Supplementary Information

Synthesis, Characterisation and Computational Studies on a Novel One-Dimensional Arrangement of Schiff-base Mn_3 Single-Molecule Magnet

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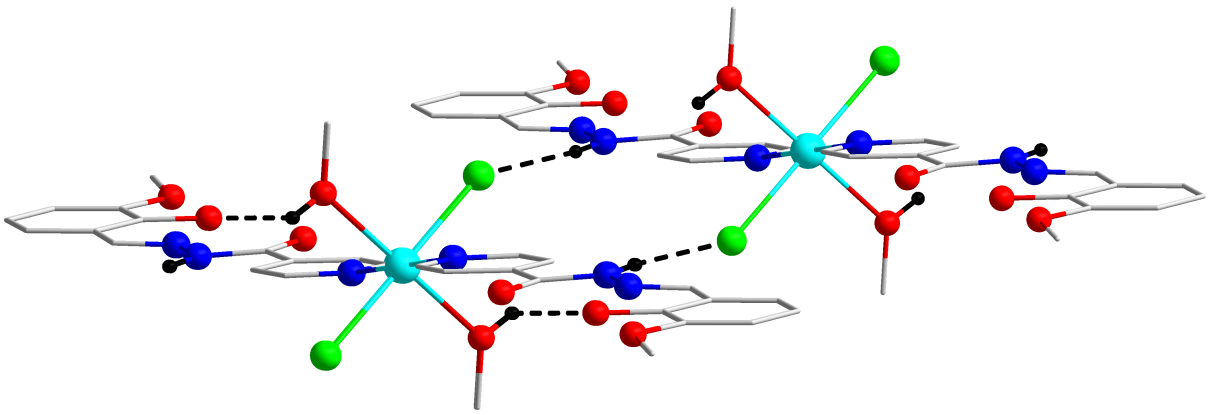

Fig. S1 The packing arrangement of **1** viewed along the *b* axis. The black dotted lines represent the hydrogen bonds between the units. The hydrogen atoms and solvent molecules are omitted for clarity. Color code: Turquoise (Mn^{II}), Red (O), Blue (N), Gray (C), Green (Cl).

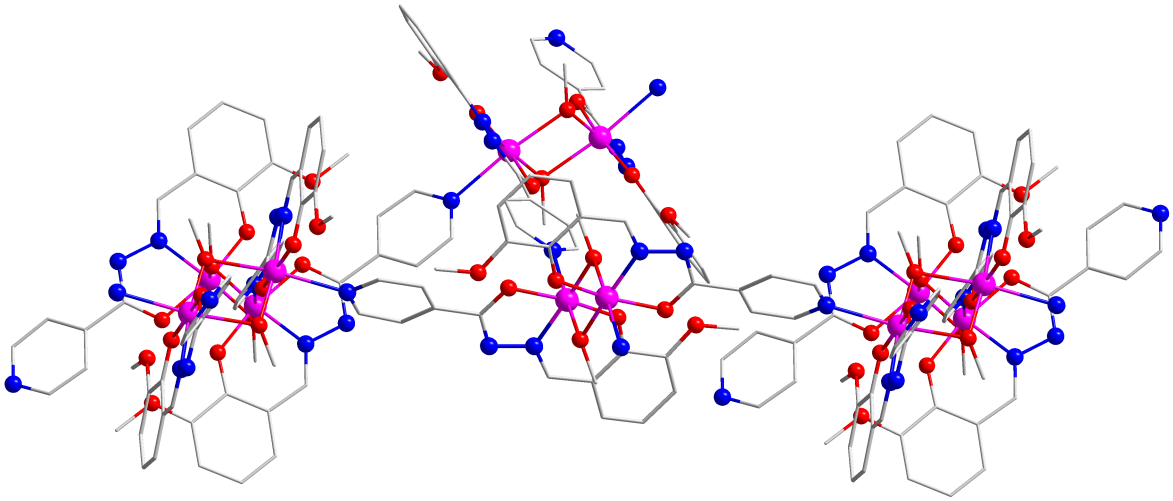

Fig. S2 The packing arrangement of **2** viewed along the *ab* plane. The hydrogen atoms and solvent molecules are omitted for clarity. Color code: Purple (Mn^{III}), Red (O), Blue (N), Gray (C).

