Supplementary material

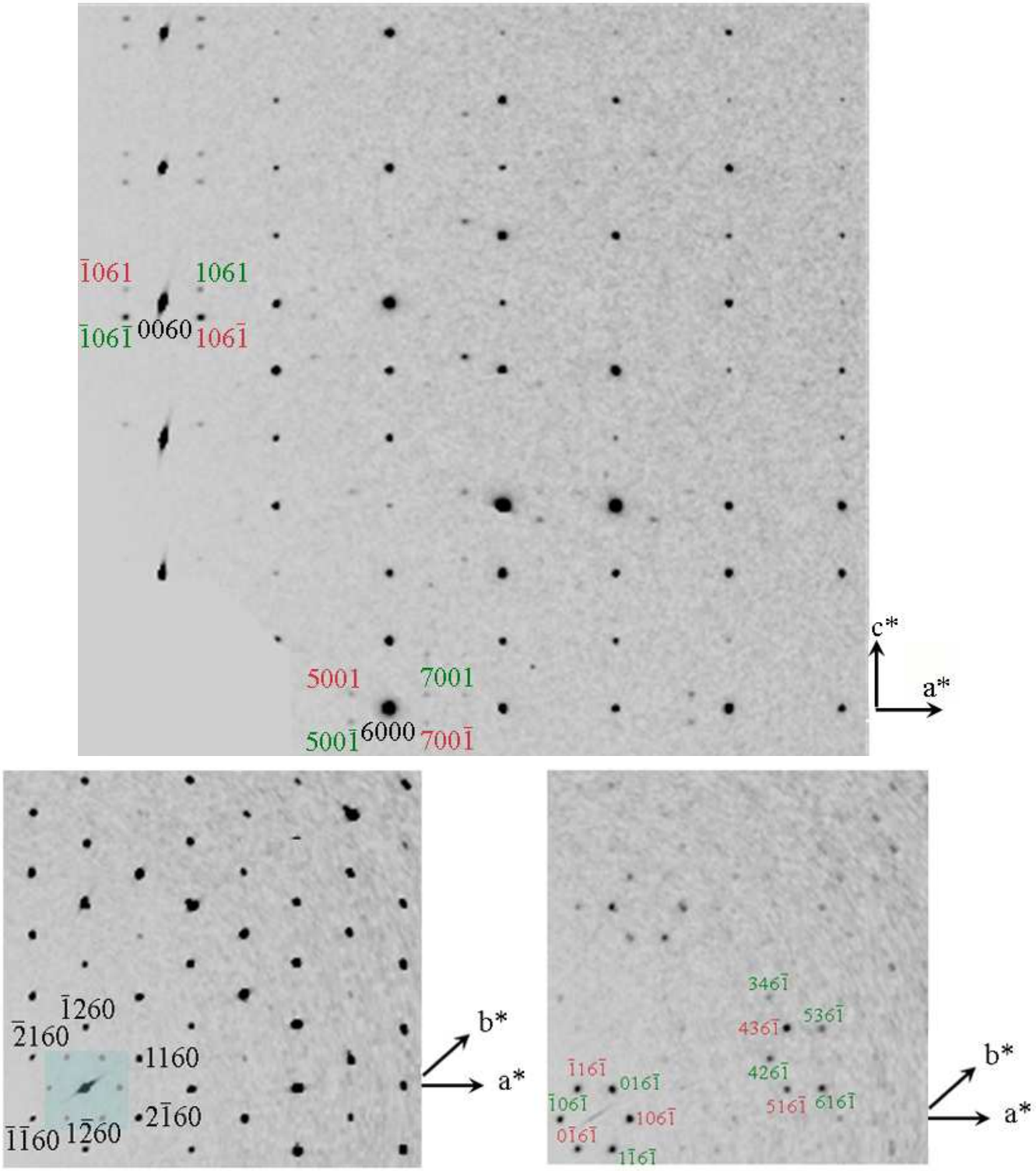

Figure 1
Reconstructions of reciprocal space on the basis of the measured frames. (top) h0l-layer (bottom,left) hk6-layer (bottom,right) hk5.8-layer. Main reflections are indexed in black, satellite reflections belonging to twin individual I are indexed in green, satellite reflections belonging to twin individual II are indexed in red.

Restrictions employed in the refinement of the modulated structure

Modulation parameters which were smaller then three times their standard deviation were set to zero and not refined.

The following local symmetry operation was used:

$$\begin{pmatrix} -1.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & -1.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & -1.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & -1.0 \end{pmatrix}$$

Coordinates, displacement and modulation parameters restricted to be equal

K1a – Na1a
K1b – Na1b

Anisotropic displacement parameters restricted to be equal, occupational modulation parameters restricted to be complementary:

O1a – O1b
O2a1 – O2a2
O2b1 – O2b2
O3a1 – O3a2
O3b1 – O3b2
O4a1 – O4a2
O4b1 – O4b2

Occupational modulation parameters restricted to be equal:

Group I: O2a1 – O2b1 – O3a1 – O3b1 – O4a1 – O4b1
Group II: O2a2 – O2b2 – O3a2 – O3b2 – O4a2 – O4b2

x and *y* coordinates restricted to be related via the local symmetry operation:

K1a – K1b

Anisotropic displacement parameters restricted to be equal via the local symmetry operation:

K1a – K1b
Na2a – Na2b
O5a – O5b
O6a – O6b
O2a1 – O2a2 – O2b1 – O2b2
O3a1 – O3a2 – O3b1 – O3b2
O4a1 – O4a2 – O4b1 – O4b2
O5a – O5b
O6a – O6b

Table 1
Fractional atomic coordinates and isotropic atomic displacement parameters (Å^2) for the average structure of nepheline in space group $P6_3$ (small primitive unit cell).

