Supplementary Materials: Tetramer Compound of Manganese Ions with Mixed Valence [MnII MnIII MnIV] and Its Spatial, Electronic, Magnetic, and Theoretical Studies

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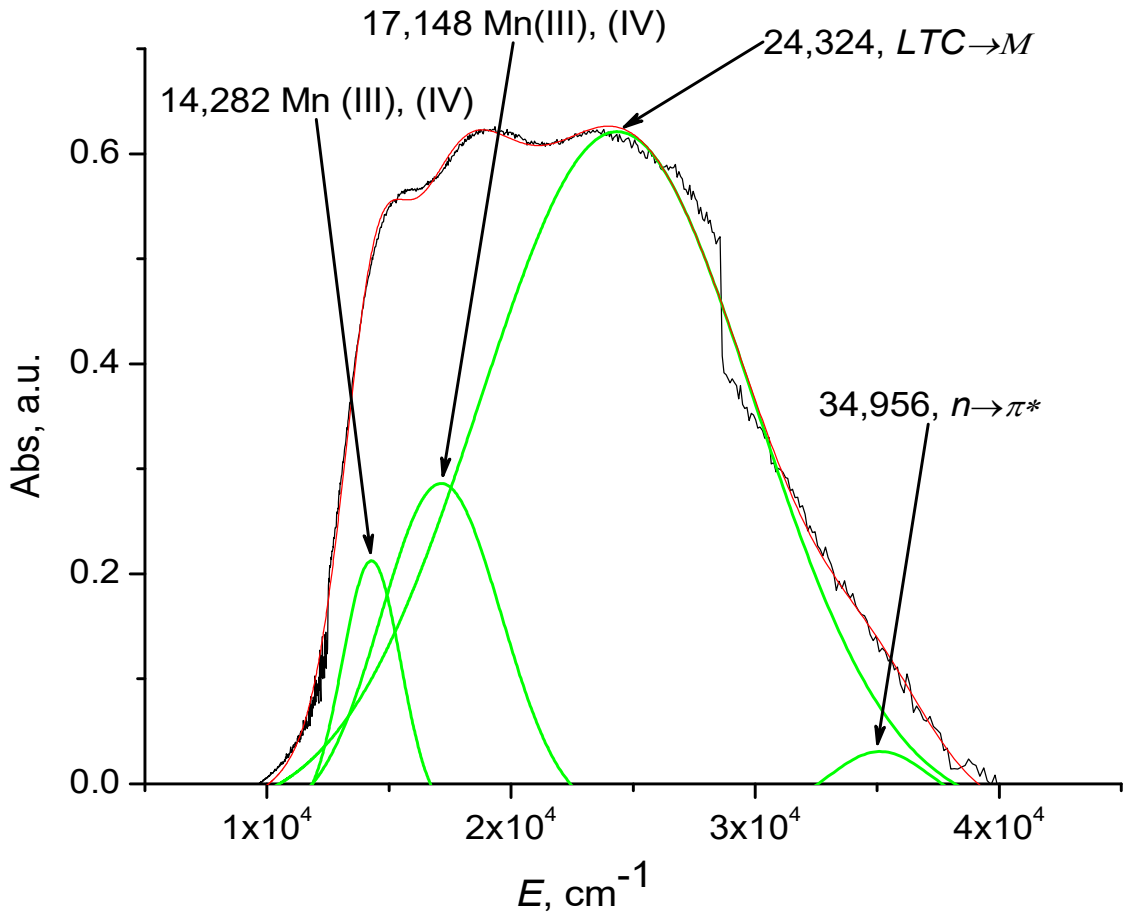

Figure SI-1. UV-Vis spectrum of **1** on polycrystalline sample showing the electronic transitions at typical reported energies for Mn(III) and Mn(IV). .

