Support Information

LiNi_{0.8}Co_{0.15}Al_{0.05}O₂ (NCA) Cathode Material: New Insights via ⁷Li and ²⁷Al MAS NMR Spectroscopy

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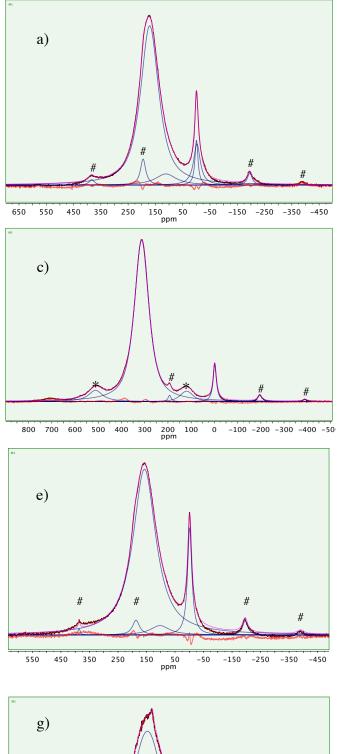
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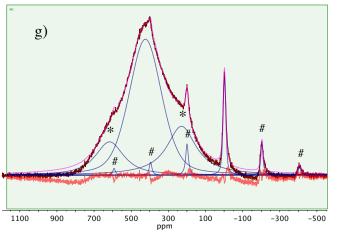
	Sample	Main Resonances (ppm)		Sample	Main Resonances (ppm)
a)	1A	0, ~500	b)	1B	0, ~500
	2A	0, 171, 111		2B	0, 36
	3A	0, 313		3B	0, 376
	4A	0, ~450		4B	0, ~500
	5A	0, 157, 102		5B	0, 84
	6A	0, ~430		6B	0, ~500
	7A	0, ~430			

Table S1: ⁷Li resonance shift values of NCA samples from (a) protocol A and (b) protocol B. The values listed for samples 1A, 4A, 6A, 7A, 1B, 4B and 6B are approximate measurements of the centers of the broad signals. The values given for samples 2A, 3A, 5A, 2B, 3B and 5B are precise.

	<u>-</u> Sample	Main Resonances (ppm)		sample	Main Resonances (ppm)
a)	1A	-970, -1180	b)	1B	-979, -1084
/	2A	0, -40	,	2B	-36, 20
	3A	0, -86, -338		3B	-81
	4A	-4 -575		4B	-972, -1077
	5A	-8, -100		5B	-21, 19
	6A	-32, -440		6B	-969, -1075
	7A	0, -484			

Table S2: Approximate ²⁷Al resonance shift values of NCA samples from (a) protocol A and (b) protocol B.





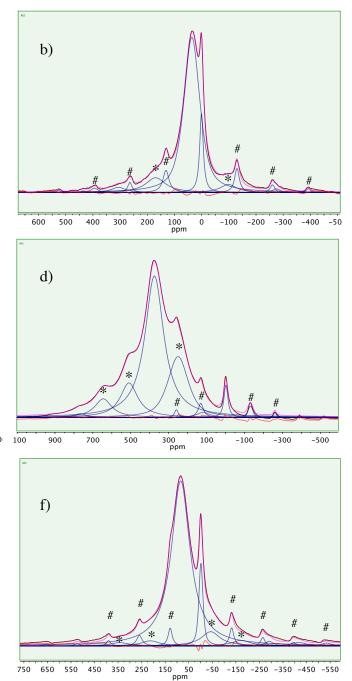


Figure S1: Line deconvolutions of samples 2A, 3A, 5A, 2B, 3B & 5B. Main peaks & peak widths (aside from the 0 ppm peak seen in all samples): a) 2A: 171 ppm (6.2kHz) + shoulder 111 ppm (ratio to main peak 1:12); b) 2B: 36 ppm (5.4kHz); c) 3A: 313 ppm (5.9kHz); d) 3B: 376 ppm (9.3kHz); e) 5A: 157 ppm (7.5kHz) + shoulder at 102 ppm (ratio to main peak 1:20); f) 5B 84 ppm (7.4kHz); g) example of 'approximate' fitting of re-lithiated sample (7A). Sidebands of the broad peaks are indicated by asterisks (*), sidebands of the 0 ppm peak indicated by crosshatch (#). Spectra in dark red, line deconvolutions in blue, line fit summary in pink, line/fitting difference in light red.

