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Hydrogen-bond system and dehydration behavior of the natural zeolite parthéite

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Abstract

The crystal structure, including H positions, of the monoclinic zeolite mineral parthéite (space group *C*2/*c*) of framework type **-PAR** from Denezhkin Kamen (Urals, Russia) was refined, from single-crystal X-ray data to R_1 = 3.46%. In addition, in situ single-crystal X-ray data have been measured in steps of 25 °C up to 375 °C to analyze dehydration behavior. In situ Raman spectra of the natural (room temperature) and partly dehydrated varieties of parthéite have been recorded at 100, 150, and 275 °C.

The structure of parthéite, $Ca_2Al_4Si_4O_{15}(OH)_2{\cdot}4H_2O$, is characterized by a tetrahedral framework interrupted by an OH-group forming the apex of one AlO_4 tetrahedron. In addition, this OH-group coordinates extraframework Ca together with two H_2O molecules and four framework oxygen sites. The structure has four strong hydrogen bonds with H···O interactions below 2 Å. The fifth hydrogen associated with a H_2O molecule, exhibits two potential acceptors of weak hydrogen bonds with H···O distances of ca. 2.5 Å. This softly bound H_2O molecule is released at 150 °C without severe impact on framework distortions but with decrease of Ca coordination from seven to six. Concurrently with loss of the second H_2O molecule at 250 °C, the structure further compacts and becomes severely distorted. The space group *C*2/*c* and the tetrahedral connectivity are preserved but β changes from 91 to 79° and the volume drops from 1730 to 1600 Å^3. Ca is still six-coordinated by five framework O atoms and OH.

Keywords: Zeolite, parthéite, hydrogen bonding, dehydration, Raman spectroscopy, crystal structure

Introduction

The atlas of zeolite framework types (Baerlocher and McCusker, August 2011) lists 197 tetrahedral frameworks characterized by a three letter framework-type code. Among these structure types eight examples have a minus sign (–) in front of their code name indicating that the framework is interrupted by an OH group. Parthéite (**-PAR**), simplified $Ca_2Al_4Si_4O_{15}(OH)_2{\cdot}4H_2O$ is one of the latter representatives described from two occurrences. The first type locality is rodingitic rocks from an ophiolitic zone in the Taurus Mountains, southwest Turkey (Sarp et al. 1979). A second occurrence has been described from gabbro-pegmatites of the Denezhkin Kamen intrusive complex in the Urals, Russia (Ivanov and Mozzherin 1982). The analog of the mineral has not been synthesized and other compositions with **-PAR** framework type have not been reported. In the original description of parthéite, based on electron-microprobe analyses, Sarp et al. (1979) could not recognize the OH-bearing nature of this mineral and the formula was given as $CaAl_2Si_2O_8{\cdot}2H_2O$ (*Z* = 8). A few years later when the crystal structure was solved (Engel and Yvon 1984), the formula was correctly rewritten as $Ca_2Al_4Si_4O_{15}(OH)_2{\cdot}4H_2O$, *Z* = 4 (Sarp 1985). The assumption that parthéite is a dimorph of lawsonite $CaAl_2Si_2O_7(OH)_2{\cdot}H_2O$ is not correct. Although these two minerals have similar stoichiometry, containing both OH-groups as well as H_2O, they have different OH/H_2O ratios and they are classified as zeolite and sorosilicate, respectively.

The **-PAR** structure (Engel and Yvon 1984) is characterized by essentially complete order of tetrahedral Si and Al and oblate 10-membered ring channels running parallel to the **c** axis. The apex of one AlO_4 tetrahedron is terminated by an OH group. Pockets within the channels host extraframework Ca coordinated by four framework O atoms, one OH-group and two H_2O molecules. In the existing structural data of parthéite (Engel and Yvon 1984), H sites have not been located. This study aims for understanding the hydrogen bond system and the dehydration behavior of parthéite based on new X-ray single-crystal diffraction data collected on crystals from Denezhkin Kamen (Urals Region, Russia). Parthéite from this locality has been used before for calorimetric determination of the enthalpy of formation (Ogorodova et al. 2007) yielding good agreement with corresponding calculations based on crystal structure data (Vieillard 1995).