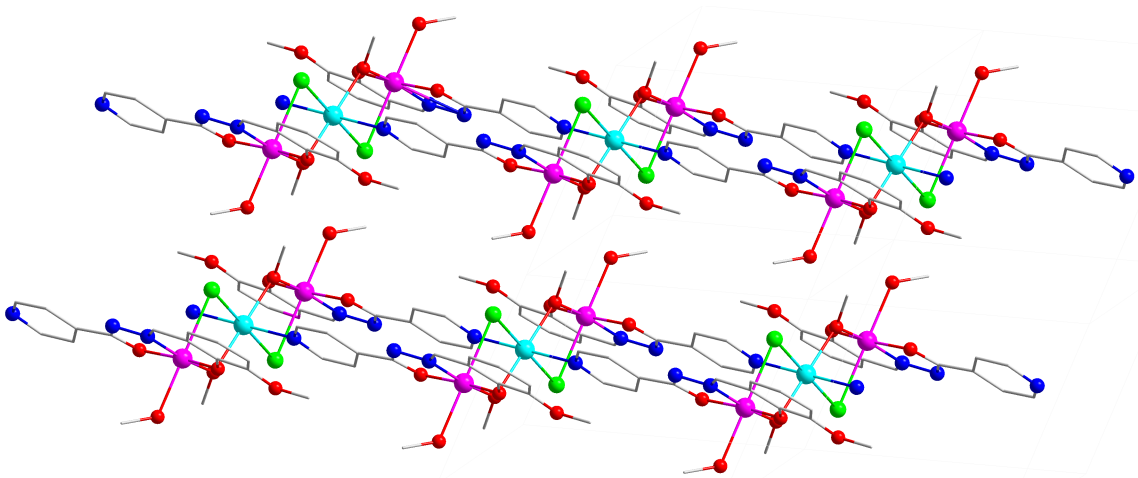

Fig. S3 The packing arrangement of **3** viewed along the *c* axis. The hydrogen atoms and solvent molecules are omitted for clarity. Color code: Turquoise (Mn^{II}), Purple (Mn^{III}), Red (O), Blue (N), Gray (C), Green (Cl).

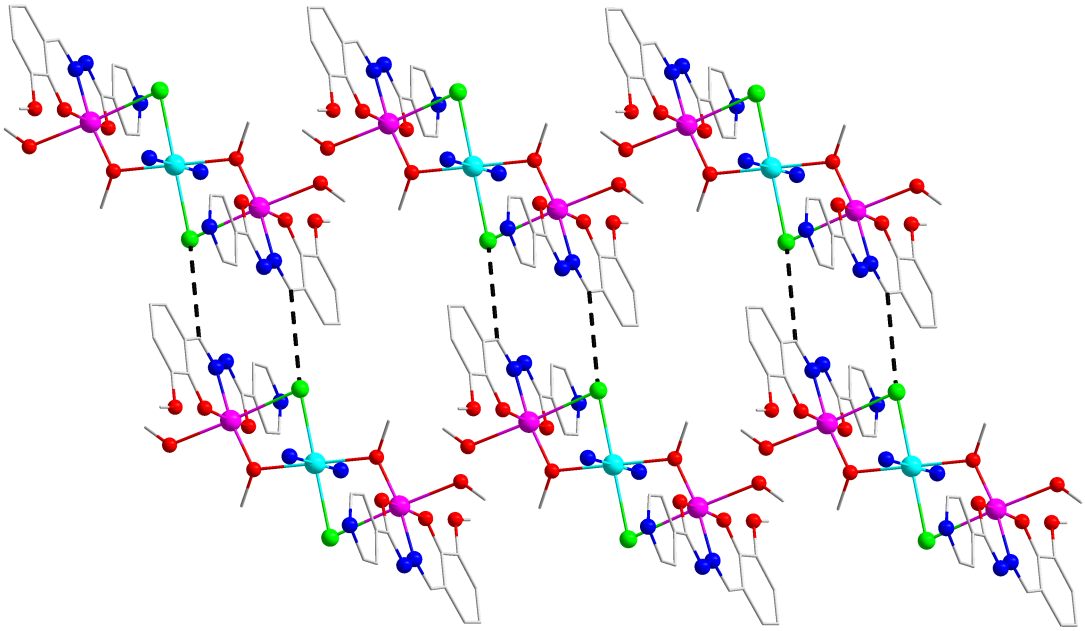

Fig. S4 The packing arrangement of **3** viewed along the *b* axis. The hydrogen atoms and solvent molecules are omitted for clarity. The black dotted lines represent the hydrogen bonds between the polymeric chains. Color code: Turquoise (Mn^{II}), Purple (Mn^{III}), Red (O), Blue (N), Gray (C), Green (Cl).

