Table 3. (deposited). Relevant inter-tetrahedral angles (°), voids diameters (Å), bond distances (Å) and the ditrigonal rotation angle (°) at different pressures of cancrinite-group minerals

P (GPa)	Si-O1-Al	Si-O2-Al	Si-O3-Al	Si-O4-Al	O3-O4-O3	$\alpha_{S6R\perp[0001]}$	O3-O4$_{S4R}$	O1-O1$_{12R}$	O3-O4$_{12R}$	(Na,Ca)-O1	(Na,Ca)-O2
Cancrinite (Lotti et al. 2012)											
0.0001	147.5(7)	151.8(6)	131.4(6)	132.5(5)	142.9(4)	8.8(2)	4.15(1)	9.16(1)	8.48(1)	2.888(8)	2.441(7)
0.76(2)	145.4(7)	149.0(5)	131.3(6)	132.6(5)	141.1(4)	9.6(2)	4.08(1)	9.12(1)	8.51(2)	2.883(8)	2.397(6)
0.99(2)	145.9(7)	149.5(5)	132.2(5)	131.5(5)	143.1(3)	9.5(2)	4.13(1)	9.08(1)	8.41(1)	2.879(8)	2.403(6)
1.39(2)	143.9(6)	148.3(5)	131.3(4)	129.9(5)	140.3(3)	10.0(2)	4.09(1)	9.04(1)	8.432(9)	2.886(7)	2.380(6)
2.33(2)	143.6(6)	148.5(4)	130.4(4)	129.4(4)	140.1(3)	9.8(2)	4.07(1)	9.00(1)	8.388(8)	2.867(7)	2.374(6)
3.59(2)	141.4(7)	144.2(5)	128.9(5)	128.6(5)	136.5(3)	11.6(2)	3.99(1)	8.88(1)	8.405(8)	2.894(7)	2.312(6)
4.30(3)	140.7(6)	143.3(5)	128.6(5)	127.8(5)	135.7(3)	12.2(2)	3.97(1)	8.81(1)	8.380(8)	2.902(7)	2.286(7)
5.00(2)	139.6(6)	143.6(5)	127.7(4)	127.2(4)	135.1(3)	11.6(2)	3.98(1)	8.837(9)	8.351(8)	2.874(7)	2.291(6)
5.73(3)	137.6(7)	140.9(5)	126.0(5)	126.5(5)	133.1(4)	13.2(2)	3.91(1)	8.68(1)	8.377(9)	2.931(8)	2.262(7)
6.16(2)	138.3(6)	140.7(5)	126.8(5)	126.9(5)	132.8(3)	13.2(2)	3.89(1)	8.70(1)	8.386(8)	2.914(7)	2.252(6)
6.63(3)	137.3(6)	138.6(5)	126.4(5)	126.8(5)	133.0(3)	14.3(2)	3.87(1)	8.636(9)	8.379(8)	2.932(7)	2.219(6)
