ELECTRONIC SUPPLEMENTARY INFORMATION (ESI)

Title:

A 2D rhomboidal system of manganese(II) $[Mn(3\text{-}MeC_6H_4COO)_2(H_2O)_2]_n$ with spin canting: rationalization of the magnetic exchange

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Content:

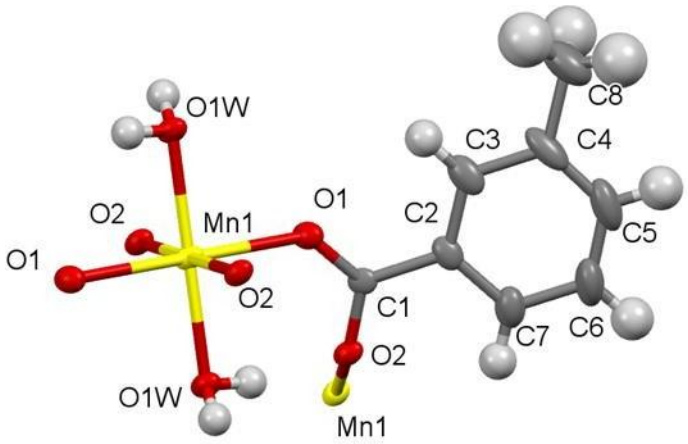

Figure S1. Asymmetric unit of compound **1**.

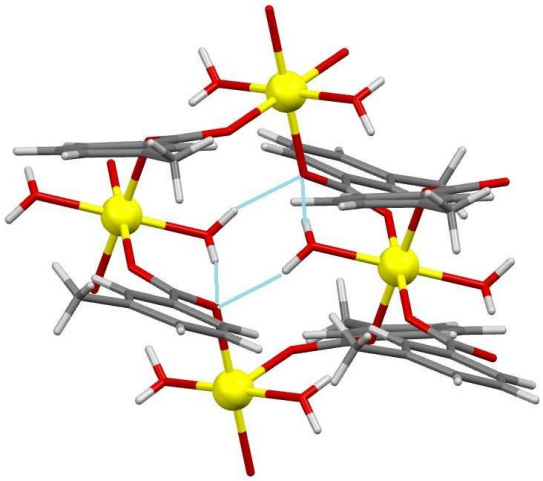

Figure S2. Hydrogen bonds between the water ligand and the carboxylate group.

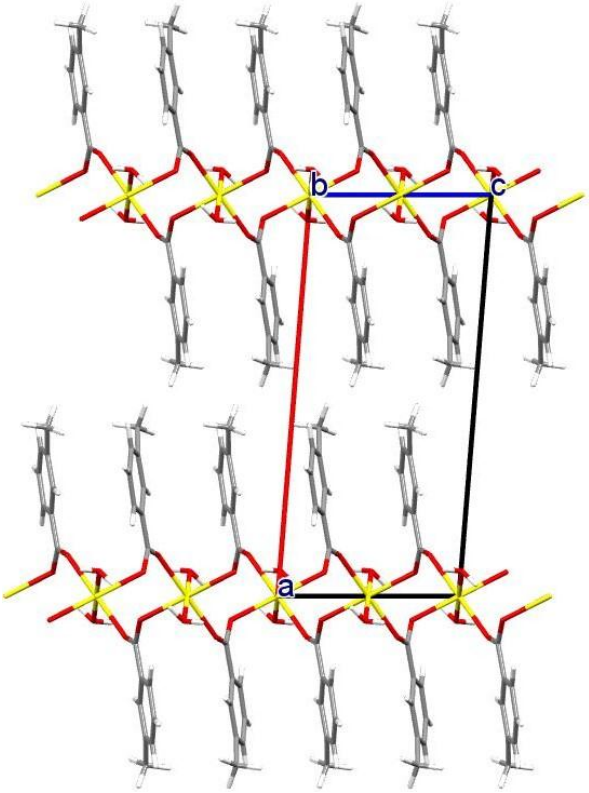

Figure S3. View down through crystallographic *b* axis of two layers of compound **1.**

