Electronic Supplementary Information (ESI)

Structural, electrochemical and magnetic analyses of a new octanuclear $Mn^{III}_2Mn^{II}_6$ cluster with linked-defect cubane topology

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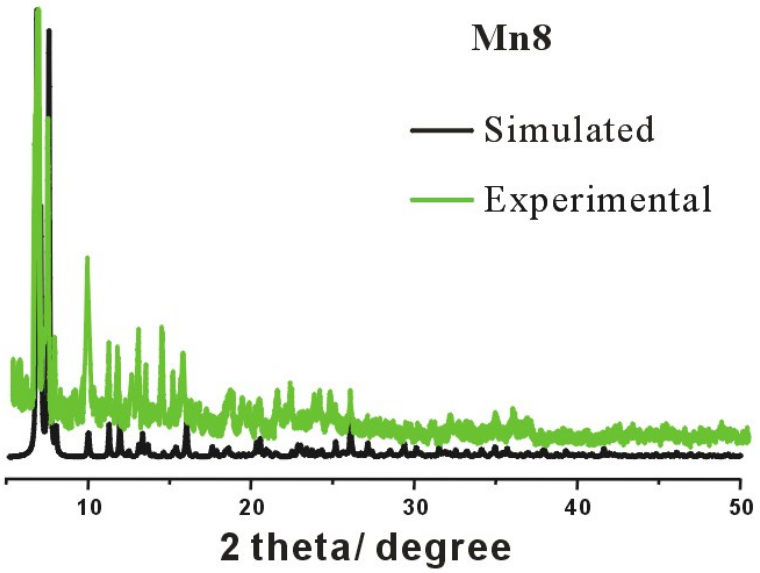
Table S1. Selected bond lengths and angles for 1.

Mn1—O7	2.049 (4)	Mn3—O3	2.119 (4)
Mn1—O5	2.153 (4)	Mn3—O12	2.151 (4)
Mn1—O9	2.179 (4)	Mn3—O1W	2.153 (4)
Mn1—N1	2.187 (5)	Mn3—O9	2.202 (4)
Mn1—O12	2.222 (4)	Mn3—O11	2.236 (4)
Mn1—O10	2.431 (4)	Mn3—O1^{i}	2.238 (4)
Mn2—O11^{i}	1.878 (3)	Mn4—O2	2.081 (4)
Mn2—O11	1.879 (4)	Mn4—O6	2.145 (4)
Mn2—O4^{i}	1.956 (4)	Mn4—N3	2.187 (5)
Mn2—O10	1.967 (3)	Mn4—O11	2.225 (3)
Mn2—O13	2.242 (4)	Mn4—O9	2.230 (4)
Mn2—O1	2.462 (4)	Mn4—O10	2.276 (4)
O7—Mn1—O5	93.33 (17)	O3—Mn3—O12	172.71 (16)
O7—Mn1—O9	97.65 (16)	O3—Mn3—O1W	88.08 (16)
O5—Mn1—O9	89.83 (15)	O12—Mn3—O1W	86.57 (16)
O7—Mn1—N1	109.03 (18)	O3—Mn3—O9	96.04 (14)
O5—Mn1—N1	92.21 (17)	O12—Mn3—O9	79.04 (13)
O9—Mn1—N1	153.07 (17)	O1W—Mn3—O9	90.21 (14)
O7—Mn1—O12	94.00 (16)	O3—Mn3—O11	91.49 (15)
O5—Mn1—O12	166.54 (15)	O12—Mn3—O11	92.80 (14)
O9—Mn1—O12	78.01 (13)	O1W—Mn3—O11	168.94 (14)
N1—Mn1—O12	96.05 (16)	O9—Mn3—O11	78.83 (13)
O7—Mn1—O10	176.85 (15)	O3—Mn3—O1^{i}	91.03 (15)
O5—Mn1—O10	89.79 (14)	O12—Mn3—O1^{i}	95.62 (14)
O9—Mn1—O10	81.89 (13)	O1W—Mn3—O1^{i}	113.03 (14)
N1—Mn1—O10	71.27 (15)	O9—Mn3—O1^{i}	155.95 (15)
O12—Mn1—O10	82.85 (13)	O11—Mn3—O1^{i}	78.03 (13)

