magnetochemistry

Supplementary Material

DFT Protocol for EPR Prediction of Paramagnetic Cu(II) Complexes and Application to Protein Binding Sites

1. Supplementary Tables

Table S1. Values of A_x, A_y, A_z and g_z for the fourteen Cu(II) complexes examined in this study.

Complex	A_x^{exptl} [1]	A_y^{exptl} [1]	A_z^{exptl} [1]	g_z^{exptl}	Ref.
[Cu(H$_{-2}$P1)]$^{4-}$	11.0	14.0	202.5	2.211	[1]
[Cu(acac)$_2$]	-27.1	-19.5	-190.8	2.117	[2]
[Cu(bipy)$_2$(NCS)]$^+$	-8.8	-8.8	-180.7	2.267	[3]
[Cu(en)$_2$]$^{2+}$	22.0	22.0	205.0	2.204	[2]
[Cu(H$_{-2}$GGG)]$^-$	21.0	21.0	201.0	2.202	[2]
[Cu(H$_{-2}$GGH)]$^-$	22.0	22.0	206.8	2.173	[2]
[Cu(H$_2$O)$_6$]$^{2+}$	8.0	8.0	137.0	2.407	[2]
[Cu(mnt)$_2$]$^{2-}$	41.2	41.2	166.3	2.086	[4]
[Cu(OH)$_4$]$^{2-}$	28.0	28.0	186.0	2.261	[5]
[Cu(salen)]	30.7	30.7	203.7	2.212	[6]
[Cu(salicylaldehydeiminato)$_2$]	21.0	21.0	185.0	2.2	[7]
[Cu(salpn)]	15.7	15.7	175.7	2.261	[8]
[Cu(*S*,*S*)-mnpala)]	20.0	20.0	192.0	2.24	[9]
[Cu(ttcn)$_2$]$^{2+}$	19.1	19.1	148.3	2.217	[10]

[1] Values given in 10^{-4} cm^{-1}. [2] This work.

Table S2. Values of A_{iso}, A_x, A_y, A_z and g_z and percent deviation (PD) calculated at the level of theory B2PLYP/6-311g(d,p).

Complex	A_{iso} [1]	A_x [1]	A_y [1]	A_z [1]	g_z	PD (A_z)	PD (g_z)
[Cu(H$_{-2}$P1)]$^{4-}$	-7.5	-32.7	-103.3	113.5	1.935	-44.0	-12.5
[Cu(acac)$_2$]	-86.4	-18.4	-18.7	-222.2	2.297	16.5	8.5
[Cu(bipy)$_2$(NCS)]$^+$	-53.6	12.8	15.7	-189.4	2.301	4.8	1.5
[Cu(en)$_2$]$^{2+}$	-96.5	-29.1	-29.4	-230.9	2.249	12.6	2.0
[Cu(H$_{-2}$GGG)]$^-$	-102.7	-29.8	-34.5	-243.7	2.211	21.3	0.4
[Cu(H$_{-2}$GGH)]$^-$	-98.8	-25.2	-37.0	-234.1	2.220	13.2	2.2
[Cu(H$_2$O)$_6$]$^{2+}$	4.7	-16.0	-82.9	113.1	2.408	-17.5	0.0
[Cu(mnt)$_2$]$^{2-}$	-62.5	-2.7	-5.9	-178.8	2.238	7.5	7.3
[Cu(OH)$_4$]$^{2-}$	-93.2	-25.4	-33.2	-221.0	2.311	18.8	2.2
[Cu(salen)]	-90.2	-19.3	-20.7	-230.7	2.251	13.3	1.8
[Cu(salicylaldehydeiminato)$_2$]	-85.0	-12.7	-13.6	-228.7	2.244	23.6	2.0
[Cu(salpn)]	-79.7	-7.7	-13.7	-217.8	2.273	24.0	0.5
[Cu(*S*,*S*)-mnpala)]	-98.8	-30.2	-31.9	-234.4	2.259	22.1	0.8
[Cu(ttcn)$_2$]$^{2+}$	-45.4	9.5	16.2	-161.9	2.275	9.2	2.6
					MAPD [2]	17.4 (9.4)	3.1 (3.5)
					MPD [3]	9.0	1.4

[1] Values given in 10^{-4} cm^{-1}. [2] Mean absolute percent deviation (MAPD) and standard deviation (SD) in parenthesis. [3] Mean percent deviation (MPD).

Table S3. Values of A_{iso}, A_x, A_y, A_z and g_z and percent deviation (PD) calculated at the level of theory B3LYP/6-311g(d,p).

Complex	A_{iso} [1]	A_x [1]	A_y [1]	A_z [1]	g_z	PD (A_z)	PD (g_z)
[Cu(H$_{-2}$P1)]$^{4-}$	-116.7	-80.7	-86.3	-183.0	2.078	-9.6	-6.0
[Cu(acac)$_2$]	-80.6	-18.9	-19.2	-203.7	2.178	6.8	2.9
[Cu(bipy)$_2$(NCS)]$^+$	-47.3	9.0	16.7	-167.5	2.172	-7.3	-4.2
[Cu(en)$_2$]$^{2+}$	-86.4	-25.4	-25.6	-208.3	2.142	1.6	-2.8
[Cu(H$_{-2}$GGG)]$^-$	-84.3	-20.3	-24.5	-208.1	2.124	3.5	-3.6
[Cu(H$_{-2}$GGH)]$^-$	-74.8	-14.6	-31.7	-178.2	2.108	-13.8	-3.0
[Cu(H$_2$O)$_6$]$^{2+}$	-0.3	-27.4	-93.8	120.1	2.290	-12.3	-4.8
[Cu(mnt)$_2$]$^{2-}$	-58.0	-13.6	-13.9	-146.7	2.113	-11.8	1.3
[Cu(OH)$_4$]$^{2-}$	-86.9	-26.8	-28.1	-205.7	2.185	10.6	-3.4
[Cu(salen)]	-79.0	-15.6	-16.9	-204.4	2.148	0.4	-2.9
[Cu(salicylaldehydeiminato)$_2$]	-73.0	-4.7	-10.8	-203.6	2.147	10.0	-2.4
[Cu(salpn)]	-71.9	-8.0	-11.8	-196.0	2.160	11.5	-4.5
[Cu(*S*,*S*)-mnpala)]	-89.7	-28.1	-30.4	-210.6	2.148	9.7	-4.1
[Cu(ttcn)$_2$]$^{2+}$	-46.9	0.2	-1.9	-138.9	2.135	-6.3	-3.7
					MAPD [2]	8.6 (4.2)	3.5 (1.1)
					MPD [3]	-0.5	-2.9

[1] Values given in 10^{-4} cm^{-1}. [2] Mean absolute percent deviation (MAPD) and standard deviation (SD) in parenthesis. [3] Mean percent deviation (MPD).

Table S4. Values of A_{iso}, A_x, A_y, A_z and g_z and percent deviation (PD) calculated at the level of theory B3P86/6-311g(d,p).

Complex	A_{iso} [1]	A_x [1]	A_y [1]	A_z [1]	g_z	PD (A_z)	PD (g_z)
[Cu(H$_{-2}$P1)]$^{4-}$	-123.0	-87.5	-93.5	-188.1	2.077	-7.1	-6.1
[Cu(acac)$_2$]	-87.8	-26.8	-27.2	-209.4	2.179	9.8	2.9
[Cu(bipy)$_2$(NCS)]$^+$	-53.8	2.0	9.5	-172.9	2.174	-4.3	-4.1
[Cu(en)$_2$]$^{2+}$	-93.9	-33.3	-33.5	-214.8	2.143	4.8	-2.8
[Cu(H$_{-2}$GGG)]$^-$	-91.3	-27.7	-31.8	-214.3	2.124	6.6	-3.5
[Cu(H$_{-2}$GGH)]$^-$	-80.2	-20.2	-37.1	-183.2	2.109	-11.4	-3.0
[Cu(H$_2$O)$_6$]$^{2+}$	-7.5	-34.7	-99.0	111.2	2.294	-18.8	-4.7
[Cu(mnt)$_2$]$^{2-}$	-63.8	-19.4	-19.9	-152.1	2.114	-8.5	1.3
[Cu(OH)$_4$]$^{2-}$	-94.9	-35.1	-36.6	-213.1	2.188	14.6	-3.2
[Cu(salen)]	-86.1	-23.3	-24.6	-210.4	2.149	3.3	-2.8
[Cu(salicylaldehydeiminato)$_2$]	-80.2	-12.9	-18.1	-209.7	2.148	13.3	-2.4
[Cu(salpn)]	-78.9	-15.5	-19.4	-201.8	2.161	14.9	-4.4
[Cu(*S*,*S*)-mnpala)]	-96.6	-35.5	-37.7	-216.5	2.150	12.7	-4.0
[Cu(ttcn)$_2$]$^{2+}$	-51.6	-3.3	-8.1	-143.5	2.138	-3.2	-3.6
					MAPD [2]	9.7 (4.7)	3.5 (1.1)
					MPD [3]	1.9	-2.9

[1] Values given in 10^{-4} cm^{-1}. [2] Mean absolute percent deviation (MAPD) and standard deviation (SD) in parenthesis. [3] Mean percent deviation (MPD).

Table S5. Values of A_{iso}, A_x, A_y, A_z and g_z and percent deviation (PD) calculated at the level of theory B3PW91/6-311g(d,p).