	occ.	x	y	z	U_{iso}
K1	0.57	0	0	0	0.0346(2)
Na1	0.24	0	0	0	0.0346(2)
Na2		0.55381(6)	0.99696(6)	0.5043(2)	0.02522(19)
Si1		2/3	1/3	0.3095(2)	0.01325(12)
Al1		2/3	1/3	0.6978(3)	0.01301(13)
Si2		0.90557(4)	0.66607(4)	0.8190(2)	0.01242(10)
Al2		0.90621(4)	0.66771(5)	0.1924(2)	0.01253(12)
O1	1/3	0.6615(9)	0.2887(5)	0.4998(6)	0.0354(18)
O2		0.97226(12)	0.68311(17)	-0.0018(3)	0.0333(4)
O3		0.82611(14)	0.47710(14)	0.2482(3)	0.0374(5)
O4		0.83682(14)	0.48963(14)	0.7601(3)	0.0335(4)
O5		0.77296(12)	0.71372(13)	0.8207(3)	0.0191(3)
O6		0.77594(13)	0.73328(13)	0.1973(3)	0.0213(3)

Table 2
Anisotropic atomic displacement parameters (Å^2) in the average structure of nepheline in space group $P6_3$ (small, primitive unit cell)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
K1	0.02818(19)	0.02818(19)	0.0474(5)	0.01409(10)	0	0
Na1	0.02818(19)	0.02818(19)	0.0474(5)	0.01409(10)	0	0
Na2	0.0274(2)	0.0325(2)	0.0218(20)	0.0196(2)	-0.0004(3)	-0.0008(4)
Si1	0.01361(14)	0.01361(14)	0.0125(2)	0.00681(7)	0	0
Al1	0.01285(15)	0.01285(15)	0.0133(3)	0.00642(8)	0	0
Si2	0.00902(11)	0.01232(12)	0.01565(14)	0.00514(9)	-0.00047(13)	0.00061(13)
Al2	0.00892(13)	0.01207(14)	0.01644(18)	0.00511(11)	-0.00014(15)	-0.00106(15)
O1	0.0551(19)	0.043(2)	0.0152(8)	0.030(3)	-0.005(3)	-0.0068(18)
O2	0.0291(4)	0.0706(7)	0.0158(3)	0.0367(5)	-0.0005(5)	-0.0004(6)
O3	0.0118(4)	0.0114(4)	0.0866(11)	0.0041(3)	0.0054(5)	0.0064(5)
O4	0.0125(4)	0.0111(3)	0.0755(9)	0.0049(3)	-0.0005(5)	-0.0042(5)
O5	0.0174(3)	0.0238(4)	0.0220(4)	0.0147(3)	-0.0022(3)	-0.0014(4)
O6	0.0211(4)	0.0265(5)	0.0238(4)	0.0175(4)	0.0053(4)	0.0027(4)

Table 3
Fractional atomic coordinates and isotropic atomic displacement parameters (Å^2) for the average structure of nepheline in space group $P3$. Note the origin shift with respect to the model in $P6_3$.

atom	occ.	x	y	z	U_{iso}
K1a	0.57	0.0011(7)	0.9991(9)	0.25	0.0415(7)
Na1a	0.24	0.0011(7)	0.9991(9)	0.25	0.0415(7)
K1b	0.57	0.0029(7)	0.0044(9)	0.7500(10)	0.0415(7)
Na1b	0.24	0.0029(7)	0.0044(9)	0.7500(10)	0.0415(7)
Na2a		0.5545(3)	0.9970(3)	0.2453(6)	0.02523(11)
Na2b		0.4466(2)	0.0029(3)	0.7460(6)	0.02523(11)
Si1		1/3	2/3	0.9399(6)	0.0136(3)
Al1		2/3	1/3	0.0526(7)	0.0136(4)
Al2		1/3	2/3	0.5517(6)	0.0125(3)
Si2		2/3	1/3	0.4408(7)	0.0130(3)
Al3		0.09379(12)	0.33222(13)	0.0572(6)	0.0123(3)
Si3		0.90523(11)	0.66604(11)	0.9317(6)	0.0124(2)
Si4		0.09416(11)	0.33384(12)	0.4309(6)	0.0125(2)
Al4		0.90626(12)	0.66757(13)	0.5586(6)	0.0127(3)
O1a	1/3	0.2840(10)	0.6404(13)	0.7523(10)	0.0280(12)
O1b	1/3	0.6752(8)	0.2927(12)	0.2534(12)	0.0280(12)
O2a1	0.6686	0.0264(8)	0.3235(10)	0.2573(11)	0.0282(8)
O2a2	0.3314	0.0291(17)	0.301(2)	0.2456(19)	0.0282(8)
O2b1	0.6686	0.9726(9)	0.6758(11)	0.7488(10)	0.0282(8)
O2b2	0.3314	0.971(2)	0.699(2)	0.7541(17)	0.0282(8)
O3a1	0.6686	0.1613(5)	0.5130(5)	0.4718(7)	0.0211(8)
O3a2	0.3314	0.1696(9)	0.5072(9)	0.5190(12)	0.0211(8)
O3b1	0.6686	0.8319(5)	0.4775(5)	0.4942(7)	0.0211(8)
O3b2	0.3314	0.8144(8)	0.4716(9)	0.5371(13)	0.0211(8)
O4a1	0.6686	0.1744(4)	0.5203(4)	0.9779(6)	0.0178(6)
O4a2	0.3314	0.1761(8)	0.5241(8)	0.0339(10)	0.0178(6)
O4b1	0.6686	0.8418(5)	0.4926(4)	0.0043(6)	0.0178(6)
O4b2	0.3314	0.8255(7)	0.4861(7)	0.9570(10)	0.0178(6)
O5a		0.2239(4)	0.2671(4)	0.0553(6)	0.0199(6)
O5b		-0.2279(4)	-0.2856(4)	0.9298(8)	0.0199(6)
O6a		0.2259(4)	0.2856(4)	0.4305(6)	0.0215(7)
O6b		0.7748(4)	0.7321(4)	0.5512(7)	0.0215(7)

