301581	2.379962993	-0.006045414
6	-0.736648725	2.408364629	0.116945579
7	-1.311748843	1.230604719	0.267433292
7	-2.637547576	1.120695885	0.214957987
6	-3.044825226	-0.145803800	0.050342993
7	-4.376050274	-0.357758235	0.252056452
7	1.218101208	1.229093484	-0.357732776
7	2.577627116	1.089462929	-0.307759980
6	2.904356485	-0.118208160	0.031765762
7	4.400074508	-0.313048823	-0.148106716
16	2.013427504	-1.479695219	0.537623722
29	-0.057737496	-0.423294691	-0.071817704
16	-2.058663147	-1.496090749	-0.445576359
1	-4.962632427	0.448867551	0.411961247
1	-4.796420933	-1.199420791	-0.107445952
1	-1.313783498	3.329933127	0.070708450
1	1.309840673	3.249476266	0.204981668
1	4.804692291	0.582674460	-0.448992342
1	4.828608282	-0.624282492	0.728049949
1	4.573555638	-1.038370289	-0.853298748

Cu(I)PTSH-*syn in vacuo*

29	-0.208173558	-0.657388017	-0.045640720
16	-2.328375540	-1.492307386	-0.394527310
6	-3.150584220	-0.025004802	0.045877858
7	-2.606014073	1.202550774	0.148450772
7	-1.280259881	1.172147969	0.175333636
6	-0.587590861	2.275423477	-0.004100824
6	0.840553630	2.112229590	-0.090857329
7	1.229938919	0.895578491	-0.411304501
7	2.562075983	0.555094737	-0.283078650
6	2.884759967	-0.727309784	-0.001456962
16	1.735633785	-1.866503494	0.511680164
7	4.216013881	-1.039765173	-0.103419907
1	4.782726197	-0.571517906	-0.799794732
1	4.440029433	-2.012989917	0.049415653
6	1.777662709	3.253075354	0.202297886
1	1.218150549	4.176351697	0.366070889
1	2.358844831	3.048424552	1.110882166
1	2.485719791	3.435569193	-0.617082369
1	-1.064370227	3.250700497	-0.090203686
7	-4.490584075	-0.071319960	0.267151906
1	-4.981242062	0.796266575	0.429565656
1	-5.009933814	-0.892389728	0.002643077
1	3.283973876	1.244320602	-0.464858014

Cu(I)PTSH-*anti in vacuo*

29	-0.208173090	-0.657388001	-0.045640933
16	-2.328375107	-1.492307444	-0.394526960
6	-3.150584427	-0.025005474	0.045878074
7	-2.606014602	1.202550716	0.148451082
7	-1.280260495	1.172147948	0.175334084
6	-0.587591639	2.275423154	-0.004100930
6	0.840553503	2.112229394	-0.090857937
7	1.229938745	0.895578370	-0.411304961
7	2.562075909	0.555095578	-0.283077951
6	2.884760163	-0.727309461	-0.001456930
16	1.735634272	-1.866503753	0.511679110
7	4.216014315	-1.039764253	-0.103418938
1	4.782726281	-0.571517112	-0.799793991
1	4.440029507	-2.012989287	0.049416074
6	1.777661370	3.253075651	0.202298086
1	1.218149168	4.176352623	0.366067099
1	2.358840455	3.048426737	1.110884156
1	2.485721395	3.435567786	-0.617079977
1	-1.064370846	3.250700148	-0.090203936
7	-4.490584525	-0.071320715	0.267152091
1	-4.981242713	0.796266262	0.429566104
1	-5.009933417	-0.892390871	0.002644071
1	3.283973845	1.244321761	-0.464856965

Cu(I)ATSH *in vacuo*

29	-0.043343074	-0.849606091	-0.040677893
16	-2.045493470	-1.926475596	-0.391001920
6	-3.023452476	-0.558315680	0.058003066
7	-2.617641399	0.716204697	0.168980536
7	-1.288409491	0.837797680	0.200212385
6	-0.748313427	2.028445935	0.010284428
6	0.702327077	2.000142165	-0.046654047
7	1.207289286	0.839605165	-0.417293759
7	2.572273790	0.635609648	-0.280466000
6	3.025968677	-0.611418199	-0.022265517
16	2.004125700	-1.856757441	0.511117411
7	4.377665614	-0.795977602	-0.163688053
1	4.880192719	-0.268237125	-0.866769860
1	4.695449670	-1.745781579	-0.030914271
6	1.556060909	3.181105375	0.334914356
1	0.953580112	4.005810052	0.715718966
1	2.259038477	2.888610499	1.124948476
1	2.144551821	3.563003341	-0.511089956
6	-1.576909424	3.271486002	-0.161997748
1	-2.256416484	3.146141523	-1.012605252
1	-2.210808157	3.444016069	0.715461637
1	-0.964925085	4.158465099	-0.339146143
7	-4.351136815	-0.760390077	0.284684474
1	-4.937327076	0.048612380	0.432371110
1	-4.774237839	-1.624970090	-0.011381424
1	3.215360389	1.376014774	-0.539496544

Cu(I)GTSMH *in vacuo*

29	-0.041962104	-0.522412823	-0.069867462
16	-2.031189015	-1.573324169	-0.566799836
6	-3.045635581	-0.227260757	-0.109603773
7	-2.641689764	1.047373276	0.060709553
7	-1.324986821	1.153254802	0.165126968
6	-0.741417099	2.334218901	0.056773936
6	0.684776638	2.290511120	0.019838256
7	1.224335736	1.146513978	-0.344420956
7	2.587236070	0.968571889	-0.134090679
6	3.036945089	-0.270084261	0.166114700
16	1.973318017	-1.532803738	0.609713332
7	4.377637933	-0.476227546	0.116451914
6	5.377175771	0.492044684	-0.301692200
1	5.416468928	1.358974764	0.371871612
1	6.354784912	0.009226978	-0.278130490
1	5.198922727	0.839924841	-1.327458550
1	4.671471506	-1.400077475	0.396301751
1	1.289139931	3.153320252	0.308392394
1	-1.308746657	3.260074448	-0.011674160
7	-4.376602571	-0.447011213	0.019491995
6	-5.336280213	0.561006144	0.442756055
1	-5.345326656	1.410614685	-0.248135333
1	-6.327414859	0.102741816	0.461888099
1	-5.098610639	0.939503399	1.442316593
1	-4.698581087	-1.375037919	-0.207242562
1	3.215827235	1.718811282	-0.396592275

Cu(I)PTSMH-*syn in vacuo*

29	-0.156690259	-0.707207806	-0.056475407
16	-2.193331972	-1.686281450	-0.510140135
6	-3.139801387	-0.273612825	-0.112482416
7	-2.676346476	0.985756809	0.008058150
7	-1.353672514	1.035101698	0.101105117