Complex	A_{iso} [1]	A_x [1]	A_y [1]	A_z [1]	g_z	PD (A_z)	PD (g_z)
[Cu(H$_{-2}$P1)]$^{4-}$	-121.2	-85.5	-91.6	-186.5	2.078	-7.9	-6.0
[Cu(acac)$_2$]	-85.7	-24.6	-25.0	-207.5	2.180	8.8	3.0
[Cu(bipy)$_2$(NCS)]$^+$	-52.2	3.6	11.4	-171.5	2.175	-5.1	-4.1
[Cu(en)$_2$]$^{2+}$	-91.8	-31.1	-31.3	-213.1	2.144	3.9	-2.7
[Cu(H$_{-2}$GGG)]$^-$	-89.4	-25.8	-29.7	-212.8	2.125	5.9	-3.5
[Cu(H$_{-2}$GGH)]$^-$	-78.5	-18.4	-35.2	-181.9	2.110	-12.0	-2.9
[Cu(H$_2$O)$_6$]$^{2+}$	-6.2	-33.4	-97.7	112.5	2.295	-17.9	-4.6
[Cu(mnt)$_2$]$^{2-}$	-62.3	-17.6	-18.1	-151.2	2.115	-9.1	1.4
[Cu(OH)$_4$]$^{2-}$	-92.8	-32.7	-34.4	-211.2	2.189	13.6	-3.2
[Cu(salen)]	-84.2	-21.2	-22.5	-208.8	2.150	2.5	-2.8
[Cu(salicylaldehydeiminato)$_2$]	-78.4	-11.0	-16.1	-208.1	2.149	12.5	-2.3
[Cu(salpn)]	-77.0	-13.4	-17.3	-200.2	2.162	13.9	-4.4
[Cu(*S*,*S*)-mnpala)]	-94.5	-33.3	-35.5	-214.7	2.151	11.8	-4.0
[Cu(ttcn)$_2$]$^{2+}$	-49.9	-1.4	-6.0	-142.4	2.140	-4.0	-3.5
					MAPD [2]	9.4 (4.5)	3.4 (1.1)
					MPD [3]	1.2	-2.8

[1] Values given in 10^{-4} cm^{-1}. [2] Mean absolute percent deviation (MAPD) and standard deviation (SD) in parenthesis. [3] Mean percent deviation (MPD).

Table S6. Values of A_{iso}, A_x, A_y, A_z and g_z and percent deviation (PD) calculated at the level of theory BHandHLYP/6-311g(d,p).

Complex	A_{iso} [1]	A_x [1]	A_y [1]	A_z [1]	g_z	PD (A_z)	PD (g_z)
[Cu(H$_{-2}$P1)]$^{4-}$	-19.5	-44.5	100.3	-114.2	1.938	-43.6	-12.4
[Cu(acac)$_2$]	-81.5	-13.5	-13.9	-217.1	2.288	13.8	8.1
[Cu(bipy)$_2$(NCS)]$^+$	-49.0	17.1	20.5	-184.4	2.291	2.1	1.1
[Cu(en)$_2$]$^{2+}$	-91.5	-24.4	-24.7	-225.4	2.238	10.0	1.6
[Cu(H$_{-2}$GGG)]$^-$	-97.3	-25.1	-29.2	-237.5	2.202	18.2	0.0
[Cu(H$_{-2}$GGH)]$^-$	-94.5	-21.3	-33.8	-228.4	2.209	10.4	1.6
[Cu(H$_2$O)$_6$]$^{2+}$	10.1	-9.6	-78.1	118.1	2.405	-13.8	-0.1
[Cu(mnt)$_2$]$^{2-}$	-60.9	-2.7	-5.6	-174.3	2.219	4.8	6.4
[Cu(OH)$_4$]$^{2-}$	-88.8	-21.2	-28.5	-216.6	2.300	16.5	1.7
[Cu(salen)]	-84.9	-14.1	-15.6	-224.9	2.242	10.4	1.4
[Cu(salicylaldehydeiminato)$_2$]	-79.3	-7.1	-8.2	-222.7	2.236	20.4	1.6
[Cu(salpn)]	-74.7	-2.9	-8.8	-212.5	2.264	20.9	0.1
[Cu(*S*,*S*)-mnpala)]	-93.9	-25.5	-27.3	-229.0	2.249	19.3	0.4
[Cu(ttcn)$_2$]$^{2+}$	-44.1	9.9	16.4	-158.5	2.256	6.9	1.8
					MAPD [2]	14.8 (9.8)	2.7 (3.5)
					MPD [3]	6.9	1.0

[1] Values given in 10^{-4} cm^{-1}. [2] Mean absolute percent deviation (MAPD) and standard deviation (SD) in parenthesis. [3] Mean percent deviation (MPD).

Table S7. Values of A_{iso}, A_x, A_y, A_z and g_z and percent deviation (PD) calculated at the level of theory CAM-B3LYP/6-311g(d,p).

Complex	A_{iso} [1]	A_x [1]	A_y [1]	A_z [1]	g_z	PD (A_z)	PD (g_z)
[Cu(H$_{-2}$P1)]$^{4-}$	-29.0	-58.2	77.3	-106.1	1.946	-47.6	-12.0
[Cu(acac)$_2$]	-81.7	-16.2	-16.6	-212.2	2.196	11.2	3.7
[Cu(bipy)$_2$(NCS)]$^+$	-81.7	-16.2	-16.6	-212.2	2.193	17.4	-3.2
[Cu(en)$_2$]$^{2+}$	-90.2	-26.7	-26.7	-217.1	2.156	5.9	-2.2
[Cu(H$_{-2}$GGG)]$^-$	-89.5	-22.4	-26.5	-219.6	2.135	9.2	-3.1
[Cu(H$_{-2}$GGH)]$^-$	-90.0	-22.1	-39.8	-208.1	2.127	0.6	-2.1
[Cu(H$_2$O)$_6$]$^{2+}$	0.7	-25.4	-94.1	121.6	2.305	-11.2	-4.2
[Cu(mnt)$_2$]$^{2-}$	-69.9	-20.8	-21.8	-167.1	2.130	0.5	2.1
[Cu(OH)$_4$]$^{2-}$	-89.5	-26.2	-28.4	-213.9	2.202	15.0	-2.6
[Cu(salen)]	-81.8	-14.9	-16.3	-214.1	2.163	5.1	-2.2
[Cu(salicylaldehydeiminato)$_2$]	-75.1	-4.1	-9.5	-211.7	2.161	14.4	-1.8
[Cu(salpn)]	-74.5	-6.8	-11.1	-205.6	2.176	17.0	-3.7
[Cu(*S*,*S*)-mnpala)]	-92.9	-27.9	-30.1	-220.7	2.165	15.0	-3.4
[Cu(ttcn)$_2$]$^{2+}$	-56.6	-3.7	-9.0	-157.2	2.155	6.0	-2.8
					MAPD [2]	11.8 (11.5)	3.4 (2.5)
					MPD [3]	4.2	-2.7

[1] Values given in 10^{-4} cm^{-1}. [2] Mean absolute percent deviation (MAPD) and standard deviation (SD) in parenthesis. [3] Mean percent deviation (MPD).

Table S8. Values of A_{iso}, A_x, A_y, A_z and g_z and percent deviation (PD) calculated at the level of theory M06/6-311g(d,p).

Complex	A_{iso} [1]	A_x [1]	A_y [1]	A_z [1]	g_z	PD (A_z)	PD (g_z)
[Cu(H$_{-2}$P1)]$^{4-}$	-70.0	-37.2	-45.3	-127.3	2.090	-37.1	-5.5
[Cu(acac)$_2$]	64.0	-16.0	102.9	105.1	2.351	-44.9	11.1
[Cu(bipy)$_2$(NCS)]$^+$	93.3	16.9	127.5	135.4	2.342	-25.1	3.3
[Cu(en)$_2$]$^{2+}$	46.3	-47.3	92.9	93.2	2.253	-54.5	2.2
[Cu(H$_{-2}$GGG)]$^-$	38.5	-67.7	89.0	94.2	2.198	-53.1	-0.2
[Cu(H$_{-2}$GGH)]$^-$	21.8	59.0	-68.6	75.1	2.161	-63.7	-0.6
[Cu(H$_2$O)$_6$]$^{2+}$	342.2	248.4	371.5	406.6	3.069	196.8	27.5
[Cu(mnt)$_2$]$^{2-}$	29.9	-43.3	64.8	68.4	2.162	-58.9	3.6
[Cu(OH)$_4$]$^{2-}$	63.8	-7.6	98.2	100.6	2.379	-45.9	5.2
[Cu(salen)]	55.3	-41.5	101.9	105.5	2.265	-48.2	2.4
[Cu(salicylaldehydeiminato)$_2$]	64.4	-39.4	114.5	118.1	2.261	-36.2	2.8
[Cu(salpn)]	67.2	-22.8	109.0	115.4	2.302	-34.3	1.8
[Cu(*S*,*S*)-mnpala)]	43.1	-46.3	86.0	89.4	2.270	-53.4	1.3
[Cu(ttcn)$_2$]$^{2+}$	50.7	-19.4	81.9	89.6	2.206	-39.6	-0.5
					MAPD [2]	57.0 (40.3)	4.6 (6.9)
					MPD [3]	-28.4	3.9

[1] Values given in 10^{-4} cm^{-1}. [2] Mean absolute percent deviation (MAPD) and standard deviation (SD) in parenthesis. [3] Mean percent deviation (MPD).

Table S9. Values of A_{iso}, A_x, A_y, A_z and g_z and percent deviation (PD) calculated at the level of theory PBE0/6-311g(d,p).

Complex	A_{iso} [1]	A_x [1]	A_y [1]	A_z [1]	g_z	PD (A_z)	PD (g_z)
[Cu(H$_{-2}$P1)]$^{4-}$	-136.3	-101.0	-106.4	-201.4	2.079	-0.5	-6.0
[Cu(acac)$_2$]	-90.4	-27.5	-28.0	-215.7	2.198	13.1	3.8
[Cu(bipy)$_2$(NCS)]$^+$	-56.8	2.1	8.6	-181.1	2.196	0.2	-3.1
[Cu(en)$_2$]$^{2+}$	-96.4	-34.2	-34.3	-220.6	2.159	7.6	-2.0
[Cu(H$_{-2}$GGG)]$^-$	-95.5	-30.3	-33.7	-222.4	2.137	10.7	-2.9
[Cu(H$_{-2}$GGH)]$^-$	-87.4	-23.9	-40.5	-197.8	2.124	-4.3	-2.2
[Cu(H$_2$O)$_6$]$^{2+}$	-8.3	-35.0	-99.2	109.3	2.314	-20.2	-3.9
[Cu(mnt)$_2$]$^{2-}$	-66.3	-18.9	-20.0	-160.0	2.131	-3.8	2.1
[Cu(OH)$_4$]$^{2-}$	-97.7	-36.0	-38.6	-218.5	2.207	17.5	-2.4
[Cu(salen)]	-89.2	-24.4	-25.8	-217.5	2.165	6.8	-2.1
[Cu(salicylaldehydeiminato)$_2$]	-83.5	-14.9	-19.1	-216.4	2.163	17.0	-1.7
[Cu(salpn)]	-81.6	-16.0	-20.4	-208.5	2.179	18.7	-3.6
[Cu(*S*,*S*)-mnpala)]	-99.7	-36.8	-38.8	-223.4	2.167	16.4	-3.3
[Cu(ttcn)$_2$]$^{2+}$	-53.0	-2.0	-7.0	-150.0	2.158	1.2	-2.7
					MAPD [2]	9.5 (7.1)	2.9 (1.1)
					MPD [3]	5.7	-2.1

[1] Values given in 10^{-4} cm^{-1}. [2] Mean absolute percent deviation (MAPD) and standard deviation (SD) in parenthesis. [3] Mean percent deviation (MPD).