Table 4
Anisotropic atomic displacement parameters (Å^2) in the average structure of nepheline in space group *P*3

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
K1a	0.0059(4)	0.0613(10)	0.0487(5)	0.0103(9)	-0.0020(19)	-0.0249(14)
Na1a	0.0059(4)	0.0613(10)	0.0487(5)	0.0103(9)	-0.0020(19)	-0.0249(14)
K1b	0.0059(4)	0.0613(10)	0.0487(5)	0.0103(9)	-0.0020(19)	-0.0249(14)
Na1b	0.0059(4)	0.0613(10)	0.0487(5)	0.0103(9)	-0.0020(19)	-0.0249(14)
Na2a	0.02759(14)	0.03248(15)	0.02173(12)	0.01961(12)	-0.0013(6)	-0.0004(7)
Na2b	0.02759(14)	0.03248(15)	0.02173(12)	0.01961(12)	-0.0013(6)	-0.0004(7)
Si1	0.0126(4)	0.0126(4)	0.0157(6)	0.00629(18)	0	0
Al1	0.0146(5)	0.0146(5)	0.0118(6)	0.0073(2)	0	0
Al2	0.0116(4)	0.0116(4)	0.0143(6)	0.0058(2)	0	0
Si2	0.0141(4)	0.0141(4)	0.0108(5)	0.00706(18)	0	0
Al3	0.0090(3)	0.0124(4)	0.0152(4)	0.0051(3)	0.0002(3)	-0.0010(3)
Si3	0.0093(3)	0.0114(3)	0.0167(4)	0.0053(3)	0.0005(3)	-0.0001(3)
Si4	0.0086(3)	0.0133(3)	0.0151(3)	0.0051(3)	0.0002(2)	0.0011(3)
Al4	0.0092(3)	0.0117(4)	0.0171(4)	0.0053(3)	-0.0001(2)	0.0011(3)
O1a	0.0349(16)	0.0417(16)	0.0142(6)	0.0243(15)	-0.0016(14)	0.0028(10)
O1b	0.0349(16)	0.0417(16)	0.0142(6)	0.0243(15)	-0.0016(14)	0.0028(10)
O2a1	0.0287(3)	0.0613(14)	0.0143(7)	0.0372(7)	-0.0004(11)	-0.0011(15)
O2a2	0.0287(3)	0.0613(14)	0.0143(7)	0.0372(7)	-0.0004(11)	-0.0011(15)
O2b1	0.0287(3)	0.0613(14)	0.0143(7)	0.0372(7)	-0.0004(11)	-0.0011(15)
O2b2	0.0287(3)	0.0613(14)	0.0143(7)	0.0372(7)	-0.0004(11)	-0.0011(15)
O3a1	0.0093(7)	0.0122(7)	0.0413(17)	0.0049(6)	0.0004(8)	0.0007(9)
O3a2	0.0093(7)	0.0122(7)	0.0413(17)	0.0049(6)	0.0004(8)	0.0007(9)
O3b1	0.0093(7)	0.0122(7)	0.0413(17)	0.0049(6)	0.0004(8)	0.0007(9)
O3b2	0.0093(7)	0.0122(7)	0.0413(17)	0.0049(6)	0.0004(8)	0.0007(9)
O4a1	0.0108(7)	0.0098(6)	0.0298(8)	0.0029(6)	-0.0030(6)	0.0026(6)
O4a2	0.0108(7)	0.0098(6)	0.0298(8)	0.0029(6)	-0.0030(6)	0.0026(6)
O4b1	0.0108(7)	0.0098(6)	0.0298(8)	0.0029(6)	-0.0030(6)	0.0026(6)
O4b2	0.0108(7)	0.0098(6)	0.0298(8)	0.0029(6)	-0.0030(6)	0.0026(6)
O5a	0.0175(7)	0.0252(9)	0.0237(8)	0.0157(7)	0.0031(6)	0.0010(7)
O5b	0.0175(7)	0.0252(9)	0.0237(8)	0.0157(7)	0.0031(6)	0.0010(7)
O6a	0.0206(8)	0.0266(9)	0.0233(8)	0.0163(7)	-0.0050(7)	-0.0045(7)
O6b	0.0206(8)	0.0266(9)	0.0233(8)	0.0163(7)	-0.0050(7)	-0.0045(7)

Table 5
Anisotropic atomic displacement parameters (Å^2) in the modulated structure of nepheline

