

Electronic Supporting Information (ESI)

Isomeric Chain Structures of $\{[\text{Mn}(\text{H}_2\text{O})_4]_2\text{Ru}_2(\text{CO}_3)_4\text{Br}_2\}_n^{n-}$:

Syntheses, Structural Diversity and Magnetic Properties

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Table S1. Selected bond angles (°) of complexes **1** and **2**

1			
Ru(1A)–Ru(1)–Br(1)	178.40(5)	O(3)–Mn(1)–O(5)	167.2(2)
Ru(1A)–Ru(1)–O(1)	90.01(14)	O(3)–Mn(1)–O(5D)	89.2(2)
Ru(1A)–Ru(1)–O(2A)	89.19(14)	O(4)–Mn(1)–O(5)	92.7(2)
O(3)–Mn(1)–O(3D)	91.3(2)	O(4)–Mn(1)–O(5D)	77.4(2)
O(3)–Mn(1)–O(4)	100.0(2)	O(5)–Mn(1)–O(5D)	93.1(3)
O(3)–Mn(1)–O(4D)	90.0(2)	Mn(1)–O(3)–C(1)	129.7(5)
2			
Ru(1A)–Ru(1)–Br(1)	177.75(5)	Ru(2B)–Ru(2)–Br(2)	176.65(6)
Ru(1A)–Ru(1)–O(1)	89.03(16)	Ru(2B)–Ru(2)–O(4)	89.44(12)
Ru(1A)–Ru(1)–O(3)	90.06(16)	Ru(2B)–Ru(2)–O(6)	89.79(12)
O(2)–Mn(1)–O(5)	88.9(2)	O(5)–Mn(1)–O(10)	91.5(2)
O(2)–Mn(1)–O(7)	89.6(2)	O(7)–Mn(1)–O(8)	88.3(2)
O(2)–Mn(1)–O(8)	91.6(2)	O(7)–Mn(1)–O(9)	88.3(2)
O(2)–Mn(1)–O(9)	94.3(2)	O(7)–Mn(1)–O(10)	90.1(3)
O(5)–Mn(1)–O(8)	94.32(19)	O(8)–Mn(1)–O(10)	86.7(2)
O(5)–Mn(1)–O(9)	89.29(19)	O(9)–Mn(1)–O(10)	87.4(3)
Mn(1)–O(2)–C(1)	131.2(5)	Mn(1)–O(5)–C(2)	128.8(4)

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

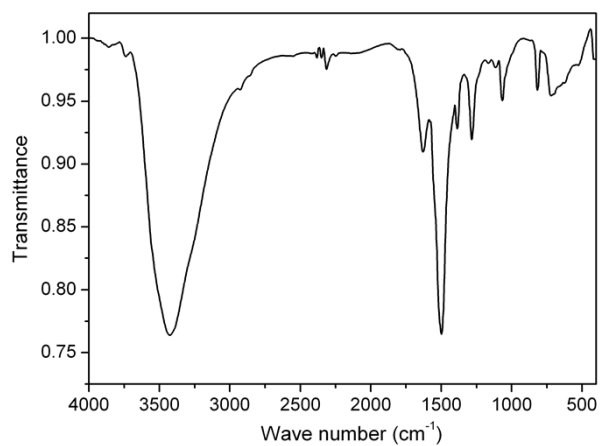


Fig S1. IR spectra of complex 1.

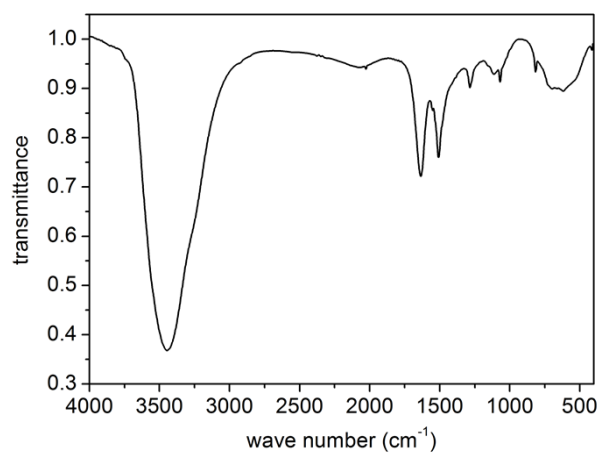


Fig S2. IR spectra of complex 2.

