Electronic Supplementary Material (ESI) for Dalton Transactions.

Achieving Selectivity for Copper over Zinc with Luminescent Terbium Probes Bearing Phenanthridine Antennas

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SUPPORTING INFORMATION

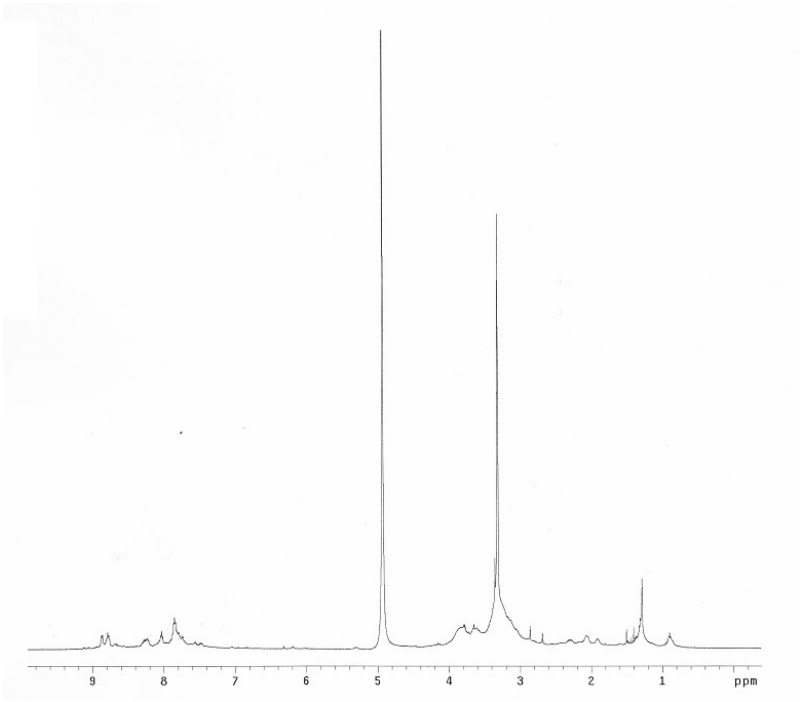

Figure S1. ^{1}H NMR spectrum of the deprotected ligand 1Phen (**9**, CD_3OD, 500 MHz).

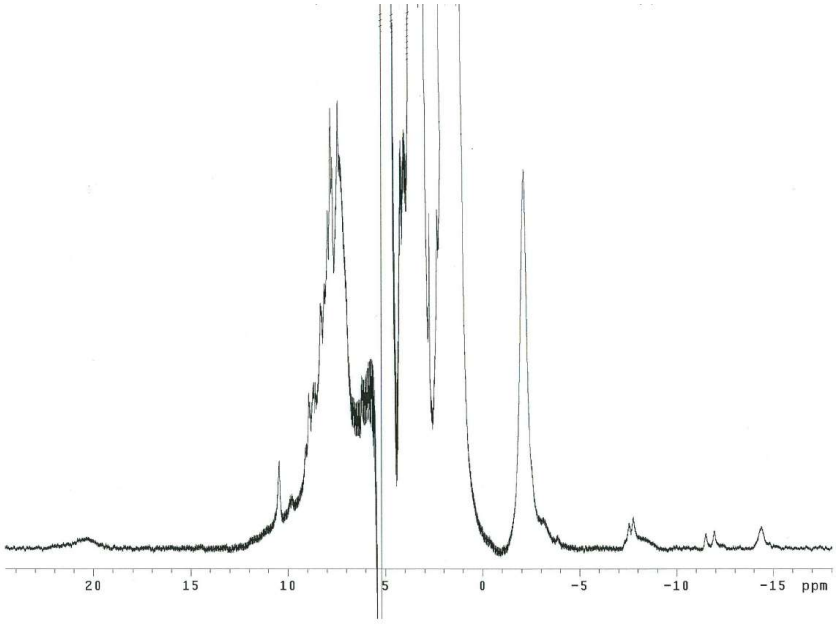

Figure S2. ^{1}H NMR spectrum of Tb-1Phen (**1**, D_2O, 500 MHz).

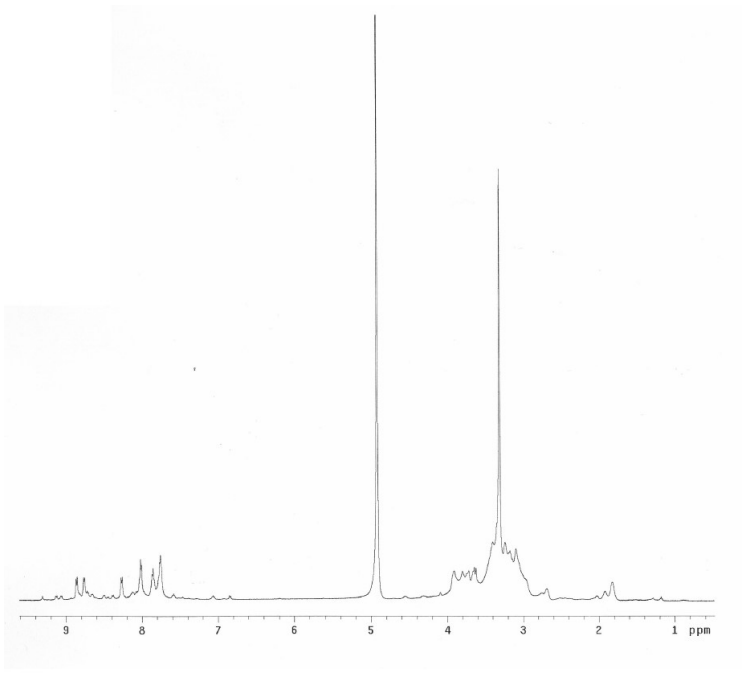

Figure S3. ^{1}H NMR spectrum of the deprotected ligand 2Phen (**12**, CD_3OD, 500 MHz).

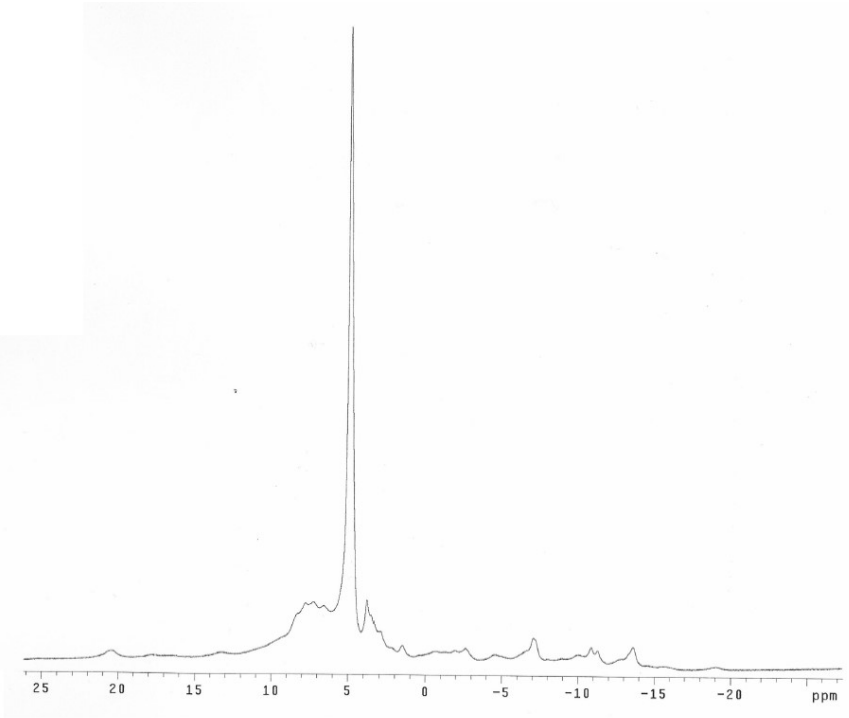

Figure S4. ^{1}H NMR spectrum of Tb-2Phen (**2**, D_2O, 500 MHz).

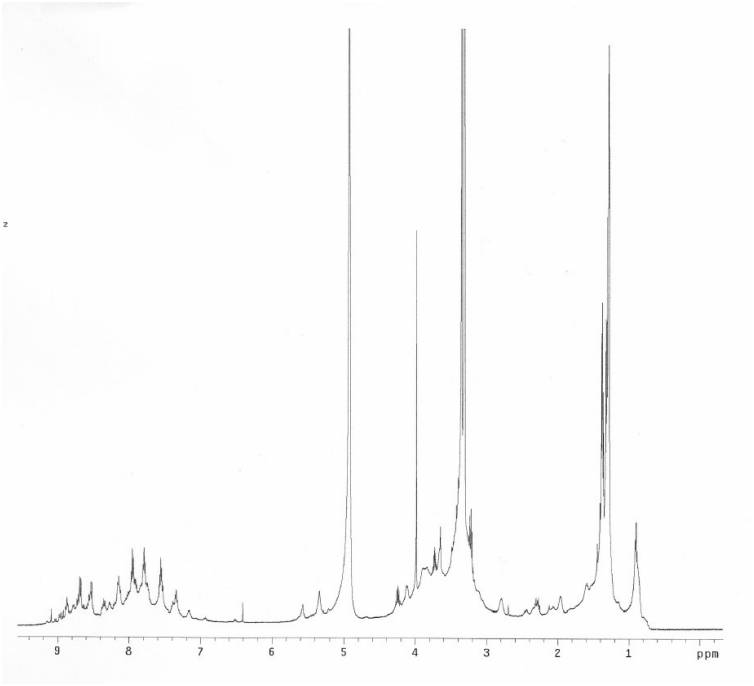

Figure S5. ^{1}H NMR spectrum of the deprotected ligand 3Phen (**17**, CD_3OD, 500 MHz).

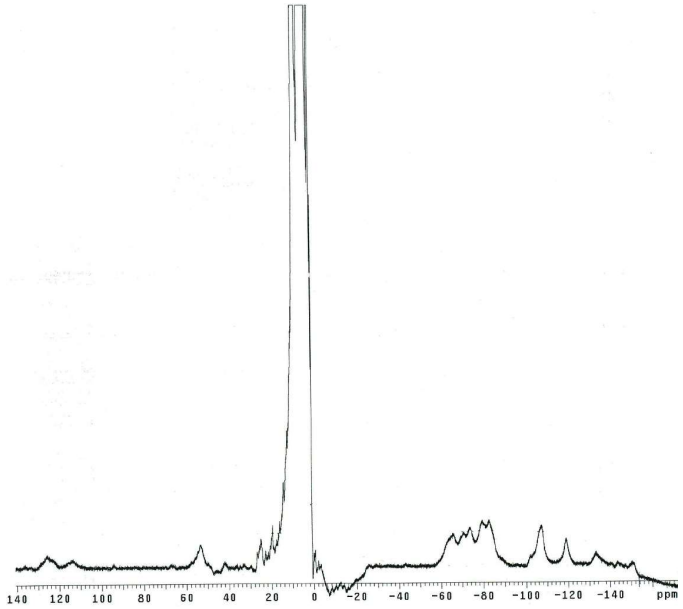

Figure S6. ^{1}H NMR spectrum of Tb-3Phen (**3**, in CD_3OD, 500 MHz).

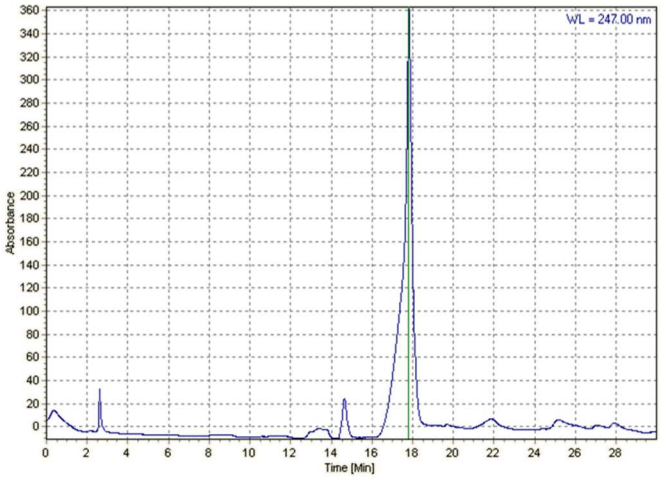

Figure S7. HPLC trace of Tb-1Phen (**1**). Experimental conditions: ZORBAX Eclipse XDB-C18 9.4 × 250 mm, 5 mμ column, 1.0 mL/min flow rate, solvent gradient: 100% water to 85% water/ 15% CH_3CN in 2 min then to 100% CH_3CN in 20 min and holding at 100% CH_3CN until 25 min then back to 85% water/ 15% CH_3CN till 30 min. At 17.80 min the product appeared and was identified by ESI MS.

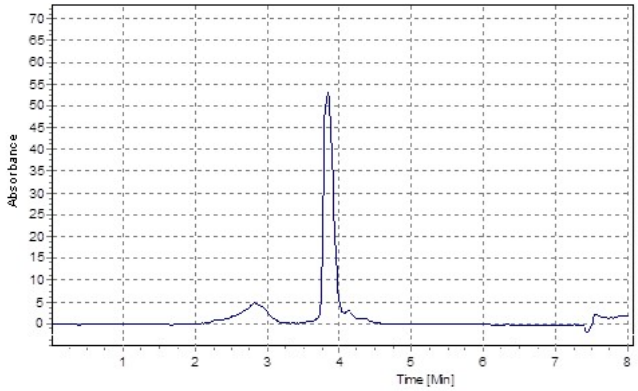

Figure S8. HPLC trace of Tb-3Phen (**3**). Experimental conditions: Varian Microsorb 300-5 C18 250 mm × 4.6 mm column, 1.0 mL/min flow rate, solvent gradient: 100% water to 40% water/ 60% CH_3CN in 10 min then to 100% CH_3CN in 13 min. At 3.84 min the product appeared and was identified by ESI-MS. The peak at 2.8 min is the solvent front.

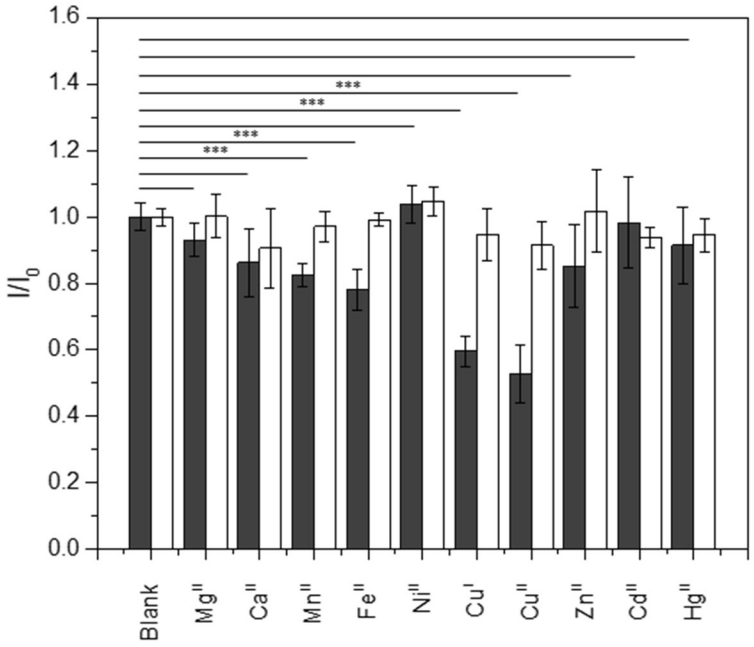

Figure S9. Integrated time-gated luminescence intensity (black bars) and fluorescence intensity (white bars) of Tb-1Phen (**1**) in the absence (blank) and presence of 1 eq. of metal ions. Experimental conditions: [Tb-1Phen] = 20 μM in 20 mM HEPES (*aq*) + 2 % CH_3CN, pH 7.0, T = 20 °C. Metal salts: $MgCl_2{\cdot}6H_2O$, $CaCl_2{\cdot}2H_2O$, $MnSO_4{\cdot}H_2O$, $FeSO_4{\cdot}7H_2O$, $Ni(NO_3)_2{\cdot}6H_2O$, $C_8H_{12}CuF_6N_4P$, $CuSO_4{\cdot}5H_2O$, $ZnSO_4{\cdot}7H_2O$, $Cd(NO_3)_2{\cdot}4H_2O$, $Hg(C_2H_3O_2)_2$. Excitation wavelength = 310 nm, excitation and emission slit widths 20 nm, delay time 0.1 ms, gate time 50.0 ms, I = integrated emission intensity from 450 nm – 700 nm (time-gated luminescence) or 335 nm – 550 nm (fluorescence). I_0 = integrated emission intensity of Tb-1Phen in the absence of metal ion. Results are mean ± SD (n = 3). * indicates a statistically significant difference (2 samples t-test, *: $p < 0.05$, **, $p < 0.03$, ***, $p < 0.02$)