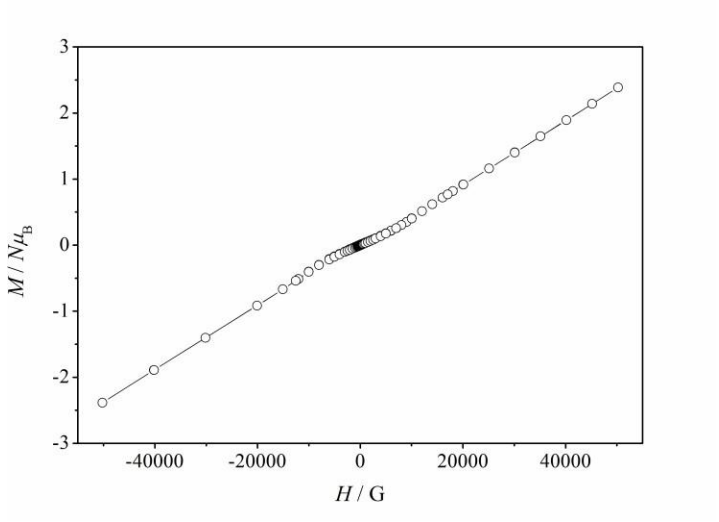

Figure S4. The whole field dependence of the magnetization of **1** between -50.2 to 50.2 kG at 2 K.

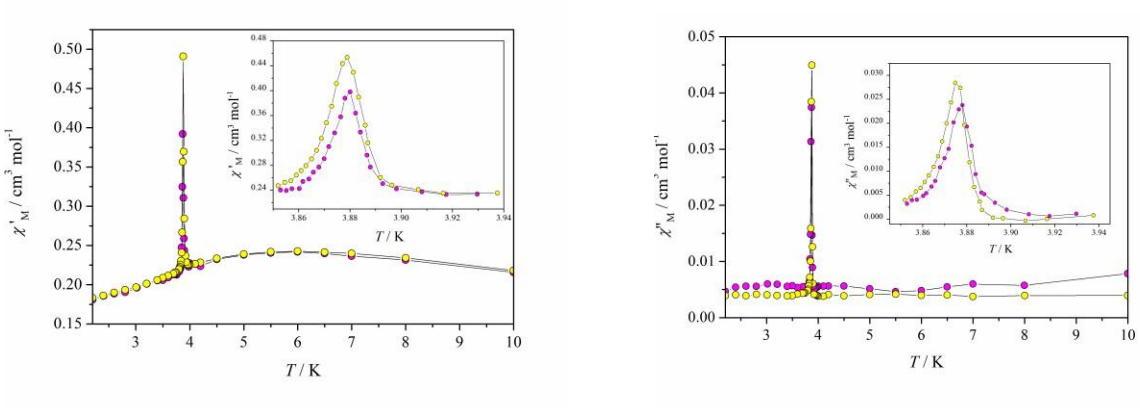

Figure S5. AC susceptibility measurements at 997 Hz (900 Hz in the inset) (yellow) and 10 Hz (magenta). Real (χ'_M) and imaginary (χ''_M) AC susceptibility components are shown in the left and right respectively.