Vishnevite (Lotti 2014)											
0.0001	153.0(7)	147.6(6)	139.9(6)	141.2(6)	152.5(4)	10.2(2)	4.025(12)	8.943(7)	8.750(8)	2.942(6)^{Na1} 2.901(4)^{Na2}	2.465(7)^{Na1} 2.365(5)^{Na2}
0.52(2)	151.9(9)	149.1(6)	138.3(9)	137.2(8)	147.5(5)	9.0(2)	4.01(2)	8.978(13)	8.725(17)	2.897(10)^{Na1} 2.859(9)^{Na2}	2.485(10)^{Na1} 2.388(7)^{Na2}
1.20(3)	150.2(8)	148.6(6)	137.4(9)	136.0(9)	146.2(5)	9.3(2)	3.99(3)	8.913(14)	8.695(18)	2.898(10)^{Na1} 2.865(9)^{Na2}	2.463(11)^{Na1} 2.375(7)^{Na2}
1.78(5)	149.0(9)	146.8(7)	135.8(8)	136.0(9)	145.1(5)	10.0(3)	3.98(2)	8.874(15)	8.670(18)	2.899(10)^{Na1} 2.866(10)^{Na2}	2.432(11)^{Na1} 2.341(8)^{Na2}
2.47(2)	147.8(10)	146.3(7)	135.5(9)	136.2(8)	144.8(5)	10.3(3)	3.96(2)	8.816(15)	8.642(18)	2.892(12)^{Na1} 2.868(10)^{Na2}	2.402(17)^{Na1} 2.327(10)^{Na2}
3.24(9)	147.4(9)	144.3(7)	132.6(8)	132.6(8)	141.5(5)	10.8(3)	3.98(2)	8.768(14)	8.558(16)	2.903(11)^{Na1} 2.858(9)^{Na2}	2.408(15)^{Na1} 2.304(9)^{Na2}
3.43(4)	145.0(8)	145.9(7)	134.4(8)	133.5(7)	141.5(5)	10.5(2)	3.93(2)	8.737(15)	8.594(17)	2.889(10)^{Na1} 2.861(9)^{Na2}	2.401(13)^{Na1} 2.316(9)^{Na2}
4.23(7)	143.1(8)	144.5(7)	131.5(7)	130.0(7)	137.7(4)	11.4(3)	3.92(2)	8.596(13)	8.513(15)	2.905(9)^{Na1} 2.881(9)^{Na2}	2.367(11)^{Na1} 2.274(9)^{Na2}
5.74(6)	142.5(9)	143.4(7)	128.9(7)	130.7(7)	136.0(4)	12.4(3)	3.90(2)	8.506(15)	8.493(17)	2.943(10)^{Na1} 2.901(10)^{Na2}	2.371(12)^{Na1} 2.244(9)^{Na2}
6.10(8)	143.3(9)	142.6(7)	128.0(8)	129.5(8)	135.0(5)	12.7(3)	3.87(3)	8.449(15)	8.473(18)	2.956(11)^{Na1} 2.900(9)^{Na2}	2.367(13)^{Na1} 2.229(9)^{Na2}

