Synthesis, Structural, and Investigation of Unique Magnetic Properties in Two novel Mn-Based Coordination Polymers

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Table S1. Crystal data and structure refinement parameters of **1**

Compound	**1**
Formula	$C_{30}H_{18}MnN_4O_4$
Formula weight	553.42
Temperature (*K*)	193.0
Crystal system	Monoclinic
Space group	*P*2/n
a (Å), *b* (Å), *c* (Å)	7.9590(6), 10.7872(8), 29.582(2)
α (°), β (°), γ (°)	90, 93.461(4), 90
V (Å^3)	2535.1(3)
Z	4
*D*calc (Mg m^{-3})	1.450
μ (mm^{-1})	3.146
F (000)	1132.0
Crystal size (mm)	0.12× 0.1× 0.1
2θ range (°)	7.59 to 120.092
Index ranges	-10 ≤h ≤9
	-13 ≤K ≤13
	-38 ≤L ≤37
Reflections collected	24117
Independent reflection	5632 [R_{int} = 0.0558]
Data/restraints/parameters	5632/126/398
Final R_1, wR_2 indices [$I > 2\sigma(I)$]	0.0360, 0.0876
R_1, wR_2 indices (all data)	0.0500, 0.0943
*GO*F	1.032
$\Delta r_{max,min}$ (*e* Å^{-3})	0.26/-0.47

Table S1. Crystal data and structure refinement parameters of **2**

Compound	**2**
Formula	$C_{24}H_{17}MnN_4O_5$
Formula weight	496.35
Temperature (*K*)	173.0
Crystal system	triclinic
Space group	*P*-1
a (Å), *b* (Å), *c* (Å)	9.5840(2), 10.5520(3), 11.7635(3)
α (°), *β* (°), *γ* (°)	93.8320(10), 111.2460(10), 108.9600(10)
V (Å^3)	1025.39(5)
Z	2
*D*calc (Mg m^{-3})	1.608
μ (mm^{-1})	5.653
F (000)	508.0
Crystal size (mm)	0.25× 0.23× 0.21
2θ range (°)	10.51 to 144.192
Index ranges	-11 ≤h ≤11
	-13 ≤K ≤13
	-14 ≤L ≤14
Reflections collected	12217
Independent reflection	3960 [R_{int} = 0.0381]
Data/restraints/parameters	3960/27/357
Final R_1, wR_2 indices [I> 2σ (I)]	0.0299,0.0763
R_1, wR_2 indices (all data)	0.0327,0.0786
*GO*F	1.049
$\Delta r_{max,min}$ (*e* Å^{-3})	0.37/-0.21

Table S3. Bond length (Å) and bond angle (°) of **1**

1					
Mn1-O(3)	2.1025(13)	Mn1-O(1)#1	2.2670(13)	Mn1-O(4)#2	2.1156(12)
Mn1-O(2)#1	2.2638(12)	Mn1-N(1)	2.2638(15)	Mn1-N(2)	2.2658(15)
O(3)-Mn(1)-O(1)#1		148.33(5)	O(3)-Mn(1)-O(4)#2		95.73(5)
O(3)-Mn(1)-O(2)#1		91.47(5)	O(3)-Mn(1)-N(1)		85.13(5)
O(2)#1-Mn(1)-N(1)		144.08(5)	O(4)#2-Mn(1)-O(1)#1		100.34(5)
O(4)#2-Mn(1)-O(2)#1		105.09(7)	O(4)#2-Mn(1)-N(1)		95.02(5)
O(4)#2-Mn(1)-N(2)		166.33(5)	O(2)#1-Mn(1)-O(1)#1		58.09(7)
O(2)#1-Mn(1)-N(2)		88.51(5)	N(2)-Mn(1)-O(1)#1		85.52(5)
N(2)-Mn(1)-N(1)		72.54(5)			

Symmetry codes for #1: 2-x, 1-y, 1-z; #2: 3/2-x, +y, 1/2-z.