Experimental methods

A prismatic parthéite crystal 20 × 30 × 76 μm in size from Denezhkin Kamen (Urals Region, Russia) was mounted on a glass needle and used for data collection at room temperature. The crystals originated from the very same sample investigated by Ivanov and Mozzherin (1982). Their chemical analysis showed $Ca_2Al_4Si_4O_{15}(OH)_2{\cdot}4H_2O$ stoichiometry, with traces of Mg^{2+} and Na^{1+}. Measurements were made with an Oxford Diffraction SuperNova area-detector equipped diffractometer using mirror optics and monochromatized Mo*K*α radiation (λ = 0.71073 Å). The unit-cell constants were obtained from least-squares refinement of the setting angles of 3120 reflections in the range 1.88° < θ < 29.73°. A total of 1366 frames were collected using ω scans, 60 s exposure time, rotation angle of 0.5° per frame, and a crystal-detector distance of 65.0 mm.

Data reduction was performed using the CrysAlisPro program (Oxford Diffraction 2010). The intensities were corrected for Lorentz and polarization effects, and an absorption correction based on the multi-scan method using SCALE3 ABSPACK in CrysAlisPro was applied. Data-collection parameters and refinement parameters

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are given in Table 1. Neutral atom scattering factors and starting coordinates from Engel and Yvon (1984) in space group *C*2/*c* were used for structure refinement with SHELXL-97 (Sheldrick 2008). Hydrogen positions were extracted from difference-Fourier maps applying the restraint H-O = 0.95(2) Å (Franks 1973) and refined with isotropic displacement parameters. The final refinement, based on 1897 observed reflections and 162 parameters with 5 restraints, converged to R_1 = 0.0346. Bond-valence calculations were performed using the parameters summarized by Brown and Altermatt (1985).

To study in situ dehydration, a second crystal from the same locality was attached to a glass fiber by two-component epoxy-glue. The crystal was too small and fragile to be mounted in a capillary. X-ray diffraction data were collected with ω scans at different φ settings (φ-ω scan) (Bruker 1999) using a Bruker APEX II SMART diffractometer and a self-constructed temperature controlled gas flow heater. The heater was mounted on the ω-axis, its gas nozzle was located 3 mm underneath the sample position. Temperature stability was ensured by using a constant flow of N_2 regulated by a mass flow controller. The heating power was controlled by an Eurotherm controller, which kept the temperature at a thermocouple in the nozzle constant. Powder measurements of well-known phase transitions as described by Krüger and Breil (2009) were utilized to obtain a temperature calibration function for temperatures at the sample position. Complete data sets were collected in steps of 25 °C up to 375 °C. Prior to the data collection, which took ca. 20 h, the crystal was equilibrated in situ for 1 h at the corresponding temperature. Data were processed using SAINT (Bruker 1999). An empirical absorption correction using SADABS (Sheldrick 1996) was applied. The refinement procedure using the program SHELXL97 (Sheldrick 2008) was the same as for the crystal measured under ambient conditions. All sites except hydrogen were refined with anisotropic displacement parameters. The isotropic displacement parameters of the hydrogen atoms were treated differently. For room-temperature data, all U_{iso} of H atoms were refined. For 150 °C data, U_{iso} of the hydrogen atom forming the hydroxyl group was refined, but those belonging to H_2O were fixed at U_{iso} = 0.05. From the data obtained at 275 °C, positions of the hydrogen atoms were not located.

After the final heating excursion to 375 °C, the crystal was cooled under nitrogen atmosphere to room temperature and subsequently exposed to humidity under ambient conditions. After allowing for rehydration for 48 h, a long exposure diffraction pattern was collected.

