Supporting Information for the manuscript

Dehydration studies of natrolites with monovalent extra framework cations

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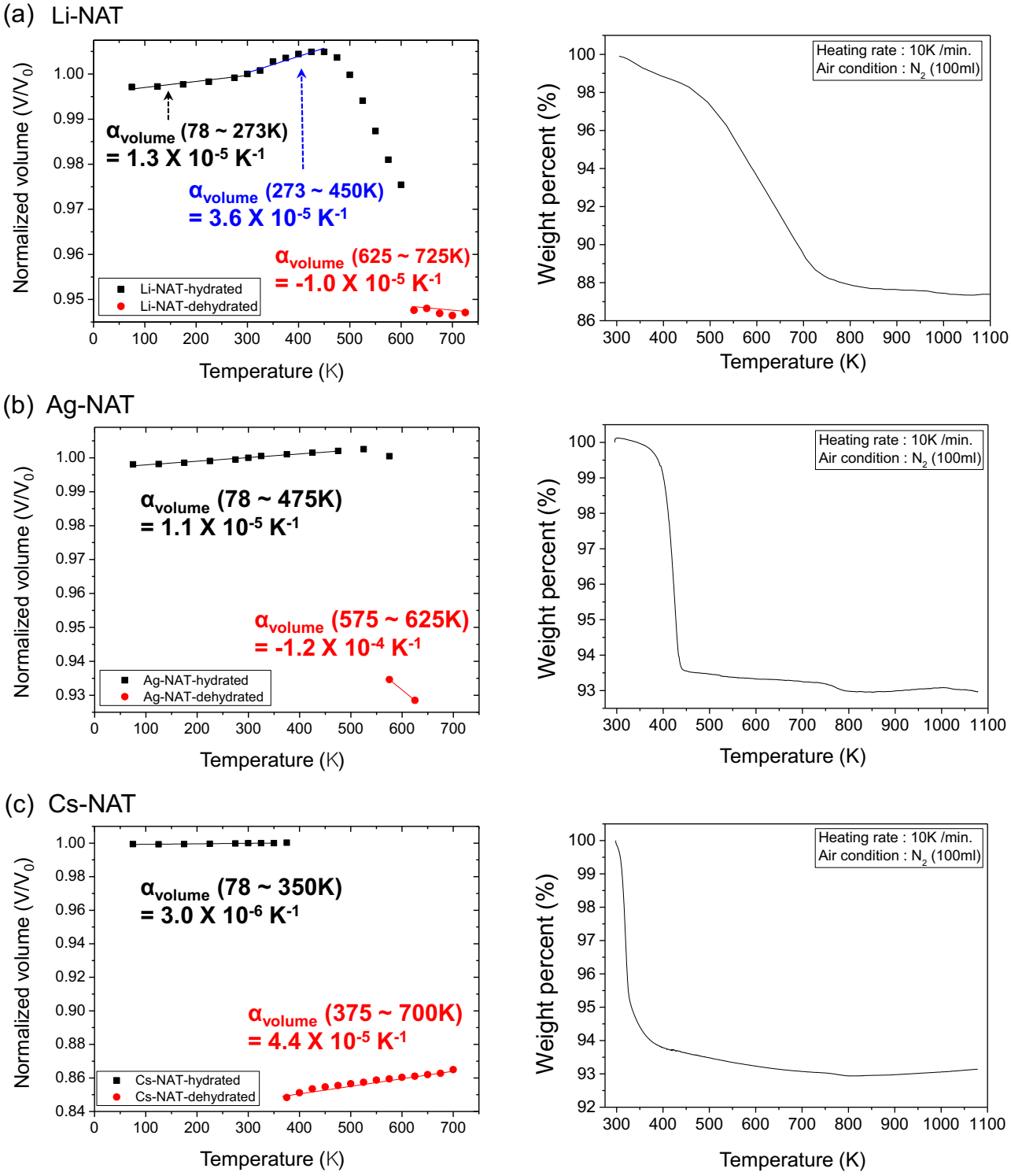
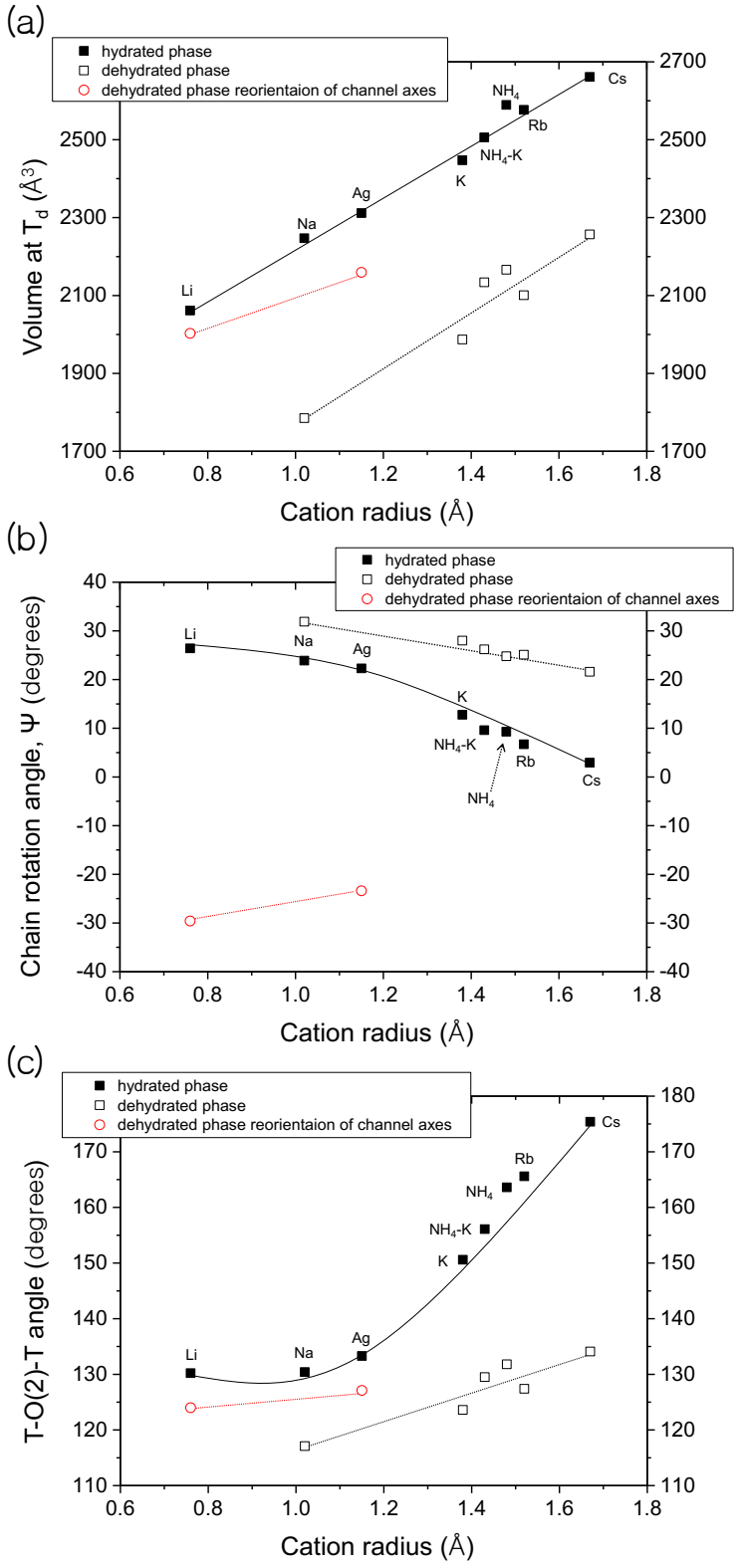
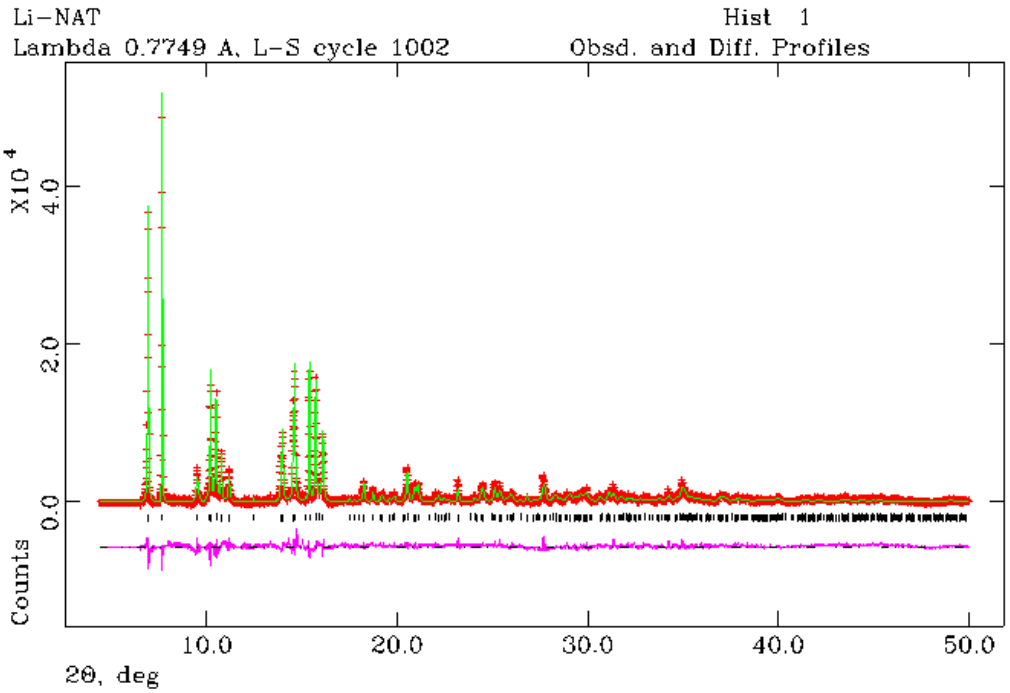
Supporting Figure 1. (Left) Temperature-induced unit cell volume (Å^3) changes of the (a) Li-NAT, (b) Ag-NAT, (c) Cs-NAT. From 75 K to 725 K, the temperature was increased by 25 K or 50 K increments under a low vacuum. The increment (or decrement) was achieved by a heating (or cooling) rate of ca. 25K/min and the temperature was then stabilized during ca. 10 min before a measurement. All the unit cell volumes are normalized to that at 300K. (Right) Thermal Gravity Analysis results of the (a) Li-NAT, (b) Ag-NAT, (c) Cs-NAT. A heating rate of 10K/min under nitrogen atmosphere was used. Black and red symbols indicate hydrated and dehydrated states, respectively. Estimated standard deviations (esd's) are smaller than the size of each symbol.

