

Structural and Thermal Properties of $\text{Na}_2\text{Mn}(\text{SO}_4)_2 \cdot 4\text{H}_2\text{O}$ and $\text{Na}_2\text{Ni}(\text{SO}_4)_2 \cdot 10\text{H}_2\text{O}$

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Supplementary Information

Table S1. Anisotropic displacement parameters (in Å²) for Na₂Mn(SO₄)₂•4H₂O and Na₂Ni(SO₄)₂•10H₂O.

Atom	<i>U</i> ₁₁	<i>U</i> ₂₂	<i>U</i> ₃₃	<i>U</i> ₁₂	<i>U</i> ₁₃	<i>U</i> ₂₃
Na ₂ Mn(SO ₄) ₂ •4H ₂ O						
Na1	0.0237(3)	0.0203(3)	0.0176(3)	0.00056(19)	0.0016(2)	-0.00062(19)
Mn1	0.01556(16)	0.01332(17)	0.01288(16)	-0.00115(8)	0.00297(10)	-0.00116(8)
S1	0.01026(16)	0.01219(17)	0.01116(17)	0.00034(9)	0.00097(10)	-0.00111(9)
O1	0.0265(5)	0.0260(5)	0.0172(4)	0.0133(4)	0.0022(4)	0.0046(3)
O2	0.0180(4)	0.0200(5)	0.0318(5)	-0.0051(3)	0.0041(4)	-0.0134(4)
O3	0.0137(4)	0.0210(4)	0.0324(5)	-0.0051(3)	0.0057(3)	-0.0045(4)
O4	0.0274(5)	0.0252(5)	0.0127(4)	0.0027(4)	0.0051(4)	0.0032(3)
O5	0.0191(4)	0.0202(4)	0.0165(4)	0.0013(3)	0.0069(3)	0.0012(3)
O6	0.0190(4)	0.0170(5)	0.0193(4)	0.0013(3)	-0.0034(3)	-0.0009(3)
Na ₂ Ni(SO ₄) ₂ •10H ₂ O						
Na1	0.0229(2)	0.0244(2)	0.0271(2)	-0.00162(16)	0.00538(19)	0.00195(17)
Ni1	0.01359(9)	0.01279(9)	0.0148(1)	0.00197(5)	0.00365(7)	0.00037(5)
S1	0.01432(11)	0.01336(10)	0.01625(12)	0.00044(7)	0.00523(9)	-0.00046(7)
O1	0.0270(4)	0.0195(3)	0.0293(4)	0.0047(3)	0.0177(3)	0.0018(3)
O2	0.0216(4)	0.0275(4)	0.0188(4)	0.0037(3)	0.0019(3)	0.0020(3)
O3	0.0236(4)	0.0404(5)	0.0273(4)	-0.0147(3)	0.0114(3)	-0.0109(4)
O4	0.0318(4)	0.0150(3)	0.0280(4)	0.0062(3)	0.0061(3)	0.0022(3)
O5	0.0205(4)	0.0191(3)	0.0283(4)	0.0016(3)	-0.0035(3)	0.0030(3)
O6	0.0255(4)	0.0207(3)	0.0231(4)	0.0075(3)	0.0028(3)	-0.0051(3)
O7	0.0254(4)	0.0235(4)	0.0250(4)	0.0030(3)	0.0054(3)	0.0036(3)
O8	0.0284(4)	0.0297(4)	0.0289(5)	0.0038(3)	0.0097(4)	-0.0042(3)
O9	0.0233(4)	0.0195(3)	0.0260(4)	-0.0027(3)	0.0117(3)	-0.0018(3)

