

Electronic Supporting Information (ESI)

Chlorine and Temperature Directed Self-assembly of Mg-Ru₂(II,III)

Carbonates and Particle Size Dependent Magnetic Properties

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Table S1. Selected bond angles (°) of compounds **1–4**

1	2		
Ru(1A)–Ru(1)–Cl(1)	176.95(4)	Ru(2)–Ru(1)–Cl(1)	180.00(2)
Ru(1A)–Ru(1)–O(1)	89.44(9)	Ru(2)–Ru(1)–O(1)	89.35(6)
Ru(1A)–Ru(1)–O(4)	89.63(10)	Ru(1)–Ru(2)–O(3)	90.54(6)
Ru(1A)–Ru(1)–O(2A)	90.04(10)	Ru(1)–Ru(2)–O(4)	180.00(2)
Ru(1A)–Ru(1)–O(5A)	89.86(10)	Cl(1)–Ru(1)–O(1)	90.65(6)
O(1)–Ru(1)–O(2A)	179.46(13)	O(1)–Ru(1)–O(1A)	178.70(9)
O(1)–Ru(1)–O(5A)	90.54(14)	O(1)–Ru(1)–O(1B)	91.08(7)
O(2A)–Ru(1)–O(4)	90.87(15)	O(1)–Ru(1)–O(1C)	88.91(7)
O(4)–Ru(1)–O(5A)	179.45(13)	O(3)–Ru(2)–O(4)	89.46(6)
O(2A)–Ru(1)–O(5A)	89.32(15)	O(3)–Ru(2)–O(3A)	178.92(9)
Cl(1)–Ru(1)–O(1)	88.74(10)	O(3)–Ru(2)–O(3B)	89.94(8)
Cl(1)–Ru(1)–O(4)	87.90(10)	O(3)–Ru(2)–O(3C)	90.05(8)
Cl(1)–Ru(1)–O(2A)	91.79(10)	Mg(1)–O(2)–C(1)	132.8(3)
Cl(1)–Ru(1)–O(5A)	92.61(10)	Ru(1)–O(1)–C(1)	119.35(18)
O(7)–Mg(1)–O(8)	91.35(19)	Ru(2)–O(3)–C(1)	120.77(19)
O(7)–Mg(1)–O(9)	92.25(18)	O(2)–Mg(1)–O(5)	95.60(9)
O(7)–Mg(1)–O(10)	88.39(18)	O(2)–Mg(1)–O(6)	91.13(8)
O(7)–Mg(1)–O(11)	174.1(2)	O(2)–Mg(1)–O(2D)	84.48(11)
O(7)–Mg(1)–O(12)	92.24(19)	O(2)–Mg(1)–O(5D)	176.34(7)
O(8)–Mg(1)–O(9)	90.67(18)	O(2)–Mg(1)–O(6D)	92.87(8)
O(8)–Mg(1)–O(10)	177.98(18)	O(5)–Mg(1)–O(6)	90.79(9)

