ELECTRONIC SUPPLEMENTARY INFORMATION

to

A new twist on an old ligand: a [Mn_{16}] double square wheel and a [Mn_{10}] contorted wheel

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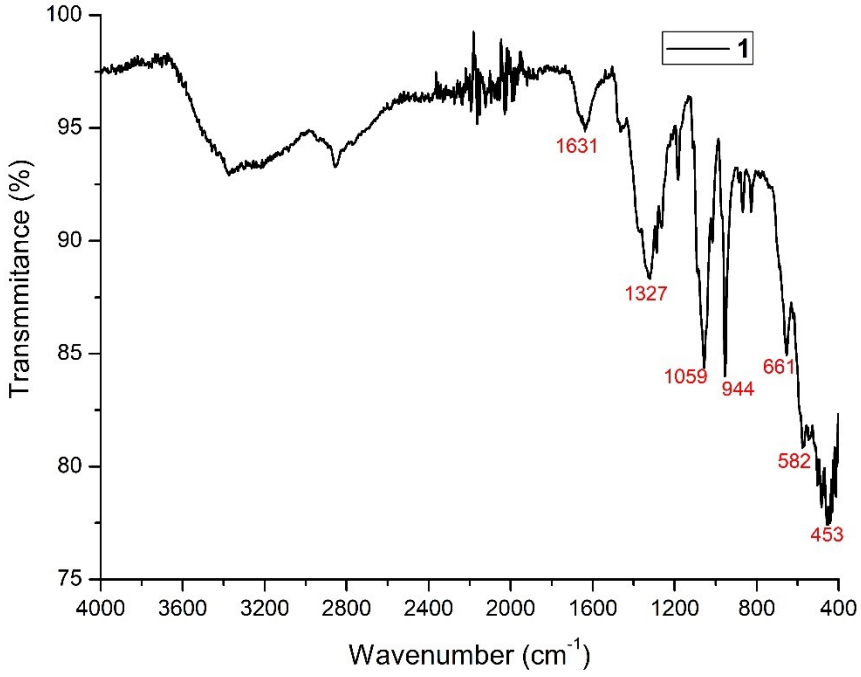
***Electronic Supplementary Information (ESI) contains*:**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Transmmitance (%)
Wavenumber (cm-1)
1631
1327
1059
944
661
582
453

