

SUPPLEMENTAL TABLES

TABLE 1. Unit-cell parameters of gmelinite-Na vs. temperature by XRPD in situ procedure

T (°C)	a	c	V	a/a ₀	c/c ₀	V/V ₀
25	13.744(1)	10.055(1)	1644.7(1)	1.000	1.000	1.000
52	13.737(1)	10.050(1)	1642.5(1)	1.000	1.000	0.999
79	13.744(1)	10.055(1)	1644.7(1)	1.000	1.000	1.000
105	13.738(1)	10.049(1)	1642.6(1)	1.000	0.999	0.999
158	13.729(1)	10.037(1)	1638.5(1)	0.999	0.998	0.996
184	13.730(1)	10.031(1)	1637.7(1)	0.999	0.998	0.996
211	13.734(1)	10.026(1)	1637.7(1)	0.999	0.997	0.996
237	13.744(1)	10.012(1)	1637.9(1)	1.000	0.996	0.996
263	13.756(1)	10.000(1)	1638.7(1)	1.001	0.995	0.996
290	13.767(1)	9.969(1)	1636.1(1)	1.002	0.991	0.995
316	13.789(1)	9.948(1)	1638.2(1)	1.003	0.989	0.996
343	13.969(7)	9.191(10)	1553.0(16)	1.016	0.914	0.944
369	13.970(7)	9.148(10)	1546.0(16)	1.016	0.910	0.940
395	13.799(1)	8.485(1)	1399.2(1)	1.004	0.844	0.851
422	13.800(1)	8.490(1)	1400.1(1)	1.004	0.844	0.851
448	13.802(1)	8.495(1)	1401.4(1)	1.004	0.845	0.852
475	13.802(1)	8.499(1)	1402.2(1)	1.004	0.845	0.853
501	13.804(1)	8.505(1)	1403.6(1)	1.004	0.846	0.853
527	13.805(1)	8.510(1)	1404.6(1)	1.004	0.846	0.854
554	13.804(1)	8.521(1)	1406.2(1)	1.004	0.847	0.855
580	13.802(1)	8.530(1)	1407.3(1)	1.004	0.848	0.856
606	13.801(1)	8.538(1)	1408.5(1)	1.004	0.849	0.856
633	13.799(1)	8.547(1)	1409.3(1)	1.004	0.850	0.857
659	13.792(1)	8.559(1)	1410.0(1)	1.004	0.851	0.857
686	13.782(1)	8.575(1)	1410.5(1)	1.003	0.853	0.858
712	13.769(1)	8.586(1)	1409.8(1)	1.002	0.854	0.857
738	13.762(1)	8.596(1)	1410.0(1)	1.001	0.855	0.857
765	13.759(1)	8.605(1)	1410.7(1)	1.001	0.856	0.858
791	13.758(1)	8.612(1)	1411.8(1)	1.001	0.857	0.858
818	13.759(1)	8.618(1)	1412.8(1)	1.001	0.857	0.859

TABLE 2. Unit-cell parameters and space groups

	a (Å)	c (Å)	V (Å ³)	Space group
Gmelinite 25 °C in situ data	13.744(1)	10.055(1)	1644.7(1)	P63/mmc
"transient" phase 343 °C in situ data	13.969(7)	9.191(10)	1553.0(16)	P31c
AFI-type phase 448 °C "in situ" data	13.802(1)	8.495(1)	1401.4(1)	P6/mcc
Δc 35 °C – transient 8.6% Δc transient – AFI 7.6% Δc 35 °C – AFI 15.5%.				
ΔV 35 °C – transient 5.6% ΔV transient – AFI 9.7% ΔV 35 °C – AFI 14.8%.				