O(8)–Mg(1)–O(11)	94.57(19)	O(5)–Mg(1)–O(5D)	84.56(9)
O(8)–Mg(1)–O(12)	88.47(18)	O(5)–Mg(1)–O(6D)	85.22(9)
O(9)–Mg(1)–O(10)	87.34(18)	O(6)–Mg(1)–O(6D)	174.61(11)
O(9)–Mg(1)–O(11)	87.43(19)		
O(9)–Mg(1)–O(12)	175.4(2)		
O(10)–Mg(1)–O(11)	85.69(19)		
O(10)–Mg(1)–O(12)	93.55(18)		
O(11)–Mg(1)–O(12)	88.18(18)		
3		4	
Ru(2)–Ru(1)–O(1)	89.44(15)	Ru(1A)–Ru(1)–O(2)	90.4(3)
Ru(2)–Ru(1)–O(4)	90.15(15)	Ru(1A)–Ru(1)–O(5)	89.7(2)
Ru(2)–Ru(1)–O(7)	90.64(15)	Ru(1A)–Ru(1)–O(3B)	175.0(2)
Ru(2)–Ru(1)–O(10)	89.23(15)	Ru(1A)–Ru(1)–O(1A)	89.3(2)
Ru(2)–Ru(1)–O(6A)	176.04(15)	Ru(1A)–Ru(1)–O(4A)	89.9(2)
Ru(1)–Ru(2)–O(2)	90.27(15)	O(2)–Ru(1)–O(5)	89.4(4)
Ru(1)–Ru(2)–O(5)	89.70(15)	O(2)–Ru(1)–O(3B)	84.7(3)
Ru(1)–Ru(2)–O(8)	88.82(15)	O(2)–Ru(1)–O(4A)	90.6(4)
Ru(1)–Ru(2)–O(11)	90.56(15)	O(3B)–Ru(1)–O(5)	91.5(4)
Ru(1)–Ru(2)–O(12B)	174.63(15)	O(1A)–Ru(1)–O(5)	90.9(4)
O(1)–Ru(1)–O(4)	88.5(2)	O(4A)–Ru(1)–O(5)	179.6(3)
O(1)–Ru(1)–O(7)	178.5(2)	O(1A)–Ru(1)–O(3B)	95.5(3)
O(1)–Ru(1)–O(10)	91.2(2)	O(3A)–Ru(1)–O(4B)	88.9(4)
O(1)–Ru(1)–O(6A)	89.6(2)	O(1A)–Ru(1)–O(4B)	89.2(4)
O(4)–Ru(1)–O(7)	93.0(2)	Ru(1A)–O(1)–C(1)	120.6(8)
O(4)–Ru(1)–O(10)	179.32(19)	Ru(1)–O(2)–C(1)	118.8(8)
O(4)–Ru(1)–O(6A)	86.0(2)	Ru(1C)–O(3)–C(1)	136.5(9)
O(7)–Ru(1)–O(10)	87.3(2)	Ru(1A)–O(4)–C(2)	120.2(9)
O(6A)–Ru(1)–O(7)	90.4(2)	Ru(1)–O(5)–C(2)	120.3(8)
O(6A)–Ru(1)–O(10)	94.6(2)	Mg(1)–O(6)–C(2)	130.8(8)
O(2)–Ru(2)–O(5)	90.51(19)	O(6)–Mg(1)–O(7)	87.8(4)
O(2)–Ru(2)–O(8)	177.8(2)	O(6)–Mg(1)–O(8)	88.9(4)
O(2)–Ru(2)–O(11)	88.79(18)	O(6)–Mg(1)–O(6D)	92.4(4)
O(2)–Ru(2)–O(12B)	86.4(2)	O(6)–Mg(1)–O(7D)	89.7(4)
O(5)–Ru(2)–O(8)	91.5(2)	O(6)–Mg(1)–O(8D)	176.2(4)
O(5)–Ru(2)–O(11)	179.25(18)	O(7)–Mg(1)–O(8)	94.0(5)
O(5)–Ru(2)–O(12B)	94.5(2)	O(7)–Mg(1)–O(7D)	176.4(5)
O(8)–Ru(2)–O(11)	89.2(2)	O(7)–Mg(1)–O(8D)	88.6(5)
O(8)–Ru(2)–O(12B)	94.4(2)	O(8)–Mg(1)–O(8D)	90.1(5)

O(11)–Ru(2)–O(12B)	85.2(2)
Ru(1)–O(1)–C(1)	119.2(4)
Ru(1)–O(4)–C(2)	120.2(5)
Ru(1)–O(7)–C(3)	119.6(4)
Ru(1)–O(10)–C(4)	120.6(5)
Ru(2)–O(2)–C(1)	119.4(4)
Ru(2)–O(5)–C(2)	121.0(5)
Ru(2)–O(8)–C(3)	121.9(4)
Ru(2)–O(11)–C(4)	119.9(5)
Ru(1C)–O(6)–C(2)	134.2(6)
Ru(2D)–O(12)–C(4)	132.7(5)
Mg(1)–O(3)–C(1)	124.2(5)
O(3)–Mg(1)–O(13)	87.8(2)
O(3)–Mg(1)–O(14)	94.8(2)
O(3)–Mg(1)–O(15)	88.0(2)
O(3)–Mg(1)–O(16)	87.3(2)
O(3)–Mg(1)–O(17)	174.4(2)
O(13)–Mg(1)–O(14)	90.3(2)
O(13)–Mg(1)–O(15)	175.6(2)
O(13)–Mg(1)–O(16)	92.4(2)
O(13)–Mg(1)–O(17)	88.2(2)
O(14)–Mg(1)–O(15)	88.5(2)
O(14)–Mg(1)–O(16)	176.6(2)
O(14)–Mg(1)–O(17)	89.2(2)
O(15)–Mg(1)–O(16)	89.0(2)
O(15)–Mg(1)–O(17)	96.1(2)
O(16)–Mg(1)–O(17)	88.9(2)

