

Supporting Information for

Li₁₃Mn(SeO₃)₈: Lithium-Rich Transition Metal Selenite Containing Jahn-Teller Distortive Cations

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Figure S1. Experimental and Calculated Powder X-ray Diffraction Patterns for $\text{Li}_{13}\text{Sc}(\text{SeO}_3)_8$

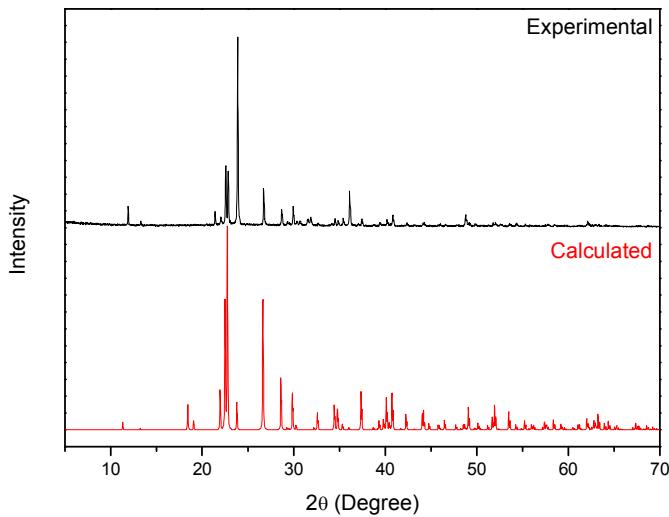


Figure S2. Experimental and Calculated Powder X-ray Diffraction Patterns for $\text{Li}_{13}\text{Mn}(\text{SeO}_3)_8$

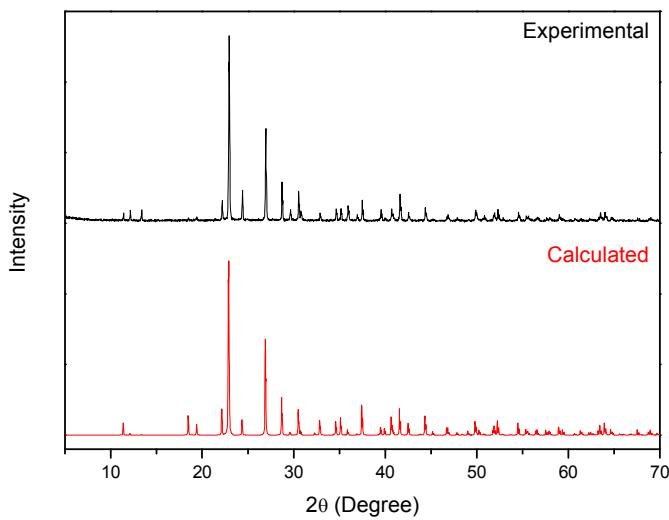


Figure S3. Experimental and Calculated Powder X-ray Diffraction Patterns for $\text{Li}_{13}\text{Fe}(\text{SeO}_3)_8$