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6	-0.721070784	2.179526177	-0.059097745
6	0.713716273	2.100059376	-0.078425132
7	1.188346969	0.907837099	-0.389104658
7	2.547214760	0.667308090	-0.175495493
6	2.926316875	-0.591794830	0.151999237
16	1.807280373	-1.766182933	0.683810842
7	4.249107473	-0.885429216	0.061173631
6	5.297992916	0.013374916	-0.389106592
1	5.382320909	0.898907424	0.255104763
1	6.248396948	-0.520103610	-0.349093574
1	5.140248543	0.336032354	-1.426802286
1	4.493816326	-1.816290643	0.364219639
6	1.570938331	3.288703536	0.262488382
1	0.952176808	4.166351359	0.460529090
1	2.164694482	3.080117417	1.161420859
1	2.268839750	3.546940245	-0.544903598
1	-1.252988901	3.122291833	-0.178010945
7	-4.480301780	-0.423416849	0.023618156
6	-5.391471495	0.648634679	0.392596298
1	-5.367404831	1.458543052	-0.344363654
1	-6.401961699	0.237041241	0.441556489
1	-5.130464892	1.071156306	1.368296957
1	-4.846715585	-1.342556485	-0.169048496
1	3.209721894	1.310576330	-0.593166256

Cu(I)ATSMH *in vacuo*

29	-0.035697018	-0.873067037	-0.049143859
16	-2.006297126	-1.967406197	-0.507513894
6	-3.025546256	-0.607243133	-0.098078863
7	-2.631073277	0.669513981	0.040019148
7	-1.305265179	0.794725044	0.136256155
6	-0.761825179	1.990068154	-0.020687857
6	0.687867928	1.967568210	-0.010401856
7	1.215546012	0.813571136	-0.377401884
7	2.589778126	0.635044174	-0.165663868
6	3.029251206	-0.612464901	0.135733155
16	1.973202175	-1.838124035	0.674729198
7	4.361312317	-0.847345869	0.011626145
6	5.362067337	0.106210241	-0.435520889
1	5.411913347	0.984429309	0.222051162
1	6.336567456	-0.383088760	-0.414908887
1	5.178027333	0.437906259	-1.466148969
1	4.652730376	-1.770538930	0.296319167
6	1.514495952	3.149659329	0.422312177
1	0.895647872	3.934911365	0.857585211
1	2.241450017	2.829871332	1.178155237
1	2.077425978	3.592119387	-0.411329887
6	-1.586250291	3.231226218	-0.222668872
1	-2.214625335	3.116824188	-1.113565942
1	-2.271453351	3.387020208	0.618686194
1	-0.968857279	4.123303313	-0.349501882
7	-4.357458351	-0.834191200	0.033999147
6	-5.329852455	0.186594843	0.387226174
1	-5.368492502	0.979375905	-0.368702884
1	-6.311814502	-0.286192230	0.461087180
1	-5.083370461	0.648570887	1.348552248
1	-4.672874339	-1.766731283	-0.182667869
1	3.211331149	1.290712249	-0.625205901

Optimised Cartesian coordinates for the protonated Cu(II)AH$^+$ complexes in solution phase using the water solvation model.

Cu(II)GTSH$^+$-X in water

6	-0.694585685	2.421782728	-0.000511071
6	0.760081016	2.433535384	0.000244156
7	1.334717867	1.261943819	0.000152940
7	2.655331778	1.103531804	0.001118983
6	3.015090433	-0.194164498	0.000261312
7	4.323814362	-0.448065778	0.002286191
7	-1.246613728	1.250744729	-0.000512807
7	-2.577420843	1.024746620	-0.000853276
6	-3.000650948	-0.264109786	0.000358919
7	-4.309220225	-0.473843237	-0.000124006
16	-1.878378379	-1.590548158	0.002163463
29	0.035818019	-0.281428587	-0.000430858
16	1.903472928	-1.571591854	-0.002734641
1	4.992161910	0.325448972	0.004806811
1	4.680802388	-1.402893100	0.000755938
1	1.327688149	3.362684341	0.001074123
1	-1.272239724	3.348396571	-0.000868530
1	-4.978821341	0.302696861	-0.001846178
1	-4.679574215	-1.426070947	0.002396749
1	-3.254125819	1.829737809	-0.001281238

Cu(II)GTSH$^+$-Y in water

6	-0.677839887	2.420030601	-0.013550003
6	0.771622118	2.429893285	-0.013366827
7	1.349964008	1.260021259	-0.004351157
7	2.670011954	1.092401175	-0.001685905
6	3.021724030	-0.203745010	0.015516529
7	4.326501567	-0.475255775	0.019182997
7	-1.253818297	1.253609616	-0.007909936
7	-2.603363625	1.141252977	0.004069997
6	-3.058119487	-0.080306790	0.009832548
7	-4.356749460	-0.358099952	0.105592729
16	-1.947893532	-1.554579134	-0.156169815
29	0.058434400	-0.257086090	-0.005018219
16	1.892522372	-1.571102984	0.031921719
1	5.005038962	0.289385381	0.008921860
1	4.671685045	-1.434448542	0.030531143
1	1.344622080	3.356093438	-0.016420444
1	-1.256980136	3.343594139	-0.013774714
1	-5.026434815	0.410268881	0.208063703
1	-4.722376818	-1.304666531	-0.004249091
1	-2.096356945	-1.986553893	1.125540863

Cu(II)GTSH$^+$-Z in water

6	-0.655951115	2.419094000	-0.000523699
6	0.790953709	2.438680580	-0.000655617
7	1.363727146	1.260605154	-0.000657928
7	2.674253231	1.095650365	-0.000357058
6	3.029022792	-0.212139389	-0.000178520
7	4.336305882	-0.458073816	0.000809325
7	-1.219484372	1.246959355	0.000903858
7	-2.577125784	1.104157578	0.000906288
6	-2.905133471	-0.150760987	0.000473840
7	-4.367295878	-0.355940915	0.000991281
16	-1.914203388	-1.569578287	-0.000822445
29	0.045788078	-0.282822183	0.000153245
16	1.916478887	-1.581184308	-0.000471864
1	5.000772444	0.319572459	0.001907647
1	4.698880644	-1.411453224	0.000240460
1	1.362362420	3.365161028	-0.000648049
1	-1.243260242	3.339030779	-0.001569410
1	-4.858120926	0.558894192	0.001168727
1	-4.675769267	-0.890022226	-0.834932090
1	-4.675140324	-0.889887344	0.837231170

Cu(II)PTSH$^+$-*syn* in water

29	-0.173922914	-0.474653771	0.000663967
16	-2.173494440	-1.557903848	0.003154625
6	-3.125394986	-0.065804992	-0.000550695
7	-2.623006060	1.181737889	-0.000236738
7	-1.290021942	1.190418068	0.000908041
6	-0.592495614	2.288684791	0.001333338
6	0.867162462	2.146809826	0.001031909
7	1.272789079	0.910311627	-0.000866394
7	2.570689131	0.513132753	-0.002708767
6	2.827044239	-0.820221894	-0.002179077
16	1.554905990	-2.001101098	0.003036755
7	4.099402107	-1.194148619	-0.005449237
1	4.862600597	-0.509492397	-0.007046456
1	4.346030551	-2.185458588	-0.005426484
6	1.754607493	3.349941901	0.002522133
1	1.161816233	4.266777553	0.006376758
1	2.404195215	3.349479357	0.887957085
1	2.400357199	3.354620076	-0.885712701
1	-1.062381114	3.271454569	0.001422419
7	-4.455012500	-0.173456624	-0.006805301
1	-5.033872423	0.668738758	-0.011136837
1	-4.914802774	-1.082862861	-0.008154358
1	3.367815836	1.183358616	-0.003433418

