

Supplementary materials

A diruthenium soft ferromagnet showing $T_c = 3.0$ K

$\text{Mn}_4(\text{H}_2\text{O})_{16}\text{H}[\text{Ru}_2(\text{CO}_3)_4]_2[\text{Ru}_2(\text{CO}_3)_4(\text{H}_2\text{O})_2]\cdot 11\text{H}_2\text{O}$

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Crystal data for **1**: $\text{C}_{12}\text{H}_{59}\text{O}_{65}\text{Mn}_4\text{Ru}_6$, $M_r = 2069.77$, red-brown plate, Monoclinic, space group P21/c, $a = 13.664(3)$ Å, $b = 13.618(3)$ Å, $c = 16.954(3)$ Å, $\beta = 110.74(3)^\circ$, $V = 2950.3(10)$ Å³, $Z = 2$, $\rho_{\text{calcd}} = 2.330$ g cm⁻³, $(\text{Mo K}\alpha) = 2.455$ mm. A single crystal of dimensions $0.25 \times 0.10 \times 0.10$ mm³ for **1** was selected for indexing and intensity data collection on a Rigaku SCX mini CCD diffractometer using graphite-monochromatized Mo K α radiation ($\lambda = 0.71073$ Å) at room temperature. Numbers of collected and observed independent [$I > 2\sigma(I)$] reflections are 29983 and 6113 ($R_{\text{int}} = 0.040$). Full matrix least-squares refinements were based on F2 and converged at $R_1 = 0.0395$ and $wR_2 = 0.0889$. GOOF = 1.160. The eight coordination water H atoms were located in a difference Fourier map and refined with restrained O-H bond lengths [$0.85(2)$ Å] and fixed isotropic displacement parameters [$U(\text{iso})\text{H} = 1.5U(\text{eq})\text{O}$].

Table S1. Selected bond lengths [Å] and angles (deg) for **1**

Ru1-Ru1E	2.2575(8)	Ru3-O17	2.028(4)
Ru1-O1	2.023(4)	Ru3-O16G	2.019(5)
Ru1-O4	2.018(4)	Ru3-O18G	2.027(4)
Ru1-O7	2.310(5)	Mn1-O13	2.196(6)
Ru1-O2E	2.037(4)	Mn1-O20	2.191(6)
Ru1-O5E	2.035(4)	Mn1-O21	2.163(8)
Ru2-Ru2F	2.2588(8)	Mn1-O22	2.172(7)

Ru2-O6	2.264(4)	Mn1-O23	2.221(7)
Ru2-O8	2.028(5)	Mn1-O19	2.187(6)
Ru2-O11G	2.026(5)	Mn2-O15	2.121(5)
Ru2-O9F	2.016(5)	Mn2-O24	2.176(7)
Ru2-O12A	2.029(5)	Mn2-O25	2.240(6)
Ru3-Ru3G	2.2570(8)	Mn2-O26	2.187(8)
Ru3-O3	2.261(4)	Mn2-O27	2.225(6)
Ru3-O14	2.029(5)	Mn2-O10C	2.167(4)
O1-Ru1-O4	88.76(17)	O13-Mn1-O20	97.0(2)
O1-Ru1-O7	83.38(17)	O13-Mn1-O21	85.9(3)
Ru1E-Ru1-O1	89.46(10)	O13-Mn1-O22	86.6(2)
O1-Ru1-O2E	179.50(17)	O13-Mn1-O23	94.5(2)
O1-Ru1-O5E	91.19(17)	O13-Mn1-O19	167.7(2)
O4-Ru1-O7	88.31(17)	O19-Mn1-O20	92.8(2)
Ru1E-Ru1-O4	90.11(10)	O19-Mn1-O21	86.5(3)
O2E-Ru1-O4	90.74(17)	O19-Mn1-O22	84.4(2)
O4-Ru1-O5E	179.92(18)	O19-Mn1-O23	94.0(3)
Ru1E-Ru1-O7	172.70(15)	O20-Mn1-O21	90.2(3)
O2E-Ru1-O7	96.63(17)	O20-Mn1-O22	173.6(2)
O5E-Ru1-O7	91.63(17)	O20-Mn1-O23	84.3(2)
Ru1E-Ru1-O2E	90.52(10)	O21-Mn1-O22	95.3(3)
Ru1E-Ru1-O5E	89.96(10)	O21-Mn1-O23	174.5(3)
O2E-Ru1-O5E	89.31(17)	O22C-Mn1-O23	90.1(3)
O6-Ru2-O8	88.98(16)	O15-Mn2-O24	177.2(2)
O6-Ru2-O12A	84.98(16)	O15-Mn2-O25	86.0(2)
Ru2F-Ru2-O6	174.74(10)	O15-Mn2-O26	91.8(3)
O6-Ru2-O9F	91.27(16)	O15-Mn2-O27	90.2(2)
O6-Ru2-O11G	95.42(16)	O10C-Mn2-O15	91.1(2)
O8-Ru2-O12A	89.98(19)	O24-Mn2-O25	94.2(3)
Ru2F-Ru2-O8	90.13(12)	O24-Mn2-O26	87.9(3)
O8-Ru2-O9F	179.6(2)	O24-Mn2-O27	87.0(2)
O8-Ru2-O11G	90.85(19)	O10C-Mn2-O24	91.7(2)
Ru2F-Ru2-O12A	89.84(12)	O25-Mn2-O26	176.9(3)
O9F-Ru2-O12A	90.41(19)	O25-Mn2-O27	86.3(2)
O11G-Ru2-O12A	179.08(19)	O10C-Mn2-O25	89.13(19)
Ru2F-Ru2-O9F	89.65(12)	O26-Mn2-O27	91.6(2)
Ru2F-Ru2-O11G	89.77(12)	O10C-Mn2-O26	93.0(2)
O9F-Ru2-O11G	88.76(19)	O10C-Mn2-O27	175.1(2)
O3-Ru3-O14	88.11(16)	Ru1-O1-C1	120.7(3)
O3-Ru3-O17	85.97(16)	Ru1E-O2-C1	119.1(4)
Ru3G-Ru3-O3	175.33(10)	Ru3-O3-C1	134.1(3)
O3-Ru3-O16G	91.96(16)	Ru1-O4-C2	119.9(3)
O3-Ru3-O18G	94.29(16)	Ru1E-O5-C2	119.3(3)

