

ELECTRONIC SUPPLEMENTARY INFORMATION for

Copper(II) cubanes with {Cu₄O₄} core and well defined S = 1 ground state.

Table S1. Magnetic and structural data for the complexes plotted in Figure 9.

<i>Refcode</i>	<i>S</i>	<i>J</i>	<i>Mean angle</i>	α	β	γ	δ	<i>DIST1</i>	<i>DIST2</i>	<i>DIST3</i>	<i>DIST4</i>
DARKOW	2	57	104.28	104.283	104.283	104.283	104.283	2.474	2.474	2.474	2.474
XINYUP	2	61	106.32	106.647	106.476	105.273	106.88	2.452	2.4	2.413	2.415
XEXZUX	2	54.6	107.12	105.701	109.112	105.167	108.49	2.479	2.502	2.447	2.454
LIJQEA	---	0	109.39	110.013	108.262	109.575	109.695	2.859	2.785	2.838	2.787
JELPUL	0	-130	109.52	111.033	109.318	109.898	107.84	2.752	2.723	2.636	2.693
HAKXIB	2	10.4	109.70	110.859	108.694	108.92	110.34	2.608	2.573	2.644	2.541
LIJQIE	---	0	109.95	109.994	109.07	108.956	111.785	2.86	2.804	2.833	2.8
WEMSUE	0	-4.5	110.04	109.885	110.197	109.885	110.197	2.544	2.544	2.573	2.573
NINPEG	0	-74.8	110.10	110.102	110.102	110.102	110.102	2.577	2.577	2.577	2.577
BOQZUD	0	-69.8	111.29	112.092	110.483	112.092	110.483	2.697	2.697	2.679	2.679
DARKUC	2	34.8	112.06	112.055	112.055	112.055	112.055	2.748	2.748	2.748	2.748
UFATOL	0	-117	112.10	112.099	112.099	112.099	112.099	2.706	2.706	2.706	2.706
BOGCOP	2	34.2	112.44	112.439	112.439	112.439	112.439	2.734	2.734	2.734	2.734
UFATUR	0	-111	112.54	112.952	112.328	111.869	112.996	2.705	2.703	2.753	2.753
LOCPIE	0	-73.6	112.93	112.932	112.932	112.932	112.932	2.686	2.686	2.686	2.686
VAVGUW	0	-75	113.07	113.068	113.068	113.068	113.068	2.724	2.724	2.724	2.724
POLKEH	0	-136	113.35	113.55	113.509	113.085	113.259	2.692	2.696	2.672	2.665
NODHEV	0	-80.5	114.05	114.009	114.086	114.009	114.086	2.722	2.722	2.73	2.73
NILDAP	0	-118.8	117.00	117	117	117	117	2.865	2.865	2.865	2.865

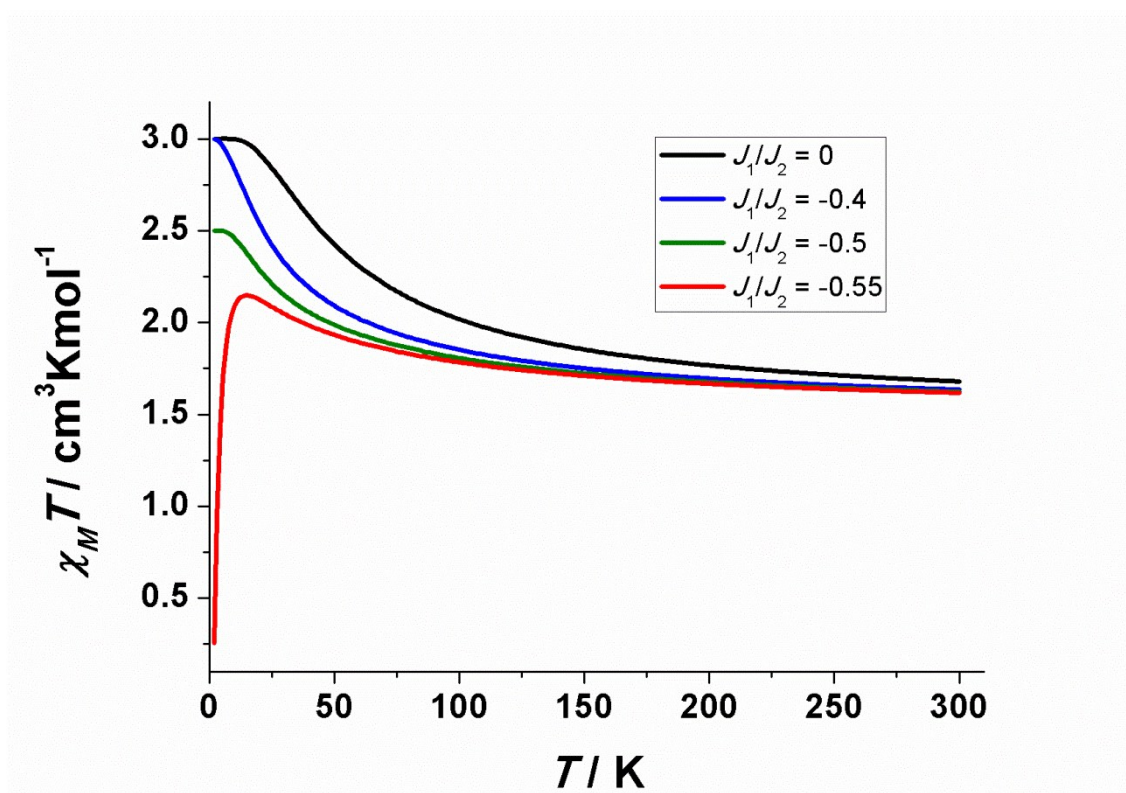


Figure S1. Simulation of the coupling constants for the (2:4) model and ratios around $-1/2$ for ferromagnetic J_2 constants. The similar shape of these simulations with those due to the effect of D in the ground state, leads erroneously to $J_1 \approx -J_2/2$ fit values. For a correct analysis of Cu^{II} cubes exhibiting this kind of plots see reference 21 (E. A. Buvaylo, V. N. Kozay, O. Yu. Vassilyeva, B. W. Skelton, J. Jezierska, L. C. Brunel and A. Ozarowski, *Inorg.Chem.*, 2005, **44**, 206).