Confocal Raman spectra of randomly oriented single crystals were recorded in the range of 100–4000 cm^{-1} with a Horiba Jobin Yvon Labram-HR 800 Raman micro-spectrometer. The samples were excited using the 532 nm emission line of a frequency-doubled 100 mW Nd:YAG laser and the 633 nm line of a 17 mW helium-neon laser using an Olympus 100× objective lens. The size of the laser spot on the surface was approximately 1 µm in diameter. The scattered light was dispersed by an optical grating with 1800 lines mm^{-1} and collected by a 1024 × 256 open electrode CCD detector. The spectral resolution, determined by measuring the Rayleigh line, was about 2 cm^{-1}. Unpolarized spectra were recorded. The accuracy of the Raman line shifts, calibrated by regularly measuring the Rayleigh line, was in the order of 0.5 cm^{-1}. In situ high-temperature Raman experiments were performed on a Linkam TS1500 heating-stage. The sample was loaded into the ceramic crucible on a 7 mm sapphire disk. Measurements were performed at 25, 100, 150, and 275 °C.

Results

Atomic coordinates and displacement parameters for the parthéite structure at room temperature, at 150 and at 275 °C are given in Tables 2 and 3[1], respectively. Results of bond valence calculations for fully hydrated parthéite are given in Table 4[1] and selected distances and angles of hydrogen bonds under ambient conditions are in Table 5. Table 6 compares Ca-O and selected O-O distances at room temperature, 150, and 275 °C. T-O distances and T-O-T angles are summarized in Table 7. Raman spectra between 100 and 1300 cm^{-1} at different temperatures are displayed in Figure 1. Unpolarized Raman spectra of parthéite at ambient conditions are given as a deposited item. Those characteristic of the OH-stretching region are given in Figures 2 and 3.

[1] Deposit item AM-12-077, Tables 3 and 4; CIFs. Deposit items are available two ways: For a paper copy contact the Business Office of the Mineralogical Society of America (see inside front cover of recent issue) for price information. For an electronic copy visit the MSA web site at http://www.minsocam.org, go to the *American Mineralogist* Contents, find the table of contents for the specific volume/issue wanted, and then click on the deposit link there.

Table 1. Parameters for X-ray data collection and crystal-structure refinement

Crystal data for	Parthéite (RT)	Parthéite (150 °C)	Parthéite (275 °C)
Cell dimensions (Å)	*a* = 21.5474(4)	*a* = 21.524(7)	*a* = 20.82(4)
	b = 8.75638(15)	*b* = 8.667(3)	*b* = 9.350(16)
	c = 9.30578(16)	*c* = 9.292(3)	*c* = 8.359(14)
	ß = 91.5524(18)°	ß = 91.067(5)°	ß = 78.86(2)°
Cell volume	1755.15(5) Å^3	1733.1(10) Å^3	1596.3(5) Å^3
Space group	*C*2/*c*	*C*2/*c*	*C*2/*c*
Z	4	4	4
Chemical formula	$Ca_2Al_4Si_4O_{15}(OH)_2{\cdot}4H_2O$	$Ca_2Al_4Si_4O_{15}(OH)_2{\cdot}2H_2O$	$Ca_2Al_4Si_4O_{15}(OH)_2$
Diffractometer	Oxford SuperNova	Bruker Apex II	Bruker Apex II
X-ray radiation	Mo*K*α (0.71073 Å)	Mo*K*α (0.71073 Å)	Mo*K*α (0.71073 Å)
X-ray power	50 kV, 0.8 mA	50 kV, 35 mA	50 kV, 35 mA
Temperature	296 K	423 K	548 K
Crystal size (mm)	0.08 × 0.03 × 0.02	0.10 × 0.05 × 0.01	0.10 × 0.05 × 0.01
Time per frame (s)	60	60	60
Number of frames	1366	1080	1080
Completeness	100%	99.5%	99.4%
Reflections collected	10172	8183	3829
Max. θ (°)	29.73	28.45	20.5
Index range	$-29 \le h \le 29$	$-28 \le h \le 25$	$-20 \le h \le 20$
	$-12 \le k \le 12$	$-11 \le k \le 11$	$-9 \le k \le 9$
	$-12 \le l \le 12$	$-12 \le l \le 12$	$-8 \le l \le 8$
Unique reflections	2375	2182	807
Reflections >2σ(*I*)	1897	1234	399
Restraints	5	3	0
Number of parameters	162	155	123
R_{int}	0.049	0.1299	0.2547
R_σ	0.050	0.1401	0.1855
GooF	1.039	0.960	0.986
*R*1, *I* > 2σ(*I*)	0.0346	0.0536	0.0727
*R*1, all data	0.0522	0.1173	0.1757
w*R*2 (on F^2)	0.0732	0.1148	0.1982
$\Delta\rho_{min}$ (−e·Å^{-3})	−0.40 close to Si2	−0.56 close to Si2	−0.63 close to Al2
$\Delta\rho_{max}$ (e·Å^{-3})	0.51 close to O10	0.76 close to O10	0.61 close to O9