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
K1a	0.0673(9)	0.0363(8)	0.0434(3)	0.0485(8)	-0.0235(9)	-0.0192(8)
Na1a	0.0673(9)	0.0363(8)	0.0434(3)	0.0485(8)	-0.0235(9)	-0.0192(8)
K1b	0.0673(9)	0.0363(8)	0.0434(3)	0.0485(8)	-0.0235(9)	-0.0192(8)
Na1b	0.0673(9)	0.0363(8)	0.0434(3)	0.0485(8)	-0.0235(9)	-0.0192(8)
Na2a	0.01942(11)	0.02504(11)	0.02000(10)	0.00708(9)	-0.0004(3)	0.0010(4)
Na2b	0.01942(11)	0.02504(11)	0.02000(10)	0.00708(9)	-0.0004(3)	0.0010(4)
Si1	0.0116(3)	0.0116(3)	0.0137(5)	0.00581(16)	0	0
Al1	0.0107(3)	0.0107(3)	0.0120(5)	0.00535(17)	0	0
Si2	0.0118(3)	0.0118(3)	0.0108(5)	0.00590(15)	0	0
Al2	0.0113(3)	0.0113(3)	0.0116(5)	0.00567(18)	0	0
Si3	0.0116(3)	0.0087(3)	0.0131(3)	0.0066(2)	-0.00048(19)	-0.00040(18)
Al3	0.0097(3)	0.0097(3)	0.0128(3)	0.0054(3)	-0.0004(2)	-0.0009(2)
Si4	0.0104(3)	0.0103(3)	0.0126(3)	0.0056(2)	0.00046(19)	-0.00006(18)
Al4	0.0116(3)	0.0088(3)	0.0124(3)	0.0065(3)	0.0014(2)	0.0001(2)
O1a	0.0298(13)	0.0351(16)	0.0126(4)	0.0095(11)	-0.0068(9)	-0.0027(8)
O1b	0.0298(13)	0.0351(16)	0.0126(4)	0.0095(11)	-0.0068(9)	-0.0027(8)
O2a1	0.0344(6)	0.0391(5)	0.0115(2)	0.0316(5)	0.0022(4)	0.002022
O2a2	0.0344(6)	0.0391(5)	0.0115(2)	0.0316(5)	0.0022(4)	0.002022
O2b1	0.0344(6)	0.0391(5)	0.0115(2)	0.0316(5)	0.0022(4)	0.002022
O2b2	0.0344(6)	0.0391(5)	0.0115(2)	0.0316(5)	0.0022(4)	0.002022
O3a1	0.0099(5)	0.0085(5)	0.0382(7)	0.0044(3)	-0.0056(6)	-0.0005(5)
O3a2	0.0099(5)	0.0085(5)	0.0382(7)	0.0044(3)	-0.0056(6)	-0.0005(5)
O3b1	0.0099(5)	0.0085(5)	0.0382(7)	0.0044(3)	-0.0056(6)	-0.0005(5)
O3b2	0.0099(5)	0.0085(5)	0.0382(7)	0.0044(3)	-0.0056(6)	-0.0005(5)
O4a1	0.0132(5)	0.0094(4)	0.0292(5)	0.0048(3)	0.0032(4)	-0.0003(4)
O4a2	0.0132(5)	0.0094(4)	0.0292(5)	0.0048(3)	0.0032(4)	-0.0003(4)
O4b1	0.0132(5)	0.0094(4)	0.0292(5)	0.0048(3)	0.0032(4)	-0.0003(4)
O4b2	0.0132(5)	0.0094(4)	0.0292(5)	0.0048(3)	0.0032(4)	-0.0003(4)
O5a	0.0185(6)	0.0263(6)	0.0201(4)	0.0173(5)	0.0010(3)	0.0039(3)
O5b	0.0185(6)	0.0263(6)	0.0201(4)	0.0173(5)	0.0010(3)	0.0039(3)
O6a	0.0174(6)	0.0223(6)	0.0197(4)	0.0133(5)	0.0000(3)	-0.0029(3)
O6b	0.0174(6)	0.0223(6)	0.0197(4)	0.0133(5)	0.0000(3)	-0.0029(3)

Table 6
Average, minimum, and maximum O-T-O angles in the modulated structure of nepheline at room temperature

