Electronic Supplementary Material (ESI) for Dalton Transactions

Supporting Information

Discrete dinuclear complex to extended 2D compound in Cu-azido system by controlling coligand stoichiometry: Synthesis and magneto-structural correlations

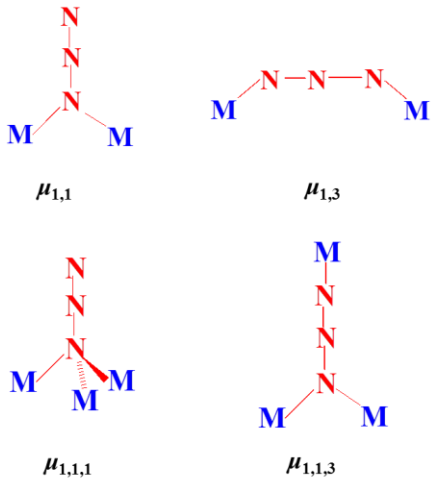
Anindita Chakraborty,[a] Lingampalli Srinivasa Rao,[a] Arun Kumar Manna,[b] Swapan K. Pati,[b] Joan Ribas[c] and Tapas Kumar Maji[*a]

[a]*Molecular Materials Laboratory, Chemistry and Physics of Materials Unit, Jawaharlal Nehru Centre for Advanced Scientific Research, Jakkur, Bangalore – 560 064, India.*

**E-mail: tmaji@jncasr.ac.in, Phone: +91 80 2208 2826, FAX: +91 80 2208 2766*

[b]*Theoretical Sciences Unit, Jawaharlal Nehru Centre for Advanced Scientific Research, Jakkur, Bangalore, 560 064, India*

[c]*Departament de Quimica Inorganica, Universitat de Barcelona, Diagonal 645, 08028 Barcelona, Spain*



Scheme S1 The observed binding modes for azido ligand in **1** and **2**.

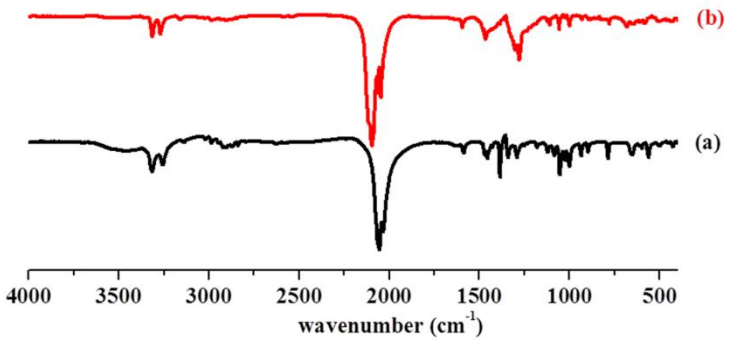


Fig. S1. IR spectra of compounds **1**(a), **2** (b).

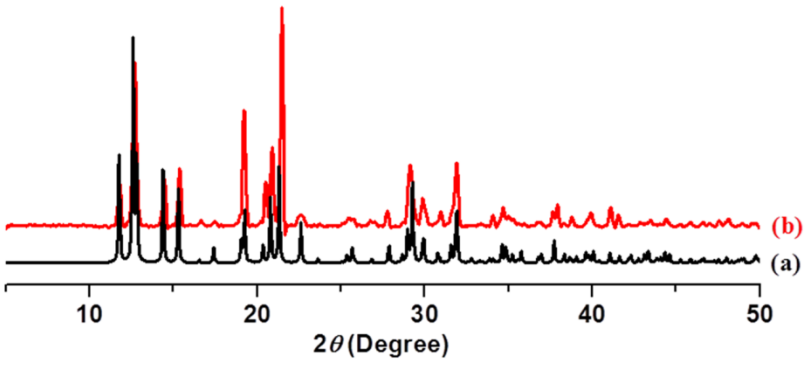


Fig. S2. PXRD patterns of compound **1**: (a) simulated; (b) bulk as-synthesized. Similarity in simulated and as-synthesized pattern indicates high purity of the compound.

