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Supplementary Material

Alkali-Metal Modification of $Li(Ni_{0.33}Mn_{0.33}Co_{0.33})O_2$

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Table S1. *Full refinement parameters of the $Li(Ni_{0.33}Mn_{0.33}Co_{0.33})O_2$ model with the observed lab XRD data. Space group = R-3m and the number of refinable parameters = 5. Values with no error in brackets () were not refined.*

$Li_{1.0}(Ni_{0.33}Mn_{0.33}Co_{0.33})O_2$

a = 2.86459(6) Å	*c* = 14.26034(35) Å	wR = 3.221 %	Zero = 1.2905(6)		
Atom	**x**	**y**	**Z**	**SOF**	**ADP**
Li1	0.0000	0.0000	0.0000	1.000	0.01
Co1	0.0000	0.0000	0.5000	0.333	0.0156(7)
Ni1	0.0000	0.0000	0.5000	0.333	0.0156(7)
Mn1	0.0000	0.0000	0.5000	0.333	0.0156(7)
O1	0.0000	0.0000	0.2446(2)	1.000	0.0037(11)

Table S2. *Refinement parameters of the NMC111 model, with (a) K introduced onto the Li site; (b) 0.1 K introduced onto the TM site and 0.1 Ni cation mixing onto the Li site; (c) no K in the system, with 0.05 Ni cation mixing onto the Li site; and (d) no Ni cation mixing onto the Li site and 0.9 Li site occupancy factor (SOF) Space group = R-3m and the number of refinable parameters = 5. Values with no error in brackets () were not refined.*

(a) "$Li_{0.9}K_{0.1}(Ni_{0.33}Mn_{0.33}Co_{0.33})O_2$" (Li site)

a = 2.86576(4) Å *c* = 14.27406(16) Å wR = 3.730 % Zero = 1.2743(16)

Atom	x	y	Z	SOF	ADP
Li1	0.0000	0.0000	0.0000	0.890(2)	0.0679(27)
Co1	0.0000	0.0000	0.5000	0.333	0.0148(5)
Ni1	0.0000	0.0000	0.5000	0.333	0.0148(5)
Mn1	0.0000	0.0000	0.5000	0.333	0.0148(5)
O1	0.0000	0.0000	0.2437(1)	1.000	0.0028(9)
K1	0.0000	0.0000	0.0000	0.110(2)	0.0679(27)

(b) "$Li_{0.9}K_{0.1}(Ni_{0.33}Mn_{0.33}Co_{0.33})O_2$" (TM site)

a = 2.86577(5) Å *c* = 14.27478(17) Å wR = 3.808 % Zero = 1.2743(16)

Atom	x	y	Z	SOF	ADP
Li1	0.0000	0.0000	0.0000	0.900	0.1057(26)
Ni2	0.0000	0.0000	0.0000	0.100	0.1057(26)
Co1	0.0000	0.0000	0.5000	0.333	0.0084(5)
Ni1	0.0000	0.0000	0.5000	0.233	0.0084(5)
Mn1	0.0000	0.0000	0.5000	0.333	0.0084(5)
O1	0.0000	0.0000	0.2439(1)	1.000	0.0066(9)
K1	0.0000	0.0000	0.5000	0.100	0.0099(10)

(c) "$Li_{0.9}K_{0.1}(Ni_{0.33}Mn_{0.33}Co_{0.33})O_2$" (No site)

a = 2.86576(5) Å *c* = 14.27383(17) Å wR = 3.715 % Zero = 1.2743(16)

Atom	x	y	Z	SOF	ADP
Li1	0.0000	0.0000	0.0000	0.900	0.0342(26)
Ni2	0.0000	0.0000	0.0000	0.050	0.0342(26)
Co1	0.0000	0.0000	0.5000	0.333	0.0084(5)
Ni1	0.0000	0.0000	0.5000	0.283	0.0084(5)
Mn1	0.0000	0.0000	0.5000	0.333	0.0084(5)
O1	0.0000	0.0000	0.2439(1)	1.000	0.0066(9)

(d) "$Li_{0.9}K_{0.1}(Ni_{0.33}Mn_{0.33}Co_{0.33})O_2$" (No site, no mixing)

a = 2.86565(5) Å *c* = 14.27438(17) Å wR = 4.140 % Zero = 1.2743(16)