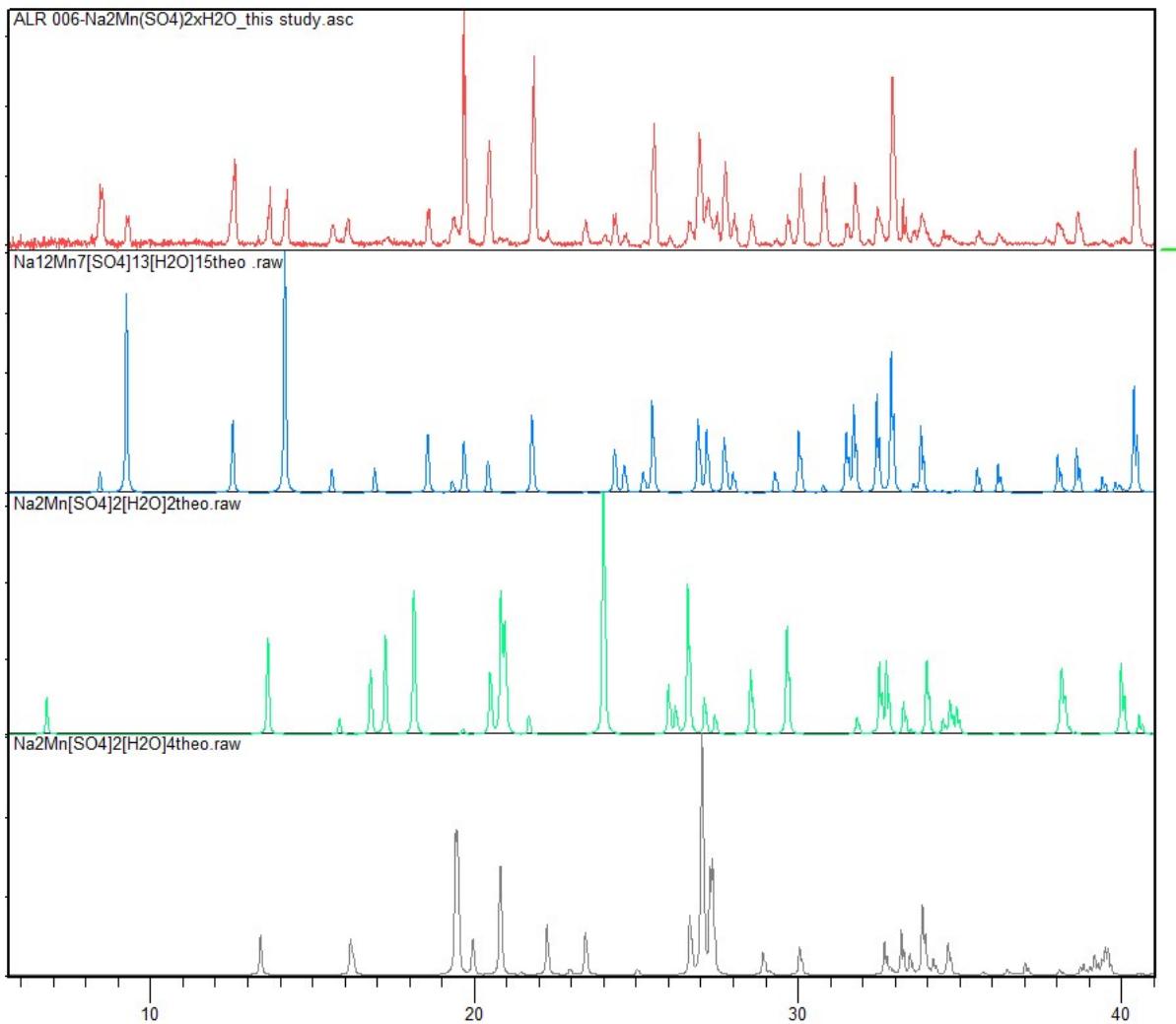


Figure S1. Theoretical powder X-ray diffraction patterns of $\text{Na}_{12}\text{Mn}_7(\text{SO}_4)_{13} \cdot 15\text{H}_2\text{O}$, $\text{Na}_2\text{Mn}(\text{SO}_4)_2 \cdot 2\text{H}_2\text{O}$, and $\text{Na}_2\text{Mn}(\text{SO}_4)_2 \cdot 4\text{H}_2\text{O}$ and experimental PXRD pattern of the sample containing manganese that was prepared during this study (Cu-K α radiation).

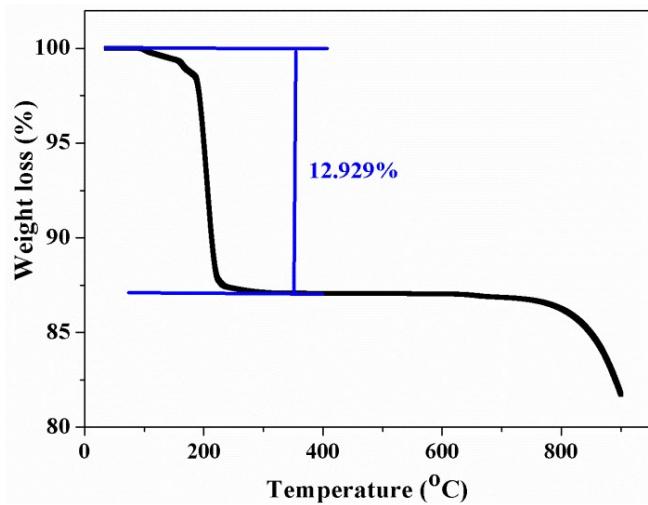


Figure S2. TGA thermal analysis of the sample containing manganese.