Electronic Supplementary Material (ESI) for Dalton Transactions

Supporting information

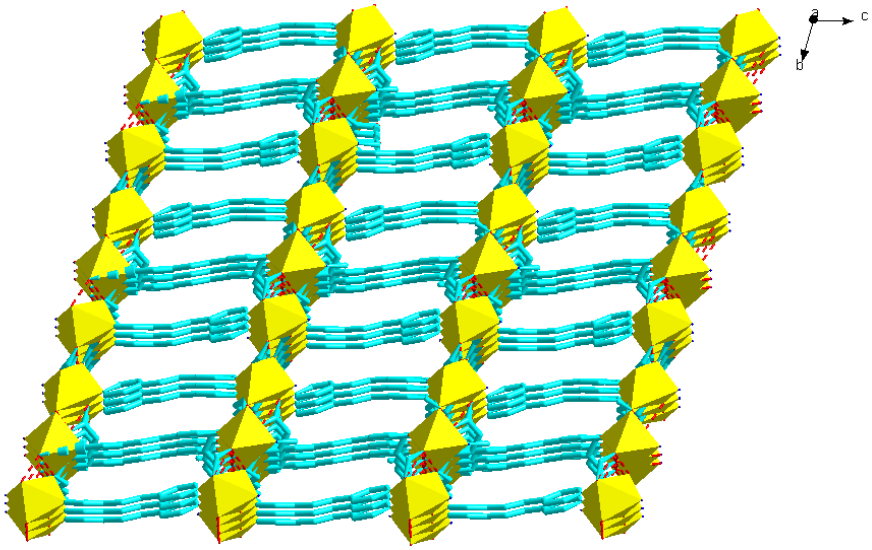

Fig S1. The 3D supermolecular strucuture constructed by the 2D network *via* the hydrogen bond.

Fitted equations of magnetism

The best fits above 40 K was fitted based on the Hamiltonian $H = -2J(S_1S_2 + S_2S_{1A})$

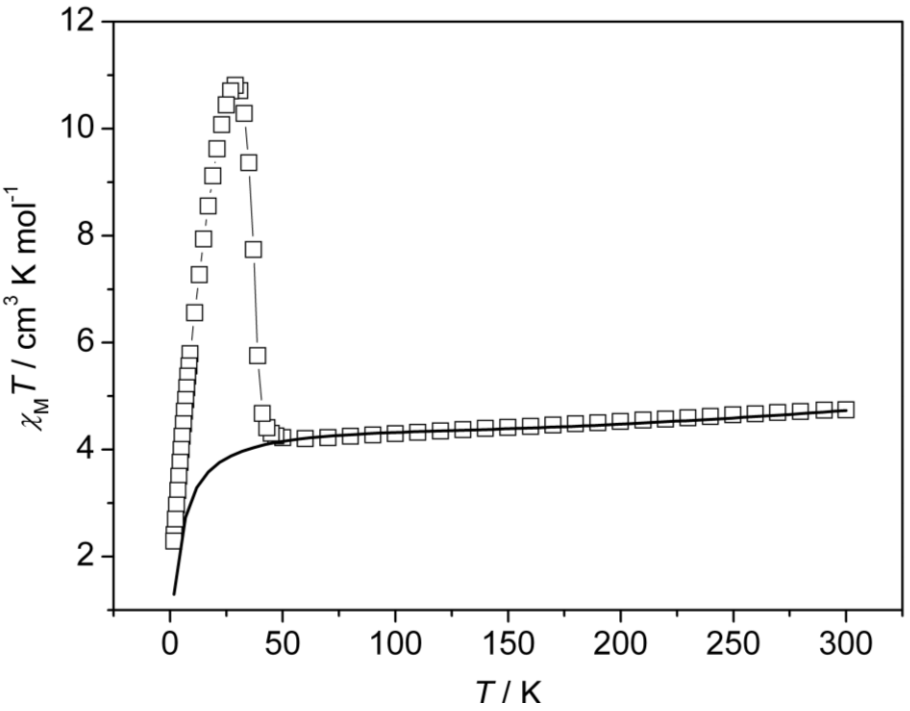

Figure S2. χ_MT plot of **1**. The solid lines represent the best fit obtained from the Hamiltonian given in the text.

