Supplementary materials

A trimanganese cluster-based 2D layer framework with facile single-crystal-to-single-crystal transformation to afford a 1D chain structure

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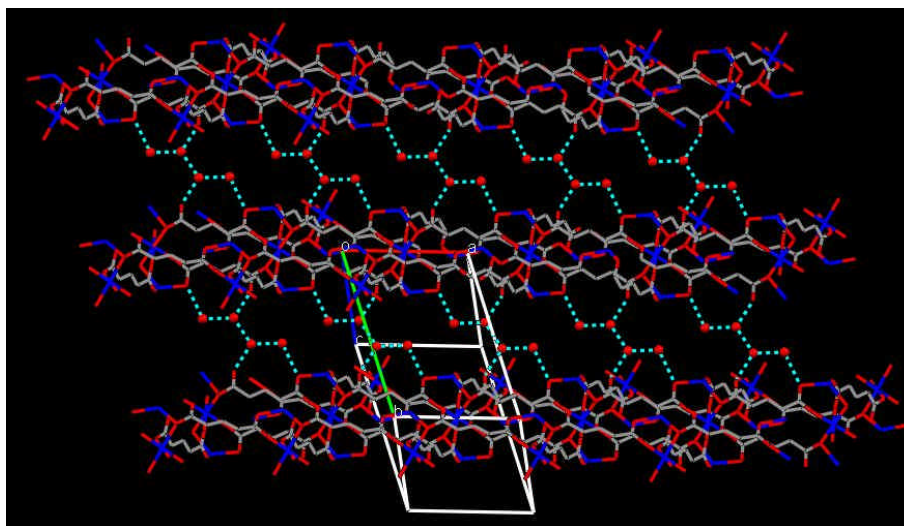E-mail: mcb@fjirsm.ac.cn and ccn@fjirsm.ac.cn*

Fig. S1 A view of 3D layer-stacked supramolecular framework for **1**, showing the zigzag-shaped water tetramers contacted to the Mn-ip host layers via hydrogen-bonds, and sandwiched between the ribbon-shaped inter-layer regions; all hydrogen atoms, bipy ligands and C4-C6/C12-C14/C20-C22 atoms of ip ligands are omitted for clarity.
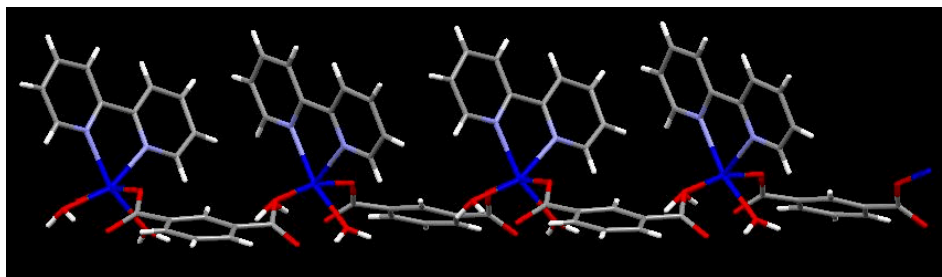
Fig. S2 The view of 1D chain structure in **2** with the metal ions uniformly separated by 7.635(2) Å, showing all bipy ligands, with a dihedral angle of 90.8(1)° for the adjacent couple, located on the same side of the chain.
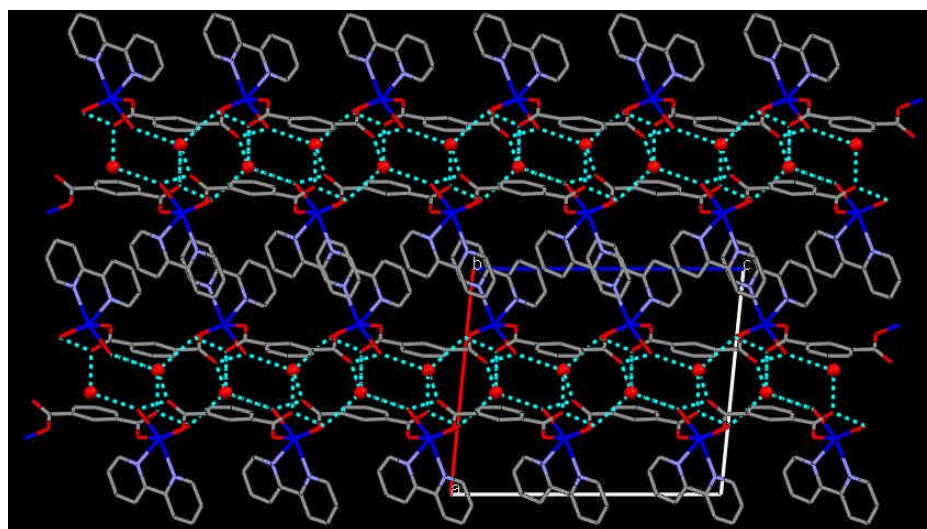