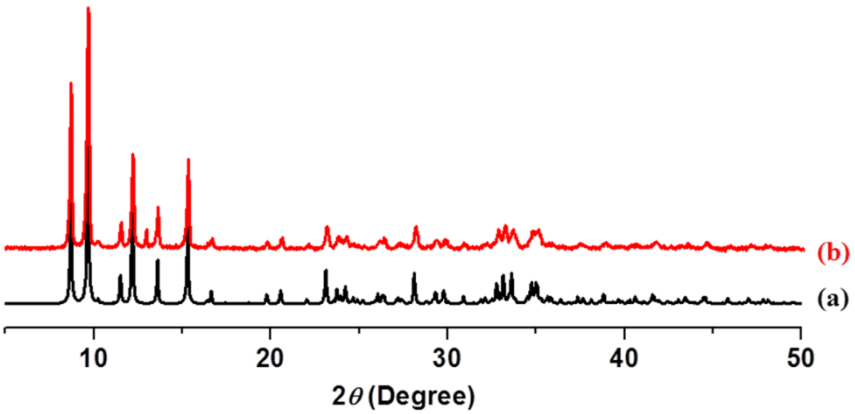


Fig. S3. PXRD patterns of compound **2**: (a) simulated; (b) bulk as-synthesized. Similarity in simulated and as-synthesized pattern indicates high purity of the compound.

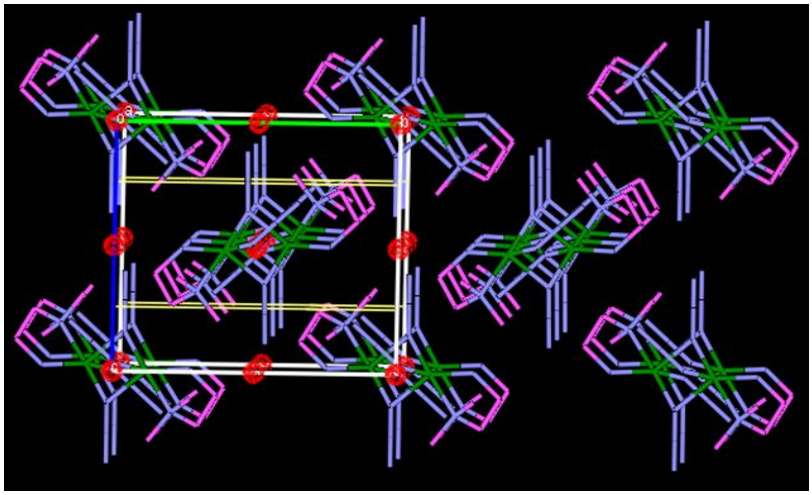


Fig. S4. Packing diagram of dimers in the lattice with the application of 2_1-screw axis along *c* direction. The 2_1-screw axis(shown in yellow line) is along *b* axis at *c* =1/4. Colour code: C, pink; Cu, green; N, blue; centre of symmetry, red circle.

