Electronic Supplementary Information

Cu^{II}-Azide polynuclear complexes of Cu_4 building clusters with Schiff-Base co-ligands: synthesis, structures, magnetic behavior and DFT studies

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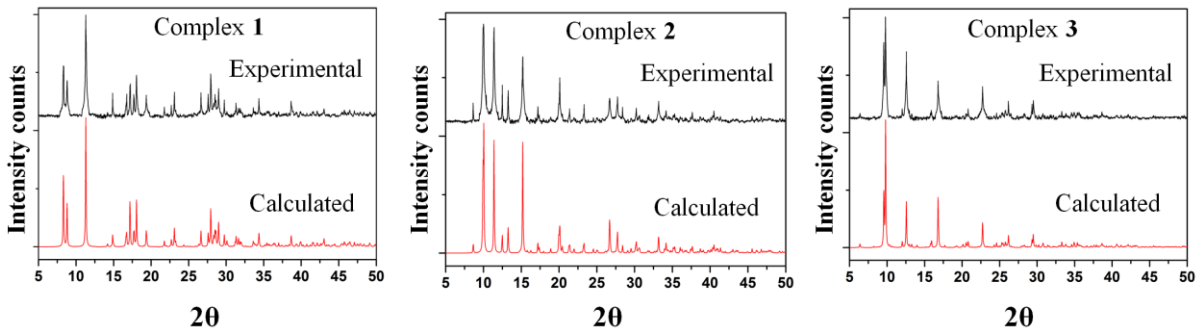


Fig. S1. Powder XRD of the complexes carried out in D8 Advance X-ray diffractometer. The experimental patterns match very well with the simulated ones obtained from X-ray single crystal structure.

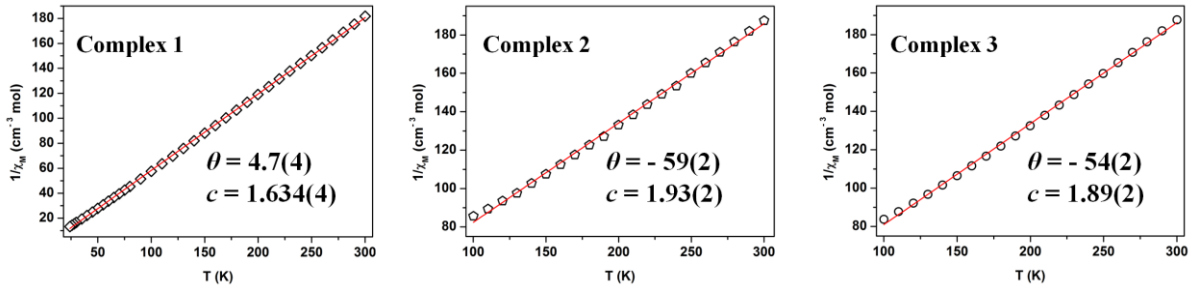


Fig. S2. Curie-Weiss fitting of complex **1-3**. The data presented corresponds to Cu^{II}_4 units. The red solid lines indicate the fitting using theoretical model (see text).

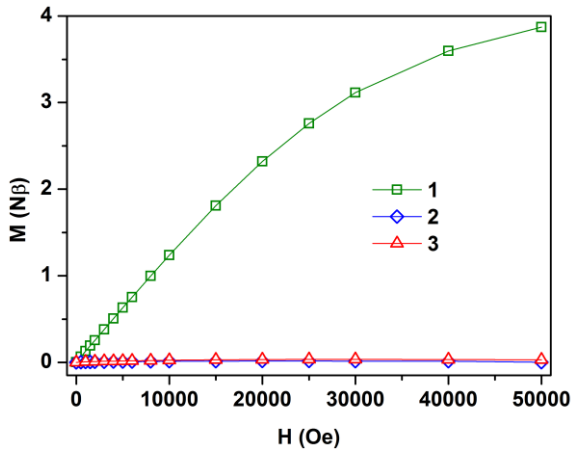


Fig. S3. Magnetization *versus* field up to H = 50 kOe (5 T) at 2 K for **1-3.** The data presented corresponds to Cu^{II}_4 units. Solid lines are only guides for the eye.