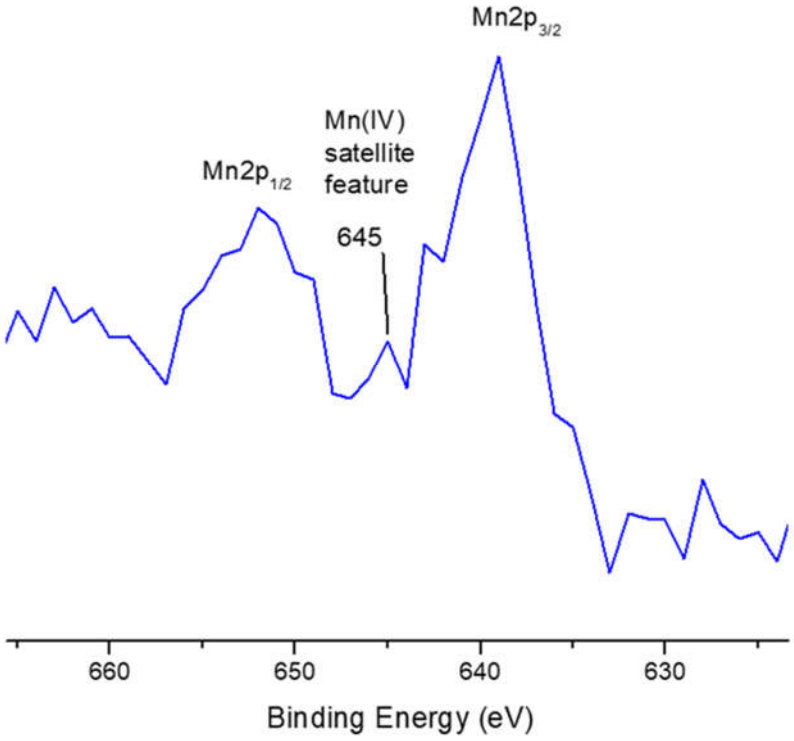

Figure SI-2. Mn2p spectra of Mn complex. MnO has a satellite feature (~647 eV), which is not present for either Mn_2O_3 or MnO_2.

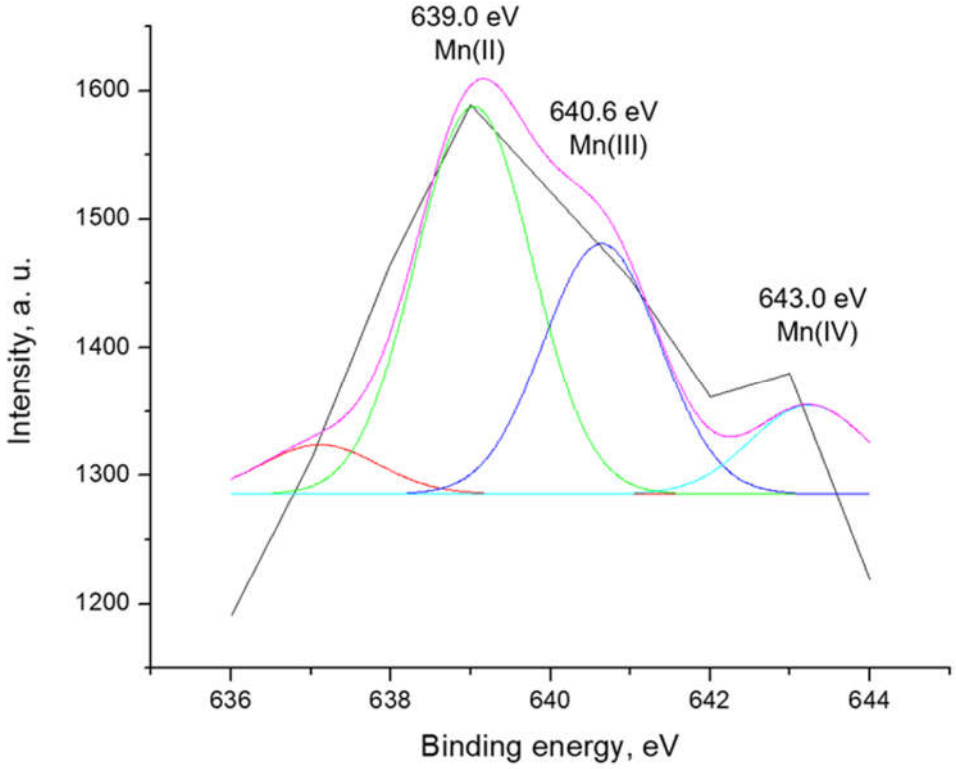

Figure SI-3. Mn2p 3/2 spectra of Mn complex. A model of three gaussian curves fit to reproduce the experimental results.

