# Supporting Information

# A homochiral diamond framework constructed from Fe(III) and Mn(II) oxo-clusters supported by Sb(III) tartrate scaffolds

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# Section 4 Additional References for the Introduction

## Section 1 Experimental Section

**Materials and Methods:** All of the reactants were reagent grade and were used as purchased without further purification. TPOM was synthesized according to literature.[1] The IR spectra were measured on a Galaxy Series FTIR 5000 spectrometer with pressed KBr pellets. Thermogravimetric analysis (TGA) measurements were carried out using a TA Instruments Hi-Res 2950 system in $N_2$ flow, with a heating rate of 3 °C $min^{-1}$. Elemental analyses were performed by Galbraith Laboratories (Knoxville, TN). The powder X-ray diffraction (PXRD) patterns were collected at room temperature on a Phillps X'pert Pro diffractometer.

**Synthesis of $(H_4TPOM)\ [Fe_4Mn_3Sb_6(\mu_4\text{-}O)_6(\mu_3\text{-}O)_2(L\text{-tartrate})_6(H_2O)]\cdot 16H_2O$ (1): 1** was synthesized by hydrothermal reaction from a mixture of $Fe(ClO_4)_3$, $Mn(OAc)_2$, $K_2Sb_2(L\text{-tartrate})_2$, TPOM, HCOOH, HCOOK, $H_2O$ and DMF (molar ratio = 4:3:3:2:4:4:4440:516). The mixture was heated at 100 °C in a sealed teflon vessel for 3 d. By using vacuum filtration and drying in air, yellow block crystals of **1** were recovered with a few yellow inpurities. Yield: 50% based on Fe. Element analysis (%): calc. for $Fe_4Mn_3Sb_6C_{49}N_4O_{62}H_{72}$: H 2.48, C 20.71, N 1.97, Fe 7.86, Mn 5.80, Sb 25.7; obs. H 2.58, C 20.21, N 1.86, Fe 7.76, Mn 5.70, Sb 24.3. IR (KBr): 3423(br. s), 2909(w), 1641(s), 1509(m), 1324(s), 1199(m), 1106(s), 1075(m), 1029(w), 996(w), 907(w), 809(w), 743(m), 591(s).

**Crystallography:** Single-crystal X-ray analysis was performed at room temperature on a Siemens SMART platform diffractometer outfitted with an Apex II area detector and monochromatized graphite Mo Kα radiation (λ = 0.71073 Å). The structure was solved by direct methods and refined using SHELXTL software package.[2] Crystallographic data and structural refinement for compound **1** are summarized in Table S1. More details on the crystallographic studies as well as atomic displacement parameters are given in CIF file. Carbon-bonded hydrogen atoms on tartrate ligands were placed in geometrically calculated positions; hydrogen atoms on water molecules and TPOM cations were not assigned and directly included in the molecule formula. Some constraints were applied to confine the geometry of TPOM. Only partial lattice water molecules were assigned, the remaining water molecules were based on elemental analysis and TG analysis.

## References

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Table S1. Crystallographic data for **1**

| Identification code | **1** |
|---|---|
| Empirical formula | $C_{49}H_{53}Fe_4Mn_3N_4O_{54.5}Sb_6$ |
| Formula weight | 2688.67 |
| Crystal system | Orthorhombic |
| Space group | $P2_12_12_1$ |
| $a$ [Å] | 20.0376(18) |
| $b$ [Å] | 20.8740(19) |
| $c$ [Å] | 20.9807(19) |
| $V$ [Å$^3$] | 8775.5(14) |
| Z | 4 |
| $D$c [g/cm$^{-3}$] | 2.035 |
| $\mu$ [mm$^{-1}$] | 2.971 |
| Flack x | 0.010(18) |
| Goodness-of-fit on $F$ | 1.025 |
| Final $R$ indices | $R_1 = 0.0390$, |
| $[I > 2\sigma(I)]^a$ | $wR_2 = 0.1131$ |
| R indices (all data) | $R_1 = 0.0438$ |
| | $wR_2 = 0.1159$ |