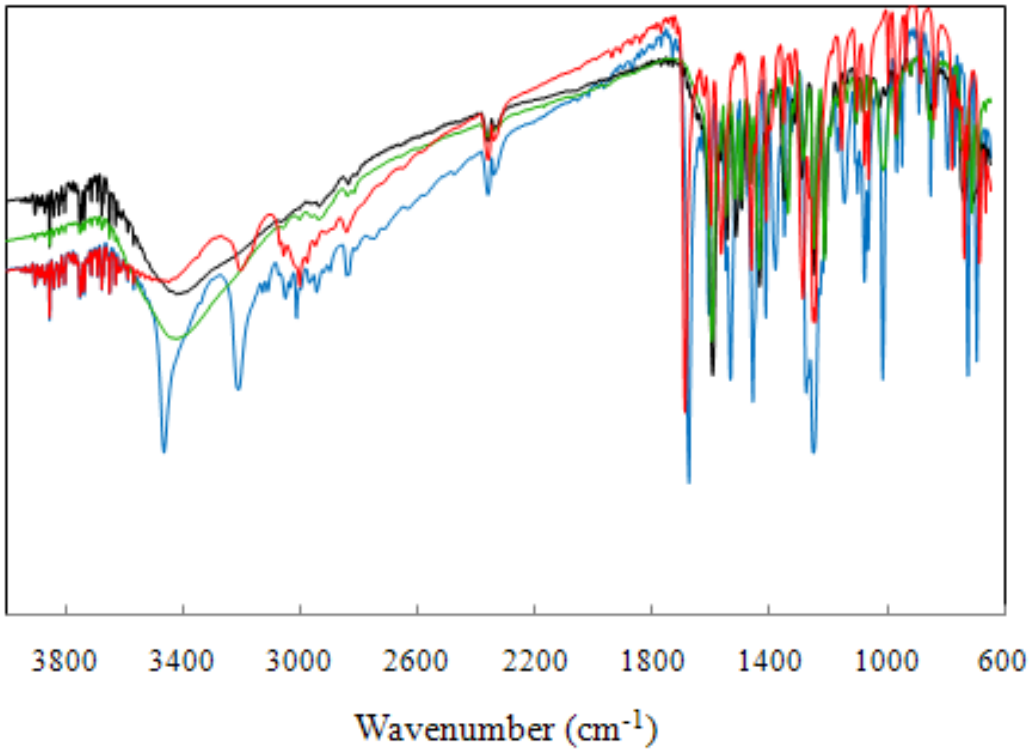

Fig. S5 Infrared spectra of H_2hmi(red), complex **1**(blue), complex **2**(black) and complex **3**(green) from 4000 to 600 cm^{-1}.