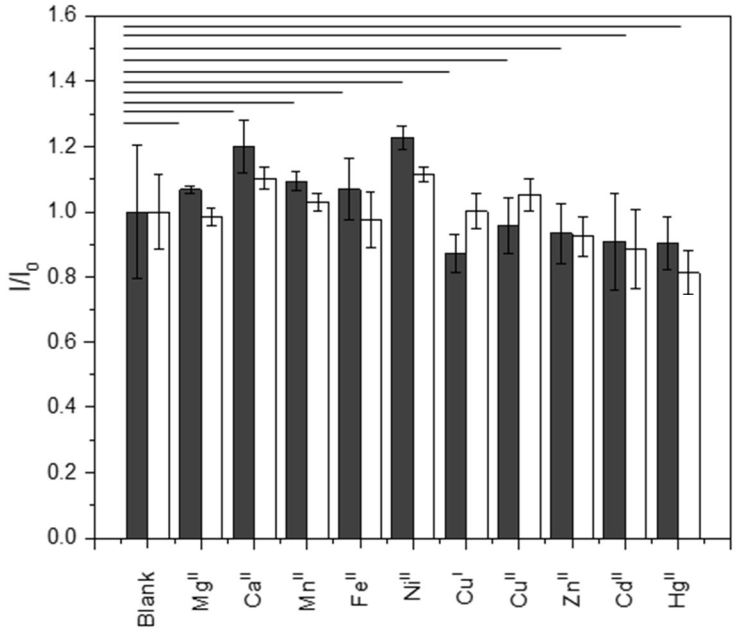

Figure S10. Integrated time-gated luminescence intensity (black bars) and fluorescence intensity (white bars) of Tb-2Phen (**2**) in the absence (blank) and presence of 1 eq. of metal ions. Experimental conditions: [Tb-2Phen] = 20 μM in 20 mM HEPES (*aq*) + 2 % CH_3CN, pH 7.0, T = 20°C. Metal salts: $MgCl_2·6H_2O$, $CaCl_2·2H_2O$, $MnSO_4·H_2O$, $FeSO_4·7H_2O$, $Ni(NO_3)_2·6H_2O$, $C_8H_{12}CuF_6N_4P$, $CuSO_4·5H_2O$, $ZnSO_4·7H_2O$, $Cd(NO_3)_2·4H_2O$, $Hg(C_2H_3O_2)_2$. Excitation wavelength = 315 nm, excitation and emission slit widths 20 nm, delay time 0.1 ms, gate time 50.0 ms, I = integrated emission intensity from 450 nm – 700 nm (time-gated luminescence) or 335 nm – 550 nm (fluorescence). I_0 = integrated emission intensity of Tb-2Phen in the absence of metal ion. Results are mean ± SD (n = 3). * indicates a statistically significant difference (2 samples t-test, *: $p < 0.05$, **, $p < 0.03$, ***, $p < 0.02$)

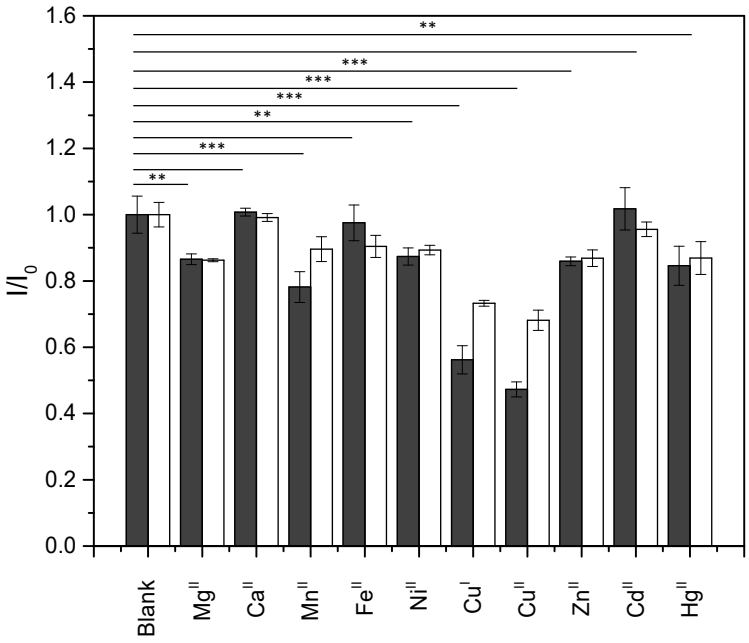

Figure S11. Integrated time-gated luminescence intensity (black bars) and fluorescence intensity (white bars) of Tb-3Phen (**3**) in the absence (blank) and presence of 1 eq. of metal ions. Experimental conditions: [Tb-3Phen] = 20 μM in 20 mM HEPES (*aq*) + 4 % CH_3CN, pH 7.0, T = 20 °C. Metal salts: $MgCl_2{\cdot}6H_2O$, $CaCl_2{\cdot}2H_2O$, $MnSO_4{\cdot}H_2O$, $FeSO_4{\cdot}7H_2O$, $Ni(NO_3)_2{\cdot}6H_2O$, $C_8H_{12}CuF_6N_4P$, $CuSO_4{\cdot}5H_2O$, $ZnSO_4{\cdot}7H_2O$, $Cd(NO_3)_2{\cdot}4H_2O$, $Hg(C_2H_3O_2)_2$. Excitation wavelength = 300 nm, excitation and emission slit widths 20 nm, delay time 0.1 ms, gate time 50.0 ms, I = integrated emission intensity from 450 nm – 700 nm (time-gated luminescence) or 335 nm – 550 nm (fluorescence). I_0 = integrated emission intensity of Tb-3Phen in the absence of metal ion. Results are mean ± SD (n = 3). * indicates a statistically significant difference (2 samples t-test, *: $p < 0.05$, **, $p < 0.03$, ***, $p < 0.02$)

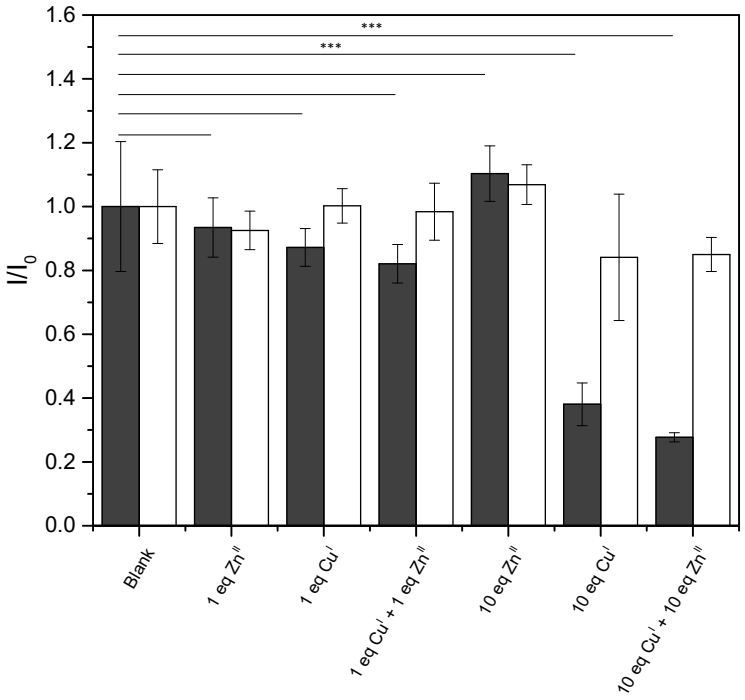

Figure S12. Integrated time-gated luminescence intensity (black bars) and fluorescence intensity (white bar) of Tb-2Phen (**2**) in the presence of either 1 or 10 equivalents of $C_8H_{12}CuF_6N_4P$ and/or $ZnSO_4 \cdot 7H_2O$. Experimental conditions: [Tb-2Phen] = 20 μM in 20 mM HEPES (*aq*) + 2 % CH_3CN, pH 7.0, T = 20 °C. Excitation wavelength = 310 nm, excitation and emission slit widths 20 nm, delay time 0.1 ms, gate time 50.0 ms, I = integrated emission intensity from 450 nm – 700 nm (time-gated luminescence) or 335 nm – 550 nm (fluorescence). I_0 = integrated emission intensity of Tb-1Phen in the absence of metal ion. Results are mean ± SD (n = 3). * indicates a statistically significant difference (2 samples t-test, *: $p < 0.05$, **, $p < 0.03$, ***, $p < 0.02$)

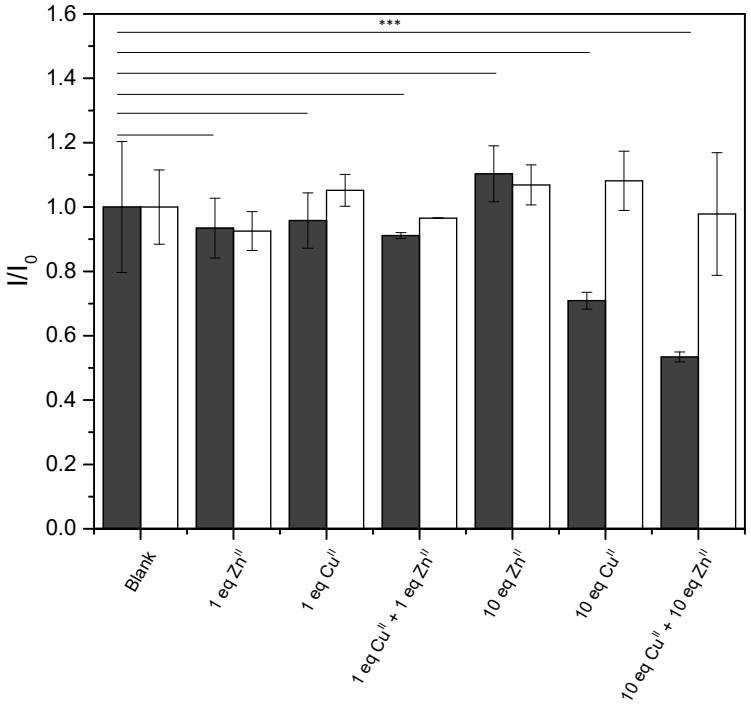

Figure S13. Integrated time-gated luminescence intensity (black bars) and fluorescence intensity (white bar) of Tb-2Phen (**2**) in the presence of either 1 or 10 equivalents of $CuSO_4$ and/or $ZnSO_4 \cdot 7H_2O$. Experimental conditions: [Tb-2Phen] = 20 μM in 20 mM HEPES (*aq*) + 2 % CH_3CN, pH 7.0, T = 20 °C. Excitation wavelength = 310 nm, excitation and emission slit widths 20 nm, delay time 0.1 ms, gate time 50.0 ms, I = integrated emission intensity from 450 nm – 700 nm (time-gated luminescence) or 335 nm – 550 nm (fluorescence). I_0 = integrated emission intensity of Tb-1Phen in the absence of metal ion. Results are mean ± SD (n = 3). * indicates a statistically significant difference (2 samples t-test, *: $p < 0.05$, **, $p < 0.03$, ***, $p < 0.02$)

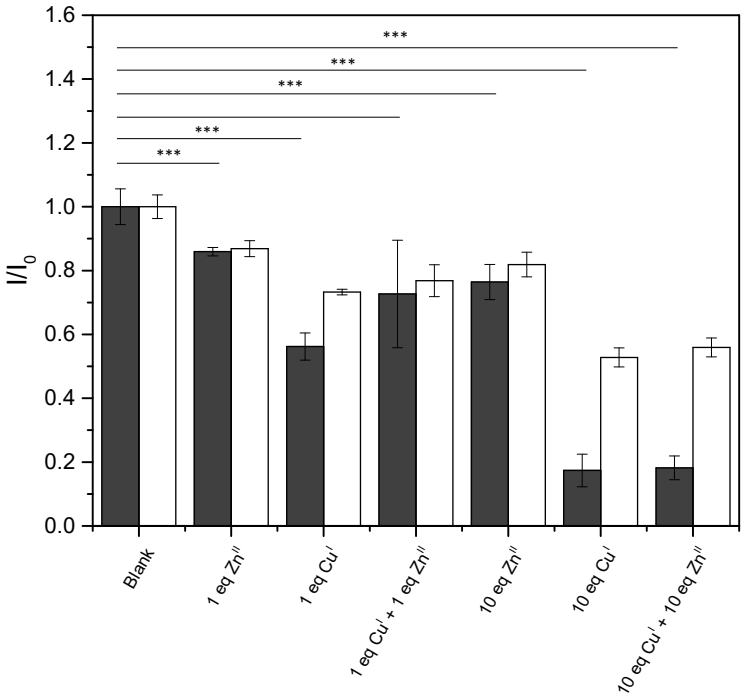

Figure S14. Integrated time-gated luminescence intensity (black bars) and fluorescence intensity (white bar) of Tb-3Phen (**3**) in the presence of either 1 or 10 equivalents of $C_8H_{12}CuF_6N_4P$ and/or $ZnSO_4 \cdot 7H_2O$. Experimental conditions: [Tb-3Phen] = 20 μM in 20 mM HEPES (*aq*) + 2.6 % CH_3CN, pH 7.0, T = 20 °C. Excitation wavelength = 300 nm, excitation and emission slit widths 20 nm, delay time 0.1 ms, gate time 50.0 ms, I = integrated emission intensity from 450 nm – 700 nm (time-gated luminescence) or 335 nm – 550 nm (fluorescence). I_0 = integrated emission intensity of Tb-3Phen in the absence of metal ion. Results are mean ± SD (n = 3). * indicates a statistically significant difference (2 samples t-test, *: $p < 0.05$, **, $p < 0.03$, ***, $p < 0.02$)

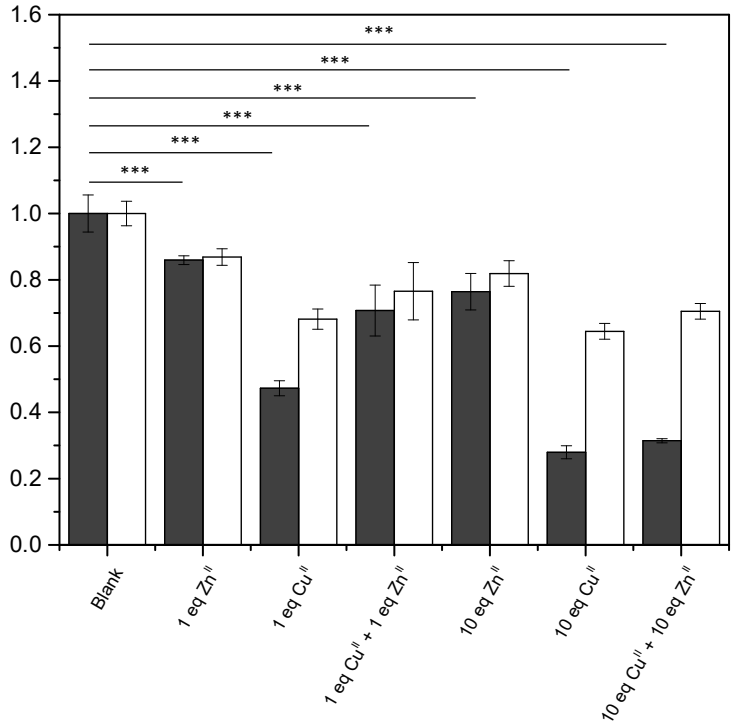

Figure S15. Integrated time-gated luminescence intensity (black bars) and fluorescence intensity (white bar) of Tb-3Phen (**3**) in the presence of either 1 or 10 equivalents of $CuSO_4$ and/or $ZnSO_4{\cdot}7H_2O$. Experimental conditions: [Tb-3Phen] = 20 μM in 20 mM HEPES (*aq*) + 2.6 % CH_3CN, pH 7.0, T = 20 °C. Excitation wavelength = 300 nm, excitation and emission slit widths 20 nm, delay time 0.1 ms, gate time 50.0 ms, I = integrated emission intensity from 450 nm – 700 nm (time-gated luminescence) or 335 nm – 550 nm (fluorescence). I_0 = integrated emission intensity of Tb-3Phen in the absence of metal ion. Results are mean ± SD (*n* = 3). * indicates a statistically significant difference (2 samples t-test, *: $p < 0.05$, **, $p < 0.03$, ***, $p < 0.02$)

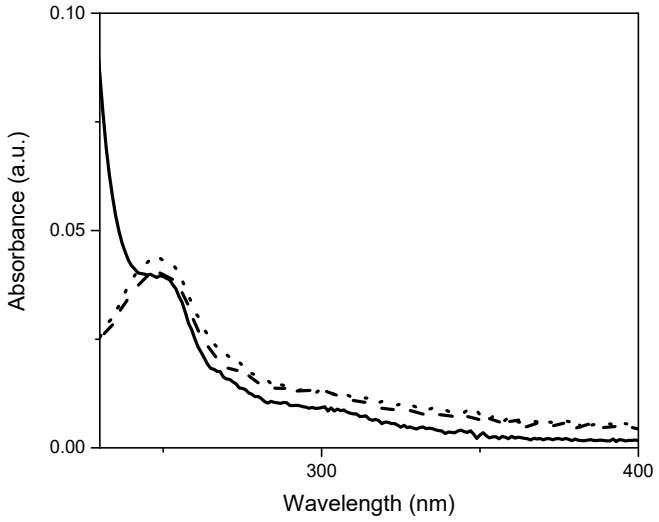

Figure S16. UV-vis absorbances of Tb-1Phen (solid line), Tb-2Phen (dotted line), Tb-3Phen (dashed line). Experimental conditions: [Tb probe] = 20 μM in 20 mM HEPES (*aq*) + 2 % CH_3CN (4 % CH_3CN for Tb-3Phen), pH 7.0, T = 20 °C.

