

Inorganic Chemistry

Inorganic-Metalorganic Hybrids Based on Copper(II)-Monosubstituted Keggin Polyanions and Dinuclear Copper(II)-Oxalate Complexes. Synthesis, X-ray Structural Characterization and Magnetic Properties.

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Supporting Information

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Scheme I.

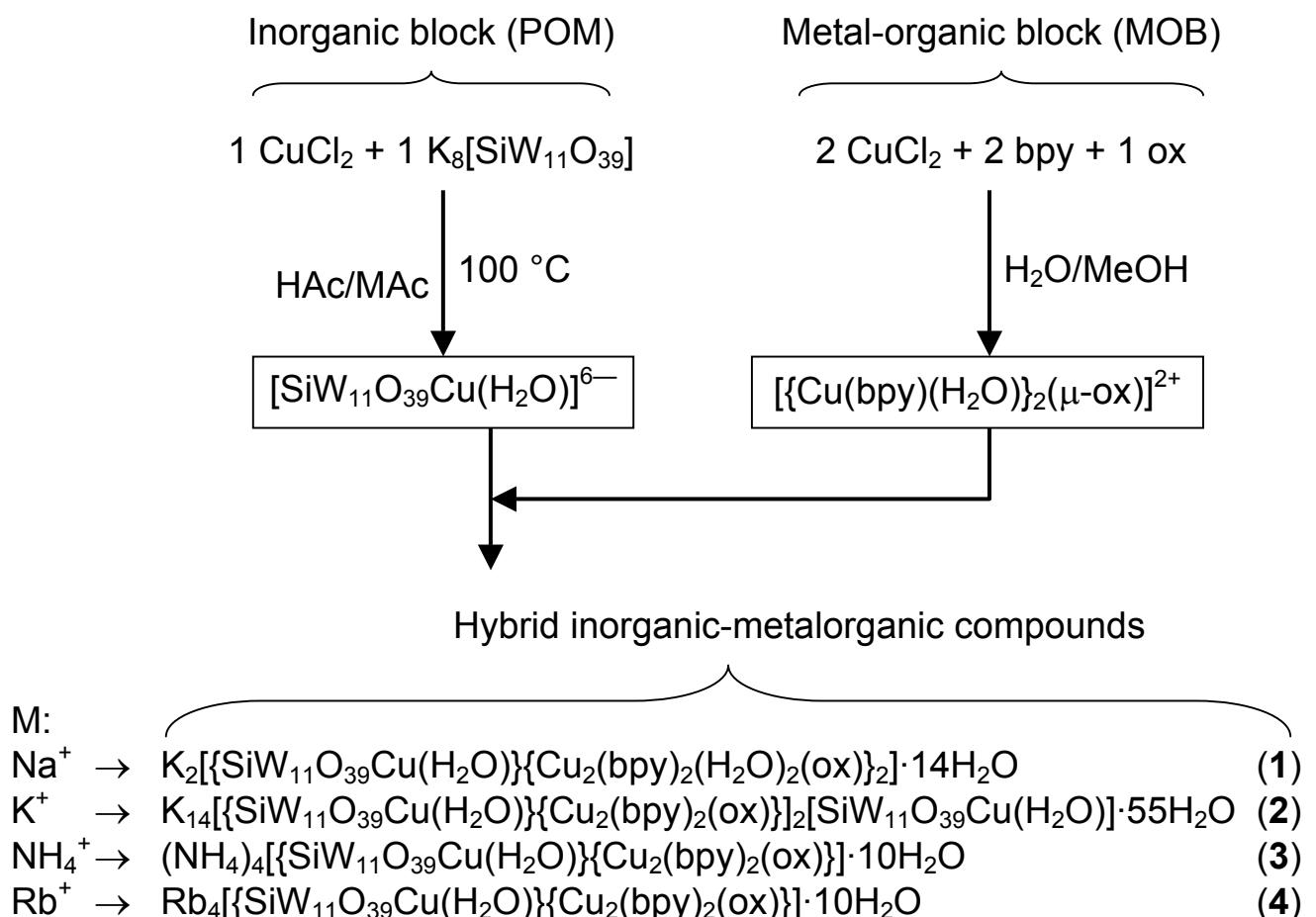


Table S1. Intermolecular π interactions (\AA , $^\circ$) for compounds **1 - 4**.

Compound		DZ	ANG	DC	DXY
1	CgN1'-CgN12 ⁽ⁱ⁾	3.52(5)	4.8(9)	3.77(5)	1.37(5)
	CgN12'-CgN1 ⁽ⁱ⁾	3.47(5)	4.8(9)	3.77(5)	1.48(5)
	CgN32-CgN32' ⁽ⁱⁱ⁾	3.41(5)	0.0(9)	3.64(5)	1.28(5)
2	CgN1-CgN12' ⁽ⁱⁱⁱ⁾	3.50(2)	1.0(6)	3.95(2)	1.83(2)
	CgN12-CgN1' ⁽ⁱⁱⁱ⁾	3.49(2)	1.0(6)	3.95(2)	1.85(2)
3	CgN1-CgN12' ^(iv)	3.45(1)	1.3(4)	3.96(1)	1.94(1)
	CgN12-CgN1' ^(iv)	3.49(1)	1.3(4)	3.96(1)	1.86(1)
	CgN2I-CgN32' ^(v)	3.44(1)	1.9(4)	3.97(1)	1.98(1)
	CgN32-CgN2I' ^(v)	3.46(1)	1.9(4)	3.97(1)	1.95(1)
4	CgN1-CgN12' ^(iv)	3.47(1)	1.7(5)	3.91(1)	1.81(1)
	CgN12-CgN1' ^(iv)	3.51(1)	1.7(5)	3.91(1)	1.72(1)
	CgN2I-CgN32' ^(v)	3.49(1)	1.0(5)	3.98(1)	1.91(1)
	CgN32-CgN2I' ^(v)	3.48(1)	1.0(5)	3.98(1)	1.95(1)

Symmetry codes. (i) 1-x, -y, -z; (ii) -x, -y, 1-z; (iii) 1-x, 1/2-y, 1/2-z; (iv) 3-x, -y, -z; (v) 1-x, 1-y, -z.

Cgi: ring i centroid, which contains the following atoms: i = N1: N1, C2, C3, C4, C5, C6; i = N12: C7, C8, C9, C10, C11, N12; i = N2I: N21, C22, C23, C24, C25, C26; i = N32: C27, C28, C29, C30, C31, N32.

DZ: Distance between planes (\AA) defined as the perpendicular distance from Cgi to the ring j plane; **ANG:** angle ($^\circ$) between the planes of ring i and ring j; **DC:** Distance (\AA) between the centroids Cgi y Cgj; **DXY:** Lateral displacement (\AA) between rings defined as the distance between Cgj and the projection of centroid Cgi on the plane j.

Fig. S1. Thermal evolution of the magnetic susceptibility and $\chi_m T$ product for compounds **2** and **4**.