O14-Ru3-O17	91.21(18)	Ru2-O6-C2	133.2(3)
Ru3G-Ru3-O14	89.94(13)	Ru2-O8-C3	118.9(4)
O14-Ru3-O16G	179.85(19)	Ru2F-O9-C3	120.4(4)
O14-Ru3-O18G	89.92(18)	Ru2G-O11-C4	120.3(4)
Ru3G-Ru3-O17	89.83(13)	Ru2B-O12-C4	119.7(3)
O16G-Ru3-O17	88.67(18)	Ru3-O14-C5	120.1(4)
O17-Ru3-O18G	178.85(18)	Ru3G-O16-C5	120.3(4)
Ru3G-Ru3-O16G	89.98(13)	Ru3-O17-C6	120.3(4)
Ru3G-Ru3-O18G	89.95(13)	Ru3G-O18-C6	120.3(4)
O16G-Ru3 -O18G	90.20(18)	Mn1-O19-C6	131.4(5)
		Mn1-O13-C4	123.1(4)
		Mn2-O15-C5	136.0(5)
		Mn2D-O10-C3	124.8(4)

Symmetry transformations used to generate equivalent atoms: A: $-1+x, 1+y, z$, B: $1+x, -1+y, z$, C: $1-x, -1/2+y, 3/2-z$, D: $1-x, 1/2+y, 3/2-z$, E: $-x, 1-y, 1-z$, F: $-x, 2-y, 1-z$, G: $1-x, 1-y, 1-z$.

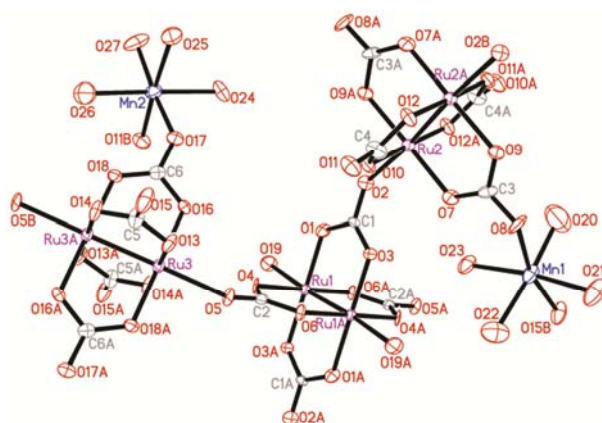


Figure S1. ORTEP diagram showing the coordination environment of **1** with thermal ellipsoids at 30% probability. All H atoms are omitted for clarity. Symmetry transformations used to generate equivalent atoms for **1**: A: $-1+x, 1+y, z$, B: $1+x, -1+y, z$, C: $1-x, -1/2+y, 3/2-z$, D: $1-x, 1/2+y, 3/2-z$, E: $-x, 1-y, 1-z$, F: $-x, 2-y, 1-z$, G: $1-x, 1-y, 1-z$.