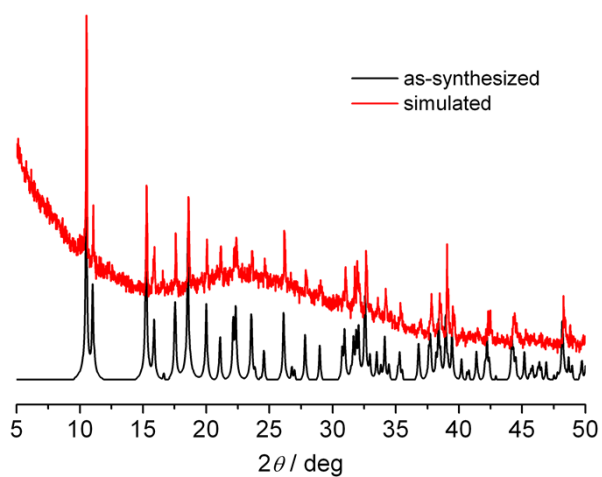


Fig S3. Comparison of XRPD patterns of the simulated pattern from the single-crystal structure determination and as-synthesized product of 1.

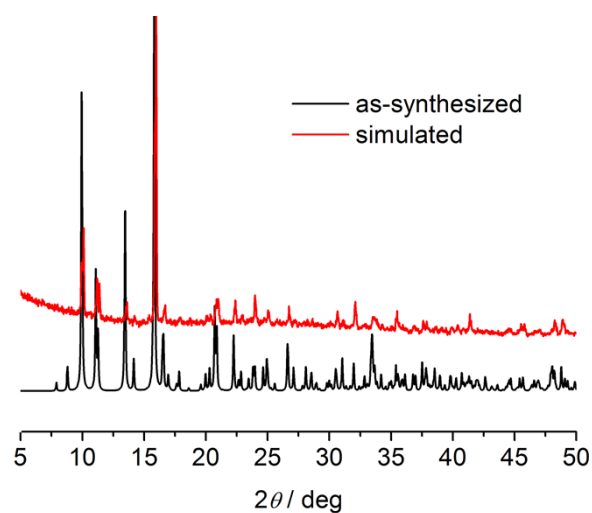


Fig S4. Comparison of XRPD patterns of the simulated pattern from the single-crystal structure determination and as-synthesized product of **2**.

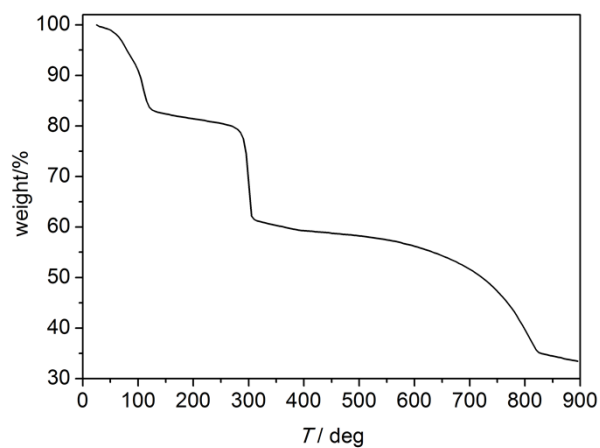


Fig S5. TG curve of complex **1**.

