

Supporting Information

Table 1.
Elemental analysis data for the various samples

Sample	Na/Al	Li/Al	(Na+Li)/Al	Na/(Na+Li)	Li/(Na+Li)
100% Li	0.00	0.96±.03	0.96±0.03	0.00	1.00±.03
86% Li : 14%Na	0.13±.01	0.80±.03	0.93±0.03	0.14±.01	0.86±.02
76% Li : 24% Na	0.23±.01	0.71±.03	0.94±0.03	0.24±.01	0.76±.02
61% Li : 39% Na	0.38±.01	0.59±.02	0.97±0.03	0.39±.01	0.61±.02
58% Li : 42% Na	0.39±.01	0.54±.02	0.93±0.03	0.42±.01	0.58±.01
20% Li : 80% Na	0.73±.03	0.19±.01	0.92±0.03	0.80±.02	0.20±.01
9% Li : 91% Na	0.90±.03	0.09±.01	0.99±0.03	0.91±.02	0.09±.01
100% Na	1.02±.04	0.00	1.02±0.04	1.00±.03	0.00

Table 2.
Selected bond distances and angles for lithium chabazite

Bond distances (Å)		Bond angles (degrees)	
T-O(1)	1.601 (10)	T-O(1)-T	138.1 (8)
T-O(2)	1.640 (8)	T-O(2)-T	171.0 (8)
T-O(3)	1.674 (11)	T-O(3)-T	134.9 (8)
T-O(4)	1.679 (9)	T-O(4)-T	128.0 (8)
Li(1)- O(4)	1.960 (10)		
Li(1)-O(3)	2.986 (8)		
Li(1)-Li(2)	3.98 (7)		
Li(2)-O(1)	2.02 (10)		
Li(2)-O(1)	3.13 (12)		
Li(2)-O(2)	2.88 (10)		
Li(2)-O(2)	3.45 (11)		
Li(2)-O(3)	2.32 (10)		
Li(2)-O(4)	3.74 (12)		

Table 3.

Selected bond distances and angles for mixed sodium-lithium
chabazite

Bond distances (Å)		Bond angles (degrees)	
T-O(1)	1.633 (10)	T-O(1)-T	139.5 (7)
T-O(2)	1.634 (8)	T-O(2)-T	170.1 (8)
T-O(3)	1.642 (10)	T-O(3)-T	137.2 (8)
T-O(4)	1.668 (8)	T-O(4)-T	130.0 (8)
Li(1)-O(4)	1.957 (9)		
Li(1)-O(3)	2.983 (8)		
Li(1)-Li(2)	4.929 (10)		
Li(1)-Na(1)	4.26 (9)		
Li(2)-O(1)	2.04		
Li(2)-O(2)	2.87		
Li(2)-O(3)	2.31		
Na(1)-O(1)	2.55 (8)		
Na(1)-O(2)	2.32 (8)		
Na(1)-O(2)	3.78 (8)		
Na(1)-O(3)	2.32 (8)		
Na(1)-O(4)	3.65 (9)		
Na(1)-Li(2)	2.58 (8)		

Table 4.
Isotropic chemical shift and quadrupolar coupling data from
 ^{23}Na MQMAS spectra

	SIII'a	SIII'b	SII
100% Na			
δ_{iso} (ppm)	-25.2 ± 2.1	$-10 \pm 2 - -21 \pm 2^a$	-11.7 ± 2.1
P_q (MHz)	4.0 ± 0.4	1.8 ± 0.3	5.1 ± 0.2
80% Na : 20% Li			
δ_{iso} (ppm)	-25.0 ± 1.4	$-10 \pm 1 - -18 \pm 1^a$	-11.0 ± 1.4
P_q (MHz)	3.8 ± 0.2	1.8 ± 0.4	5.0 ± 0.1
39% Na : 61% Li			
δ_{iso} (ppm)	-25.4 ± 1.4	$-15 \pm 1 - -22 \pm 1^a$	—
P_q (MHz)	4.1 ± 0.2	2.0 ± 0.3	
24% Na : 76% Li			
δ_{iso} (ppm)	-21.2 ± 1.4	—	—
P_q (MHz)	4.0 ± 0.1		

^arange of chemical shifts, see text

Figure 1.

^7Li MAS NMR spectra showing the satellite transitions belonging to the two peaks in lithiated chabazite with the central transitions truncated for clarity: a) spectral component with $\delta_{\text{iso}} = -0.37$ ppm and b) spectral component with $\delta_{\text{iso}} = -1.22$ ppm.

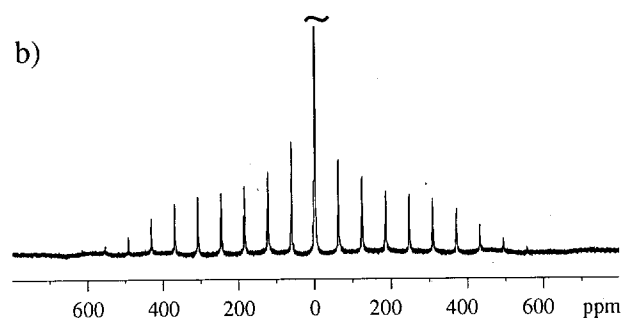
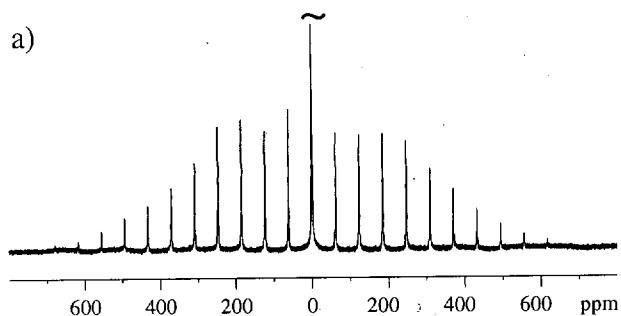


Fig 1

supporting
information