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Is Copper(I) Hard or Soft? A Density Functional Study of Mixed Ligand Complexes

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Tables S1-S7 Total Energy (E) (Zero point Energy corrected), Ionization potential (IP) and Electron affinity (EA) of Ni(0), Cu(I) and Zn(II) complexes of H_2S, H_2O, PH_3 and NH_3.

Table S1 Energies (Hartree)

Systems	E	IP	EA
S (H_2S)	-11.2755414	0.3875043	0.129087
W (H_2O)	-76.3935513	0.4578389	0.1679682
P (PH_3)	-8.2465947	0.3840.712	0.1345815
N (NH_3)	-56.5143517	0.366396	0.1922655

Table S2 Energies (Hartree)

Systems	E	IP	EA
NiS_3	-203.1059329	0.1919522	0.0328653
NiS_2W	-268.2219504	0.1663549	0.0322743
NiS_4	-214.3786714	0.1635793	0.0413731

Ni = Ni(0), S = H_2S, W = H_2O

Table S3 Energies (Hartree)

Systems	E	IP	EA
CuS_3	-229.7969856	0.5054003	0.1289577
CuS_2W	-294.9319724	0.5000981	0.1242178
CuSW_2	-360.065509	0.49955	0.1204292
CuW_3	-425.1982756	0.5012568	0.1133734
CuS_4	-241.0890628	0.4742501	0.1099928
CuS_3W	-306.2227281	0.469012	0.1049437
CuS_2W_2	-371.3550943	0.4604211	0.1013979
CuSW_3	-436.4860357	0.4646355	0.0976437
CuW_4	-501.6157262	0.4538439	0.0877684

Cu = Cu(I), S = H_2S, W = H_2O

Table S4 Energies (Hartree)

Systems	E	IP	EA
ZnS_3	-98.7790877	0.7110139	0.3628225
ZnS_2W	-163.9292467	0.7245112	0.3567685
ZnSW_2	-229.0779418	0.7622352	0.3511484
ZnW_3	-294.2272689	0.8319197	0.3460078
ZnS_4	-110.1038431	0.6740344	0.3172943
ZnS_3W	-175.2538937	0.6803614	0.3097532
ZnS_2W_2	-240.4040006	0.6909088	0.3025391
ZnSW_3	-305.5541811	0.7203428	0.2965467
ZnW_4	-370.704691	0.7835886	0.2903615

Zn = Zn(II), S = H_2S, W = H_2O

Table S5 Energies (Hartree)

Systems	E	IP	EA
NiP_3	-194.060785	0.2009925	0.0419825
NiP_2N	-242.3236863	0.1703726	0.035982
NiPN_2	-290.5810887	0.1408571	0.036447
NiP_4	-202.3217475	0.1934532	0.046828
NiP_3N	-250.5806171	0.1692964	0.0395696
NiP_2N_2	-298.8383613	0.1489447	0.0384231
NiPN_3	-347.0887026	0.1282377	0.042502

Ni = Ni(0), P = PH_3, N = NH_3

Table S6 Energies (Hartree)

Systems	E	IP	EA
CuP_3	-220.7450272	0.4887765	0.1140405
CuP_2N	-269.0287613	0.4788629	0.0981292
CuPN_2	-317.3110108	0.471244	0.096437
CuN_3	-365.591394	0.4645418	0.0904202
CuP_4	-229.0101392	0.4579169	0.0700275
CuP_3N	-277.2908259	0.4496145	0.0900171

CuP_2N_2	-325.5705088	0.4405296	0.0876685
CuPN_3	-373.8475967	0.4300554	0.0841425
CuN_4	-422.1233301	0.4146616	0.0684476

Cu = Cu(I), *P* = PH_3, *N* = NH_3

Table S7 Energies (Hartree)

Systems	E	IP	EA
ZnP_3	-89.7571322	0.7082913	0.300054
ZnP_2N	-138.051844	0.7161157	0.3034507
ZnPN_2	-186.3462742	0.7447929	0.3016653
ZnN_3	-234.6400918	0.7990283	0.3010362
ZnP_4	-98.0540388	0.6657612	0.2571632
ZnP_3N	-146.3484241	0.673536	0.2530844
ZnP_2N_2	-194.6429284	0.6790783	0.249849
ZnPN_3	-242.9364522	0.700612	0.2472617
ZnN_4	-291.2302167	0.739395	0.2462019

Zn = Zn(II), *P* = PH_3, *N* = NH_3