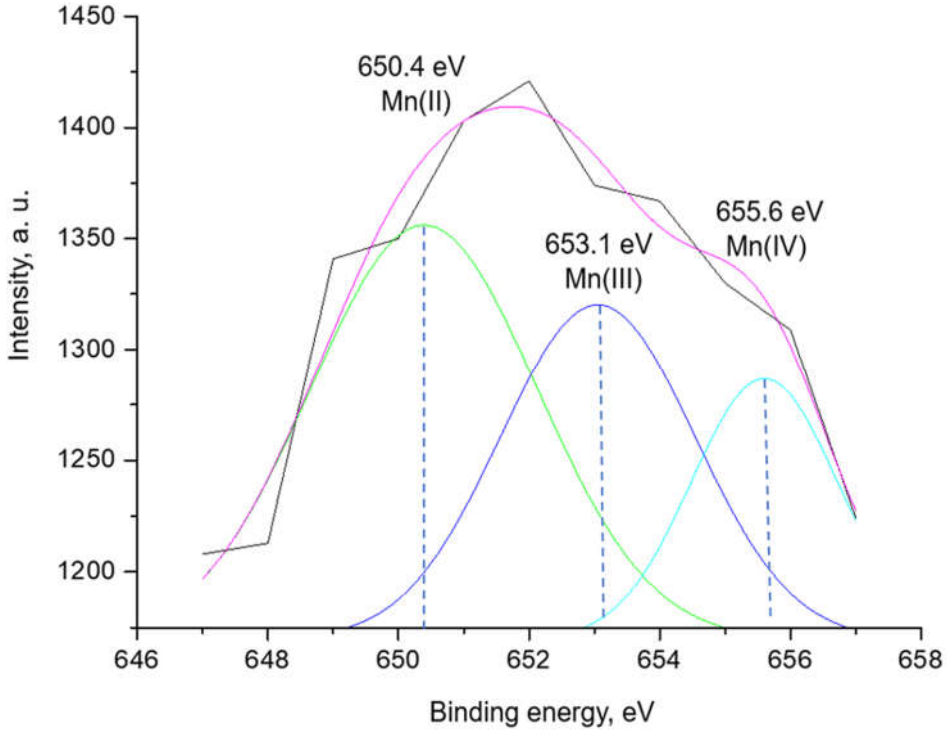

Figure SI4. Mn2p 1/2 spectra of Mn complex. A model of three Gaussian curves fit to reproduce the experimental results.

Table SI1. X-ray photoelectron spectroscopy (XPS) resumed information of energies corresponding manganese oxidation states present in **1**.

	Peak (eV) $Mn2p_{1/2}$	[45–58]	Peak (eV) $Mn2p_{3/2}$	[45–58]
Mn			640.6	[48]
			640.7	[49]
Mn(II)	649.5	[53]	639.7	[55]
	649.5	[54]	639.0	[56]
Mn(III)	653.4	[50]	640.3	[51]
	653.1	[51]	640.6	[52]
Mn(IV)			642.7	[50]
			642.6	[51]
Compound **1**	650.4		639.0	
	653.1		640.6	This work
			643.0	