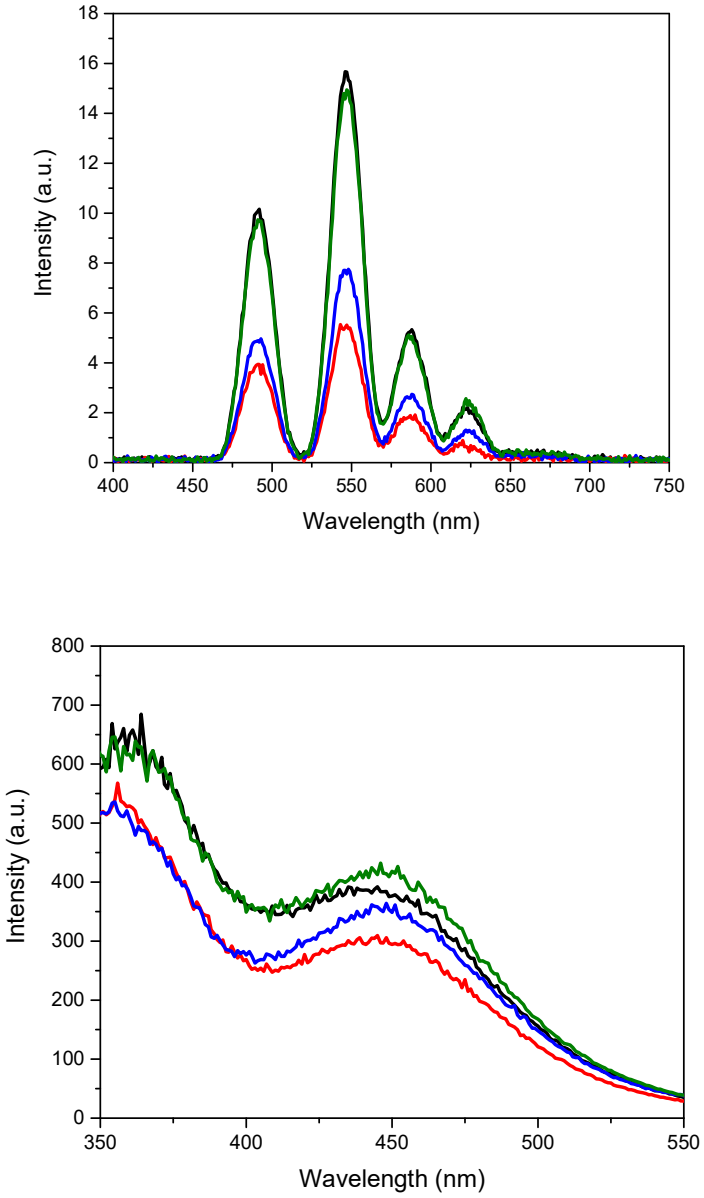

Figure S17. Time-gated luminescence intensity (top) and fluorescence intensity (bottom) of Tb-2Phen (**2**) in the absence (black line) in the presence of 10 equivalents of $C_8H_{12}CuF_6N_4P$ (red line), $CuSO_4 \cdot 5H_2O$ (blue line), or $ZnSO_4 \cdot 7H_2O$ (green line). Experimental conditions: [Tb-2Phen] = 20 μM in 20 mM HEPES (*aq*) + 2 % CH_3CN, pH 7.0, T = 20 °C. Excitation wavelength = 310 nm, excitation and emission slit widths 20 nm, delay time 0.1 ms, gate time 50.0 ms.

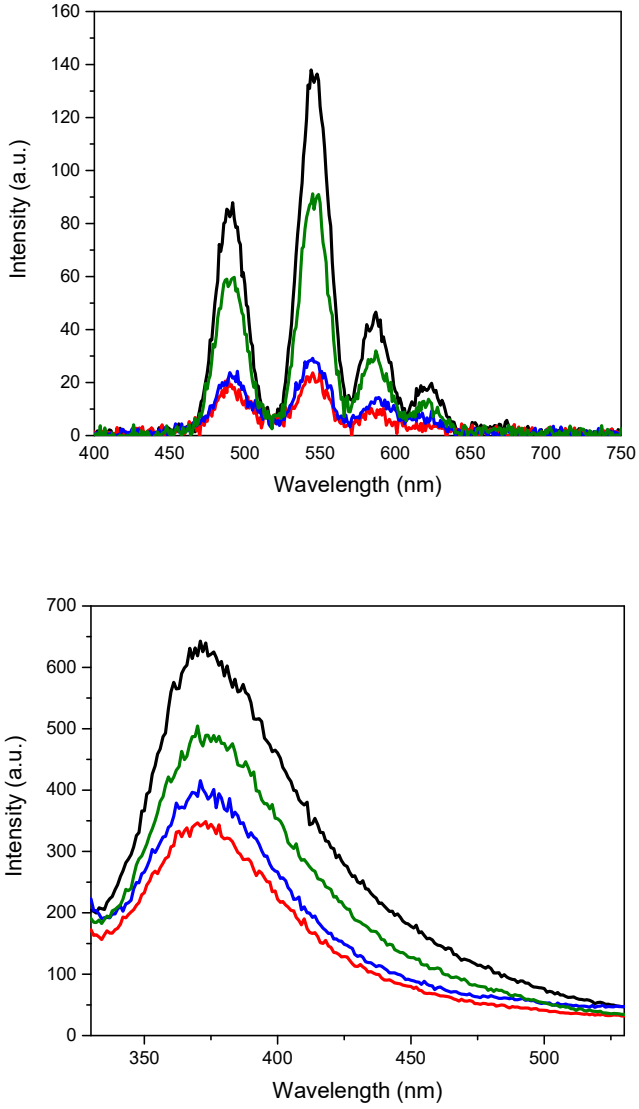

Figure S18. Time-gated luminescence intensity (top) and fluorescence intensity (bottom) of Tb-3Phen (**3**) in the absence (black line) and presence of 10 eq. of $C_8H_{12}CuF_6N_4P$ (red line), $CuSO_4 \cdot 5H_2O$ (blue line), or $ZnSO_4 \cdot 7H_2O$ (green line). Experimental conditions: [Tb-3Phen] = 20 μM in 20 mM HEPES (*aq*) + 4 % CH_3CN, pH 7.0, T = 20°C. Excitation wavelength = 300 nm, excitation and emission slit widths 20 nm, delay time 0.1 ms, gate time 50.0 ms.

Computational Methods

Geometry optimizations on selected structures were performed using the M06-L functional[1,2] in the Gaussian '09 software package.[3] Pople 6-31G(d) basis sets were employed for organic atom types,[4] and SDD basis sets and psuedopotentials were used for metals.[5] Thermal free energies were obtained from frequency calculations performed at the same level of theory. Unless otherwise specified, all calculations employed the SMD continuum solvation model, with parameters set for water.

Density fitting basis sets automatically generated by the Gaussian software package were used, together with the resolution of the identity approximation, to reduce the computational cost of the calculations. For numerical integration, most calculations employed the pruned (99,590) UltraFine grid most commonly used for DFT in Gaussian. However, severe geometry convergence difficulties when dealing with solvated metal aquo clusters necessitated the use of the larger SuperFine grid, which entails a pruned (175,974) grid for first-row atoms and a pruned (250,974) grid for larger atoms. The use of the larger grid helped to eliminate imaginary frequencies, and was found to affect the electronic energies by < 0.1 kcal/mol.

The standard states of the metals and ligand were assumed to be 200 μM and 20 μM, respectively, and consequently the free energy of each species was adjusted by a change of standard state correction: -3.2 kcal/mol for metals, and -4.5 kcal/mol for the ligand and bound species. Note that, because of cancellation, this correction affects only the absolute ΔG values for metal binding, and not the relative binding free energies between metals. Hence, the magnitude of this term does not affect any of the binding trends reported here.

For the sake of reducing computational cost and allowing for a more thorough study of the possible binding configurations of the metals, the portion of the **2** used to chelate the lanthanide – along with the lanthanide itself – was removed from the structures prior to optimization. The bond between the carbons alpha and beta to the amide nitrogen was severed, and the beta carbon was capped with a proton. We believe that this approximation is not detrimental to the computational study, because the portion of the ligand chelating the lanthanide is not expected to participate in binding the transition metals, and because we currently have no plans to carry out a theoretical study of exciton transfer within the probe.

References

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Structures from the main text:

L(H_2O)$_3$ in SMD water
E= -1724.963 28 a.u.

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H	4.838024	0.619759	-1.117892
O	4.321512	1.424593	-1.385341
H	3.481546	1.097301	-1.750064

$[Cu(I)(H_2O)_2]^+$ in SMD water
E= -350.121 98 a.u.

Cu	0.000015	-0.018123	-0.000456
O	-1.924938	-0.019906	0.103857
H	-2.218110	0.900716	-0.015817
O	1.924975	-0.020043	-0.102540
H	2.218307	0.900634	0.016271
H	-2.261461	-0.478467	-0.686028
H	2.260544	-0.477719	0.688254

$[Cu(II)(H_2O)_6]^{2+}$ in SMD water
E= -655.679 21 a.u.

Cu	0.000000	0.000000	0.000000
O	1.750093	-0.666551	1.290375
H	2.414660	-0.783270	0.591809
O	-1.401845	-1.094941	1.268600
H	-1.822291	-1.691359	0.625588
O	-0.275717	1.614613	1.186495
H	-0.600272	2.308023	0.583016
O	-1.750093	0.666551	-1.290375
H	-1.488833	1.577640	-1.504500
O	0.275717	-1.614613	-1.186495
H	-0.620615	-1.913142	-1.426022
O	1.401845	1.094941	-1.268600
H	1.822291	1.691359	-0.625588
H	-2.088131	-0.426609	1.436916
H	1.488833	-1.577640	1.504500
H	0.600272	-2.308023	-0.583016
H	-2.414660	0.783270	-0.591809
H	0.620615	1.913142	1.426022
H	2.088131	0.426609	-1.436916

$[Zn(II)(H_2O)_6]^{2+}$ in SMD water
E= -685.512 15 a.u.

Zn	0.000000	0.000000	0.000000
H	-1.276559	2.155736	0.624830
H	-0.123033	1.994489	1.613709
H	-0.144716	-2.200265	1.298462
H	-0.902616	-1.149726	2.105457

H	1.991689	0.941020	1.395588
H	1.387475	-0.229997	2.166539
H	0.902616	1.149726	-2.105457
H	0.144716	2.200265	-1.298462
H	0.123033	-1.994489	-1.613709
H	1.276559	-2.155736	-0.624830
H	-1.387475	0.229997	-2.166539
H	-1.991689	-0.941020	-1.395588
O	0.862365	1.549126	-1.219908
O	1.787415	-0.005226	1.309757
O	-0.901556	1.527672	1.265316
O	0.901556	-1.527672	-1.265316
O	-0.862365	-1.549126	1.219908
O	-1.787415	0.005226	-1.309757

$[Cu(I)L(H_2O)_3]^+$ tetrahedral, in SMD water
E= -1922.268 29 a.u.

N	5.821398	0.282172	0.200540
N	1.606915	0.975352	-0.084520
C	0.802058	1.208655	1.129689
H	0.436898	2.245549	1.167598
H	1.479433	1.086309	1.987666
C	-0.324511	0.212178	1.278196
C	-1.602528	0.579353	1.817699
C	-1.023820	-2.000743	0.930928
C	-2.644993	-0.393164	1.832487
C	-1.872942	1.879895	2.305384
C	-0.682913	-3.291252	0.484027
C	-2.344604	-1.725649	1.364378
C	-3.921527	-0.014131	2.290395
H	-1.085906	2.629176	2.325349
C	-3.129738	2.217754	2.762400
C	-1.630497	-4.294492	0.444026
H	0.346297	-3.463164	0.158727
C	-3.293330	-2.767708	1.306143
C	-4.163572	1.268018	2.744127
H	-4.732396	-0.738815	2.293776
H	-3.320234	3.224837	3.128348
C	-2.945875	-4.027086	0.855386
H	-1.359370	-5.287662	0.091964
H	-4.319366	-2.582399	1.616821

H	-5.157866	1.539220	3.093341
H	-3.697203	-4.813377	0.819244
N	-0.039902	-1.022310	0.896136
C	7.131626	0.514879	0.822937
H	7.014257	1.357733	1.518339
Cu	1.621450	-1.345119	-0.114216
H	5.908215	-0.532747	-0.409190
C	2.966118	1.505814	0.117722
H	3.353130	1.040120	1.032097
H	2.928297	2.596869	0.305754
C	3.907143	1.223631	-1.040679
H	3.690256	1.890249	-1.885241
H	3.742823	0.195060	-1.403636
C	5.364411	1.397277	-0.637463
H	5.483783	2.321765	-0.052579
H	5.988260	1.514111	-1.537861
C	1.014764	1.622669	-1.286650
C	-0.449211	1.318403	-1.454052
C	-1.478545	2.259311	-1.087323
C	-2.013293	-0.334921	-1.949522
C	-2.836565	1.826392	-1.137390
C	-1.196457	3.580720	-0.672741
C	-2.228712	-1.666041	-2.363421
C	-3.108905	0.466326	-1.533807
C	-3.853183	2.734552	-0.780669
H	-0.168070	3.929690	-0.626756
C	-2.213257	4.449247	-0.331185
C	-3.496686	-2.208060	-2.338746
H	-1.367573	-2.255458	-2.676141
C	-4.392897	-0.116686	-1.514107
C	-3.548883	4.022977	-0.387809
H	-4.894213	2.422181	-0.817920
H	-1.977983	5.465113	-0.021157
C	-4.583003	-1.428166	-1.904549
H	-3.655105	-3.241744	-2.640561
H	-5.248496	0.465448	-1.177596
H	-4.350042	4.709095	-0.119996
H	-5.581174	-1.860353	-1.872161
N	-0.715623	0.120117	-1.921706
H	1.549363	1.231656	-2.159913
H	1.203466	2.706544	-1.249129
H	7.354774	-0.367865	1.437336
C	8.279363	0.784505	-0.132801

H	8.384769	-0.029276	-0.862311
H	8.138847	1.718977	-0.688986
H	0.672737	-1.013565	-2.308725
O	1.449350	-1.636746	-2.343750
H	2.187940	-1.063203	-2.604792
H	9.224984	0.866668	0.415759
O	3.418713	-2.344101	-0.066201
H	3.966606	-1.968746	-0.774991
H	4.848696	-0.459668	1.505247
H	3.806070	-1.959003	0.770847
O	4.326222	-1.049481	2.127345
H	5.009021	-1.582306	2.563358

$[Cu(II)L(H_2O)_2]^{2+}$ trigonal bipyramidal, in SMD water
E= -1845.712 96 a.u.

N	-4.119394	-0.448872	-0.441766
N	-1.507437	-1.744150	0.468487
C	-0.447153	-1.626054	1.495689
H	0.260303	-2.459646	1.414487
H	-0.927446	-1.721688	2.478114
C	0.232081	-0.286767	1.435530
C	1.620541	-0.117798	1.745464
C	-0.027535	1.996344	0.945671
C	2.205903	1.165252	1.545723
C	2.425476	-1.190864	2.192011
C	-0.903517	3.037803	0.586239
C	1.354523	2.255868	1.137636
C	3.592402	1.310538	1.751994
H	1.984304	-2.168081	2.372271
C	3.775474	-1.012333	2.402770
C	-0.417712	4.313726	0.385576
H	-1.960693	2.811393	0.458337
C	1.819218	3.568079	0.917142
C	4.361965	0.242050	2.166271
H	4.068369	2.273532	1.584663
H	4.387621	-1.846338	2.739132
C	0.952585	4.576547	0.543512
H	-1.096810	5.115328	0.103525
H	2.875397	3.794978	1.042241
H	5.431230	0.376223	2.316701
H	1.334610	5.581466	0.377512

N	-0.539287	0.719509	1.079674
C	-5.106585	0.655074	-0.567163
H	-5.629781	0.728226	0.393310
Cu	-2.389151	0.213889	0.392281
H	-3.844847	-0.727409	-1.388212
C	-2.492925	-2.761141	0.920798
H	-2.760760	-2.503191	1.952948
H	-1.989470	-3.741124	0.944833
C	-3.757288	-2.844649	0.088741
H	-4.306527	-3.727202	0.436153
H	-3.530450	-3.031789	-0.970540
C	-4.677143	-1.646946	0.217909
H	-4.847594	-1.391466	1.272973
H	-5.655496	-1.882464	-0.224177
C	-0.971055	-2.127485	-0.885236
C	0.355437	-1.494634	-1.223512
C	1.603698	-2.176208	-0.988134
C	1.446741	0.439626	-1.935765
C	2.817188	-1.467447	-1.233671
C	1.669492	-3.501311	-0.499319
C	1.310904	1.770177	-2.385034
C	2.735866	-0.100420	-1.685289
C	4.043597	-2.119923	-0.994729
H	0.754941	-4.055566	-0.301486
C	2.884870	-4.110250	-0.265646
C	2.424986	2.563393	-2.558386
H	0.309630	2.157931	-2.566867
C	3.856094	0.736588	-1.869845
C	4.077843	-3.415175	-0.518969
H	4.979969	-1.600252	-1.182934
H	2.917331	-5.130513	0.109853
C	3.703752	2.042860	-2.292119
H	2.314777	3.594204	-2.889298
H	4.856043	0.360192	-1.666010
H	5.035940	-3.898647	-0.339001
H	4.581482	2.673236	-2.418758
N	0.294766	-0.279534	-1.718698
H	-1.709317	-1.810370	-1.629181
H	-0.912798	-3.222104	-0.933765
H	-4.546313	1.589074	-0.702956
C	-6.072373	0.447635	-1.713028
H	-5.535916	0.392777	-2.668774
H	-6.658717	-0.471097	-1.595459

H	-1.226782	0.674722	-1.771022
O	-2.053898	1.212240	-1.610012
H	-2.677300	0.879317	-2.276242
H	-6.774066	1.286623	-1.769912
O	-3.388694	1.254712	2.003969
H	-3.834761	2.020230	1.603096
H	-4.124627	0.679516	2.275773

[Zn(II)L(H_2O)$_3$]$^{2+}$ tetrahedral, in SMD water
E= -1951.952 68 a.u.