Table S4. Bond length (Å) and bond angle (°) of **2**

2					
Mn1-O(2)#1	2.1475(12)	Mn1-O(1)	2.1010(12)	Mn1-O(5)	2.1634(13)
Mn1-O(4)#2	2.3104(12)	Mn1-O(3)#2	2.2430(14)	Mn1-N(1)#3	2.3351(14)
O(2)#1-Mn(1)-O(5)		167.45(5)	O(2)#1-Mn(1)-O(4)#2		88.12(5)
O(2)#1-Mn(1)-O(3)#2		91.03(5)	O(2)#1-Mn(1)-N(1)#3		84.46(5)
O(1)-Mn(1)-O(2)#1		102.29(5)	O(1)-Mn(1)-O(5)		88.41(5)
O(1)-Mn(1)-O(4)#2		154.51(5)	O(1)-Mn(1)-O(3)#2		98.46(5)
O(1)-Mn(1)-N(1)#3		110.07(5)	O(5)-Mn(1)-O(4)#2		84.77(5)
O(5)-Mn(1)-O(3)#2		93.88(6)	O(5)-Mn(1)-N(1)#3		85.72(5)
O(4)#2-Mn(1)-N(1)#3		93.90(5)	O(3)#2-Mn(1)-O(4)#2		57.69(5)
O(3)#2 -Mn(1)-N(1)#3		151.43(5)			

Symmetry codes for #1: 2-x, 2-y, 2-z; #2: 2+x, 1+y, 1+z; #3: 1+x, 1+y, +z.

Table S5. Structural parameters of π…π interactions of **1**.

π···π	α	DC	β	DZ
Cg(4)···Cg(4)#1	4.29(9)	3.6206(9)	18.2	3.4393(7)
Cg(9)···Cg(10)#2	6.31(9)	3.6379(5)	22.4	-3.4860(4)
Cg(8)···Cg(8)#3	2.93(9)	3.6884(12)	22.9	-3.3974(8)
Cg(4)···Cg(8)#3	3.85(11)	3.7165(11)	24	-3.4869(7)
Cg(4)···Cg(5)#3	3.43(8)	3.7519(11)	20.1	-3.4803(7)
Cg(3)···Cg(4)#3	5.92(7)	3.7846(9)	24.2	-3.5637(6)
Cg(3)···Cg(3)#3	7.49(6)	3.8060(9)	20.1	-3.5745(6)
Cg(9)···Cg(2)#4	1.88(8)	4.1994(10)	36.7	-3.4465(7)
Cg(3)···Cg(8)#3	5.25(8)	4.4003(11)	40.6	-3.5405(6)
Cg(4)···Cg(4)#3	4.29(8)	4.4789(10)	39.6	-3.4497(7)
Cg(3)···Cg(4)#1	5.92(7)	4.7630(10)	43.2	3.3253(6)
Cg(4)···Cg(8)#1	3.85(8)	4.8731(11)	44.2	3.4942(7)
Cg(3)···Cg(5)#3	4.70(8)	5.0108(11)	46	-3.5075(6)
Cg(5)···Cg(8)#3	2.33(9)	5.0496(12)	47.8	-3.4641(8)
Cg(6)···Cg(6)#2	0.03(13)	5.3509(16)	42	-3.9795(11)
Cg(6)···Cg(6)#2	0.03(13)	5.3509(16)	52.6	3.939(8)
Cg(9)···Cg(4)#4	19.8	5.3160(11)	81.1	5.0005(7)
Cg(10)···Cg(10)#4	0.02(9)	5.7653(12)	44.9	4.0861(8)

α: dihedral angle between mean planes of the rings (°), DC: distance between ring centroids (nm), β: angle between DC vector and normal to plane (I) (°), DZ: perpendicular distance of the centroids of ring(I) on plane of ring(II) (nm). Symmetry codes: #1 5/2-x, y, 1/2-z; #2 1-x, 1-y, 1-z, #3: 3/2-x, y, 1/2-z, #4: 1+x, y, z, #5: 1-x, 2-y, 1-z, #6: 1+x, -1+y, z. Rings: Cg(2): O1, C30, O2, Mn1; Cg(3): Mn1, N1, C5, C6, N2; Cg(4): N1, C1, C2, C3, C4, C5; Cg(5): N2, C6, C7, C10, C11, C12; Cg(6): N3, C20, C21, N4, C22 C23; Cg(8): C4, C5, C6, C7, C8, C9; Cg(9): C14, C15, C16, C17, C18, C19; Cg(10): C24, C25, C26, C27, C28, C29.

Table S6. Structural parameters of π…π interactions of **2**.

