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Electronic Supplementary Information

Effect of the apical ligand in the geometry and magnetic properties of copper(II)/mesoxalate trinuclear units

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Theoretical calculations

Spin-unrestricted DFT calculations were performed at the B3LYP level by means of the Gaussian09 with a triple-ξ all-electron Gaussian basis set for all the elements.[1, 2] In previous studies in which the geometry of the trinuclear complex was close to either equilateral or isosceles-triangular,[3, 4] the geometry of the complexes was symmetrized to their ideal geometry in order to compare the values of the theoretical magnetic coupling constants with the results obtained by means of the magnetic susceptibility data.[5] However, in this study the geometries were not symmetrized and the coordinates of all atoms were directly taken form CIF files. The general zero-field Hamiltonian for a triangular system can be written as $\boldsymbol{H} = -J_{12}(\boldsymbol{S}_1\boldsymbol{S}_2) - J_{13}(\boldsymbol{S}_1\boldsymbol{S}_3) - J_{23}(\boldsymbol{S}_2\boldsymbol{S}_3)$, where 1, 2 and 3 refer to the three copper(II) centers and J_{12}, J_{13}, and J_{23} correspond to the magnetic coupling constants between two adjacent copper(II) centers. All compounds (except **2**) exhibit scalene-triangular structure, and single-point calculations were performed for the quartet $S = 3/2$ (HS = +++), with mean $S^2 \approx 3.75$ and the three non-degenerated broken-symmetry doublet states $S = ½$ (LS1 = +−+, LS2=++−, LS3 −++) with mean $S^2 \approx 1.75$. The values of the magnetic coupling constants are obtained from the differences of energy of these four energy states as $E_{HS}-E_{LS1}=-J_{12}-J_{23}$, $E_{HS}-E_{LS2}=-J_{23}-J_{13}$, $E_{HS}-E_{LS3}=-J_{12}-J_{13}$. Because of the equilateral-triangular structure of the trinuclear unit in **2** the magnetic coupling constant can be calculated as $E_{HS}-E_{LS}=-2J$.[6-8] In addition to **1**-**3** we have recalculated with this method the magnetic coupling constants of all these compounds: $\{(Ph_4P)_2[MCu_3(Hmesox)_3Cl]\}_n$ (with M(II)= Mn and Co), $K_3[Cu_3(Hmesox)_3(H_2O)]$, $\{[La(H_2O)_3Cu_3(Hmesox)_3(H_2O)_5]\cdot 8H_2O\}_n$, $\{[La(H_2O)_2Cu_3(Hmesox)_3(H_2O)_3]\cdot 7H_2O\}_n$.[3, 4, 9] The values for compounds $\{[LnCu_3(Hmesox)_3DMSO]\}_n$, with Ln(III)= La, Ce, Pr, Nd and Eu were taken from the corresponding publication.[8]

The knowledge of the values of the J constants is crucial since it comes from the energy of the $S = 3/2$ and the $S = ½$ magnetic states of the copper(II) trinuclear units, and therefore, it is possible to know the population of each state at each temperature and the total spin of the ground state.[5, 10] It has to be noted that the $S = 3/2$ ground state needs, at least, two ferromagnetic coupling constants within the triangle and that a $S = ½$ ground state can be achieved with two antiferromagnetic coupling constants within the triangle. Three antiferromagnetic coupling constants may lead to spin frustrated systems.[5] The calculated values (J_{theo}) are shown in Table S5 and plotted in Fig. 9 together with the experimental values (J_{exp}). It can be observed that in many cases calculated and experimental values are very close, but not always (especially those of compound **3** for which a bad approximation to the model is performed, blue circles).