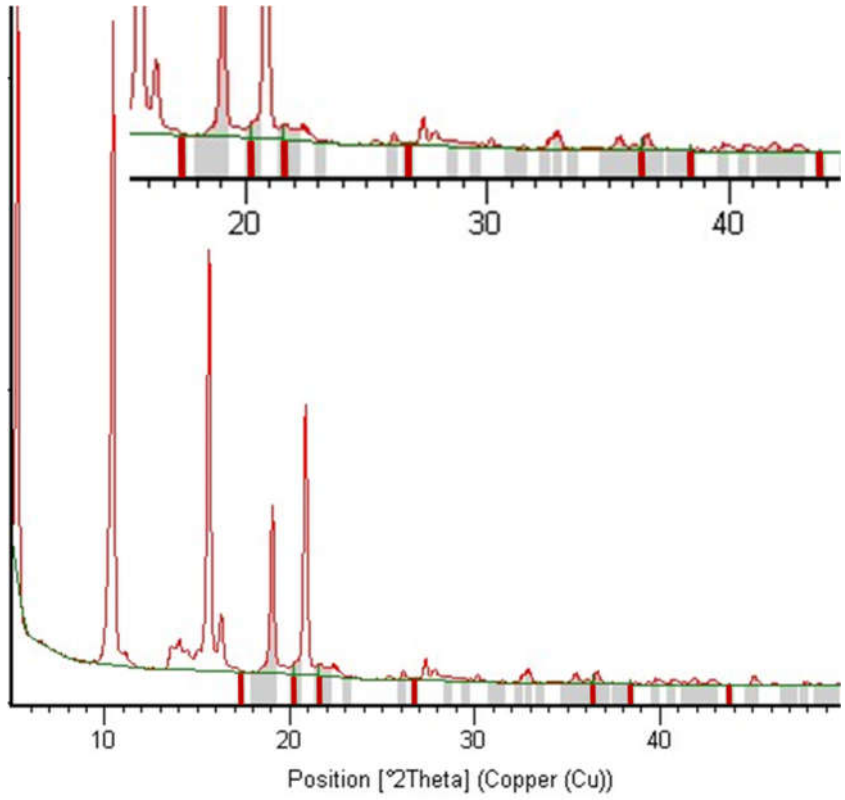

Figure SI 5. Powder X-ray diffraction (PXRD) of **1** compared with Mn(II) in MnO pattern. Inset: a zoom of the spectrum is placed for clarity.