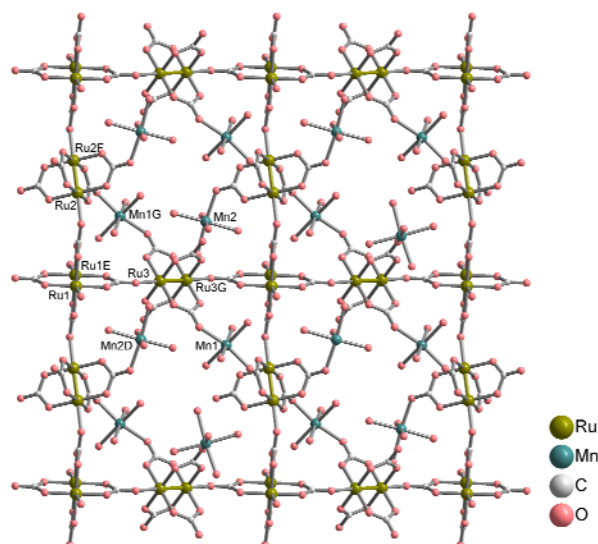


Figure S2. Perspective views of the 2D layer with the (4,4) net-work $[\text{Ru}_2(\text{CO}_3)_4]_n^{3n-}$ and $\text{Mn}(\text{H}_2\text{O})_4^{2+}$ cations bridges in the *ab* plane. Symmetry transformations used to generate equivalent atoms for **1**: A: $-1+x, 1+y, z$, B: $1+x, -1+y, z$, C: $1-x, -1/2+y, 3/2-z$, D: $1-x, 1/2+y, 3/2-z$, E: $-x, 1-y, 1-z$, F: $-x, 2-y, 1-z$, G: $1-x, 1-y, 1-z$.

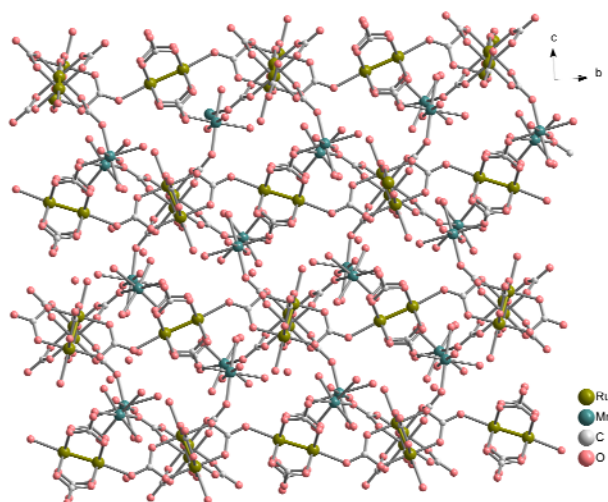


Figure S3. Packing diagram of complex **1** in the *bc* plane. The hydrogen atoms and lattice water molecules are omitted.

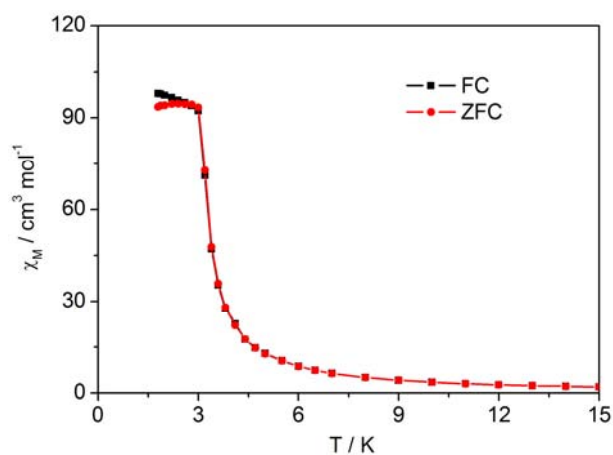


Figure S4. Plots of field-cooled magnetization (FCM, ■) and zero-field-cooled magnetization (ZFCM, ●) vs temperature measured at 30 Oe for complex **1**.

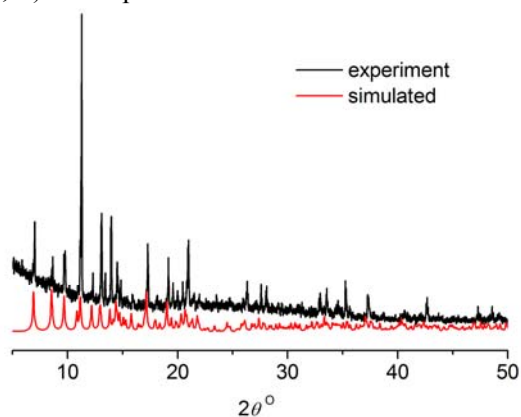


Figure S4. Comparison of XRPD pattern from the single-crystal structure determination and as-synthesized product of complex **1**