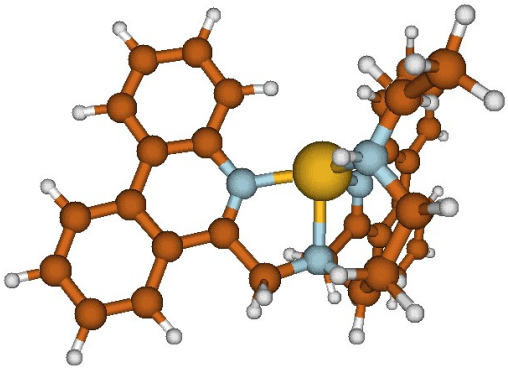
N	5.785933	0.251632	0.269937
N	1.604464	0.953927	-0.168719
C	0.815736	1.246282	1.046947
H	0.433966	2.274341	1.020469
H	1.496354	1.185783	1.906926
C	-0.293887	0.239694	1.247635
C	-1.555070	0.593618	1.831799
C	-0.981402	-1.982805	0.913212
C	-2.581165	-0.395001	1.878900
C	-1.820156	1.896124	2.310978
C	-0.634526	-3.262764	0.443002
C	-2.285306	-1.725596	1.404663
C	-3.848210	-0.025720	2.371281
H	-1.040534	2.653349	2.293253
C	-3.066223	2.222442	2.802258
C	-1.568033	-4.279003	0.444203
H	0.378862	-3.425211	0.070897
C	-3.218404	-2.782091	1.387095
C	-4.086724	1.257539	2.821132
H	-4.652008	-0.757072	2.401995
H	-3.261590	3.230048	3.162777
C	-2.867038	-4.033649	0.917871
H	-1.299109	-5.266527	0.075875
H	-4.231445	-2.616728	1.746716
H	-5.073875	1.521306	3.195179
H	-3.604510	-4.833363	0.913569
N	-0.030200	-0.984149	0.848129
C	7.091969	0.582527	0.858742
H	6.984547	1.557944	1.353278
Zn	1.693570	-1.219585	-0.299107
H	5.871613	-0.661840	-0.179450

C	2.983804	1.476106	-0.030011
H	3.357165	1.123490	0.936287
H	2.955910	2.577996	0.016506
C	3.906145	1.016810	-1.144682
H	3.703522	1.572947	-2.068929
H	3.714720	-0.047249	-1.372713
C	5.369210	1.203082	-0.769398
H	5.524340	2.216457	-0.370501
H	5.994454	1.122281	-1.672276
C	0.983585	1.558864	-1.395907
C	-0.492188	1.275546	-1.522370
C	-1.495775	2.230543	-1.123835
C	-2.097194	-0.359557	-1.961482
C	-2.860276	1.812274	-1.122888
C	-1.183185	3.550369	-0.725699
C	-2.339685	-1.690757	-2.358673
C	-3.164854	0.454834	-1.502532
C	-3.852391	2.732831	-0.730949
H	-0.150611	3.890024	-0.721532
C	-2.176933	4.430454	-0.349498
C	-3.609369	-2.221434	-2.273073
H	-1.497944	-2.289025	-2.705465
C	-4.451800	-0.116734	-1.422749
C	-3.518454	4.018123	-0.353523
H	-4.897456	2.432565	-0.729490
H	-1.919726	5.445011	-0.053573
C	-4.668537	-1.429118	-1.795588
H	-3.789777	-3.255660	-2.559906
H	-5.286864	0.473840	-1.051861
H	-4.301068	4.713842	-0.057611
H	-5.667430	-1.853153	-1.715362
N	-0.795755	0.082942	-1.982140
H	1.499799	1.127590	-2.259744
H	1.195461	2.635653	-1.388989
H	7.282897	-0.150098	1.654275
C	8.258132	0.611938	-0.111779
H	8.345148	-0.341011	-0.650124
H	8.152910	1.410439	-0.855952
H	0.543966	-1.075400	-2.374357
O	1.358217	-1.658479	-2.286910
H	2.052979	-1.166198	-2.758563
H	9.200948	0.781563	0.421351
O	3.260525	-2.288108	0.381326

H	3.956993	-2.178799	-0.289180
H	4.740895	-0.236087	1.647396
H	3.595015	-1.751118	1.168064
O	4.136152	-0.682514	2.313736
H	4.743376	-1.186659	2.877828

Alternative binding topologies:

$[Cu(I)L]^+$ trigonal pyramidal, in SMD water
E= -1692.991 19 a.u.

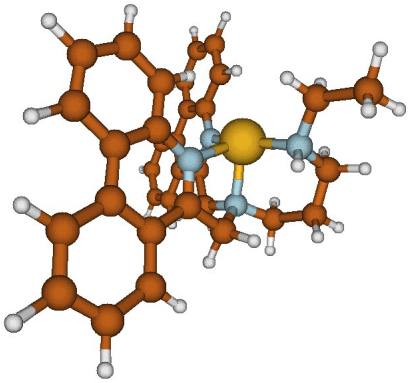


N	-0.157288	2.070950	-2.211602
C	-0.155939	0.037504	-3.688993
N	0.129676	-1.181980	-1.507264
C	1.543642	-1.543170	-1.551276
H	1.669843	-2.636829	-1.509033
H	1.952585	-1.235454	-2.524605
C	2.361687	-0.870405	-0.471981
C	3.666752	-1.368106	-0.134137
C	4.228715	-2.492157	-0.781021
C	4.421756	-0.696237	0.869437
C	2.557051	0.884090	1.067591
C	5.487309	-2.945501	-0.442878
H	3.672447	-3.004667	-1.561781
C	5.699759	-1.186283	1.198793
C	3.840943	0.468072	1.496640
C	1.957107	2.024219	1.632931
C	6.224088	-2.291272	0.556194
H	5.907067	-3.810270	-0.952165
H	6.288512	-0.689166	1.966010
C	4.481672	1.221574	2.501352
H	0.967241	2.313288	1.265960
C	2.607403	2.745345	2.613920
H	7.214604	-2.653013	0.824603

C	3.877852	2.336771	3.050720
H	5.467524	0.926240	2.853732
H	2.137594	3.625807	3.047157
H	4.391628	2.901662	3.825734
N	1.845469	0.205088	0.091273
H	0.934237	0.188619	-3.728774
H	-0.453709	-0.202993	-4.717468
C	-0.499885	-1.176388	-2.836937
H	-0.244977	-2.103960	-3.381521
H	-1.586910	-1.200718	-2.675915
C	-0.613659	-2.036582	-0.578935
H	0.056514	-2.311889	0.249336
H	-0.899203	-2.979069	-1.069750
Cu	0.013837	0.843482	-0.549651
C	-1.810354	-1.333402	0.021284
C	-2.991003	-2.053655	0.410087
C	-2.678315	0.680772	0.843955
C	-4.062476	-1.335799	1.018619
C	-3.126258	-3.447487	0.212762
C	-2.454847	2.051167	1.072651
C	-3.895942	0.079897	1.247495
C	-5.228853	-2.035086	1.382831
H	-2.316478	-4.016098	-0.235984
C	-4.278116	-4.107308	0.588205
C	-3.421240	2.827225	1.679514
H	-1.493434	2.465785	0.757742
C	-4.867663	0.897311	1.860834
C	-5.337349	-3.395628	1.171641
H	-6.057961	-1.501571	1.841218
H	-4.365003	-5.179771	0.427989
C	-4.637335	2.243457	2.071181
H	-3.242491	3.885911	1.855738
H	-5.814108	0.466301	2.179349
H	-6.247165	-3.916893	1.462419
H	-5.402572	2.852701	2.547630
N	-1.669577	-0.037254	0.226391
C	-0.836793	1.348300	-3.310815
H	-1.873293	1.166628	-2.989808
H	-0.889530	1.987920	-4.204633
C	-0.815997	3.358132	-1.891550
H	-1.843696	3.126024	-1.580921
H	-0.302356	3.763012	-1.009976
C	-0.812470	4.383330	-3.009601

H	-1.193153	5.342223	-2.640032
H	0.204827	4.551393	-3.386385
H	0.777542	2.299041	-2.555816
H	-1.442816	4.084995	-3.854845

[Cu(II)L]$^{2+}$ trigonal pyramidal, in SMD water
E= -1692.844 48 a.u.



N	0.919646	3.015106	-0.809730
C	0.565797	2.571055	-3.242823
N	0.219424	0.367045	-2.042490
C	1.631550	-0.057221	-2.082053
H	1.742828	-0.863660	-2.819321
H	2.249421	0.776256	-2.438703
C	2.126574	-0.483890	-0.721609
C	3.258772	-1.357011	-0.585373
C	3.971860	-1.840950	-1.703273
C	3.670563	-1.727718	0.727114
C	1.855914	-0.323899	1.592727
C	5.056579	-2.676450	-1.534792
H	3.675179	-1.547962	-2.707599
C	4.775578	-2.589882	0.865965
C	2.938679	-1.200501	1.855177
C	1.109189	0.226853	2.650056
C	5.454045	-3.055671	-0.243141
H	5.601432	-3.042058	-2.402152
H	5.105239	-2.892535	1.856751
C	3.235820	-1.498792	3.200058
H	0.280412	0.892225	2.398873
C	1.422935	-0.083266	3.957681
H	6.305658	-3.720304	-0.112897
C	2.493154	-0.951699	4.229728
H	4.059155	-2.168309	3.438391

H	0.843922	0.340750	4.775180
H	2.740050	-1.197755	5.260251
N	1.486563	0.010619	0.308809
H	1.644772	2.432762	-3.395518
H	0.208538	3.076109	-4.147566
C	-0.155437	1.234929	-3.187655
H	0.024764	0.680773	-4.121877
H	-1.237865	1.394493	-3.105485
C	-0.665116	-0.826165	-1.986026
H	-0.062639	-1.700076	-1.702529
H	-1.043837	-1.033897	-2.995185
Cu	-0.123880	1.430031	-0.256914
C	-1.792696	-0.706805	-1.003052
C	-2.881415	-1.638037	-1.021544
C	-2.684196	0.416498	0.864580
C	-3.910420	-1.505613	-0.046694
C	-2.945234	-2.681043	-1.971476
C	-2.538177	1.470925	1.782537
C	-3.811543	-0.439494	0.922139
C	-4.977651	-2.423778	-0.070240
H	-2.154755	-2.795560	-2.708796
C	-4.000765	-3.567967	-1.965432
C	-3.494832	1.682066	2.754307
H	-1.659517	2.113768	1.710283
C	-4.771544	-0.196849	1.925034
C	-5.021659	-3.433510	-1.011599
H	-5.779980	-2.344640	0.658538
H	-4.041350	-4.369330	-2.699358
C	-4.617050	0.841822	2.822906
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H	-5.650694	-0.832242	1.997809
H	-5.855840	-4.131979	-1.011778
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H	-0.733549	3.679069	-1.897900
H	0.781130	4.490975	-2.319086
C	0.869788	4.006840	0.296775
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H	1.121992	3.470083	1.219743
C	1.804982	5.181132	0.101555
H	1.773807	5.827110	0.985261
H	2.839363	4.840804	-0.028152

H	1.899230	2.767226	-0.975576
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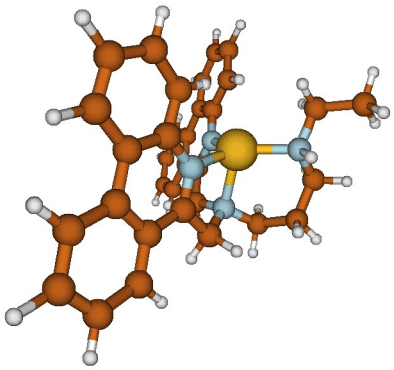
[Zn(II)L]$^{2+}$ trigonal pyramidal, in SMD water
E= -1722.667 93 a.u.



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H	1.775223	-2.035504	-2.207283
H	2.068625	-0.392097	-2.753088
C	2.346938	-0.634961	-0.662053
C	3.623593	-1.208898	-0.348808
C	4.260883	-2.120248	-1.218834
C	4.264251	-0.829095	0.866000
C	2.357070	0.647928	1.307828
C	5.492310	-2.651468	-0.898100
H	3.786803	-2.402897	-2.155247
C	5.518063	-1.394250	1.168519
C	3.604493	0.124336	1.727409
C	1.676670	1.595069	2.093106
C	6.119178	-2.287786	0.303874
H	5.976456	-3.350920	-1.575462
H	6.028349	-1.123348	2.089321
C	4.128304	0.575762	2.955421
H	0.719814	1.980559	1.733845
C	2.215827	2.020398	3.289787
H	7.089179	-2.710419	0.557607
C	3.447723	1.502958	3.721383
H	5.081793	0.193721	3.311533
H	1.688597	2.752406	3.897366
H	3.872494	1.834492	4.666249

N	1.769858	0.246683	0.123912
H	1.045542	1.151297	-3.726904
H	-0.292038	0.947413	-4.830966
C	-0.392050	-0.395957	-3.201628
H	-0.082181	-1.190681	-3.898280
H	-1.481675	-0.472151	-3.093587
C	-0.538919	-1.783685	-1.214496
H	0.153677	-2.326885	-0.555866
H	-0.863735	-2.502520	-1.977221
Zn	-0.030281	1.052846	-0.567207
C	-1.694997	-1.317016	-0.367312
C	-2.771903	-2.203035	-0.031316
C	-2.607042	0.410951	0.939718
C	-3.815269	-1.720402	0.810647
C	-2.820998	-3.531168	-0.509792
C	-2.454680	1.722797	1.422155
C	-3.727255	-0.370390	1.315624
C	-4.881586	-2.585883	1.122055
H	-2.022421	-3.915144	-1.138718
C	-3.874753	-4.357200	-0.181214
C	-3.404744	2.268407	2.260897
H	-1.570096	2.289668	1.121381
C	-4.682181	0.215622	2.170548
C	-4.911403	-3.877488	0.634231
H	-5.694075	-2.240721	1.756196
H	-3.902449	-5.377770	-0.555567
C	-4.525749	1.508543	2.632160
H	-3.285110	3.282900	2.634322
H	-5.555699	-0.353999	2.478043
H	-5.745540	-4.528548	0.887419
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C	-0.776185	2.156851	-3.156501
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H	-0.097340	5.314443	-2.477054
H	0.738749	2.978159	-2.073668
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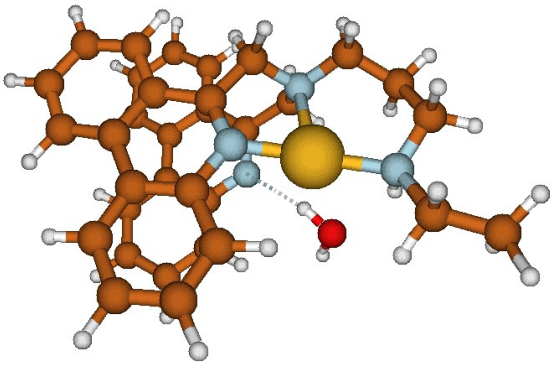
[Cu(I)LH$_2$O]$^+$ t-shape, one phen bound, in SMD water
E= -1769.420 94 a.u.



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C	-0.207899	-0.462741	-1.494135
C	-1.599915	-0.285711	-1.790793
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C	-2.163875	1.018215	-1.670137
C	-2.438487	-1.365947	-2.154938
C	0.980640	2.887885	-0.842526
C	-1.290319	2.117635	-1.338085
C	-3.549382	1.178633	-1.868214
H	-2.022530	-2.361806	-2.283113
C	-3.788692	-1.174671	-2.357420
C	0.522126	4.181484	-0.697132
H	2.036432	2.634501	-0.710042
C	-1.730409	3.447846	-1.177203
C	-4.349414	0.103236	-2.199275
H	-4.000213	2.162447	-1.761755
H	-4.420575	-2.017830	-2.629424
C	-0.844311	4.460202	-0.862152
H	1.217053	4.982488	-0.454048
H	-2.784710	3.686073	-1.299493
H	-5.417578	0.249914	-2.346230
H	-1.209409	5.478182	-0.742673
N	0.593085	0.555485	-1.225136
C	5.126602	0.939529	-0.243720
H	5.175995	1.020525	-1.337134

Cu	2.344060	0.127842	-0.478794
H	4.135581	-0.218243	1.098592
C	2.564954	-2.848680	-0.814861
H	2.790572	-2.645197	-1.870102
H	2.227625	-3.899806	-0.757961
C	3.839536	-2.673502	0.002900
H	4.438902	-3.581286	-0.141486
H	3.616676	-2.640117	1.079629
C	4.731561	-1.496963	-0.370158
H	4.860950	-1.444273	-1.460128
H	5.726946	-1.664999	0.064963
C	0.871643	-2.403150	0.857882
C	-0.303843	-1.552054	1.261369
C	-1.665774	-2.006935	1.129246
C	-0.982215	0.577626	1.911213
C	-2.715252	-1.075827	1.387794
C	-2.000805	-3.323760	0.738979
C	-0.585401	1.881935	2.275918
C	-2.360254	0.275031	1.747905
C	-4.051408	-1.504916	1.259338
H	-1.216557	-4.046779	0.531512
C	-3.318716	-3.714625	0.618924
C	-1.525713	2.875918	2.447426
H	0.478548	2.083561	2.392195
C	-3.297978	1.314285	1.923125
C	-4.349149	-2.800373	0.885562
H	-4.864159	-0.810765	1.459991
H	-3.556931	-4.733785	0.321901
C	-2.889916	2.589333	2.262776
H	-1.212227	3.884627	2.710151
H	-4.358474	1.118685	1.777848
H	-5.388139	-3.111325	0.794904
H	-3.629983	3.377865	2.384371
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H	1.644971	-2.318256	1.630342
H	0.605888	-3.468560	0.781460
H	4.639251	1.851556	0.122240
C	6.516477	0.818986	0.349968
H	6.468982	0.624306	1.429278
H	7.104403	0.019844	-0.114649
H	1.813914	0.257972	2.049099
O	2.634622	0.652730	2.431420
H	2.333252	0.957260	3.301030

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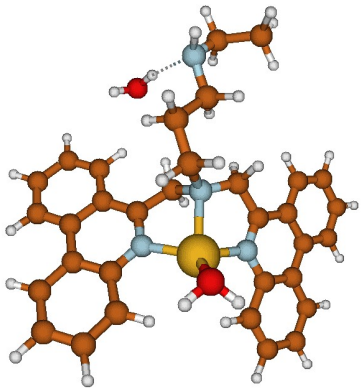
[Cu(I)LH$_2$O]$^+$ see-saw, one phen bound, in SMD water
E= -1769.420 92 a.u.



