Electronic Supplementary Material (ESI) for Dalton Transactions

Supporting Information

Cu^{II}-azide polymers with various molar equivalents of blocking diamine ligands: synthesis, structures, magnetic properties with DFT studies

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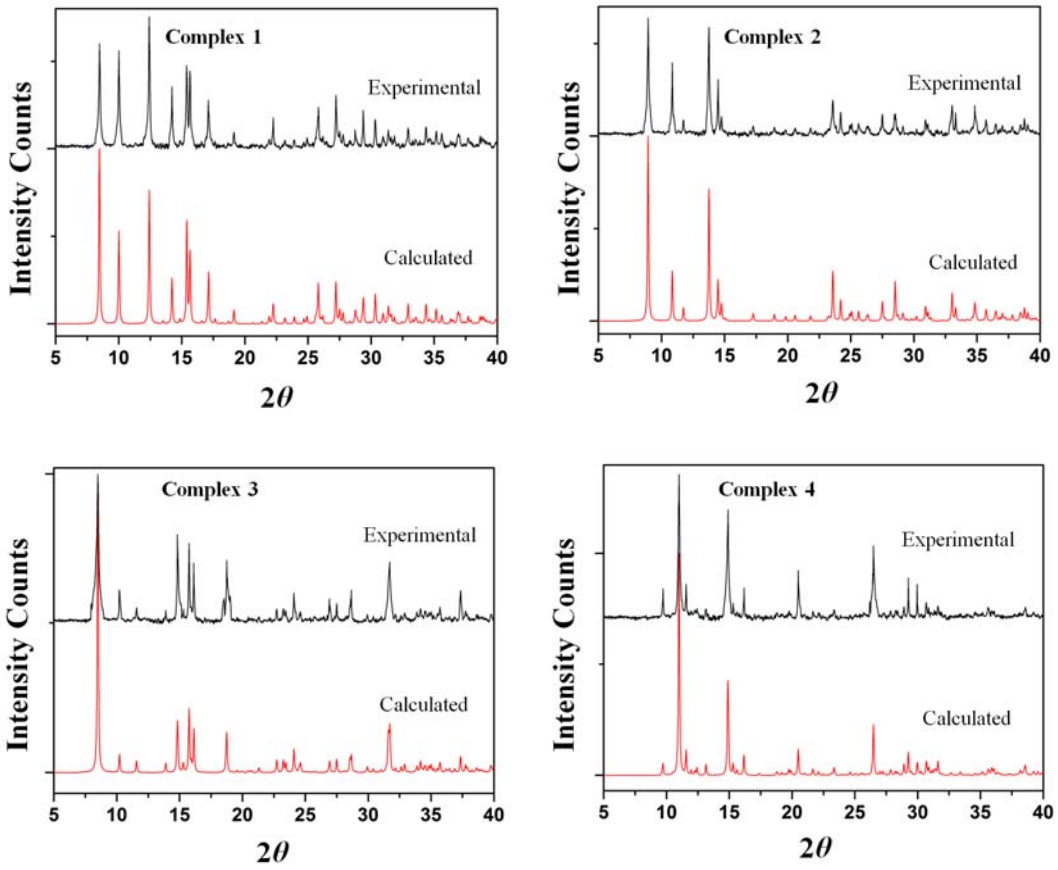

Fig. S1. Powder XRD of the complexes carried out in a D8 Advance X-ray diffractometer. The experimental patterns match very well with the simulated ones obtained from X-ray single crystal structure.

