Combining oxime-based [Mn₆] clusters with cyanometalates: 1D chains of [Mn₆] SMMs from [M(CN)₂]⁻ (M= Au, Ag)

Sergio Sanz, Jamie M. Frost, Giulia Lorusso, Marco Evangelisti, Mateusz B. Pitak, Simon J. Coles, Gary S. Nichol and Euan K. Brechin

Experimental Procedures

Solvents and reagents were used as received from commercial suppliers.

**Synthesis of compound 1:** Mn(NO₃)₂·4H₂O (125 mg, 0.5 mmol), 2-hydroxypropiophenone oxime (80 mg, 0.5 mmol), 3-ethynlypyridine (50 mg, 0.25 mmol) and KAu(CN)₂ (144 mg, 0.5 mmol) were dissolved in MeOH (20 ml). After 5 minutes of stirring LiOMe (37 mg, 1 mmol) was added, and the solution stirred for a further 1 h, before being filtered and allowed to stand. Black rod-like X-ray quality crystals were obtained after room temperature evaporation of the mother liquor over 4 days. Elemental analysis (%) calculated (found) for C₃₈H₃₉AuMn₃N₆O₉ (1085.23): C 42.03 (41.92), H 3.62 (3.49), N 7.74 (7.58).

**Synthesis of compound 2:** Mn(NO₃)₂·4H₂O (125 mg, 0.5 mmol), 2-hydroxyacetophenone Oxime (75 mg, 0.5 mmol), 3-ethynlypyridine (50 mg, 0.25mmol), KAg(CN)₂ (128 mg, 0.5 mmol), were dissolved in MeOH (20 ml). After 5 minutes of stirring LiOMe (37 mg, 1 mmol) was added, and the solution stirred for a further 1 h, before being filtered. The filtrate was collected and allowed to stand for 24 h before being filtered again. Black rod-like X-ray quality crystals were obtained after room temperature evaporation of the mother liquor over 4 days. Elemental analysis (%) calculated (found) for C₃₄H₃₀AgMn₃N₆O₈ (923.33): C 44.21 (44.14), H 3.28 (3.24), N 9.10 (9.01).

**Figure S1.** Plot of magnetisation versus field for 1 and 2 in the 2.0 to 20 K temperature range, in fields up to 5 T.
**Figure S2.** Plot of $\chi_M''$ vs. $T$ for compound compound 1 (left) and 2 (right) in the indicated temperature and frequency ranges.

**Figure S3.** Arrhenius analysis of the ac susceptibility data for 1; $\tau_0 = 1.5 \times 10^{-10}$ s and $U_{\text{eff}} = 39.9$ K.

**Figure S4.** Arrhenius analysis of the ac susceptibility data for 2; $\tau_0 = 5.4 \times 10^{-10}$ s and $U_{\text{eff}} = 50.7$ K.
Figure S5. Packing of the chains of 1 in the crystal. H-atoms omitted for clarity.

Figure S6. Packing of the chains of 2 in the crystal. H-atoms omitted for clarity.