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Actylenedicarboxylato bridged Mn(II)-based 1D coordination polymer: electrochemical CO_2 reduction and magnetic properties

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Supporting Information

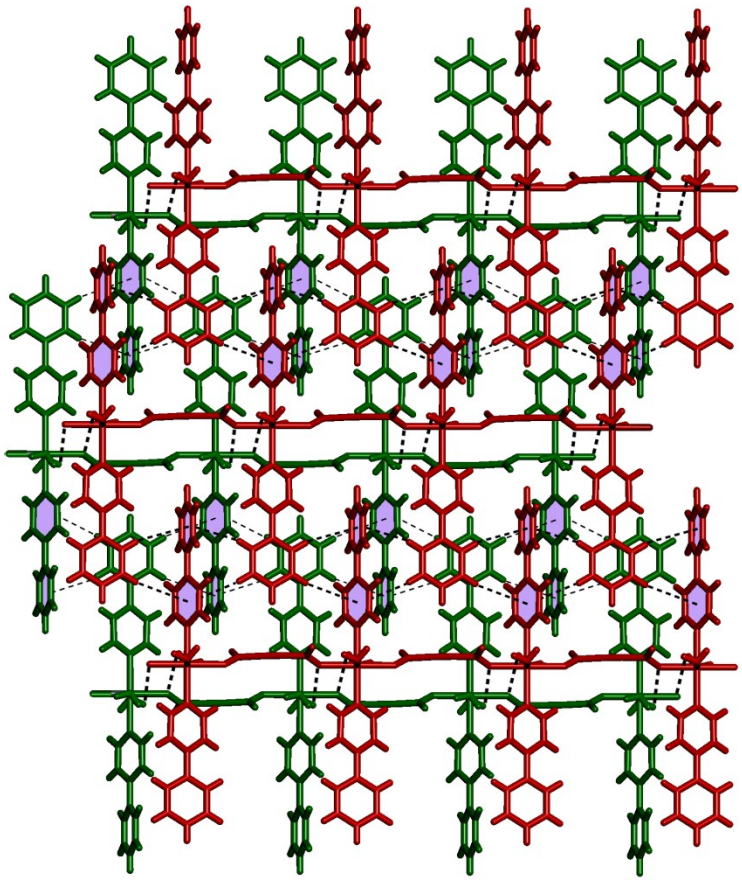

Fig. S1 3D supramolecular architecture of compound **1** generated by intermolecular hydrogen bonding and C–H···π interactions.

Table S1 Crystal data and refinement parameters for compound **1**

Formula	$C_{26}H_{22}MnN_2O_6$
Fw	512.95
crystsyst	triclinic
space group	*C*2/*c*
a (Å)	9.9338(6)
b (Å)	27.9007(17)
β(deg)	115.055(2)
γ (deg)	64.936(2)
V (Å^3)	2376.5(2)
Z	4
D_{calcd}(g/cm^3)	1.434
μ(mm^{-1})	0.596
λ(Å)	0.71073
data[$I > 2\sigma(I)$]/params	2072/202
GOF on F^2	1.109
final *R* indices[$I > 2\sigma(I)$][a,b]	*R*1 = 0.0769
	*wR*2 = 0.2228

[a] $R1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$, [b] $wR2 = [\Sigma w(F_o^2 - F_c^2)^2/\Sigma w(F_o^2)^2]^{1/2}$

Table S2 Selected bond lengths and bond angles in **1**

Mn(1)-O(2)	2.181(4)	O(5)-Mn(1)-N(1)	93.69(17)	O(2)-Mn(1)- N(1)	90.00(17)
Mn(1)-N(2)	2.269(4)	O(6)-Mn(1)-N(1)	93.66(17)	O(5)- Mn(1)-O(6)	172.66(16)
Mn(1)-O(5)	2.176(4)	N(1)-Mn(1)-N(2)	179.9(2)	O(5)-Mn(1)-O(4)b	88.35(15)
Mn(1)-O(4)b	2.181(4)	O(2)-Mn(1)-O(6)	88.44(17)	O(6)-Mn(1)-O(4)b	91.60(17)
Mn(1)-O(6)	2.177(5)	O(2)-Mn(1)-O(4)b	179.94(19)	N(2)-Mn(1)-O(4)b	89.96(17
Mn(1)-N(1)	2.292(6)	O(5) - Mn(1)-N(2)	86.32(17)	Mn(1)-O(2)C(23)	128.5(4)
O(2)-Mn(1)-O(5)	91.62(15)	O(6)-Mn(1)-N(2)	86.34(17)	Mn(1)-N(1)-C(5)	121.3(4)
O(2)-Mn(1)-N(2)	90.08(17)	N(1)-Mn(1)-O(4)b	89.96(17)	Mn(1)-N(2)-C(16)	121.8(4)

Symmetry Code: b = x, 1+y, z

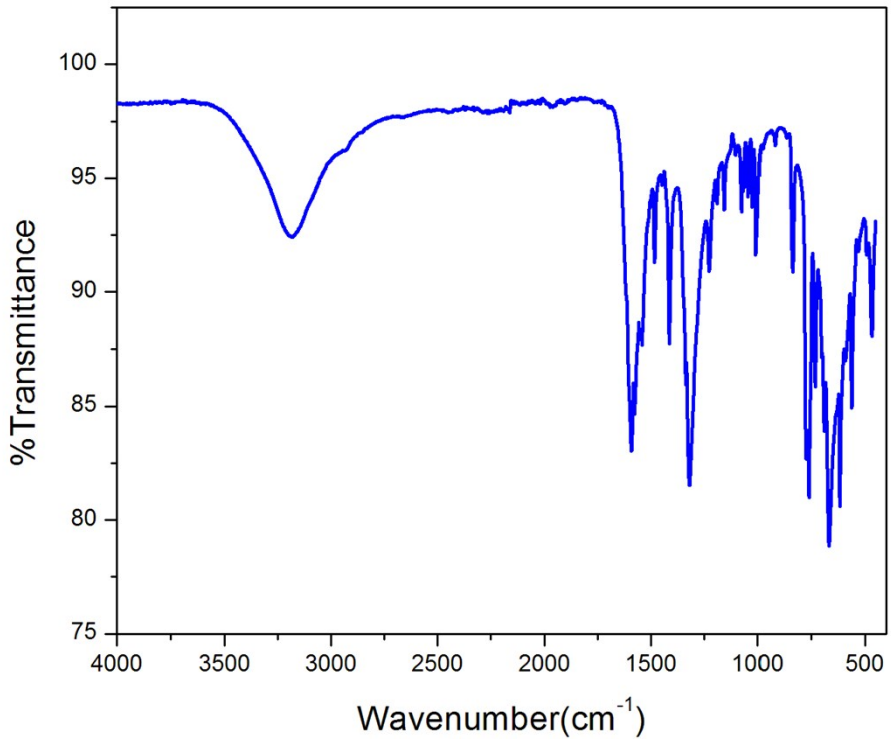

Fig. S2 FT-IR spectrum of compound **1**.