Cu(II)PTSH$^+$-*anti* in water

29	0.113273062	-0.488884719	-0.001797179
16	2.168708096	-1.565634747	-0.002889389
6	3.127189945	-0.117392992	0.002150652
7	2.557258031	1.115220679	0.000908128
7	1.208348054	1.181587983	-0.000956050
6	0.521347105	2.276489092	-0.001282687
6	-0.936919009	2.133635138	-0.001691601
7	-1.345855164	0.890165220	-0.001460506
7	-2.645890346	0.572507510	0.000295215
6	-2.850495031	-0.752894329	0.002241099
16	-1.583295186	-1.993170191	-0.002550304
7	-4.121017754	-1.166499611	0.008006550
1	-4.878109681	-0.480614555	0.009873458
1	-4.357924736	-2.157220367	0.009492927
6	-1.850962050	3.317373481	-0.000908015
1	-1.281134982	4.249764748	-0.005963629
1	-2.505990397	3.294615366	-0.880118652
1	-2.498123045	3.299559485	0.884294178
1	0.989852614	3.263209644	-0.000660481
7	4.451083946	-0.175951524	0.007087115
1	5.027728738	0.671758820	0.011793976
1	4.927447977	-1.079696063	0.006888569
1	3.136275056	1.994684596	0.003333099

Cu(II)ATSH$^+$ in water

29	-0.031788193	-0.678116033	0.000137593
16	-1.870515705	-1.999140136	0.001717301
6	-2.995277624	-0.627799388	0.000258623
7	-2.651894142	0.663580036	-0.000427015
7	-1.320842977	0.850374012	-0.000262129
6	-0.780438777	2.039611067	-0.000065106
6	0.706044764	2.041775820	-0.000848831
7	1.240152839	0.857236451	-0.000096116
7	2.574710545	0.609532560	0.000019801
6	2.984792364	-0.685723834	-0.000395360
16	1.859772370	-2.004365693	-0.001586356
7	4.292805750	-0.904878480	0.001244409
1	4.970037845	-0.135233539	0.003570190
1	4.654782298	-1.860079160	0.000127242

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6	1.502226226	3.308068264	-0.001131459
1	0.865823797	4.191441991	-0.016569398
1	2.137587224	3.357555602	0.893678433
1	2.160914532	3.343376795	-0.879437225
6	-1.564339935	3.315370238	0.000954010
1	-1.331632700	3.916404423	-0.887005217
1	-2.631794953	3.097169598	0.006971291
1	-1.322205063	3.920862001	0.883265214
7	-4.304563238	-0.906116464	-0.000834406
1	-4.985369269	-0.145194901	-0.001481384
1	-4.643397611	-1.866119248	0.001439190
1	3.288381341	1.365364828	-0.000786713

Cu(II)GTSMH$^+$ in water

29	0.035781008	-0.349582129	0.002226139
16	1.896004152	-1.645586116	-0.002533731
6	3.022896930	-0.271560629	0.000218295
7	2.663379443	1.028064117	-0.000753201
7	1.344431185	1.186454996	-0.006386107
6	0.771572550	2.359957982	-0.004239100
6	-0.680206537	2.350862144	-0.004974968
7	-1.243305116	1.184120483	0.013151155
7	-2.584647769	0.978967142	-0.001620945
6	-3.015738422	-0.311746202	-0.000895230
16	-1.881804559	-1.639641693	-0.002713282
7	-4.317099309	-0.556944693	-0.002454156
6	-5.388429466	0.440932037	0.004744433
1	-5.329994010	1.068760663	0.902432549
1	-5.339768179	1.072143381	-0.891178663
1	-6.338143875	-0.095990094	0.008748248
1	-4.598868456	-1.547862377	-0.007449829
1	-1.251949232	3.281442102	-0.021963025
1	1.340269486	3.288323443	-0.001114705
7	4.326947806	-0.542106499	0.001246248
6	5.382330646	0.471623204	0.003937936
1	5.311246848	1.102236378	0.896415666
1	6.341620464	-0.049255992	0.001741277
1	5.310379103	1.107869454	-0.884418466
1	4.615253456	-1.527848052	0.002585192
1	-3.207386222	1.811407792	-0.001433204

Cu(II)PTSMH$^+$-*syn* in water

29	0.137156069	-0.527530009	0.060215704
16	2.058008083	-1.738856866	0.037726933
6	3.113215003	-0.310701612	-0.005849798
7	2.688405812	0.968781887	-0.015749873
7	1.361658677	1.060776701	0.013311786
6	0.732946072	2.201167145	-0.020436774
6	-0.730786801	2.143086778	0.010712627
7	-1.210765891	0.937955529	0.125189155
7	-2.561925512	0.665652226	0.152691565
6	-2.893562433	-0.663710711	0.029788295
16	-1.689881829	-1.911721743	-0.116019638
7	-4.178358110	-0.976339623	-0.016276927
6	-5.293351396	-0.029783647	-0.106085658
1	-5.091500015	0.715060886	-0.883980090
1	-6.187691480	-0.597584934	-0.367764207
1	-5.461502600	0.478525517	0.851752799
1	-4.410966056	-1.979838327	-0.052459471
6	-1.546286534	3.389328368	-0.108727296
1	-0.931453253	4.218314654	-0.466061437
1	-2.383030745	3.231182286	-0.799173298
1	-1.967041938	3.670935549	0.866686250
1	1.260550521	3.152080792	-0.081953663
7	4.429303714	-0.516611943	-0.034656353
6	5.433238026	0.546895003	-0.075489644
1	5.359896705	1.184338943	0.812023145
1	6.416406491	0.073169814	-0.102413315
1	5.303055343	1.168153946	-0.967817171
1	4.765435780	-1.487018423	-0.025941753
1	-3.130407226	1.241115984	0.808494120

Cu(II)ATSMH in water

29	-0.033473188	-0.700789394	0.000402768
16	-1.868442680	-2.018751985	0.001010708
6	-3.001007450	-0.644157496	0.000309979
7	-2.652936209	0.647882649	-0.000059275
7	-1.323229286	0.830067549	0.000426358
6	-0.781073684	2.020083702	-0.000008331
6	0.702845480	2.018131863	0.000413823
7	1.234749834	0.832052546	-0.000516390
7	2.574996788	0.596636601	-0.000472671
6	2.998309424	-0.699105081	-0.000410666
16	1.863425677	-2.016861621	0.000024343
7	4.301861619	-0.935500851	-0.000887435
6	5.360292054	0.076435528	-0.000919437
1	5.301652705	0.704182955	0.897703117
1	6.317591583	-0.446966348	-0.001039049
1	5.301465800	0.704294616	-0.899445915
1	4.593570736	-1.923975630	-0.001208615
6	1.508485885	3.279240349	0.002167474
1	0.877691787	4.167012052	0.000844877
1	2.151770233	3.320079397	0.892261143
1	2.155693521	3.320409905	-0.885033185
6	-1.565478947	3.295586031	-0.001290545
1	-1.329686735	3.898616379	-0.887109369
1	-2.631987643	3.073195778	-0.001231558
1	-1.329953731	3.900387450	0.883376786
7	-4.306253303	-0.933197517	-0.000827246
6	-5.368610085	0.070593370	-0.001112431
1	-5.301921475	0.707311985	-0.889917904
1	-6.324693512	-0.456672753	-0.002846896
1	-5.304182596	0.705507951	0.889162778
1	-4.582581809	-1.920993986	-0.001089035
1	3.229663373	1.373883841	-0.001210833

Optimised Cartesian coordinates for the reduced, protonated Cu(I)AH complexes in solution phase using the water solvation model.