π···π	α	DC	β	DZ
Cg(2)···Cg(3)#1	14.55(9)	4.5999(11)	41.6	3.5008(7)
Cg(3)···Cg(2)#1	14.55(9)	5.5120(11)	50.7	-3.4931(7)
Cg(4)···Cg(4)#2	0.00(8)	4.244(12)	22.0	3.9341(8)
Cg(5)···Cg(3)#1	11.4(3)	3.745(3)	19.9	3.647(3)
Cg(5)···Cg(5)#1	0.00(4)	4.850(5)	43	3.547(4)
Cg(5)···Cg(5)#3	0.00(12)	5.410(5)	38.2	-4.251(3)
Cg(7)···Cg(4)#4	13.88(11)	4.1329(13)	29.5	-3.0020(9)

α: dihedral angle between mean planes of the rings (°), DC: distance between ring centroids (nm), β: angle between DC vector and normal to plane (I) (°), DZ: perpendicular distance of the centroids of ring(I) on plane of ring(II) (nm), S: distance between ring centroid(I) and perpendicular projection of ring centroid(II) on ring (I) (nm). Symmetry codes: #1 -x, -y, 1-z; #2 1-x, 1-y, 2-z; #3 -1-x, -y, 1-z. Rings: Cg(2): Mn1, O3, C18, O4; Cg(3): N1, C9, C8, N2, C11, C10; Cg(4): C2, C3, C4, C5, C6, C7; Cg(5): C12, C13, C14, C15, C16, C17; Cg(7): N3, C19, N4, C21, C20.

Table S7. Hydrogen bond parameters of **1** and **2**.

D−H···A	d(D−H)/Å	d(H···A)/Å	d(D···A)/Å	∠DHA / (°)
		1		
C1−H1···O1	0.95	2.45	3.192(2)	135
		2		
O5−H5A···O4#1	0.85(3)	1.85(3)	2.695(2)	174(2)
O5−H5B···N3#1	0.848(17)	1.895(19)	2.734(2)	171(3)
C4−H4···O5#2	0.95	2.51	3.368(2)	150)s
C7−H7···O4#3	0.95	2.42	3.301(2)	154)s

Symmetry codes: ; #1: 1/2+x, 1-y, -1/2-z for **1**. #1: -1+x, -1+y, z; #2: 2-x, 1-y, 2-z; #3: -x, 1-y, 1-z for **2**

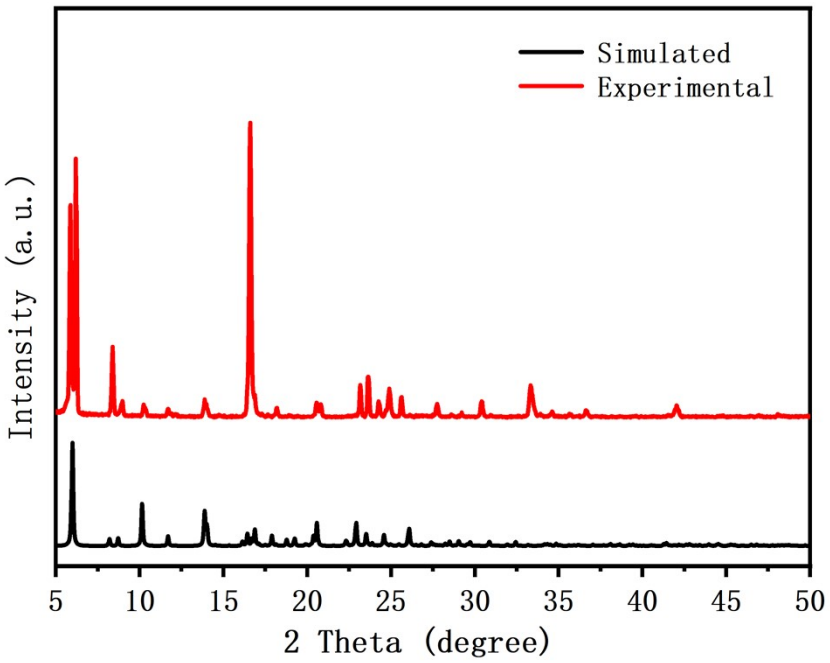

Figure S1. PXRD simulation pattern of **1**, PXRD pattern of **1**.