Table S10. Values of A_{iso}, A_x, A_y, A_z and g_z and percent deviation (PD) calculated at the level of theory TPSSh/6-311g(d,p).

Complex	A_{iso} [1]	A_x [1]	A_y [1]	A_z [1]	g_z	PD (A_z)	PD (g_z)
[Cu(H$_{-2}$P1)]$^{4-}$	-96.1	-56.5	-67.2	-164.7	2.070	-18.7	-6.4
[Cu(acac)$_2$]	-75.3	-14.3	-14.4	-197.3	2.140	3.4	1.1
[Cu(bipy)$_2$(NCS)]$^+$	-79.0	-17.8	-18.0	-201.3	2.134	11.4	-5.9
[Cu(en)$_2$]$^{2+}$	-73.8	-10.9	-15.1	-195.3	2.115	-4.7	-4.1
[Cu(H$_{-2}$GGG)]$^-$	-59.1	-2.1	-19.0	-156.2	2.101	-22.3	-4.6
[Cu(H$_{-2}$GGH)]$^-$	-8.7	-42.3	-109.1	125.1	2.087	-39.5	-3.9
[Cu(H$_2$O)$_6$]$^{2+}$	-48.9	-4.4	-4.4	-137.9	2.216	0.6	-7.9
[Cu(mnt)$_2$]$^{2-}$	-80.9	-20.3	-21.6	-200.7	2.095	20.7	0.4
[Cu(OH)$_4$]$^{2-}$	-65.0	-2.3	-5.3	-187.5	2.147	0.8	-5.0
[Cu(salen)]	-71.4	-9.2	-10.1	-194.8	2.118	-4.4	-4.2
[Cu(salicylaldehydeiminato)$_2$]	-41.1	14.5	21.7	-159.6	2.118	-13.7	-3.7
[Cu(salpn)]	-66.7	1.2	-6.0	-195.4	2.126	11.2	-6.0
[Cu(*S*,*S*)-mnpala)]	-65.0	-2.3	-5.3	-187.5	2.118	-2.3	-5.4
[Cu(ttcn)$_2$]$^{2+}$	-36.2	8.4	13.2	-130.2	2.116	-12.2	-4.6
					MAPD [2]	13.7 (12.6)	4.5 (1.9)
					MPD [3]	-5.0	-4.3

[1] Values given in 10^{-4} cm^{-1}. [2] Mean absolute percent deviation (MAPD) and standard deviation (SD) in parenthesis. [3] Mean percent deviation (MPD).

Table S11. Values of A_{iso}, A_x, A_y, A_z and g_z and percent deviation (PD) calculated at the level of theory ω-B97-xD/6-311g(d,p).

Complex	A_{iso} [1]	A_x [1]	A_y [1]	A_z [1]	g_z	PD (A_z)	PD (g_z)
[Cu(H$_{-2}$P1)]$^{4-}$	-6.3	-37.3	-84.4	102.7	1.954	-49.3	-11.6
[Cu(acac)$_2$]	-95.9	-31.0	-31.5	-225.2	2.206	18.0	4.2
[Cu(bipy)$_2$(NCS)]$^+$	-71.9	-5.5	-8.6	-201.7	2.204	11.6	-2.8
[Cu(en)$_2$]$^{2+}$	-105.9	-42.9	-43.0	-231.7	2.164	13.0	-1.8
[Cu(H$_{-2}$GGG)]$^-$	-106.0	-39.1	-43.5	-235.4	2.139	17.1	-2.8
[Cu(H$_{-2}$GGH)]$^-$	-107.7	-39.2	-56.8	-227.2	2.134	9.9	-1.8
[Cu(H$_2$O)$_6$]$^{2+}$	-14.7	-37.0	99.6	-106.8	2.325	-22.0	-3.4
[Cu(mnt)$_2$]$^{2-}$	-84.9	-34.0	-35.8	-185.0	2.143	11.2	2.7
[Cu(OH)$_4$]$^{2-}$	-102.7	-40.1	-42.2	-225.9	2.213	21.4	-2.1
[Cu(salen)]	-98.7	-32.4	-33.8	-230.0	2.170	12.9	-1.9
[Cu(salicylaldehydeiminato)$_2$]	-92.6	-22.5	-27.4	-227.9	2.167	23.2	-1.5
[Cu(salpn)]	-91.3	-24.2	-28.5	-221.3	2.185	25.9	-3.4
[Cu(*S*,*S*)-mnpala)]	-108.0	-43.5	-45.7	-234.8	2.173	22.3	-3.0
[Cu(ttcn)$_2$]$^{2+}$	-73.9	-20.0	-25.3	-176.5	2.170	19.0	-2.1
					MAPD [2]	19.1 (9.9)	3.1(2.5)
					MPD [3]	9.6	-2.2

[1] Values given in 10^{-4} cm^{-1}. [2] Mean absolute percent deviation (MAPD) and standard deviation (SD) in parenthesis. [3] Mean percent deviation (MPD).

Table S12. Values of A_{iso}, A_x, A_y, A_z and g_z and percent deviation (PD) calculated at the level of theory MPW1PW91/6-311g(d,p).

Complex	A_{iso} [1]	A_x [1]	A_y [1]	A_z [1]	g_z	PD (A_z)	PD (g_z)
[Cu(H$_{-2}$P1)]$^{4-}$	[2]	[2]	[2]	[2]	[2]	[2]	[2]
[Cu(acac)$_2$]	-65.7	-13.4	-13.9	-169.9	2.125	-10.9	0.4
[Cu(bipy)$_2$(NCS)]$^+$	-36.5	9.3	15.6	-134.4	2.112	-25.6	-6.8
[Cu(en)$_2$]$^{2+}$	-70.2	-15.4	-15.6	-179.7	2.101	-12.3	-4.7
[Cu(H$_{-2}$GGG)]$^-$	-62.3	-5.7	-12.5	-168.7	2.088	-16.1	-5.2
[Cu(H$_{-2}$GGH)]$^-$	-44.7	2.9	-12.9	-124.0	2.071	-40.0	-4.7
[Cu(H$_2$O)$_6$]$^{2+}$	[2]	[2]	[2]	[2]	[2]	[2]	[2]
[Cu(mnt)$_2$]$^{2-}$	-43.8	-5.8	-6.4	-119.1	2.077	-28.4	-0.4
[Cu(OH)$_4$]$^{2-}$	-66.3	-10.7	-17.3	-171.0	2.134	-8.1	-5.6
[Cu(salen)]	-63.5	-9.4	-10.7	-170.4	2.102	-16.3	-5.0
[Cu(salicylaldehydeiminato)$_2$]	-59.4	1.9	-7.7	-172.5	2.103	-6.8	-4.4
[Cu(salpn)]	-58.1	-4.2	-6.2	-163.7	2.109	-6.8	-6.7
[Cu(*S*,*S*)-mnpala)]	-68.4	-15.0	-17.7	-172.5	2.103	-10.2	-6.1
[Cu(ttcn)$_2$]$^{2+}$	-34.3	3.3	7.6	-113.9	2.099	-23.2	-5.3
					MAPD [3]	17.1 (11.7)	4.6 (2.1)
					MPD [4]	-17.1	-4.5

[1] Values given in 10^{-4} cm^{-1}. [2] With MPW1PW91 functional the structures of [Cu(H$_2$O)$_6$]$^{2+}$ and [Cu(H$_{-2}$P1)$_2$]$^{4-}$ did not give a converged wavefunction during the ORCA simulations. [3] Mean absolute percent deviation (MAPD) and standard deviation (SD) in parenthesis. [4] Mean percent deviation (MPD).

Table S13. Selected bond distances (Å) and angles (degree) for the models of HSA and PrP and for the X-ray structures of similar Cu(II)-peptide complexes.[1,2]

Complex	**GGGG** [3]	**GGHR** [4]	**HGGGW** [5]	**HSA(1-5)** [6]	**PrP(108-112)** [6]	**PrP(108-112)** [6]	**PrP(184-188)** [6]
Donors	NH_2, N^-, N^-, N^-	NH_2, N^-, N^-, N_{His}	N_{His}, N^-, N^-, CO	NH_2, N^-, N^-, N_{His}	S_{Met}, N^-, N^-, N_{His}	N^-, N^-, N^-, N_{His}	N^-, N^-, N^-, N_{His}
Cu–D(1)	2.033	2.039	1.991	2.085	2.541	1.991	2.001
Cu–N^-(1)	1.912	1.877	1.996	1.944	1.917	1.899	1.906
Cu–N^-(2)	1.913	1.958	1.921	1.943	1.970	1.990	1.993
Cu–D(2)	1.951	1.961	2.066	2.005	1.993	2.019	2.055
D(1)–Cu–N^-(1)	84.6	82.7	91.0	80.3	93.4	84.0	83.5
N^-(1)–Cu–N^-(2)	83.5	83.9	106.3	83.6	83.4	83.5	82.9
N^-(1)–Cu–D(2)	82.9	94.6	82.1	95.5	94.7	92.8	92.4
D(1)–Cu–D(2)	109.1	98.6	80.4	99.6	93.9	104.2	106.2

[1] Distances in Å and angles in degrees. [2] D stands for donor and could be: D(1) = NH_2, N_{His}, S_{Met}, N^- and D(2) = N^-, N_{His}, CO. [3] GlyGlyGlyGly; experimental data taken from ref. [11]. [4] GlyGlyHis-*N*-methylamide; experimental data taken from ref. [12]. [4] HisGlyGlyGlyTrp; experimental data taken from ref. [13]. [6] Structure DFT optimized at the level of theory B3LYP-D3 (this work).

