

Supporting Information

Interesting cationic ($\text{Li}^+/\text{Fe}^{3+}/\text{Te}^{6+}$) variations in new rocksalt ordered structures

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Table S1. Crystallographic parameters of $\text{Li}_{4.5}\text{Fe}_{0.5}\text{TeO}_6$.

Crystal data	
Empirical formula	$\text{Li}_{4.5}\text{Fe}_{0.5}\text{TeO}_6$
Crystal system	Monoclinic
Space Group	$C2/m$ (#12)
a [Å]	5.1413(4)
b [Å]	8.8424(5)
c [Å]	5.1468(4)
β [°]	110.395(8)
V [Å³]	219.31(3)
Z	2
Molecular Weight	281.972
ρ_{calc} [g/cm³]	4.282
Morphology	Irregular
Colour	Green
Dimensions (mm)	$0.07 \times 0.07 \times 0.06$
Temperature [K]	293(2)
Wavelength [MoKα][Å]	0.71073
Monochromator	Graphite
Scan mode	ω scan
Min/Max Bragg angle [°]	4.22-29.33
hkl range	$-6 \rightarrow 6, -11 \rightarrow 11,$ $-6 \rightarrow 6$
F(000)	253.0
μ (mm⁻¹)	8.308
R_{int}	0.0279
R_{sigma}	0.0225
Refinement	F^2
No. reflections used	1565
Unique reflections	295
Number of parameters	26
GoF	1.065

R[F² > 2σ(F²)]	0.0192
wR₂	0.0467
Extinction Coefficient	0.0
Δρ/e[Å⁻³]	2.256/-0.996

Table S2. Anisotropic Displacement Parameters (SXR) of $\text{Li}_{4.5}\text{Fe}_{0.5}\text{TeO}_6$

<i>Anisotropic Displacement Parameters</i>						
Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Te1	0.0062(2)	0.0052(2)	0.0062(2)	0	-0.00015(14)	0
Li1	0.020(5)	0.020(5)	0.018(4)	0	0.013(4)	0
Li2/Fe1	0.013(4)	0.011(4)	0.014(4)	0	-0.005(3)	0
Li3/Fe2	0.0063(10)	0.0036(10)	0.0091(10)	0	-0.0003(8)	0

Table S3. Crystallographic (PXRD) parameters of $\text{Li}_{4.5}\text{Fe}_{0.5}\text{TeO}_6$ and $\text{Li}_{3.75}\text{Fe}_{1.75}\text{Te}_{0.5}\text{O}_6$

	$\text{Li}_{4.5}\text{Fe}_{0.5}\text{TeO}_6$	$\text{Li}_{3.75}\text{Fe}_{1.75}\text{Te}_{0.5}\text{O}_6$
Crystal system	Monoclinic	Monoclinic
Space group	<i>C 1 2/m 1</i>	<i>C 1 2/m 1</i>
Lattice constants:		
<i>a</i> (Å)	5.1834(1)	5.1686(2)
<i>b</i> (Å)	8.8858(2)	8.8362(1)
<i>c</i> (Å)	5.16840(8)	5.1508(1)
β (°)	110.660(1)	110.610(3)
Cell volume (Å³)	222.742(5)	220.19(1)
Formula weight	284.61	281.52
Z	2	2
Density (calc.)	4.22 g cm ⁻³	4.33g cm ⁻³
Radiation	CuK α	CuK α
2θ range	10 - 70°	10 - 70°
No. of data points	4570	4570
No. of reflections	53	53
No. of parameters	21	27
Agreement factors:		
R _p	2.13%	1.13%
R _{wp}	2.94%	2.05 %
χ^2	7.830	9.972