Cu(I)GTSH-X in water

6	-0.701648323	2.378772455	0.025368737
6	0.742376550	2.401434323	-0.042875877
7	1.313127387	1.244670039	-0.258181857
7	2.656894381	1.145320106	-0.217266419
6	3.084610655	-0.109275658	-0.046412206
7	4.412065109	-0.321780573	-0.219023846
7	-1.237346120	1.224609967	0.303587442
7	-2.591868742	1.054581681	0.213462634
6	-3.074234474	-0.190579068	0.001425600
7	-4.402861637	-0.345770399	0.080755890
16	-2.036560111	-1.511885579	-0.397476451
29	0.037827610	-0.480463511	0.014958285
16	2.082843128	-1.480489265	0.421825787
1	5.019339712	0.471874673	-0.418802374
1	4.839385125	-1.179853737	0.116564872
1	1.308219718	3.323155488	0.098198310
1	-1.296041704	3.275900177	-0.165350998
1	-5.012798674	0.406383813	0.407914220
1	-4.818470373	-1.254652703	-0.113951235
1	-3.233861817	1.875103518	0.303673136

Cu(I)GTSH-Y in water

6	0.710613501	2.362256622	0.003028650
6	-0.732259824	2.388427130	0.116536295
7	-1.310272809	1.230674317	0.286267234
7	-2.654674122	1.126019324	0.257738702
6	-3.074295451	-0.123603887	0.039122720
7	-4.400976988	-0.349631530	0.186148296
7	1.260924343	1.215901376	-0.284658237
7	2.629981458	1.137470492	-0.315380421
6	3.108859658	-0.043549886	-0.066347733
7	4.393579466	-0.380370030	-0.335231143
16	2.057859274	-1.326855340	0.673393517
29	-0.068197875	-0.451190045	-0.081889902
16	-2.066486874	-1.486034640	-0.464072496
1	-5.017662697	0.434284064	0.395882782
1	-4.816873893	-1.205469213	-0.169563349
1	-1.292190558	3.320776090	0.026258623
1	1.308817990	3.263354697	0.148429838
1	4.989734066	0.358833230	-0.713714172
1	4.864668002	-1.073730140	0.245637762
1	2.571850353	-2.368925239	-0.025491305

Cu(I)GTSH-Z in water

6	0.702985305	2.362584135	-0.012192837
6	-0.728314215	2.389152653	0.108499446
7	-1.300083200	1.219394025	0.289954155
7	-2.645572967	1.121032432	0.248166462
6	-3.073233546	-0.127106017	0.049665357
7	-4.399961106	-0.353858518	0.236764879
7	1.223200101	1.217406653	-0.387554330
7	2.586497561	1.079093351	-0.345985741
6	2.939497850	-0.118851733	-0.001111268
7	4.406202598	-0.335409123	-0.123692189
16	1.986192550	-1.447533498	0.542895799
29	-0.046436854	-0.429677557	-0.057154184
16	-2.066899425	-1.479880224	-0.460964397
1	-5.006791978	0.442869570	0.426300479
1	-4.828156624	-1.182219514	-0.166545894
1	-1.301871570	3.313746807	0.037162166
1	1.324301584	3.227756821	0.224527414
1	4.867785761	0.524623063	-0.471574711
1	4.830713201	-0.587590210	0.786473324
1	4.614405063	-1.108203720	-0.782510702

Cu(I)PTSH-*syn* in water

29	-0.196282274	-0.674892761	-0.016976235
16	-2.330350134	-1.486009647	-0.397033562
6	-3.182083205	-0.007652081	0.031704020
7	-2.628519172	1.202491321	0.168014085
7	-1.281375731	1.166668461	0.192596973
6	-0.598977945	2.257107531	-0.027199034
6	0.848759831	2.111164245	-0.085385061
7	1.242330705	0.898358376	-0.378134969
7	2.583225473	0.576789194	-0.272111428
6	2.911075935	-0.712839273	-0.027617823
16	1.744073167	-1.859051212	0.521675977
7	4.193377621	-1.060534888	-0.211312647
1	4.890785911	-0.385584545	-0.531585265
1	4.514416080	-1.981412862	0.080017172

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6	1.758518066	3.267738364	0.211466148
1	1.181424632	4.172142304	0.418049997
1	2.376388443	3.040118131	1.090398990
1	2.439673264	3.474832325	-0.623725935
1	-1.074279447	3.229821385	-0.164868625
7	-4.523333632	-0.077293194	0.218973625
1	-5.043531124	0.785174559	0.375040748
1	-5.038331910	-0.889811703	-0.107425542
1	3.302378651	1.209116689	-0.681858332

Cu(I)PTSH-*anti* in water

29	-0.196282413	-0.674893989	-0.016974603
16	-2.330350504	-1.486010150	-0.397031509
6	-3.182083575	-0.007651777	0.031703473
7	-2.628519537	1.202491495	0.168012733
7	-1.281375964	1.166668487	0.192597317
6	-0.598978538	2.257107372	-0.027200035
6	0.848759439	2.111164769	-0.085385312
7	1.242330890	0.898358815	-0.378133503
7	2.583225854	0.576790485	-0.272109577
6	2.911076819	-0.712838495	-0.027618219
16	1.744074458	-1.859052371	0.521671722
7	4.193379161	-1.060532666	-0.211311394
1	4.890787419	-0.385581571	-0.531582508
1	4.514417488	-1.981411645	0.080015364
6	1.758516626	3.267739761	0.211465746
1	1.181422679	4.172149517	0.418022749
1	2.376367075	3.040131365	1.090415718
1	2.439690547	3.474817275	-0.623715050
1	-1.074280452	3.229820586	-0.164872759
7	-4.523334251	-0.077292525	0.218971878
1	-5.043531738	0.785175591	0.375036796
1	-5.038332154	-0.889811147	-0.107427480
1	3.302378105	1.209117551	-0.681858850

Cu(I)ATSH in water

29	-0.036049617	-0.873856691	-0.016306007
16	-2.067247201	-1.910038837	-0.388291011
6	-3.065112172	-0.527912349	0.053761495
7	-2.642890091	0.727638038	0.202668791
7	-1.292107170	0.840964129	0.222768970
6	-0.749103975	2.012019501	-0.000048401
6	0.720948830	1.986794680	-0.019949771
7	1.223322008	0.838334298	-0.394555807
7	2.597998308	0.648795395	-0.296129116
6	3.054325259	-0.601095655	-0.057085552
16	2.013512151	-1.852680421	0.513158796
7	4.361136741	-0.822897817	-0.264241636
1	4.985599858	-0.082903996	-0.590654072
1	4.772693266	-1.710624127	0.016077788
6	1.534609148	3.177218944	0.401885432
1	0.935132184	3.890814851	0.970267314
1	2.374102413	2.847964548	1.024971706
1	1.957628795	3.702454304	-0.465581822
6	-1.535785949	3.271495014	-0.234393767
1	-2.234729604	3.122202190	-1.065547975
1	-2.140282440	3.528529745	0.644522982
1	-0.889142119	4.117797690	-0.474698761
7	-4.394033035	-0.745037412	0.250432993
1	-5.000491244	0.063772735	0.381128111
1	-4.819033439	-1.592550829	-0.114386147
1	3.230447820	1.332197850	-0.762735465

