Supplementary Information

Synthesis, Characterisation and Computational Studies on a Novel One-Dimensional Arrangement of Schiff-base Mn₃ Single-Molecule Magnet

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Fig. S1 The packing arrangement of 1 viewed along the b axis. The black dotted lines represent the hydrogen bonds between the units. The hydrogen atoms and solvent molecules are omitted for clarity. Color code: Turquoise (MnII), Red (O), Blue (N), Gray (C), Green (Cl).

Fig. S2 The packing arrangement of 2 viewed along the ab plane. The hydrogen atoms and solvent molecules are omitted for clarity. Color code: Purple (MnIII), Red (O), Blue (N), Gray (C).
**Fig. S3** The packing arrangement of 3 viewed along the c axis. The hydrogen atoms and solvent molecules are omitted for clarity. Color code: Turquoise (Mn\(^{II}\)), Purple (Mn\(^{III}\)), Red (O), Blue (N), Gray (C), Green (Cl).

**Fig. S4** The packing arrangement of 3 viewed along the b axis. The hydrogen atoms and solvent molecules are omitted for clarity. The black dotted lines represent the hydrogen bonds between the polymeric chains. Color code: Turquoise (Mn\(^{II}\)), Purple (Mn\(^{III}\)), Red (O), Blue (N), Gray (C), Green (Cl).
Fig. S5 Infrared spectra of H$_2$hmi (red), complex 1 (blue), complex 2 (black) and complex 3 (green) from 4000 to 600 cm$^{-1}$. 
Fig. S6 Infrared spectra of H$_2$hmi (red), complex 1 (blue), complex 2 (black) and complex 3 (green) from 1800-800 cm$^{-1}$.

![Infrared spectra of H$_2$hmi and complexes](image)

Fig. S7 The IR comparison of DFT calculated absorbance (red) and experimental transmittance (blue) of H$_2$hmi.
Fig. S8 The IR comparison of DFT calculated absorbance (red) and experimental transmittance (blue) of complex 2