Structure Refinement details

For all the compounds, all non-hydrogen positions were refined with anisotropic temperature factors (except atom C1 in compound **2**). The phenyl rings of the Ph_4P^+ cations, in **1** and **3**, were refined with a rigid group constraint for the phenyl rings (AFIX 66). Additionally, an “equal Uij” restraint (EADP) was fixed for **3**. Hydrogen atoms on the mesoxalate-OH were positioned geometrically for **1**-**3** (O-H=0.83 Å) and refined using a riding model (AFIX 83) with Uiso (H)=1.5 Ueq(O). The aromatic hydrogen atoms of **1** and **3** were positioned geometrically (C-H=0.94 Å) and refined using a riding model (AFIX 43) with Uiso (H)=1.2 Ueq(CH). Hydrogen atoms of water molecules of **1** were found, but not refined since a suitable geometry around the oxygen atom was not found. In the case of compound **3**, only four hydrogen atoms of two water molecules were found and allowed to ride on the oxygen atom with Uiso(H)= 1.2 Ueq(O). The rest of hydrogen atoms of three additional water molecules could not be found nor calculated. Although they could not be located, they have been included in the unit card for calculation of the correct sum formula, density, and F(000), because of their large number.

Although crystals of **2** were of good quality, the high absorption coefficient of Co atoms resulted in low diffraction at high angles. As a consequence, attempts to identify the tetraphenylphosphonium cations and crystallization water molecules failed. Instead, a new set of F^2(hkl) values was obtained by SQUEEZE procedure implemented in PLATON[11-15] which reduced R_1 to 0.0450.

The number of tetraphenylphosphonium cations in the structure was estimated by the charge balance of the chemical formula and elemental analysis. The C1 atom could not be refined anisotropically. The C3-O6 distance was refined using DFIX. Because of the slightly high value of the Flack parameter, 0.14(3), the structure was refined as an inversion twin by means of TWIN/BASF refinement, however no improvement was achieved. Nevertheless, the refinement of the inverse of the structure gives a Flack parameter of 0.88(3) which means the correct absolute configuration was solved.

FIGURES

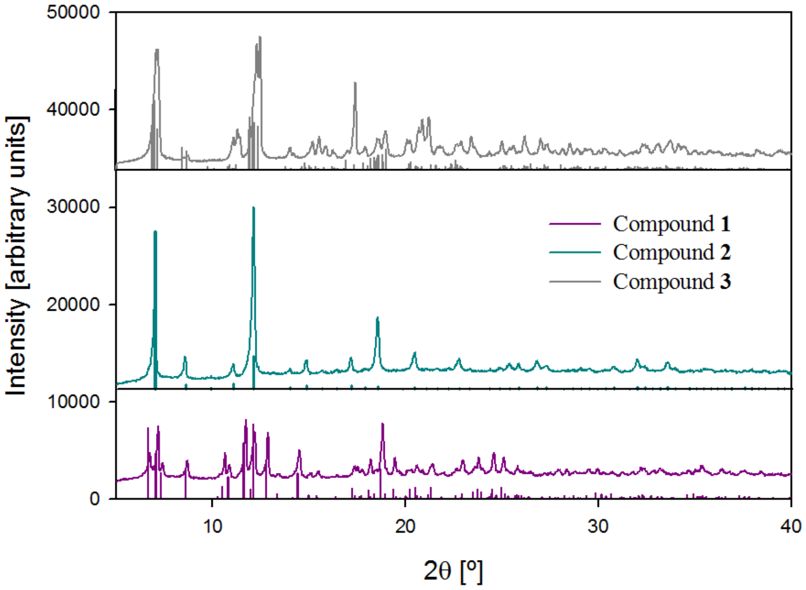

Fig. S1. Simulated and experimental X-ray powder diffraction patterns of compounds **1-3**.