Symmetry codes: **1.** A, 2 - x, -y, 1 - z; **2.** A, 2 - x, 1 - y, z; B, 2 - x, y, z; C. x, 1 - y, z; D, 3/2 - x, 3/2 - y, z; **3.** A, 1 - x, 1/2 + y, 2 - z; B, 2 - x, -1/2 + y, 2 - z; C, 1 - x, -1/2 + y, 2 - z; D, 2 - x, 1/2 + y, 2 - z; **4.** A, 1 - x, -y, 1 - z; B, 1 - x, 1/2 + y, 3/2 - z; C, 1 - x, -1/2 + y, 3/2 - z; D, 3/2 - x, 1/2 - y, z.

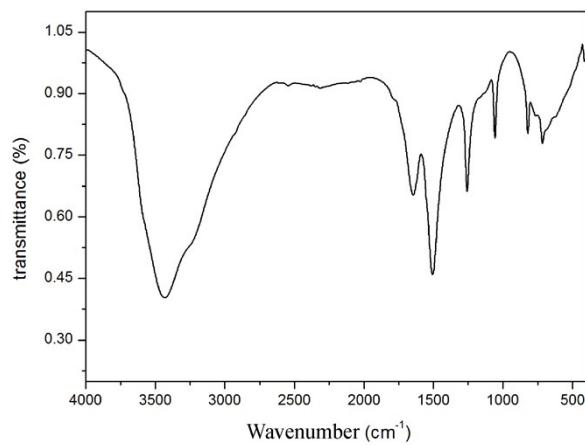


Fig. S1 IR spectra of compound **1**.

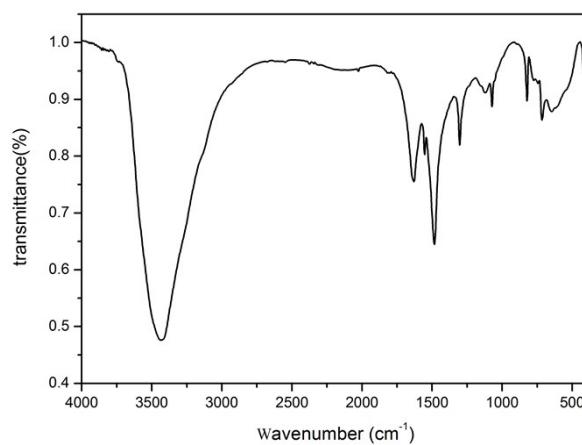


Fig S2. IR spectra of compound **2**.

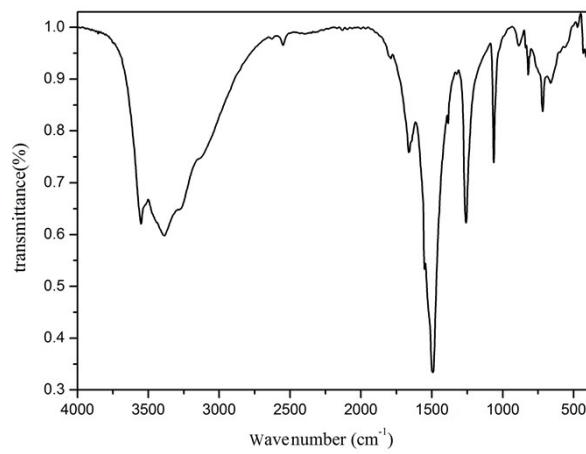


Fig S3. IR spectra of compound **3**.

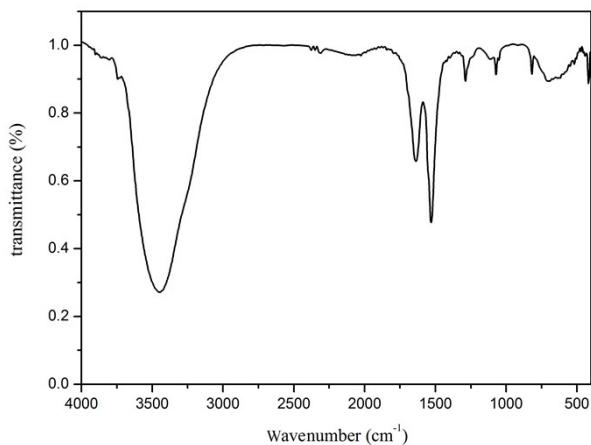


Fig S4. IR spectra of compound 4.