Result of IR

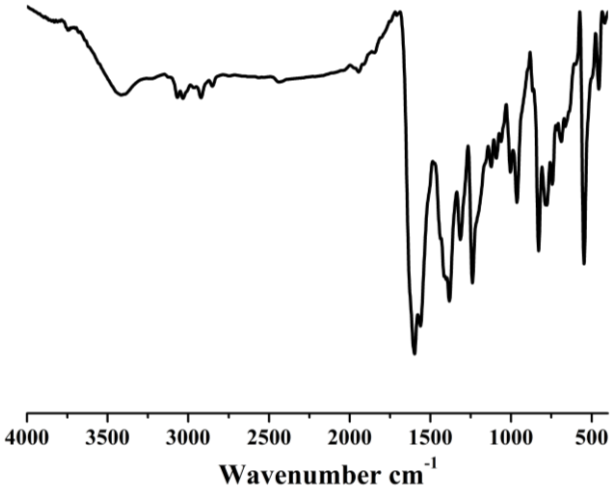

Fig S3. The IR of complex **1**.

Result of TGA and X-ray powder diffraction of 1

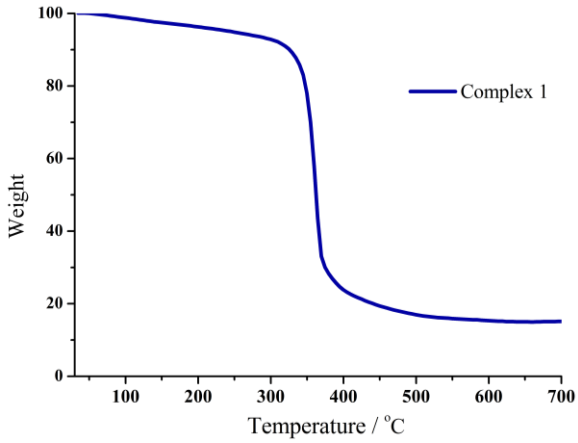

Fig S4. The TGA curve of complex **1**

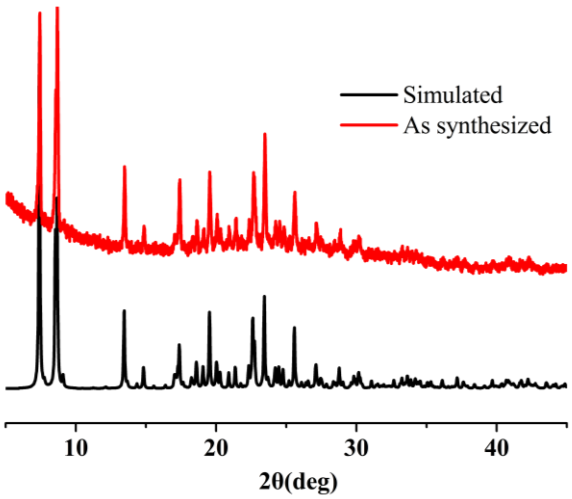

Fig S5. Comparison of XRPD patterns of the simulated pattern from the single-crystal structure determination and the as-synthesized of compound **1**.

Table 1. Crystal data and structure refinement information for complexes **1**(296K) **and 1'**(100K)

1		**1'**	
Formula	$C_{78}H_{54}Mn_3N_8O_{14}$	Formula	$C_{78}H_{54}Mn_3N_8O_{14}$
Fw	1492.11	Fw	1492.11
Temp (K)	296(2)	Temp (K)	100(2)
Cryst system	Triclinic	Cryst system	Triclinic
Space group	*P*$\bar{1}$	Space group	*P*$\bar{1}$
a (Å)	11.4021(15)	a (Å)	11.313(2)
b (Å)	11.888(3)	b (Å)	11.826(2)
c (Å)	13.5025(16)	c (Å)	13.416(3)
α (°)	103.486(3)	α (°)	103.917(4)
β (°)	112.845(2)	β (°)	112.404(3)
γ (°)	93.903(3)	γ (°)	93.820(3)
V (Å^3)	1614.3(5)	V (Å^3)	1585.4(5)
Z	1	Z	1
F (000)	765	F (000)	765
D_c(g/cm^3)	1.535	D_c(g/cm^3)	1.563
GOF	0.980	GOF	1.836
R_1^{α}(I>2σ(I))	0.0639	R_1^{α}(I>2σ(I))	0.0947
${}_wR_2^{\alpha}$ (all data)	0.2131	${}_wR_2^{\alpha}$ (all data)	0.3351