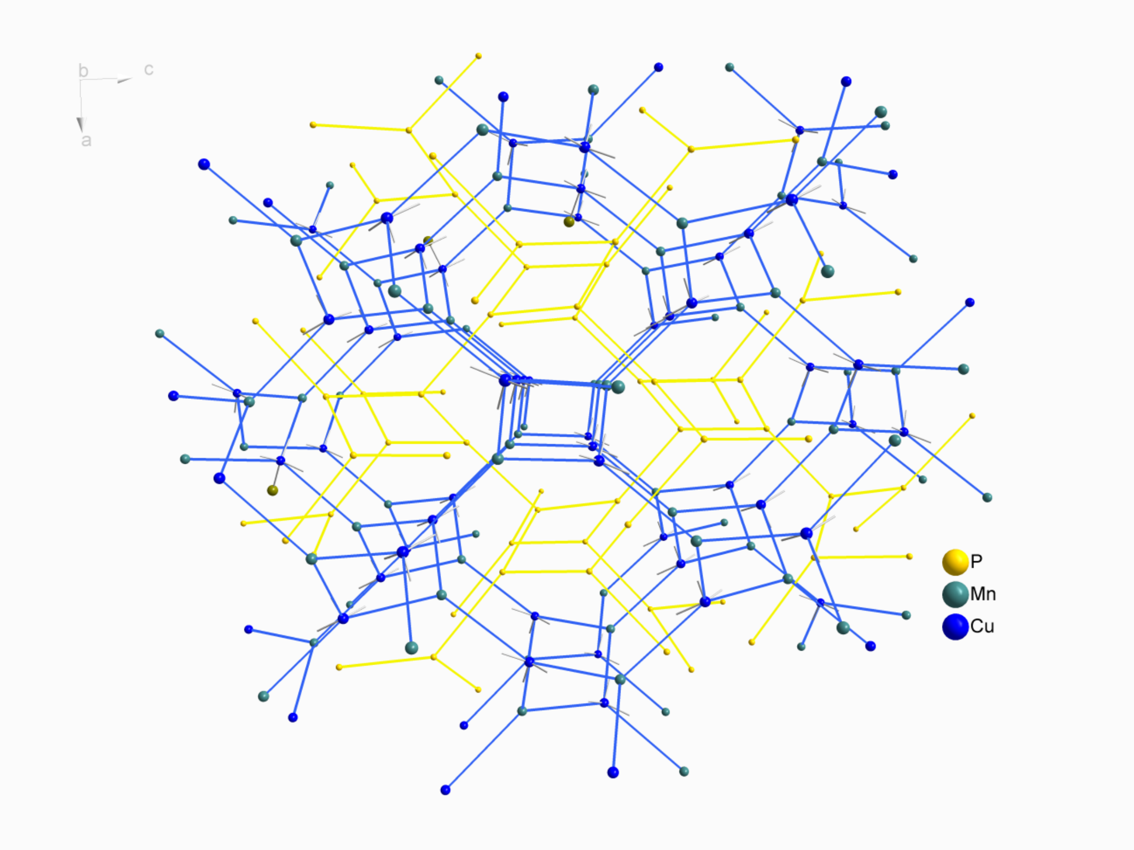

Fig. S2. Schematic representation of the interpenetrated anionic and cationic networks in **1**. Cu means Cu_3 centroid.

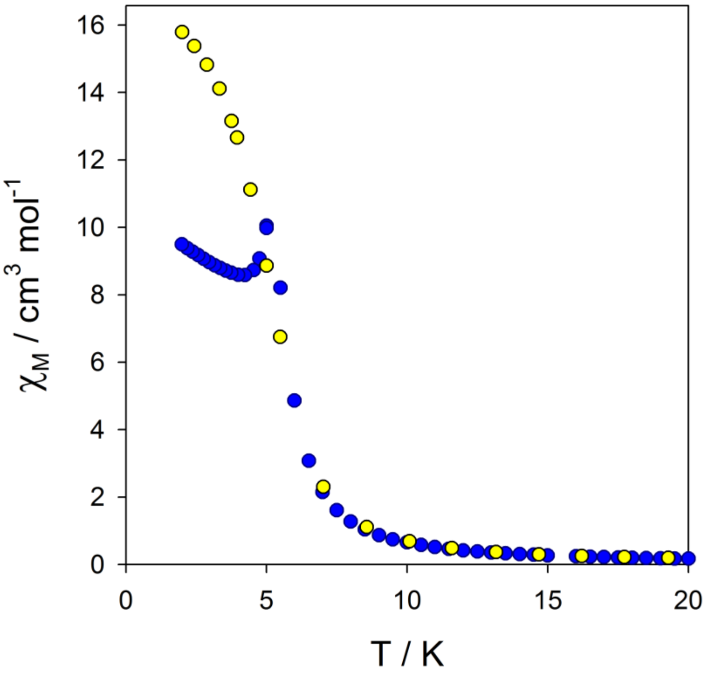

Fig. S3. χ_M vs. T plot for **1**. ZFC blue plot, FC yellow plot.