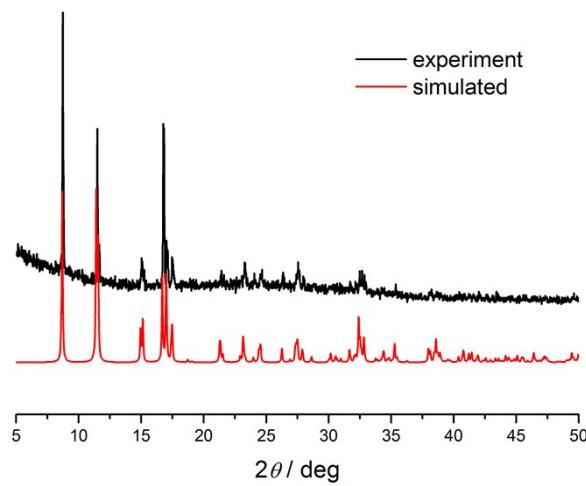


Fig. S5 Comparison of XRPD patterns of the simulated pattern from the single-crystal structure determination and as-synthesized product of **1**.

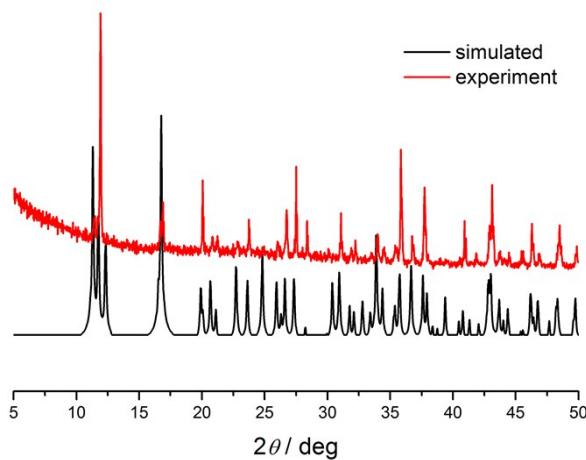


Fig. S6 Comparison of XRPD patterns of the simulated pattern from the single-crystal structure determination and as-synthesized product of **2**.

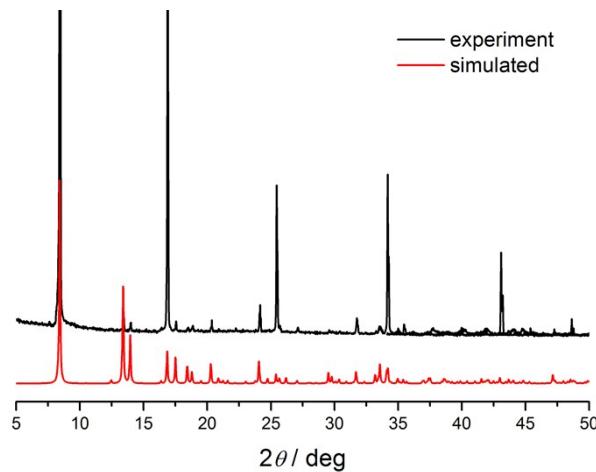


Fig. S7 Comparison of XRPD patterns of the simulated pattern from the single-crystal structure determination and as-synthesized product of **3**

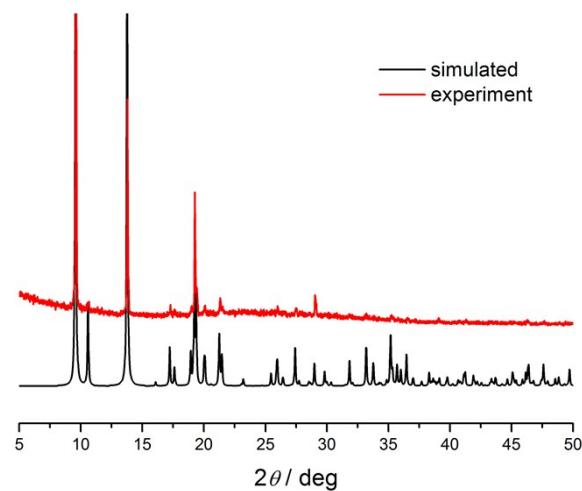


Fig. S8 Comparison of XRPD patterns of the simulated pattern from the single-crystal structure determination and as-synthesized product of **4**.