2. Supporting Figures

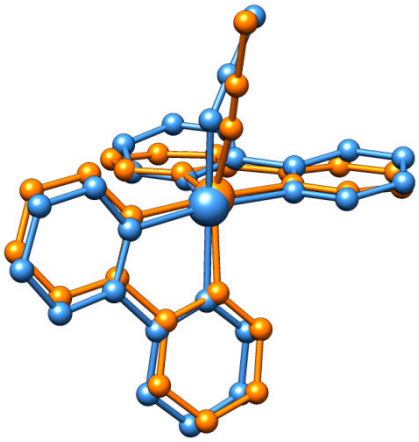

Figure S1. Superimposition of the optimized structure of $[Cu(bipy)_2(NCS)]^+$ complex at B3LYP-D3 level of theory (in blue) and X-ray structure from ref. [14] (in orange).

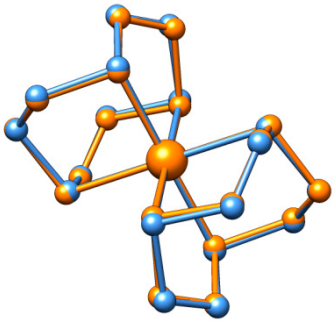

Figure S2. Superimposition of the optimized structure of $[Cu(ttcn)]^{2+}$ complex at B3LYP-D3 level of theory (in blue) and X-ray structure from ref. [10] (in orange).

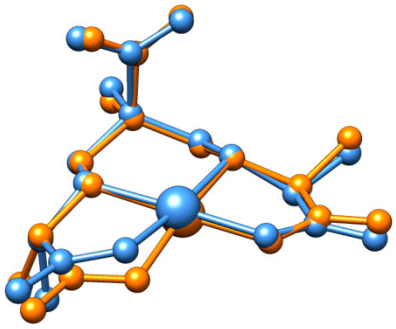

Figure S3. Superimposition of the optimized structure of [Cu(*S*,*S*-mnpala)] complex at B3LYP-D3 level of theory (in blue) and X-ray structure from ref. [15] (in orange).

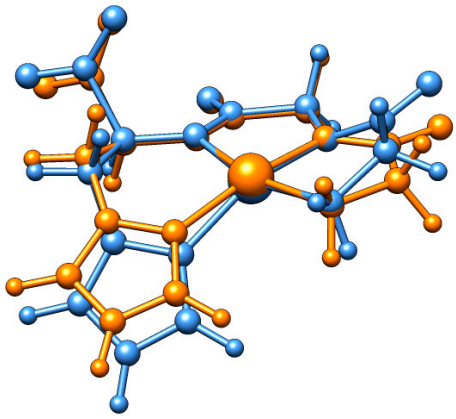

Figure S4. Superimposition of the optimized structure of $[CuH_{-2}GGH]^-$ complex at B3LYP-D3 level of theory using 6-311g(d,p) for the main group elements and SDD [ECP] for Cu (in blue), and *def*2-TZVP for all atoms in SMD continuum model for water (in orange).

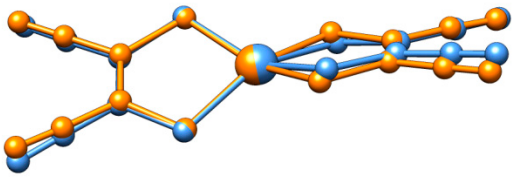

Figure S5. Superimposition of the optimized structure of $[Cu(mnt)]^{2-}$ complex at B3LYP-D3 level of theory using 6-311g(d,p) for the main group elements and SDD [ECP] for Cu (in blue), and X-ray structure from ref. [16] (in orange).

3. Cartesian Coordinates

$[Cu(H_{-1}P1)_2]^{4-}$

	Value
Charge	-2
Electronic Energy (a.u.)	-1218.118651
Gibbs energy (a.u.)	-1218.029674
Number of Imaginary Frequencies	0

Molecular Geometry in Cartesian Coordinates

O	0.375047	2.136137	0.000480
C	1.581228	2.463214	0.000160
N	1.951555	0.015222	-0.000306
C	2.733929	-1.050932	-0.000295
C	4.182609	-1.020669	-0.000257
C	4.821799	0.345883	-0.000028
C	3.885922	1.450306	-0.000043
C	2.526435	1.282742	-0.000128
H	4.284526	2.459599	0.000092
C	-3.885883	-1.450327	0.000186
C	-2.526402	-1.282727	0.000038
N	-1.951566	-0.015187	-0.000250
C	-2.733961	1.050952	-0.000283
C	-4.182640	1.020649	-0.000193
C	-4.821787	-0.345926	0.000157
H	-4.284469	-2.459627	0.000409
C	-1.581159	-2.463195	0.000380
O	-0.374981	-2.136083	0.000626
H	2.239049	-2.018530	-0.000342
H	-2.239100	2.018560	-0.000413
O	4.850065	-2.077092	-0.000403
O	6.056141	0.498951	0.000112
O	-6.056125	-0.499026	0.000353
O	-4.850133	2.077049	-0.000392
Cu	-0.000020	0.000015	-0.000008

[Cu(acac)$_2$]

	Value
Charge	0
Electronic Energy (a.u.)	-730.697837
Gibbs energy (a.u.)	-730.621447
Number of Imaginary Frequencies	0

Molecular Geometry in Cartesian Coordinates

C	-3.276837	0.000083	0.004091
Cu	0.000031	0.000022	-0.002132
O	-1.348694	-1.408352	-0.001562
C	-2.601661	-1.222549	0.001643
C	-2.601548	1.222585	0.002158
O	-1.348501	1.408154	-0.001225
H	-4.358489	0.000081	0.006824
H	-3.207778	2.138103	0.003466
H	-3.208127	-2.137928	0.002235
C	3.276840	0.000172	0.005010
O	1.348386	1.408013	-0.002763
C	2.601472	1.222621	0.001509
C	2.601699	-1.222496	0.002274
O	1.348742	-1.408312	-0.002708
H	4.358488	0.000220	0.008879
H	3.208182	-2.137860	0.004128
H	3.207570	2.138216	0.002257

$[Cu(bipy)_2(NCS)]^+$

	Value
Charge	1
Electronic Energy (a.u.)	-1679.404520
Gibbs energy (a.u.)	-1679.131341
Number of Imaginary Frequencies	0

Molecular Geometry in Cartesian Coordinates

Cu	0.279733	0.189307	-0.557624
N	2.100911	1.113455	-0.484417
C	2.281154	2.408096	-0.761700
C	3.539217	2.999055	-0.708014
C	4.631393	2.210222	-0.364403
C	4.438641	0.859676	-0.085513
C	3.150660	0.333211	-0.152734
C	2.809490	-1.084680	0.110855
C	3.729956	-2.045061	0.529384
C	3.298872	-3.347884	0.753044
C	1.957639	-3.663083	0.559077
C	1.095864	-2.655508	0.145528
N	1.510410	-1.404091	-0.076793
N	-1.417827	-0.932986	-0.877787
C	-1.649687	-1.522917	-2.057562
C	-2.855075	-2.138887	-2.357563
C	-3.853826	-2.133485	-1.387807
C	-3.616830	-1.509361	-0.170488
C	-2.383673	-0.896837	0.064167
C	-2.058359	-0.169870	1.322231
C	-2.985565	0.031447	2.347329
C	-2.602616	0.749159	3.474175
C	-1.307148	1.249535	3.554347
C	-0.444069	1.005830	2.492020
N	-0.806460	0.313828	1.410686
N	-0.584802	1.739891	-1.392574
C	-1.719734	2.077491	-1.254459
S	-3.252841	2.504877	-1.055599
H	-0.839534	-1.483176	-2.775600
H	-3.004897	-2.598760	-3.325339
H	-4.812012	-2.600015	-1.581309
H	-4.391776	-1.490301	0.581898
H	-3.996561	-0.342172	2.269240
H	-3.311915	0.923361	4.274056
H	-0.973484	1.820476	4.411068

H	1.383094	2.946150	-1.039916
H	0.573500	1.381318	2.496884
H	3.651218	4.050334	-0.938347
H	5.626383	2.636164	-0.318753
H	5.281981	0.233941	0.171550
H	4.767681	-1.784430	0.683893
H	4.002101	-4.105279	1.077332
H	1.582016	-4.664277	0.724332
H	0.041959	-2.838842	-0.015597

$[Cu(en)_2]^{2+}$

	Value
Charge	2
Electronic Energy (a.u.)	-578.078382
Gibbs energy (a.u.)	-577.883320
Number of Imaginary Frequencies	0

Molecular Geometry in Cartesian Coordinates

C	2.809634	-0.669253	0.358955
N	1.533799	1.380466	-0.009028
C	2.809525	0.669420	-0.358802
N	1.533995	-1.380530	0.009325
H	1.625255	-1.805806	-0.915854
H	1.383917	2.159812	-0.650138
H	1.624932	1.805304	0.916377
H	3.681141	1.265830	-0.083439
H	2.822982	0.529978	-1.441919
H	2.823227	-0.529802	1.442057
H	3.681305	-1.265526	0.083491
H	1.384141	-2.159588	0.650791
C	-2.809375	0.669320	0.359313
Cu	-0.000002	-0.000074	-0.000262
N	-1.534098	-1.380549	-0.009145
C	-2.809626	-0.669107	-0.358875
N	-1.533857	1.380498	0.009094
H	-1.625379	1.805363	-0.916264
H	-1.384414	-2.159868	-0.650358
H	-1.625403	-1.805492	0.916204
H	-3.681448	-1.265369	-0.083908
H	-2.822852	-0.529258	-1.441938
H	-2.822216	0.529486	1.442384
H	-3.681174	1.265775	0.084649
H	-1.383774	2.159838	0.650180

[Cu(H$_{-2}$GGG)]$^{-}$

	Value
Charge	-1
Electronic Energy (a.u.)	-896.336286
Gibbs energy (a.u.)	-896.223319
Number of Imaginary Frequencies	0