Fig. S3 A partial packing diagram of **2**, showing the formation of the 3D supramolecular framework derived from the parallel stacking of the H-bonded double-layers. The interlayer bipy ligands display partial π-π stacking interactions with a perpendicular ring distance of 3.473(5) Å
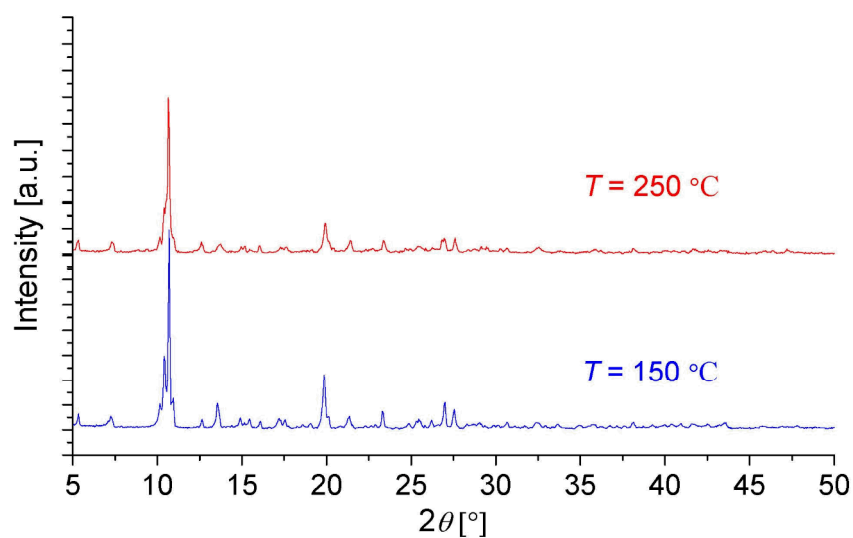
Fig. S4 A comparison of powder X-ray diffraction patterns for **1** recorded at 250 ℃ and 150 ℃, respectively, showing the stability of polymeric framework at higher temperature.
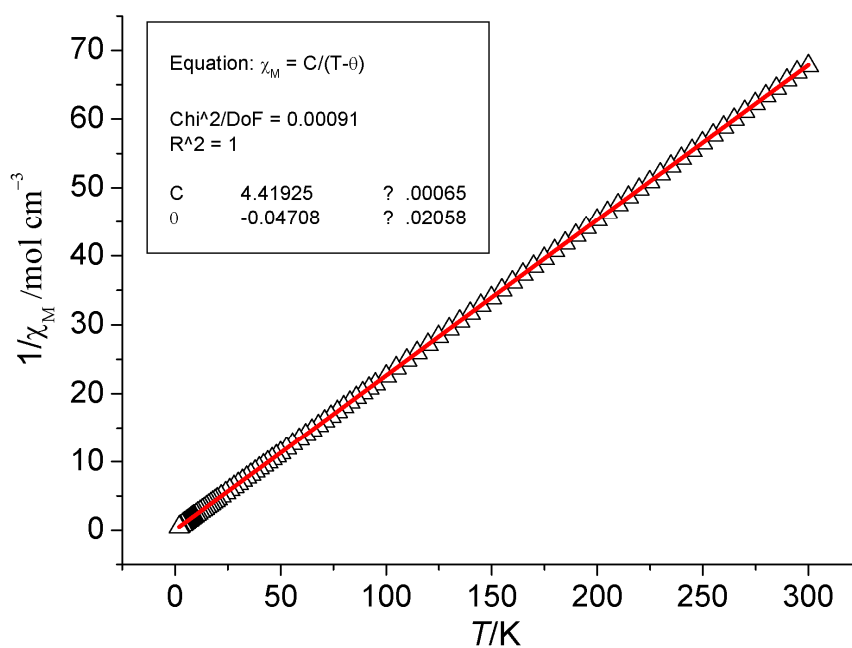

Fig. S5 The inverse molar magnetic susceptibility ($1/\chi_M$) vs. T for complex **2** (the red solid line represents the calculated values; the fitting results are listed in the inset).

Eq. S1 The fit equation for $S = 5/2$ trimer (the interaction between both ends is neglected)

$$\chi_M = \frac{Ng^2\beta^2}{3kT}\left[\frac{A}{B}\right]$$

$$A = 2040e^{-32x} + 1860e^{-17x} + 858e^{-4x} + 495e^{7x} + 252e^{16x} + 105e^{23x} + 1365e^{-27x} + 858e^{-14x}$$
$$+ 495e^{-3x} + 252e^{6x} + 105e^{13x} + 30e^{18x} + 858e^{-22x} + 492e^{-11x} + 252e^{-2x} + 105e^{5x} + 30e^{10x}$$
$$+ 3e^{13x} + 252e^{-8x} + 105e^{-x} + 30e^{4x} + 252e^{-12x} + 105e^{-5x} + 30 + 105e^{-7x}$$

$$B = 32e^{-32x} + 48e^{-17x} + 24e^{-4x} + 24e^{7x} + 16e^{16x} + 12e^{23x} + 28e^{-27x} + 24e^{-14x}$$
$$+ 20e^{-3x} + 16e^{6x} + 12e^{13x} + 8e^{18x} + 24e^{-22x} + 20e^{-11x} + 16e^{-2x} + 12e^{5x} + 8e^{10x}$$
$$+ 4e^{13x} + 16e^{-8x} + 12e^{-x} + 8e^{4x} + 16e^{-12x} + 12e^{-5x} + 8 + 12e^{-7x}$$

$$x = \frac{-J}{kT}$$