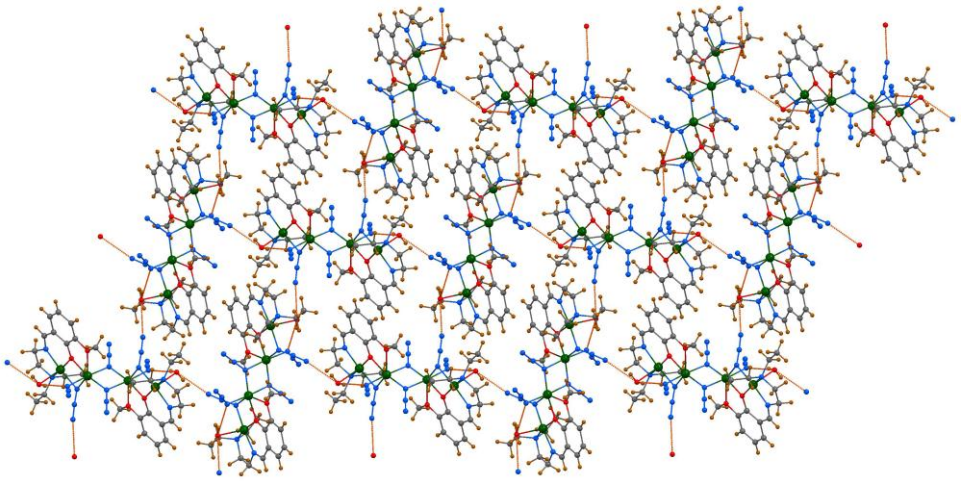
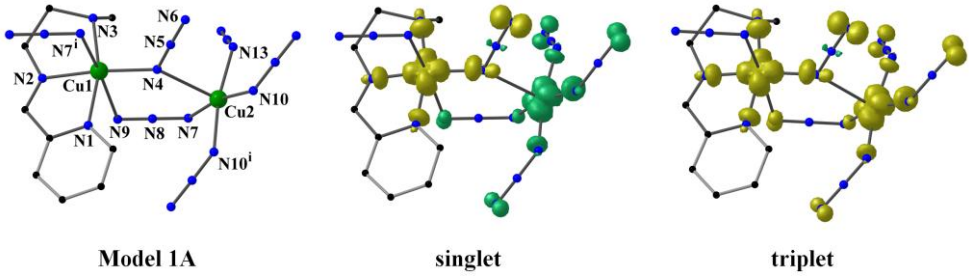


Fig. S4. 2D arrangement of the H-bonded clusters of complex **2**.

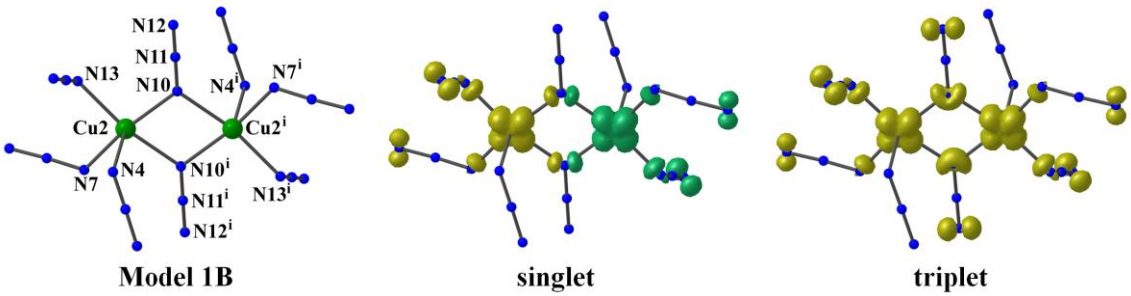
Mulliken Atomic spin density plots and tables (in au) of all the model systems in all of their spin states (for lanl2dz basis set).

Positive and negative spin populations are represented as yellow and green surfaces. The isodensity surfaces correspond to a value of 0.01 e/b^3.