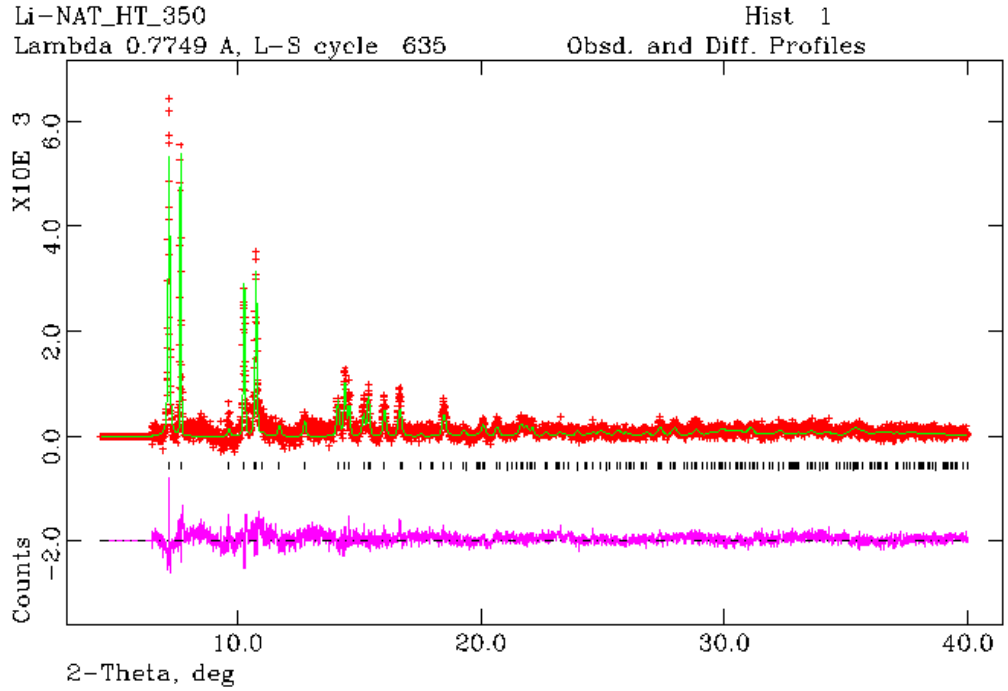


Supporting Figure 2. Changes in the (a) unit cell volume at T_d, (b) chain rotation angle and (c) T-O(2)-T angle of cation-substituted natrolite as a function of cation size. Labels indicate each cation-substituted natrolite. Filled and opened symbols represent hydrated and dehydrated phases, respectively. All straight and curved lines are guides to the eyes.