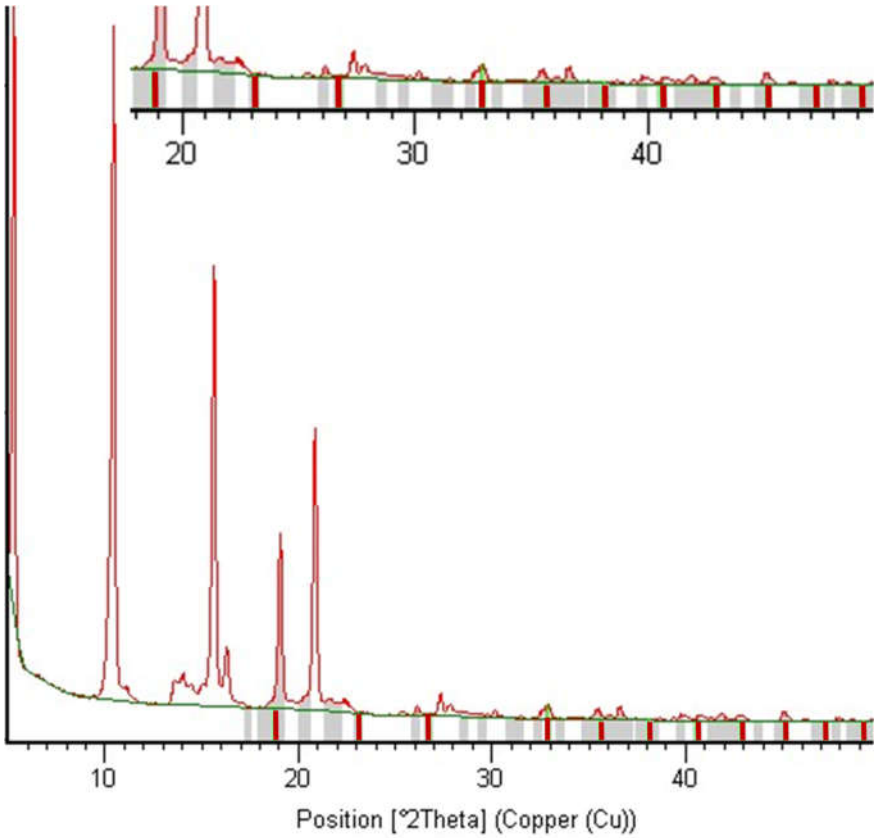

Figure SI 6. PXRD of **1** compared with Mn(III) in Mn_2O_3 pattern. Inset: a zoom of the spectrum is placed for clarity.

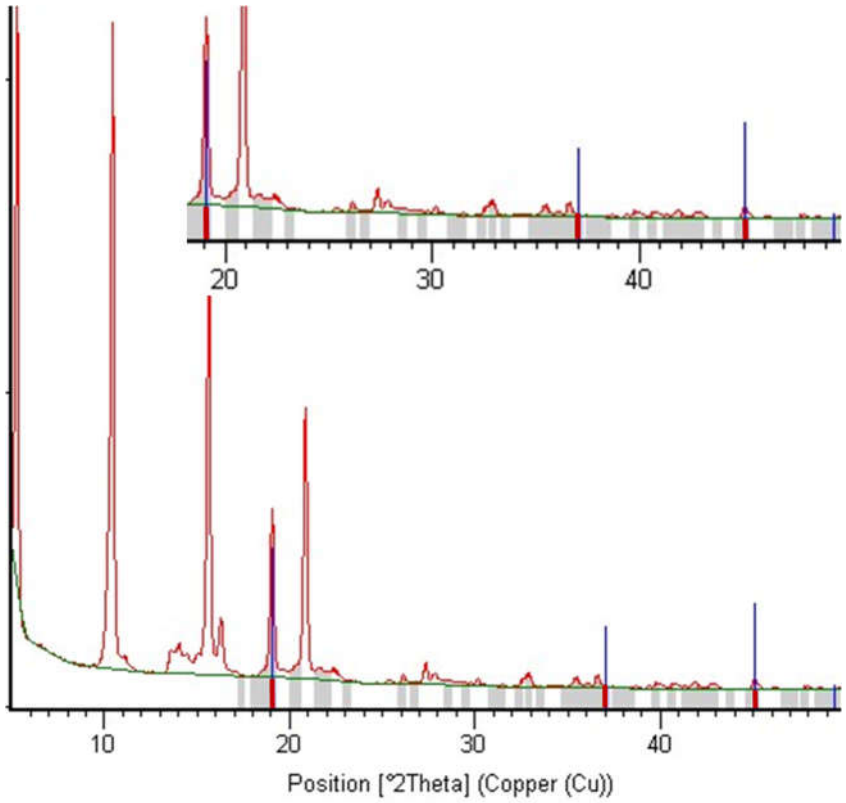

Figure SI 7. PXRD of **1** compared with Mn(IV) in MnO_2 pattern. Inset: a zoom of the spectrum is placed for clarity.