Molecular Geometry in Cartesian Coordinates

N	1.434301	-2.141540	-0.183349
H	1.271515	-2.964591	0.387574
C	2.740764	-1.488101	0.126598
C	2.704461	0.063516	0.040940
H	3.015984	-1.736365	1.154434
H	3.543269	-1.849356	-0.522379
O	3.777195	0.669082	0.145258
N	1.471240	0.524469	-0.100157
C	1.123040	1.934806	-0.075652
C	-0.419031	2.118075	-0.020345
H	1.564641	2.446198	0.788911
H	1.486453	2.462819	-0.965656
O	-0.919359	3.244843	-0.087703
N	-1.060741	0.948701	0.101443
C	-2.485907	0.751625	0.090628
C	-2.796397	-0.771895	0.039698
H	-2.980496	1.160498	0.981477
H	-2.971096	1.224472	-0.773586
O	-3.960747	-1.142387	0.049997
H	1.403641	-2.446380	-1.151615
O	-1.760836	-1.574810	-0.013867
Cu	-0.053073	-0.649679	-0.020186

[Cu(H$_{-2}$GGH)]$^{-}$

	Value
Charge	-1
Electronic Energy (a.u.)	-1160.700824
Gibbs energy (a.u.)	-1160.515887
Number of Imaginary Frequencies	0

Molecular Geometry in Cartesian Coordinates

N	-2.176715	-0.512508	-0.446891
C	-1.746122	-1.757363	-1.052199
C	-0.207243	-1.876166	-1.032289
H	-2.159804	-2.622740	-0.522095
H	-2.069914	-1.837923	-2.096142
O	0.337619	-2.761197	-1.686645
C	-3.387776	-0.365235	0.077061
C	-3.520403	0.915267	0.937954
O	-4.373883	-1.105548	0.006342
N	-2.344802	1.825315	0.835242
H	-3.598937	0.576757	1.973634
H	-4.458885	1.415933	0.682020
H	-2.198260	2.345645	1.694371
N	0.418196	-0.954902	-0.251835
C	1.851251	-1.041824	-0.120978
H	2.349249	-1.077162	-1.096986
C	2.397498	0.141327	0.703440
C	2.394854	-2.327156	0.713815
H	1.951110	0.072359	1.703559
H	3.474525	-0.004006	0.798240
C	2.103993	1.487999	0.144695
O	1.593717	-2.856862	1.492090
N	0.798576	1.951333	0.038998
C	2.938796	2.451248	-0.357469
C	0.844801	3.149549	-0.513377
N	2.127439	3.498158	-0.769465
H	4.009673	2.477314	-0.459563
H	-0.002282	3.771233	-0.753684
H	2.432424	4.354851	-1.200783
H	-2.497056	2.505677	0.097033
O	3.609205	-2.520734	0.496878
Cu	-0.701443	0.574453	0.133270

$[Cu(H_2O)_6]^{2+}$

	Value
Charge	2
Electronic Energy (a.u.)	-655.599583
Gibbs energy (a.u.)	-655.496642
Number of Imaginary Frequencies	0

Molecular Geometry in Cartesian Coordinates

Cu	0.001611	-0.000129	-0.000670
O	2.129291	-0.001331	-0.435829
O	-0.505488	-0.306641	-1.906099
O	-2.130006	0.001062	0.430821
O	0.512251	0.306967	1.903435
O	0.063440	-2.093031	0.275952
O	-0.071992	2.094380	-0.264956
H	0.666286	2.662306	-0.520745
H	2.792748	0.133167	0.252732
H	-0.459573	0.372217	-2.593565
H	-2.606422	0.114165	1.262556
H	0.427510	1.178120	2.316253
H	-0.680172	-2.655571	0.527992
H	2.602833	-0.118020	-1.268696
H	-0.426962	-1.178481	-2.318571
H	-2.791163	-0.135524	-0.259545
H	0.462486	-0.372844	2.589773
H	0.862214	-2.636305	0.268783
H	-0.876487	2.629253	-0.264121

$[Cu(mnt)_2]^{2-}$

	Value
Charge	-2
Electronic Energy (a.u.)	-2314.363831
Gibbs energy (a.u.)	-2314.350111
Number of Imaginary Frequencies	0

Molecular Geometry in Cartesian Coordinates

Cu	-0.000062	-0.000284	-0.000220
S	1.654224	-1.565642	0.557406
S	1.653914	1.565129	-0.558152
S	-1.654345	-1.565543	-0.557807
S	-1.653752	1.565373	0.557621
N	5.330778	-1.917560	0.630977
N	5.330425	1.918364	-0.629898
N	-5.330915	-1.917552	-0.630089
N	-5.330218	1.918387	0.630922
C	3.115262	-0.653022	0.223104
C	3.115102	0.653121	-0.223119
C	4.344614	-1.335799	0.442857
C	4.344344	1.336264	-0.442404
C	-3.115262	-0.652980	-0.222958
C	-3.115060	0.653172	0.223212
C	-4.344683	-1.335797	-0.442324
C	-4.344207	1.336323	0.442952

$[Cu(OH)_4]^{2-}$

	Value
Charge	-2
Electronic Energy (a.u.)	-500.696516
Gibbs energy (a.u.)	-500.681608
Number of Imaginary Frequencies	0

Molecular Geometry in Cartesian Coordinates

Cu	-0.065441	-0.078506	-0.011850
O	1.821726	0.845627	-0.140264
O	0.912317	-1.776649	0.067206
O	-1.903315	-0.791427	-0.030455
O	-0.781665	1.776381	0.073924
H	1.753667	-1.321349	-0.077685
H	0.100606	2.127275	-0.111090
H	1.951973	0.951361	0.810486
H	-2.300949	0.087920	-0.041329

[Cu(salen)]

	Value
Charge	0
Electronic Energy (a.u.)	-1075.026637
Gibbs energy (a.u.)	-1074.911087
Number of Imaginary Frequencies	0

Molecular Geometry in Cartesian Coordinates

Cu	-0.000749000	0.181460000	-0.001133000
O	1.397439000	-1.183755000	-0.039149000
O	-1.396520000	-1.182908000	0.029403000
N	1.318702000	1.627913000	0.200084000
N	-1.319049000	1.626642000	-0.197932000
C	2.598049000	1.513447000	0.190396000
C	0.650706000	2.924234000	0.404248000
C	-0.651066000	2.923072000	-0.403584000
C	-2.598855000	1.512070000	-0.190165000
C	2.653860000	-1.037271000	-0.033792000
C	3.470875000	-2.229661000	-0.128864000
C	4.842581000	-2.149386000	-0.137687000
C	5.470519000	-0.893547000	-0.048600000
C	4.705042000	0.291885000	0.053179000
C	3.322301000	0.261652000	0.063347000
C	-2.654067000	-1.037314000	0.031544000
C	-3.468383000	-2.229554000	0.131373000
C	-4.840107000	-2.149827000	0.142494000
C	-5.469605000	-0.894270000	0.053295000
C	-4.706503000	0.290889000	-0.050710000
C	-3.323072000	0.261139000	-0.063660000
H	3.210498000	2.412115000	0.295210000
H	0.424474000	3.010222000	1.471382000
H	-0.424918000	3.007332000	-1.470897000
H	-3.210554000	2.411005000	-0.295779000
H	2.944406000	-3.173822000	-0.195708000
H	5.442300000	-3.048293000	-0.212298000
H	6.551825000	-0.825787000	-0.054734000
H	5.224804000	1.241148000	0.126954000
H	-2.941372000	-3.173423000	0.197670000
H	-5.439091000	-3.049041000	0.219316000
H	-6.550992000	-0.828116000	0.062001000
H	-5.226640000	1.239976000	-0.123263000
H	1.290119000	3.760997000	0.113883000

H	-1.291714000	3.759429000	-0.114872000

[Cu(salicylaldehydeiminato)$_2$]

	Value
Charge	0
Electronic Energy (a.u.)	-998.331649
Gibbs energy (a.u.)	-998.142363
Number of Imaginary Frequencies	0

Molecular Geometry in Cartesian Coordinates

C	5.257858	-1.128033	-0.000194
C	3.939674	-1.526027	0.000244
C	2.875189	-0.581973	0.000347
C	3.239328	0.809165	-0.000072
C	4.607144	1.177345	-0.000443
C	5.610731	0.236813	-0.000532
H	6.039313	-1.881114	-0.000253
H	3.665931	-2.574277	0.000556
H	4.855856	2.234744	-0.000698
H	6.651460	0.535758	-0.000872
O	1.654777	-1.020684	0.000903
O	-1.654790	1.020674	0.000931
C	2.261247	1.852285	-0.000088
N	0.977388	1.684371	-0.000422
C	-2.875199	0.581967	0.000364
C	-3.939689	1.526016	0.000264
C	-3.239335	-0.809175	-0.000071
C	-5.257871	1.128012	-0.000183
H	-3.665955	2.574267	0.000588
C	-4.607147	-1.177363	-0.000451
C	-5.610738	-0.236835	-0.000536
H	-6.039331	1.881088	-0.000240
H	-4.855853	-2.234764	-0.000717
H	-6.651466	-0.535784	-0.000883
C	-2.261240	-1.852282	-0.000095
N	-0.977385	-1.684339	-0.000427
H	-2.654003	-2.872540	0.000123
H	2.654032	2.872535	0.000139
H	-0.421781	-2.534011	-0.000298
H	0.421810	2.534059	-0.000285
Cu	0.000012	0.000014	0.000096

[Cu(salpn)]

	Value
Charge	2
Electronic Energy (a.u.)	-1115.079620
Gibbs energy (a.u.)	-11114.830341
Number of Imaginary Frequencies	0