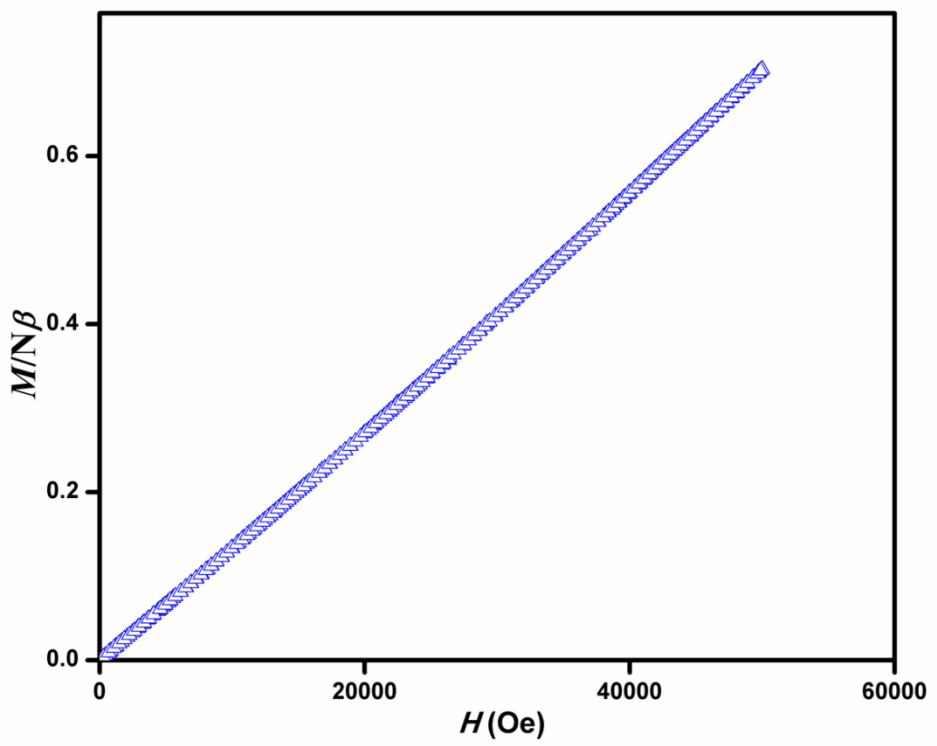


Fig. S5 The M *vs.* *H* curve for **1** at 3 K.

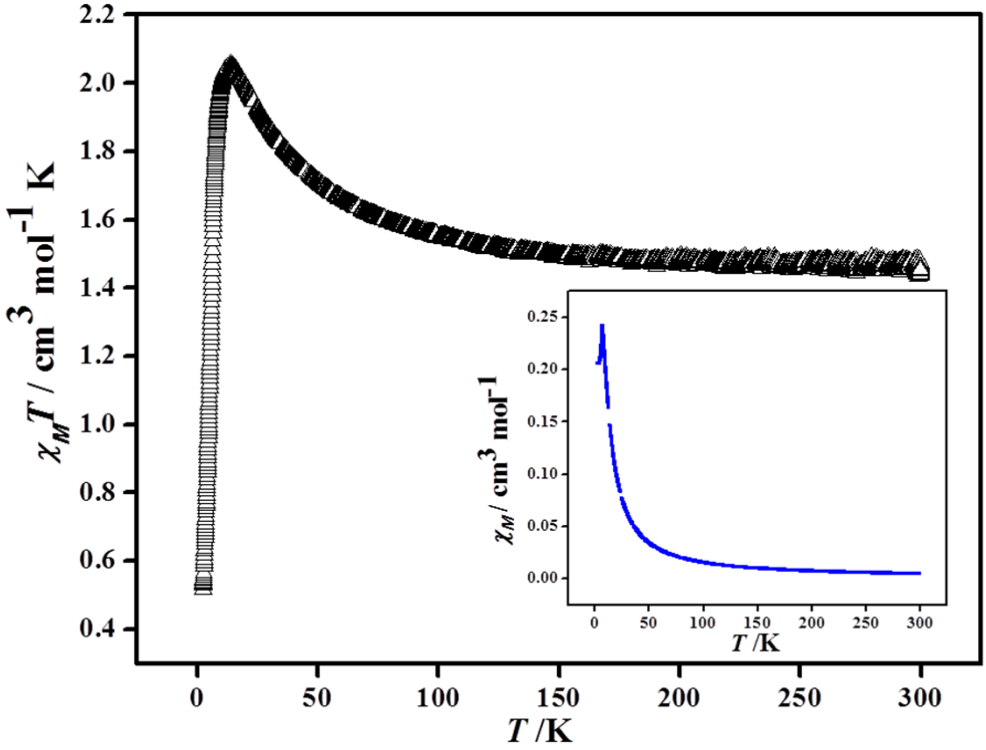


Fig. S6. The plots of $\chi_M T$ *vs.* *T* (per Cu3 unit) and χ_M *vs.* *T* (inset) for **2**.

