

Support Information

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

Nicole Leifer, Onit Srur-Lavi, Irina Matlahov, Boris Markovsky, Doron Aurbach, Gil Goobes*

Department of Chemistry, Bar Ilan University, Ramat Gan 5290002, Israel.

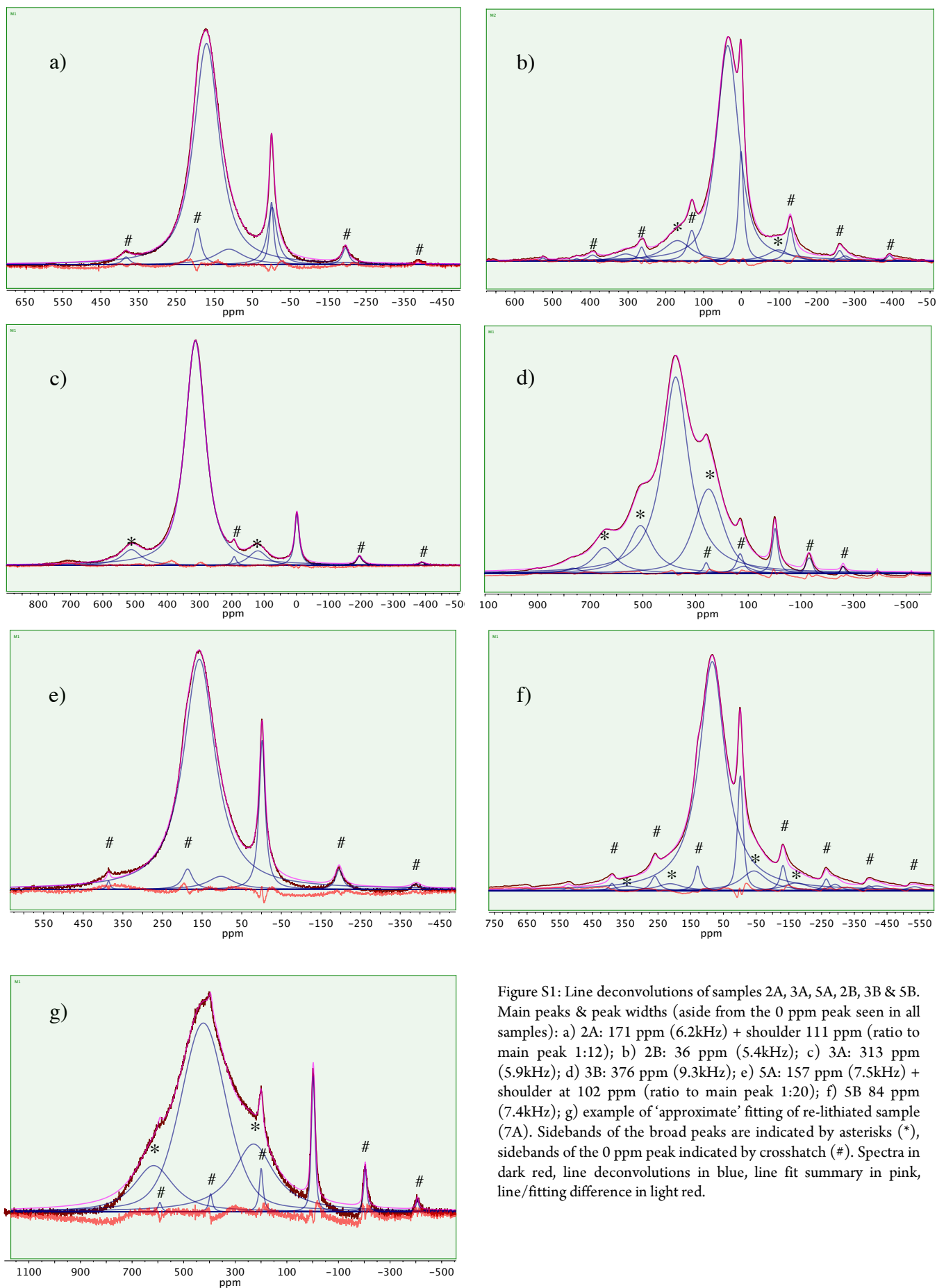
Corresponding Author *Email: gil.goobes@biu.ac.il

a)	□		b)	□	
	Sample	Main Resonances (ppm)		Sample	Main Resonances (ppm)
	1A	0, ~500		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.

a)	□		b)	□	
	Sample	Main Resonances (ppm)		Sample	Main Resonances (ppm)
	1A	-970, -1180		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 ^{27}Al resonance shift values of NCA samples from (a) protocol A and (b) protocol B.