Table S1 Summary of crystallographic data for complexes **1-3**

Compound	(**1**)	(**2**)[a]	(**3**)
M / g mol^{-1}	1439.36	1407.31	2917.59
Temp. / K	293(2)	150(2)	150(2)
λ/Å	1.54184	1.54184	1.54184
Crystal system	Orthorhombic	Cubic	Monoclinic
Space group	$P\ 2_1\ 2_1\ 2_1$	$P\ 2_1\ 3$	$P\ 2_1$
a / Å	16.21700(10)	17.9181(7)	17.5123(5)
b / Å	17.98310(10)	17.9181(7)	18.1004(6)
c / Å	19.64020(10)	17.9181(7)	18.1084(5)
α / °	90.00	90.00	90.00
β / °	90.00	90.00	92.118(2)
γ / °	90.00	90.00	90.00
V / $Å^3$	5727.71(6)	5752.8(7)	5736.1(3)
Z	4	4	2
D_{calc} / g/cm^3	1.669	1.625	1.693
μ / mm^{-1}	5.015	5.423	3.741
Unique reflections	51667	8265	21167
R(int)	0.0375	0.1140	0.0740
R_1 [$I > 2\sigma(I)$][b]	0.0354	0.0450	0.0754
wR_2 [$I > 2\sigma(I)$]	0.0955	0.1155	0.1853
GOF on F^2 [c]	1.022	1.065	1.031
Abs.struc. param. (Flack value)[16-18]	0.081(4)	0.14(3)	-0.06(4)

[a] Set of data generated with SQUEEZE. [b] $R_1 = [\Sigma(||F_o| - |F_c||)/\Sigma|F_o|]$; $wR_2 = [\Sigma[w(F_o^2 - F_c^2)^2]/\Sigma[w(F_o^2)^2]]^{1/2}$. [c] Goodness-of-fit = $[\Sigma[w(F_o^2 - F_c^2)^2]/(n - p)]^{1/2}$. [d] $w = 1/[\sigma^2(F_o^2) + (aP)^2 + bP]$ where $P = (\max(F_o^2 \text{ or } 0) + 2F_c^2)/3$.

Empirical formulae: $C_{57}H_{47}BrCu_3MnO_{20}P_2$ (**1**), $C_{57}H_{43}BrCu_3CoO_{18}P_2$ (**2**) and $C_{114}H_{96}Br_2Cu_6Zn_2O_{41}P_4$ (**3**).

Table S2-S4. Main distances and angles compounds **1, 2, 3**. Addison parameters for Cu(II) ions[19] and distortion parameters from the octahedral geometry for Mn(II), Co(II) and Zn(II) ions[20]

Table S2. Main distances and angles for compound **1**. Addison parameters for Cu(II) ions and distortion parameters from the octahedral geometry for Mn(II) ion.