[a] $R_1=\sum||F_0|-|F_c||/\sum|F_0|$. [b] ${}_wR_2=\{\sum[w(F_0^2-F_c^2)^2]/\sum(F_0^2)^2\}^{1/2}$

Table 2. The contradistinction to the 1(296K) and 1'(100K) of selected bond distances (Å) and angles (°)

1		**1'**	
Mn(1)-O(4)	2.219(4)	Mn(1)-O(4)	2.214(7)
Mn(1)-O(6)	2.099(4)	Mn(1)-O(6)	2.101(6)
Mn(1)-N(3)	2.295(5)	Mn(1)-N(3)	2.294(8)
Mn(2)-O(1)#4	2.174(4)	Mn(2)-O(1)#2	2.188(6)
Mn(2)-O(2)	2.182(4)	Mn(2)-O(2)	2.195(7)
Mn(2)-O(4)	2.372(4)	Mn(2)-O(4)	2.335(7)
Mn(2)-O(5)#3	2.246(5)	Mn(2)-O(5)#1	2.261(7)
Mn(2)-N(1)	2.253(5)	Mn(2)-N(1)	2.254(8)
Mn(2)-N(2)#5	2.305(5)	Mn(2)-N(2)#3	2.304(8)
O(6)#3-Mn(1)-O(6)	180.0	O(6)#1-Mn(1)-O(6)	180.0
O(6)-Mn(1)-O(4)	94.62(17)	O(6)-Mn(1)-O(4)	94.7(3)
O(6)-Mn(1)-O(4)#3	85.38(17)	O(6)-Mn(1)-O(4)#1	85.3(3)
O(6)-Mn(1)-N(3)	87.81(18)	O(6)-Mn(1)-N(3)	87.6(3)
O(4)-Mn(1)-N(3)	85.99(17)	O(4)-Mn(1)-N(3)	86.5(3)
O(6)-Mn(1)-N(3)#3	92.19(18)	O(6)-Mn(1)-N(3)#1	92.4(3)
O(4)#3-Mn(1)-O(4)	180.0(2)	O(4)-Mn(1)-O(4)#1	180.0
O(4)-Mn(1)-N(3)#3	94.01(17)	O(4)-Mn(1)-N(3)#1	93.5(3)
N(3)#3-Mn(1)-N(3)	180.0(3)	N(3)-Mn(1)-N(3)#1	180.0(4)
O(1)#4-Mn(2)-O(2)	94.80(16)	O(1)#2-Mn(2)-O(2)	94.3(2)
O(1)#4-Mn(2)-O(5)#3	78.25(17)	O(1)#2-Mn(2)-O(5)#1	77.5(3)
O(1)#4-Mn(2)-N(1)	83.98(17)	O(1)#2-Mn(2)-N(1)	83.4(3)
O(2)-Mn(2)-O(5)#3	170.82(16)	O(2)-Mn(2)-O(5)#1	169.7(2)
O(2)-Mn(2)-N(1)	92.22(18)	O(2)-Mn(2)-N(1)	92.8(3)
O(5)#3-Mn(2)-N(1)	92.97(19)	O(5)#1-Mn(2)- N(1)	92.5(3)
O(1)#4-Mn(2)-N(2)#5	92.25(17)	O(1)#2-Mn(2)-N(2)#3	92.7(3)
O(2)-Mn(2)-N(2)#5	91.41(17)	O(2)-Mn(2)-N(2)#3	92.1(3)
O(5)#3-Mn(2)-N(2)#5	82.98(19)	O(5)#1-Mn(2)-N(2)#3	82.1(3)

N(1)-Mn(2)-N(2)#5	174.97(19)	N(1)-Mn(2)-N(2)#3	174.0(3)
O(1)#4-Mn(2)-O(4)	168.59(15)	O(1)#2-Mn(2)-O(4)	167.9(3)
O(2)-Mn(2)-O(4)	75.29(14)	O(2)-Mn(2)-O(4)	75.3(2)
O(5)#3-Mn(2)-O(4)	112.19(15)	O(5)#1-Mn(2)-O(4)	113.5(2)
N(1)-Mn(2)-O(4)	90.67(16)	N(1)-Mn(2)-O(4)	90.9(3)
N(2)#5-Mn(2)-O(4)	93.62(17)	N(2)#3-Mn(2)-O(4)	93.8(3)
Mn(1)-O(4)-Mn(2)	112.38(17)	Mn(1)-O(4)-Mn(2)	112.4(3)