Supplementary Information for

In-situ dehydration studies of fully K-, Rb-, and Cs-exchanged natrolite

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Supplementary Table 1. Chemical composition calculated from Energy Dispersive Spectroscopy (EDS) method.

Energy Dispersive Spectroscopy (EDS)					
K-NAT					
Elements		K	Al	Si	O
Atomic percent (%)	*1*	11.85	11.15	18.12	58.89
	2	11.53	11.00	18.40	59.07
	3	11.68	11.58	17.84	58.90
	4	11.44	11.17	18.31	59.09
	5	11.37	11.41	18.14	59.08
Unit cell composition		$K_{15.69}Al_{15.26}Si_{24.62}O_{80}$ xH_2O			

Supplementary Table 2. Concentration of elements from samples investigated by Inductively Coupled Plasma (ICP).

ICP				
		K-NAT	Rb-NAT	Cs-NAT
Concentration of elements (ppm)	Al	155900	137960	104800
	Na	≤ 3*		
	K	162500	≤ 1*	≤ 1*
	Rb		273600	
	Cs			224839

*Detection limit: hundreds ppb

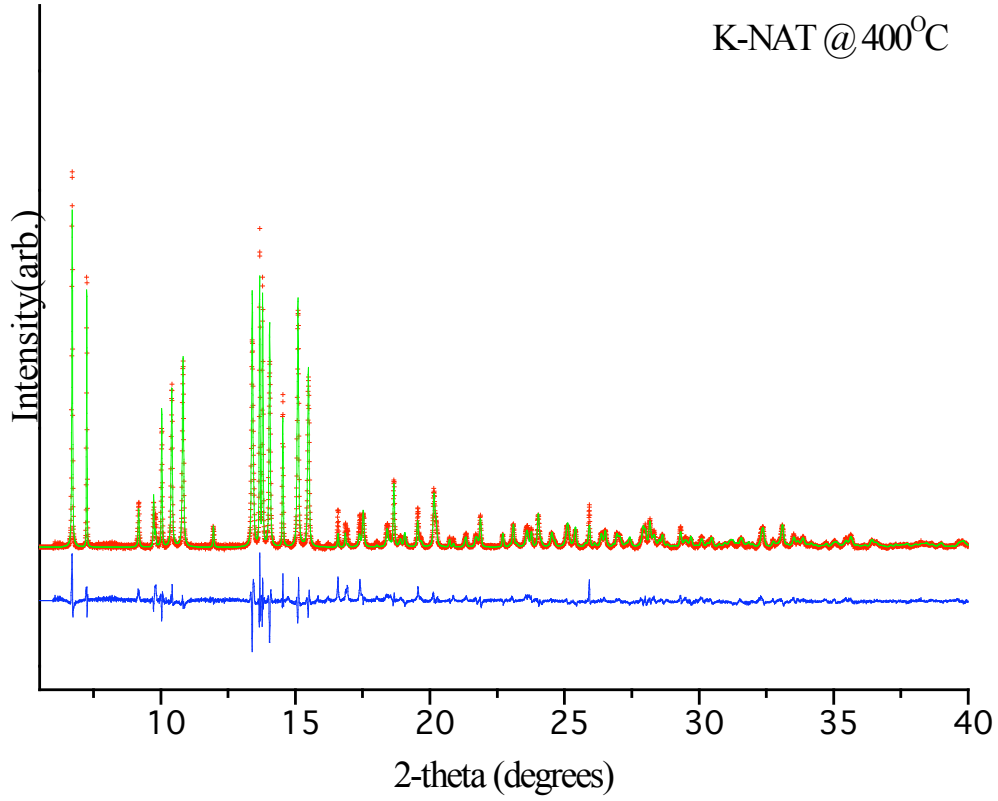
Supplementary Table 3. Final refined cell parameters for K-, Rb- and Cs-exchanged natrolite at different temperatures (* dehydrated phases)