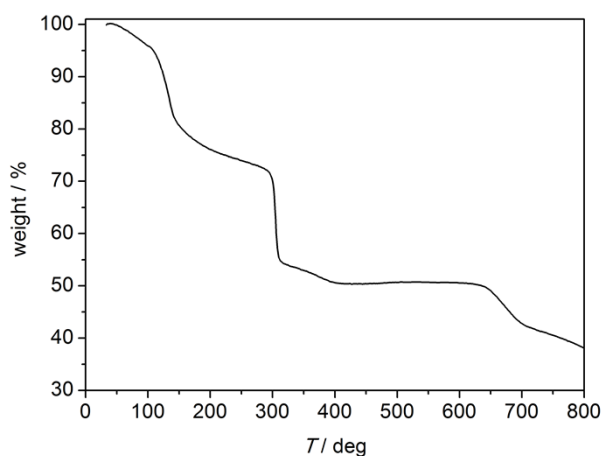


Fig S6. TG curve of complex **2**.

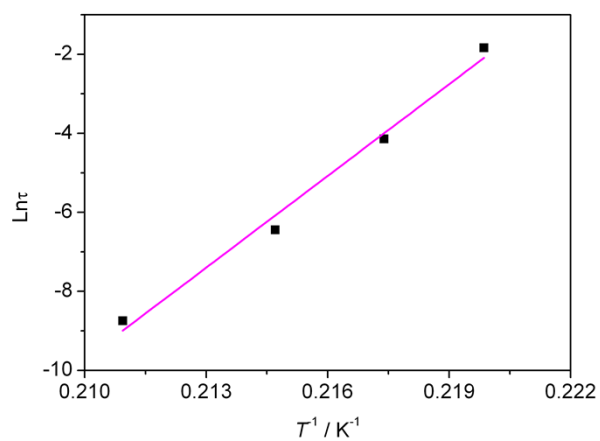


Fig S7. Plot of $\ln\tau$ against $1/T$ for **1**, the solid line is least-squares fits to the Arrhenius law.

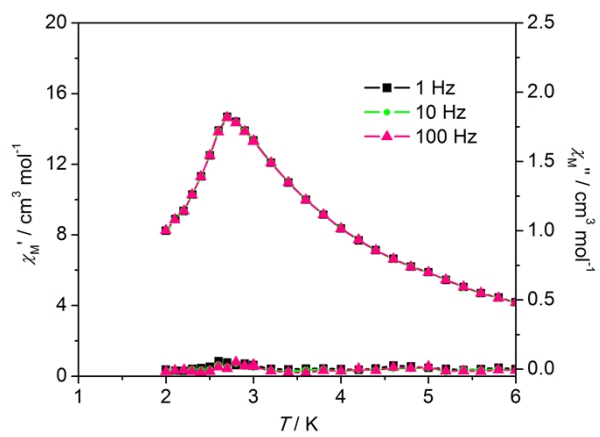


Fig S8. AC magnetic susceptibilities at 1,10,100 Hz of **2**.

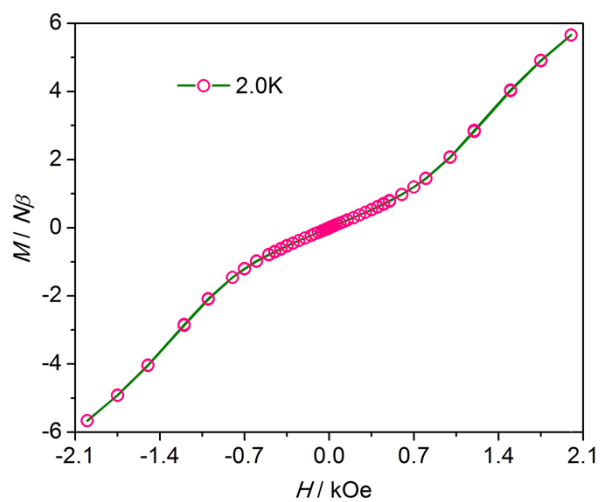


Fig S9. Magnetization M in $N\beta$ units vs H plot for complex **2**.