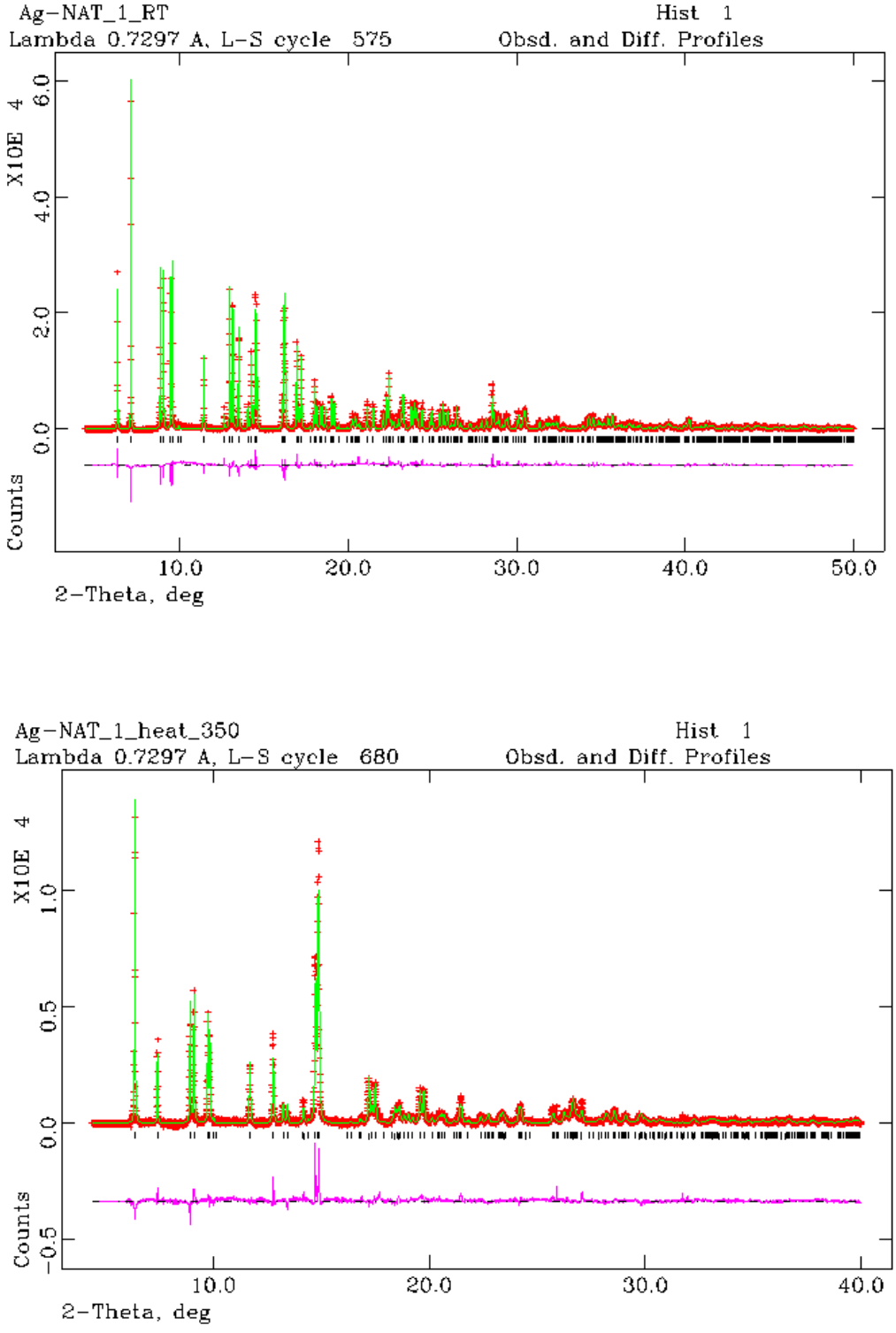


Supporting Figure 3. Rietveld refinement fits of the structural models of the Li-NAT at ambient (Li-NAT-hyd, top) and at 350˚C (625K, Li-NAT-deh, bottom) using synchrotron X-ray powder diffraction data. Backgrounds were subtracted. Red points shown represent the observed data. The green continuous lines through the sets of points are the calculated profiles from the structure refinements summarized in Supporting Tables 1 and 2. The sets of black tic marks below the data indicate the positions of the allowed reflections. The lower purple curves represents the differences between observed and calculated profiles (I_{obs} - I_{calc}) plotted on the same scale as the observed data.





Supporting Figure 4. Rietveld refinement fits of the structural models of the Ag-NAT at ambient (Ag-NAT-hyd, upper) and at 350˚C (625K, Ag-NAT-deh, lower) using synchrotron X-ray powder diffraction data. Backgrounds were subtracted. Red points shown represent the observed data. The green continuous lines through the sets of points are the calculated profiles from the structure refinements summarized in Supporting Tables 1 and 2. The sets of black tic marks below the data indicate the positions of the allowed reflections. The lower purple curves represents the differences between observed and calculated profiles (I_{obs} - I_{calc}) plotted on the same scale as the observed data.



Supporting Table 1. Refined atomic coordinates for Li- , Ag-, K-, NH_4K-, NH_4-, Rb- and Cs-NAT under ambient condition (-hyd) and at 625K (-deh).[a]