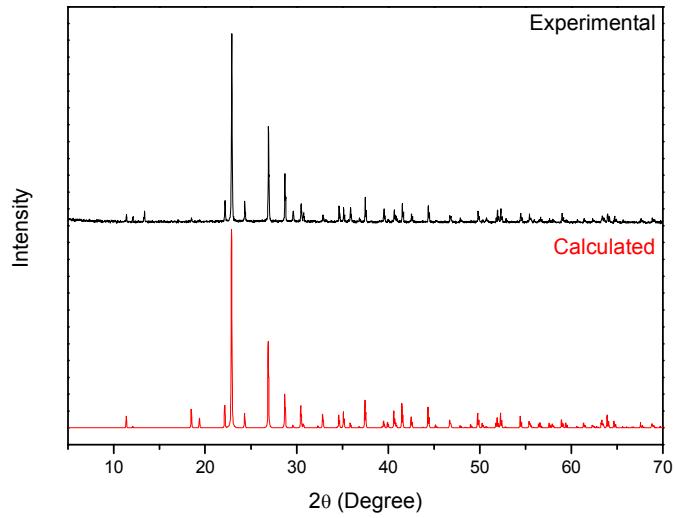


Figure S4. Final Rietveld plot of $\text{Li}_{13}\text{Cr}(\text{SeO}_3)_8$

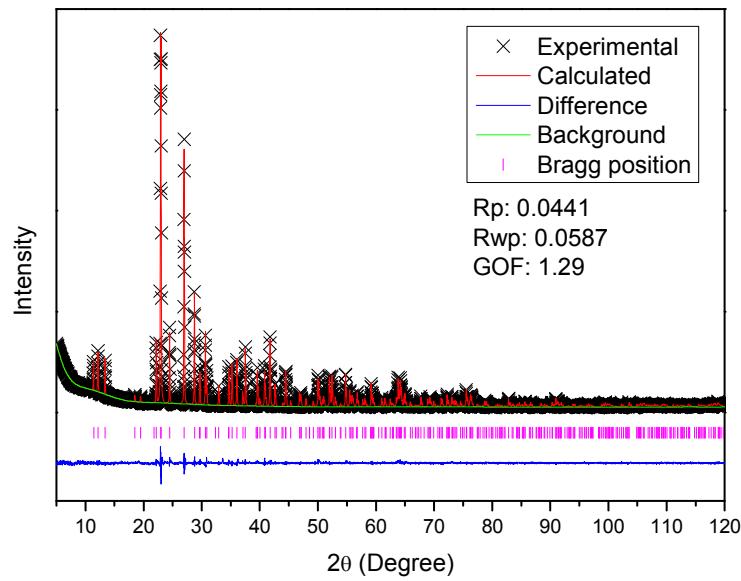


Table S1. Atomic Coordinates and Isotropic Displacement Parameters for $\text{Li}_{13}\text{Cr}(\text{SeO}_3)_8$

| | x | y | z | B_{iso} |
|-------|-------------|------------|-------------|------------------|
| Li(1) | 0.856(4) | 1.121(4) | 0.1068(8) | 0.4(3) |
| Li(2) | 0.480(4) | 0.497(4) | 0.1328(8) | 0.4(3) |
| Li(3) | 1/3 | 2/3 | 1/6 | 0.4(3) |
| O(1) | 0.8148(8) | 0.8535(10) | 0.0558(3) | 0.6(2) |
| O(2) | 0.6508(10) | 1.0085(11) | 0.0737(3) | 0.5(2) |
| O(3) | 0.5485(8) | 0.7169(8) | 0.1171(3) | 0.3(2) |
| O(4) | 0.4934(8) | 0.1905(11) | 0.1419(3) | 0.7(2) |
| Cr(1) | 1 | 1 | 0 | 0.27(12) |
| Se(1) | 0.62103(15) | 0.8270(2) | 0.05182(6) | 0.20(4) |
| Se(2) | 2/3 | 1/3 | 0.10878(11) | 0.30(6) |

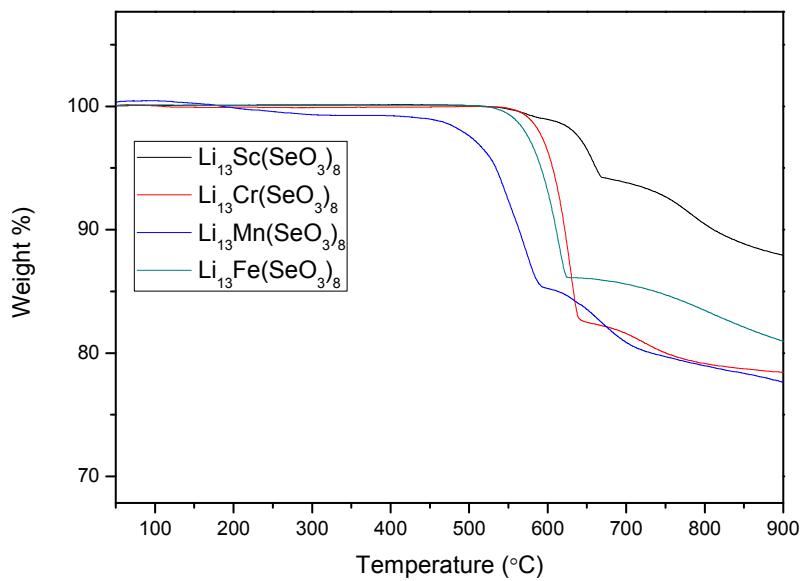
Figure S5. Thermogravimetric Analysis Diagrams for $\text{Li}_{13}\text{M}(\text{SeO}_3)_8$ ($\text{M} = \text{Sc}, \text{Cr}, \text{Mn}, \text{and Fe}$)

Figure S6. EDX Result for $\text{Li}_{13}\text{M}(\text{SeO}_3)_8$ ($\text{M} = \text{Sc, Cr, Mn, and Fe}$)

| | $\text{Li}_{13}\text{Sc}(\text{SeO}_3)_8$ | $\text{Li}_{13}\text{Cr}(\text{SeO}_3)_8$ | $\text{Li}_{13}\text{Mn}(\text{SeO}_3)_8$ | $\text{Li}_{13}\text{Fe}(\text{SeO}_3)_8$ |
|------|---|---|---|---|
| O K | 69.75 % | 77.67 % | 67.64 % | 71.31 % |
| M K | 3.24 % | 2.53 % | 4.39 % | 2.88 % |
| Se L | 27.01 % | 19.79 % | 27.97 % | 25.80 % |