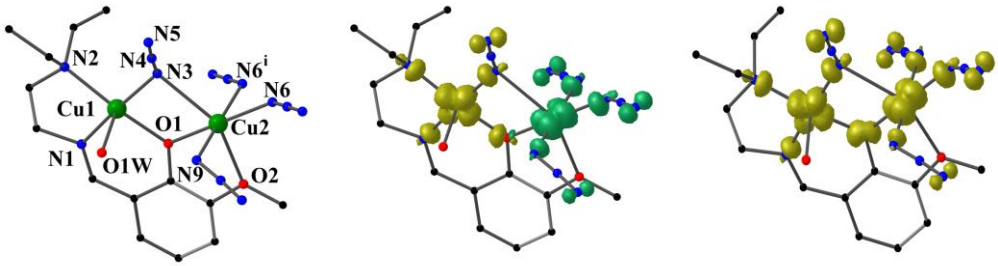
Model 1A

Atoms	Singlet	Triplet
Cu1	0.530464	0.549435
Cu2	-0.474973	0.484776
N1	0.060328	0.068834
N2	0.076553	0.081838
N3	0.085017	0.088143
N4	0.118431	0.110404
N5	-0.053002	-0.051549
N6	0.174106	0.168383
N7	-0.016812	0.018535
$N7^i$	0.000275	0.001786
N8	0.002765	-0.005633
N9	-0.074792	0.082749
N10	-0.081947	0.082596
$N10^i$	-0.047410	0.041133
N13	-0.042005	0.040169



Model 1B

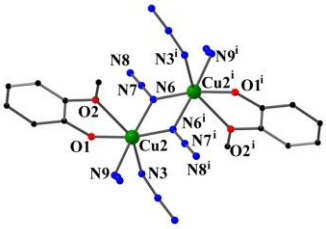
Atoms	Singlet	Triplet
Cu2	0.538118	0.522375
Cu2^{i}	-0.537858	0.524325
N4	0.003284	0.002169
N4^{i}	-0.003279	0.002138
N7	0.036206	0.041072
N7^{i}	-0.036276	0.038086
N10	0.002245	0.108286
N10^{i}	-0.002290	0.102965
N11	0.000573	-0.025322
N11^{i}	-0.000568	-0.029415
N12	0.001134	0.113042
N12^{i}	-0.001181	0.122787
N13	0.057720	0.060826
N13^{i}	-0.057809	0.062558



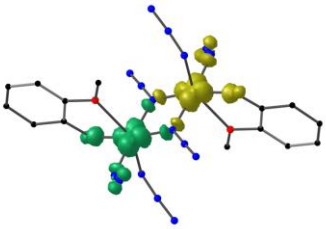
Model 2A singlet triplet

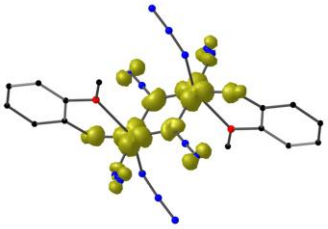
Model 2A

Atoms	Singlet	Triplet
Cu1	0.491357	0.527375
Cu2	-0.434156	0.523253
N1	0.071908	0.085432
N2	0.076355	0.090700
N3	0.082235	0.103746
N4	-0.016130	-0.044393
N5	0.096305	0.147569
N6	-0.082172	0.102519
N6^{i}	-0.064614	0.069370
N9	-0.098168	0.128459
O1	0.047679	0.108362
O2	-0.000242	0.000314
O1W	0.000468	0.000890



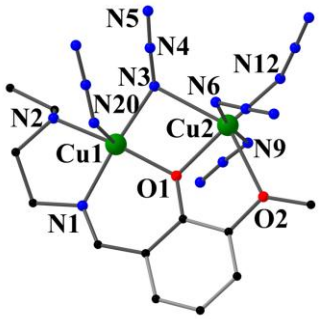
Model 2B


singlet

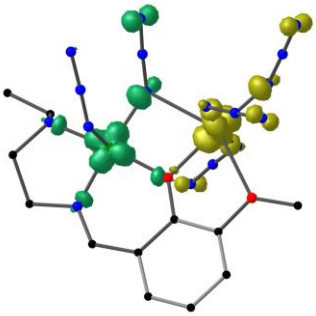

triplet

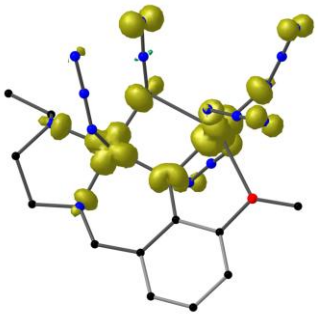
Model 2B

Atoms	Singlet	Triplet
Cu2	-0.599619	0.589511
Cu2^{i}	0.599619	0.596978
N3	-0.004009	0.011441
N3^{i}	0.004009	0.003465
N6	0.002221	0.106320
N6^{i}	-0.002221	0.105227
N7	0.003695	-0.027694
N7^{i}	-0.003695	-0.027343
N8	-0.011387	0.114984
N8^{i}	0.011387	0.113964
N9	-0.050560	0.052039
N9^{i}	0.050560	0.050481
O1	-0.086125	0.091716
O1^{i}	0.086125	0.090886
O2	-0.000112	0.000099
O2^{i}	0.000112	0.000054