O4a1-Si1-O4a1^{iii}	115.0(2)	113.1(2)	117.0(2)
O4a1-Si1-O4a1^{v}	115.07(18)	113.15(18)	117.01(19)
O4a1-Si1-O4a2^{iii}	107.8(5)	106.2(5)	109.6(5)
O4a1-Si1-O4a2^{v}	108.8(3)	107.5(3)	110.2(3)
O4a1-Si1-O1a^{viii}	113.5(3)	111.1(3)	116.0(4)
O4a1-Si1-O1a^{ix}	107.9(4)	106.4(4)	109.6(4)
O4a1-Si1-O1a^{x}	86.5(3)	83.5(3)	89.5(3)
O4a1^{iii}-Si1-O4a1^{v}	115.1(2)	113.1(2)	117.0(2)
O4a1^{iii}-Si1-O4a2	108.8(4)	107.5(4)	110.2(4)
O4a1^{iii}-Si1-O4a2^{v}	107.9(4)	106.2(4)	109.6(4)
O4a1^{iii}-Si1-O1a^{viii}	86.5(2)	83.5(3)	89.5(3)
O4a1^{iii}-Si1-O1a^{ix}	113.5(3)	111.1(3)	116.0(3)
O4a1^{iii}-Si1-O1a^{x}	107.9(4)	106.4(4)	109.6(4)
O4a1^{v}-Si1-O4a2	107.9(4)	106.2(4)	109.6(4)
O4a1^{v}-Si1-O4a2^{iii}	108.8(5)	107.5(5)	110.2(5)
O4a1^{v}-Si1-O1a^{viii}	108.0(4)	106.4(4)	109.6(4)
O4a1^{v}-Si1-O1a^{ix}	86.5(4)	83.5(4)	89.5(5)
O4a1^{v}-Si1-O1a^{x}	113.5(4)	111.1(4)	116.0(4)
O4a2-Si1-O4a2^{iii}	98.2(5)	96.8(5)	99.5(5)
O4a2-Si1-O4a2^{v}	98.2(4)	96.8(4)	99.5(4)
O4a2-Si1-O1a^{viii}	129.4(4)	128.4(4)	130.4(4)
O4a2-Si1-O1a^{ix}	123.2(4)	122.6(4)	123.8(4)
O4a2-Si1-O1a^{x}	102.7(3)	100.5(3)	104.9(3)
O4a2^{iii}-Si1-O4a2^{v}	98.2(5)	96.8(5)	99.5(5)
O4a2^{iii}-Si1-O1a^{viii}	102.7(3)	100.5(3)	104.9(3)
O4a2^{iii}-Si1-O1a^{ix}	129.4(3)	128.4(3)	130.4(3)
O4a2^{iii}-Si1-O1a^{x}	123.2(5)	122.6(4)	123.8(5)
O4a2^{v}-Si1-O1a^{viii}	123.2(5)	122.6(5)	123.8(4)
O4a2^{v}-Si1O1a^{ix}	102.7(5)	100.5(5)	104.9(5)
O4a2^{v}-Si1-O1a^{x}	129.4(5)	128.4(5)	130.4(5)
O4b2-Al1-O4b2^{vi}	101.5(3)	99.4(3)	103.6(3)
O4b2-Al1-O4b2^{vii}	101.5(3)	99.4(3)	103.6(3)
O4b2-Al1-O4b1^{vi}	110.4(3)	109.3(3)	111.5(3)
O4b2-Al1-O4b^{vii}	108.0(3)	105.9(3)	110.2(3)
O4b2-Al1-O1b^{xi}	104.7(5)	103.8(5)	105.6(5)
O4b2-Al1-O1b^{xii}	119.6(6)	116.3(6)	122.7(6)
O4b2-Al1-O1b^{xiii}	124.5(3)	121.1(3)	128.0(3)
O4b2^{vi}-Al1-O4b2^{vii}	101.5(4)	99.4(3)	103.6(4)
O4b2^{vi}-Al1-O4b1	108.0(3)	105.9(3)	110.2(3)
O4b2^{vi}-Al1-O4b1^{vii}	110.4(3)	109.3(3)	111.5(3)
O4b2^{vi}-Al1-O1b^{xi}	124.5(3)	121.1(3)	128.0(3)
O4b2^{vi}-Al1-O1b^{xii}	104.7(5)	103.8(5)	105.6(5)
O4b2^{vi}-Al1-O1b^{xiii}	119.5(5)	116.3(5)	122.7(5)
O4b2^{vii}-Al1-O4b1	110.3(2)	109.3(2)	111.5(3)
O4b2^{vii}-Al1-O4b1^{vi}	108.0(3)	105.9(3)	110.2(3)
O4b2^{vii}-Al1-O1b^{xi}	119.6(5)	116.3(5)	122.7(5)
O4b2^{vii}-Al1-O1b^{xii}	124.5(7)	121.1(7)	128.0(7)
O4b2^{vii}-Al1-O1b^{xiii}	104.7(6)	103.8(6)	105.6(5)
O4b1-Al1-O4b1^{vi}	114.6(3)	113.2(3)	116.0(3)
O4b1-Al1-O4b1^{vii}	114.6(2)	113.2(2)	116.0(2)
O4b1-Al1-O1b^{xi}	91.8(4)	90.0(4)	93.6(4)
O4b1-Al1-O1b^{xii}	106.6(5)	105.3(5)	107.9(5)
O4b1-Al1-O1b^{xiii}	112.0(2)	110.3(2)	113.7(2)
O4b1^{vi}-Al1-O4b1^{vii}	114.6(2)	113.2(2)	116.0(2)
O4b1^{vi}-Al1-O1b^{xi}	112.0(3)	110.3(2)	113.7(2)
O4b1^{vi}-Al1-O1b^{xii}	91.8(4)	90.0(4)	93.6(4)
O4b1^{vi}-Al1-O1b^{xiii}	106.6(4)	105.3(4)	107.9(4)
O4b1^{vii}-Al1-O1b^{xi}	106.6(5)	105.3(5)	107.9(5)
O4b1^{vii}-Al1-O1b^{xii}	112.0(6)	110.3(6)	113.7(6)
O4b1^{vii}-Al1-O1b^{xiii}	91.8(5)	90.0(5)	93.6(5)