Cu1 O1A	1.956 (2)	Cu3 O3B	1.988(2)
Cu1 O3A	1.964(2)	Cu3 O6B	1.936(2)
Cu1 O1B	1.958 (2)	Cu3 O1C	1.949(2)
Cu1 O3B	1.978 (2)	Cu3 O3C	1.915(2)
Cu1 Br1	2.7339(8)	Cu3 Br1	2.7235(7)
Cu2 O3A	1.925 (2)	Mn1 O2A	2.175(2)
Cu2 O6A	1.931(2)	Mn1 O5A^{ii}	2.087(2)
Cu2 O3C	1.914(2)	Mn1 O2B^{i}	2.185(2)
Cu2 O6C	1.943(3)	Mn1 O5B^{i}	2.129(2)
Cu2 O1W	2.4582(2)	Mn1 O2C	2.133(3)
		Mn1 O5C	2.227(2)
O1A Cu1 O3A	82.85(10)	O6B Cu3 O1C	91.17(11)
O1A Cu1 O1B	95.80(11)		
O1A Cu1 O3B	171.92(12)	O6B Cu3 Br1	99.20(9)
O1A Cu1 Br1	100.01(11)	O1C Cu3 O3B	164.15(11)
O3A Cu1 O3B	94.14(9)	O1C Cu3 Br1	107.92(9)
O3A Cu1 Br1	94.95(7)	O3C Cu3 O3B	94.46(9)
O1B Cu1 O3A	156.42(12)	O3C Cu3 O6B	165.00(12)
O1B Cu1 O3B	83.94(9)	O3C Cu3 O1C	84.30(10)
O1B Cu1 Br1	108.41(10)	O3C Cu3 Br1	95.80(7)
O3B Cu1 Br1	87.70(7)		
		O2A Mn1 O2B^{i}	96.74(11)
O3A Cu2 O6A	84.47(9)	O2A Mn1 O5C	90.37(10)
O3A Cu2 O6C	164.47(13)	O5A^{ii} Mn1 O2A	83.22(9)
O6A Cu2 O6C	91.44(11)	O5A^{ii} Mn1 O2B^{i}	103.88(10)
O3C Cu2 O3A	100.12(9)	O5A^{ii} Mn1 O5B^{i}	170.46(10)
O3C Cu2 O6A	175.40(10)	O5A^{ii} Mn1 O2C	89.56(10)
O3C Cu2 O6C	84.07(10)	O5A^{ii} Mn1 O5C	90.35(9)
		O2B^{i} Mn1 O5C	164.72(10)
Cu1 O3B Cu3	107.85(10)	O5B^{i} Mn1 O2A	90.24(10)
Cu2 O3A Cu1	129.85(11)	O5B^{i} Mn1 O2B^{i}	83.73(9)
Cu2 O3C Cu3	129.72(11)	O5B^{i} Mn1 O2C	95.93(11)
Cu3 Br1 Cu1	71.949(17)	O5B^{i} Mn1 O5C	82.73(9)
		O2C Mn1 O2A	169.50(10)
O3B Cu3 Br1	87.79(7)	O2C Mn1 O2B^{i}	92.38(11)
O6B Cu3 O3B	84.05(10)	O2C Mn1 O5C	82.03(9)
τ-Cu1[b]	0.26	Trigonal distortion Mn1	4.06°
τ-Cu2[b]	0.18	Mean Oh quadratic elongation Mn1	1.000
τ-Cu3[b]	0.01	Octahedral distortion Mn1	58.68°
Mean square relative deviation from average bond length x 10.000 Mn1			4.397

a) Symmetry codes: i= (-0.5+x,0.5-y,2-z); ii=(2-x,0.5+y,1.5-z)

b) Addison τ parameter

Table S3. Main distances and angles for compound **2**. Addison parameters for Cu(II) ion and distortion parameters from the octahedral geometry for Co(II) ion.