## Section 2 Supplementary Structural Figures

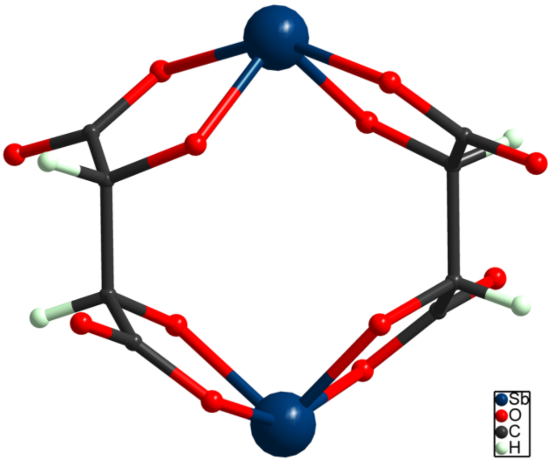


**Figure S1:** Ball-and-stick representation of the $Sb_2(tartrate)_2^{2-}$ ligand.

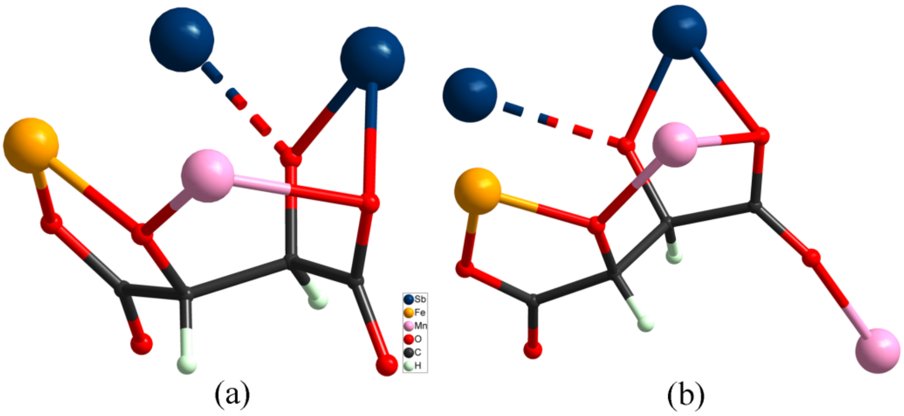


**Figure S2:** Schematic view of the coordination modes of the tartrate ligands in **1**. (a) mode A, (b) mode B. In mode A, the ligand coordination is $\mu_4$-$\eta^2$:$\eta^2$:$\eta^2$:$\eta^1$. Each ligand uses one oxygen atom from a carboxylate group and the oxygen atom of the neighbouring hydroxyl group to chelate either one $Fe^{3+}$ ion or one $Sb^{3+}$ ion. The hydroxyl group which coordinates to the $Fe^{3+}$ ion is also bonded to one $Mn^{2+}$ ion. The other hydroxyl group, which bonded to the $Sb^{3+}$ ion, is further weakly bonded to a second $Sb^{3+}$ ion. In mode B, the ligand coordination is $\mu_5$-$\eta^2$:$\eta^2$:$\eta^2$:$\eta^1$:$\eta^1$. The carboxylate group bonded to the $Sb^{3+}$ ion in mode A utilizes the other oxygen atom to bond to another $Mn^{2+}$ ion.

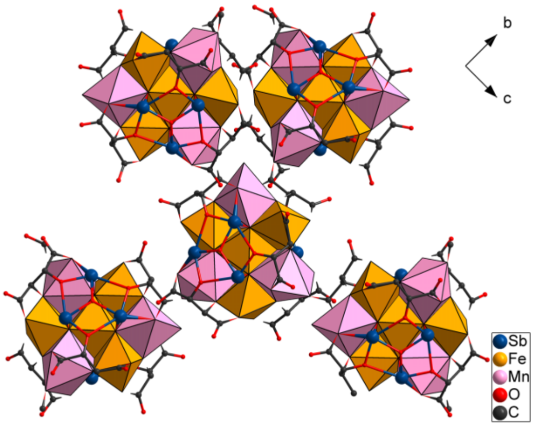
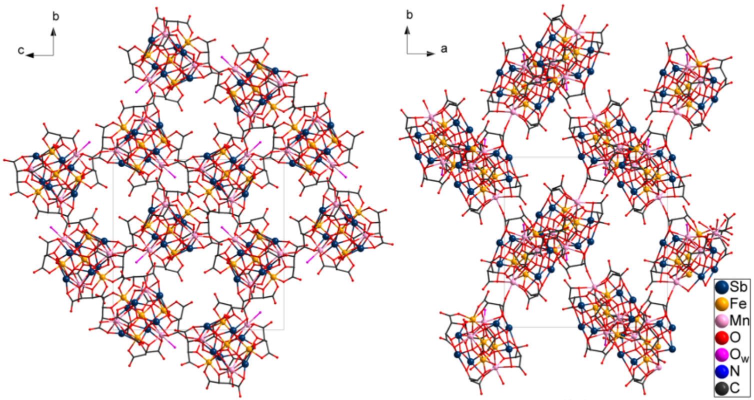
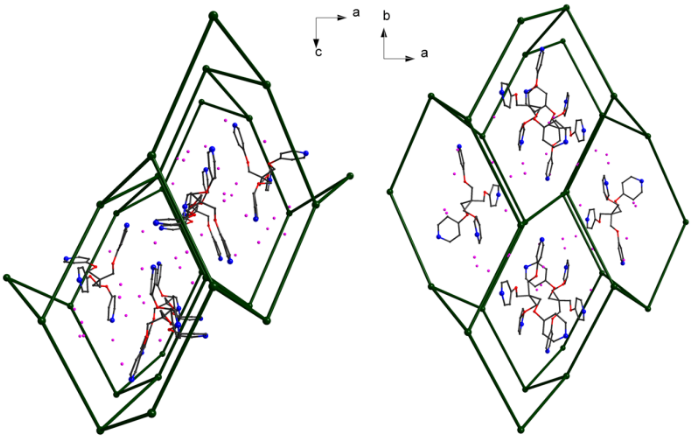