Model 3A

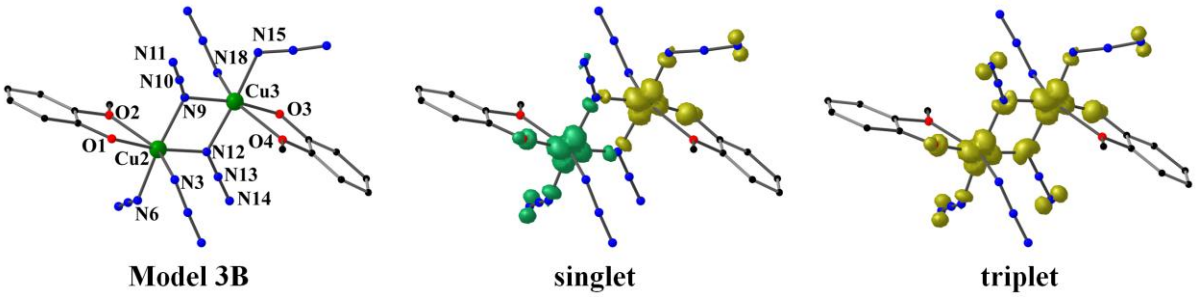

singlet


triplet

Model 3A

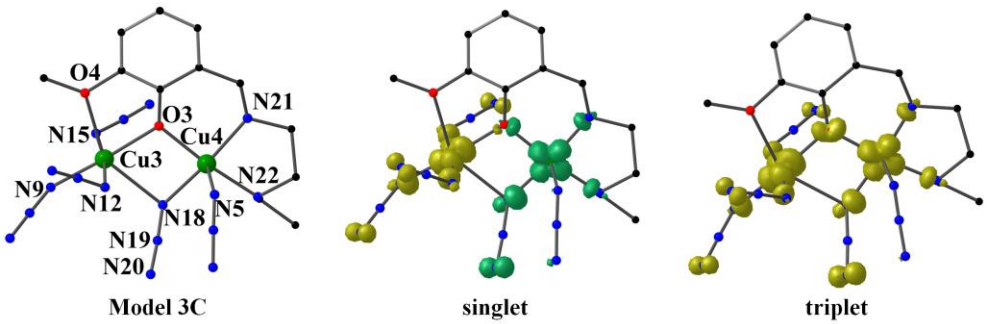
Atoms	Singlet	Triplet
Cu1	-0.501257	0.524104
Cu2	0.546198	0.526433
N1	-0.039778	0.078267
N2	-0.040231	0.075153
N3	-0.081615	0.126114

N4	0.007669	-0.049564
N5	-0.076619	0.150868
N6	0.053654	0.060023
N9	0.049686	0.052552
N12	0.066529	0.081769
N20	-0.021886	0.021815
O1	-0.014914	0.094726
O2	0.000172	0.000168



Model 3B

Atoms	Singlet	Triplet
Cu2	-0.513226	0.580812
Cu3	0.509989	0.585710
N3	-0.004907	0.012835
N6	-0.050926	0.044506
N9	-0.009072	0.094423
N10	0.005527	-0.023555
N11	-0.018086	0.120093
N12	0.002954	0.110786
N13	-0.005315	-0.026327
N14	0.010296	0.119512
N15	0.054629	0.046144
N18	0.007614	0.010439
O1	-0.066506	0.086041
O2	-0.000204	0.000315
O3	0.081589	0.095636
O4	0.000214	0.000212



Model 3C

Atoms	Singlet	Triplet
Cu3	0.572122	0.521234
Cu4	-0.507112	0.527711
N5	-0.021554	0.022434
N9	0.067634	0.081123
N12	0.052643	0.060432
N15	0.047671	0.052675
N18	-0.083654	0.126555
N19	0.007334	-0.049876
N20	-0.071122	0.150111
N21	-0.039322	0.078534
N22	-0.040998	0.075768
O3	-0.014665	0.094635
O4	0.000154	0.000155