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C	0.024521	-0.444712	1.360840
C	1.373196	-0.292178	1.822658
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C	2.129379	-1.381077	2.317051
C	-0.995827	2.911295	0.505522
C	1.180497	2.103507	1.283088
C	3.330124	1.131277	2.127526
H	1.673457	-2.363311	2.409600
C	3.444883	-1.213720	2.695804
C	-0.487905	4.188248	0.373326
H	-2.036875	2.681125	0.263091
C	1.672067	3.417004	1.135537
C	4.052693	0.047330	2.587215
H	3.815760	2.102216	2.063135
H	4.013355	-2.063151	3.069549
C	0.857162	4.439342	0.687257
H	-1.127802	4.996754	0.026072
H	2.711848	3.634278	1.369891
H	5.094747	0.175030	2.873379
H	1.261918	5.443529	0.578269
N	-0.722573	0.584080	0.993043
C	-5.238943	0.864049	0.758339

H	-5.028980	0.624517	1.808590
Cu	-2.442412	0.181184	0.120310
H	-4.605277	0.184105	-1.044799
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H	-2.937788	-2.751012	1.362635
H	-2.335062	-3.840557	0.110055
C	-3.897774	-2.479625	-0.540221
H	-4.455215	-3.413326	-0.687799
H	-3.607757	-2.142933	-1.547710
C	-4.859055	-1.475531	0.084766
H	-4.953881	-1.670595	1.162314
H	-5.859110	-1.607159	-0.352626
C	-0.805853	-2.270892	-1.144220
C	0.459694	-1.483108	-1.361454
C	1.758710	-2.018292	-1.033434
C	1.363215	0.587623	-1.934584
C	2.891706	-1.159064	-1.147094
C	1.949981	-3.345856	-0.587403
C	1.107766	1.902129	-2.378760
C	2.681046	0.203224	-1.572911
C	4.165605	-1.666869	-0.822301
H	1.099188	-4.015470	-0.491045
C	3.209239	-3.814888	-0.272939
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C	4.323142	-2.970494	-0.394925
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C	3.428120	2.465139	-2.049535
H	1.920323	3.847858	-2.761613
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H	-1.479647	-2.095036	-1.991617
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O	-2.290815	0.800746	-2.182863

H	-2.809523	0.069936	-2.554817
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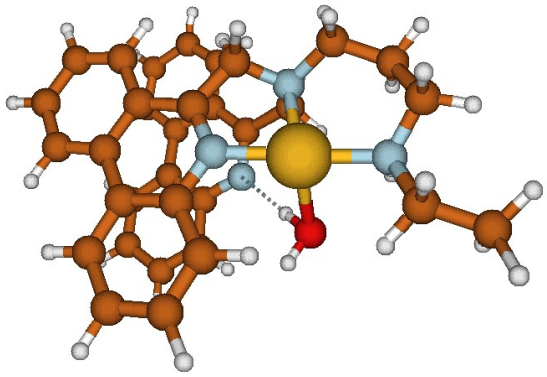
$[Cu(II)LH_2O]^{2+}$ see-saw, one phen bound, in SMD water
E= -1769.282 97 a.u.



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H	2.034927	2.789124	-0.723534
C	-1.770676	3.468902	-1.107679
C	-4.273126	0.045787	-2.181871
H	-4.006884	2.107666	-1.701526
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C	-0.912875	4.505028	-0.791974
H	1.136905	5.097112	-0.424935
H	-2.832502	3.675226	-1.220886
H	-5.346155	0.155146	-2.324868
H	-1.308364	5.509447	-0.658257
N	0.628620	0.655194	-1.184749

C	5.088240	0.935440	-0.003947
H	5.308971	0.951072	-1.077891
Cu	2.405808	0.208514	-0.402354
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H	2.201946	-3.745960	-0.775446
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H	4.508507	-3.607173	-0.261549
H	3.715427	-2.803842	1.074872
C	4.819174	-1.509838	-0.255257
H	4.999539	-1.382644	-1.330512
H	5.794456	-1.666200	0.224745
C	1.123373	-2.049622	0.943280
C	-0.196228	-1.396269	1.269946
C	-1.449852	-2.081216	1.077870
C	-1.268341	0.571580	1.914008
C	-2.656482	-1.355130	1.304920
C	-1.529095	-3.427548	0.653717
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C	-2.750549	-4.040297	0.465948
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C	-3.676868	0.880403	1.849733
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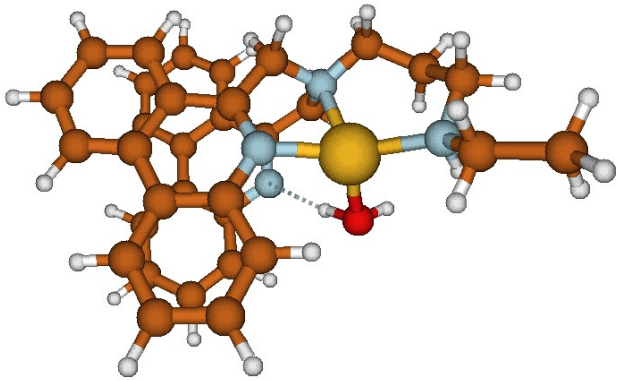
H	-4.819794	-1.475018	1.284256
H	-2.792520	-5.077335	0.140778
C	-3.514413	2.202812	2.213343
H	-2.112638	3.769873	2.734259
H	-4.679904	0.499991	1.669581
H	-4.899317	-3.812518	0.553525
H	-4.387548	2.843530	2.317760
N	-0.122473	-0.163524	1.719161
H	1.876850	-1.691653	1.652183
H	1.069588	-3.139970	1.049715
H	4.480730	1.821504	0.218735
C	6.356510	0.951169	0.821786
H	6.127148	0.879820	1.892284
H	7.033443	0.130868	0.559401
H	1.447348	0.770782	1.782472

O	2.303859	1.250533	1.603314
H	2.016131	2.161337	1.428893
H	6.893415	1.891183	0.655915

[Zn(II)LH$_2$O]$^{2+}$ see-saw, one phen bound, in SMD water

E= -1799.098 11 a.u.

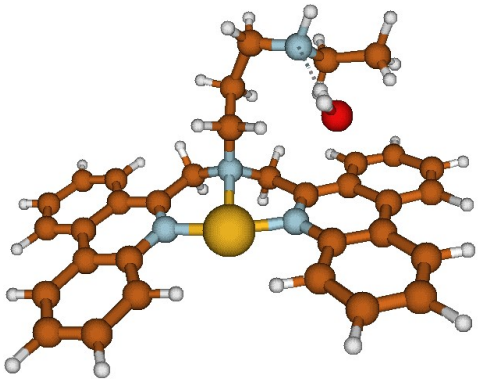


N	4.465675	-0.028704	0.049162
N	1.591731	-1.805516	-0.064316
C	0.669528	-1.788751	-1.220706
H	-0.043294	-2.619693	-1.160481
H	1.266034	-1.953154	-2.127126
C	-0.033758	-0.457385	-1.356336
C	-1.375097	-0.354551	-1.852307
C	0.082918	1.857683	-0.964185
C	-2.020268	0.915642	-1.806967
C	-2.080378	-1.478222	-2.339223
C	0.863407	2.936841	-0.511838
C	-1.270155	2.056154	-1.338075
C	-3.367991	0.999170	-2.208456
H	-1.588308	-2.445010	-2.406919
C	-3.392563	-1.359810	-2.744182
C	0.313211	4.198175	-0.409882
H	1.901888	2.750311	-0.233017
C	-1.805241	3.354612	-1.216859
C	-4.041472	-0.116797	-2.663888
H	-3.888745	1.952433	-2.166038
H	-3.927487	-2.231550	-3.114743
C	-1.030437	4.404403	-0.761307
H	0.917643	5.028724	-0.052245
H	-2.844245	3.539167	-1.479814
H	-5.082302	-0.029592	-2.968679
H	-1.466827	5.396874	-0.671802

N	0.654961	0.600381	-0.986907
C	5.180512	0.929084	-0.833092
H	4.912919	0.673708	-1.865229
Zn	2.428720	0.213738	0.039934
H	4.697767	0.222639	1.014304
C	2.712881	-2.761223	-0.289096
H	2.954337	-2.728971	-1.357999
H	2.358578	-3.780469	-0.070841
C	3.971756	-2.449457	0.511606
H	4.532525	-3.385496	0.618125
H	3.724412	-2.134172	1.537059
C	4.904031	-1.436103	-0.138659
H	4.959250	-1.615475	-1.220338
H	5.918626	-1.551883	0.262582
C	0.890068	-2.172913	1.208639
C	-0.404252	-1.427701	1.419363
C	-1.680126	-2.010542	1.084150
C	-1.385926	0.616591	1.969219
C	-2.841224	-1.185417	1.167941
C	-1.822358	-3.351032	0.657831
C	-1.179659	1.941890	2.405515
C	-2.682910	0.185419	1.586422
C	-4.091481	-1.734862	0.819705
H	-0.951459	-3.998135	0.591494
C	-3.059867	-3.861876	0.325137
C	-2.228832	2.836024	2.435337
H	-0.174657	2.242298	2.698539
C	-3.734288	1.124789	1.620815
C	-4.199950	-3.047602	0.406503
H	-4.987177	-1.120848	0.875536
H	-3.150230	-4.896408	0.001616
C	-3.511604	2.424058	2.033377
H	-2.062408	3.861912	2.758054
H	-4.735369	0.831183	1.312873
H	-5.175177	-3.451341	0.141698
H	-4.336451	3.133529	2.046088
N	-0.286469	-0.206299	1.888828
H	1.573885	-1.942067	2.032422
H	0.729883	-3.258371	1.212716
H	4.761630	1.920606	-0.625968
C	6.682090	0.936766	-0.647170
H	6.949649	1.119926	0.401158
H	7.142241	-0.007773	-0.958244

H	1.307307	0.525969	2.131730
O	2.231492	0.903500	2.006974
H	2.800596	0.318089	2.536776
H	7.126763	1.735507	-1.250465

$[Cu(I)LH_2O]^+$ t-shape, two phen bound, in SMD water
E= -1769.405 91 a.u.



C	-4.862055	-2.652757	1.338868
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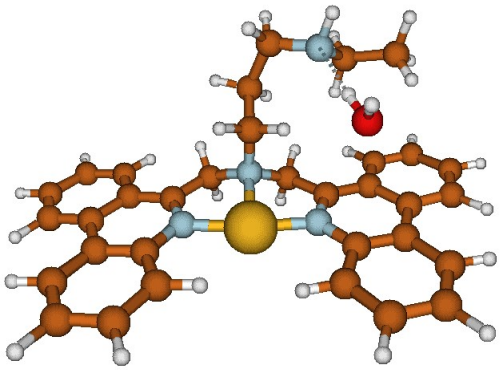
H	-5.493703	-2.953355	0.495290
C	-3.462128	-3.204823	1.187179
H	-3.002538	-2.805243	0.271149
H	-3.494461	-4.304400	1.064477
N	-2.617583	-2.822995	2.325273
H	-3.114523	-3.116285	3.165605
C	-1.332008	-3.538484	2.331484
H	-1.490764	-4.631780	2.354747
H	-0.814580	-3.271850	3.263049
C	-0.453416	-3.199927	1.136281
H	0.466324	-3.794847	1.208907
H	-0.950482	-3.529519	0.213127
C	-0.122978	-1.710709	1.051200
H	-0.992201	-1.118306	1.363959
H	0.685894	-1.461584	1.752674
N	0.268855	-1.219497	-0.275358
C	1.549945	-1.720301	-0.740739
C	-0.833148	-1.209740	-1.226751
H	1.761190	-2.710277	-0.310630
H	-0.423965	-1.088649	-2.239419
H	-1.379268	-2.164689	-1.228026
C	-1.802887	-0.066224	-0.970250
C	-3.197258	-0.188671	-1.293206

C	-2.111296	2.135545	-0.197722
C	-4.070489	0.900306	-1.002952
C	-3.728874	-1.351600	-1.898717
C	-1.509866	3.286877	0.342104
C	-3.507434	2.100079	-0.431793
C	-5.442220	0.765898	-1.293626
H	-3.075910	-2.181714	-2.153467
C	-5.074005	-1.447782	-2.186897
C	-2.273523	4.393615	0.651056
H	-0.428773	3.269600	0.506498
C	-4.263074	3.243591	-0.101203
C	-5.936349	-0.386291	-1.872288
H	-6.124633	1.581938	-1.069632
H	-5.465003	-2.348297	-2.655384
C	-3.659860	4.367949	0.428337
H	-1.803924	5.281839	1.067984
H	-5.337946	3.246752	-0.265604
H	-6.999237	-0.467072	-2.090812
H	-4.264509	5.238104	0.674882
N	-1.296554	1.050413	-0.474994
H	1.519787	-1.876409	-1.827962
C	2.720724	-0.797872	-0.434582
C	4.062961	-1.293298	-0.575432
C	3.511491	1.321273	0.210995
C	5.155608	-0.427614	-0.287587
C	4.323759	-2.613738	-1.007112
C	3.179691	2.632151	0.596804
C	4.867771	0.924195	0.128909
C	6.466667	-0.921785	-0.428282
H	3.501280	-3.281914	-1.247415
C	5.618965	-3.068883	-1.141518
C	4.169601	3.544756	0.899780
H	2.120347	2.897345	0.645764
C	5.858283	1.875904	0.446745
C	6.695035	-2.217978	-0.846267
H	7.314853	-0.277680	-0.210774
H	5.804880	-4.086654	-1.477075
C	5.517740	3.160463	0.824833
H	3.905906	4.557425	1.197004
H	6.909004	1.600599	0.394624
H	7.716280	-2.579147	-0.948990
H	6.300301	3.876823	1.065330
N	2.471111	0.448691	-0.078218

Cu	0.609181	1.017234	-0.122432
H	-5.335143	-3.024156	2.257586
H	-2.776298	-0.949535	2.364432
O	-2.942536	0.029725	2.376308
H	-2.619563	0.290618	3.250920

$[Cu(II)LH_2O]^{2+}$ t-shape, two phen bound, in SMD water
E= -1769.257 90 a.u.

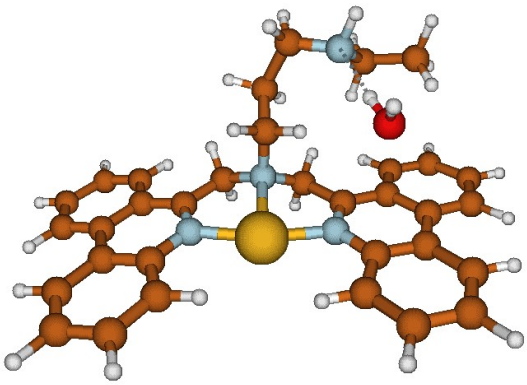


C	-4.626227	-2.822594	1.569224
H	-4.709248	-1.728933	1.536228
H	-5.282845	-3.236575	0.795673
C	-3.199383	-3.277170	1.355799
H	-2.831990	-2.900711	0.389337
H	-3.152162	-4.380961	1.297479
N	-2.311357	-2.768108	2.409254
H	-2.729080	-3.035447	3.299811
C	-0.984655	-3.397188	2.367391
H	-1.066039	-4.496803	2.430573
H	-0.431769	-3.066732	3.256218
C	-0.195715	-3.056080	1.110199
H	0.767330	-3.578190	1.158452
H	-0.716584	-3.458465	0.231647
C	0.018217	-1.552810	0.975896
H	-0.867852	-1.008468	1.320781
H	0.857621	-1.227327	1.601216
N	0.287692	-1.070498	-0.411379
C	1.546860	-1.601494	-0.972186
C	-0.892614	-1.211064	-1.289981
H	1.677623	-2.646967	-0.668153
H	-0.562254	-1.112168	-2.331505
H	-1.327675	-2.211268	-1.187425
C	-1.889753	-0.123454	-0.996652

C	-3.291208	-0.277460	-1.227826
C	-2.167120	2.111330	-0.289488
C	-4.154348	0.817875	-0.929338
C	-3.834318	-1.480093	-1.734397
C	-1.540634	3.291552	0.147025
C	-3.572692	2.051889	-0.457535
C	-5.539216	0.648810	-1.117977
H	-3.178588	-2.309675	-1.987080
C	-5.193915	-1.609165	-1.919134
C	-2.298577	4.410497	0.423860
H	-0.452984	3.303736	0.250120
C	-4.317317	3.210901	-0.161782
C	-6.048160	-0.541648	-1.598986
H	-6.221463	1.462620	-0.886523
H	-5.604206	-2.538315	-2.307501
C	-3.693791	4.365560	0.270232
H	-1.815692	5.325789	0.758088
H	-5.397769	3.203084	-0.280449
H	-7.121966	-0.649863	-1.736344
H	-4.289721	5.248540	0.489566
N	-1.377117	1.010718	-0.555578
H	1.476946	-1.597732	-2.067144
C	2.719871	-0.756201	-0.556000
C	4.063863	-1.231288	-0.666850
C	3.443759	1.333853	0.263057
C	5.129402	-0.362965	-0.289870
C	4.351332	-2.522731	-1.161762
C	3.065164	2.602127	0.733767
C	4.807038	0.955328	0.203312
C	6.450756	-0.831040	-0.419551
H	3.542814	-3.183698	-1.463776
C	5.656409	-2.950090	-1.278984
C	4.028000	3.502188	1.140866
H	2.002533	2.843968	0.776808
C	5.765708	1.896801	0.628580
C	6.707902	-2.098529	-0.904125
H	7.284092	-0.190881	-0.142443
H	5.870761	-3.944488	-1.663027
C	5.384618	3.143949	1.085252
H	3.736821	4.483847	1.507233
H	6.822522	1.643383	0.602520
H	7.737091	-2.438807	-0.996778
H	6.143776	3.852497	1.408428

N	2.446354	0.464587	-0.135772
Cu	0.545691	0.952524	-0.233301
H	-5.007142	-3.158868	2.542553
H	-2.638944	-0.911851	2.340164
O	-2.879855	0.048986	2.290105
H	-2.814696	0.336169	3.212245

[Zn(II)LH$_2$O]$^{2+}$ t-shape, two phen bound, in SMD water
E= -1799.070 02 a.u.