		Li-NAT -hyd	Li-NAT -deh	Ag-NAT -hyd	Ag-NAT -deh	K-NAT -hyd[c]	K-NAT -deh[d]	NH_4K-NAT -hyd[c]	NH_4K –NAT -deh[d]	NH_4-NAT -hyd[c]	NH_4 –NAT -deh[d]	Rb-NAT -hyd[c]	Rb-NAT -deh[d]	Cs-NAT -hyd[c]	Cs-NAT -deh[d]
Space Group		**F***dd2*	**F***dd2*	**F***dd2*	**F***dd2*	**F***dd2*	**F***dd2*	**F***dd2*	**F***dd2*	**F***dd2*	**F***dd2*	**F***dd2*	**F***dd2*	**F***dd2*	**F***dd2*
$_wR_p$ (%), χ^2		4.99, 12.6	3.18, 3.32	6.74, 11.9	3.84, 3.24	10.7, 6.2	7.1, 5.5	14.8, 2.6	7.3, 11.9	12.0, 14.1	8.6, 5.5	9.6, 2.87	1.4, 2.4	13.0, 3.83	6.1, 6.5
Unit cell composition		$Li_{16}Al_{16}Si_{24}O_{80}$ x $16H_2O$	$Li_{16}Al_{16}Si_{24}O_{80}$	$Ag_{15.4(1)}Al_{16}Si_{24}O_{80}$ x $16H_2O$	$Ag_{16}Al_{16}Si_{24}O_{80}$	$K_{15.5(2)}Al_{16}Si_{24}O_{80}$ x $14.0(2)H_2O$	$K_{16}Al_{16}Si_{24}O_{80}$	$(NH4)_{5.1(1)}K_{10.9(1)}Al_{16}Si_{24}O_{80}$ x$15.7(3)H_2O$	$(NH4)_{5.3(1)}K_{10.7(1)}Al_{16}Si_{24}O_{80}$	$(NH4)_{16(2)}Al_{16}Si_{24}O_{80}$ x$14.1(9)H_2O$	$(NH_4)_{16}Al_{16}Si_{24}O_{80}$	$Rb_{14.8(2)}Al_{16}Si_{24}O_{80}$ x$17.6(9)H_2O$	$Rb_{16}Al_{16}Si_{24}O_{80}$	$Cs_{14.6(5)}Al_{16}Si_{24}O_{80}$ x$14.7(1)H_2O$	$Cs_{16}Al_{16}Si_{24}O_{80}$
Cell Parameters (Å)	*a*	17.5535(7)	16.645(2)	18.5560(2)	18.3568(6)	19.2743(2)	17.0764(4)	19.5553(2)	17.4722(5)	19.8423(1)	17.8804(6)	19.8409(1)	17.608(1)	19.9776(1)	18.2685(5)
	b	18.6567(5)	18.373(2)	18.9264(2)	18.7419(6)	19.7527(2)	18.2357(4)	19.9442(2)	18.5303(4)	20.0652(1)	18.5782(6)	20.0115(1)	18.687(2)	20.2977(1)	19.0488(5)
	c	6.4767(1)	6.5491(6)	6.57899(6)	6.2356(2)	6.4807(1)	6.5046(1)	6.4951(1)	6.5429(1)	6.51942(5)	6.5525(2)	6.5378(1)	6.5544(5)	6.5570(1)	6.6020(1)
($Å^3$)	*V*	2121.1(1)	2002.7(5)	2310.53(4)	2145.3(2)	2467.33(7)	2025.5(1)	2533.19(5)	2118.4(1)	2595.65(4)	2176.6(1)	2595.79(5)	2156.7(5)	2658.84(3)	2297.4(2)
Si(1) 8a	*x*	0	0	0	0	0	0	0	0	0	0	0	0	0	0
	y	0	0	0	0	0	0	0	0	0	0	0	0	0	0
	z	0	0	0	0	0	-0.0005(6)	0.006(1)	-0.0610(8)	-0.018(1)	-0.0560(7)	0	0.0072(5)	0	0.0045(7)
	U_{iso}[b]	0.0109(4)	0.004(2)	0.0041(8)	0.002(1)	0.0142(5)	0.0117(4)	0.0043(5)	0.0165(6)	0.0154(4)	0.0205(7)	0.0145(4)	0.016(3)	0.0089(6)	0.013(1)
Si(2) 16b	*x*	0.1454(3)	0.2219(4)	0.1555(2)	0.2047(3)	0.1687(1)	0.1444(3)	0.1723(1)	0.1459(2)	0.1734(1)	0.1486(3)	0.1743(1)	0.1460(3)	0.1784(1)	0.1548(3)
	y	0.2206(2)	0.1477(3)	0.2089(2)	0.1590(3)	0.1971(1)	0.2224(2)	0.1935(1)	0.2186(2)	0.1898(1)	0.2166(2)	0.1916(1)	0.2151(3)	0.1892(1)	0.2094(3)
	z	0.6264(9)	0.6135(8)	0.6171(9)	0.6206(9)	0.6210(5)	0.6200(5)	0.6271(9)	0.5514(7)	0.6015(8)	0.5638(5)	0.6194(5)	0.6256(5)	0.6231(8)	0.6231(5)
Al(1) 16b	*x*	0.0325(2)	0.1085(3)	0.0392(2)	0.0962(3)	0.0542(1)	0.0357(2)	0.057(1)	0.0339(2)	0.0593(1)	0.0351(2)	0.0581(1)	0.0385(3)	0.0612(1)	0.0430(3)
	y	0.0944(2)	0.0224(3)	0.0917(2)	0.0385(3)	0.0786(1)	0.0961(2)	0.0747(1)	0.0936(2)	0.0729(1)	0.0933(3)	0.0736(1)	0.0903(3)	0.0718(1)	0.0888(2)
	z	0.6153(9)	0.6092(8)	0.6147(8)	0.6058(9)	0.6165(5)	0.6136(5)	0.6198(9)	0.5475(7)	0.5952(8)	0.5553(5)	0.6121(5)	0.6142(4)	0.6141(8)	0.6158(4)
O(1) 16b	*x*	0.0081(4)	0.0796(2)	0.0287(4)	0.0546(4)	0.0505(2)	0.0303(3)	0.0505(2)	0.0222(3)	0.0473(2)	0.0168(4)	0.0430(2)	0.0294(6)	0.0347(3)	0.0311(4)
	y	0.0749(2)	-0.0018(5)	0.0668(2)	0.0481(3)	0.0479(2)	0.0688(2)	0.0467(2)	0.069(1)	0.0471(2)	0.0707(2)	0.0523(1)	0.0660(3)	0.0568(2)	0.0625(3)
	z	0.873(1)	0.8571(9)	0.869(1)	0.8562(9)	0.8681(6)	0.8668(6)	0.8715(9)	0.8002(8)	0.8475(9)	0.8077(6)	0.8656(6)	0.8682(5)	0.8627(9)	0.8645(5)
	U_{iso}[b]	0.028(1)	0.009(3)	0.001(1)	0.010(2)	0.0110(7)	0.054(2)	0.019(1)	0.014(1)	0.0158(7)	0.025(1)	0.0204(7)	0.041(6)	0.011(1)	0.027(2)
O(2) 16b	*x*	0.0615(3)	0.2047(3)	0.0747(3)	0.1835(3)	0.0978(1)	0.0565(2)	0.1049(2)	0.0617(3)	0.1108(2)	0.0662(3)	0.1120(1)	0.0627(3)	0.1194(2)	0.0749(3)
	y	0.1846(3)	0.0609(3)	0.1774(3)	0.0751(3)	0.1544(2)	0.1892(2)	0.1472(2)	0.1832(2)	0.1412(2)	0.1815(3)	0.1414(1)	0.1800(3)	0.1347(2)	0.1741(2)
	z	0.596(2)	0.607(1)	0.601(2)	0.610(2)	0.6081(10)	0.604(1)	0.603(1)	0.529(1)	0.585(1)	0.54(1)	0.6008(9)	0.597(1)	0.6194(15)	0.6054(9)
O(3) 16b	*x*	0.1065(4)	0.1020(5)	0.0974(3)	0.0995(4)	0.0958(2)	0.1094(3)	0.0965(2)	0.1042(3)	0.0961(2)	0.1035(3)	0.0988(2)	0.1086(5)	0.0988(2)	0.1027(4)
	y	0.0378(3)	-0.0530(4)	0.0333(3)	-0.0519(3)	0.0220(1)	0.0511(2)	0.0175(2)	0.0415(3)	0.0086(2)	0.0365(3)	0.0087(1)	0.0413(3)	0.0020(2)	0.0328(3)
	z	0.536(1)	0.447(1)	0.490(1)	0.538(1)	0.4549(8)	0.4821(8)	0.46(1)	0.4363(9)	0.4572(9)	0.4593(8)	0.4855(8)	0.492(1)	0.5058(12)	0.492(1)
O(4)	*x*	0.2030(3)	0.2946(4)	0.2090(3)	0.2907(3)	0.2203(1)	0.1977(3)	0.2257(2)	0.2037(3)	0.2299(2)	0.2067(3)	0.2333(1)	0.2026(4)	0.2430(2)	0.2102(3)