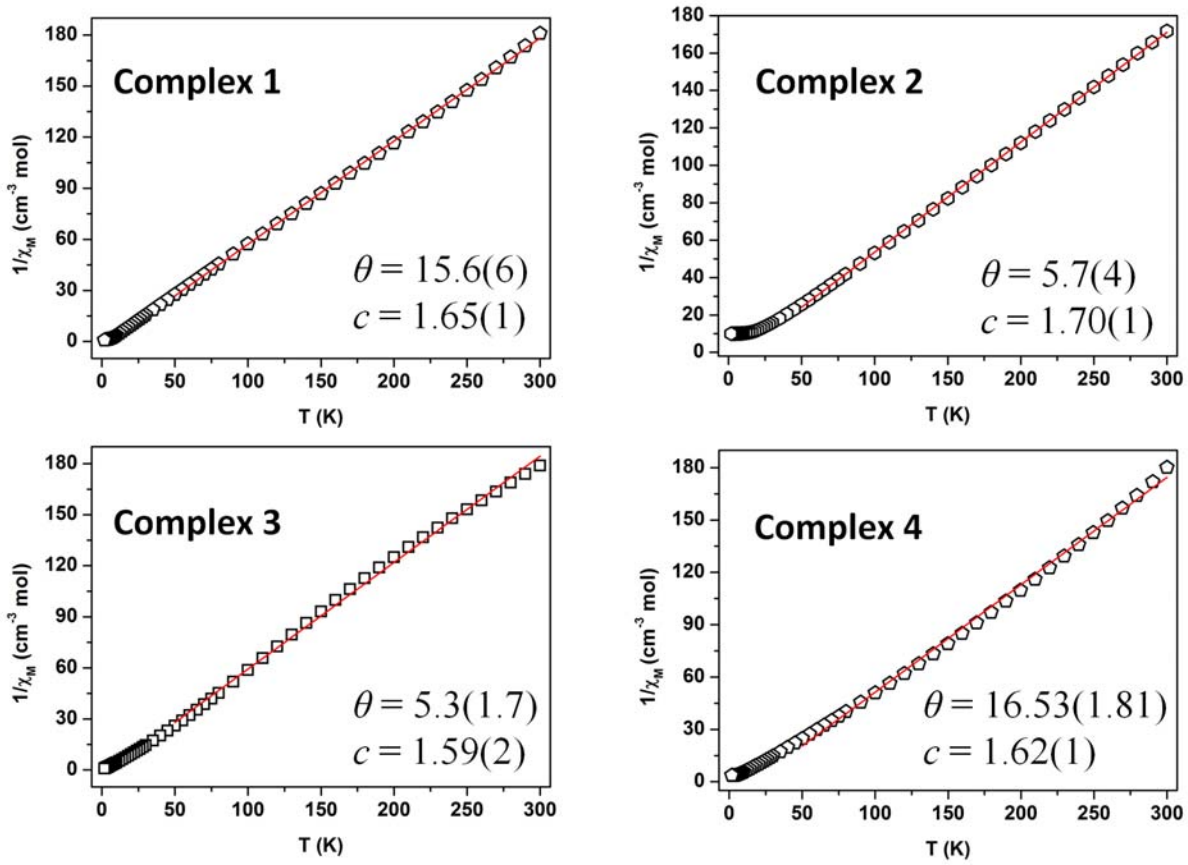

Fig. S2. Curie-Weiss fitting of complex **1-4**. The data presented corresponds to Cu^{II}_4 units for **1-2** and Cu^{II}_5 units for **3-4**. The red solid lines indicate the fitting using theoretical model (see text).

Table S1. Atomic spin densities (in au) of all the model systems in all of their spin states (for LanL2DZ basis set).

Model 1

Atoms	Quintet	Triplet	Singlet
Cu1	0.507554	0.529232	-0.496224
Cu2	0.457543	-0.478230	0.451863
Cu3	0.446814	0.472828	0.451863
Cu4	0.499103	0.536085	-0.496224
N1	0.072256	0.075687	-0.074512
N2	0.089413	0.089505	-0.087798
N3	0.130487	0.125231	-0.059016

N4	0.091311	0.090346	-0.024819
N5	0.092356	0.083733	0.085799
N6	0.092919	-0.084404	0.085799
N7	0.091754	0.024689	-0.024819
N8	0.137474	0.050138	-0.059016
N9	0.075195	0.078419	-0.074512
N10	0.089708	0.088184	-0.087798