C	-4.731632	-2.921931	1.353404
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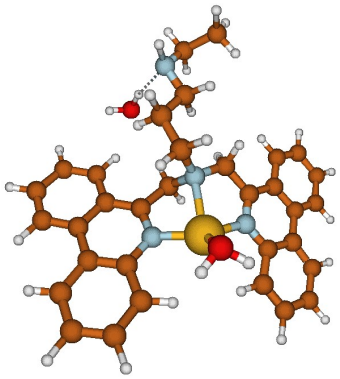
H	-5.307583	-3.345441	0.522977
C	-3.281139	-3.342310	1.264928
H	-2.845968	-2.967870	0.326494
H	-3.202158	-4.445417	1.225614
N	-2.499500	-2.796437	2.382170
H	-2.986728	-3.066717	3.235776
C	-1.155890	-3.385391	2.466099
H	-1.212598	-4.486313	2.539525
H	-0.696113	-3.028007	3.396990
C	-0.265334	-3.030797	1.283795
H	0.695034	-3.542963	1.421218
H	-0.696161	-3.447849	0.363094
C	-0.052319	-1.526467	1.140409
H	-0.956503	-0.984980	1.443672
H	0.753359	-1.188432	1.804934
N	0.280871	-1.054579	-0.229224
C	1.529769	-1.625926	-0.738533
C	-0.858042	-1.185114	-1.143168
H	1.690671	-2.635437	-0.338672
H	-0.489756	-1.135305	-2.176183
H	-1.345222	-2.161791	-1.034398

C	-1.859965	-0.071037	-0.947367
C	-3.246081	-0.251142	-1.267460
C	-2.230386	2.158048	-0.277699
C	-4.149972	0.822654	-1.020793
C	-3.733865	-1.456790	-1.820818
C	-1.665374	3.352791	0.200726
C	-3.625684	2.063180	-0.502848
C	-5.516302	0.630820	-1.301239
H	-3.051282	-2.273397	-2.039903
C	-5.075111	-1.607784	-2.102735
C	-2.467483	4.442806	0.468622
H	-0.585955	3.397045	0.355255
C	-4.419761	3.190748	-0.213362
C	-5.969981	-0.561573	-1.829403
H	-6.226091	1.431467	-1.110286
H	-5.438608	-2.538527	-2.531936
C	-3.853499	4.357032	0.263283
H	-2.026375	5.364497	0.841040
H	-5.495065	3.147092	-0.367307
H	-7.029848	-0.686865	-2.041079
H	-4.486997	5.213869	0.481241
N	-1.395034	1.079137	-0.506263
H	1.458875	-1.743962	-1.827623
C	2.735223	-0.765943	-0.438867
C	4.057289	-1.282392	-0.648627
C	3.588005	1.309675	0.277534
C	5.174746	-0.447564	-0.364995
C	4.266915	-2.582803	-1.157862
C	3.292814	2.602411	0.742210
C	4.931224	0.885081	0.134942
C	6.467708	-0.955019	-0.595774
H	3.418517	-3.220709	-1.391565
C	5.545180	-3.049865	-1.379545
C	4.312373	3.472602	1.069880
H	2.245408	2.896469	0.838947
C	5.950729	1.794517	0.480325
C	6.648231	-2.230273	-1.094282
H	7.338832	-0.338346	-0.390491
H	5.697567	-4.049973	-1.778286
C	5.648330	3.061989	0.939726
H	4.080903	4.471786	1.431628
H	6.992954	1.498952	0.388477
H	7.656149	-2.600567	-1.269588

H	6.452722	3.745369	1.202138
N	2.533076	0.465341	-0.025383
Zn	0.592183	1.113264	-0.038360
H	-5.188405	-3.272257	2.288394
H	-2.831393	-0.953039	2.275872
O	-3.081657	0.006552	2.225578
H	-3.039345	0.287498	3.150870

$[Cu(I)L(H_2O)_2]^+$ distorted tetrahedral, two phen bound, in SMD water
E= -1845.829 76 a.u.



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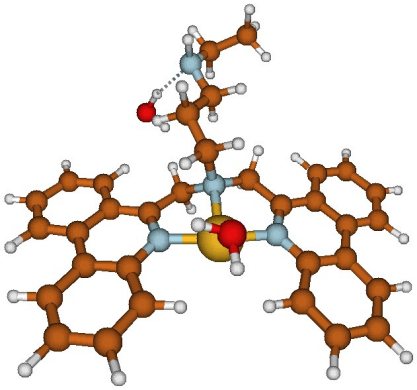
C	1.344757	1.296872	0.272258
H	1.355437	2.021196	-0.557897
H	1.691390	1.855915	1.152783
C	2.365637	0.216952	-0.021805
C	3.691562	0.610299	-0.415057
C	4.056924	1.970686	-0.530547
C	4.662177	-0.395487	-0.679391
C	2.938248	-2.053994	-0.130658
C	5.336302	2.327784	-0.904100
H	3.328770	2.750367	-0.319686
C	5.957521	-0.001622	-1.066176
C	4.268706	-1.777559	-0.530942
C	2.513874	-3.386083	0.030698
C	6.289106	1.334871	-1.178548
H	5.604492	3.378673	-0.987743
H	6.713331	-0.753525	-1.279483
C	5.135827	-2.866162	-0.755159
H	1.478633	-3.566398	0.333967
C	3.383807	-4.433556	-0.198112

H	7.296218	1.617051	-1.478691
C	4.704249	-4.168761	-0.592799
H	6.163849	-2.684784	-1.060050
H	3.046009	-5.460158	-0.073377
H	5.392723	-4.991634	-0.773173
N	2.014622	-1.045974	0.117157
H	-2.086130	2.784797	0.662692
H	-1.810333	3.109625	2.364653
C	-0.705213	1.438082	1.656860
H	-1.515917	0.755722	1.952800
H	0.004387	1.457414	2.494238
C	-0.813813	0.764439	-0.699636
H	-0.172114	0.355290	-1.494223
H	-1.108109	1.772941	-1.025441
Cu	0.151349	-1.489932	0.696731
C	-1.992495	-0.168858	-0.547530
C	-3.338248	0.187951	-0.885130
C	-2.634040	-2.352092	0.033232
C	-4.366246	-0.789503	-0.727395
C	-3.683663	1.476655	-1.353815
C	-2.219579	-3.623352	0.472649
C	-3.998006	-2.105688	-0.261775
C	-5.692883	-0.432794	-1.036440
H	-2.914507	2.232572	-1.487940
C	-4.992617	1.796315	-1.646565
C	-3.137767	-4.640420	0.633890
H	-1.155414	-3.772799	0.669959
C	-4.914166	-3.163060	-0.082523
C	-6.003505	0.835880	-1.486155
H	-6.489599	-1.163567	-0.921675
H	-5.238081	2.795316	-2.002439
C	-4.494555	-4.403764	0.357321
H	-2.812801	-5.622237	0.971593
H	-5.969676	-3.006911	-0.293678
H	-7.036224	1.088351	-1.718006
H	-5.221037	-5.203308	0.486343
N	-1.667907	-1.371973	-0.101479
C	-0.297104	3.900718	1.064125
H	0.161581	3.683397	0.087431
H	0.526839	3.911009	1.801045
C	-0.052375	6.260865	0.482633
H	0.272280	5.994731	-0.533920
H	-0.646801	7.178289	0.387775

C	1.158229	6.519625	1.361959
H	1.722707	7.384978	0.995089
H	0.857824	6.731769	2.396474
H	-1.316235	5.458149	1.856477
H	1.844643	5.664327	1.379633
H	-0.587449	-2.885460	2.771307
H	0.923893	-2.692456	2.820662
O	0.093342	-2.192962	2.756541
H	-1.881232	4.792575	-0.638137
O	-2.143226	4.533895	-1.557990
H	-3.101925	4.421540	-1.485267

$[Cu(II)L(H_2O)_2]^{2+}$ see-saw, two phen bound, in SMD water
E= -1845.682 99 a.u.



N	-0.889950	4.968900	1.356307
C	-0.976303	2.543424	1.612113
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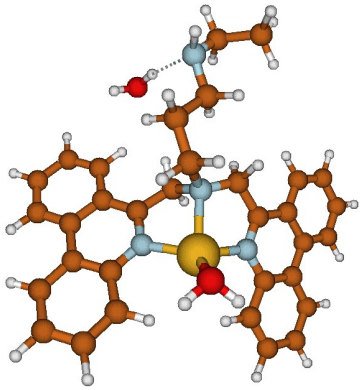
C	1.296547	1.270746	-0.403705
H	1.185775	1.649359	-1.427755
H	1.591351	2.129292	0.211044
C	2.395446	0.246193	-0.367324
C	3.741927	0.629534	-0.667503
C	4.069511	1.962174	-1.001266
C	4.761663	-0.361332	-0.623537
C	3.027895	-1.998856	-0.030030
C	5.373672	2.310523	-1.281168
H	3.291724	2.721156	-1.041570
C	6.084609	0.026995	-0.909128
C	4.390968	-1.718843	-0.299111
C	2.611497	-3.310360	0.260013
C	6.383300	1.336127	-1.232205
H	5.619438	3.338119	-1.538078

H	6.885772	-0.706749	-0.877197
C	5.306607	-2.788677	-0.251074
H	1.553515	-3.507066	0.438156
C	3.533921	-4.336534	0.298011
H	7.412487	1.613483	-1.450073
C	4.888505	-4.071311	0.045364
H	6.359038	-2.608428	-0.455654
H	3.208656	-5.350500	0.519162
H	5.613816	-4.881277	0.074894
N	2.073457	-0.995012	-0.062184
H	-1.965255	2.556420	1.130531
H	-1.169018	2.669522	2.686785
C	-0.333497	1.173418	1.467815
H	-1.013348	0.420770	1.885564
H	0.602884	1.107746	2.034007
C	-1.115836	0.935282	-0.876492
H	-0.732676	0.752079	-1.888658
H	-1.467899	1.974237	-0.854991
Cu	0.159345	-1.318514	0.258693
C	-2.206381	-0.063964	-0.600926
C	-3.586795	0.192110	-0.871650
C	-2.665967	-2.273146	0.083001
C	-4.533449	-0.845968	-0.626104
C	-4.030111	1.439740	-1.364014
C	-2.141470	-3.503396	0.517304
C	-4.056589	-2.118470	-0.140908
C	-5.894038	-0.585655	-0.876902
H	-3.318474	2.239904	-1.546614
C	-5.369383	1.662090	-1.601713
C	-2.983356	-4.571153	0.749498
H	-1.063740	-3.589376	0.653733
C	-4.890220	-3.226713	0.111413
C	-6.303427	0.643596	-1.354659
H	-6.636967	-1.357909	-0.695516
H	-5.700684	2.628344	-1.975138
C	-4.365836	-4.426930	0.550081
H	-2.576204	-5.523283	1.081933
H	-5.962481	-3.143062	-0.046099
H	-7.360600	0.822561	-1.539579
H	-5.029763	-5.268192	0.735636
N	-1.788780	-1.229866	-0.142713
C	-0.159095	3.723577	1.117138
H	0.006810	3.658697	0.029704

H	0.839183	3.709542	1.590749
C	-0.175097	6.153411	0.862879
H	-0.083357	6.043402	-0.227398
H	-0.827971	7.018495	1.033588
C	1.187790	6.410544	1.480388
H	1.600315	7.361149	1.122377
H	1.118881	6.467606	2.574661
H	-1.010005	5.067759	2.364476
H	1.909884	5.624085	1.229983
H	-0.654129	-1.920427	2.630859
H	0.383430	-3.000272	2.344794
O	0.267917	-2.035614	2.344063
H	-2.137567	4.671666	0.000793
H	-1.860469	4.196834	-1.425060
O	-2.592817	4.474550	-0.856335

[Zn(II)L(H_2O)$_2$]$^{2+}$ distorted tetrahedral, two phen bound, in SMD water
E= -1875.505 43 a.u.



N	-0.730020	5.232102	1.143049
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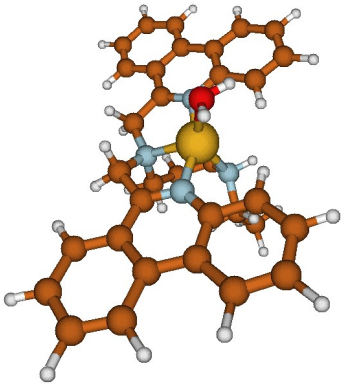
C	1.395009	1.285602	0.326063
H	1.386389	2.030231	-0.481027
H	1.791334	1.802487	1.210078
C	2.358949	0.181073	-0.034746
C	3.662718	0.511330	-0.537772
C	4.069459	1.852266	-0.711790
C	4.562004	-0.545068	-0.855924
C	2.828592	-2.121102	-0.128856
C	5.325899	2.144896	-1.199385
H	3.393693	2.665070	-0.455807
C	5.835654	-0.214639	-1.357378

C	4.130550	-1.906992	-0.643168
C	2.361594	-3.426282	0.106245
C	6.208966	1.104128	-1.526686
H	5.631614	3.180245	-1.329921
H	6.539588	-1.002012	-1.613968
C	4.930517	-3.036428	-0.908475
H	1.352246	-3.558762	0.501352
C	3.168291	-4.513529	-0.160797
H	7.198057	1.336293	-1.916032
C	4.459816	-4.314095	-0.672642
H	5.935134	-2.907915	-1.303818
H	2.802382	-5.521220	0.022601
H	5.096023	-5.170255	-0.885480
N	1.983525	-1.061792	0.155620
H	-2.013227	2.862373	0.968326
H	-1.524911	3.166789	2.623581
C	-0.593541	1.451895	1.808920
H	-1.410490	0.791994	2.130007
H	0.162731	1.423105	2.602345
C	-0.823341	0.888042	-0.580858
H	-0.213667	0.594544	-1.446727
H	-1.144370	1.919765	-0.766259
Zn	0.106678	-1.369888	0.974067
C	-1.987868	-0.069465	-0.503150
C	-3.279875	0.238842	-1.039007
C	-2.680809	-2.228961	0.135608
C	-4.306665	-0.748108	-0.952649
C	-3.565464	1.488655	-1.632473
C	-2.315698	-3.453756	0.724144
C	-3.997086	-2.021132	-0.346244
C	-5.581508	-0.437029	-1.464081
H	-2.795648	2.251482	-1.705510
C	-4.825618	1.765116	-2.117670
C	-3.246622	-4.463924	0.850088
H	-1.287172	-3.586301	1.066451
C	-4.925141	-3.072026	-0.199406
C	-5.836459	0.794749	-2.033911
H	-6.381193	-1.171317	-1.412365
H	-5.032459	2.734693	-2.565890
C	-4.558474	-4.267087	0.388540
H	-2.965546	-5.410760	1.305541
H	-5.946279	-2.947018	-0.550877
H	-6.830252	1.013122	-2.419265

H	-5.292774	-5.062758	0.492523
N	-1.724617	-1.239013	0.042188
C	-0.136601	3.893049	1.154597
H	0.167472	3.677528	0.118879
H	0.781434	3.837825	1.766909
C	0.145056	6.227183	0.507131
H	0.215849	5.959556	-0.557429
H	-0.376912	7.191014	0.551002
C	1.537096	6.367073	1.097660
H	2.078218	7.189757	0.615549
H	1.492250	6.580717	2.173683
H	-0.875813	5.512507	2.112860
H	2.134576	5.457231	0.960415
H	-0.526105	-2.690383	3.022260
H	0.999774	-2.513576	3.007262
O	0.167761	-2.016460	2.914393
H	-1.985219	4.895799	-0.191948
O	-2.478909	4.619048	-1.005725
H	-3.276986	4.212029	-0.639727

[Cu(II)LH$_2$O]$^{2+}$ distorted square pyramidal, in SMD water
E= -1769.269 34 a.u.



