Supporting Information of

"$Mn(C_2O_4)(H_2O)_{0.25}$: An Antiferromagnetic Oxalate-based Cage Compound"

By Zhang et al.,

Synthesis:

All reagents are commercially avaible and used as received without further purification unless otherwise stated. $MnCl_2.4H_2O$ 1.0mmol, $H_2C_2O_4{\cdot}2H_2O$ 1.0mmol and 8.0ml 1,3-$CH_2OHCH_2CHOHCH_3$ were sealed in a Telfon-lined stainless steel vessel, heated to 120ºC for 72 hours under autogenous pressure, and then cooled to room-temperature. The resulting pink crystals were collected and washed with methanol and then dried in the air at ambient temperature.

Physical Characterizations:

Element analysis of carbon and hydrogen were performed on an Elementar Vario EL analyzer. IR spectra were recorded on a Bio-rad FTS6000 spectrometer for KBr pellet. X-ray diffraction data was collected at 173K on Rigaku diffractometer with confused monochromated Mo Kα (λ = 0.71073 Å) radiation. The structure was solved by direct method and refined by full-matrix least-squares on F^2 using SHELX program, with anisotropic thermal parameters for all non-hydrogen atoms. Hydrogen atoms of H_2O were located by different Fourier map and refined with constrains for the ideal geometry. Powder X-ray diffraction pattern was obtained on a Rigaku RINT2000 diffractometer at room temperature with Cu Kα (λ = 1.54056 Å) radiation in a flat-plate geometry. Magnetization measurements were performed against tightly packed polycrystalline sample in capsule on a Quantum Design MPMS 7XL SQUID system. Susceptibility data were corrected for diamagnetism of sample by Pascal constants (-42.25×10^{-6} cm^3mol^{-1}) and background by experimental measurement on the sample holder. The ac susceptibility measurement was carried out on a Quantum Design MPMS 5XL SQUID system for polycrystalline sample. Specific heat measurement was carried out on a Quantum Design PPMS 9XL system for polycrystalline sample fixed on sample holder by N-grease. The data was corrected for the contribution of N-grease and sample holder.

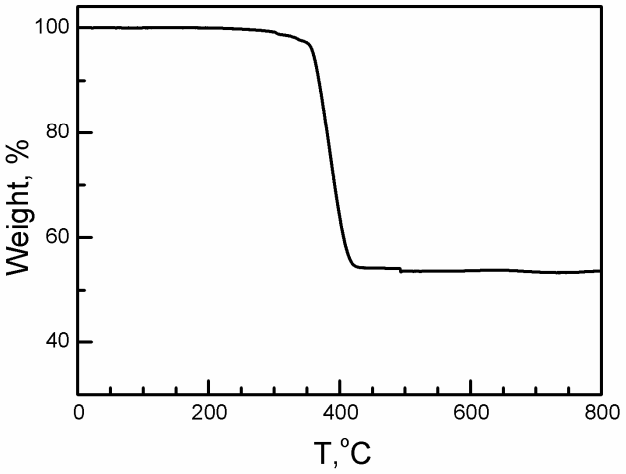

Figure S1. Thermogravimetric analysis plot of $Mn(C_2O_4)(H_2O)_{0.25}$ (black) measured at a heating rate of 10 °C/min.

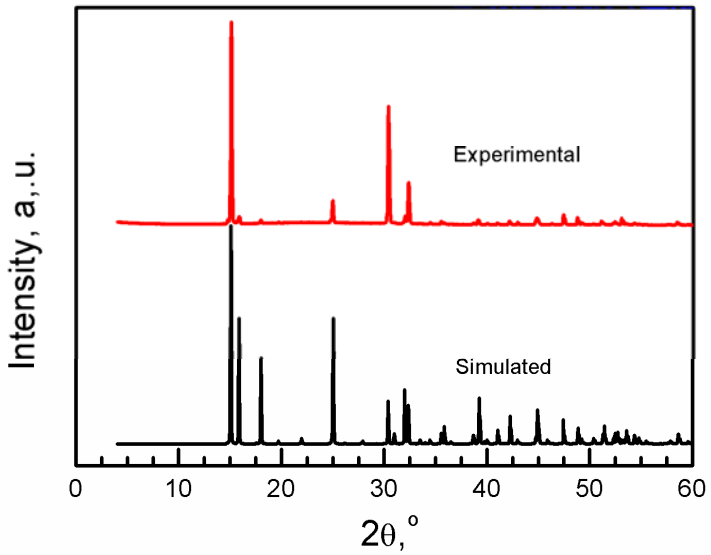

Figure S2. X-ray powder diffraction pattern**.** Black line: the simulated one based on the single crystal structure of $Mn(C_2O_4)(H_2O)_{0.25}$; red line: the experiment data from polycrystals.