Molecular Geometry in Cartesian Coordinates

Cu	-0.008144000	0.255419000	0.164944000
O	1.216887000	-1.194204000	-0.213975000
O	-1.298659000	-1.110592000	0.590921000
N	1.500069000	1.546253000	0.355970000
N	-1.478034000	1.612234000	-0.151468000
C	2.756753000	1.218574000	0.292214000
C	1.185659000	2.962543000	0.544374000
C	0.195793000	3.455044000	-0.514820000
C	-1.245406000	3.066195000	-0.214120000
C	-2.716267000	1.248456000	-0.331225000
C	2.503927000	-1.220947000	-0.186435000
C	3.177969000	-2.454512000	-0.423744000
C	4.550848000	-2.532842000	-0.413146000
C	5.351774000	-1.395615000	-0.166079000
C	4.734594000	-0.190063000	0.064749000
C	3.321353000	-0.067602000	0.064288000
C	-2.552740000	-1.162007000	0.308161000
C	-3.261416000	-2.384273000	0.497762000
C	-4.599046000	-2.487687000	0.196677000
C	-5.328938000	-1.386439000	-0.304793000
C	-4.680264000	-0.188870000	-0.483123000
C	-3.300240000	-0.040621000	-0.186831000
H	3.484476000	2.026917000	0.420771000
H	0.751106000	3.099532000	1.541952000
H	0.241171000	4.547765000	-0.561940000
H	-1.907762000	3.511893000	-0.965759000
H	-3.424175000	2.037239000	-0.609271000
H	2.558802000	-3.323030000	-0.611730000
H	5.028978000	-3.489636000	-0.597412000
H	6.431651000	-1.476097000	-0.160483000
H	5.330989000	0.697945000	0.254419000
H	-2.695488000	-3.225490000	0.878627000
H	-5.104560000	-3.436538000	0.345497000
H	-6.381651000	-1.487161000	-0.537810000
H	-5.225298000	0.673687000	-0.856031000

H	2.105709000	3.556773000	0.503568000
H	0.499542000	3.073316000	-1.494518000
H	-1.523480000	3.498690000	0.756204000

[Cu((*S*,*S*)-mnpala)]

	Value
Charge	0
Electronic Energy (a.u.)	-1204.567793
Gibbs energy (a.u.)	-1204.324814
Number of Imaginary Frequencies	0

Molecular Geometry in Cartesian Coordinates

Cu	0.277971	-0.980721	-0.254193
O	1.933078	-1.823473	-0.743111
O	4.163341	-1.619290	-0.533977
O	-0.842255	-2.517196	-0.415629
O	-2.913854	-3.281973	-0.024907
O	0.507891	2.874268	-1.670015
O	-1.610299	2.418069	-1.607679
N	1.488948	0.664088	-0.002778
N	-1.504301	0.007668	0.070346
N	-0.510445	2.531842	-1.091881
C	3.026773	-1.230605	-0.369506
C	2.805426	0.084540	0.432232
C	2.836454	-0.251189	1.922048
C	1.018151	1.825238	0.771992
C	-0.410228	2.273665	0.430914
C	-1.500585	1.268757	0.836587
C	-2.425733	-1.033691	0.635194
C	-3.901830	-0.690769	0.485529
C	-2.067632	-2.413548	-0.000032
C	-0.695050	3.633034	1.085222
H	1.629604	0.986070	-0.960642
H	-1.848492	0.226074	-0.866118
H	3.613798	0.777811	0.184517
H	1.986750	-0.887457	2.191937
H	2.839121	0.633684	2.562916
H	3.751273	-0.810520	2.119731
H	1.705021	2.666069	0.641725
H	1.009948	1.559572	1.828490
H	-2.473601	1.757457	0.761463
H	-1.329787	1.022177	1.887034
H	-2.161162	-1.125995	1.694488
H	-4.486224	-1.551534	0.808400
H	-4.194072	0.180529	1.076886
H	-4.148168	-0.505425	-0.564416
H	-0.647369	3.529530	2.171615

H	-1.688984	3.989812	0.812137
H	0.044057	4.372024	0.773081

$[Cu(ttcn)_2]^{2+}$

	Value
Charge	2
Electronic Energy (a.u.)	-3058.098458
Gibbs energy (a.u.)	-3057.798303
Number of Imaginary Frequencies	0

Molecular Geometry in Cartesian Coordinates

Cu	0.000000	0.000000	0.000000
S	-0.054261	-0.544914	2.640466
S	2.239634	0.834354	0.357214
S	0.933426	-2.226158	-0.272301
C	1.340528	0.582915	3.049876
C	2.577275	0.533018	2.152568
C	3.163856	-0.523750	-0.480453
C	2.750570	-1.937305	-0.086916
C	0.455116	-3.005636	1.329334
C	0.732783	-2.211868	2.607084
H	1.650861	0.388877	4.078459
H	0.881508	1.573484	3.033226
H	3.272779	1.313578	2.466508
H	3.098160	-0.419237	2.236745
H	4.227904	-0.373163	-0.286790
H	2.990011	-0.335982	-1.541391
H	3.256025	-2.654542	-0.736105
H	3.026829	-2.174117	0.939110
H	0.957550	-3.974313	1.375749
H	-0.612388	-3.197430	1.204981
H	0.331702	-2.779977	3.448437
H	1.800726	-2.095049	2.786362
S	0.054261	0.544914	-2.640466
S	-2.239634	-0.834354	-0.357214
S	-0.933426	2.226158	0.272301
C	-1.340528	-0.582915	-3.049876
C	-0.732783	2.211868	-2.607084
C	-2.577275	-0.533018	-2.152568
C	-3.163856	0.523750	0.480453
C	-2.750570	1.937305	0.086916
C	-0.455116	3.005636	-1.329334
H	-1.650861	-0.388877	-4.078459
H	-0.881508	-1.573484	-3.033226
H	-0.331702	2.779977	-3.448437
H	-1.800726	2.095049	-2.786362

H	-3.272779	-1.313578	-2.466508
H	-3.098160	0.419237	-2.236745
H	-4.227904	0.373163	0.286790
H	-2.990011	0.335982	1.541391
H	-3.256025	2.654542	0.736105
H	-3.026829	2.174117	-0.939110
H	-0.957550	3.974313	-1.375749
H	0.612388	3.197430	-1.204981

$[Cu(mnt)_2]^{2-}$ (B3LYP-D3-*def*2-TZVP)

	Value
Charge	-2
Electronic Energy (a.u.)	-3757.671174
Gibbs energy (a.u.)	-3757.657362
Number of Imaginary Frequencies	0

Molecular Geometry in Cartesian Coordinates

Cu	-0.000006000	0.000105000	0.000017000
S	1.650068000	-1.553774000	0.567408000
S	1.650217000	1.553816000	-0.567307000
S	-1.650111000	-1.553757000	-0.567373000
S	-1.650251000	1.553822000	0.567346000
N	5.308984000	-1.919257000	0.640123000
N	5.308850000	1.919323000	-0.640452000
N	-5.308730000	-1.919644000	-0.640366000
N	-5.308765000	1.919581000	0.640383000
C	3.100313000	-0.650948000	0.228281000
C	3.100373000	0.650795000	-0.228314000
C	4.327457000	-1.334748000	0.449464000
C	4.327584000	1.334454000	-0.449561000
C	-3.100356000	-0.650924000	-0.228263000
C	-3.100410000	0.650819000	0.228332000
C	-4.327501000	-1.334722000	-0.449438000
C	-4.327618000	1.334481000	0.449585000

$[Cu(mnt)_2]^{2-}$ (B3LYP-D3-*def*2-TZVP , SMD for CH_2Cl_2)

	Value
Charge	-2
Electronic Energy (a.u.)	-3757.858073
Gibbs energy (a.u.)	-3757.843726
Number of Imaginary Frequencies	0

Molecular Geometry in Cartesian Coordinates

Cu	0.000023000	0.000007000	0.000020000
S	1.636940000	1.560004000	0.559850000
S	1.637009000	-1.559922000	-0.559785000
S	-1.636922000	-1.559913000	0.559982000
S	-1.636940000	1.559881000	-0.560009000
N	5.298011000	1.902926000	0.625409000
N	5.297664000	-1.903292000	-0.625686000
N	-5.298089000	-1.902673000	0.625383000
N	-5.298035000	1.902788000	-0.625220000
C	3.082967000	0.651050000	0.224494000
C	3.082993000	-0.650934000	-0.224330000
C	4.311660000	1.327373000	0.441063000
C	4.311721000	-1.327160000	-0.440975000
C	-3.082932000	-0.650997000	0.224455000
C	-3.082940000	0.650943000	-0.224497000
C	-4.311634000	-1.327309000	0.441002000
C	-4.311654000	1.327158000	-0.441275000

[Cu(H$_{-2}$GGH)]$^{-}$ (B3LYP-D3-*def*2-TZVP)

	Value
Charge	-1
Electronic Energy (a.u.)	-2604.054000
Gibbs energy (a.u.)	-2603.869058
Number of Imaginary Frequencies	0

Molecular Geometry in Cartesian Coordinates

N	2.158505000	-0.583153000	0.395667000
C	1.706552000	-1.811392000	1.008587000
C	0.169466000	-1.892906000	1.001226000
H	2.092866000	-2.689355000	0.481724000
H	2.039144000	-1.893465000	2.047911000
O	-0.389097000	-2.770870000	1.654341000
C	3.387656000	-0.421874000	-0.061175000
C	3.562559000	0.857985000	-0.906585000
O	4.374540000	-1.157856000	0.061462000
N	2.393493000	1.774957000	-0.851242000
H	3.688248000	0.525997000	-1.938106000
H	4.488287000	1.353006000	-0.605947000
H	2.252225000	2.258152000	-1.730369000
N	-0.442670000	-0.960073000	0.233187000
C	-1.877413000	-0.999261000	0.121248000
H	-2.360091000	-1.011811000	1.103802000
C	-2.392347000	0.198277000	-0.699340000
C	-2.475078000	-2.261515000	-0.695392000
H	-1.949255000	0.120151000	-1.698338000
H	-3.472379000	0.090806000	-0.795790000
C	-2.063552000	1.531330000	-0.135861000
O	-1.729628000	-2.774320000	-1.537747000
N	-0.749819000	1.957930000	-0.022969000
C	-2.871760000	2.514494000	0.364860000
C	-0.765215000	3.153301000	0.530062000
N	-2.035672000	3.534620000	0.781307000
H	-3.940745000	2.569526000	0.463738000
H	0.095929000	3.751934000	0.774211000
H	-2.317894000	4.397286000	1.211992000
H	2.534657000	2.482802000	-0.139770000
O	-3.672741000	-2.466598000	-0.411489000
Cu	0.711460000	0.555914000	-0.145691000

[Cu(H$_{-2}$GGH)]$^{-}$ (B3LYP-D3-*def*2-TZVP, SMD for H$_2$O)