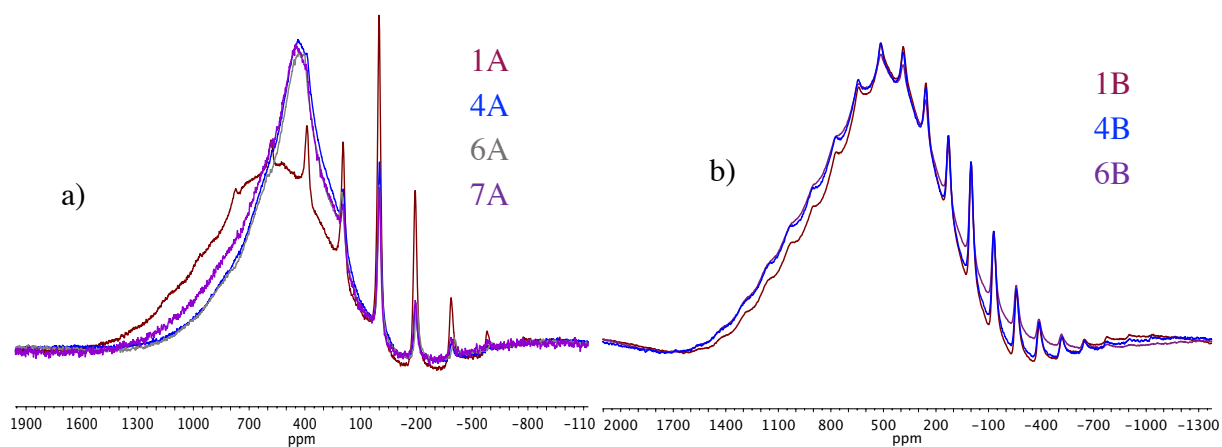


Figure S2: ^7Li single pulse spectra of pristine and re-lithiated samples a) 1A, 4A, 6A and 7A; and b) 1B, 4B & 6B, normalized to equal intensities and superimposed to highlight similarities/differences in spectra upon cycling and re-lithiation.

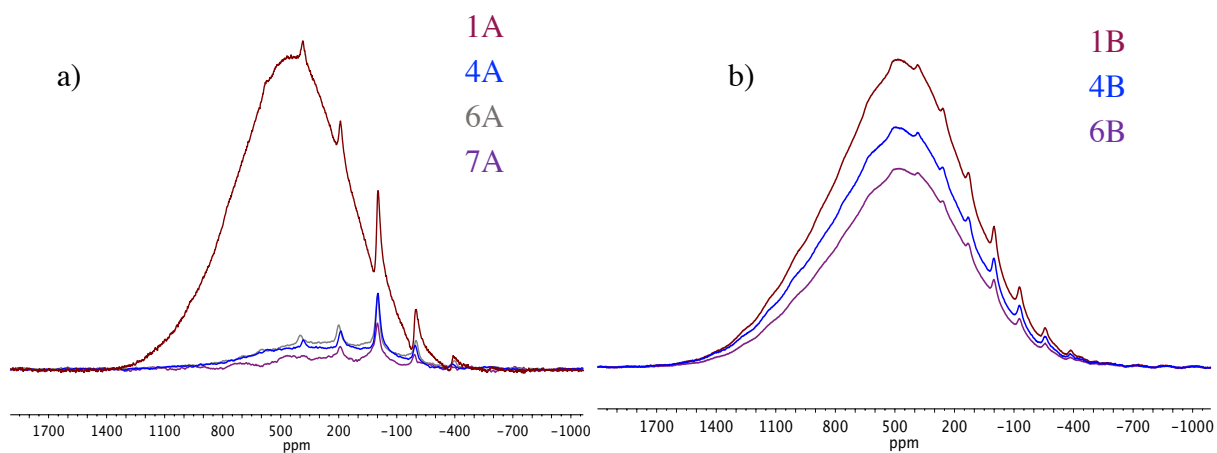


Figure S3: ^7Li Hahn-echo spectra of pristine and re-lithiated samples a) 1A, 4A, 6A and 7A; and b) 1B, 4B & 6B, collected with identical parameters including number of scans, and normalized to mass of sample, superimposed to highlight similarities/differences in each group of spectra.