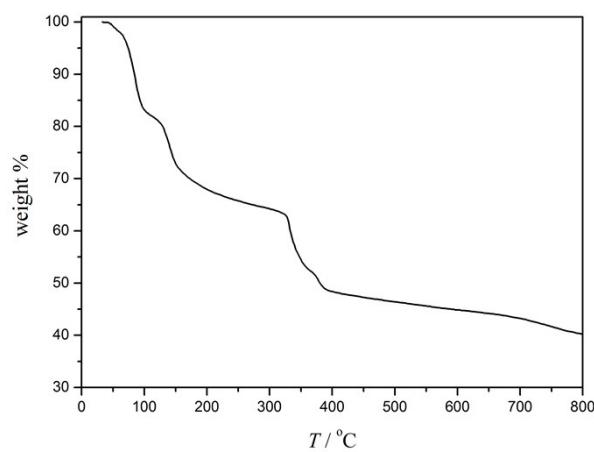


Fig. S9 TG curve of compound **1**

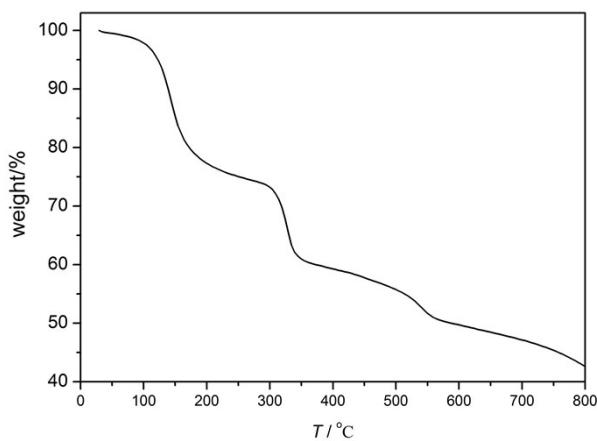


Fig. S10 TG curve of compound 2.