C	-1.024874	2.205245	3.903754
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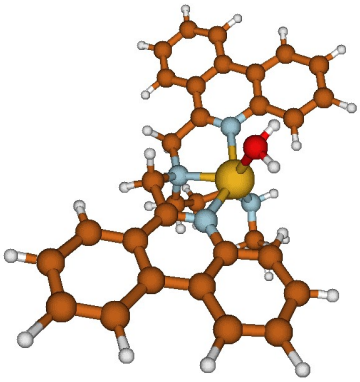
H	-2.003782	2.492961	4.303134
C	-1.197856	1.568076	2.538578
H	-1.797981	2.222621	1.896912
H	-1.752457	0.626210	2.626074
N	0.064160	1.307416	1.808894
H	0.482259	2.221933	1.628073
C	1.070477	0.548833	2.581871
H	1.263920	1.038669	3.546882

H	2.006389	0.624974	2.022158
C	0.717843	-0.920406	2.833572
H	1.656492	-1.490594	2.869299
H	0.278051	-1.025209	3.834333
C	-0.268575	-1.617780	1.911510
H	-0.347974	-2.672312	2.223371
H	-1.270121	-1.186841	2.025835
N	0.023827	-1.589287	0.456986
C	1.322840	-2.193439	0.121200
C	-1.114626	-2.188174	-0.261409
H	1.640581	-2.874708	0.922303
H	-0.804646	-2.413778	-1.290972
H	-1.400388	-3.139930	0.206290
C	-2.273931	-1.223966	-0.325155
C	-3.632028	-1.665853	-0.438678
C	-2.915956	1.039762	-0.479863
C	-4.660696	-0.685333	-0.555139
C	-3.972842	-3.037299	-0.442627
C	-2.492715	2.381330	-0.544860
C	-4.289930	0.709635	-0.586818
C	-5.996136	-1.121926	-0.650048
H	-3.196137	-3.792985	-0.364558
C	-5.289172	-3.432485	-0.547779
C	-3.418946	3.391434	-0.702686
H	-1.425280	2.599976	-0.464889
C	-5.210701	1.766570	-0.739851
C	-6.303988	-2.467838	-0.645488
H	-6.801024	-0.396304	-0.731335
H	-5.540110	-4.490491	-0.549995
C	-4.784957	3.079254	-0.795810
H	-3.091010	4.427152	-0.753492
H	-6.273312	1.552653	-0.822973
H	-7.342962	-2.781710	-0.720579
H	-5.514447	3.876778	-0.917512
N	-1.958007	0.057028	-0.330615
H	1.214580	-2.815964	-0.776836
C	2.385139	-1.157374	-0.143515
C	3.765367	-1.534352	-0.240963
C	2.902959	1.105245	-0.546446
C	4.737385	-0.525550	-0.492652
C	4.170746	-2.880342	-0.108313
C	2.416459	2.419758	-0.677782
C	4.292029	0.840304	-0.640757

C	6.089447	-0.906821	-0.589647
H	3.431545	-3.657096	0.069157
C	5.502047	-3.223579	-0.214260
C	3.289650	3.463758	-0.907126
H	1.340978	2.596234	-0.594554
C	5.156734	1.927923	-0.875802
C	6.463425	-2.229344	-0.453491
H	6.853847	-0.157687	-0.778233
H	5.806013	-4.262807	-0.114017
C	4.666889	3.213165	-1.006743
H	2.910087	4.477980	-1.008074
H	6.228042	1.760146	-0.954185
H	7.513748	-2.501329	-0.534107
H	5.355332	4.035812	-1.186410
N	1.994197	0.089441	-0.309135
Cu	0.010915	0.420532	-0.242930
H	-0.563995	1.523316	4.627531
H	-0.891364	1.004838	-2.649651
H	0.468089	1.685002	-2.498532
O	0.022543	0.830389	-2.366890

[Zn(II)LH$_2$O]$^{2+}$ distorted square pyramidal, in SMD water
E= -1799.090 37 a.u.

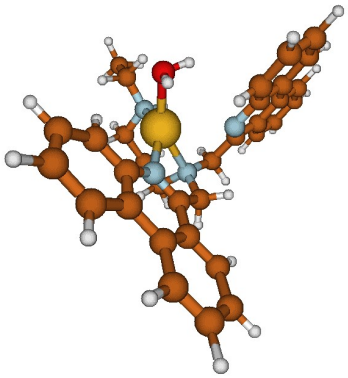


C	-0.759368	3.227368	3.673867
H	-0.037058	4.033367	3.492252
H	-1.695579	3.686700	4.009063
C	-1.006367	2.421535	2.415973
H	-1.495226	3.044131	1.659536
H	-1.683144	1.581793	2.616920
N	0.222542	1.875671	1.786690
H	0.798581	2.675700	1.516894
C	1.058167	1.065356	2.709174

H	1.426444	1.693618	3.531126
H	1.942757	0.762286	2.139743
C	0.362990	-0.150900	3.305447
H	1.150518	-0.753752	3.775085
H	-0.293631	0.162766	4.128420
C	-0.493020	-1.021465	2.391926
H	-0.652219	-2.001047	2.871573
H	-1.485802	-0.570539	2.274125
N	0.021610	-1.225715	1.014521
C	1.349854	-1.858237	0.976421
C	-0.956455	-2.024311	0.256749
H	1.728290	-1.986668	2.000321
H	-0.482848	-2.350851	-0.680163
H	-1.210847	-2.932492	0.821582
C	-2.193133	-1.237430	-0.094304
C	-3.444032	-1.887384	-0.363607
C	-3.096167	0.877796	-0.549573
C	-4.564840	-1.080505	-0.714338
C	-3.588073	-3.291060	-0.302441
C	-2.852955	2.258580	-0.668415
C	-4.385827	0.349459	-0.807322
C	-5.795881	-1.714834	-0.970171
H	-2.735372	-3.916817	-0.051510
C	-4.804482	-3.883767	-0.567997
C	-3.875144	3.116466	-1.019520
H	-1.841434	2.623587	-0.480943
C	-5.411025	1.251287	-1.156969
C	-5.913220	-3.088726	-0.897671
H	-6.667525	-1.121647	-1.234672
H	-4.904511	-4.965570	-0.519606
C	-5.161963	2.606688	-1.257899
H	-3.685440	4.183526	-1.112042
H	-6.414061	0.880683	-1.355002
H	-6.873753	-3.557883	-1.100774
H	-5.969630	3.282773	-1.529564
N	-2.044757	0.063452	-0.185459
H	1.272776	-2.874694	0.569783
C	2.379409	-1.069159	0.204375
C	3.691940	-1.618938	-0.000108
C	2.987730	0.953338	-0.803566
C	4.666101	-0.829679	-0.673066
C	4.028698	-2.915608	0.443168
C	2.603282	2.271157	-1.116202

C	4.307137	0.511483	-1.072174
C	5.942448	-1.381962	-0.894321
H	3.290913	-3.520171	0.964814
C	5.290178	-3.427466	0.219714
C	3.499352	3.136643	-1.711809
H	1.592204	2.593490	-0.859165
C	5.197097	1.415139	-1.685686
C	6.247834	-2.655950	-0.456633
H	6.701987	-0.802927	-1.413562
H	5.540726	-4.427997	0.564565
C	4.800445	2.700063	-2.005396
H	3.199204	4.155243	-1.947386
H	6.216708	1.105934	-1.903791
H	7.241018	-3.062355	-0.636451
H	5.506820	3.380340	-2.475926
N	2.050968	0.129988	-0.208221
Zn	-0.028237	0.760776	0.017747
H	-0.381931	2.609897	4.497102
H	-0.779418	1.465573	-2.443472
H	0.734338	1.258365	-2.518266
O	-0.077942	0.848590	-2.175183

[Cu(I)LH$_2$O]$^+$ distorted trigonal bipyramidal, in SMD water
E= -1769.404 56 a.u.



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C	0.444977	2.928333	-2.591945
N	0.200200	0.508268	-1.850760
C	1.598328	0.150894	-2.033695
H	1.741086	-0.487500	-2.926963
H	2.168528	1.064526	-2.238789
C	2.214750	-0.527049	-0.835379
C	3.625125	-0.830849	-0.863743

C	4.431895	-0.532172	-1.982779
C	4.213989	-1.432744	0.281338
C	1.977736	-1.429705	1.288784
C	5.783350	-0.812748	-1.972436
H	3.987507	-0.077593	-2.865261
C	5.596614	-1.704474	0.266213
C	3.357131	-1.749524	1.400660
C	1.097047	-1.772525	2.334997
C	6.366992	-1.400454	-0.839229
H	6.395300	-0.577584	-2.840655
H	6.068618	-2.161901	1.132559
C	3.808921	-2.372657	2.581211
H	0.037518	-1.548366	2.210772
C	1.565060	-2.389649	3.478688
H	7.432921	-1.619530	-0.830355
C	2.931982	-2.683239	3.603851
H	4.862490	-2.620702	2.693291
H	0.875816	-2.650745	4.279145
H	3.303505	-3.165958	4.505442
N	1.439598	-0.801807	0.183121
H	1.527760	2.841306	-2.762342
H	0.081336	3.560369	-3.412197
C	-0.241842	1.580708	-2.761306
H	-0.124721	1.251676	-3.811426
H	-1.320864	1.703311	-2.590828
C	-0.669846	-0.656592	-1.995770
H	-0.109018	-1.559288	-1.720467
H	-0.949204	-0.789061	-3.056093
Cu	-0.319124	1.338575	0.229244
C	-1.915875	-0.595394	-1.149709
C	-2.915120	-1.615019	-1.278449
C	-3.150425	0.504535	0.509891
C	-4.069269	-1.562483	-0.445226
C	-2.769232	-2.687102	-2.188910
C	-3.242645	1.616268	1.367725
C	-4.194316	-0.453817	0.474092
C	-5.032137	-2.582762	-0.557735
H	-1.890177	-2.739355	-2.827215
C	-3.726775	-3.676949	-2.272127
C	-4.335052	1.775571	2.198115
H	-2.422981	2.339124	1.353114
C	-5.293411	-0.269903	1.337476
C	-4.865799	-3.622656	-1.453455

H	-5.922433	-2.558986	0.066462
H	-3.599785	-4.498849	-2.973667
C	-5.362799	0.820053	2.185301
H	-4.398775	2.638097	2.858236
H	-6.104237	-0.995063	1.341307
H	-5.622718	-4.401306	-1.522646
H	-6.223302	0.938525	2.840602
N	-2.014888	0.397726	-0.282616
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H	-0.866835	3.813066	-1.105985
H	0.620036	4.710321	-1.435997
C	0.855332	3.941350	1.062629
H	-0.178897	4.241425	1.280832
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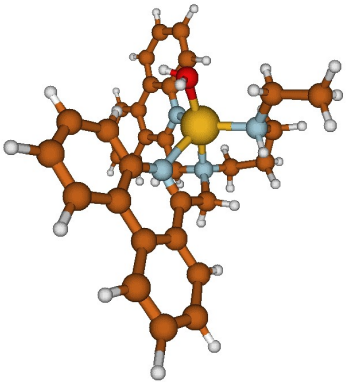
C	1.753087	5.154615	0.912385
H	1.809470	5.700183	1.861267
H	2.773761	4.856318	0.640205
H	1.771378	2.807454	-0.355816
H	1.391935	5.858316	0.154075
O	-0.249734	1.223810	2.509786
H	0.576034	0.742880	2.686874
H	-0.930945	0.541584	2.626811

[Cu(II)LH$_2$O]$^{2+}$ trigonal bipyramidal, in SMD water
E= -1769.274 96 a.u.



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C	1.586283	-0.243488	1.969896
H	1.700252	0.385361	2.866807
H	2.087186	-1.191450	2.198298
C	2.243558	0.403944	0.782643

C	3.619199	0.806417	0.863781
C	4.387663	0.598062	2.028831
C	4.218110	1.395002	-0.283235
C	2.039719	1.187503	-1.400636
C	5.719178	0.957164	2.061317
H	3.931129	0.144161	2.905652
C	5.579804	1.749619	-0.220949
C	3.393410	1.614354	-1.448696
C	1.184946	1.439391	-2.490094
C	6.314946	1.534698	0.928665
H	6.306862	0.791322	2.961290
H	6.064647	2.197049	-1.084979
C	3.851913	2.247620	-2.621051
H	0.139484	1.147547	-2.406617
C	1.659298	2.071518	-3.622210
H	7.365758	1.815779	0.954712
C	3.004114	2.467563	-3.690066
H	4.884689	2.582673	-2.686095
H	0.989746	2.268904	-4.456577
H	3.379402	2.963353	-4.582725
N	1.508756	0.552289	-0.294046
H	1.205641	-2.879830	2.939303
H	-0.367844	-3.420696	3.470013
C	-0.413269	-1.452767	2.733030
H	-0.247638	-1.029863	3.735226
H	-1.495924	-1.467978	2.559542
C	-0.601968	0.779107	1.819085
H	0.030158	1.588018	1.434569
H	-0.796144	1.003622	2.877443
Cu	-0.116622	-1.185105	-0.187287
C	-1.875890	0.726067	1.032245
C	-2.883886	1.732666	1.182707
C	-3.139959	-0.435088	-0.560780
C	-4.055440	1.642251	0.379715
C	-2.715539	2.824217	2.061713
C	-3.256713	-1.589745	-1.355284
C	-4.201103	0.504202	-0.498148
C	-5.021038	2.661313	0.487971
H	-1.816310	2.899878	2.668807
C	-3.677739	3.808783	2.143170
C	-4.393766	-1.802761	-2.108698
H	-2.439686	-2.310410	-1.345064
C	-5.344745	0.262420	-1.284870

C	-4.834193	3.723095	1.351808
H	-5.922683	2.622893	-0.117949
H	-3.540886	4.650795	2.817582
C	-5.437330	-0.864500	-2.079381
H	-4.483192	-2.699257	-2.718144
H	-6.176656	0.962314	-1.259481
H	-5.591807	4.501389	1.416362
H	-6.332684	-1.030973	-2.674240
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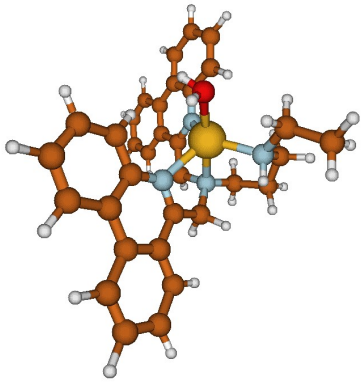
C	-0.064990	-3.614500	1.374236
H	-1.117615	-3.594043	1.058304
H	0.205649	-4.666787	1.533753
C	0.840646	-3.944177	-0.902983
H	-0.181918	-4.138502	-1.248298
H	1.349165	-3.382282	-1.692682
C	1.585489	-5.236065	-0.634203
H	1.712083	-5.787688	-1.572150
H	2.584675	-5.037439	-0.226826
H	1.693435	-2.908557	0.627239
H	1.056293	-5.893957	0.063333
O	-0.273381	-1.535088	-2.214516
H	0.606455	-1.319749	-2.574143
H	-0.855700	-0.851971	-2.591941

[Zn(II)LH$_2$O]$^{2+}$ trigonal bipyramidal, in SMD water
E= -1799.091 30 a.u.



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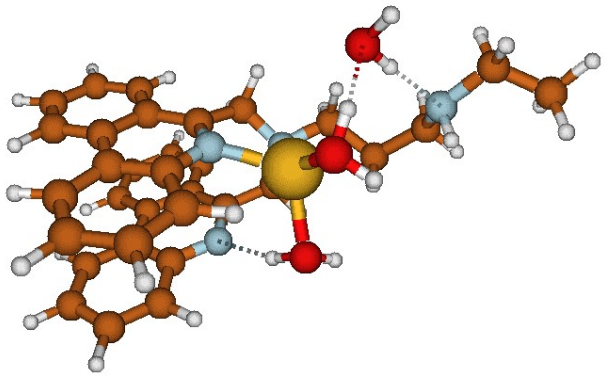
C	1.597979	0.110273	-2.023624
H	1.756141	-0.582268	-2.866761
H	2.088458	1.050659	-2.306815

C	2.256286	-0.434118	-0.784426
C	3.622363	-0.872750	-0.841110
C	4.383202	-0.766955	-2.024914
C	4.223547	-1.378868	0.343080
C	2.064727	-1.032858	1.463694
C	5.710261	-1.142521	-2.039175
H	3.925649	-0.377073	-2.931088
C	5.581172	-1.751810	0.299375
C	3.404970	-1.496344	1.527264
C	1.216850	-1.179083	2.576441
C	6.309639	-1.633904	-0.868514
H	6.292224	-1.053908	-2.953638
H	6.069545	-2.132266	1.192975
C	3.856567	-2.065038	2.734748
H	0.179505	-0.862902	2.483237
C	1.684422	-1.747848	3.744384
H	7.357879	-1.925385	-0.879486
C	3.015467	-2.184997	3.824691
H	4.877715	-2.431651	2.811093
H	1.018669	-1.866161	4.596504
H	3.385117	-2.634707	4.743634
N	1.537167	-0.471376	0.314248
H	1.195021	2.733146	-3.036574
H	-0.360917	3.202787	-3.671994
C	-0.393513	1.264082	-2.853621
H	-0.212913	0.823564	-3.848160
H	-1.479877	1.265351	-2.697467
C	-0.583978	-0.897956	-1.822765
H	0.039307	-1.697608	-1.401900
H	-0.808669	-1.194652	-2.858741
Zn	-0.104113	1.158074	0.234496
C	-1.853416	-0.799341	-1.020701
C	-2.860754	-1.815259	-1.124977
C	-3.118433	0.409957	0.537602
C	-4.030879	-1.700721	-0.323378
C	-2.693078	-2.937929	-1.964171
C	-3.228184	1.582929	1.304574
C	-4.175179	-0.534994	0.517052
C	-4.994837	-2.724981	-0.393103
H	-1.796766	-3.034058	-2.571882
C	-3.653447	-3.926579	-2.009744
C	-4.353866	1.811543	2.070404
H	-2.412482	2.303869	1.265497

C	-5.309325	-0.276373	1.312098
C	-4.808662	-3.815725	-1.219976
H	-5.895262	-2.666925	0.212993
H	-3.515965	-4.790740	-2.655431
C	-5.395083	0.870222	2.078678
H	-4.435904	2.721165	2.661121
H	-6.137393	-0.981251	1.319233
H	-5.565416	-4.596715	-1.256566
H	-6.281938	1.047920	2.682971
N	-1.967133	0.227075	-0.207711
C	-0.179068	3.501009	-1.577153
H	-1.235897	3.413529	-1.287624
H	0.005384	4.560795	-1.797922
C	0.692729	4.111596	0.646666
H	-0.343677	4.330478	0.932384
H	1.174316	3.659490	1.519035
C	1.432485	5.373949	0.253694
H	1.496315	6.047408	1.115647
H	2.456834	5.143969	-0.065769
H	1.597828	2.945673	-0.755923
H	0.939687	5.925856	-0.554101
O	-0.244880	1.771258	2.281119
H	0.629368	1.582462	2.664565
H	-0.833055	1.127122	2.711468

[Cu(II)L(H$_2$O)$_3$]$^{2+}$ tetrahedral, in SMD water
E= -1922.122 09 a.u.