16b	*y*	0.1577(4)	0.1581(5)	0.1533(3)	0.1639(4)	0.1585(2)	0.1634(3)	0.1563(2)	0.1601(3)	0.156(1)	0.1577(3)	0.1536(2)	0.1590(5)	0.1526(2)	0.1575(4)
	z	0.702(1)	0.776(1)	0.727(1)	0.679(1)	0.7755(8)	0.7380(8)	0.778(1)	0.647(1)	0.745(1)	0.6514(8)	0.7419(7)	0.735(1)	0.7201(12)	0.740(1)
O(5)	*x*	0.1746(3)	0.2507(6)	0.1820(2)	0.1968(3)	0.2038(2)	0.1778(3)	0.2034(2)	0.1743(2)	0.2036(2)	0.1773(2)	0.1975(1)	0.1793(3)	0.1947(2)	0.1849(3)
16b	*y*	0.2456(4)	0.1781(2)	0.2233(4)	0.2001(4)	0.2004(2)	0.2228(3)	0.2009(2)	0.2333(3)	0.2032(2)	0.2341(4)	0.2081(2)	0.2249(6)	0.2134(3)	0.2206(5)
	z	0.396(1)	0.3930(8)	0.385(1)	0.3932(9)	0.3924(6)	0.3890(6)	0.3967(9)	0.3208(8)	0.3732(8)	0.3339(6)	0.3881(6)	0.3974(5)	0.3910(9)	0.3957(7)
M1	*x*	0.237(2)	0.187(3)	0.22170(6)	0.1152(2)	0.1597(2)	0.0511(2)	0.1579(2)	0.0341(3)	0.1701(8)	0.0423(5)	0.1703(1)	0.0453(3)	0.1724(3)	0.0444(1)
	y	0.001(2)	0.069(4)	0.03069(6)	0.1357(2)	0.0932(2)	0.1863(2)	0.0936(2)	0.1885(3)	0.082(1)	0.1960(5)	0.0800(2)	0.1933(3)	0.0813(2)	0.19799(9)
16b	*z*	0.645(5)	0.269(8)	0.6193(8)	0.137(1)	0.1227(8)	0.1284(6)	0.127(1)	0.064(1)	0.087(3)	0.071(2)	0.1203(7)	0.1361(9)	0.1186(10)	0.1252(7)
	Occu.	1.0	1.0	0.965(4)	1.0	0.591(6)	1.0	0.683(8)	0.667(7)	0.73(6)	1.00	0.501(6)	1.0	0.486(16)	1.0
	U_{iso} [b]	0.021(3)	0.05(3)	0.0190(3)	0.0427(8)	0.027(1)	0.052(1)	0.064(2)	0.03(1)	0.025(2)	0.007(3)	0.019(1)	0.045(2)	0.013(1)	0.0390(5)
M2	*x*					0.1331(3)		0.128(2)	0.1(1)	0.155(2)		0.1538(2)		0.1573(3)	
	y					0.1224(4)		0.135(2)	0.181(2)	0.105(3)		0.0997(2)		0.0914(2)	
16b	*z*					0.1242(14)		0.129(8)	0.096(5)	0.111(8)		0.1203(8)		0.1199(12)	
	Occu.					0.377(6)		0.317(8)	0.333(7)	0.27(6)		0.370(5)		0.425(16)	
M3	*x*											0.1132(6)			
	y											0.1450(6)			
16b	*z*											0.0982(31)			
	Occu.											0.057(1)			
OW1	*x*	0.0445(5)		0.0635(4)		0.2511(5)		0.2505(7)		0.2371(6)		0.2404(10)		0.2476(4)	
	y	0.1943(4)		0.1802(4)		-0.0178(5)		0.0027(7)		0.004(1)		0.0004(17)		0.0372(3)	
16b	*z*	0.117(2)		0.103(2)		0.6489(20)		0.597(3)		0.574(3)		0.671(7)		0.5477(17)	
	Occu.	1.0		1.0		0.462(7)		0.63(1)		0.45(3)		0.39(3)		0.918(7)	
	U_{iso} [b]	0.021(3)		0.0190(3)		0.025(4)		0.062(2)		0.022(2)		0.125(5)		0.013(1)	
OW2	*x*					0.2722(5)		0.277(1)		0.2452(7)		0.2403(6)			
	y					0.0271(5)		0.046(1)		0.035(2)		0.0246(8)			
16b	*z*					0.4895(22)		0.482(4)		0.544(3)		0.529(5)			
	Occu.					0.413(7)		0.35(1)		0.43(3)		0.71(3)			