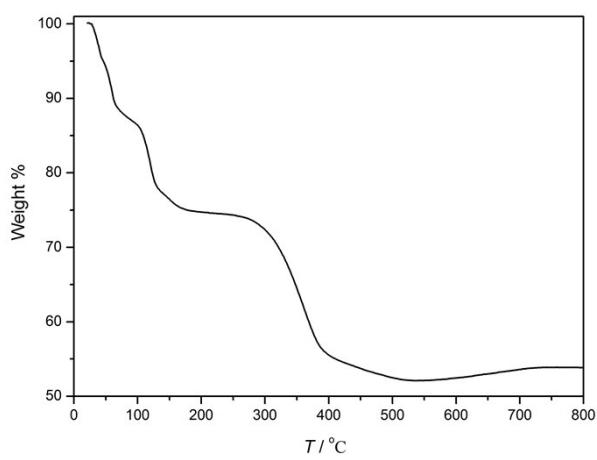


Fig. S11 TG curve of compound 3

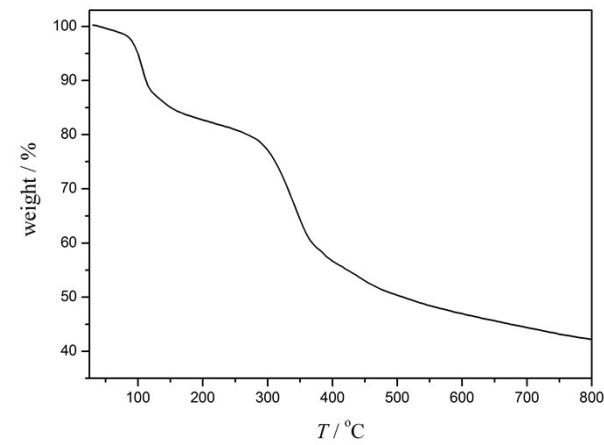


Fig. S12 TG curve of compound 4

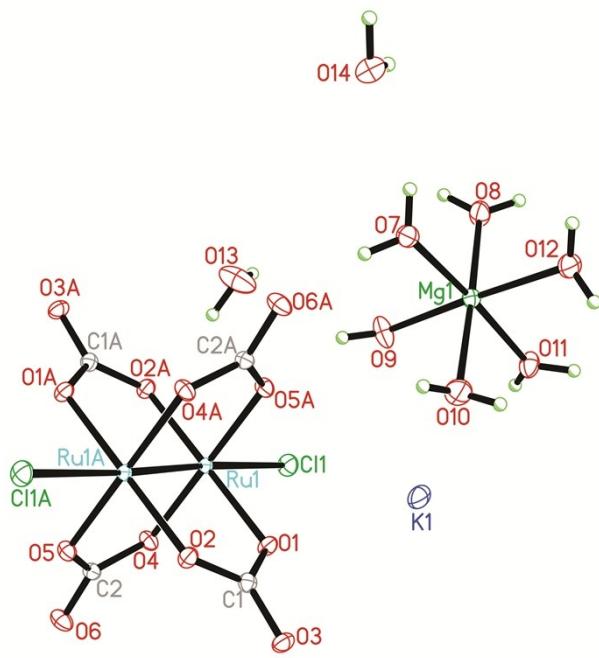


Fig. S13 ORTEP representation (30% thermal probability ellipsoids) of the crystal structure of **1**

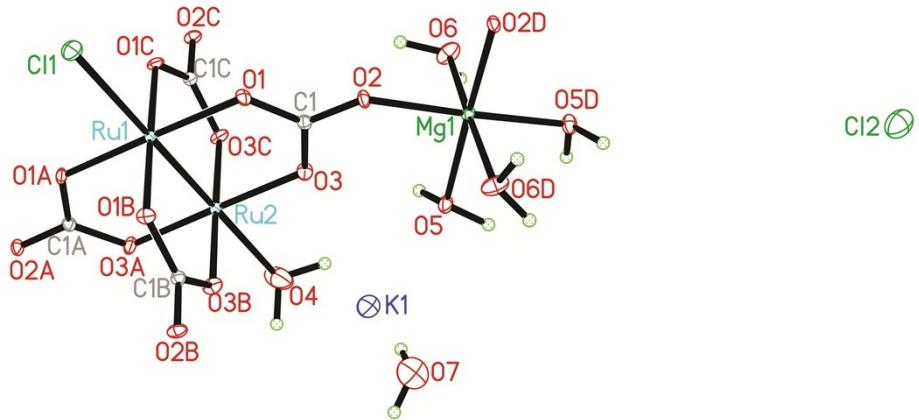


Fig. S14 ORTEP representation (30% thermal probability ellipsoids) of the crystal structure of **2**

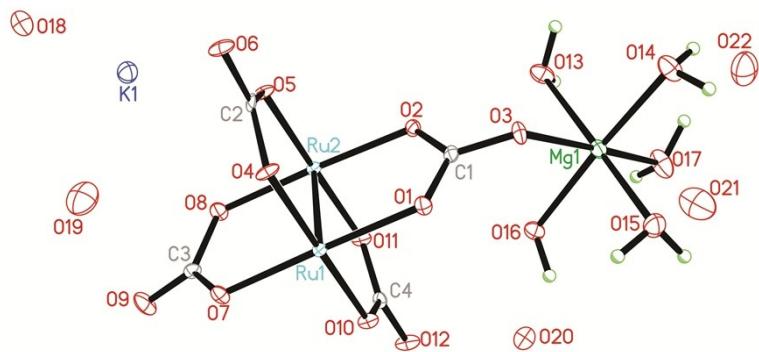


Fig. S15 ORTEP representation (30% thermal probability ellipsoids) of the crystal structure of **3**

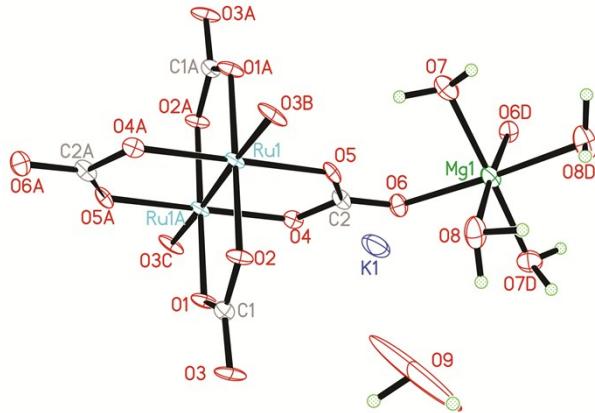


Fig. S16 ORTEP representation (30% thermal probability ellipsoids) of the crystal structure of **4**.

