Supplementary Information: S3

Results of refinements from the neutron powder data using anisotropic atomic displacement parameters

	Volume ($Å^3$)	*a*(Å)	*b*(Å)	*c*(Å)	Na *y*	Na U_{iso}	Co/Ni U_{iso}	F1 *y*	F1 U_{iso}	F2 *y*	F2 *z*	F2 U_{iso}		
(a)													R_{wp}	χ^2
$NaCoF_3$	231.627(8)	3.06749(6)	10.1241(2)	7.4584(1)	0.2547(2)			0.9236(1)		0.62908(7)	0.05985(8)		0.0251	3.273
$NaNiF_3$	225.104(8)	3.02784(6)	10.0505(2)	7.3971(1)	0.2544(2)			0.9268(2)		0.6264(1)	0.0588(1)		0.0286	2.314
	U_{11}	U_{22}	U_{33}	U_{23}										
Na	1.8(1)	1.11(8)	1.91(18)											
Co	0.44(9)	0.8(1)	0.16(7)	0.28(7)										
F1	1.53(5)	1.01(5)	0.22(4)											
F2	0.94(3)	0.65(3)	1.13(3)	-0.08(3)										
Na	1.3(1)	1.6(1)	1.5(1)											
Ni	0.55(3)	0.63(4)	0.58(3)	-0.01(4)										
F1	0.99(6)	1.34(8)	0.21(5)											
F2	0.41(5)	0.68(5)	1.37(5)	-0.23(4)										

The table above is presented in the same form as Table 1 in the main text of the paper.

Comparing these values with those in the main text, it can be seen that:

a/. the introduction of anisotropic displacement parameters produces only a very slight improvement in the agreement factors (e.g. R_{wp} decreases from 0.0259 to 0.0251 for $NaCoF_3$ and from 0.0296 to 0.0286 for $NaNiF_3$)

b/. all fractional coordinates are essentially unchanged with respect to those listed in Table 1 of the main text

c/. for $NaNiF_3$, the agreement of the anisotropic displacement parameters with those from the single-crystal X-ray refinement (Table 1, main text) is poor, with, for example, F1 showing a much larger degree of anisotropy in the refinement from the neutron powder data.

d/. in the Table above, there are sometimes marked differences between the displacement parameters for the two compounds, which seems unlikely to be the case in reality (compare e.g. the U_{ij} values for the Co and Ni atoms).