6.11(4)	138.9(9)	140.0(7)	128.4(8)	128.3(8)	135.3(5)	14.4(3)	3.84(3)	8.260(16)	8.43(2)	2.984(11)^{Na1} 2.956(10)^{Na2}	2.290(14)^{Na1} 2.173(9)^{Na2}
7.40(4)	136.2(10)	130.0(7)	125.1(13)	125.2(14)	129.9(10)	17.5(4)	3.71(3)	8.18(2)	8.916(16)	2.942(12)^{Na1} 2.96(2)^{Na2}	2.078(17)^{Na1} 2.008(15)^{Na2}
Balliranoite (Lotti et al. 2014b)											
0.0001	155.4(3)	160.3(3)	136.1(4)	137.9(4)	161.4(2)	1.2(1)	4.400(10)	9.400(7)	8.279(11)	2.614(4)	2.560(4)
0.85(3)	152.9(3)	160.2(3)	133.7(4)	136.4(5)	157.7(2)	1.4(1)	4.399(10)	9.323(8)	8.202(11)	2.610(5)	2.551(4)
1.73(3)	150.3(3)	159.4(3)	132.5(4)	134.7(4)	154.4(2)	1.8(1)	4.392(10)	9.255(8)	8.173(10)	2.623(4)	2.544(4)
2.62(4)	148.4(3)	159.4(3)	131.7(4)	133.3(4)	152.8(2)	1.9(1)	4.390(10)	9.189(8)	8.120(11)	2.624(4)	2.542(4)
3.80(5)	146.4(3)	158.5(3)	130.5(4)	131.6(4)	148.8(2)	2.4(1)	4.357(10)	9.087(8)	8.077(9)	2.631(5)	2.525(4)
4.95(3)	144.6(3)	159.3(3)	129.0(4)	130.2(4)	146.9(2)	2.3(2)	4.354(11)	9.008(8)	8.015(11)	2.632(5)	2.536(4)
4.95(4)	143.6(3)	157.9(4)	128.6(5)	128.5(5)	145.3(3)	2.7(2)	4.333(12)	8.940(10)	7.964(13)	2.626(7)	2.513(5)
6.77(2)	142.3(3)	156.7(3)	127.5(4)	128.1(4)	143.8(2)	2.9(2)	4.339(10)	8.927(8)	7.947(11)	2.625(6)	2.504(5)
Davyne (Lotti et al. 2014a)											
0.0001[a]	167.7(3)	158.1(3)	142.0(2)	–	180	2.5(1)	4.361(6)	9.451(6)	8.439(4)	2.661(4)	2.533(4)
0.38(2)	169.1(6)	157.1(4)	139.9(5)	142.6(5)	170.1(4)	3.0(2)	4.328(11)	9.414(11)	8.460(11)	2.676(7)^{Ca1} 2.681(7)^{Ca2}	2.521(6)^{Ca1} 2.522(6)^{Ca2}
0.91(3)	164.2(6)	157.6(4)	140.1(5)	139.9(5)	168.6(3)	2.9(2)	4.344(8)	9.377(10)	8.403(8)	2.680(7)^{Ca1} 2.672(7)^{Ca2}	2.517(5)^{Ca1} 2.532(6)^{Ca2}
1.57(5)	159.3(6)	156.2(4)	139.0(4)	138.2(4)	162.6(3)	3.6(2)	4.325(8)	9.301(9)	8.373(8)	2.683(7)^{Ca1} 2.680(7)^{Ca2}	2.490(5)^{Ca1} 2.510(6)^{Ca2}
2.05(6)	157.5(5)	156.7(4)	137.3(4)	137.7(4)	160.8(2)	3.4(2)	4.328(7)	9.280(9)	8.329(7)	2.700(7)^{Ca1} 2.668(7)^{Ca2}	2.487(5)^{Ca1} 2.513(6)^{Ca2}
3.07(2)	154.6(5)	155.2(4)	134.5(3)	137.2(4)	157.3(2)	4.0(2)	4.327(11)	9.192(9)	8.264(7)	2.674(7)^{Ca1} 2.674(7)^{Ca2}	2.462(5)^{Ca1} 2.491(6)^{Ca2}
3.49(2)	153.4(5)	156.0(4)	134.4(3)	137.0(3)	156.2(2)	3.5(2)	4.304(11)	9.187(8)	8.254(7)	2.655(5)^{Ca1} 2.656(7)^{Ca2}	2.473(5)^{Ca1} 2.495(6)^{Ca2}
4.56(7)	151.1(6)	155.7(5)	132.9(4)	136.0(4)	153.2(2)	3.6(2)	4.287(14)	9.129(9)	8.207(8)	2.649(7)^{Ca1} 2.650(7)^{Ca2}	2.460(6)^{Ca1} 2.490(7)^{Ca2}
5.33(8)	149.9(6)	156.2(5)	131.7(4)	134.4(4)	152.0(3)	3.6(2)	4.293(14)	9.064(9)	8.160(8)	2.656(6)^{Ca1} 2.658(7)^{Ca2}	2.470(6)^{Ca1} 2.505(7)^{Ca2}
6.10(8)	148.8(7)	155.6(5)	129.9(4)	133.8(4)	150.2(3)	3.9(2)	4.290(15)	9.011(9)	8.113(9)	2.655(6)^{Ca1} 2.659(6)^{Ca2}	2.455(6)^{Ca1} 2.494(7)^{Ca2}
7.18(6)	148.0(7)	155.1(6)	129.2(5)	133.3(5)	147.9(3)	4.1(2)	4.254(16)	8.953(11)	8.090(10)	2.647(8)^{Ca1} 2.655(8)^{Ca2}	2.443(8)^{Ca1} 2.483(9)^{Ca2}