Cu(I)GTSMH in water

29	-0.038845989	-0.556987154	-0.025536185
16	-2.050990082	-1.568295127	-0.530153957
6	-3.085478051	-0.199820755	-0.095232017
7	-2.664520608	1.055691318	0.092287505
7	-1.323193339	1.154787796	0.190031244
6	-0.746612228	2.314263786	-0.003296542
6	0.696946863	2.297833091	-0.009074919
7	1.252414823	1.148922300	-0.275737694
7	2.606429927	0.992636785	-0.122294285
6	3.076690597	-0.254194468	0.144837675
16	2.003456503	-1.565008783	0.510099731
7	4.399852767	-0.446511215	0.120808447
6	5.401374835	0.524003656	-0.314139414
1	5.493408866	1.356816145	0.395953970
1	6.361968176	0.008850520	-0.372473680
1	5.149056254	0.922598245	-1.304271791
1	4.730413152	-1.372608265	0.413953277
1	1.277810584	3.194912488	0.221479505
1	-1.310915522	3.233103533	-0.167099033
7	-4.413698812	-0.429455289	0.006824481
6	-5.391531450	0.583727639	0.382775207
1	-5.429736301	1.397963502	-0.352130433
1	-6.371708424	0.103706190	0.434600543
1	-5.152798865	1.016122232	1.360789684
1	-4.758478020	-1.347150976	-0.280570399
1	3.188714246	1.843796906	-0.007472486

Cu(I)PTSMH-*syn* in water

29	-0.152745788	-0.724691939	-0.071966308
16	-2.218325130	-1.675969077	-0.510651201
6	-3.173455737	-0.249507922	-0.095639693
7	-2.687728936	0.993288096	0.049611467
7	-1.344674898	1.025244190	0.100138110
6	-0.709903885	2.155906351	-0.071726679
6	0.739603159	2.071486456	-0.100448155
7	1.196425076	0.894719647	-0.461583228
7	2.577814376	0.668493500	-0.306410611
6	2.952598162	-0.569822274	0.103981172
16	1.796826577	-1.707286421	0.716162279
7	4.252102267	-0.892889747	0.066474226
6	5.348434144	0.004947153	-0.284339200
1	5.357181867	0.889435246	0.366085361
1	6.283727573	-0.541892547	-0.152010180
1	5.281683313	0.330301488	-1.330874743
1	4.496745375	-1.819781842	0.430421422
6	1.586189637	3.243080514	0.306772216
1	0.961198989	4.098791717	0.572316773
1	2.199452198	2.970771262	1.175260103
1	2.272378676	3.546566884	-0.493429300
1	-1.227423692	3.110036532	-0.182353625
7	-4.507694926	-0.405934206	0.040127574
6	-5.427601442	0.661821379	0.412458741
1	-5.442698498	1.459107731	-0.341146111
1	-6.427873657	0.230215413	0.495547337
1	-5.147669318	1.104659344	1.374756402
1	-4.901615364	-1.318963815	-0.195022829
1	3.169632553	1.200986447	-0.965558097

Cu(II)ATSMH

29	-0.036713730	-0.900740832	-0.052654618
16	-2.041379101	-1.957376589	-0.502849600
6	-3.066871729	-0.577868964	-0.081225042
7	-2.649129519	0.680792812	0.085874673
7	-1.302251932	0.790117853	0.140714054
6	-0.751014702	1.968666792	-0.029123896
6	0.715901124	1.936234789	-0.018121540
7	1.225925904	0.801196602	-0.432447141
7	2.619095080	0.634736929	-0.291029032
6	3.058683092	-0.592942674	0.085704037
16	1.967939232	-1.789372020	0.700765988
7	4.370490981	-0.855588847	0.010912100
6	5.414615855	0.094055019	-0.361978769
1	5.408679757	0.968436044	0.302087586
1	6.376513935	-0.413622269	-0.270665438
1	5.297533378	0.431556218	-1.400161228
1	4.667209655	-1.775352850	0.353364549
6	1.519537985	3.106751950	0.474320623
1	0.916885072	3.769594244	1.098588511
1	2.375033427	2.748032350	1.055928120
1	1.917986402	3.696628698	-0.362589221
6	-1.532942801	3.236573099	-0.229308708
1	-2.202332690	3.127445024	-1.090827518
1	-2.170851369	3.446119056	0.638320660
1	-0.881304856	4.095242266	-0.403597187
7	-4.395062014	-0.807333714	0.043071772
6	-5.372428416	0.220040227	0.378169780
1	-5.405244232	1.008017052	-0.384967263
1	-6.353563571	-0.256566228	0.444054227
1	-5.136502169	0.688209951	1.340165053
1	-4.740777909	-1.730551921	-0.223435463
1	3.174109403	1.209761518	-0.946237561

Optimised Cartesian coordinates for the Cu(II)AH$^+$ complexes in solution phase using the DMSO solvation model.

Cu(II)GTSH$^+$-X in DMSO

6	-0.685611000	2.426109000	-0.000343000
6	0.766547000	2.436399000	-0.000047000
7	1.339051000	1.261329000	0.000055000
7	2.653560000	1.099159000	0.000311000
6	3.005429000	-0.202737000	0.000454000
7	4.316529000	-0.452363000	-0.000487000
7	-1.244005000	1.257019000	-0.000268000
7	-2.579193000	1.030370000	-0.000601000
6	-2.997496000	-0.263242000	-0.000243000
7	-4.308322000	-0.481020000	0.000166000
16	-1.879628000	-1.583244000	-0.000363000
29	0.037055000	-0.280615000	0.000055000
16	1.898868000	-1.575746000	0.000903000
1	4.976298000	0.319092000	-0.000808000
1	4.673942000	-1.399465000	-0.001526000
1	1.336663000	3.361525000	0.000150000
1	-1.257034000	3.354770000	-0.000705000
1	-4.987737000	0.276156000	-0.000501000
1	-4.663998000	-1.430742000	0.000548000
1	-3.237134000	1.819701000	-0.000533000

Cu(II)GTSH$^+$-Y in DMSO

6	-0.673722000	2.418414000	-0.012143000
6	0.774186000	2.432103000	-0.011828000
7	1.353833000	1.261253000	-0.005142000
7	2.668987000	1.091772000	-0.002585000
6	3.015457000	-0.205884000	0.014439000
7	4.322994000	-0.473185000	0.018091000
7	-1.248667000	1.250759000	-0.005620000
7	-2.598668000	1.140943000	0.001152000
6	-3.057112000	-0.074142000	0.007355000
7	-4.361636000	-0.345781000	0.106847000
16	-1.957273000	-1.558969000	-0.150342000

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29	0.063327000	-0.259307000	-0.005259000
16	1.892446000	-1.572698000	0.030738000
1	4.992905000	0.289411000	0.008172000
1	4.668707000	-1.424539000	0.030140000
1	1.347679000	3.355533000	-0.012883000
1	-1.256601000	3.337388000	-0.013555000
1	-5.020135000	0.423449000	0.196574000
1	-4.732200000	-1.275785000	-0.046536000
1	-2.110382000	-1.982172000	1.128101000