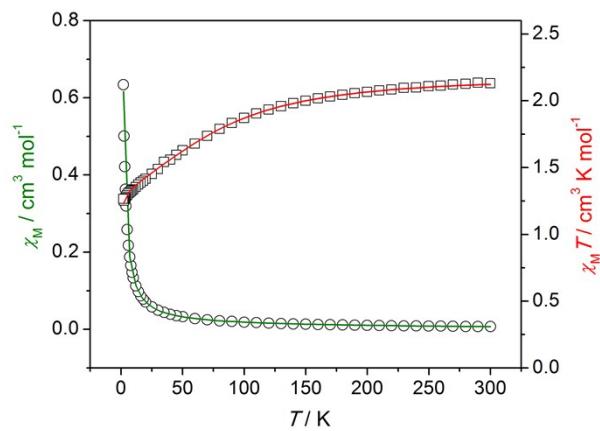


Fig S17. χ_M and $\chi_M T$ vs T plots for **2**.

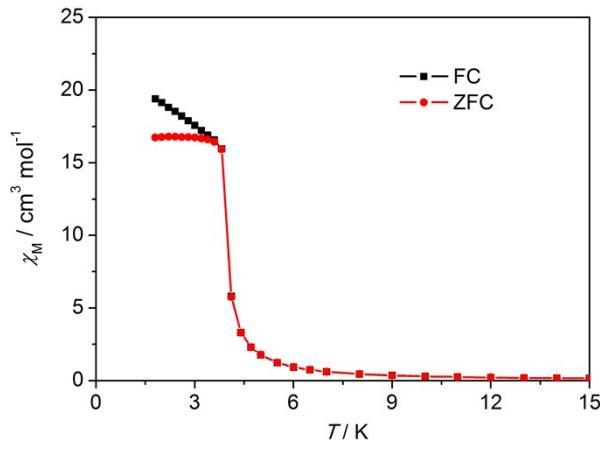


Fig S18. FC and ZFC vs T plots for **3**.

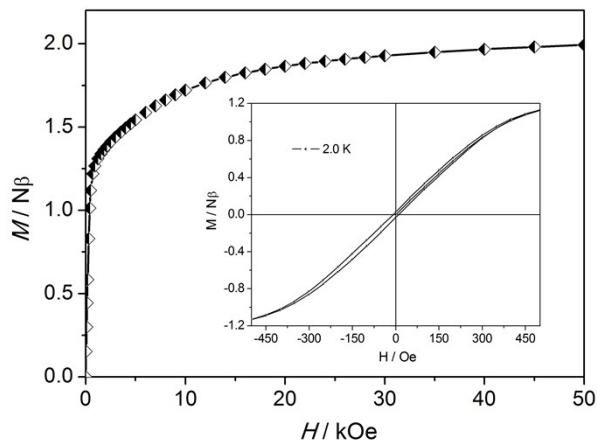


Fig S19. M and $\chi_M T$ vs H plots for **3**.

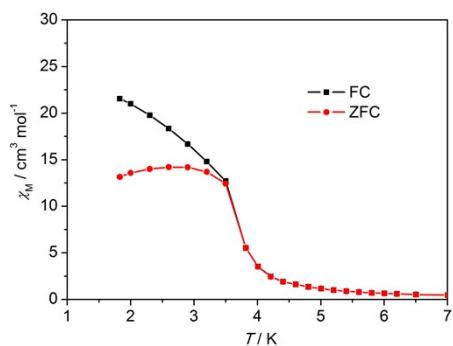


Fig S20. FC and ZFC vs T plots for **4** (large crystals)

