chemistry

MDPI

ESI for:

Nature inspired manganese(III)-calcium complexes: towards synthetic models for the WOC of PSII

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Table S1. Crystallographic and data collection parameters for complexes **1** and **2**.

	Complex 1·1MeCN·2H$_2$O	**Complex 2·18MeOH·4H$_2$O**	**Complex 3**
CSD	2245032	2245034	2245033
T (K)	100	100	118
Wavelength (Å)	0.71073	0.71073	0.71073
System	Trigonal	Trigonal	Orthorhombic
Space group	R3-	P3-	Pbca
Unit cell a, b, c (Å)	24.6538(12), 24.6538(12), 47.334(3)	19.814(2), 19.814(2), 14.978(2)	6.324(3), 21.172(3) 26.320(4)
Unit cell α, β, γ (°)	90, 90, 120	90, 90, 120	90, 90, 90
R1, wR2	0.096, 0.26	0.063, 0.17	0.070, 0.183

Table S2. Bond Valence sum calculations for complexes **1** and **2**.

Complex 1

	Mn(II)	Mn(III)	Mn(IV)
Mn1	3.33967	**3.054704**	3.206986
disorder 1			
Mn2	2.943517	**2.692354**	2.826572
disorder 2			
Mn2	3.839489	**3.511875**	3.686947
AVERAGE		**3.10211**	

Ca7	**2.113881**	
O2	1.281149	**MeO-**
O1	1.758343	**O2-**

Complex 2

	Mn(II)	Mn(III)	Mn(IV)
Mn1	3.07042	**2.808428**	2.948433
Mn2	3.51897	**3.218705**	3.379162
Mn3	3.839489	**3.511875**	3.686947

Ca4	**2.279328**	
O2	2.095931	**O2-**
O1	1.133629	**OH**
O3	1.620074	**MeO-**
O4	1.874023	**O2-**
O5	1.657655	**MeO-**

Figure S1. XPS spectrum for complex **1**.

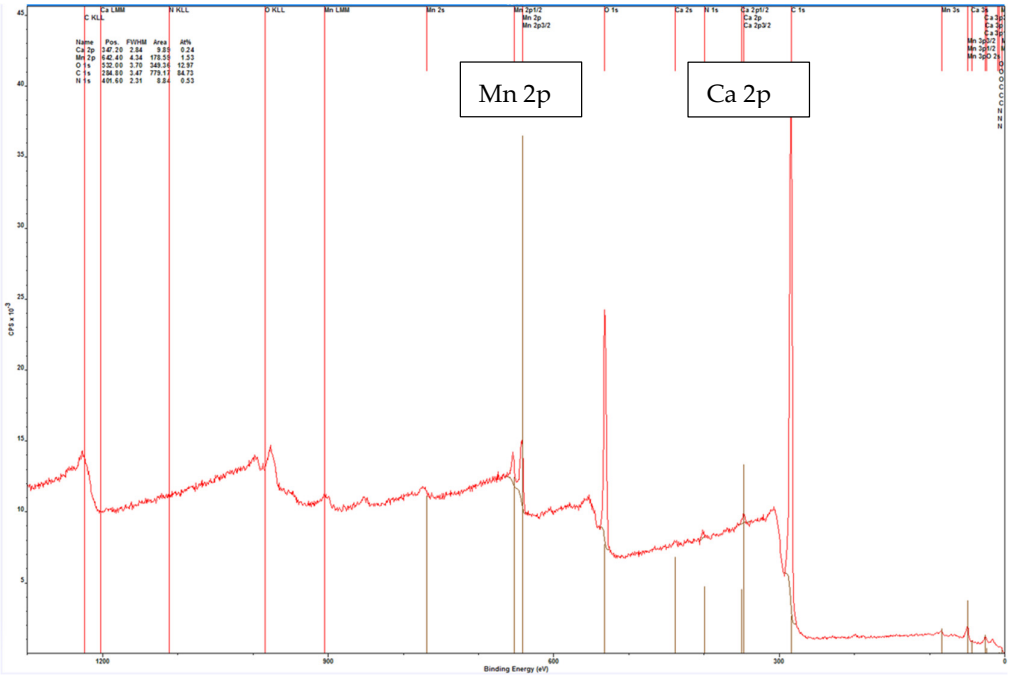
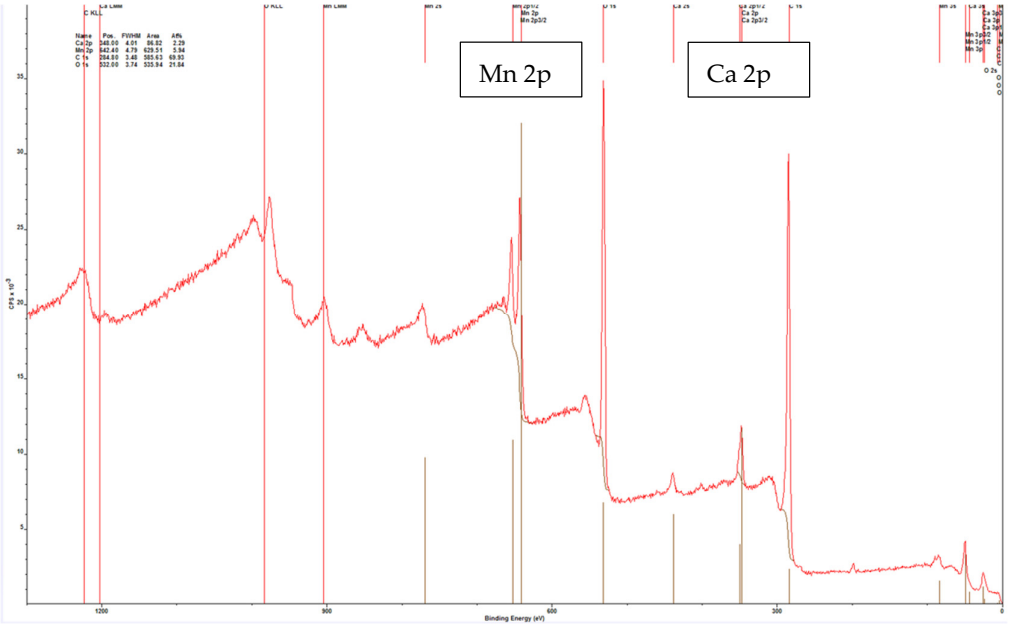


Figure S2. XPS spectrum for complex **2**.


Mn 2p
Ca 2p
Binding Energy (eV)