Cu1 O1	1.931(1)	Co1 O2	2.096(1)
Cu1 O3	1.907(1)	Co1 O2^{iii}	2.096(1)
Cu1 O3^{ii}	2.017(1)	Co1 O2^{iv}	2.096(1)
Cu1 O6	1.965(1)	Co1 O5^{i}	2.067(1)
Cu1 Br1	2.840(1)	Co1 O5^{v}	2.067(1)
Cu1^{i} Br1	2.840(1)	Co1 O5^{vi}	2.067(1)
Cu1^{ii} Br1	2.840(1)	O5 Co1^{ii}	2.067(1)
O3 Cu1^{i}	2.002(1)		
O1 Cu1 Br1	102.914(1)	O2 Co1 O2^{iii}	90.478(1)
O1 Cu1 O3	82.578(1)	O2 Co1 O2^{iv}	90.478(1)
O1 Cu1 O3^{ii}	172.946(1)	O2^{iii} Co1 O2^{iv}	90.478(1)
O1 Cu1 O6	91.466(1)	O5^{i} Co1 O2	86.354(1)
O3 Cu1 Br1	84.779(1)	O5^{i} Co1 O2^{iii}	92.694(1)
O3^{ii} Cu1 Br1	83.160(1)	O5^{i} Co1 O2^{iv}	175.534(1)
O3 Cu1 O3^{ii}	101.726(1)	O5^{v} Co1 O2	175.534(1)
O3 Cu1 O6	161.450(1)	O5^{v} Co1 O2^{iii}	86.354(1)
O6 Cu1 Br1	113.720(1)	O5^{v} Co1 O2^{iv}	92.694(1)
O6 Cu1 O3^{ii}	82.718(1)	O5^{vi} Co1 O2	92.694(1)
		O5^{vi} Co1 O2^{iii}	175.534(1)
Cu1 O3 Cu1^{i}	115.881(1)	O5^{vi} Co1 O2^{iv}	86.354(1)
Cu1 Br1 Cu1^{i}	71.369(1)	O5^{i} Co1 O5^{v}	90.646(1)
Cu1 Br1 Cu1^{ii}	71.369(1)	O5^{i} Co1 O5^{vi}	90.646(1)
Cu1^{i} Br1 Cu1^{ii}	71.369(1)	O5^{v} Co1 O5^{vi}	90.646(1)
τ-Cu1[b]	0.19	Trigonal distortion Co1	1.51°
Mean Oh quadratic elongation Co1	1.000	Octahedral distortion Co1	23.17°
Mean square relative deviation from average bond length x 10.000 Co1			0.489

a)Symmetry codes: i= (y,z,x) ii=(z,x,y) iii=(-y,-0.5+z,0.5-x) iv=(0.5-z,-x,0.5+y) v=(-z,-0.5+x,0.5-y) vi=(0.5-x,-y,0.5+z) b)Addison parameter

Table S4. Main distances and angles for compound **3**. Addison parameters for Cu(II) ion and distortion parameters from the octahedral geometry for Zn(II) ions.

Cu1 O1A	1.960 (11)	Cu5 O1E	1.898(13)
Cu1 O3A	1.912(10)	Cu5 O3E	1.977(11)
Cu1 O3C	1.977 (10)	Cu5 Br2	2.862(4)
Cu1 O5C	1.906 (12)	Cu6 O3E	1.930(11)
Cu1 Br1	2.825(3)	Cu6 O6E	1.938(13)
Cu2 O3A	1.918 (11)	Cu6 O1F	1.927(11)
Cu2 O6A	1.940(11)	Cu6 O3F	2.000(11)
Cu2 O1B	1.914(12)	Cu6 Br2	2.705(3)
Cu2 O3B	1.949(10)		
Cu2 Br1	2.913(3)	Zn1 O2A	2.138(10)
Cu3 O3B	1.905(10)	Zn1 O5A	2.023(11)
Cu3 O6B	1.950(11)	Zn1 O2B	2.053(10)
Cu3 O1C	1.925(10)	Zn1 O5B	2.094(11)
Cu3 O3C	1.955(11)	Zn1 O2F	2.090(10)
Cu3 Br1	2.822(3)	Zn1 O5F	2.000(10)
Cu4 O1D	1.954(11)		
Cu4 O3D	1.924(9)	Zn2 O2C	2.150(11)
Cu4 O3F	1.950(10)	Zn2 O6C	2.046(11)
Cu4 O6F	1.881(11)	Zn2 O2D	2.099(10)
Cu4 O1W^{i}	2.6038(242)	Zn2 O5D	2.065(12)
Cu5 O3D	1.934(10)	Zn2 O2E	2.112(11)
Cu5 O6D	1.950(11)	Zn2 O5E	2.028(11)