Table 7
O-T-O angles continued

O3b1-Si2-O3b1^{vi}	113.0(3)	111.1(3)	115.0(3)
O3b1-Si2-O3b1^{vii}	112.9(2)	111.1(2)	115.0(2)
O3b1-Si2-O3b2^{vi}	105.3(4)	103.0(4)	107.3(4)
O3b1-Si2-O3b2^{vii}	108.9(3)	107.4(3)	110.3(3)
O3b1-Si2-O1b	93.4(5)	88.3(5)	98.6(5)
O3b1-Si2-O1b^{vi}	108.3(6)	106.0(5)	110.7(6)
O3b1-Si2-O1b^{vii}	114.6(3)	111.5(3)	117.8(3)
O3b1^{vi}-Si2-O3b1^{vii}	112.9(2)	111.1(2)	115.0(2)
O3b1^{vi}-Si2-O3b2	108.9(4)	107.4(4)	110.3(4)
O3b1^{vi}-Si2-O3b2^{vii}	105.2(3)	103.0(3)	107.3(3)
O3b1^{vi}-Si2-O1b	114.7(3)	111.5(3)	117.8(3)
O3b1^{vi}-Si2-O1b^{vi}	93.5(4)	88.3(4)	98.6(4)
O3b1^{vi}-Si2-O1b^{vii}	108.3(5)	106.0(5)	110.7(4)
O3b1^{vii}-Si2-O3b2	105.2(4)	103.0(4)	107.3(4)
O3b1^{vii}-Si2-O3b2^{vi}	108.9(4)	107.4(4)	110.3(4)
O3b1^{vii}-Si2-O1b	108.4(5)	106.0(5)	110.7(5)
O3b1^{vii}-Si2-O1b^{vi}	114.6(7)	111.5(7)	117.8(7)
O3b1^{vii}-Si2-O1b^{vii}	93.5(6)	88.3(5)	98.6(6)
O3b2-Si2-O3b2^{vi}	99.1(4)	98.3(4)	100.0(4)
O3b2-Si2-O3b2^{vii}	99.2(4)	98.3(4)	100.0(4)
O3b2-Si2-O1b	106.0(5)	102.6(5)	109.5(5)
O3b2-Si2O1b^{vi}	121.2(6)	118.5(6)	123.9(6)
O3b2-Si2-O1b^{vii}	126.7(3)	126.2(3)	127.3(3)
O3b2^{vi}-Si2-O3b2^{vii}	99.2(4)	98.3(4)	100.0(4)
O3b2^{vi}-Si2-O1b	126.7(3)	126.2(3)	127.3(3)
O3b2^{vi}-Si2-O1b^{vi}	106.1(5)	102.6(5)	109.5(5)
O3b2^{vi}-Si2-O1b^{vii}	121.2(5)	118.5(5)	123.9(5)
O3b2^{vii}-Si2-O1b	121.3(5)	118.5(5)	123.9(5)
O3b2^{vii}-Si2-O1b^{vi}	126.7(7)	126.2(7)	127.3(7)
O3b2^{vii}-Si2-O1b^{vii}	106.1(6)	102.6(6)	109.5(6)
O3a2-Al2-O3a2^{iii}	117.6(4)	114.7(4)	120.5(4)
O3a2-Al2-O3a2^{v}	117.6(4)	114.7(4)	120.5(4)
O3a2-Al2-O3a1^{iii}	118.5(3)	114.8(3)	122.2(3)
O3a2-Al2-O3a1^{v}	108.7(3)	107.4(3)	110.1(3)
O3a2-Al2-O1a	102.6(4)	100.5(4)	104.6(4)
O3a2-Al2-O1a^{iii}	83.6(5)	83.4(5)	83.8(5)
O3a2-Al2-O1a^{v}	110.1(5)	109.0(5)	111.3(5)
O3a2^{iii}-Al2-O3a2^{v}	117.6(5)	114.7(5)	120.5(5)
O3a2^{iii}-Al2-O3a1	108.7(4)	107.4(4)	110.1(4)
O3a2^{iii}-Al2-O3a1^{v}	118.5(4)	114.8(4)	122.2(4)
O3a2^{iii}-Al2-O1a	110.2(4)	109.0(4)	111.3(4)
O3a2^{iii}-Al2-O1a^{iii}	102.6(4)	100.5(4)	104.6(4)
O3a2^{iii}-Al2-O1a^{v}	83.6(4)	83.4(4)	83.8(4)
O3a2^{v}-Al2-O3a1	118.5(4)	114.8(4)	122.2(4)
O3a2^{v}-Al2-O3a1^{iii}	108.7(3)	107.4(3)	110.1(4)
O3a2^{v}-Al2-O1a	83.6(4)	83.4(4)	83.8(4)
O3a2^{v}-Al2-O1a^{iii}	110.2(4)	109.0(4)	111.3(4)
O3a2^{v}-Al2-O1a^{v}	102.6(5)	100.5(5)	104.6(5)
O3a1-Al2-O3a1^{iii}	107.2(2)	106.0(2)	108.4(2)
O3a1-Al2-O3a1^{v}	107.2(3)	106.0(2)	108.4(3)
O3a1-Al2-O1a	116.2(4)	114.3(4)	118.2(4)
O3a1-Al2-O1a^{iii}	95.9(4)	92.1(4)	99.8(4)
O3a1-Al2-O1a^{v}	121.2(4)	117.9(4)	124.6(4)
O3a1^{iii}-Al2-O3a1^{v}	107.2(2)	106.0(2)	108.4(2)
O3a1^{iii}-Al2-O1a	121.3(3)	117.9(3)	124.6(4)
O3a1^{iii}-Al2-O1a^{iii}	116.2(4)	114.3(4)	118.2(4)
O3a1^{iii}-Al2-O1a^{v}	95.9(3)	92.1(3)	99.8(3)
O3a1^{v}-Al2-O1a	95.9(2)	92.1(2)	99.8(3)
O3a1^{v}-Al2-O1a^{iii}	121.2(3)	117.9(3)	124.6(3)
O3a1^{v}-Al2-O1a^{v}	116.2(4)	114.3(4)	118.2(4)