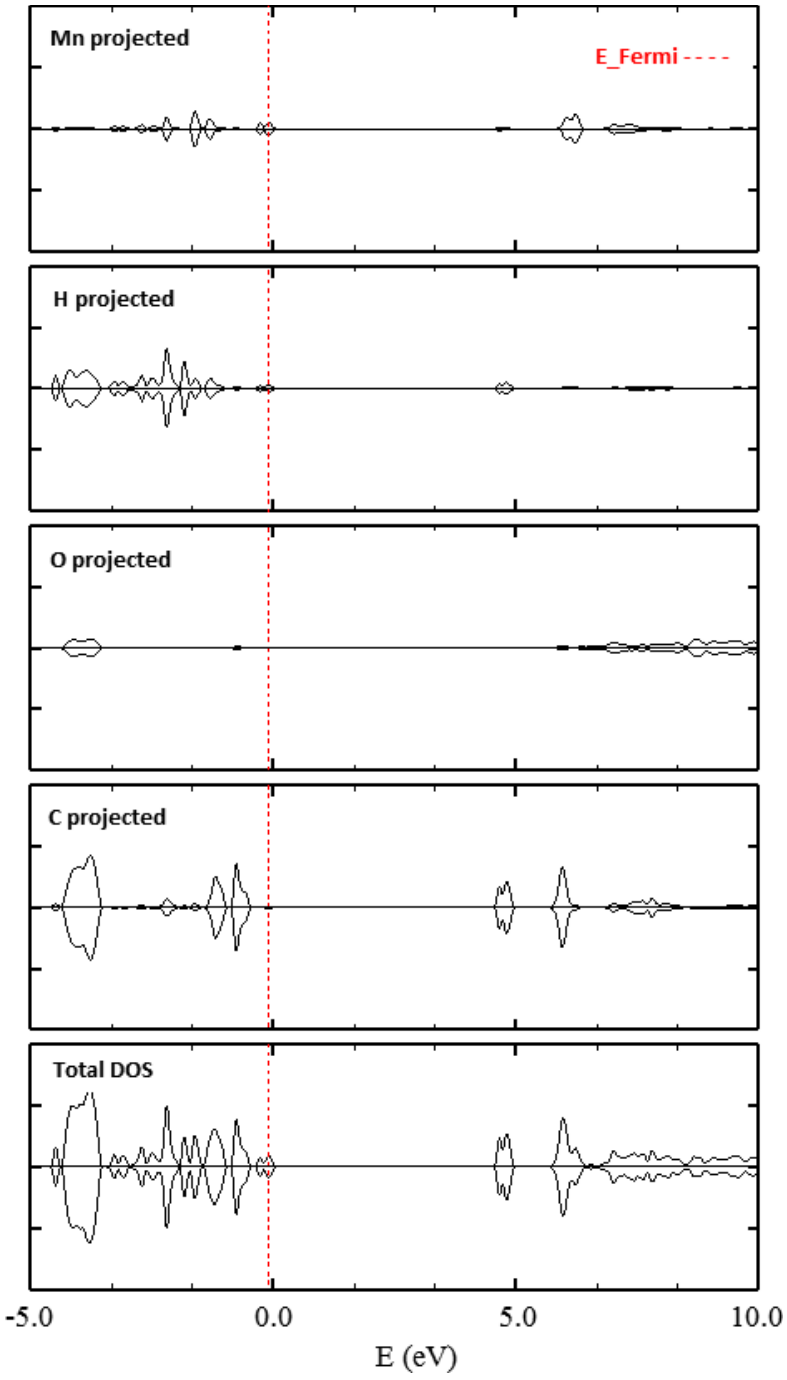

Figure S6. Total and atom projected density of states (DOS, arb. units) for AF ground state of compound **1** obtained using B3LYP functional and all electron basis sets. E_F is set at 0.0 eV.

Table S1. X-ray Crystallographic Data for compound crystallographic data collection and structure refinement details for compound $[Mn(3\text{-}MeC_6H_4COO)_2(H_2O)_2]$ (**1**).

chemical formula	$C_{16}H_{18}MnO_6$
formula weight /g mol^{-1}	361.24
T / K	100(2)
λ (Mo Kα) / Å	0.71073
crystal system	$P2_1/c$ (No. 14)
space group	Monoclinic
crystal size / mm	0.1 x 0.1 x 0.2
a / Å	16.057(2)
b / Å	6.8909(9)
c / Å	7.2259(10)
β / deg.	94.608(5)
V / $Å^3$	796.94(18)
Z	2
ρ_{calcd} / g cm^{-3}	1.505
μ / mm^{-1}	0.856
F(000)	374
Θ range / deg.	2.5 to 24.7
limiting indices	h = -18→18, k = -8→8, l = -7→8
data / restraints / parameters	1361 / 103 / 143
goodness-of-fit on F^2	1.081
final R indices [$I>2\sigma(I)$]	$R1_a$= 0.0425, $\omega R2_b$= 0.1016
R indices (all data)	$R1_a$= 0.0589, $\omega R2_b$= 0.1130

[a] $R1 = \sum(||F_o| - |F_c||)/\sum|F_o|$. [b] $\omega R2 = \{\sum[\omega(F_o^2 - F_c^2)^2] / \sum[\omega(F_o^2)^2]\}^{1/2}$, $\omega = 1/[\sigma^2(F_o^2) + (0.0675P)^2 + 1.4805P]$, where $P = (F_o^2+2F_c^2) / 3$.