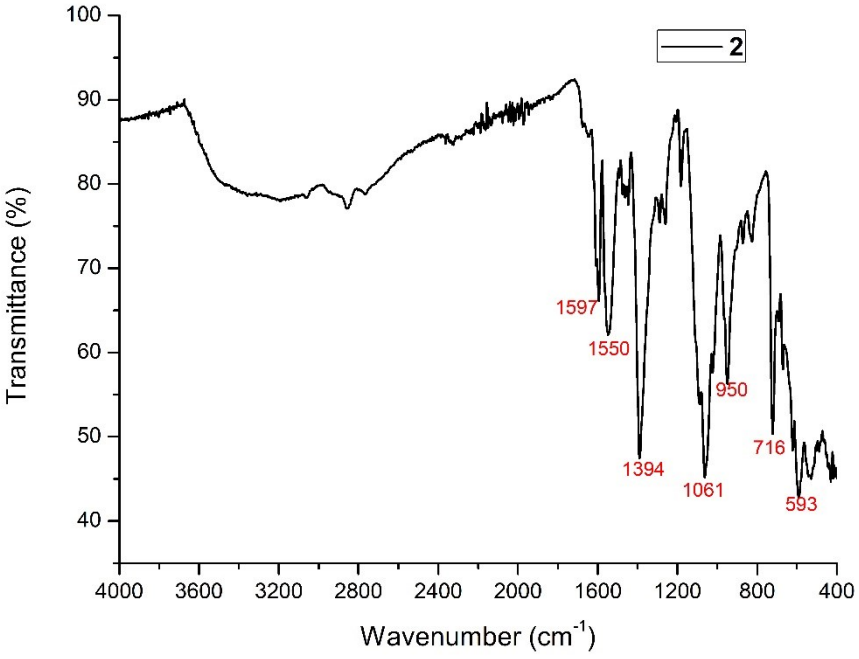
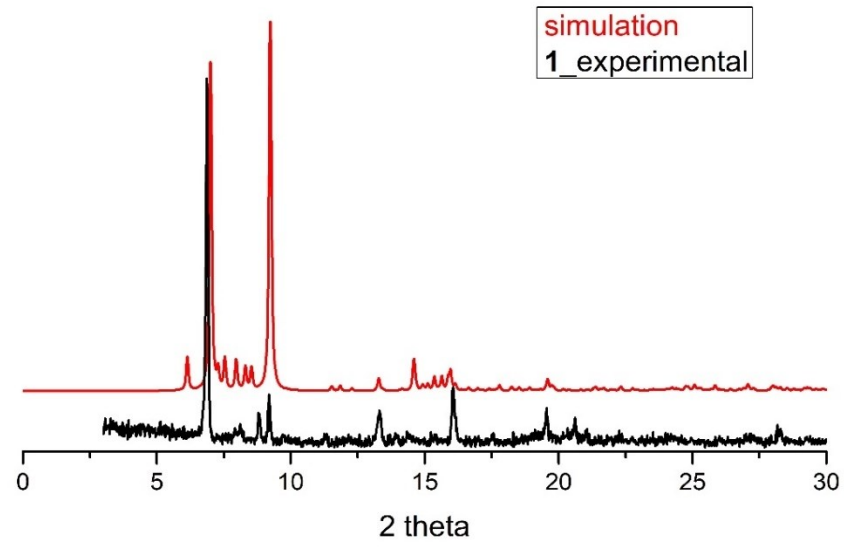
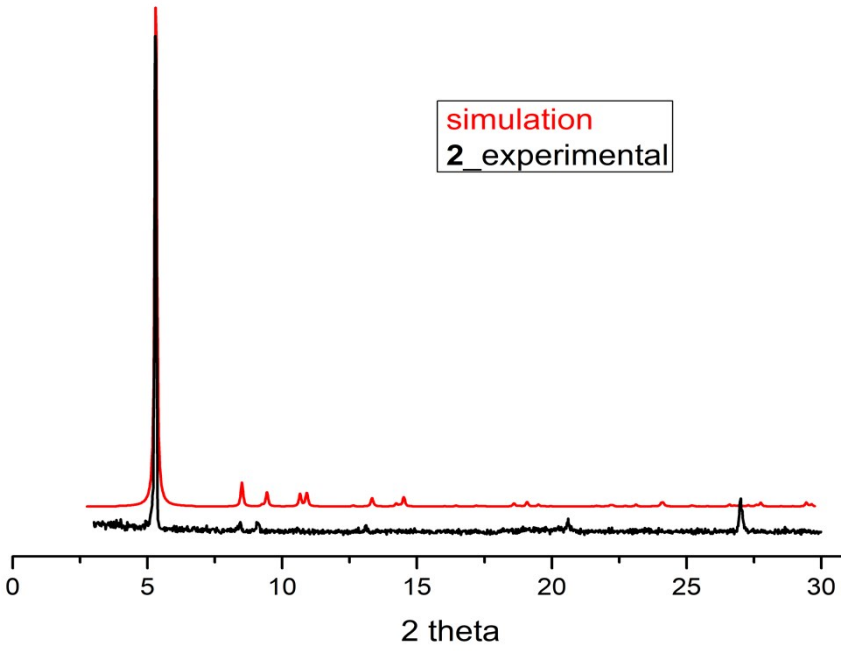

2
Transmittance (%)
Wavenumber (cm-1)
1597
1550
1394
1061
950
716
593

Fig S1. The FTIR-ATR spectra of **1** (top) and **2** (bottom).


simulation
1_experimental
0
5
10
15
20
25
30
2 theta


simulation
2_experimental
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5
10
15
20
25
30
2 theta

Fig S2. Powder XRD diagrams' comparison for **1** (top) and **2** (bottom) and their simulated pXRD diagram. The differences in the peaks' intensity are due to solvent loss and preferred crystal orientation.