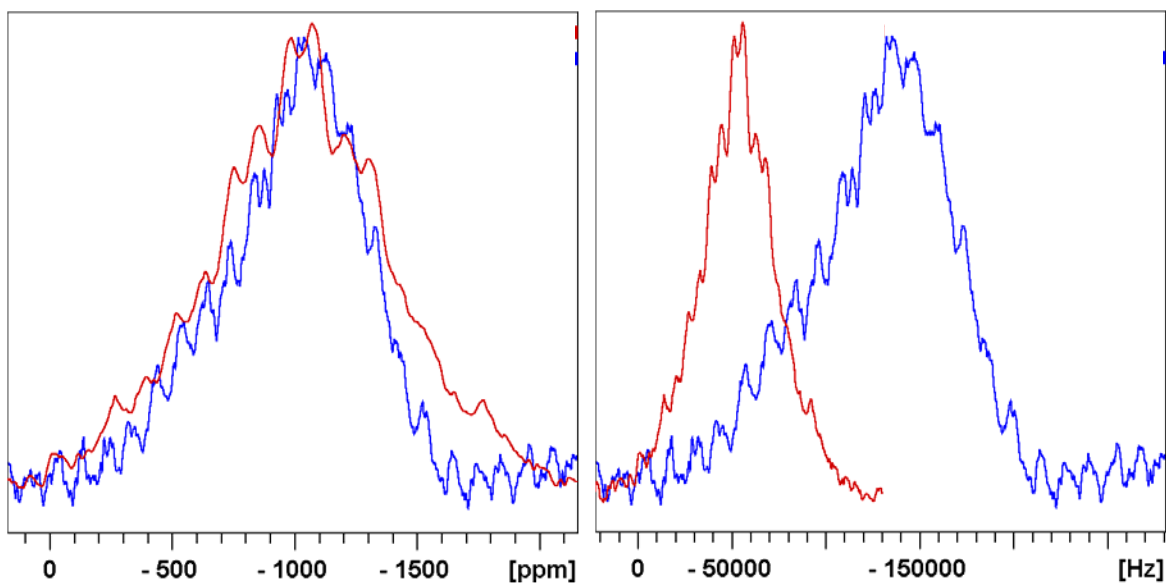


Figure S4 (left) ^{27}Al solid-echo spectra (drawn on a ppm scale) of sample 1B measured at a field of 11.74 T (blue) and at a field of 4.7 T (red). Exponential multiplication of 1000 Hz is used here to show that the spectrum at 4.7 T is identical to that shown in Figure 3 sample 1B. (right) ^{27}Al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

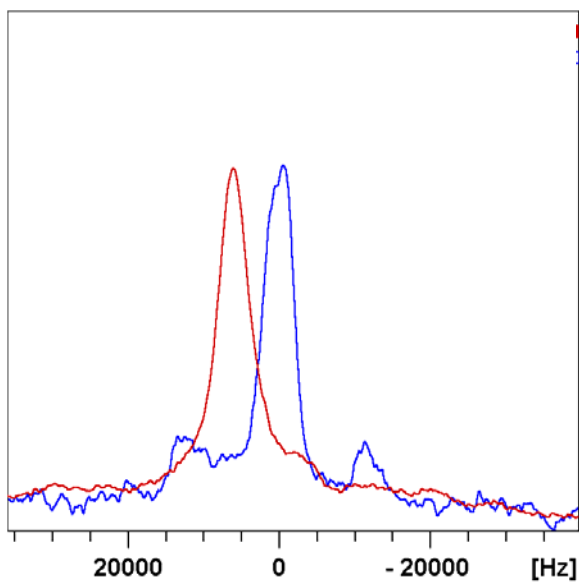


Figure S5 ^{27}Al solid-echo spectra (drawn on a Hertz scale) of sample 5B measured at a field of 11.74 T (red) and at a field of 4.7 T (blue).