Model 2

Atoms	Quintet	Triplet	Singlet
Cu1	0.435128	0.413898	-0.273807
Cu2	0.494323	-0.515583	0.279539
Cu3	0.363531	0.394309	-0.277911
Cu4	0.501806	0.506169	0.282774
N1	0.077297	0.074325	-0.042062
N2	0.059038	0.057608	-0.034628
N3	0.140160	0.046757	-0.015952
N4	0.112736	0.035900	-0.010076
N5	0.060720	-0.054543	0.057576
N6	-0.011957	0.006026	0.002064
N7	0.107479	-0.095848	0.067628
N8	0.064332	0.071614	-0.042623
N9	0.049981	0.055203	-0.035099
N10	0.101480	0.107666	-0.011263
N11	0.125878	0.133969	-0.017339
N12	0.054698	0.055848	0.056644
N13	-0.010074	-0.008779	0.002004
N14	0.105694	0.104765	0.067082

Model 3A

Atoms	Triplet	Singlet
Cu1	0.496189	-0.510865
Cu2	0.502611	0.516782
N1	0.107009	-0.109215
N2	0.070304	-0.080767
N3	0.090774	0.044110
N4	-0.016016	-0.004954
N5	0.096329	-0.007678
N6	0.098176	0.005537
N7	-0.015640	0.005517
N8	0.088318	-0.045962

N9	0.106935	0.108823
N10	0.072779	0.080641

Model 3B

Atoms	Quartet	Doublet
Cu1	0.528801	-0.524616
Cu2	0.555053	0.556690
Cu3	0.528313	0.524484
N1	0.056529	-0.059088
N2	0.063906	-0.066308
N3	0.112775	0.010377
N4	0.101845	0.019213
N5	0.101875	0.102614
N6	0.112880	0.113158
N7	0.064284	0.063124
N8	0.056677	0.057769