Cu(II)GTSH$^+$-Z in DMSO

6	0.653422000	2.420485000	0.000021000
6	-0.791376000	2.441187000	0.000210000
7	-1.364705000	1.261569000	0.000257000
7	-2.671548000	1.095500000	0.000511000
6	-3.020943000	-0.214252000	0.000102000
7	-4.332020000	-0.454660000	0.001724000
7	1.217504000	1.247391000	-0.001086000
7	2.573701000	1.103624000	-0.000567000
6	2.894273000	-0.152828000	0.000002000
7	4.367434000	-0.345245000	0.001086000
16	1.918954000	-1.575618000	0.000860000
29	-0.047428000	-0.284642000	-0.000784000
16	-1.916486000	-1.582042000	-0.001074000
1	-4.986689000	0.321582000	0.002633000
1	-4.695569000	-1.399768000	0.002637000
1	-1.364352000	3.364407000	0.000484000
1	1.242435000	3.336979000	0.000969000
1	4.838056000	0.573857000	0.001201000
1	4.678064000	-0.872194000	0.832572000
1	4.679132000	-0.872496000	-0.829811000

Cu(II)PTSH$^+$-*syn* in DMSO

29	0.178530313	-0.478734516	0.000817682
16	2.174881552	-1.560107226	0.000520271
6	3.119116848	-0.070153800	-0.001472794
7	2.621954611	1.181297089	-0.001342250
7	1.294844541	1.192569941	-0.000584356
6	0.596634198	2.293145988	-0.000542562
6	-0.859637984	2.146131124	-0.000110138
7	-1.262427947	0.907946327	0.000409845
7	-2.565153001	0.517877720	0.000501747
6	-2.828662527	-0.815820891	-0.000011160
16	-1.566891003	-1.997211290	-0.000590957
7	-4.105948580	-1.185216425	0.000053506
1	-4.869401535	-0.512902411	-0.000349807
1	-4.348476541	-2.169802768	0.000380554
6	-1.761819994	3.339772093	-0.000123446
1	-1.182123400	4.263886764	-0.001635845
1	-2.408127727	3.339184828	-0.886902969
1	-2.405869823	3.340721548	0.888313025
1	1.067570210	3.273087060	-0.001020676
7	4.450916456	-0.170666952	-0.000398313
1	5.019377321	0.670120529	-0.000071264
1	4.912353334	-1.071345487	0.000568688
1	-3.323615613	1.202346220	0.001215831

Cu(II)ATSH$^+$ in DMSO

29	-0.033472197	-0.681783009	0.000062717
16	-1.865773023	-2.004703530	-0.000043041
6	-2.985349333	-0.636212645	-0.000166524
7	-2.649622252	0.658468994	-0.000965098
7	-1.324545805	0.848492628	-0.000490049
6	-0.787001358	2.041135669	-0.000279749
6	0.696702240	2.042841133	-0.000283825
7	1.232609243	0.858299970	0.000823966
7	2.571543086	0.618628165	0.001441998
6	2.986729279	-0.677613462	0.000455487
16	1.872168416	-1.995073996	-0.000260244
7	4.298491553	-0.896179870	0.000187408
1	4.979730351	-0.140827727	0.001000720
1	4.652183440	-1.846496302	-0.000539693
6	1.497646382	3.307849470	-0.001005823
1	0.861934180	4.191282015	-0.013232117
1	2.132826179	3.360823256	0.892635488
1	2.150574615	3.349079241	-0.882271620
6	-1.579723530	3.311947186	0.000040485
1	-1.356313844	3.914807969	-0.887989116
1	-2.643902439	3.079942439	0.005768427
1	-1.347412379	3.920004844	0.882121297
7	-4.296719699	-0.911531794	0.000353974
1	-4.970089376	-0.153199321	-0.000323895
1	-4.634556001	-1.864765771	0.000645814
1	3.247077734	1.384566199	0.003192758

Cu(II)GTSMH$^+$ in DMSO

29	-0.037521269	-0.350607082	-0.000643352
16	-1.892779150	-1.648331339	-0.004296993
6	-3.011627254	-0.274679267	-0.000633782
7	-2.657553243	1.027688999	0.000507667
7	-1.343934483	1.188195423	0.000289142
6	-0.772289363	2.364949383	-0.000187170
6	0.677916781	2.356198326	-0.000389938
7	1.241013387	1.188735125	-0.001405203
7	2.581305882	0.972375625	-0.000192004
6	3.006509554	-0.322371877	0.001188010
16	1.880186372	-1.643727746	0.004148663
7	4.313878678	-0.556187334	0.000340940
6	5.374035263	0.453975977	-0.001684597
1	5.316122740	1.080829820	-0.898467820
1	5.320907402	1.079771894	0.896157237
1	6.330008833	-0.068559635	-0.004624476
1	4.594483530	-1.533625551	0.002372861
1	1.246431977	3.286946334	0.000608676
1	-1.343967440	3.288959578	-0.000302005
7	-4.318256212	-0.540929672	0.000764453
6	-5.371669841	0.475120284	0.003381949
1	-5.298761757	1.107402223	-0.885529606
1	-6.331845607	-0.041366844	0.005611487
1	-5.294453037	1.107075228	0.892128811
1	-4.598396949	-1.516688339	-0.000659480
1	3.216642914	1.771501885	0.001552988

Cu(II)PTSMH$^+$-*syn* in DMSO

29	0.142498907	-0.536507730	-0.001938419
16	2.062866502	-1.738781829	-0.001529909
6	3.107501942	-0.307360818	0.000694673
7	2.685539502	0.972724374	0.000900886
7	1.362488459	1.063483660	-0.000559897
6	0.733944375	2.207132603	0.000262020
6	-0.726587362	2.149440472	-0.000390424
7	-1.204891494	0.938054094	-0.000204708
7	-2.533109339	0.637891211	-0.000078143
6	-2.890153098	-0.676480610	0.000369017
16	-1.699165387	-1.935998167	-0.000248200
7	-4.186867635	-0.968296071	0.001919219
6	-5.284209245	0.000726071	0.003410844
1	-5.257509120	0.627033060	-0.895796280
1	-6.220608316	-0.556387538	0.004657382
1	-5.255027131	0.626778701	0.902705509
1	-4.427196435	-1.956430055	0.000256412
6	-1.560475803	3.392571769	-0.000973241
1	-0.929900123	4.282877268	0.002210238
1	-2.199736102	3.433383607	-0.892250681
1	-2.205012348	3.430750680	0.886599581
1	1.265648991	3.155308207	0.002130513
7	4.426960427	-0.506769892	0.000077064
6	5.426742481	0.561208464	0.003909429
1	5.318399102	1.187709564	0.893438266
1	6.412393105	0.095037201	0.005102197
1	5.321976022	1.190648424	-0.883962797
1	4.755503689	-1.466989530	0.001287898
1	-3.222036839	1.382445268	0.000210835

Cu(II)ATSMH$^+$ in DMSO

29	0.036900931	-0.708677172	-0.000368181
16	1.871723087	-2.021535865	0.000195792
6	2.994072519	-0.645668418	0.000452074
7	2.648369102	0.647986215	0.000615118
7	1.324008938	0.829339978	0.000308264
6	0.781608598	2.021313663	0.000370039
6	-0.699315386	2.014834274	-0.000079557
7	-1.229463850	0.827208209	-0.000419849
7	-2.570430919	0.592841818	-0.000751581
6	-2.994850287	-0.702987808	-0.000673722
16	-1.872676839	-2.020807838	-0.001029559
7	-4.305637743	-0.924605324	-0.000265020
6	-5.351370019	0.100085479	0.001705105
1	-5.292374429	0.724729976	-0.897118154
1	-6.315090956	-0.408286938	0.002365459
1	-5.290269203	0.723199182	0.901445379
1	-4.597638966	-1.898611810	-0.000340959
6	-1.513195107	3.272462911	-0.000190066
1	-0.885652539	4.162025001	0.001120981
1	-2.154197103	3.317279668	-0.890367085
1	-2.156215830	3.316161469	0.888582154
6	1.571297621	3.294279725	0.000817823
1	1.343610140	3.899055596	0.886484654
1	2.635555387	3.062641925	0.000229267
1	1.342805013	3.900197015	-0.883843372
7	4.302588999	-0.925800799	-0.000010355
6	5.358914499	0.084445027	0.000666030
1	5.287478100	0.717973134	0.889328702
1	6.318134572	-0.434299115	0.000700459
1	5.288001345	0.718717935	-0.887516852
1	4.574289454	-1.902809324	-0.000816535
1	-3.222318160	1.369783755	-0.000978984

Optimised Cartesian coordinates for the reduced, protonated Cu(I)AH complexes in solution phase using the DMSO solvation model.