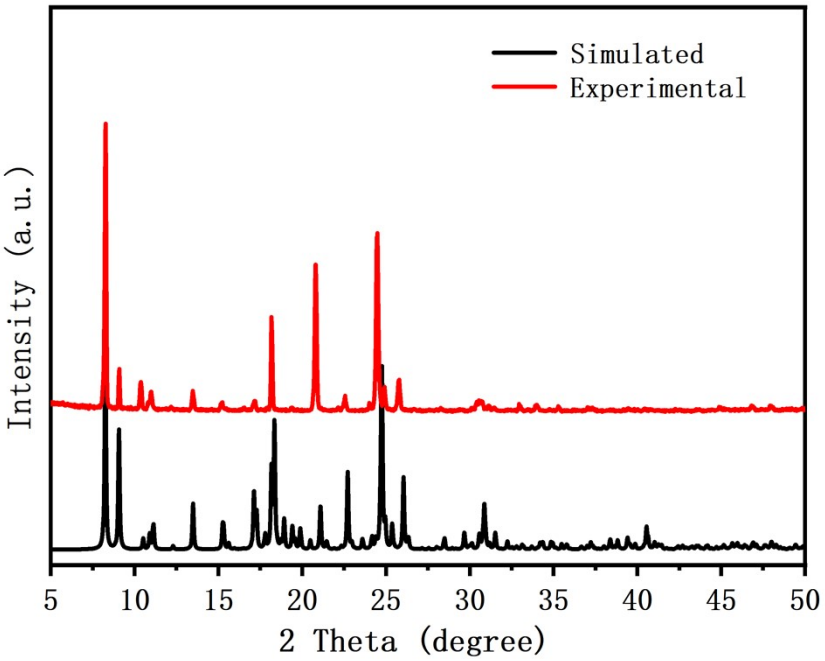

Figure S2. PXRD simulation pattern of **2**, PXRD pattern of **2**.

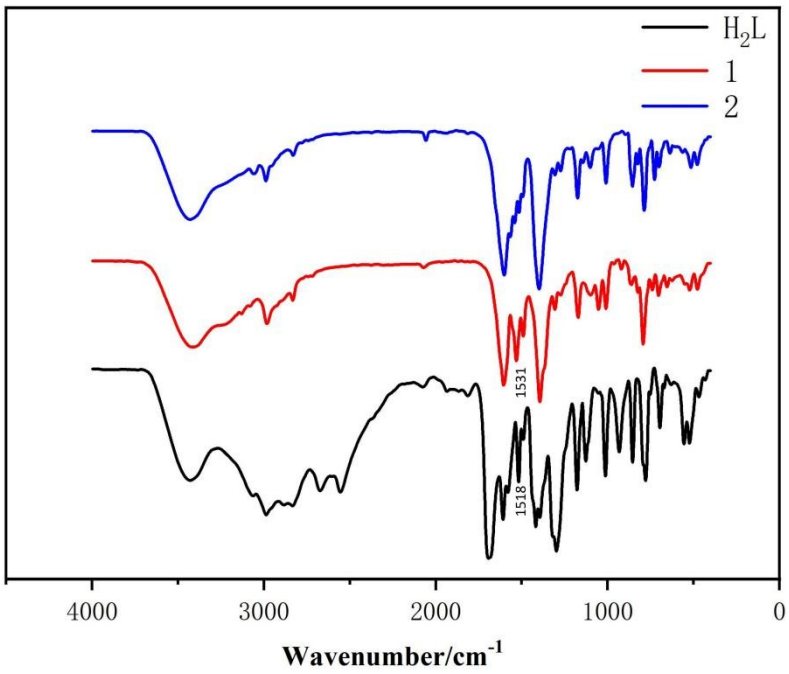

Figure S3. FT-IR of H_2L, **1** and **2**.