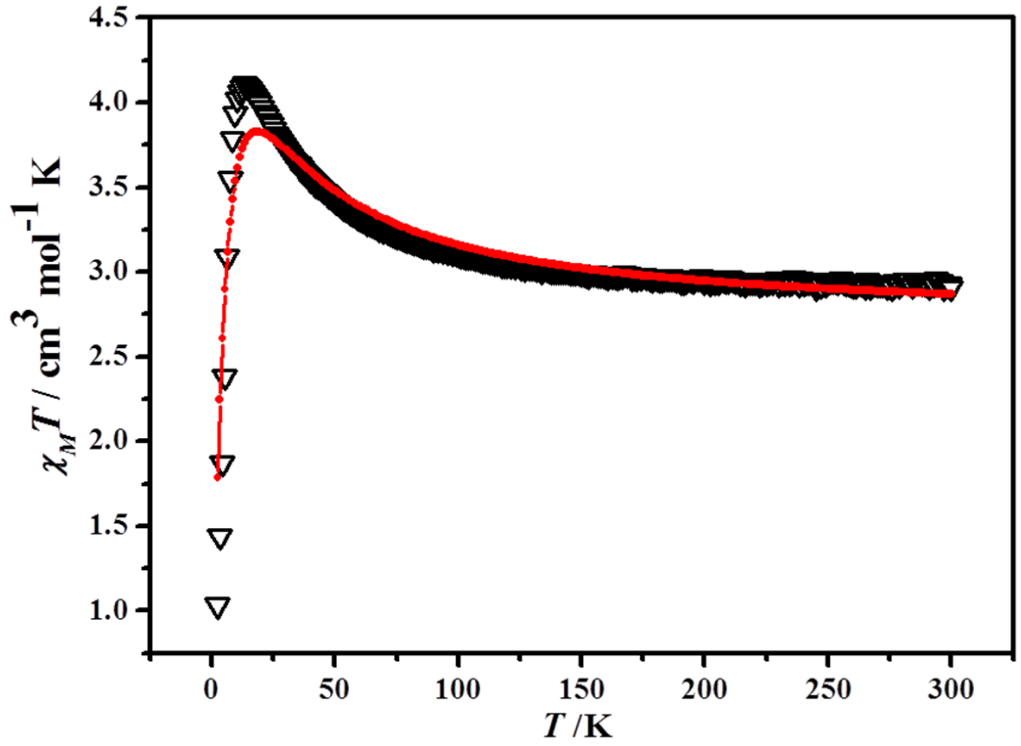


Fig. S7. The plot of $\chi_M T$ *vs.* T for **2** considering a hexanuclear unit. The solid red line indicates the best fit obtained considering one average J.

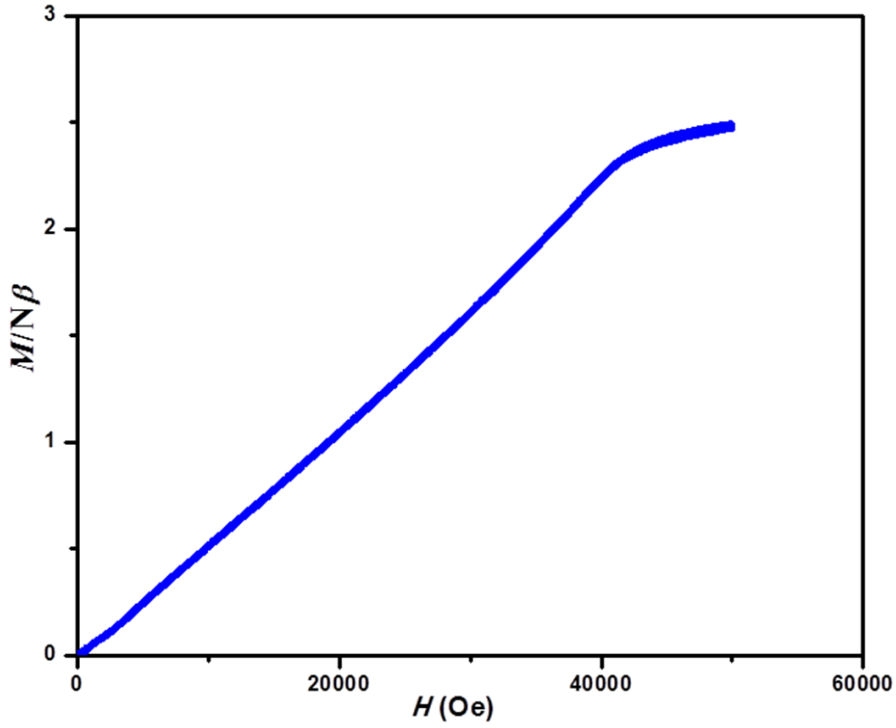


Fig. S8. The M *vs.* H curve for **2** at 3 K.

Table S1. Results for the two possible spin states of the model system **A**. (The energy (E) is scaled with respect to the lowest energy magnetic state and the spin density values for all Cu(II) centers are given only for the low energy spin state).

Model	**S**	**E (cm^{-1})**	**Spin density (e)**
A (For compound **1**)	0	0.00	Cu1 (0.48) Cu2 (-0.48)
	1	3.66	