	Value
Charge	-1
Electronic Energy (a.u.)	-2604.240362
Gibbs energy (a.u.)	-2604.051867
Number of Imaginary Frequencies	0

Molecular Geometry in Cartesian Coordinates

N	2.039622000	-0.951812000	0.054558000
C	1.462965000	-2.195655000	0.502457000
C	-0.050513000	-2.060603000	0.625677000
H	1.665857000	-3.020980000	-0.189658000
H	1.859424000	-2.500327000	1.476471000
O	-0.694650000	-3.022652000	1.122623000
C	3.334488000	-0.746631000	-0.005719000
C	3.734037000	0.666908000	-0.414242000
O	4.245182000	-1.583985000	0.234634000
N	2.575567000	1.582072000	-0.556903000
H	4.277707000	0.602724000	-1.357174000
H	4.429515000	1.047090000	0.334294000
H	2.566025000	2.006547000	-1.477844000
N	-0.566547000	-0.923642000	0.178310000
C	-2.012403000	-0.759611000	0.226606000
H	-2.347241000	-0.670495000	1.264406000
C	-2.447209000	0.503282000	-0.546536000
C	-2.811250000	-1.929470000	-0.410419000
H	-2.168930000	0.359342000	-1.594871000
H	-3.534430000	0.579429000	-0.505119000
C	-1.864180000	1.785874000	-0.067686000
O	-2.388764000	-2.417834000	-1.490918000
N	-0.497404000	2.005915000	-0.052593000
C	-2.483460000	2.926303000	0.355590000
C	-0.302244000	3.243360000	0.372008000
N	-1.480876000	3.831965000	0.625462000
H	-3.524035000	3.169998000	0.474667000
H	0.650908000	3.724312000	0.509952000
H	-1.603299000	4.777767000	0.955855000
H	2.633467000	2.340001000	0.115256000
O	-3.886103000	-2.253569000	0.165957000
Cu	0.794338000	0.496375000	-0.201133000

Cu(II)-HSA model (AspAlaHisLysSer–NHCH$_3$ with NH$_2$, N$^-$, N$^-$, His3-N coordination)

	Value
Electronic Energy (Eh)	-2136.096560
Sum of electronic and thermal Free Energies (Eh)	-2135.546024
Number of Imaginary Frequencies	0

Molecular Geometry in Cartesian Coordinates

N	3.302594	0.327105	1.291590
H	4.142528	0.476878	0.734078
H	3.594753	0.419892	2.263673
C	2.824124	-1.064170	1.068674
H	2.578971	-1.123389	0.002072
C	3.896788	-2.118922	1.364781
H	4.444032	-1.859946	2.273148
H	3.415356	-3.084582	1.501692
C	4.843493	-2.078486	0.171911
O	4.547656	-2.891218	-0.834392
O	5.730073	-1.251444	0.104576
C	1.464179	-1.292934	1.761731
O	1.008283	-2.441633	1.819219
N	0.885331	-0.146489	2.126271
C	-0.529789	-0.123088	2.476848
H	-1.005822	-1.047345	2.130717
C	-0.769966	0.005886	3.983511
H	-0.325657	-0.846581	4.500609
H	-0.318015	0.924958	4.366029
H	-1.842186	0.021084	4.187039
C	-1.202849	1.019635	1.706522
O	-2.443812	1.082114	1.643452
N	-0.366559	1.863719	1.072360
C	-0.947144	2.799538	0.122559
H	-1.941934	3.096563	0.469274
C	-0.092399	4.068749	-0.024224
H	-0.630412	4.771296	-0.660863
H	0.023180	4.519876	0.965755
C	1.249166	3.809208	-0.630492
N	2.103282	2.818402	-0.162577
C	3.182297	2.831841	-0.930987
H	4.032614	2.176848	-0.846241
N	3.064493	3.789550	-1.871680
H	3.745388	3.997759	-2.585438
C	1.844313	4.414839	-1.701375
H	1.501393	5.202291	-2.349186
C	-1.196315	2.170560	-1.272405

O	-1.602486	2.848585	-2.200181
N	-0.946946	0.833123	-1.344088
H	-0.607890	0.400190	-0.500225
C	-1.415422	-0.039796	-2.404574
H	-1.776572	0.611947	-3.203776
C	-0.289602	-0.938575	-2.947591
H	-0.682368	-1.455103	-3.825810
H	0.532533	-0.294410	-3.276784
C	0.217800	-1.995097	-1.953847
H	0.590333	-1.518981	-1.038814
H	-0.628710	-2.621372	-1.655466
C	1.307326	-2.889817	-2.568210
H	2.263193	-2.355805	-2.622222
H	1.021607	-3.119308	-3.600748
C	1.512846	-4.226836	-1.853678
H	0.548747	-4.748884	-1.788503
H	2.180692	-4.852285	-2.453199
N	2.138219	-4.071874	-0.520947
H	2.250518	-4.987591	-0.092684
H	1.536679	-3.550807	0.123213
H	3.671361	-3.386327	-0.672409
C	-2.610108	-0.923270	-1.962482
O	-2.943059	-1.877812	-2.651259
N	-3.181204	-0.606014	-0.774967
H	-2.975213	0.279651	-0.332389
C	-4.290160	-1.356735	-0.222313
H	-4.503231	-2.167146	-0.927307
C	-3.934588	-1.980383	1.148857
H	-4.631333	-2.795350	1.361841
H	-2.929725	-2.417639	1.062262
O	-4.034492	-1.078460	2.231461
H	-3.467442	-0.297331	2.066741
Cu	1.516648	1.387824	1.113656
C	-5.544727	-0.472786	-0.115170
O	-5.535218	0.676423	-0.485331
C	-6.761869	-1.117685	0.508306
H	-6.585499	-1.177921	1.586609
H	-7.638422	-0.500284	0.316591
H	-6.920648	-2.132911	0.134463

Cu(II)-PrP (region 106-126, Ac–AsnMetLysHisMet–NHCH$_3$ with Met109-S, N$^-$, N$^-$, His111-N coordination)

	Value
Electronic Energy (Eh)	-3202.091124
Sum of electronic and thermal Free Energies (Eh)	-3201.382999
Number of Imaginary Frequencies	0

Molecular Geometry in Cartesian Coordinates

C	4.180305	2.565601	-0.430777
O	3.761089	2.257307	-1.554472
N	3.629069	2.132513	0.722958
C	2.389923	1.380949	0.803814
C	1.143311	2.316418	0.866034
O	1.322119	3.489354	1.231695
C	2.389315	0.536249	2.099748
C	2.383456	1.440522	3.323947
O	3.385452	2.058024	3.676521
N	1.192743	1.515308	3.990160
H	3.941416	2.525097	1.604386
H	2.342487	0.698603	-0.046708
H	1.516745	-0.113195	2.074969
H	3.289528	-0.080415	2.147558
H	0.350438	1.230470	3.510641
H	1.105207	2.269955	4.656640
N	-0.048233	1.704628	0.710010
C	-1.200099	2.418726	1.289900
C	-2.369467	1.443966	1.532624
O	-3.321217	1.760568	2.268160
C	-1.676402	3.621539	0.440618
C	-2.093570	3.241189	-0.984169
S	-1.983637	4.627379	-2.187809
C	-0.163462	4.650908	-2.384092
H	-0.910502	2.837878	2.262415
H	-2.514034	4.103220	0.955609
H	-0.843547	4.326431	0.421679
H	-3.125843	2.880373	-1.015976
H	-1.463845	2.437989	-1.377612
H	0.097694	5.530658	-2.976645
H	0.335855	4.714089	-1.413119
H	0.177736	3.752937	-2.908250
N	-2.243595	0.308717	0.825803
C	-3.236647	-0.733434	0.769570
C	-2.749245	-1.856474	-0.184066
O	-3.483392	-2.836328	-0.403360

C	-4.604614	-0.195029	0.288204
C	-5.749845	-1.178401	0.535115
C	-7.082212	-0.636246	-0.000224
C	-8.190187	-1.643364	0.240636
N	-9.523613	-1.111457	-0.314437
H	-3.385205	-1.193414	1.761145
H	-4.528497	0.038128	-0.782790
H	-4.789502	0.737611	0.828803
H	-5.501082	-2.133717	0.062532
H	-5.842434	-1.358890	1.614966
H	-7.326143	0.317536	0.489414
H	-6.989071	-0.440123	-1.077904
H	-8.007131	-2.592085	-0.268787
H	-8.362259	-1.833092	1.302636
H	-10.303025	-1.761440	-0.172301
H	-9.436651	-0.928442	-1.319516
H	-9.760309	-0.220831	0.135120
N	-1.525372	-1.635947	-0.726194
C	-1.010000	-2.630734	-1.667347
C	0.104788	-3.449013	-0.992528
O	0.061354	-4.666734	-0.882325
C	-0.555842	-1.984952	-3.001827
C	0.474426	-0.898338	-2.909745
C	1.617338	-0.695981	-3.643515
N	0.332057	0.172331	-2.031834
C	1.337668	1.004539	-2.258966
N	2.139400	0.516199	-3.221666
H	-1.793383	-3.357532	-1.896380
H	-0.183986	-2.771529	-3.667733
H	-1.457288	-1.565781	-3.467281
H	2.080679	-1.286932	-4.417454
H	1.533124	1.925181	-1.741545
H	3.041157	0.926992	-3.425454
N	1.129304	-2.691917	-0.475140
C	1.993025	-3.148890	0.596611
C	1.466106	-2.752161	1.999110
O	2.174768	-2.892641	2.992210
C	3.416303	-2.602655	0.400825
C	4.054634	-3.115897	-0.890073
S	5.623441	-2.284145	-1.343414
C	6.677800	-2.772705	0.067816
H	1.060541	-1.689713	-0.578625
H	1.995789	-4.242879	0.554426

H	3.377782	-1.507027	0.367520
H	4.004750	-2.874457	1.279687
H	4.219904	-4.198668	-0.839840
H	3.385336	-2.927094	-1.735633
H	7.684213	-2.403519	-0.142760
H	6.329888	-2.330111	1.004105
H	6.714749	-3.861674	0.166888
N	0.216183	-2.218309	2.038921
H	-0.331048	-2.130806	1.190743
C	5.385206	3.478471	-0.278368
H	6.149839	3.169467	-0.994534
H	5.081090	4.498718	-0.533329
H	5.805800	3.479743	0.730355
C	-0.382323	-1.747517	3.275964
H	-1.101416	-0.961212	3.030464
H	-0.896266	-2.553348	3.813562
H	0.398618	-1.348241	3.927575
Cu	-0.737582	0.145820	-0.320021