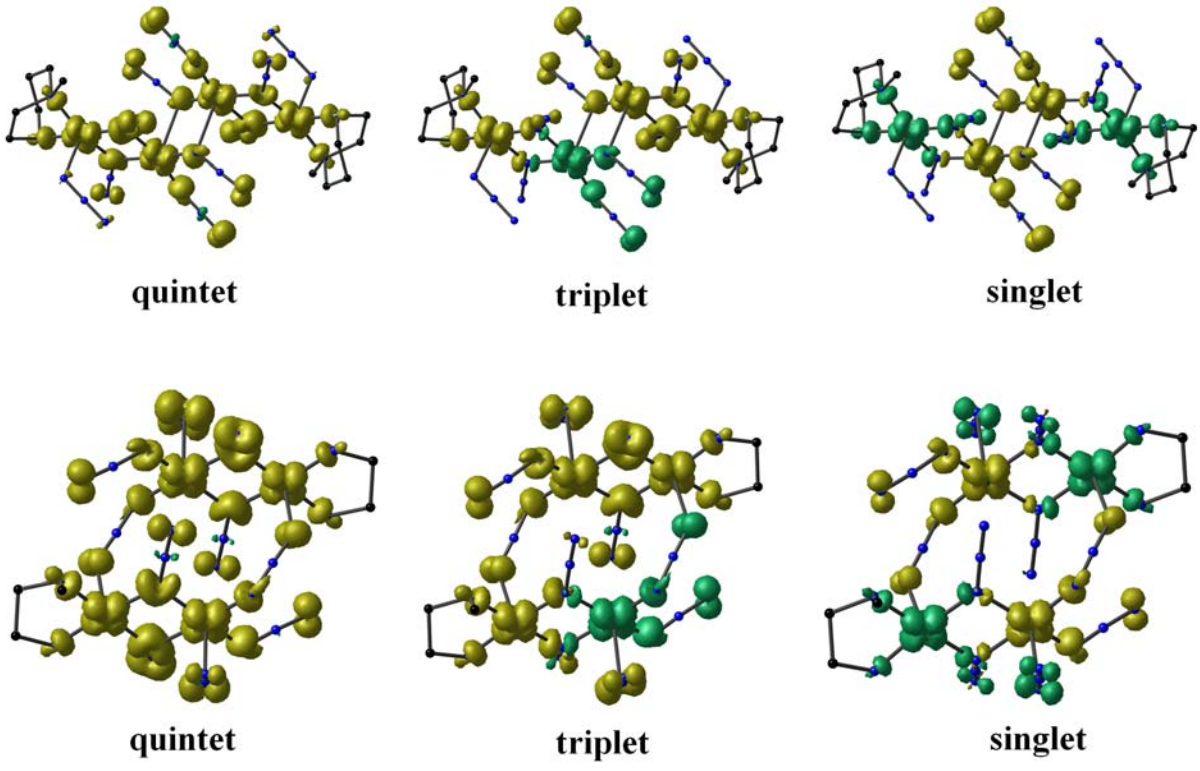

Fig. S3. Spin density maps calculated for **1** (top) and **2** (bottom) at B3LYP level (with LanL2DZ basis set) for singlet, triplet and quintet states. Positive and negative spin

populations are represented as yellow and green surfaces. The isodensity surfaces correspond to a value of 0.007 e/b^3.

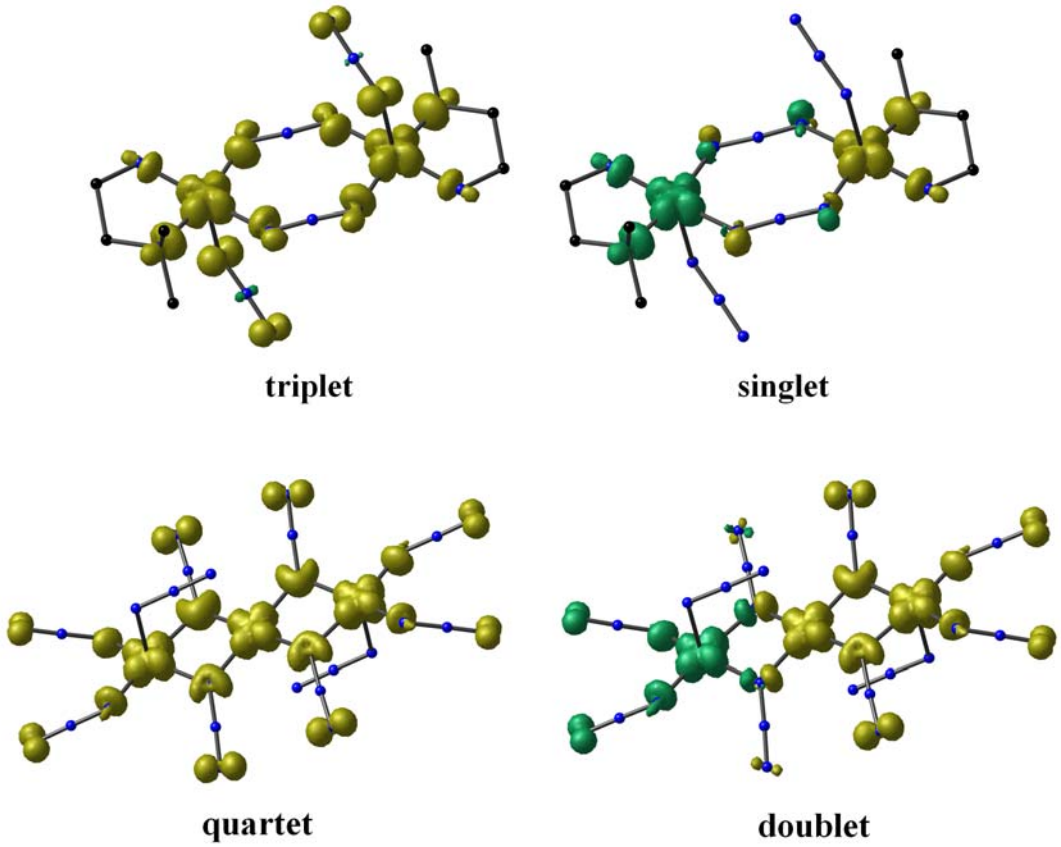

Fig. S4. Spin density maps calculated for **3A** (top) and **3B** (bottom) at B3LYP level (with LanL2DZ basis set) for the indicated states. Positive and negative spin populations are represented as yellow and green surfaces. The isodensity surfaces correspond to a value of 0.007 e/b^3.