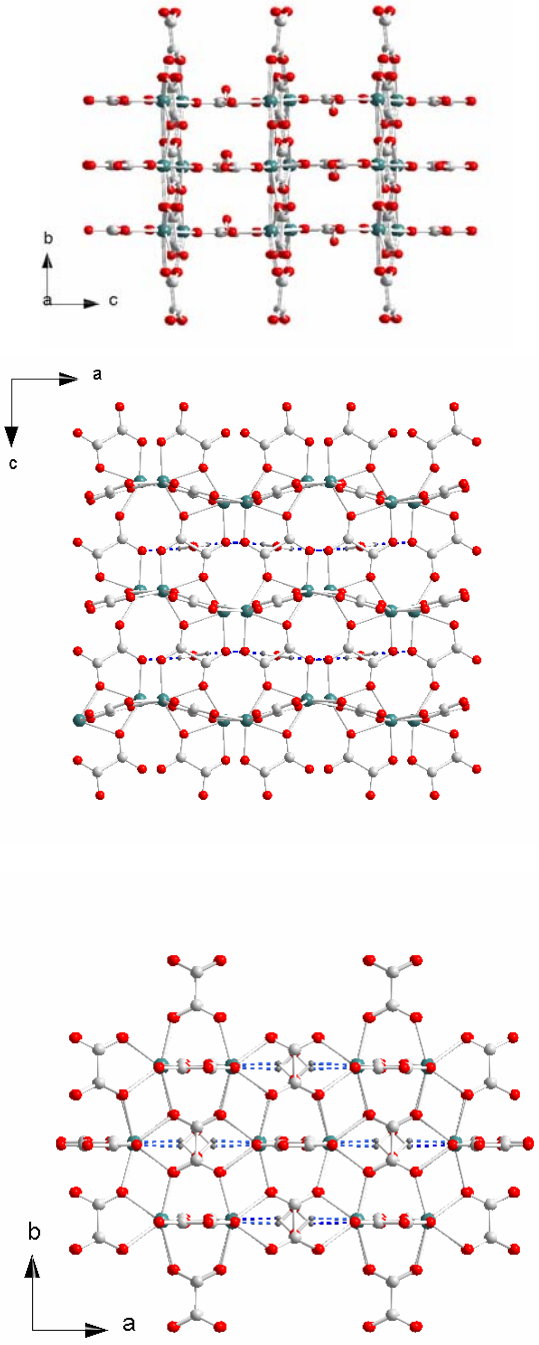

Figure S3. Crystal structure viewed along the *a*, *b*, and *c* axis. Coloro Code: Mn, grew; C, grey; O, red; H, light grey. Dashed blue sticks are hydrogen bonds.

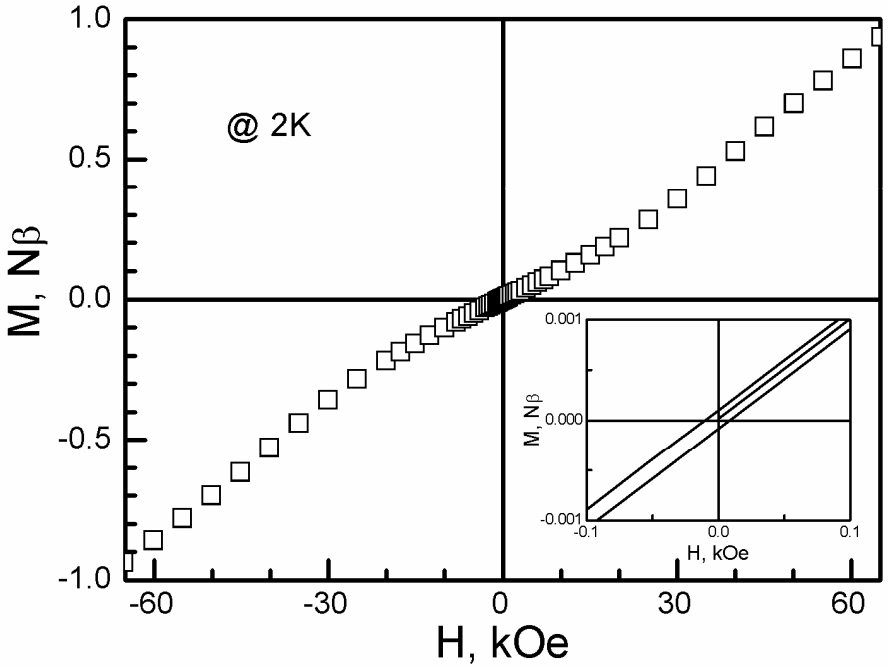

Figure S4. Isothermal magnetization of $Mn(C_2O_4)(H_2O)_{0.25}$ at 2 K. Inset: low-field of 100 Oe.