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H	0.292775	-2.417442	-1.086825
H	1.430642	-1.409035	-1.979478

C	-0.287116	-0.328861	-1.324400
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C	-2.522866	0.516909	-1.864760
C	-1.980592	-1.827380	-2.354127
C	-0.300590	3.160851	-0.386119
C	-2.097828	1.800472	-1.359166
C	-3.829561	0.270650	-2.330115
H	-1.267380	-2.647773	-2.371614
C	-3.262694	-2.031628	-2.816473
C	-1.157144	4.239981	-0.300768
H	0.728819	3.228216	-0.038002
C	-2.944759	2.922409	-1.257552
C	-4.192139	-0.978506	-2.793915
H	-4.565624	1.070648	-2.329317
H	-3.557189	-3.010805	-3.187776
C	-2.484467	4.118745	-0.741398
H	-0.804611	5.181396	0.114868
H	-3.980334	2.848781	-1.581209
H	-5.207323	-1.146475	-3.147464
H	-3.159875	4.968431	-0.668134
N	0.108558	0.863472	-0.931131
C	6.945612	-0.344607	-0.697963
H	6.965575	-1.204881	-1.381157
Cu	1.855494	0.857996	0.118979
H	5.573165	0.519888	0.516380
C	2.892646	-1.742459	-0.041664
H	3.304638	-1.320888	-0.965172
H	2.793141	-2.828684	-0.194258
C	3.814415	-1.441563	1.131387
H	3.654088	-2.159175	1.944805
H	3.592109	-0.444070	1.547922
C	5.273668	-1.466251	0.701804
H	5.476950	-2.357953	0.090980
H	5.915155	-1.540584	1.593540
C	0.875899	-1.706980	1.335382
C	-0.565826	-1.294264	1.472723
C	-1.649858	-2.164671	1.095900
C	-2.016485	0.458732	1.965863
C	-2.975602	-1.639363	1.133160
C	-1.451414	-3.499667	0.675642
C	-2.144795	1.793580	2.400818
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C	-4.045528	-2.472816	0.750111
H	-0.448879	-3.918799	0.640237
C	-2.518995	-4.292806	0.309762
C	-3.378045	2.409841	2.399386
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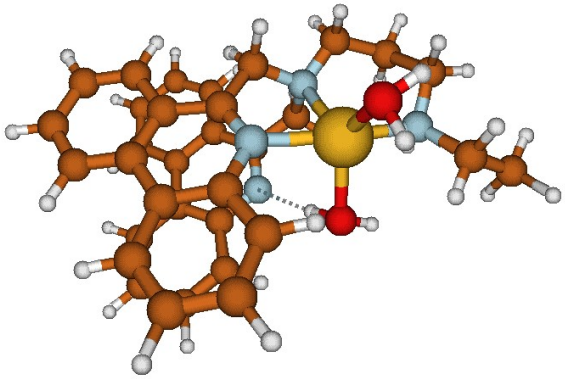
C	-4.407077	0.390968	1.546392
C	-3.822745	-3.774836	0.348312
H	-5.063673	-2.091859	0.773808
H	-2.348644	-5.319307	-0.007079
C	-4.512880	1.704158	1.961850
H	-3.471988	3.444507	2.723324
H	-5.299965	-0.132204	1.211047
H	-4.664198	-4.401248	0.058787
H	-5.483209	2.196128	1.949068
N	-0.751054	-0.076611	1.928613
H	1.441989	-1.318738	2.187633
H	1.001486	-2.796134	1.322688
H	7.061802	0.551553	-1.322110
C	8.088748	-0.434669	0.296000
H	8.045090	0.388566	1.021184
H	8.074728	-1.377385	0.855606
H	0.756336	0.962150	2.258868
O	1.640184	1.421565	2.185120
H	2.233310	0.862314	2.714625
H	9.053810	-0.373045	-0.220248
O	2.981224	2.428604	-0.482043
H	3.638266	2.553838	0.224789
H	4.634794	0.313893	-1.512444
H	3.481709	1.936422	-1.208879
O	4.129263	0.794930	-2.233166
H	4.824245	1.225062	-2.755483

$[Zn(II)L(H_2O)_2]^{2+}$ trigonal bipyramidal, in SMD water
E= -1875.526 56 a.u.



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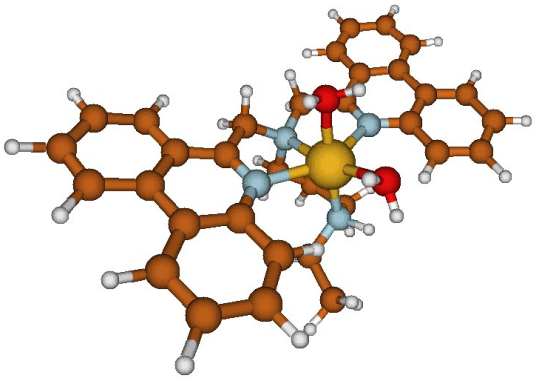
H	0.948028	-1.637919	-2.532814
C	-0.276171	-0.264195	-1.474150
C	-1.683170	-0.183293	-1.747779
C	-0.148179	2.028607	-1.012029
C	-2.343059	1.060149	-1.527420
C	-2.432562	-1.302027	-2.177903
C	0.678995	3.124216	-0.702060
C	-1.549062	2.204782	-1.151012
C	-3.741929	1.117671	-1.689621
H	-1.936695	-2.248165	-2.379946
C	-3.797086	-1.208932	-2.347969
C	0.129446	4.372066	-0.491216
H	1.753233	2.954326	-0.622535
C	-2.081902	3.488765	-0.917222
C	-4.455108	0.003993	-2.085520
H	-4.271584	2.048835	-1.503878
H	-4.364605	-2.078661	-2.672290
C	-1.260401	4.550069	-0.588697
H	0.770695	5.216071	-0.246417
H	-3.153687	3.654593	-1.000021
H	-5.534953	0.070012	-2.202329
H	-1.693881	5.532173	-0.412200
N	0.439808	0.787423	-1.148022
C	5.225138	0.627978	0.699349
H	5.729411	0.769418	-0.264682
Zn	2.428301	0.394346	-0.402776

H	3.902180	-0.733715	1.433816
C	2.545599	-2.656045	-1.003006
H	2.843372	-2.353843	-2.015780
H	2.044233	-3.635210	-1.087726
C	3.785470	-2.792867	-0.139875
H	4.323926	-3.674779	-0.507050
H	3.522246	-3.022565	0.902617
C	4.745362	-1.619504	-0.183414
H	4.956496	-1.330418	-1.222879
H	5.702428	-1.916596	0.269948
C	1.046362	-2.058195	0.822699
C	-0.288496	-1.464804	1.196081
C	-1.521251	-2.182746	0.988055
C	-1.420705	0.424347	1.965003
C	-2.749491	-1.516903	1.275806
C	-1.558221	-3.503161	0.484151
C	-1.315122	1.752565	2.428780
C	-2.698688	-0.153796	1.744168
C	-3.960505	-2.206135	1.062649
H	-0.632299	-4.023846	0.251877
C	-2.759359	-4.148803	0.276482
C	-2.448301	2.507948	2.642840
H	-0.322328	2.169750	2.590284
C	-3.839082	0.644992	1.970280
C	-3.966342	-3.496574	0.572404
H	-4.907545	-1.718994	1.282001
H	-2.769320	-5.164867	-0.111583
C	-3.716827	1.950174	2.405487
H	-2.361589	3.537264	2.985141
H	-4.832065	0.239410	1.789298
H	-4.913124	-4.008582	0.412368
H	-4.610338	2.550184	2.564889
N	-0.252182	-0.253494	1.704148
H	1.786051	-1.719265	1.556287
H	1.018251	-3.154283	0.878426
H	4.695839	1.563674	0.921000
C	6.220434	0.319275	1.797788
H	5.710575	0.184773	2.760179
H	6.800352	-0.587568	1.590645
H	1.223507	0.772794	1.701592
O	2.004788	1.356942	1.470339
H	2.682327	1.121074	2.125826
H	6.930838	1.145787	1.910369

O	3.456890	1.261106	-2.052609
H	3.722558	2.139679	-1.729504
H	4.300469	0.788587	-2.157849

[Cu(II)L(H$_2$O)$_2$]$^{2+}$ octahedral, in SMD water
E= -1845.687 52 a.u.



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H	-1.549164	4.094678	1.246633
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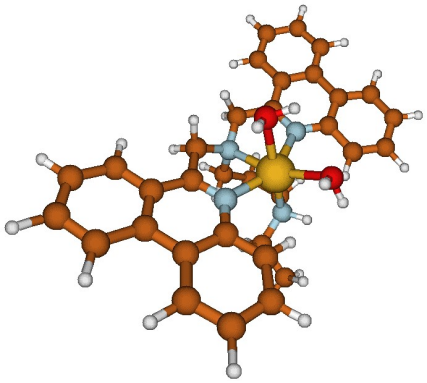
H	-2.064102	1.648950	1.693836
H	-1.162098	1.748042	3.198881
N	0.034241	1.866705	1.466201
H	0.367151	2.751358	1.074468
C	1.097740	1.404240	2.387209
H	1.112836	2.078964	3.254901
H	2.048108	1.539180	1.867179
C	0.925772	-0.047361	2.856118
H	1.892626	-0.562978	2.777879
H	0.679858	-0.055858	3.924617
C	-0.154781	-0.886195	2.195797
H	-0.220269	-1.845333	2.735047
H	-1.137114	-0.405646	2.288370
N	0.036643	-1.182510	0.752689
C	1.287261	-1.926623	0.516512
C	-1.099732	-2.003089	0.288301
H	1.520202	-2.534198	1.404519
H	-0.810128	-2.507155	-0.642148
H	-1.287694	-2.799711	1.023411
C	-2.362192	-1.230818	0.013798
C	-3.608954	-1.938450	-0.129737
C	-3.374876	0.820553	-0.422516

C	-4.782208	-1.189109	-0.422606
C	-3.693752	-3.342569	-0.008974
C	-3.214557	2.213248	-0.547389
C	-4.663626	0.243589	-0.559383
C	-6.003055	-1.876481	-0.568914
H	-2.801949	-3.927772	0.201123
C	-4.902138	-3.990085	-0.164738
C	-4.299334	3.028579	-0.798979
H	-2.216631	2.629066	-0.425213
C	-5.753270	1.098539	-0.821039
C	-6.061895	-3.250244	-0.441755
H	-6.913415	-1.324858	-0.790132
H	-4.955035	-5.072434	-0.072007
C	-5.576999	2.464315	-0.937328
H	-4.163444	4.104783	-0.885129
H	-6.752837	0.683734	-0.929744
H	-7.014966	-3.761557	-0.560783
H	-6.434589	3.103929	-1.134597
N	-2.251723	0.063316	-0.143131
H	1.120423	-2.644450	-0.295844
C	2.483011	-1.091714	0.142790
C	3.759253	-1.749539	0.006623
C	3.386206	0.973885	-0.428151
C	4.881988	-0.972515	-0.386442
C	3.913495	-3.135359	0.224364
C	3.167440	2.355502	-0.588094
C	4.693027	0.444284	-0.593125
C	6.124148	-1.616413	-0.550988
H	3.058635	-3.738906	0.519926
C	5.142564	-3.740271	0.057047
C	4.209480	3.199094	-0.919416
H	2.162719	2.743324	-0.436701
C	5.735691	1.327025	-0.937451
C	6.251722	-2.974346	-0.333416
H	6.996206	-1.042990	-0.855815
H	5.250620	-4.809524	0.224833
C	5.500148	2.678983	-1.100066
H	4.029938	4.265750	-1.037217
H	6.745672	0.945100	-1.069407
H	7.219896	-3.452643	-0.467547
H	6.321813	3.342312	-1.361816
N	2.304704	0.181360	-0.087434
Cu	-0.023484	0.745398	-0.256443

H	-0.701882	4.174678	2.805855
H	-0.742248	-0.255042	-2.484564
H	0.733880	0.142535	-2.571660
O	0.108307	-0.362990	-2.021945
H	-0.749744	2.296356	-2.156149
H	-0.127097	3.270157	-1.149718
O	0.039261	2.423557	-1.600346

$[Zn(II)L(H_2O)_2]^{2+}$ octahedral, in SMD water
E= -1875.509 80 a.u.



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H	-1.281574	1.696215	3.270184
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H	0.233755	2.796204	1.183064
C	1.007300	1.458687	2.482140
H	1.006812	2.114242	3.365619
H	1.956619	1.633337	1.968527
C	0.900278	-0.010408	2.928562
H	1.885261	-0.487105	2.828933
H	0.678033	-0.039572	4.002280
C	-0.157153	-0.900833	2.293147
H	-0.208087	-1.836542	2.874262
H	-1.148996	-0.435370	2.363929
N	0.036006	-1.258978	0.861240
C	1.291303	-1.988537	0.640168
C	-1.109003	-2.078884	0.433648
H	1.574795	-2.543342	1.548939
H	-0.816940	-2.674019	-0.440516

H	-1.369098	-2.797599	1.225372
C	-2.314693	-1.264717	0.051143
C	-3.597961	-1.898675	-0.088158
C	-3.188924	0.819007	-0.546327
C	-4.712762	-1.101625	-0.469552
C	-3.771519	-3.284113	0.121333
C	-2.937541	2.189479	-0.737413
C	-4.504666	0.310497	-0.685042
C	-5.967264	-1.723810	-0.618990
H	-2.923295	-3.904124	0.400605
C	-5.011558	-3.867405	-0.036585
C	-3.965065	3.052576	-1.059310
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C	-5.533760	1.213136	-1.019976
C	-6.113527	-3.080380	-0.405719
H	-6.833313	-1.134806	-0.910569
H	-5.134838	-4.935879	0.124565
C	-5.271012	2.557507	-1.202409
H	-3.764216	4.113109	-1.196518
H	-6.553897	0.852224	-1.128896
H	-7.091303	-3.541860	-0.528154
H	-6.083449	3.235822	-1.453643
N	-2.125125	0.009652	-0.190887
H	1.129516	-2.750513	-0.131626
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C	3.727022	-1.733958	-0.007623
C	3.260153	0.989459	-0.345470
C	4.803003	-0.918286	-0.449295
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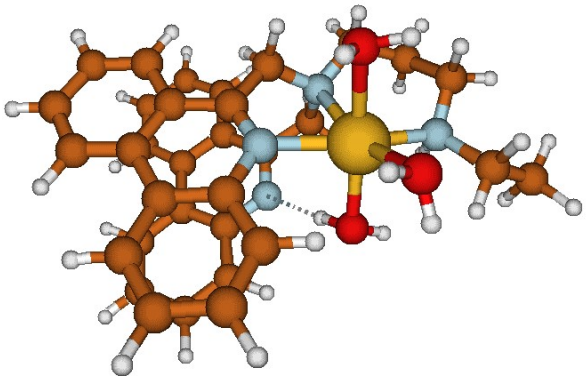
C	3.011328	2.373180	-0.412042
C	4.567544	0.498637	-0.597500
C	6.048279	-1.524781	-0.704838
H	3.110878	-3.750858	0.508384
C	5.160860	-3.686704	-0.083311
C	4.017143	3.255482	-0.752067
H	2.014701	2.733364	-0.170055
C	5.571718	1.419741	-0.956401
C	6.222908	-2.883216	-0.526096
H	6.885862	-0.923080	-1.048921
H	5.307128	-4.755568	0.054833
C	5.302829	2.772434	-1.038311
H	3.812995	4.323276	-0.792465
H	6.580146	1.066863	-1.159588

H	7.192736	-3.332249	-0.730809
H	6.095969	3.465128	-1.311269
N	2.213187	0.151043	0.004784
Zn	-0.026225	0.660982	-0.214625
H	-0.898931	4.150229	2.936483
H	-0.711000	-0.649337	-2.508142
H	0.754030	-0.243714	-2.604860
O	0.139577	-0.752043	-2.049231
H	-0.509538	2.036832	-2.354550
H	0.137095	3.022766	-1.377257
O	0.278959	2.156243	-1.796755

$[Zn(II)L(H_2O)_3]^{2+}$ octahedral, in SMD water
E= -1951.949 60 a.u.



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C	0.387859	3.081807	-0.541114
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H	1.449966	2.959763	-0.356696
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C	-4.507291	-0.248242	-2.245447
H	-4.433993	1.813533	-1.704726
H	-4.303610	-2.340183	-2.765946
C	-1.606355	4.432096	-0.601079
H	0.357700	5.170868	-0.069720
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N	0.306754	0.738146	-1.037421
C	5.227858	0.529832	0.849182
H	5.745774	0.726001	-0.097381
Zn	2.413519	0.428299	-0.410984
H	3.785625	-0.742736	1.477620
C	2.446696	-2.722832	-0.800193
H	2.733407	-2.483928	-1.830994
H	1.924495	-3.695546	-0.822602
C	3.697133	-2.840333	0.047346
H	4.212966	-3.751010	-0.280283
H	3.447375	-3.008208	1.105503
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H	-5.033096	-3.920872	0.530674

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H	1.145773	0.758610	1.741585
O	1.946500	1.323325	1.526347
H	2.607078	1.068028	2.190871
H	6.917187	0.910885	2.127607
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H	3.782324	-0.069990	-2.629394
H	3.073644	2.628033	-1.770547
H	3.704775	2.829485	-0.392003
O	2.813294	-0.121949	-2.578625
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