Atom	x	y	Z	SOF	ADP
Li1	0.0000	0.0000	0.0000	0.900	0.0100
Co1	0.0000	0.0000	0.5000	0.333	0.0047(6)
Ni1	0.0000	0.0000	0.5000	0.333	0.0047(6)
Mn1	0.0000	0.0000	0.5000	0.333	0.0047(6)
O1	0.0000	0.0000	0.2473(2)	1.000	0.0115(10)

Table S3. *Refinement parameters of the NMC111 model, with (a) Cs introduced onto the Li site; (b) 0.1 Cs introduced onto the TM site and 0.1 Ni cation mixing onto the Li site; (c) no Cs in the system, with 0.05 Ni cation mixing onto the Li site; and (d) no Ni cation mixing onto the Li site and 0.9 Li site occupancy factor (SOF) Space group = R-3m and the number of refinable parameters = 5. Values with no error in brackets () were not refined.*

(a) "$Li_{0.9}Cs_{0.1}(Ni_{0.33}Mn_{0.33}Co_{0.33})O_2$" (Li site)

a = 2.86734(9) Å	*c* = 14.26197(68) Å	wR = 4.483 %	Zero = 1.2777(11)	
Atom	**x**	**Y**	**Z**	**SOF**	**ADP**
Li1	0.0000	0.0000	0.0000	0.911(2)	0.02
Co1	0.0000	0.0000	0.5000	0.333	0.0457(15)
Ni1	0.0000	0.0000	0.5000	0.333	0.0457(15)
Mn1	0.0000	0.0000	0.5000	0.333	0.0457(15)
O1	0.0000	0.0000	0.2423(4)	1.000	0.0112(22)
Cs1	0.0000	0.0000	0.0000	0.089(2)	0.02

(b) "$Li_{0.9}Cs_{0.1}(Ni_{0.33}Mn_{0.33}Co_{0.33})O_2$" (TM site)

a = 2.86735(8) Å	*c* = 14.26190(23) Å	wR = 4.836 %	Zero = 1.2777(11)	
Atom	**x**	**y**	**Z**	**SOF**	**ADP**
Li1	0.0000	0.0000	0.0000	0.900	0.1083(86)
Ni2	0.0000	0.0000	0.0000	0.100	0.1083(86)
Co1	0.0000	0.0000	0.5000	0.333	0.0483(17)
Ni1	0.0000	0.0000	0.5000	0.233	0.0483(17)
Mn1	0.0000	0.0000	0.5000	0.333	0.0483(17)
O1	0.0000	0.0000	0.2456(4)	1.000	0.0100
Cs1	0.0000	0.0000	0.5000	0.100	0.0483(17)

(c) "$Li_{0.9}Cs_{0.1}(Ni_{0.33}Mn_{0.33}Co_{0.33})O_2$" (No site)

a = 2.86736(7) Å	*c* = 14.26177(21) Å	wR = 4.388 %	Zero = 1.2777(11)	
Atom	**x**	**y**	**Z**	**SOF**	**ADP**
Li1	0.0000	0.0000	0.0000	0.900	0.0562(54)
Ni2	0.0000	0.0000	0.0000	0.050	0.0562(54)
Co1	0.0000	0.0000	0.5000	0.333	0.0209(10)
Ni1	0.0000	0.0000	0.5000	0.283	0.0209(10)
Mn1	0.0000	0.0000	0.5000	0.333	0.0209(10)
O1	0.0000	0.0000	0.2449(3)	1.000	0.0218(18)

(d) "$Li_{0.9}Cs_{0.1}(Ni_{0.33}Mn_{0.33}Co_{0.33})O_2$" (No site, no mixing)

a = 2.86736(8) Å	*c* = 14.26165(23) Å	wR = 4.633 %	Zero = 1.2777(11)

Atom	x	y	Z	SOF	ADP
Li1	0.0000	0.0000	0.0000	0.900	0.0100
Co1	0.0000	0.0000	0.5000	0.333	0.0067(10)
Ni1	0.0000	0.0000	0.5000	0.333	0.0067(10)
Mn1	0.0000	0.0000	0.5000	0.333	0.0067(10)
O1	0.0000	0.0000	0.2453(3)	1.000	0.0100