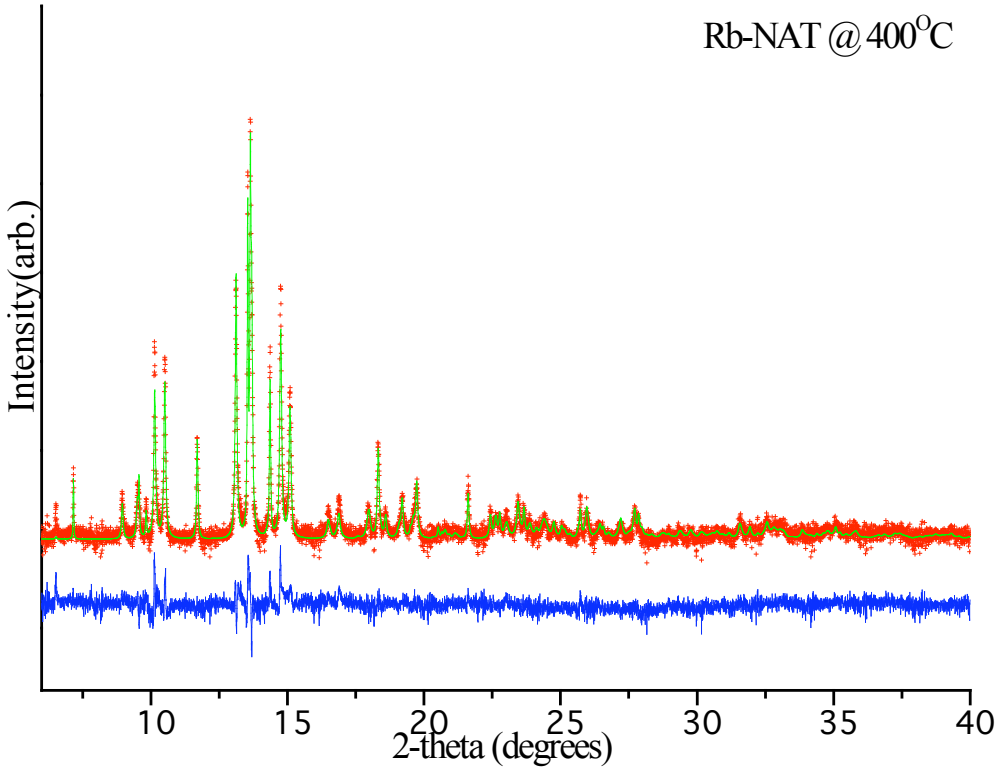
K-NAT				
Temperature (□)	cell lengths (Å)			cell volume (Å^3)
	a	*b*	*c*	*V*
25	19.2703(2)	19.7465(2)	6.48245(4)	2466.66(4)
50	19.2821(1)	19.7422(2)	6.48194(4)	2467.48(4)
75	19.2880(1)	19.7257(1)	6.48191(3)	2466.17(3)
100	19.2657(1)	19.6842(1)	6.48045(3)	2457.58(3)
125	19.2593(1)	19.6628(1)	6.47919(3)	2453.62(3)
150	19.2610(1)	19.6515(1)	6.47744(3)	2451.76(3)
175	19.2561(2) 16.9501(4)*	19.6334(2) 18.0948(4)*	6.47282(4) 6.47836(9)*	2447.14(3) 1986.96(6)*
200	19.253(1) 16.9658(3)*	19.6357(8) 18.1040(3)*	6.4693(4) 6.48236(7)*	2445.63(2) 1991.05(7)*
225	16.9796(3)*	18.1169(3)*	6.48495(7)*	1994.88(6)*
250	16.9909(2)*	18.1330(3)*	6.48732(7)*	1998.71(6)*
275	17.0087(2)*	18.1538(2)*	6.49101(6)*	2004.24(5)*
300	17.0195(3)*	18.1697(3)*	6.49393(7)*	2008.18(6)*
325	17.0305(3)*	18.1850(3)*	6.49531(8)*	2011.59(6)*
350	17.0456(3)*	18.2023(3)*	6.49911(7)*	2016.47(6)*
375	17.0624(3)*	18.2230(3)*	6.50294(7)*	2021.95(6)*
400	17.0764(4)*	18.2357(4)*	6.5046(1)*	2025.5(1)*
425	17.0934(3)*	18.2579(3)*	6.50861(8)*	2031.27(7)*
25(cooled down)	19.2205(6)	19.7537(9)	6.4860(3)	2462.6(1)