Notes: $\alpha_{S6R\perp[0001]} = \Sigma_i\{1/6\cdot[|120°-\theta_i|/2]\}$ (see Figure 6; parameter originally defined for phyllosilicates, Brigatti and Guggenheim 2002)

[a] $P6_3/m$ davyne sample at 0.0001 GPa, $P6_3$ davyne at all the other pressures (Lotti et al. 2014a).

Table 4. Relevant inter-tetrahedral angles (°), voids diameters (Å), bond distances (Å) and the ditrigonal rotation angle (°) at different temperatures of cancrinite-group minerals

T (K)	Si-O1-Al	Si-O2-Al	Si-O3-Al	Si-O4-Al	O3-O4-O3	$\alpha_{S6R\perp[0001]}$	O3-$O4_{S4R}$	O1-$O1_{12R}$	O3-$O4_{12R}$	(Na,Ca)-O1	(Na,Ca)-O2
					Cancrinite (Hassan et al. 2006)						
298	151.6(6)	155.3(5)	142.7(10)	125.2(9)	146.8[a]	7.63[a]	4.160[a]	8.793[a]	8.447[a]	2.888(7)	2.521(6)
374	152.2(6)	155.5(5)	142.8(10)	126.1(9)	147.8[a]	7.18[a]	4.157[a]	8.814[a]	8.457[a]	2.881(7)	2.524(6)
480	152.7(6)	155.8(5)	142.3(11)	127.2(11)	148.8[a]	7.08[a]	4.167[a]	8.845[a]	8.461[a]	2.871(7)	2.531(6)
571	152.8(6)	156.3(5)	140.5(12)	129.9(13)	150.9[a]	6.70[a]	4.186[a]	8.884[a]	8.456[a]	2.861(6)	2.543(6)
678	152.9(6)	156.7(4)	138.4(14)	135.3(16)	154.0[a]	6.40[a]	4.189[a]	8.931[a]	8.465[a]	2.850(7)	2.567(5)
769	153.7(6)	157.8(4)	139.2(11)	134.1(11)	154.7[a]	5.98[a]	4.189[a]	8.953[a]	8.486[a]	2.852(7)	2.587(5)
784	153.4(6)	157.6(4)	139.0(10)	134.0(11)	154.6[a]	5.95[a]	4.186[a]	8.959[a]	8.487[a]	2.847(7)	2.586(5)
830	152.2(6)	158.3(4)	140.3(9)	132.5(9)	154.3[a]	6.05[a]	4.206[a]	8.941[a]	8.478[a]	2.857(7)	2.596(5)
875	151.0(6)	157.8(4)	140.1(10)	132.9(10)	154.3[a]	5.90[a]	4.202[a]	8.989[a]	8.490[a]	2.838(7)	2.593(5)
921	151.8(6)	158.4(4)	140.1(9)	132.4(10)	155.3[a]	5.90[a]	4.229[a]	8.971[a]	8.474[a]	2.851(7)	2.599(5)
966	152.4(6)	158.9(4)	139.6(9)	132.7(10)	155.7[a]	5.78[a]	4.242[a]	8.973[a]	8.468[a]	2.852(7)	2.603(5)
1073	155.1(7)	158.7(5)	138.6(9)	133.2(10)	157.7[a]	5.75[a]	4.256[a]	8.972[a]	8.470[a]	2.866(7)	2.604(6)
1164	156.1(7)	159.5(5)	139.8(11)	133.5(11)	159.9[a]	5.60[a]	4.285[a]	8.976[a]	8.461[a]	2.876(8)	2.622(6)
1225	154.5(10)	160.6(6)	141.0(16)	134.7(15)	162.9[a]	4.78[a]	4.270[a]	9.052[a]	8.499[a]	2.837(9)	2.639(8)
					Cancrinite (Isupova et al. 2010)						
173	146.4(1)	151.1(1)	133.2(2)	133.18(8)	144.9[a]	9.03[a]	4.134[a]	8.800[a]	8.475[a]	2.877(2)	2.429(2)
293	147.4(1)	151.86(9)	133.8(2)	133.71(7)	145.7[a]	8.43[a]	4.144[a]	8.856[a]	8.493[a]	2.866(2)	2.444(2)
473	149.8(2)	153.2(2)	135.1(2)	135.0(2)	149.2[a]	7.73[a]	4.163[a]	8.923[a]	8.502[a]	2.854(2)	2.469(3)
673	151.5(2)	152.2(2)	136.6(2)	136.2(2)	151.5[a]	7.95[a]	4.146[a]	8.950[a]	8.540[a]	2.857(3)	2.461(4)
					Cancrinite (Gatta et al. 2014)						
303	147.2(2)	151.2(2)	133.4(2)	133.3(2)	144.6(3)	8.48(9)	4.145(6)	8.862(5)	8.487(4)	2.862(3)	2.437(4)
478	148.0(2)	152.5(2)	134.0(2)	134.1(2)	146.39(16)	7.99(8)	4.166(6)	8.901(5)	8.485(4)	2.854(2)	2.455(3)
748	151.2(3)	151.0(3)	136.1(3)	136.6(3)	149.8(2)	8.19(12)	4.155(8)	8.971(7)	8.536(5)	2.846(3)	2.446(4)
					Cancrinite (Gatta et al. 2012a)						
293	147.02(9)	151.79(7)	133.46(7)	133.55(7)	144.84(2)	8.45(3)	4.129(3)	8.841(2)	8.486(1)	2.858(1)	2.437(1)
250	146.46(8)	151.45(10)	133.26(7)	133.26(7)	144.42(5)	8.66(3)	4.123(2)	8.815(2)	8.471(1)	2.863(1)	2.429(1)