Cu(I)GTSH-X in DMSO

6	-0.700770841	2.380026447	0.021409366
6	0.739278958	2.407900176	-0.051868738
7	1.311736265	1.245903514	-0.248241712
7	2.648308490	1.143260601	-0.211068715
6	3.069537343	-0.116437733	-0.049330673
7	4.398802768	-0.325022155	-0.242722298
7	-1.233629544	1.227830301	0.321169593
7	-2.589855614	1.051810851	0.215240541
6	-3.065939382	-0.196212685	-0.006246323
7	-4.398373288	-0.357754732	0.079914380

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16	-2.030522596	-1.505448402	-0.407070509
29	0.041338124	-0.476250910	0.025538771
16	2.080494243	-1.483949418	0.424355085
1	4.995714726	0.474281707	-0.418030491
1	4.827017618	-1.172037339	0.101581428
1	1.305537424	3.330801835	0.065781820
1	-1.297773849	3.270359548	-0.186311464
1	-5.016430926	0.381105183	0.398558074
1	-4.805318266	-1.252914658	-0.155145763
1	-3.218658703	1.856189237	0.292564519

Cu(I)GTSH-Y in DMSO

6	0.709161613	2.355686823	0.005889524
6	-0.730617433	2.391106535	0.123516509
7	-1.314257477	1.233023398	0.280436848
7	-2.653088406	1.128146643	0.253925311
6	-3.067374183	-0.125815966	0.045976685
7	-4.397765962	-0.344822469	0.198318043
7	1.256590286	1.207961675	-0.286848562
7	2.625410313	1.132723455	-0.310937491
6	3.108717484	-0.039233533	-0.054153843
7	4.404928614	-0.368587460	-0.320327272
16	2.069441249	-1.342889729	0.664404198
29	-0.076026427	-0.444943998	-0.100046415
16	-2.071554169	-1.492023429	-0.448184149
1	-5.005133441	0.441382848	0.395028211
1	-4.812282339	-1.198156285	-0.146950921
1	-1.286371482	3.325613278	0.048255738
1	1.315029917	3.249713131	0.152483860
1	4.977770368	0.383209530	-0.693300096
1	4.887652986	-0.991067960	0.317959189
1	2.589860620	-2.358287909	-0.060992084

Cu(I)GTSH-Z in DMSO

6	0.699673031	2.366893299	-0.013900856
6	-0.729496259	2.391884997	0.109279006
7	-1.300650261	1.220681688	0.290895843
7	-2.642320659	1.118923602	0.246253053
6	-3.061860764	-0.131066318	0.049666091
7	-4.393320122	-0.356937855	0.241929951
7	1.221862605	1.219634028	-0.382416883
7	2.583062475	1.079819367	-0.338073141
6	2.925233766	-0.121341806	0.006374197
7	4.402952222	-0.329870968	-0.128784515
16	1.988902197	-1.456735948	0.541429242
29	-0.048371455	-0.425882704	-0.059290007
16	-2.063285653	-1.482354154	-0.459763163
1	-4.992237693	0.443375133	0.406630061
1	-4.816094743	-1.174251428	-0.174237961
1	-1.306277331	3.312922846	0.038741229
1	1.321710023	3.231927929	0.215162898
1	4.845449322	0.537024678	-0.467924030
1	4.830549485	-0.588823113	0.770736233
1	4.607405932	-1.090106075	-0.793496242

Cu(I)PTSH-*syn* in DMSO

29	-0.200079115	-0.672170636	-0.025730056
16	-2.333195488	-1.489377162	-0.390499002
6	-3.172447210	-0.012655177	0.038810928
7	-2.623115822	1.201328766	0.164251327
7	-1.281838967	1.167224642	0.187313972
6	-0.598333889	2.260067902	-0.028209772
6	0.844968450	2.112208598	-0.089646365
7	1.239940417	0.898654435	-0.385626975
7	2.579759203	0.573692708	-0.270094043
6	2.908780338	-0.715624142	-0.019254005
16	1.745609083	-1.865096443	0.501068372
7	4.202743402	-1.052750209	-0.172535730
1	4.899898264	-0.399363237	-0.513521532
1	4.507801216	-1.979114106	0.093480830
6	1.756524750	3.268969458	0.206818411
1	1.181038057	4.176361995	0.400089960
1	2.364487781	3.052081966	1.094381695
1	2.444824227	3.474479602	-0.622563592
1	-1.075278227	3.231264610	-0.159328315
7	-4.515838493	-0.074409724	0.239834151
1	-5.024549997	0.789998380	0.381575489
1	-5.031367493	-0.880895982	-0.081385212
1	3.288320221	1.225728674	-0.608781700

Cu(I)ATSH in DMSO

29	-0.038964805	-0.865667599	-0.026747858
16	-2.061954227	-1.910673030	-0.399325397
6	-3.049270220	-0.535492874	0.061448220
7	-2.634022684	0.722213569	0.210958661
7	-1.288884338	0.838176434	0.225295343
6	-0.749290330	2.014206955	0.003105903
6	0.715300868	1.990555934	-0.030539789
7	1.218461705	0.837880444	-0.400310040
7	2.592530689	0.646459824	-0.286921210
6	3.047325313	-0.605477374	-0.043400518
16	2.008724758	-1.854191095	0.506975629
7	4.362292263	-0.824182035	-0.235153913
1	4.993590524	-0.098033082	-0.556626435
1	4.759811843	-1.712687061	0.037836895
6	1.540864230	3.181307415	0.371436587
1	0.939134589	3.931660931	0.885694000
1	2.344322307	2.862785887	1.045250196
1	2.011531144	3.663031599	-0.495946239
6	-1.550426479	3.266956610	-0.218572837
1	-2.260521089	3.109871767	-1.037688777
1	-2.146896965	3.515672039	0.667327886
1	-0.917664905	4.120685473	-0.467877851
7	-4.379751207	-0.753148477	0.275596244
1	-4.976250137	0.056975013	0.395720296
1	-4.803307281	-1.589065477	-0.100972212
1	3.216495485	1.337151008	-0.706554563