Table 8
O-T-O angles continued

Angle	average	minimum	maximum
O5a^{i}-Si3-O5b	110.00(18)	109.50(19)	110.57(18)
O5a^{i}-Si3-O4b2	116.7(3)	112.5(3)	121.0(3)
O5a^{i}-Si3-O4b1	103.9(2)	101.6(2)	106.3(2)
O5a^{i}-Si3-O2b2	105.3(4)	100.2(4)	110.6(4)
O5a^{i}-Si3-O2b1	113.0(3)	110.5(3)	115.6(3)
O5b-Si3-O4b2	110.1(3)	109.8(3)	110.4(3)
O5b-Si3-O4b1	111.4(2)	110.7(2)	112.2(2)
O5b-Si3-O2b2	106.7(5)	105.0(5)	108.5(5)
O5b-Si3-O2b1	110.0(3)	107.8(3)	112.3(3)
O4b2-Si3-O2b2	107.3(4)	106.1(4)	108.4(4)
O4b2-Si3-O2b1	96.0(4)	91.9(4)	100.2(3)
O4b1-Si3-O2b2	119.0(4)	117.1(4)	120.8(4)
O4b1-Si3-O2b1	108.2(2)	106.4(2)	110.1(2)
O5a-Al3-O5b^{i}	110.64(16)	110.39(17)	110.93(17)
O5a-Al3-O4a1	112.62(17)	112.06(17)	113.17(17)
O5a-Al3-O4a2	112.3(4)	112.2(4)	112.5(4)
O5a-Al3-O2a2	104.5(4)	102.8(4)	106.2(4)
O5a-Al3-O2a1	110.1(3)	109.6(3)	110.5(3)
O5b^{i}-Al3-O4a1	102.85(19)	101.66(18)	104.04(19)
O5b^{i}-Al3-O4a2	115.6(3)	113.3(3)	118.0(3)
O5b^{i}-Al3-O2a2	108.6(4)	107.4(4)	109.9(4)
O5b^{i}-Al3-O2a1	109.1(3)	108.8(3)	109.5(3)
O4a1-Al3-O2a2	117.6(3)	115.3(3)	119.8(3)
O4a1-Al3-O2a1	111.3(2)	109.6(2)	113.0(2)
O4a2-Al3-O2a2	104.1(4)	103.5(4)	104.8(4)
O4a2-Al3-O2a1	98.2(3)	95.5(3)	100.9(3)
O6a-Si4-O5b^{ii}	110.42(17)	110.17(17)	110.66(17)
O6a-Si4-O3a2^{iii}	106.7(5)	105.1(5)	108.3(5)
O6a-Si4-O3a1^{iii}	112.9(3)	111.1(3)	114.7(3)
O6a-Si4-O2a2	104.6(5)	103.3(5)	105.8(5)
O6a-Si4-O2a1	110.3(4)	108.9(4)	111.6(4)
O6b^{ii}-Si4-O3a2^{iii}	101.5(4)	97.4(4)	105.6(4)
O6b^{ii}-Si4-O3a1^{iii}	110.1(2)	109.8(2)	110.4(3)
O6b^{ii}-Si4-O2a2	108.7(4)	105.5(4)	111.8(4)
O6b^{ii}-Si4-O2a1	109.6(3)	108.9(3)	110.3(3)
O3a2^{iii}-Si4-O2a2	124.7(4)	121.6(4)	127.7(4)
O3a2^{iii}-Si4-O2a1	117.9(4)	113.6(4)	122.0(4)
O3a1^{iii}-Si4-O2a2	110.0(3)	107.5(3)	112.4(4)
O3a1^{iii}-Si4-O2a1	103.3(3)	102.1(3)	104.5(3)
O6a^{iv}-Al4-O6b	111.65(15)	111.15(15)	112.12(16)
O6a^{iv}-Al4-O3b1	103.6(2)	102.4(2)	104.8(2)
O6a^{iv}-Al4-O3b2	114.8(3)	112.7(3)	117.0(3)
O6a^{iv}-Al4-O2b2	106.0(4)	102.2(4)	110.0(4)
O6a^{iv}-Al4-O2b1	113.2(2)	111.7(2)	114.7(3)
O6b-Al4-O3b1	113.65(19)	112.49(19)	114.81(19)
O6b-Al4-O3b2	111.6(3)	109.3(3)	113.8(3)
O6b-Al4-O2b2	106.2(5)	104.7(5)	107.6(5)
O6b-Al4-O2b1	109.4(3)	108.2(3)	110.5(3)
O3b1-Al4-O2b2	115.5(4)	112.5(4)	118.5(3)
O3b1-Al4-O2b1	105.1(2)	104.6(2)	105.7(2)
O3b2-Al4-O2b2	105.8(4)	104.4(4)	107.2(4)
O3b2-Al4-O2b1	95.1(3)	90.6(3)	99.6(3)

Symmetry codes:
(i)-x_2,x_1-x_2,x_3;(ii)-x_2,x_1-x_2,x_3+1;
(iii)-x_2+2/3,x_1-x_2+1/3,x_3;(iv)-x_2,x_1-x_2,x_3-1;

(v)$-x_1+x_2+1/3,-x_1+2/3,x_3$;(vi)$-x_2-2/3,x_1-x_2-1/3,x_3$;
(vii)$-x_1+x_2-1/3,-x_1-2/3,x_3$;(viii)$x_1,x_2,x_3-1$;
(ix)$-x_2+2/3,x_1-x_2+1/3,x_3-1$;(x)$-x_1+x_2+1/3,-x_1+2/3,x_3-1$;
(xi) x_1,x_2,x_3+1;(xii)$-x_2-2/3,x_1-x_2-1/3,x_3+1$;
(xiii)$-x_1+x_2-1/3,-x_1-2/3,x_3+1$;(xiv)$x_1+2/3,x_2+1/3,x_3$;
(xv)$x_1+2/3,x_2+1/3,x_3+1$;(xvi)$-x_1+x_2+1/3,-x_1-1/3,x_3+1$;
(xvii)$x_1-2/3,x_2-1/3,x_3$;(xviii)$x_1-2/3,x_2-1/3,x_3-1$.

Table 3. *Atomic coordinates and isotropic displacement parameters of nepheline (Superspace group* $X3(0\,0\,\gamma)0$*)*