220	146.14(8)	151.27(10)	133.05(6)	133.02(6)	143.98(4)	8.75(3)	4.120(2)	8.810(2)	8.475(1)	2.866(1)	2.427(1)
180	145.85(8)	150.90(9)	132.83(7)	132.85(7)	143.71(5)	8.87(3)	4.117(2)	8.802(2)	8.472(1)	2.866(1)	2.421(1)
140	145.42(8)	150.74(9)	132.78(7)	132.72(7)	143.37(5)	9.05(3)	4.111(2)	8.783(2)	8.474(1)	2.873(1)	2.418(1)
100	145.32(7)	150.56(9)	132.55(7)	132.66(7)	143.05(5)	9.09(3)	4.108(2)	8.783(1)	8.480(1)	2.875(1)	2.416(1)
Vishnevite (Lotti 2014)											
293	153.3(2)	147.4(3)	140.6(4)	140.2(4)	152.6(2)	10.2(1)	4.042(10)	8.930(5)	8.726(7)	2.920(3)	2.411(4)
110	151.6(2)	146.8(2)	139.6(4)	139.4(4)	151.2(2)	10.8(1)	4.015(10)	8.852(5)	8.715(6)	2.937(3)	2.400(4)
Balliranoite (Gatta et al. 2013b)											
293	155.98(8)	161.28(6)	136.44(6)	137.33(7)	162.68(5)	1.02(3)	4.427(1)	9.387(1)	8.251(2)	2.6218(9)	2.5761(8)
250	155.27(8)	161.28(7)	136.13(6)	137.09(6)	161.81(4)	1.03(3)	4.424(1)	9.373(2)	8.239(2)	2.620(1)	2.5752(9)
220	154.81(7)	161.21(6)	135.98(6)	136.84(6)	161.43(4)	1.04(3)	4.430(1)	9.372(2)	8.235(2)	2.6207(9)	2.5753(8)
180	154.32(8)	161.17(6)	135.70(6)	136.65(6)	160.85(4)	1.07(3)	4.428(1)	9.367(2)	8.231(2)	2.6209(9)	2.5746(9)
140	153.92(8)	161.23(7)	135.51(6)	136.42(6)	160.43(4)	1.06(6)	4.427(1)	9.356(2)	8.219(2)	2.619(1)	2.5738(9)
108	153.65(8)	161.21(7)	135.40(6)	136.29(7)	160.18(4)	1.08(3)	4.429(1)	9.352(6)	8.215(2)	2.620(1)	2.5741(9)
Davyne (Gatta et al. 2013a)											
293	166.15(7)	156.87(5)	141.83(7)	141.52(6)	171.51(4)	3.00(2)	4.331(2)	9.427(1)	8.467(1)	2.6715(8)	2.5162(7)
250	164.87(6)	156.96(5)	141.85(6)	141.24(5)	169.96(4)	3.00(2)	4.323(2)	9.413(1)	8.460(1)	2.6701(7)	2.5153(7)
220	164.02(5)	156.80(4)	141.43(5)	141.06(4)	169.00(3)	3.00(2)	4.327(1)	9.412(1)	8.4512(8)	2.6675(6)	2.5129(6)
180	163.05(5)	156.88(4)	141.24(5)	140.73(4)	167.92(3)	3.00(2)	4.327(1)	9.404(1)	8.4459(8)	2.6685(6)	2.5140(6)
140	162.45(5)	156.77(4)	141.05(5)	140.29(4)	167.22(3)	3.02(2)	4.331(1)	9.400(1)	8.4357(8)	2.6670(6)	2.5121(6)
110	161.99(5)	156.73(4)	140.86(5)	140.26(4)	166.65(3)	3.04(2)	4.329(1)	9.394(1)	8.4334(8)	2.6677(6)	2.5117(6)
Pitiglianoite[b] (Bonaccorsi et al. 2007)											
298	155.9(4)	144.9(4)	143.2(4)	144.0(4)	155.7[a]	11.25[a]	4.000[a]	8.953[a]	8.835[a]	2.954(5)^{Na}	2.394(6)^{Na}
730	152.7(5)	147.9(6)	139.3(6)	139.6(7)	152.0[a]	10.03[a]	4.051[a]	8.942[a]	8.730[a]	2.917(9)^{Na}	2.42(1)^{Na}2.82(1)^{K}
298 post-H*T*	147.9(3)	148.0(2)	136.8(2)	136.5(2)	147.6[a]	10.00[a]	4.078[a]	8.868[a]	8.646[a]	2.911(4)^{Na} 3.122(4)^{K}	2.397(8)^{Na} 2.760(5)^{K}

$\alpha_{S6R\perp[0001]} = \Sigma_i\{1/6\cdot[|120°-\theta_i|/2]\}$ (see Figure 6; parameter originally defined for phyllosilicates, Brigatti and Guggenheim 2002).

[a] Calculated from published data; [b] Structure refinements performed in the vishnevite subcell.