Cu(I)GTSMH in DMSO

29	-0.041252000	-0.544977000	-0.040474000
16	-2.044335000	-1.565805000	-0.550221000
6	-3.069632000	-0.205070000	-0.099672000
7	-2.656989000	1.055495000	0.083918000
7	-1.323639000	1.157274000	0.179911000
6	-0.744602000	2.322659000	0.007372000
6	0.694208000	2.298133000	-0.007810000
7	1.244555000	1.149534000	-0.298451000
7	2.600003000	0.979199000	-0.131391000
6	3.062391000	-0.265373000	0.150234000
16	1.991733000	-1.558862000	0.536184000
7	4.391891000	-0.457749000	0.125719000
6	5.393516000	0.517130000	-0.292226000
1	5.465126000	1.355989000	0.412033000
1	6.360904000	0.015237000	-0.321496000
1	5.171317000	0.902395000	-1.293848000
1	4.708678000	-1.374201000	0.421542000
1	1.279805000	3.187679000	0.234438000
1	-1.309437000	3.243274000	-0.131335000
7	-4.399206000	-0.435523000	0.016687000
6	-5.372957000	0.569136000	0.419013000
1	-5.412558000	1.396947000	-0.298162000
1	-6.353374000	0.091638000	0.468573000
1	-5.126890000	0.982930000	1.402014000
1	-4.730724000	-1.352070000	-0.252488000
1	3.211218000	1.791894000	-0.139146000

Cu(I)PTSMH-*syn* in DMSO

29	-0.153834331	-0.721739198	-0.050062678
16	-2.207533121	-1.674979002	-0.507415438
6	-3.161070058	-0.250945763	-0.103817648
7	-2.686183680	0.995318830	0.035265178
7	-1.349366948	1.034699899	0.113086610
6	-0.716670252	2.166145587	-0.079763755
6	0.728728683	2.090977699	-0.089324322
7	1.196947094	0.899820561	-0.387162646
7	2.556582388	0.661489490	-0.199312478
6	2.946550618	-0.594183769	0.128576920
16	1.811869171	-1.780886488	0.648632509
7	4.259639111	-0.877527631	0.062256176
6	5.314900235	0.049222915	-0.332246701
1	5.367204326	0.911832245	0.343974817
1	6.266067023	-0.481150293	-0.282114738
1	5.176167581	0.399859554	-1.362346639
1	4.526569985	-1.802212035	0.379123987
6	1.575514190	3.283737419	0.255190774
1	0.951510458	4.155686167	0.460485297
1	2.176241198	3.072251027	1.148759102
1	2.267752746	3.546986685	-0.554539122
1	-1.241584994	3.109523659	-0.227308138
7	-4.499792309	-0.408320335	0.022690520
6	-5.419305742	0.655523254	0.400605615
1	-5.405806060	1.471095575	-0.330810423
1	-6.425232215	0.234110978	0.448218484
1	-5.159623373	1.072456177	1.379041054
1	-4.876379976	-1.320727410	-0.195209373
1	3.212266787	1.313342503	-0.618018632

Cu(I)ATSMH in DMSO

29	-0.034860591	-0.897056002	-0.040291205
16	-2.032188515	-1.965260055	-0.485893738
6	-3.052606433	-0.586548974	-0.079533940
7	-2.642019229	0.675092435	0.077793033
7	-1.302525480	0.790902506	0.151802690
6	-0.758602236	1.974851107	-0.028796635
6	0.702810523	1.953794308	-0.008344342
7	1.224084922	0.807625613	-0.383236160
7	2.602030077	0.633512037	-0.203976605
6	3.053140294	-0.608962197	0.101711240
16	1.984562054	-1.846374306	0.636477192
7	4.375773350	-0.835800084	0.000637436
6	5.383260886	0.144850826	-0.386686277
1	5.403707766	0.995542524	0.306013623
1	6.357785559	-0.343123414	-0.358765000
1	5.216829551	0.510083447	-1.407706919
1	4.688942224	-1.750982095	0.303610514
6	1.512249960	3.135733517	0.449692480
1	0.891322869	3.874761613	0.957578194
1	2.290245414	2.801404967	1.144942215
1	2.013725827	3.636934593	-0.388976813
6	-1.562546950	3.224868291	-0.254353156
1	-2.210150014	3.095304285	-1.128844818
1	-2.226453468	3.422648585	0.595268921
1	-0.928228273	4.097662167	-0.420121993
7	-4.385731487	-0.808605803	0.039188649
6	-5.356707036	0.226557646	0.362322291

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1	-5.362232017	1.019304561	-0.394587622
1	-6.344906760	-0.235621437	0.406545689
1	-5.133464179	0.686442938	1.330223067
1	-4.721359183	-1.728602173	-0.211698696
1	3.209936275	1.289059168	-0.685903976

Optimised Cartesian coordinates for the reduced triplet Cu(I)A$^-$ species *in vacuo*.

Cu(I)GTS$^-$-triplet *in vacuo*

29	-0.000008000	-0.276278000	-0.011497000
16	-1.934412000	-1.574911000	-0.009989000
6	-3.010246000	-0.168647000	0.000491000
7	-2.637822000	1.083500000	0.010778000
7	-1.283367000	1.228811000	-0.011984000
6	-0.705065000	2.435786000	-0.000437000
6	0.705167000	2.435793000	-0.000889000
7	1.283478000	1.228823000	-0.012908000
7	2.637903000	1.083435000	0.009959000
6	3.010265000	-0.168717000	0.000534000
16	1.934263000	-1.574910000	-0.008615000
7	4.385891000	-0.427137000	-0.048019000
1	4.939068000	0.362918000	0.265862000
1	4.646342000	-1.300539000	0.391360000
1	1.305287000	3.342989000	0.007709000
1	-1.305199000	3.342967000	0.008331000
7	-4.385911000	-0.426872000	-0.047671000
1	-4.938808000	0.362633000	0.268056000
1	-4.646010000	-1.300994000	0.390469000

Cu(I)ATSM$^-$-triplet *in vacuo*

29	-0.004255000	-0.708374000	0.000154000
16	-1.917503000	-2.021644000	-0.000433000
6	-3.001965000	-0.614105000	-0.000404000
7	-2.634392000	0.641246000	-0.000208000
7	-1.275807000	0.801831000	-0.000086000
6	-0.708025000	2.024881000	-0.000117000
6	0.714332000	2.013954000	-0.000101000
7	1.269934000	0.787880000	0.000046000
7	2.628536000	0.635210000	0.000119000
6	2.998485000	-0.620653000	0.000206000
16	1.911950000	-2.026640000	0.000241000
7	4.350836000	-0.898150000	0.000280000
6	5.367232000	0.127637000	0.000170000
1	5.288266000	0.775445000	0.884135000
1	6.350507000	-0.353525000	0.000370000
1	5.288466000	0.775105000	-0.884070000
1	4.609092000	-1.870023000	0.000280000
6	1.569942000	3.249299000	-0.000177000
1	0.961157000	4.157464000	-0.002377000
1	2.228462000	3.271605000	0.878271000
1	2.231394000	3.269152000	-0.876424000
6	-1.536231000	3.285571000	-0.000290000
1	-1.340714000	3.906820000	-0.885291000
1	-2.593752000	3.016778000	0.001365000
1	-1.338253000	3.908627000	0.882860000
7	-4.354443000	-0.892755000	-0.000780000
6	-5.372064000	0.131514000	0.000720000
1	-5.294605000	0.780109000	-0.882903000
1	-6.354745000	-0.350819000	0.000276000
1	-5.294397000	0.778164000	0.885804000
1	-4.611510000	-1.864927000	0.000679000