

10.1071/CH09378_AC

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Australian Journal of Chemistry, 2010, 63(2), 286–292

Accessory Publication

Crystal Structures , Topological Analyses and Magnetic Properties of Two Manganese-2,5-Dihydroxyterephthalic Acid Complexes

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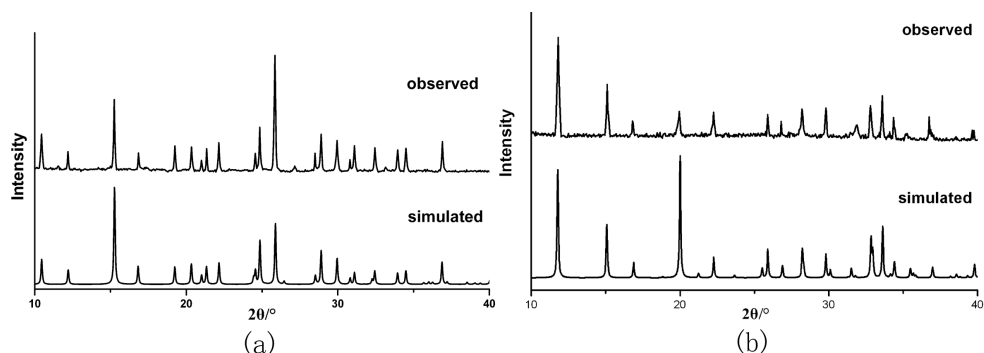


Fig. S1. Simulated and observed XRD patterns of complexes **1** (a) and **2**(b).

Table S1 Selected bond lengths (Å) and bond angles (°) for **1** and **2**.

Complex 1			
Mn1—O2 ⁱ	2.1251 (12)	Mn1—O3	2.1732 (11)
Mn1—O2 ⁱⁱ	2.1251 (12)	Mn1—O4	2.1973 (11)
Mn1—O3 ⁱⁱⁱ	2.1732 (11)	Mn1—O4 ⁱⁱⁱ	2.1973 (11)
O2 ⁱ —Mn1—O2 ⁱⁱ	174.25 (5)	O3 ⁱⁱⁱ —Mn1—O4	175.39 (3)
O2 ⁱ —Mn1—O3 ⁱⁱⁱ	96.24 (4)	O3—Mn1—O4	89.57 (5)
O2 ⁱⁱ —Mn1—O3 ⁱⁱⁱ	87.94 (4)	O2 ⁱ —Mn1—O4 ⁱⁱⁱ	89.49 (4)
O2 ⁱ —Mn1—O3	87.94 (4)	O2 ⁱⁱ —Mn1—O4 ⁱⁱⁱ	86.60 (4)
O2 ⁱⁱ —Mn1—O3	96.24 (4)	O3 ⁱⁱⁱ —Mn1—O4 ⁱⁱⁱ	89.57 (5)
O3 ⁱⁱⁱ —Mn1—O3	86.92 (6)	O3—Mn1—O4 ⁱⁱⁱ	175.39 (3)
O2 ⁱ —Mn1—O4	86.60 (4)	O4—Mn1—O4 ⁱⁱⁱ	94.10 (6)
O2 ⁱⁱ —Mn1—O4	89.49 (4)		
Complex 2			
Mn1—O3	2.1113 (15)	Mn1—O2 ⁱⁱⁱ	2.2284 (14)
Mn1—O3 ⁱ	2.1200 (14)	Mn1—O4	2.2502 (16)
Mn1—O1 ⁱⁱ	2.1600 (16)	Mn1—O2	2.2690 (15)
O3—Mn1—O3 ⁱ	104.91 (5)	O1 ⁱⁱ —Mn1—O4	162.52 (5)
O3—Mn1—O1 ⁱⁱ	93.73 (6)	O2 ⁱⁱⁱ —Mn1—O4	80.82 (6)
O3 ⁱ —Mn1—O1 ⁱⁱ	102.22 (6)	O3—Mn1—O2	78.24 (5)
O3—Mn1—O2 ⁱⁱⁱ	156.33 (5)	O3 ⁱ —Mn1—O2	163.51 (5)
O3 ⁱ —Mn1—O2 ⁱⁱⁱ	98.72 (6)	O1 ⁱⁱ —Mn1—O2	93.63 (6)
O1 ⁱⁱ —Mn1—O2 ⁱⁱⁱ	82.48 (6)	O2 ⁱⁱⁱ —Mn1—O2	78.69 (6)
O3—Mn1—O4	99.50 (6)	O4—Mn1—O2	78.07 (6)
O3 ⁱ —Mn1—O4	85.44 (6)		

Symmetry codes: (i) 1/2+x, 1/2-y, 1/2+z; (ii) 1/2-x, 1/2-y, 1-z; (iii) 1-x, y, 3/2-z. For **2**: (i) x, 3/2-y,

1/2+z; (ii) 1-x, 1/2+y, 1/2-z; (iii) 1-x, 1-y, 1-z.

Table S2 Hydrogen bonds for **1** and **2** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
1				
O4—H4A...O1 ⁱ	0.82	2.01	2.8162 (15)	168.2
O4—H4B...O1 ⁱⁱ	0.84	2.03	2.8719 (15)	174.9
O1—H1...O3	0.70	1.87	2.5202 (14)	154.7
2				
O4—H4B...O1 ⁱ	0.87	2.02	2.864 (2)	165.0

Symmetry codes, for **1**: (i) -1/2+x, 1/2-y, -1/2+z; (ii) 3/2-x, 1/2-y, 1-z. For **2**: (i) x, 1/2-y, 1/2+z.