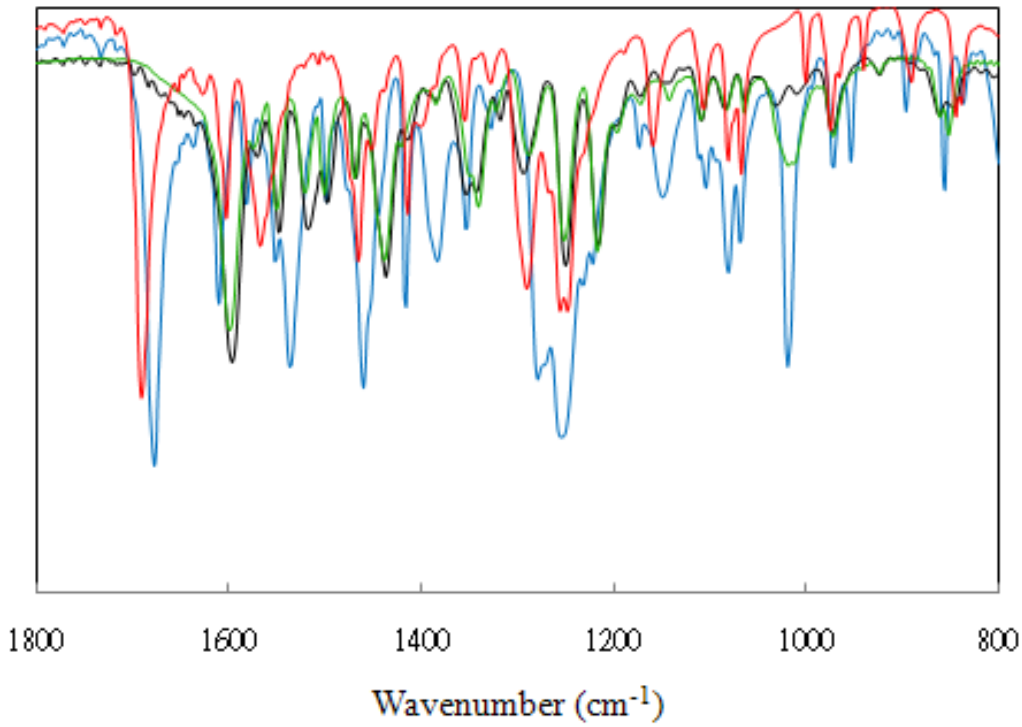

Fig. S6 Infrared spectra of H_2hmi (red), complex **1** (blue), complex **2** (black) and complex **3** (green) from 1800-800 cm^{-1}.

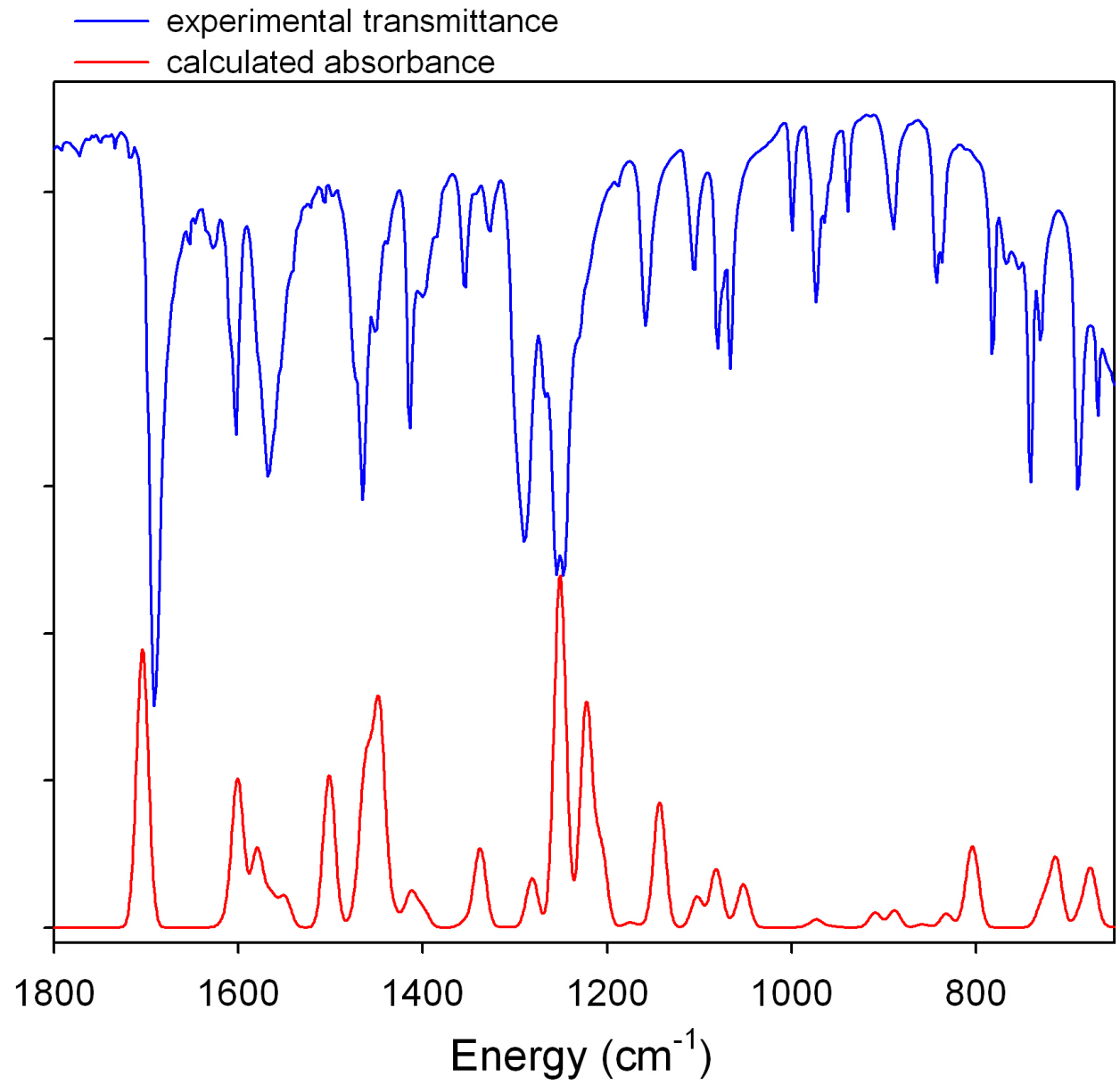

Fig. S7 The IR comparison of DFT caculated absorbance (red) and ecperimental transmittance (blue) of H_2hmi