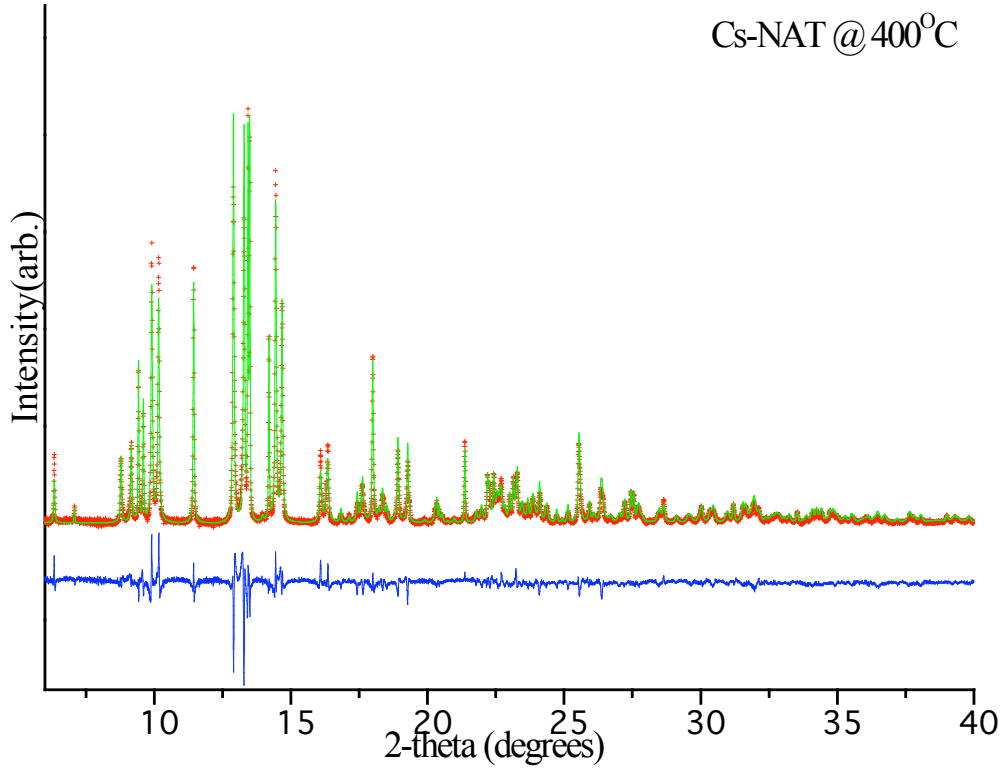
Rb-NAT				
Temperature (□)	cell lengths (Å)			cell volume (Å^3)
	a	*b*	*c*	*V*
25	19.8234(3)	19.9871(3)	6.5283(1)	2586.58(8)
50	19.8326(3)	19.9837(3)	6.5286(1)	2587.48(7)
75	19.8373(4)	19.9728(4)	6.5268(1)	2586.0(1)
100	19.8340(3)	19.9628(3)	6.5228(1)	2582.62(9)
125	19.8301(4)	19.9556(4)	6.5205(1)	2580.30(9)
150	19.8179(4) 17.418(2)*	19.9504(4) 18.511(2)*	6.5174(1) 6.5158(5)*	2576.8(3) 2100.8(2)*
175	19.809(1) 17.428(1)*	19.968(1) 18.527(1)*	6.5163(4) 6.5172(3)*	2577.6(3) 2104.3(3)*
200	17.436(1)*	18.541(1)*	6.5206(3)*	2107.9(3)*
225	17.449(1)*	18.552(1)*	6.5232(3)*	2111.6(3)*
250	17.4629(9)*	18.565(1)*	6.5262(3)*	2115.7(3)*
275	17.478(1)*	18.569(1)*	6.5291(4)*	2119.0(4)*
300	17.5013(9)*	18.595(1)*	6.5339(3)*	2126.3(3)*
325	17.519(1)*	18.604(1)*	6.5367(4)*	2130.4(4)*
350	17.542(1)*	18.626(1)*	6.5414(4)*	2137.3(4)*
375	17.562(1)*	18.645(1)*	6.5453(4)*	2143.2(4)*
400	17.608(1)*	18.687(2)*	6.5544(5)*	2156.7(5)*
425	17.625(1)*	18.706(1)*	6.5580(3)*	2162.1(3)*
25(cooled down)	17.3364(8)*	18.4601(9)*	6.5053(2)*	2081.9(2)*

Cs-NAT				
Temperature (□)	cell lengths (Å)			cell volume (Å^3)
	a	*b*	*c*	*V*
25	20.2894(1)	19.9982(1)	6.5574(1)	2660.67(3)
50	20.2802(1)	20.0051(1)	6.5581(1)	2660.66(3)
75	20.2621(1)	20.0193(1)	6.5593(1)	2660.68(4)
100	20.2874(9) 18.0872(5)*	19.9866(7) 18.9867(5)*	6.5634(3) 6.5722(1)*	2661.3(2) 2257.0(1)*
125	18.1018(4)*	19.0019(4)*	6.5843(1)*	2264.8(1)*
150	18.1208(4)*	19.0102(4)*	6.5921(1)*	2270.8(1)*
175	18.1365(4)*	19.0133(4)*	6.5943(1)*	2273.9(1)*
200	18.1495(3)*	19.0148(4)*	6.5954(1)*	2276.1(1)*
225	18.1652(3)*	19.0188(4)*	6.5966(1)*	2279.0(1)*
250	18.1792(3)*	19.0218(4)*	6.5970(1)*	2281.2(1)*
275	18.1954(5)*	19.0295(5)*	6.5983(2)*	2284.7(2)*
300	18.2074(4)*	19.0318(4)*	6.5984(1)*	2286.4(1)*
325	18.2218(3)*	19.0374(4)*	6.5988(1)*	2289.1(1)*
350	18.2338(4)*	19.0412(4)*	6.5986(1)*	2291.0(1)*
375	18.2436(4)*	19.0481(4)*	6.5994(1)*	2293.3(1)*
400	18.2685(5)*	19.0488(5)*	6.6020(1)*	2297.4(2)*
425	18.2802(4)*	19.0653(4)*	6.6031(1)*	2301.3(1)*
25(cooled down)	18.0095(3)*	18.9510(4)*	6.5658(1)*	2240.90(8)*

Supplementary Figure 1. Results of Rietveld refinements of the structural models of K-, Rb-, and Cs-NAT at 400 °C using synchrotron X-ray powder diffraction data. Points shown represent the observed data. The continuous lines through the sets of points are the calculated profiles from the structure refinements summarized in Tables 1-2. The lower curves represents the differences between observed and calculated profiles (I_{obs} - I_{calc}) plotted on the same scale as the observed data.




Rb-NAT @ 400°C
Intensity(arb.)
10
15
20
25
30
35
40
2-theta (degrees)


Cs-NAT @ 400°C
Intensity(arb.)
10
15
20
25
30
35
40
2-theta (degrees)