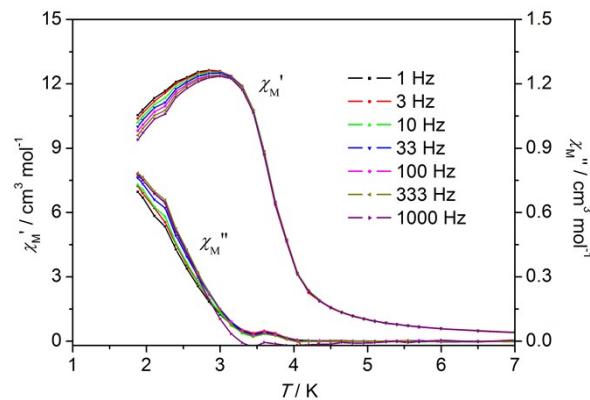


Fig S21. In-phase (χ_M') and out-of-phase (χ_M'') components for sample **4-1** with increasing frequencies

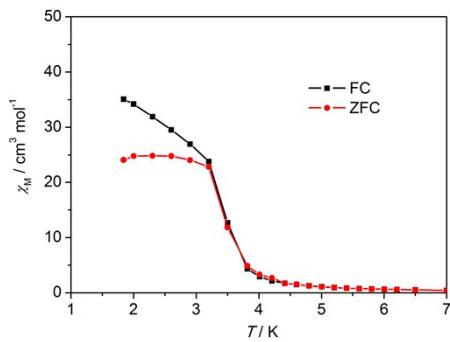


Fig S22. FC and ZFC vs T plots for sample 4-1.

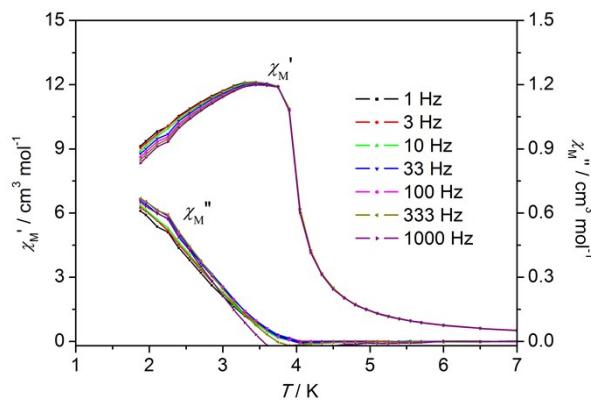


Fig S23. In-phase (χ_M') and out-of-phase (χ_M'') components for sample 4-2 with increasing frequencies

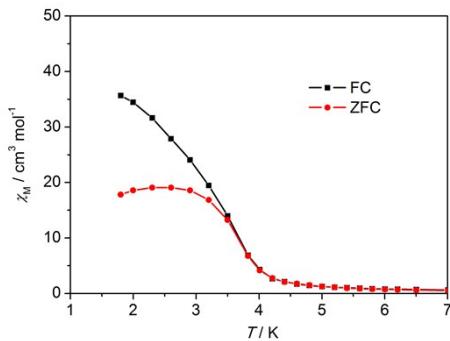


Fig S24. FC and ZFC vs T plots for sample 4-2

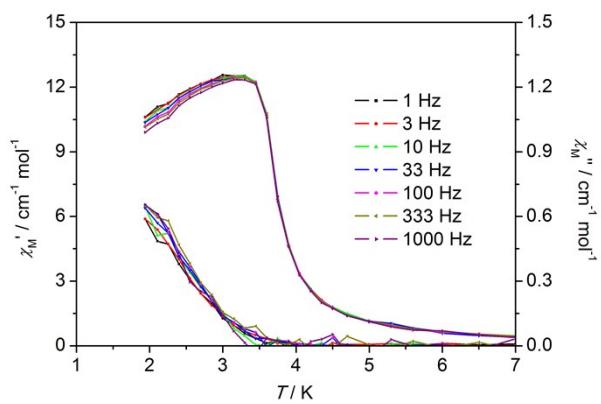


Fig S25. In-phase (χ_M') and out-of-phase (χ_M'') components for sample 4-3 with increasing frequencies

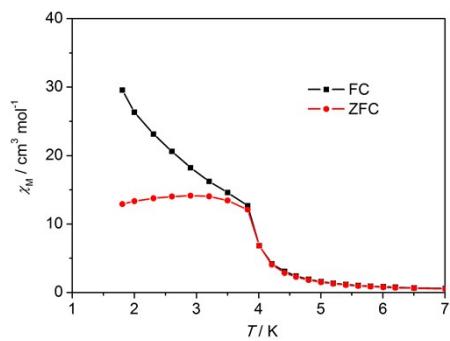


Fig S26. FC and ZFC vs T plots for sample 4-3