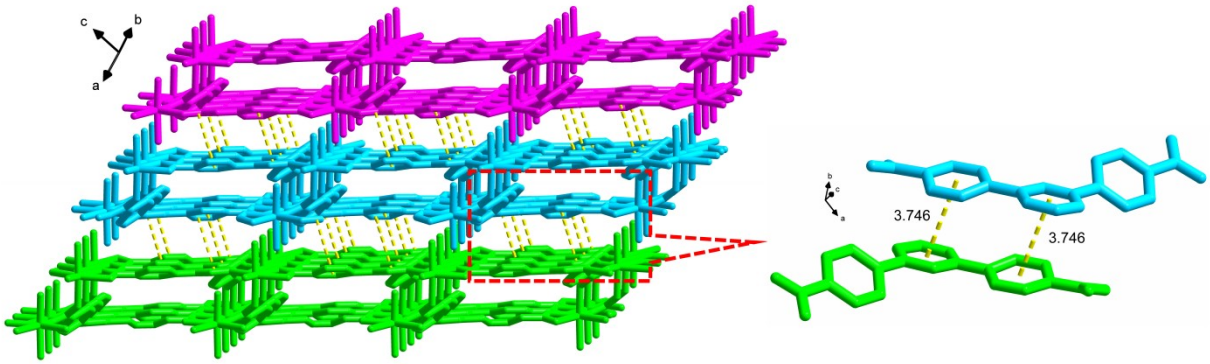

Figure S4. The 3D structure of **2** and π···π stacking interactions.

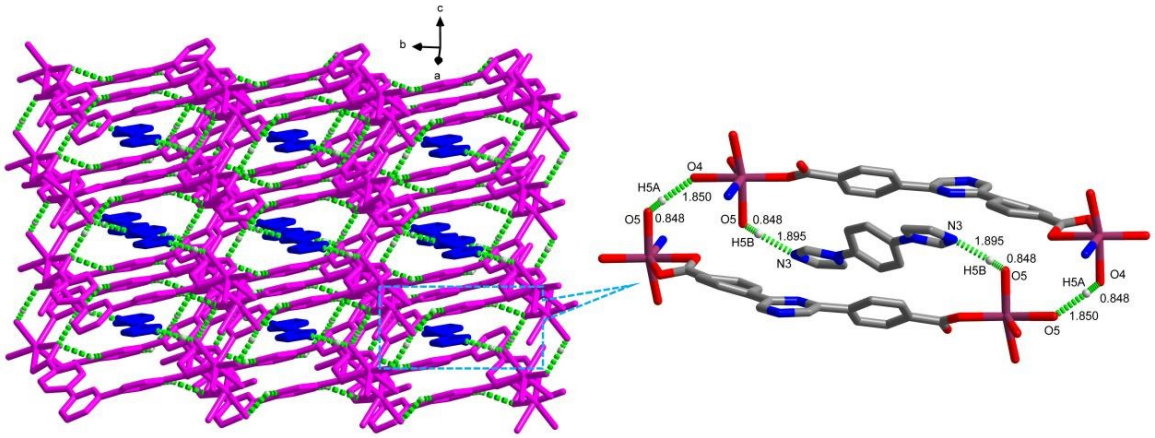

Figure S5. hydrogen bond between **2** and dib.

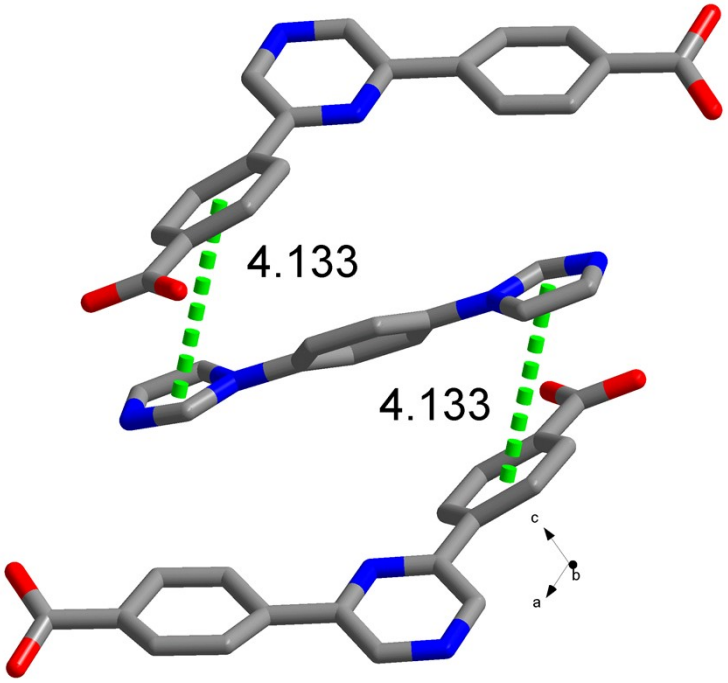

Figure S6. π···π stacking interactions between **2** and dib.