O1A Cu1 O3C	173.1(5)	O3E Cu6 O6E	83.8(5)
O1A Cu1 Br1	102.6(4)	O3E Cu6 O3F	98.8(4)
O3A Cu1 O1A	84.8(4)	O3E Cu6 Br2	85.8(3)
O3A Cu1 O3C	100.1(4)	O6E Cu6 O3F	158.0(5)
O3A Cu1 Br1	86.1(3)	O6E Cu6 Br2	114.0(4)
O3C Cu1 Br1	82.7(3)	O1F Cu6 O3E	173.8(5)
O5C Cu1 O1A	89.0(5)	O1F Cu6 O6E	91.5(5)
O5C Cu1 O3A	164.9(5)	O1F Cu6 O3F	84.0(4)
O5C Cu1 O3C	85.0(4)	O1F Cu6 Br2	99.8(4)
O5C Cu1 Br1	108.7(4)	O3F Cu6 Br2	88.0(3)
O3A Cu2 O6A	86.6(4)	Cu1 O3A Cu2	118.0(6)
O3A Cu2 O3B	96.4(4)	Cu3 O3B Cu2	119.3(5)
O3A Cu2 Br1	83.5(3)	Cu3 O3C Cu1	115.4(5)
O6A Cu2 O3B	157.8(5)	Cu4 O3D Cu5	120.4(5)
O6A Cu2 Br1	120.5(3)	Cu4 O3F Cu6	115.5(5)
O1B Cu2 O3A	174.5(5)	Cu6 O3E Cu5	116.4(5)
O1B Cu2 O6A	89.6(5)		
O1B Cu2 O3B	85.7(4)	Cu1 Br1 Cu2	69.76(8)
O1B Cu2 Br1	101.9(4)	Cu3 Br1 Cu1	72.13(8)
O3B Cu2 Br1	81.8(3)	Cu3 Br1 Cu2	70.85(8)
		Cu6 Br2 Cu5	73.17(9)
O3B Cu3 O6B	83.9(5)		
O3B Cu3 O1C	172.6(5)	O5A Zn1 O2A	87.0(4)
O3B Cu3 O3C	99.6(5)	O5A Zn1 O2B	91.3(4)
O3B Cu3 Br1	85.0(3)	O5A Zn1 O5B	93.1(4)
O6B Cu3 O3C	160.7(5)	O5A Zn1 O2F	171.8(4)
O6B Cu3 Br1	116.2(4)	O2B Zn1 O2A	90.3(4)
O1C Cu3 O6B	89.9(4)	O2B Zn1 O5B	87.4(4)
O6B Cu3 O1C	91.17(11)	O2B Zn1 O2F	90.8(4)
O1C Cu3 O3C	84.9(4)	O5B Zn1 O2A	177.7(4)
O1C Cu3 Br1	101.4(3)	O2F Zn1 O2A	85.1(4)
O3C Cu3 Br1	83.2(3)	O2F Zn1 O5B	94.9(4)

		O5F Zn1 O2A	94.2(4)
O3D Cu4 O1D	84.3(4)	O5F Zn1 O5A	89.7(4)
O1D Cu4 O1W^{i}	90.096(638)	O5F Zn1 O2B	175.4(4)
O3D Cu4 O3F	100.9(4)	O5F Zn1 O5B	88.1(4)
O3D Cu4 O1W^{i}	83.403(645)	O5F Zn1 O2F	88.9(4)
O3F Cu4 O1D	174.7(4)		
O3F Cu4 O1W^{i}	90.013(611)	O6C Zn2 O2C	86.2(4)
O6F Cu4 O1D	88.9(5)	O6C Zn2 O2D	91.2(4)
O6F Cu4 O3D	168.5(5)	O6C Zn2 O5D	90.6(5)
O6F Cu4 O3F	85.9(4)	O6C Zn2 O2E	175.0(4)
O6F Cu4 O1W^{i}	87.380(673)	O2D Zn2 O2C	87.6(4)
		O2D Zn2 O2E	89.5(4)
O3D Cu5 O6D	84.0(5)	O5D Zn2 O2C	173.2(4)
O3D Cu5 O3E	96.4(4)	O5D Zn2 O2D	86.4(4)
O3D Cu5 Br2	86.0(3)	O5D Zn2 O2E	94.4(5)
O6D Cu5 O3E	160.1(6)	O2E Zn2 O2C	88.9(4)
O6D Cu5 Br2	119.0(4)	O5E Zn2 O2C	92.9(5)
O1E Cu5 O3D	172.4(6)	O5E Zn2 O6C	91.6(5)
O1E Cu5 O6D	92.7(5)	O5E Zn2 O2D	177.2(5)
O1E Cu5 O3E	84.4(5)	O5E Zn2 O5D	93.2(5)
O1E Cu5 Br2	101.6(5)	O5E Zn2 O2E	87.8(4)
O3E Cu5 Br2	80.8(3)		
τ-Cu1^{b}	0.14	τ-Cu4^{b}	0.10
τ-Cu2^{b}	0.27	τ-Cu5^{b}	0.21
τ-Cu3^{b}	0.20	τ-Cu6^{b}	0.26
Trigonal distortion Zn1	2.29°	Octahedral distortion Zn1	28.56°
Trigonal distortion Zn2	1.65°	Octahedral distortion Zn1	27.62°