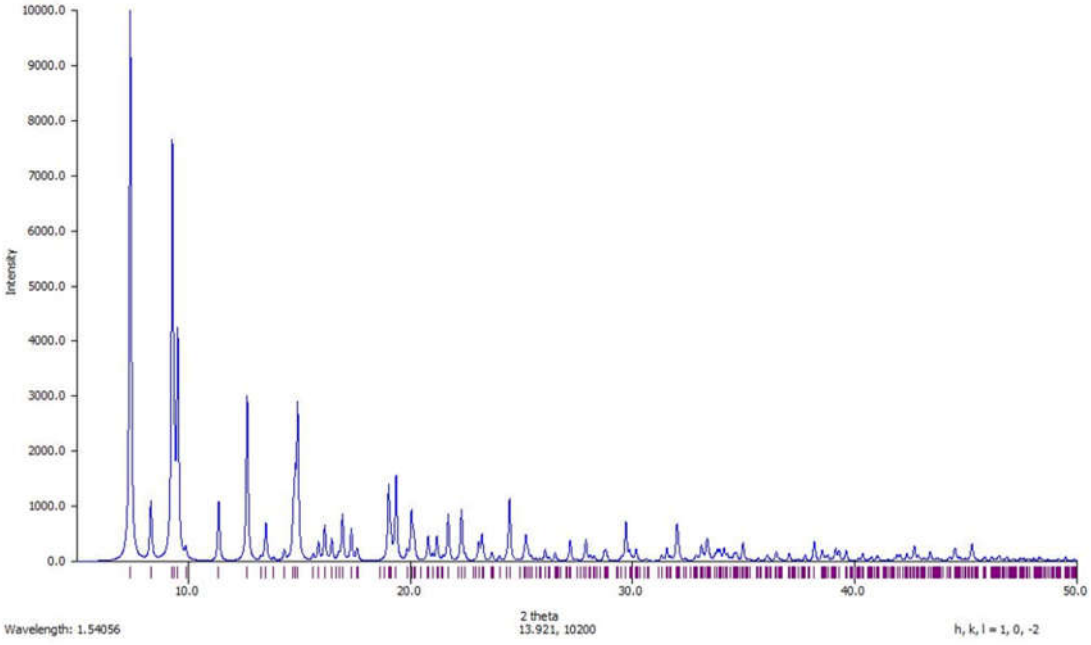

Figure SI 8. Simulation of the PXRD of **1** monocrystal structure with FWHM 0.1.

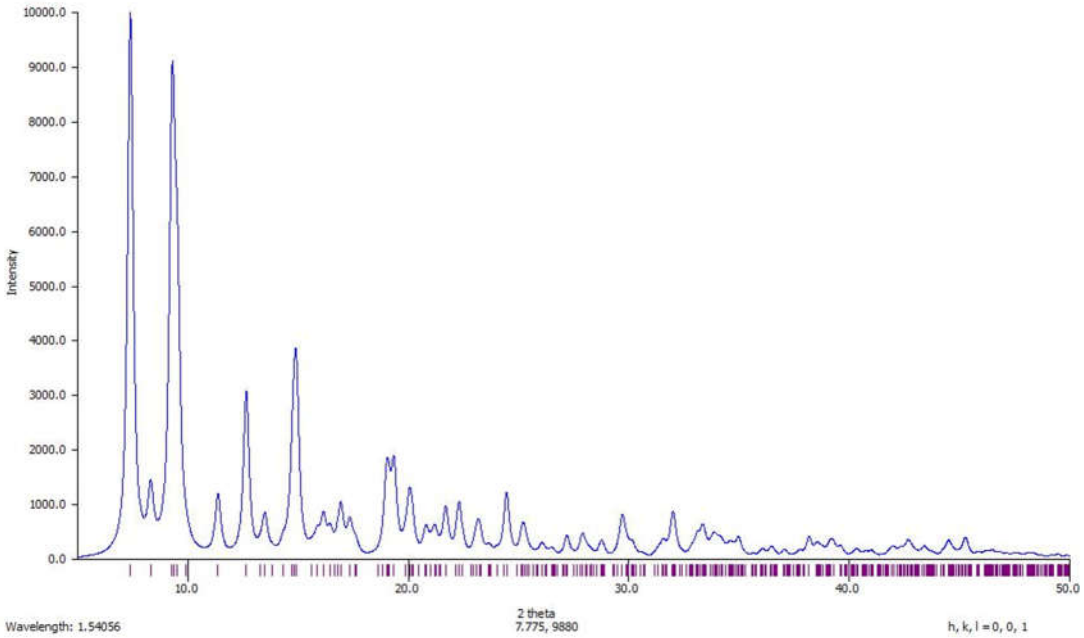

Figure SI 9. Simulation of the PXRD of **1** monocrystal structure with FWHM 0.3.