**Figure S3:** Ball-and-stick representation of connectivity between clusters of **1**. $Fe^{3+}$ and $Mn^{2+}$ ions are highlighted as light orange and rose octahedral.



(a) (b)

**Figure S4:** Ball-and-stick representation of the diamondiod network of **1**. a) viewe along *a*-axis, b) viewe along *c*-axis.



(a) (b)

**Figure S5:** Schematic representation of TMOP and guest water molecules in the framework. Projection along (a) b- and (b) c-axis. The diamond frameworks are shown in solid dark green lines.

## Section 3 Supplementary Physical Characterization Data

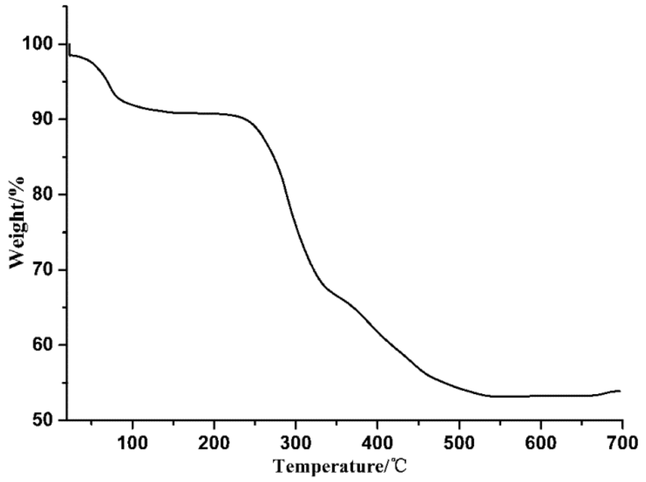


**Figure S6:** TGA of **1** in a $N_2$ flow.

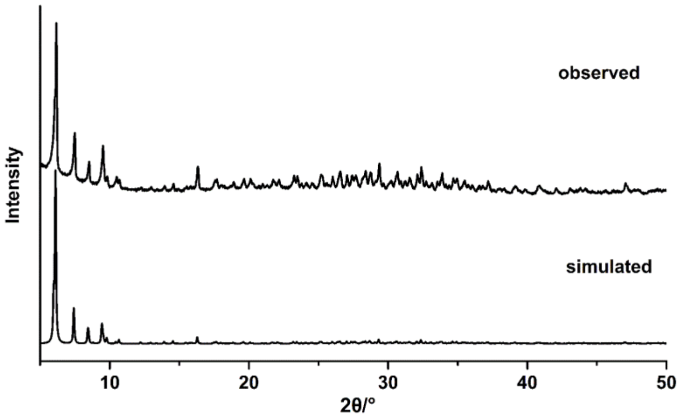


**Figure S7:** Simulated and observed powder X-ray diffraction (PXRD) of **1**.

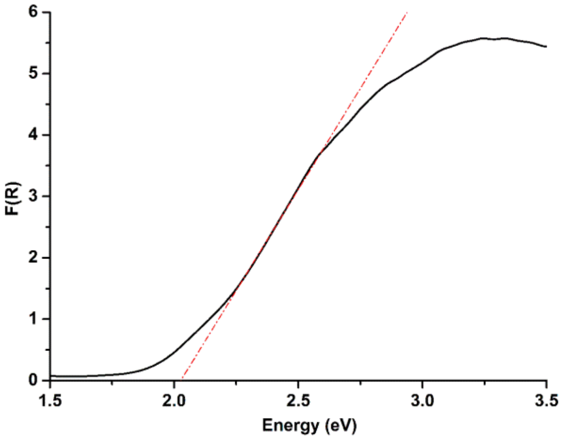


**Figure S8:** UV-VIS-NIR spectrum of **1**

## Section 4 Additional References for the Introduction

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