TABLE 2a. Atomic coordinates and displacement parameters (Å^3) of parthéite at RT (U_{equ} for Si1 to O11, U_{iso} for H sites)

Atom	x	y	z	$U_{equ/iso}$
Si1	0.06721(3)	0.18348(8)	0.28940(7)	0.00653(15)
Si2	0.23984(3)	0.00789(8)	0.46198(7)	0.00596(15)
Al1	0.11617(4)	0.08403(9)	0.60078(8)	0.00693(17)
Al2	0.19981(4)	0.31654(9)	0.28577(8)	0.00626(16)
Ca1	0.35596(3)	0.19896(6)	0.04443(6)	0.01130(13)
O1	0.06952(8)	0.0168(2)	0.21617(19)	0.0098(4)
O2	0.07252(8)	0.1721(2)	0.46320(19)	0.0099(4)
O3	0.12242(8)	0.2886(2)	0.22936(19)	0.0094(4)
O4	0.17245(8)	0.0354(2)	0.02491(19)	0.0093(4)
O5	0.20795(8)	0.46651(19)	0.40976(19)	0.0090(4)
O6	0.23450(9)	0.1559(2)	0.36083(19)	0.0109(4)
O7	0.23371(8)	0.3601(2)	0.12194(18)	0.0084(4)
O8	0.0000	0.2627(3)	0.2500	0.0082(5)
O9	0.35277(9)	0.2676(2)	0.2914(2)	0.0125(4)
O10	0.07184(11)	0.5030(3)	0.0158(3)	0.0342(6)
O11	0.45417(10)	0.3049(3)	0.0797(2)	0.0212(5)
H1	0.4552(17)	0.387(3)	0.141(3)	0.038(11)
H2	0.4911(12)	0.312(5)	0.033(4)	0.051(13)
H3	0.3205(12)	0.216(4)	0.327(4)	0.034(10)
H4	0.051(3)	0.466(8)	0.095(5)	0.18(3)
H5	0.0772(19)	0.609(2)	0.014(5)	0.060(14)

TABLE 2b. Atomic coordinates and displacement parameters (Å^3) of parthéite at 150 °C (U_{equ} for Si1 to O11, U_{iso} for H sites)

Atom	Occ.	x	y	z	$U_{equ/iso}$
Si1	1	0.06687(6)	0.18563(17)	0.28767(15)	0.0154(3)
Si2	1	0.24008(6)	0.01065(16)	0.46284(15)	0.0139(3)
Al1	1	0.11439(7)	0.09085(18)	0.60152(16)	0.0149(4)
Al2	1	0.19875(7)	0.31896(18)	0.28582(15)	0.0139(4)
Ca1	1	0.35172(5)	0.21062(13)	0.04383(11)	0.0213(3)
O1	1	0.06940(16)	0.0181(4)	0.2143(4)	0.0202(9)
O2	1	0.07327(16)	0.1748(4)	0.4609(3)	0.0208(9)
O3	1	0.12215(15)	0.2932(4)	0.2225(3)	0.0178(8)
O4	1	0.17264(15)	0.0304(4)	0.0293(3)	0.0161(8)
O5	1	0.20593(15)	0.4691(4)	0.4126(3)	0.0165(8)
O6	1	0.23476(16)	0.1580(4)	0.3608(4)	0.0184(8)
O7	1	0.23635(15)	0.3586(4)	0.1232(3)	0.0163(8)
O8	1	0.0000	0.2671(6)	0.2500	0.0185(12)
O9	1	0.35323(18)	0.2632(5)	0.2884(4)	0.0256(14)
O11a	0.27(3)	0.0402(12)	0.333(9)	–0.078(3)	0.092(17)
O11b	0.73(3)	0.4544(4)	0.2796(18)	0.0813(8)	0.037(4)
H1	0.73	0.492(2)	0.266(11)	0.033(8)	0.050
H2	0.73	0.467(4)	0.368(6)	0.132(8)	0.050
H3	1	0.3168(18)	0.224(7)	0.330(6)	0.05(2)