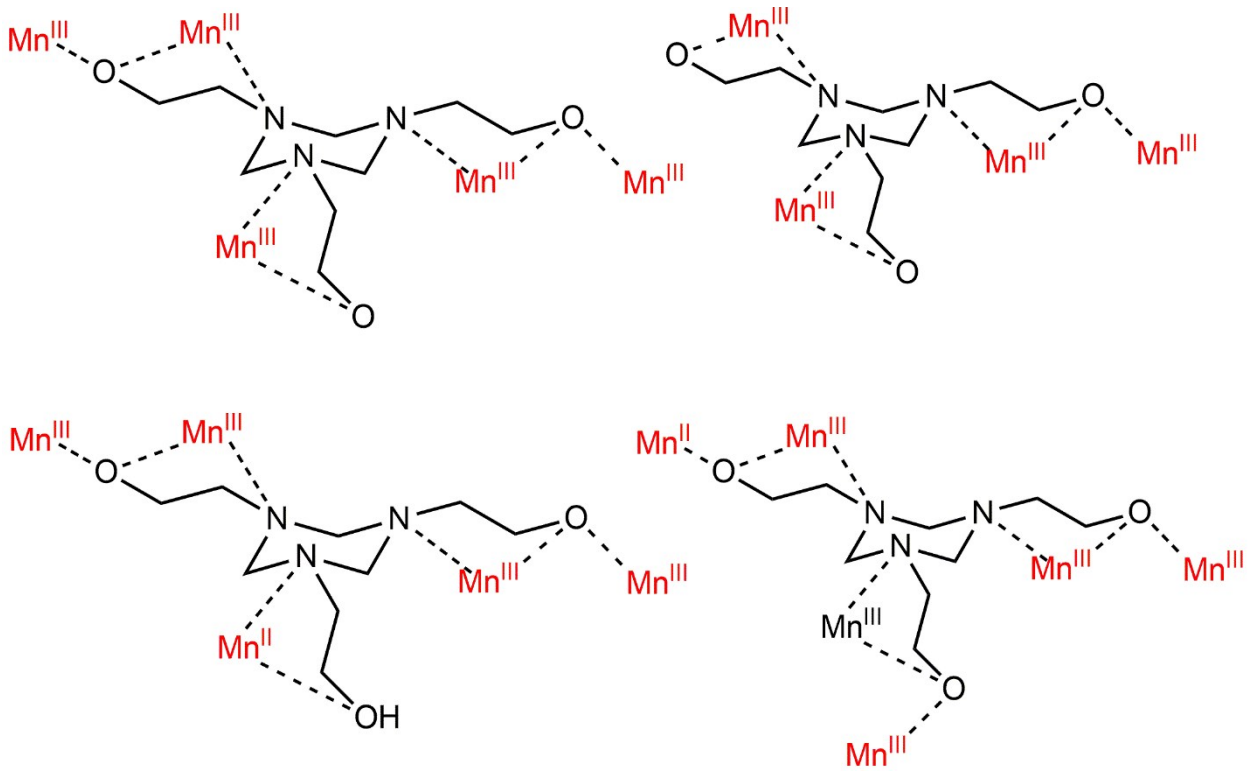

Fig S3. The coordination modes of the ligand in **1** and **2.**

Table S1. BVS calculations for the metallic centres in **1** and **2**.

1	Mn(II)	Mn(III)	Mn(IV)
Mn1	**2.18**	2.01	1.98
Mn5	**2.17**	2.00	1.96
Mn2	3.14	**2.90**	2.84
Mn3	3.34	**3.08**	3.02
Mn4	3.35	**3.11**	3.05
Mn6	3.31	**3.05**	2.99
Mn7	3.22	**2.98**	2.92
Mn8	3.20	**2.95**	2.90
2			
Mn1	3.34	**3.08**	3.02
Mn2	3.26	**3.01**	2.95
Mn3	3.36	**3.10**	3.04

Table S2. BVS calculations for the assignment of O^{2-}/OH^{-} in **1** and **2**.

1	Charge
O13	**-1.78**
O14	**-2.00**
O16	**-1.96**
O15	**-1.09**
2	
O5	**-2.03**
O7	**-0.97**