Cu(II)-PrP (region 106-126, Ac–AsnMetLysHisMet–NHCH$_3$ with N$^-$, N$^-$, N$^-$, His111-N coordination)

	Value
Electronic Energy (Eh)	-3203.190312
Sum of electronic and thermal Free Energies (Eh)	-3202.468159
Number of Imaginary Frequencies	0

Molecular Geometry in Cartesian Coordinates

C	3.241516	-3.569114	-1.600081
O	2.439989	-4.068501	-0.802119
N	3.292608	-2.231386	-1.806773
C	2.585693	-1.285074	-0.938049
C	1.163612	-1.003233	-1.471074
O	0.790316	0.082428	-1.873750
C	3.419788	-0.042954	-0.688177
C	4.681899	-0.403294	0.105694
O	4.748718	-1.417415	0.795293
N	5.704137	0.467721	-0.014082
H	3.946407	-1.860405	-2.479438
H	2.479403	-1.794913	0.014960
H	3.664014	0.476205	-1.618277
H	2.826673	0.660302	-0.096553
H	5.585488	1.378316	-0.448584
H	6.511970	0.325222	0.573956
N	0.375738	-2.121908	-1.387929
C	-0.867512	-2.313719	-2.140488
C	-2.011731	-1.352789	-1.760794
O	-2.796729	-1.024019	-2.654937
C	-1.319148	-3.791496	-2.050770
C	-0.987955	-4.571675	-0.769342
S	-1.476485	-3.872803	0.860692
C	-3.287976	-3.769169	0.674818
H	0.884761	-2.960471	-1.124974
H	-0.690379	-2.076418	-3.192088
H	-2.392446	-3.817839	-2.249549
H	-0.847984	-4.358070	-2.861183
H	0.085980	-4.741809	-0.668864
H	-1.451888	-5.559109	-0.824044
H	-3.682636	-3.453151	1.640533
H	-3.543774	-3.028133	-0.079445
H	-3.685870	-4.753249	0.425183
N	-2.084719	-0.951997	-0.484619
C	-2.897147	0.226754	-0.242071
C	-2.309146	1.020216	0.922845

O	-2.754080	2.155726	1.184241
C	-4.395369	-0.088177	-0.058741
C	-5.263362	1.166728	-0.183956
C	-6.762292	0.867949	-0.045597
C	-7.559144	2.153251	-0.184987
N	-9.064055	1.881293	-0.058365
H	-2.815322	0.884388	-1.116010
H	-4.556240	-0.574393	0.911219
H	-4.662369	-0.798263	-0.846036
H	-4.947872	1.897126	0.564798
H	-5.077325	1.618130	-1.165546
H	-7.072100	0.149185	-0.814830
H	-6.959803	0.412668	0.933068
H	-7.316094	2.876036	0.594681
H	-7.421013	2.622069	-1.160146
H	-9.622640	2.734583	-0.150278
H	-9.277979	1.459479	0.850018
H	-9.371474	1.222556	-0.779871
N	-1.271329	0.434369	1.540680
C	-0.551108	1.245816	2.505491
C	0.394136	2.292260	1.866614
O	0.935534	3.125995	2.576397
C	0.166774	0.405391	3.572062
C	1.076872	-0.658087	3.050969
C	2.391054	-0.896341	3.344894
N	0.635538	-1.668279	2.201853
C	1.655308	-2.498983	2.017701
N	2.730095	-2.068563	2.701064
H	-1.265584	1.886305	3.033303
H	0.734882	1.088070	4.205720
H	-0.597135	-0.068702	4.196999
H	3.089877	-0.351642	3.955472
H	1.665022	-3.362125	1.372276
H	3.675528	-2.381432	2.522367
N	0.511342	2.274865	0.509428
C	0.870502	3.475918	-0.247673
C	-0.122086	3.698861	-1.416668
O	0.253156	4.097164	-2.507795
C	2.313263	3.494643	-0.756588
C	3.314101	3.649287	0.384162
S	5.073144	3.713127	-0.143341
C	5.062257	5.143038	-1.279967
H	0.079546	1.514035	0.001332

H	0.738468	4.314123	0.446246
H	2.499911	2.589662	-1.337870
H	2.393547	4.329173	-1.453628
H	3.104474	4.551373	0.963161
H	3.257966	2.816222	1.088432
H	6.103008	5.357229	-1.523599
H	4.514952	4.929401	-2.197428
H	4.630863	6.011228	-0.779287
N	-1.423711	3.458430	-1.124152
H	-1.712793	3.180313	-0.193154
C	4.219915	-4.417244	-2.374973
H	5.049558	-4.670462	-1.709238
H	3.730241	-5.344676	-2.669795
H	4.622655	-3.915420	-3.256459
C	-2.455166	3.630276	-2.132641
H	-3.421110	3.694061	-1.629737
H	-2.276616	4.543091	-2.703547
H	-2.470967	2.789611	-2.834549
Cu	-0.884908	-1.402475	0.941332

Cu(II)-PrP (region 180-193, Ac–IleLysGlnHisThr–NHCH$_3$ with N$^-$, N$^-$, N$^-$, His187-N coordination)

	Value
Electronic Energy (Eh)	-2559.637440
Sum of electronic and thermal Free Energies (Eh)	-2558.863617
Number of Imaginary Frequencies	0

Molecular Geometry in Cartesian Coordinates

C	-4.234557	1.280485	2.271030
O	-4.109236	0.075180	2.534409
N	-3.563799	1.899251	1.277917
C	-2.661619	1.248819	0.326806
C	-1.512417	2.232986	0.052422
O	-1.834622	3.429004	-0.125839
C	-3.364358	0.806295	-0.979245
H	-3.652759	2.897330	1.138023
H	-2.297523	0.335312	0.794580
H	-2.677282	0.107039	-1.459506
H	-4.246541	0.220176	-0.689725
N	-0.268706	1.737443	-0.052679
C	0.693064	2.658909	-0.682566
C	1.866213	1.879128	-1.301156
O	2.688553	2.448565	-2.043471
C	1.212757	3.750031	0.287662
C	2.034650	3.203366	1.468663
H	0.192897	3.192039	-1.499211
H	1.816027	4.460153	-0.290710
H	0.331659	4.281829	0.651783
H	1.630905	2.222889	1.753737
H	1.920144	3.849057	2.348517
N	1.921634	0.604652	-0.886687
C	2.932028	-0.337336	-1.307121
C	2.626582	-1.718749	-0.684477
O	3.378287	-2.677027	-0.927170
C	4.337894	0.120265	-0.862889
C	5.491180	-0.696707	-1.432240
H	2.933786	-0.453182	-2.401586
H	4.363006	0.058662	0.231523
H	4.444961	1.164796	-1.163161
H	5.330766	-1.758516	-1.205471
H	5.512045	-0.619681	-2.526808
N	1.543603	-1.735751	0.135229
C	1.236281	-3.002552	0.800500
C	0.021398	-3.664825	0.120579

O	0.080058	-4.772485	-0.393021
C	1.061517	-2.804370	2.325021
C	-0.007723	-1.841708	2.739452
C	-1.059599	-2.030272	3.598085
N	-0.067869	-0.532946	2.256733
C	-1.112529	0.039561	2.841569
N	-1.734193	-0.824657	3.665583
H	2.058929	-3.704232	0.642744
H	0.857835	-3.774942	2.790190
H	2.028493	-2.456265	2.710592
H	-1.376887	-2.900376	4.150226
H	-2.698760	-0.676968	3.947504
N	-1.106726	-2.881737	0.074203
C	-2.171473	-3.064473	-0.890733
C	-1.955458	-2.186347	-2.145249
O	-2.853822	-2.057911	-2.990164
C	-3.546723	-2.762123	-0.227541
H	-3.507665	-1.723421	0.148760
H	-1.066912	-1.973971	0.513028
H	-2.156570	-4.109607	-1.213276
O	-4.611508	-2.928099	-1.137298
N	-0.773564	-1.541424	-2.244926
H	-0.052302	-1.702161	-1.552494
C	-5.183764	2.157808	3.071949
H	-6.209256	1.854582	2.839762
H	-5.022837	1.974866	4.137333
H	-5.078113	3.225852	2.864484
C	-0.468916	-0.633611	-3.339217
H	0.330170	0.034503	-3.013394
H	-0.155586	-1.176440	-4.238143
H	-1.354844	-0.045751	-3.586757
Cu	0.655931	0.026132	0.415950
C	-3.805507	-3.678366	0.963314
H	-3.802871	-4.724915	0.641946
H	-3.048371	-3.540880	1.739533
H	-4.788604	-3.444566	1.380210
H	-4.302319	-2.572346	-1.993425
C	6.830270	-0.259254	-0.889401
O	6.975028	0.564231	0.038509
N	7.918400	-0.822136	-1.452394
H	8.833967	-0.584138	-1.101381
H	7.834781	-1.512633	-2.181846
C	3.534543	3.073509	1.138778

H	3.659553	2.716251	0.115503
H	4.002641	4.067874	1.185616
C	4.236672	2.135121	2.106867
H	3.816664	1.128368	2.054114
H	4.165524	2.491356	3.139179
N	5.710440	2.012013	1.779286
H	6.111175	2.936961	1.606504
H	6.234222	1.594770	2.551273
H	5.964300	1.402260	0.924464
C	-3.774789	1.848139	-2.039407
H	-2.864662	2.364489	-2.374686
C	-4.377634	1.087685	-3.235423
H	-5.359136	0.673637	-2.970570
H	-3.748200	0.245458	-3.537730
H	-4.514558	1.741014	-4.101843
C	-4.735139	2.927412	-1.502349
H	-5.578722	2.438103	-0.993580
H	-4.193844	3.515485	-0.757649
C	-5.267224	3.891070	-2.570092
H	-5.918623	3.389752	-3.292517
H	-4.441468	4.349792	-3.126671
H	-5.845632	4.700341	-2.110959
H	-1.445778	1.048153	2.664368

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