TABLE 2c. Atomic coordinates and equivalent displacement parameters (Å^3) of parthéite at 275 °C

Atom	x	y	z	U_{equ}
Si1	0.0624(3)	0.2007(7)	0.2969(7)	0.0438(18)
Si2	0.2415(3)	0.0525(6)	0.4526(7)	0.0394(17)
Al1	0.0925(3)	0.1123(7)	0.6391(7)	0.0452(19)
Al2	0.2041(3)	0.3130(7)	0.2866(7)	0.0419(18)
Ca1	0.3381(2)	0.1878(5)	0.0636(5)	0.0485(15)
O1	0.0697(8)	0.0570(16)	0.3036(19)	0.090(6)
O2	0.0539(6)	0.1847(13)	0.4903(14)	0.045(4)
O3	0.1291(6)	0.2954(14)	0.2252(15)	0.050(4)
O4	0.1760(6)	–0.0984(14)	0.0659(16)	0.055(4)
O5	0.1968(6)	0.4310(13)	0.4506(14)	0.043(4)
O6	0.2525(6)	0.1574(13)	0.2924(14)	0.044(4)
O7	0.2539(6)	0.3842(13)	0.3906(13)	0.040(4)
O8	0.0000	0.2869(17)	0.2500	0.037(5)
O9	0.4178(7)	0.2720(16)	0.1886(15)	0.064(4)

TABLE 5. Hydrogen bond distances (Å) and O-H···O angles of parthéite at room temperature

Species	D-H	H···A	D···A	<(DHA)°	Hydrogen bond
H_2O II	0.917(18)	1.84(2)	2.714(3)	159(3)	O11-H1···O1
H_2O II	0.919(19)	1.89(2)	2.805(3)	172(4)	O11-H2···O2
(OH)	0.899(18)	1.96(2)	2.821(3)	160(3)	O9-H3···O6
H_2O I	0.94(2)	2.55(4)	3.429(3)	156(6)	O10-H4···O8
H_2O I	0.94(2)	2.50(4)	2.922(3)	108(6)	O10-H4···O3
H_2O I	0.936(19)	1.98(2)	2.887(3)	164(4)	O10-H5···O2

Notes: Hydrogen positions were determined with the restraint O-H is 0.95(2) Å. D: donor; A: acceptor; H1-O11-H2: 104(3)°; H4-O10-H5: 115(5)°.

TABLE 6. Ca-O and O-O (Å) distances (related to hydrogen bonding) in parthéite under ambient conditions and after partial dehydration at 150 and 275 °C

Ca coordination	RT	150 °C	275 °C
Ca-O11 (H_2O)	2.326(2)	2.310(7)	
Ca-O9 (OH)	2.3785(19)	2.317(4)	2.266(14)
Ca-O10 (H_2O)	2.431(3)		
Ca-O4	2.4862(18)	2.400(4)	
Ca-O7	2.4971(18)	2.500(4)	2.518(14)
Ca-O5	2.5005(18)	2.470(4)	2.519(13)
Ca-O3	2.6048(19)	2.549(4)	2.382 (13)
Ca-O7′			2.697(13)
Ca-O6			2.367(13)
Mean	2.461	2.425	2.458
O10-O2	2.887(3)		
O10-O8	3.429(3)		
O11-O1	2.714(3)	2.859(12)	
O11-O2	2.805(3)	2.839(8)	
O9-O6	2.821(3)	2.802(5)	3.55(2)
O9-O2			3.02(2)