[a]Esd's are in parentheses. M1, M2 and M3 denote each extra-framework cation site. M1 and M2 denote K^+ site and NH_4^+ site in NH_4K-NAT models, respectively.
[b]Isotropic displacement factors (U_{iso}) were refined by grouping the framework tetrahedral atoms, the framework oxygen atoms and the non-framework cations, respectively.
[c]Data of the hydrated phase at room temperature.[1,2]
[d]Data of the dehydrated phase at 675K.[2,3]

Supporting Table 2. Selected interatomic distances (Å) and angles (˚) for Li- , Ag-, K-, NH_4K-, NH_4-, Rb- and Cs-NAT under ambient condition (-hyd) and at 625K (-deh).[a]

	Li-NAT -hyd	Li-NAT -deh	Ag-NAT -hyd	Ag-NAT -deh	K-NAT -hyd[c]	K-NAT -deh[d]	NH_4K-NAT -hyd[c]	NH_4K –NAT -deh[d]	NH_4-NAT -hyd[c]	NH_4 –NAT -deh[d]	Rb-NAT -hyd[c]	Rb-NAT -deh[d]	Cs-NAT -hyd[c]	Cs-NAT -deh[d]
Si(1) - O(1)	1.628(2)	1.622(1)	1.621(2)	1.618(1)	1.604(2)	1.608(2)	1.615(1)	1.614(2)	1.595(2)	1.617(2)	1.610(1)	1.617(1)	1.619(2)	1.611(2)
Si(1) - O(5)	1.631(2)	1.620(1)	1.624(2)	1.621(1)	1.614(2)	1.610(2)	1.618(1)	1.609(2)	1.605(2)	1.619(2)	1.613(1)	1.616(1)	1.621(2)	1.611(2)
mean[b]	1.630(1)	1.621(1)	1.623(1)	1.620(1)	1.609(1)	1.609(1)	1.6165(1)	1.612(1)	1.600(1)	1.618(1)	1.612(1)	1.617(1)	1.620(1)	1.611(1)
Si(2) - O(2)	1.632(3)	1.622(2)	1.617(3)	1.621(2)	1.609(2)	1.622(2)	1.619(2)	1.618(2)	1.582(3)	1.620(2)	1.598(1)	1.617(2)	1.617(2)	1.611(2)
Si(2) - O(3)	1.624(3)	1.622(2)	1.626(3)	1.619(2)	1.600(2)	1.610(2)	1.613(2)	1.613(2)	1.591(3)	1.611(2)	1.609(2)	1.617(2)	1.635(3)	1.608(2)
Si(2) - O(4)	1.623(3)	1.622(2)	1.615(3)	1.622(2)	1.605(2)	1.605(2)	1.614(2)	1.609(2)	1.612(3)	1.614(2)	1.608(2)	1.616(2)	1.620(2)	1.612(2)
Si(2) - O(5)	1.642(3)	1.621(2)	1.626(3)	1.621(2)	1.630(2)	1.606(2)	1.622(2)	1.612(2)	1.627(3)	1.624(2)	1.615(2)	1.617(2)	1.632(3)	1.613(2)
mean[b]	1.630(2)	1.622(1)	1.621(2)	1.621(1)	1.611(1)	1.611(1)	1.617(1)	1.613(1)	1.603(1)	1.617(1)	1.608(1)	1.617(1)	1.626(1)	1.611(1)
Al - O(1)	1.760(3)	1.751(2)	1.747(3)	1.747(2)	1.741(2)	1.723(2)	1.733(2)	1.728(2)	1.742(3)	1.738(2)	1.738(2)	1.733(2)	1.741(3)	1.730(2)
Al - O(2)	1.762(3)	1.749(2)	1.753(3)	1.745(2)	1.718(2)	1.735(2)	1.725(2)	1.733(2)	1.712(3)	1.733(2)	1.729(1)	1.733(2)	1.726(2)	1.729(2)
Al - O(3)	1.752(3)	1.752(2)	1.749(3)	1.746(2)	1.729(2)	1.730(2)	1.726(2)	1.724(2)	1.735(3)	1.734(2)	1.739(2)	1.733(2)	1.754(2)	1.731(2)
Al - O(4)	1.754(3)	1.749(2)	1.747(3)	1.747(2)	1.741(2)	1.719(2)	1.74(1)	1.714(2)	1.755(3)	1.727(2)	1.741(2)	1.733(2)	1.737(3)	1.727(2)
mean[b]	1.757(2)	1.750(1)	1.749(2)	1.746(1)	1.732(1)	1.727(1)	1.731(1)	1.725(1)	1.736(1)	1.733(1)	1.737(1)	1.733(1)	1.740(1)	1.729(1)
Si(1) - O(1) - Al	132.7(4)	139.0(4)	139.2(4)	135.1(4)	136.9(3)	139.1(4)	138(1)	141.0(4)	141.0(3)	139.2(4)	140.5(3)	140.5(4)	140.9(4)	143.4(4)
Si(2) - O(2) - Al	130.2(4)	124.0(4)	133.3(4)	127.1(3)	150.6(2)	123.6(3)	156.1(3)	129.5(3)	163.6(3)	131.8(4)	165.6(3)	127.4(4)	175.4(4)	134.1(4)
Si(2) - O(3) - Al	129.6(4)	148.5(3)	140.8(2)	132.3(2)	136.2(2)	128.2(4)	134.7(2)	134.3(4)	140.2(2)	133.5(4)	135.7(2)	130.4(5)	134.7(3)	135.4(4)
Si(2) - O(4) - Al	133.9(4)	151.7(3)	145.3(2)	137.6(5)	135.9(2)	142.3(4)	134.4(2)	139.8(4)	137.7(2)	137.5(4)	136.2(2)	138.6(5)	134.5(3)	139.1(4)
Si(1) - O(5) - Si(2)	142.6(5)	142.5(4)	143.3(5)	134.6(4)	140.6(3)	143.1(4)	141.8(3)	141.9(4)	146.3(4)	144.6(4)	144.5(3)	147.0(4)	143.7(4)	146.8(5)
Average chain rotation angle of T_5O_{10} unit, Ψ	26.4(2)	-29.6(2)	22.3(2)	-23.4(2)	12.77	28.0	9.61	26.21	9.34	24.82	6.71	25.1	2.93(1)	21.6(1)
M1 - O(1)				2.646(6)	2.821(5)	2.759(6)	2.835(6)	2.818(7)	2.98(1)	2.93(1)	3.076(4)	2.972(7)	3.260(7)	3.112(6)
											3.388(4)		3.194(6)	
M1 - O(2)	2.20(3)	2.24(5)	2.569(7)			3.095(9)		2.916(6)		2.998(9)		3.05(1)		3.251(8)
	2.45(3)		2.772(8)			2.925(5)		3.082(9)		3.11(2)		3.048(8)		3.272(6)
M1 - O(3)	2.50(3)	2.89(7)	2.458(6)	2.553(8)	2.851(5)		2.902(6)	3.263(7)	3.18(2)		3.122(5)		3.346(8)	
M1 - O(4)	3.02(3)	2.94(5)	2.438(6)	2.461(8)	2.844(5)		2.907(6)	3.169(7)	2.94(1)		3.139(5)		3.304(8)	