atom	harmonic	x	y	z	U_{iso}
K1a		-0.00185(8)	-0.00146(7)	0.25	0.0390(7)
Na1a		-0.00185(8)	-0.00146(7)	0.25	0.0390(7)
K1b		0.00185(8)	0.00146(7)	-0.2515(4)	0.0390(7)
Na1b		0.00185(8)	0.00146(7)	-0.2515(4)	0.0390(7)
Na2a		0.36891(9)	0.18630(9)	0.2465(3)	0.02327(8)
Na2b		-0.37180(9)	-0.18686(9)	-0.2570(2)	0.02327(8)
Si1		1/3	1/3	-0.0609(3)	0.0123(3)
Al1		-1/3	-1/3	0.0515(3)	0.0111(3)
Si2		-1/3	-1/3	-0.5608(3)	0.0115(3)
Al2		1/3	1/3	0.5505(3)	0.0115(3)
Si3		-0.19104(4)	-0.14272(4)	-0.0698(2)	0.0105(2)
Al3		0.19043(5)	0.14217(5)	0.0566(2)	0.0105(2)
Si4		0.19119(4)	0.14286(5)	0.4296(2)	0.0109(2)
Al4		-0.19011(5)	-0.14187(5)	-0.4436(2)	0.0104(2)
O1a		0.3639(4)	0.3563(4)	0.7501(4)	0.0288(10)
O1b		-0.3179(4)	-0.3097(5)	-0.7504(4)	0.0288(10)
O2a1		0.2045(3)	0.1142(4)	0.2505(5)	0.0226(4)
O2a2		0.1907(6)	0.1085(7)	0.2494(10)	0.0226(4)
O2b1		-0.2091(3)	-0.1220(2)	-0.2471(4)	0.0226(4)
O2b2		-0.1910(5)	-0.1027(5)	-0.2507(8)	0.0226(4)
O3a1		0.2690(2)	0.37747(18)	0.4732(5)	0.0190(4)
O3a2		0.2782(4)	0.3869(4)	0.5198(8)	0.0190(4)
O3b1		-0.29084(17)	-0.2301(2)	-0.5084(5)	0.0190(4)
O3b2		-0.2896(4)	-0.2355(3)	-0.4659(8)	0.0190(4)
O4a1		0.29077(18)	0.23168(18)	-0.0186(4)	0.0177(3)
O4a2		0.2921(5)	0.2373(4)	0.0358(6)	0.0177(3)
O4b1		-0.28482(19)	-0.2223(2)	0.0031(4)	0.0177(3)
O4b2		-0.2842(3)	-0.2264(3)	-0.0447(8)	0.0177(3)
O5a		0.10309(14)	0.16343(17)	0.0510(3)	0.0189(5)
O5b		-0.11498(14)	-0.17059(16)	-0.0709(3)	0.0189(5)
O6a		0.11491(14)	0.17146(15)	0.4284(3)	0.0183(4)
O6b		-0.10366(13)	-0.16413(15)	-0.4475(3)	0.0183(4)

Table 4. *Amplitudes of displacive modulation in nepheline (Superspace group* $X3(0\,0\,\gamma)0$*)*

atom	harmonic	x	y	z
K1a	sin1	0.0036(4)	0.0026(4)	0
	cos1	0	0	-0.0092(3)
Na1a	sin1	0.0036(4)	0.0026(4)	0
	cos1	0	0	-0.0092(3)
K1b	sin1	0.0070(4)	0.0045(4)	-0.00167(13)
	cos1	0	0	-0.0078(3)
Na1b	sin1	0.0070(4)	0.0045(4)	-0.00167(13)
	cos1	0	0	-0.0078(3)
Na2a	sin1	-0.00244(7)	0	-0.00305(13)
	cos1	0	0.00109(4)	0
Na2b	sin1	0.00299(8)	-0.00126(4)	0.00324(13)
	cos1	-0.00149(4)	0	0.00187(6)
Si1	sin1	-0.00195(6)	-0.00270(6)	0
	cos1	-0.00199(8)	0.00069(8)	0
Al1	sin1	0.00229(7)	0.00287(7)	0
	cos1	-0.00199(9)	0.00099(9)	0
Si2	sin1	0.00115(6)	0.00273(6)	0
	cos1	-0.00249(8)	-0.00025(8)	0
Al2	sin1	-0.00093(7)	-0.00255(7)	0
	cos1	-0.00241(9)	-0.00040(9)	0
Si3	sin1	0.00241(5)	0.00146(5)	-0.00245(10)
	cos1	-0.00023(5)	-0.00043(5)	-0.00718(9)
Al3	sin1	-0.00204(5)	-0.00124(6)	0.00345(10)
	cos1	-0.00036(6)	-0.00062(5)	-0.00687(10)
Si4	sin1	-0.00229(5)	-0.00145(5)	-0.00237(10)
	cos1	0	0.00017(4)	-0.00734(8)
Al4	sin1	0.00229(5)	0.00150(5)	0.00298(11)
	cos1	0.00032(3)	0.00042(5)	-0.00735(9)
O1a	sin1	0	-0.0013(3)	0
	cos1	0	0.0029(3)	0
O1b	sin1	0	0.0030(6)	0
	cos1	-0.0060(4)	0.0020(3)	0
O2a1	sin1	-0.0051(3)	-0.0061(3)	0.0029(5)
	cos1	0	0	-0.0080(4)
O2a2	sin1	0	0	-0.0050(12)
	cos1	0	0	-0.0084(8)
O2b1	sin1	0.0044(2)	0.0071(2)	0.0026(4)
	cos1	-0.00396(13)	-0.00439(15)	-0.0104(3)
O2b2	sin1	0.0027(4)	-0.0035(5)	-0.0028(9)
	cos1	0	0	0
O3a1	sin1	-0.00259(19)	-0.00147(17)	0.0066(4)
	cos1	0.00110(15)	0.00130(16)	-0.0034(4)
O3a2	sin1	-0.0020(3)	-0.0036(3)	-0.0037(7)
	cos1	0	0.0020(3)	0.0031(6)
O3b1	sin1	0	0.00134(17)	0.0117(5)
	cos1	0	0	-0.0113(4)
O3b2	sin1	0.0029(3)	0	0
	cos1	0	0.0038(3)	-0.0065(7)
O4a1	sin1	0	0	0.0042(4)
	cos1	0	0	0
O4a2	sin1	-0.0024(4)	-0.0032(3)	0
	cos1	-0.00061(19)	0.0005(2)	-0.0042(6)
O4b1	sin1	0.00085(15)	0.00201(14)	-0.0051(4)
	cos1	0	0.00119(9)	-0.00244(18)
O4b2	sin1	0	0	0.0049(7)
	cos1	0	0	-0.0062(6)
O5a	sin1	-0.00149(8)	0	0.00252(11)
	cos1	-0.00132(9)	-0.00191(11)	-0.00945(18)
O5b	sin1	0.00190(8)	0.00131(7)	0
	cos1	-0.00071(9)	-0.00125(11)	-0.00755(18)
O6a	sin1	-0.00148(8)	0	0
	cos1	-0.00034(6)	0	-0.00741(18)
O6b	sin1	0.00179(8)	0.00082(7)	0.00284(10)