Mean square relative deviation from average bond length x 10.000 Zn1 5.042

Mean square relative deviation from average bond length x 10.000 Zn2 4.022

Table S5. Cu-O-Cu angle, θ; Theoretical magnetic coupling constant, J_{theo}; Experimental magnetic coupling constant, J_{exp}.

Compound	θ/º	J_{theo} /cm^{-1}	J_{exp} / cm^{-1}	Ref
1	129.85	-178.8		This work
1	129.73	-132.6		This work
1	107.84	22.7		This work
2	115.88	-22.5		This work
3	117.93	-29.1	15.1	This work
3	119.25	-36.2	-10.8	This work
3	115.45	-17.3	15.1	This work
3	120.40	-57.9	-10.8	This work
3	115.44	-14.1	15.1	This work
3	116.40	-30.9	15.1	This work
$(Ph_4P)[MnCu_3(HL)_3Cl]$	110.94	15.3		3
$(Ph_4P)[MnCu_3(HL)_3Cl]$	117.99	-60.5		3
$(Ph_4P)[MnCu_3(HL)_3Cl]$	115.93	-23.6		3
$(Ph_4P)[CoCu_3(HL)_3Cl]$	112.80	2.1		9
$(Ph_4P)[CoCu_3(HL)_3Cl]$	114.80	-27.0		9
$(Ph_4P)[CoCu_3(HL)_3Cl]$	116.40	-27.0		9
$K_3[Cu_3(HL)_3]$	110.74	-6.8	-3.0	9
$K_3[Cu_3(HL)_3]$	129.74	-206.8	-194.0	9
$K_3[Cu_3(HL)_3]$	128.30	-179.5	-194.0	9
$[La(H_2O)_3Cu_3(HL)_3(H_2O)_5]$	125.56	-123.4	-55.0	4
$[La(H_2O)_3Cu_3(HL)_3(H_2O)_5]$	122.50	-59.5	-55.0	4
$[La(H_2O)_3Cu_3(HL)_3(H_2O)_5]$	136.17	-242.3	-224.0	4
$[La(H_2O)_3Cu_3(HL)_3(H_2O)_5]$	119.42	-49.4	-104.0	4
$[La(H_2O)_3Cu_3(HL)_3(H_2O)_5]$	129.90	-231.0	-157.0	4
$[La(H_2O)_3Cu_3(HL)_3(H_2O)_5]$	114.75	-25.8	20.0	4
$[LaCu_3(HL)_3DMSO]$	114.50	-46.5	-65.0	8
$[CeCu_3(HL)_3DMSO]$	114.60	-41.1		8
$[PrCu_3(HL)_3DMSO]$	116.00	-59.8		8
$[NdCu_3(HL)_3DMSO]$	114.60	-40.3		8
$[EuCu_3(HL)_3DMSO]$	110.70	-20.5		8
$[EuCu_3(HL)_3DMSO]$	112.90	-18.5		8
$[EuCu_3(HL)_3DMSO]$	112.90	-18.5		8
$[EuCu_3(HL)_3DMSO]$	110.30	-4.8		8
$[EuCu_3(HL)_3DMSO]$	110.10	-15.1		8
$[EuCu_3(HL)_3DMSO]$	114.60	-35.8		8

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