M1 - O(5)		2.42(7)		2.501(6)	2.874(5)	2.827(7)	2.907(6)	3.084(7)	3.14(2)	3.05(1)	3.151(4) 3.381(4)	2.975(7)	3.254(7) 3.348(6)	3.157(7)
M2 - O(1)					2.732(7)		2.87(4)	3.15(4) 3.03(4)	2.98(4)		2.916(4) 3.389(4)		3.056(7) 3.278(6)	
M2 - O(2)							3.12(5)	2.91(3)			3.355(6)		3.48(1) 3.48(1)	
M2 - O(3)					3.007(8)		3.24(5)		3.19(5)		3.194(5)		3.327(9)	
M2 - O(4)					2.905(8)		3.00(5)		2.99(5)		3.126(5)		3.368(9)	
M2 - O(5)					2.692(7)		2.63(4)	2.19(4)	2.79(6)		2.920(5)		3.139(7)	
M3 - O(1)											2.77(2)			
M3 - O(2)											3.25(2) 3.29(2)			
M3 - O(3)														
M3 - O(4)														
M3 - O(5)											2.83(2)			
OW1 - O(1)	2.81(1)		2.72(1)											
OW1 - O(2)	2.929(8) 3.12(2)				3.09(1)								3.272(9)	
OW1 - O(3)											3.06(3)		3.071(8)	
OW1 - O(4)											3.11(3)		2.603(9)	
OW1 - O(5)	3.07(1)		2.99(1)											
OW1 - M1	1.87(3) 2.30(3)		2.530(9) 2.56(1)				2.63(1)		2.52(3)				2.92(1) 3.31(1)	
OW1 – M2					3.05(1)				3.06(8)		2.92(3)		3.26(1)	
OW1 – M3											3.17(4)			
OW2 - O(1)														
OW2 - O(2)					3.11(1)									
OW2 - O(3)											2.84(1)			
OW2 - O(4)											2.94(1)			
OW2 - O(5)														
OW2 – M1					2.85(1)		3.21(2)		2.89(3)		3.21(3)			
											2.81(2)			
OW2 – M2					3.01(1)		2.49(5)		2.89(3)					
OW2 – M3											3.15(2)			
OW1– OW2									3.18(3)					

[a]Esd's are in parentheses. M1, M2 and M3 denote each extra-framework cation site. M1 and M2 denote K^+ site and NH_4^+ site in NH_4K-NAT models, respectively.
[b]Standard deviations computed using

$$\sigma = 1/n\left[\sum_{i=1}^{n}\sigma_i^{\,2}\right]^{1/2}$$

[c]Data of the hydrated phase at room temperature.[1,2]
[d]Data of the dehydrated phase at 675K.[2,3]

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