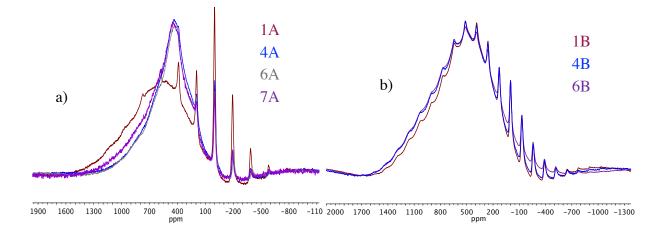


Figure S2: ⁷Li single pulse spectra of pristine and re-lithiated samples a) 1A, 4A, 6A and 7A; and b) 1B, 4B & 6B, normalized to equal intensities and superimposed to highlight similarities/differences in spectra upon cycling and re-lithiation.

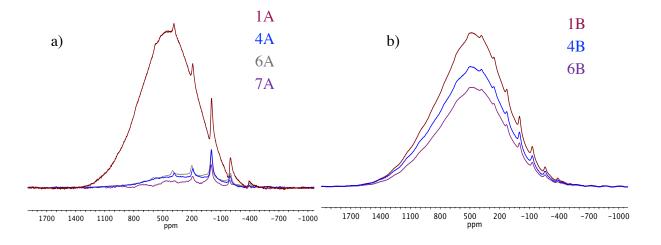


Figure S3: ⁷Li Hahn-echo spectra of pristine and re-lithiated samples a) 1A, 4A, 6A and 7A; and b) 1B, 4B & 6B, collected with identical parameters including number of scans, and normalized to mass of sample, superimposed to highlight similiarites/differences in each group of spectra.

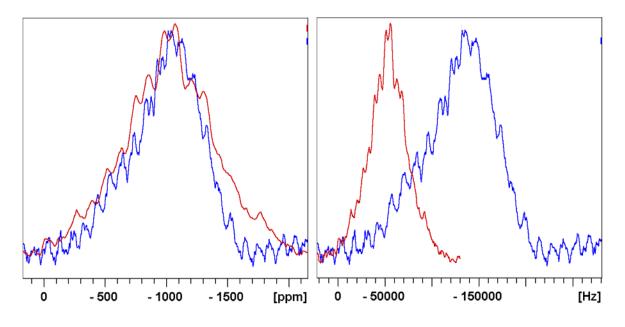


Figure S4 (left) ²⁷Al solid-echo spectra (drawn on a ppm scale) of sample 1B measured at a field of 11.74 T (blue) and at a field of 4.7 T (red). Exponential multiplication of 1000 Hz is used here to show that the spectrum at 4.7 T is identical to that shown in Figure 3 sample 1B. (right) ²⁷Al solid-echo spectra (drawn on a Hertz scale) of sample 1B measured at a field of 11.74 T (blue) and at a field of 4.7 T (red).

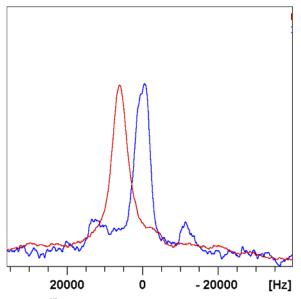


Figure S5 ²⁷Al solid-echo spectra (drawn on a Hertz scale) of sample 5B measured at a field of 11.74 T (red) and at a field of 4.7 T (blue).