O11^{i}—Mn2—O11	83.56 (16)	O2—Mn4—O6	93.48 (16)
O11^{i}—Mn2—O4^{i}	98.48 (16)	O2—Mn4—N3	105.33 (17)
O11—Mn2—O4^{i}	175.88 (17)	O6—Mn4—N3	91.27 (17)
O11^{i}—Mn2—O10	165.25 (15)	O2—Mn4—O11	95.57 (14)
O11—Mn2—O10	84.94 (15)	O6—Mn4—O11	159.61 (15)
O4^{i}—Mn2—O10	92.46 (16)	N3—Mn4—O11	103.84 (16)
O11^{i}—Mn2—O13	97.28 (15)	O2—Mn4—O9	173.86 (15)
O11—Mn2—O13	103.73 (15)	O6—Mn4—O9	92.65 (15)
O4^{i}—Mn2—O13	79.62 (15)	N3—Mn4—O9	74.95 (16)
O10—Mn2—O13	94.39 (15)	O11—Mn4—O9	78.48 (13)
O11^{i}—Mn2—O1	79.69 (14)	O2—Mn4—O10	95.10 (15)
O11—Mn2—O1	92.10 (14)	O6—Mn4—O10	90.55 (14)
O4^{i}—Mn2—O1	84.77 (15)	N3—Mn4—O10	159.34 (16)
O10—Mn2—O1	91.56 (14)	O11—Mn4—O10	70.49 (12)
O13—Mn2—O1	163.50 (14)	O9—Mn4—O10	84.41 (13)

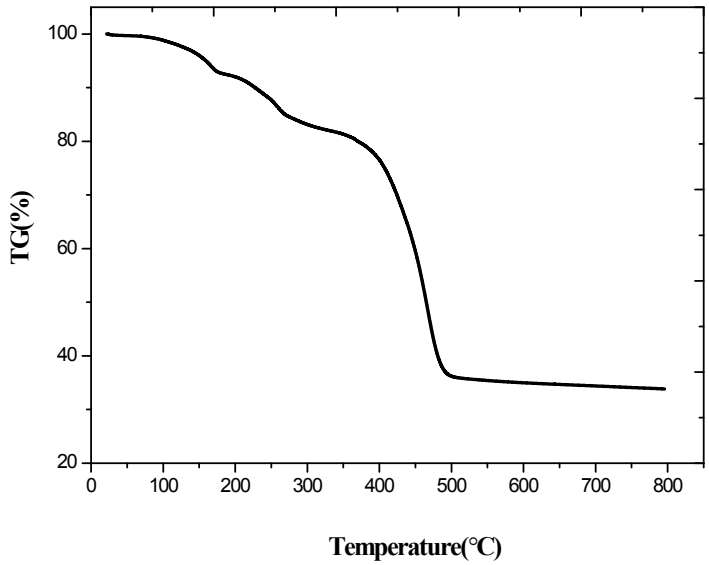
Symmetry code: (i) −x+1, −y+1, −z.

Figure S1. The XRD patterns of 1.



As shown in Fig. S1, the X-ray powder diffraction patterns measured for the as-synthesized sample of **1** is in good agreement with the PXRD patterns simulated from the respective single-crystal X-ray data, proving the purity of the bulk phases. The dissimilarity in reflection intensities between the simulated and the experimental patterns may be due to the different orientation of the microcrystals in the powder samples.

Figure S2. The TGA for 1.



The thermogravimetric analysis (TGA) for **1** is measured under the N_2 atmosphere. For **1**, the weight loss of 7.25 % in the temperature range of 20 to 180 ^oC is attributed to the removal of four lattice acetonitrile molecules (calcd 6.89 %), then the weight loss of 9.67 % in the temperature range of 180 to 300 ^oC is attributed to the removal of two $PhCOO^-$ ligands (calcd 10.15 %)

Figure S3. The IR for 1.