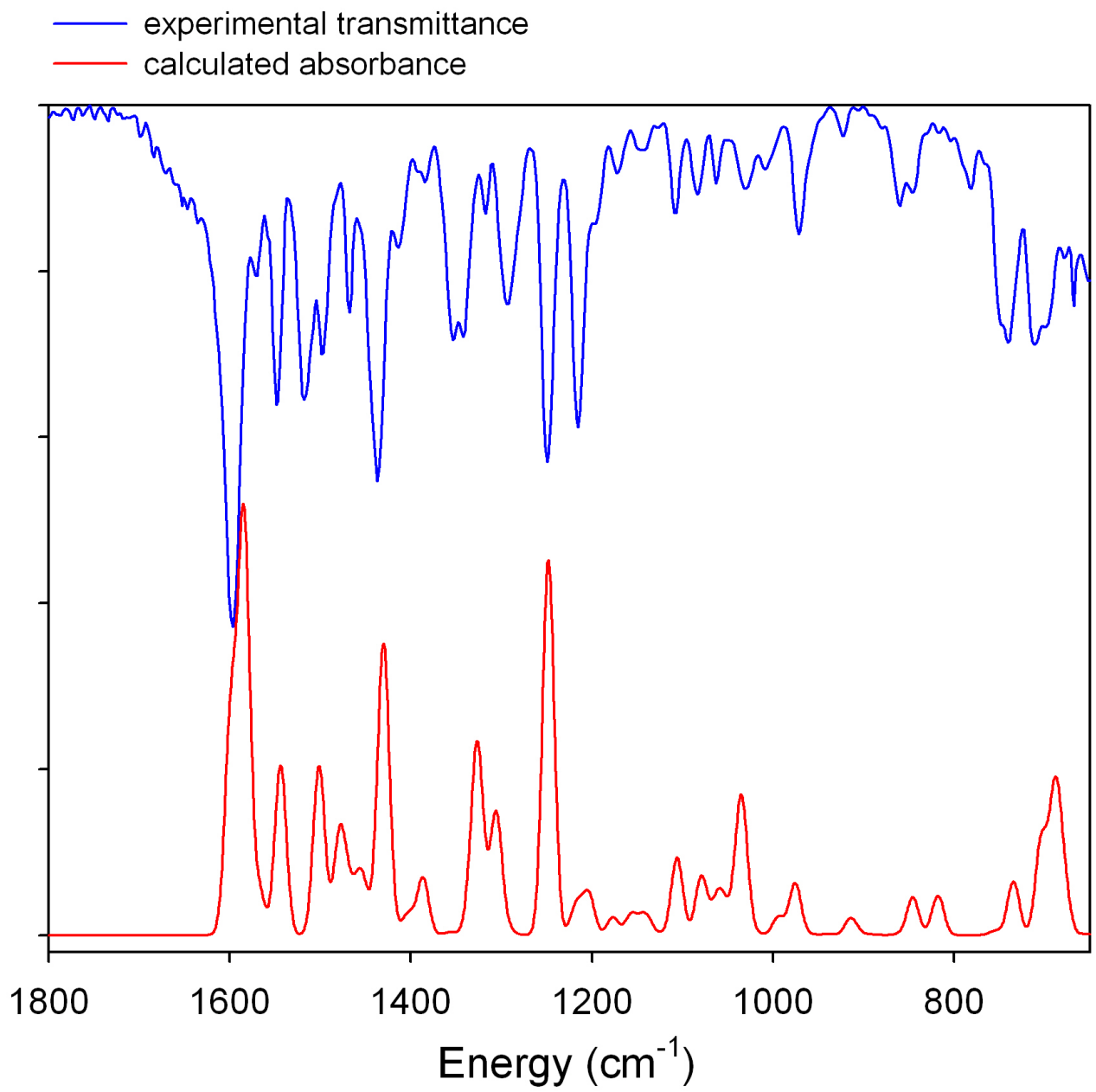

Fig. S8 The IR comparison of DFT caculated absorbance (red) and experimental transmittance (blue) of complex **2**