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Supplementary Information

Water Sensitivity of Layered P2/P3-$Na_xNi_{0.22}Co_{0.11}Mn_{0.66}O_2$ Cathode Material

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Rietveld refinement of layered P2/P3-$Na_xNi_{0.22}Co_{0.11}Mn_{0.66}O_2$

R-Values

Rexp	1.93	Rwp	4.40	Rp	3.13	GOF	2.28
Rexp`	1.45	Rwp`	3.31	Rp`	2.47	DW	0.45

Quantitative Analysis - Rietveld

Phase 1: P3	64.53(51) %
Phase 2: P2	35.47(51) %

Background

One on X		125600(4300)
Chebychev polynomial, Coefficient	0	-1000(120)
	1	2180(100)
	2	-825(44)
	3	295(17)
	4	-56.6(75)

Instrument

Primary radius (mm)	217.5
Secondary radius (mm)	217.5
Receiving slit width (mm)	0.5
Additional convolutions	
Hat, Constant	0.02147464
Gaussian, Tan(Th)	0.05309249
Lorentzian, 1/Cos(Th)	0.006755493
Circles, -Tan(Th)	0.4096129
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Corrections

Specimen displacement	0.0861(22)
LP Factor	0

Structure 1

Phase name	P3
R-Bragg	1.694
Spacegroup	R3m
Scale	0.00546(11)
Cell Mass	293.993
Cell Volume (Å^3)	119.252(20)
Wt% - Rietveld	64.53(51)

Preferred Orientation

Dir 1: 0 0 3	1.1475(74)
Dir 2: 1 0 1	0.14(66)

Lattice parameters

a (Å)	2.86095(15)
c (Å)	16.8234(21)

Site	Np	x	y	z	Atom	Occ	Beq
Na1	3	0.00000	0.00000	0.17121	Na+1	0.45	0
Ni1	3	0.00000	0.00000	0.00000	Ni+2	0.22	0
Co1	3	0.00000	0.00000	0.00000	Co+3	0.11	0
Mn1	3	0.00000	0.00000	0.00000	Mn+4	0.66	0
O1	3	0.00000	0.00000	0.39121	O-2	1	0
O2	3	0.00000	0.00000	-0.39121	O-2	1	0

Structure 2

Phase name	P2
R-Bragg	4.236
Spacegroup	$P6_3/mmc$
Scale	0.006770(60)
Cell Mass	195.995
Cell Volume (Å^3)	79.2373(76)
Wt% - Rietveld	35.47(51)

Preferred Orientation

(Dir 1: 0 0 2)	0.8836(36)

Lattice parameters

a (Å)	2.859376(98)
c (Å)	11.19069(75)

Site	Np	x	y	z	Atom	Occ	Beq
Mn1	2	0.00000	0.00000	0.00000	Mn+4	0.66	0
Ni1	2	0.00000	0.00000	0.00000	Ni+2	0.22	0
Co1	2	0.00000	0.00000	0.00000	Co+3	0.11	0
Na1	2	0.00000	0.00000	0.25000	Na+1	0.225	0
Na2	2	0.33333	0.66667	0.75000	Na+1	0.225	0
O1	4	0.33333	0.66667	0.08720	O-2	1	0