TABLE 3. Experimental and refinement parameters of gmelinite-Na heated to 343 °C ("transient" phase) by XRPD in situ procedure

Gmelinite-Na 343 °C	
Space group	P31c
a (Å)	13.972(7)
c (Å)	9.188 (10)
V (Å ³)	1553.4(19)
R _{wp}	16.75
R _p	13.81
R _c ²	18.45
No. Reflections	2861
Nobs	775
No. Variables	106

TABLE 4. Atomic coordinates, occupancy, and temperature factor of gmelinite-Na heated to 343 °C ("transient" phase) by XRPD in situ procedure

Atoms	x	y	z	Occ.	U _{iso}
T1	0.451(1)	0.117(1)	0.109	0.5	0.052(5)
T2	0.479(1)	0.352(1)	0.081(1)	1.0	0.042(3)
T3	0.444(1)	0.113(1)	0.442(1)	1.0	0.042(3)
T4	0.447(1)	0.338(1)	0.421(5)	1.0	0.042(3)
T1P	0.416(1)	0.126(1)	-0.064(1)	0.5	0.052(5)
O1	0.444(1)	0.223(1)	0.057(1)	1.0	0.063(6)
O1'	0.435(2)	0.222(1)	0.486(1)	1.0	0.063(6)
O2	0.139(1)	0.569(1)	-0.018(1)	1.0	0.063(6)
O2'	0.600(1)	0.432(1)	0.011(1)	1.0	0.063(6)
O3	0.419(1)	0.067(1)	0.275(1)	0.5	0.063(6)
O3'	0.430(2)	0.326(1)	0.250(1)	1.0	0.063(6)
O4	0.364(1)	-0.007(1)	0.517(1)	1.0	0.063(6)
O4'	0.376(1)	0.379(1)	0.521(2)	1.0	0.063(6)
O3P	0.374(2)	0.129(1)	-0.230(1)	0.5	0.063(6)
Na1	0.333	0.667	0.145(11)	1.0	0.091(11)
Na2	0.667	0.333	0.070(10)	0.241(7)	0.071(3)
W1	0.239(5)	0.166(6)	0.431(5)	0.445(9)	0.039(3)

TABLE 5. Interatomic distances (Å) and angles (°) in the framework in gmelinite-Na heated to 343 °C ("transient" phase) by XRPD in situ procedure

T1-O1	1.61(1)	T2-O1	1.63(1)
T1-O2'	1.68(1)	T2-O2'	1.63(1)
T1-O3	1.64(1)	T2-O3'	1.66(1)
T1-O4	1.62(1)	T2-O4'	1.68(1)
T3-O1'	1.63(1)	T4-O1'	1.63(1)
T3-O2	1.64(1)	T4-O2	1.63(1)
T3-O3	1.64(1)	T4-O3'	1.64(1)
T3-O4	1.63(1)	T4-O4'	1.64(1)
T1P-O1	1.64(1)	T1-T1P	1.69(1)
T1P-O2'	2.01(1)		
T1P-O4	1.64(1)		
T1P-O3P	1.64(1)		
O1-T1-O2'	87(1)	O1-T2-O2'	110(1)
O1-T1-O3	122(1)	O1-T2-O3'	91(1)
O1-T1-O4	113(1)	O1-T2-O4'	111(1)
O2-T1-O3	133(1)	O2-T2-O3'	134(1)
O2-T1-O4	101(1)	O2-T2-O4'	114(1)
O3-T1-O4	100(1)	O3-T2-O4'	94(1)
O1-T3-O2	108(1)	O1-T4-O2	104(1)
O1-T3-O3	120(1)	O1-T4-O3'	107(1)
O1-T3-O4	121(1)	O1-T4-O4'	113(1)
O2-T3-O3	107(1)	O2-T4-O3'	116(1)
O2-T3-O4	104(1)	O2-T4-O4'	97(1)
O3-T3-O4	95(1)	O3-T4-O4'	119(1)
O1-T1P-O2'	75(1)	T1-O1-T2	149(1)
O1-T1P-O4	110(1)	T3-O1'-T4	140(1)
O1-T1P-O3P	124(1)	T1-O2'-T2	109(1)
O2-T1P-O4	88(1)	T1-O3-T3	139(1)
O2-T1P-O3P	130(1)	T1-O4-T3	156(1)
O4-T1P-O3P	119(1)	T2-O4'-T4	152(1)
T2-O1-T1P	145(1)	T2-O3'-T4	152(1)
T3-O2-T4	141(1)	T3-O4-T1P	128(1)
T2-O2'-T1P	147(1)	T1-T1P-O3P	176(1)

Note: Estimated standard deviations in parentheses refer to the last digit.