TABLE 7. Selected bond-distances (Å) and T-O-T angles (°) for parthéite at different temperatures

Bond/angle	RT	150 °C	275 °C
Si1-O1	1.6122(19)	1.605(4)	1.575(15)
Si1-O3	1.6155(19)	1.637(4)	1.662(14)
Si1-O2	1.6214(18)	1.616(3)	1.598(13)
Si1-O8	1.6384(12)	1.635(3)	1.638(9)
Mean	1.6218	1.623	1.618
Si2-O6	1.6040(18)	1.594(4)	1.639(13)
Si2-O7	1.6227(18)	1.627(4)	1.653(13)
Si2-O4	1.6251(19)	1.628(3)	1.563(14)
Si2-O5	1.6333(18)	1.634(3)	1.650(13)
Mean	1.6213	1.621	1.626
Al1-O1	1.7325(19)	1.722(4)	1.698(16)
Al1-O2	1.7475(18)	1.726(4)	1.741(13)
Al1-O9	1.762(2)	1.762(4)	1.778(14)
Al1-O4	1.7632(19)	1.777(4)	1.734(14)
Mean	1.7513	1.747	1.738
Al2-O6	1.7312(19)	1.735(4)	1.776(14)
Al2-O7	1.7503(19)	1.761(3)	1.764(13)
Al2-O3	1.7519(19)	1.754(4)	1.740(14)
Al2-O5	1.7537(19)	1.761(4)	1.743(14)
Mean	1.7468	1.753	1.756
Si1-O1-Al1	138.46(12)	141.1(2)	160.0(12)
Si1-O2-Al1	141.25(12)	144.3(2)	141.6(9)
Si1-O3-Al2	132.84(11)	129.3(2)	132.8(8)
Si1-O8-Si1	129.88(16)	128.9(3)	121.1(10)
Si2-O4-Al1	129.57(11)	130.9(2)	159.0(9)
Si2-O5-Al2	129.66(11)	127.3(2)	119.3(8)
Si2-O6-Al2	156.44(13)	155.5(2)	121.6(8)
Si2-O7-Al2	138.87(12)	137.1(2)	127.7(8)
Mean	137.12	136.8	135.4

DISCUSSION

Single-crystal X-ray diffraction techniques are certainly not the best choice to analyze hydrogen-bond systems. However, for low material quantities or small crystal size, neutron diffraction is not applicable. It is the well-known disadvantage of X-ray diffraction that for hydrogen not the position of the nucleus but that of the bonding electron to the adjacent donor is located. Thus, the direction of the O-H vector is correct but not the OH-distance. This shortcoming is corrected by addition of restraints during the refinement procedure to improve the "true" crystal-chemical model. These restraints act as additional observations and define an elongate O-H vector [0.95(2) Å in

this study] corresponding to an average distance derived from neutron diffraction data (Franks 1973).

Bond-valence calculations (Brown and Altermatt 1985) were used to confirm the experimentally derived hydrogen bond systems. In a first step of calculations of bond-valence sums (bvs), hydrogen bonds contributing to the bond valence of oxygen atoms were ignored. An oxygen bvs <0.5 valence units (v.u.) characterizes a H_2O molecule and a bvs of about 1 suggests a donor of a hydrogen bond (OH group). Valence sums considerably below 2 v.u. (>1.5 v.u.) indicate that such oxygen atoms possibly participate at a hydrogen bond as acceptor. According to a model by Ferraris and Ivaldi (1988), which is here strongly simplified, the bvs for a donor of a hydrogen bond may be increased by 0.8 v.u. and the bvs of acceptor oxygen may be increased by 0.2 v.u. Corresponding calculations (Table 4) indicate that O9 represents an OH group; O10 and O11 belong to H_2O molecules. In addition, O1, O2, and O6 have low bvs making them candidates for acceptors of hydrogen bonds.

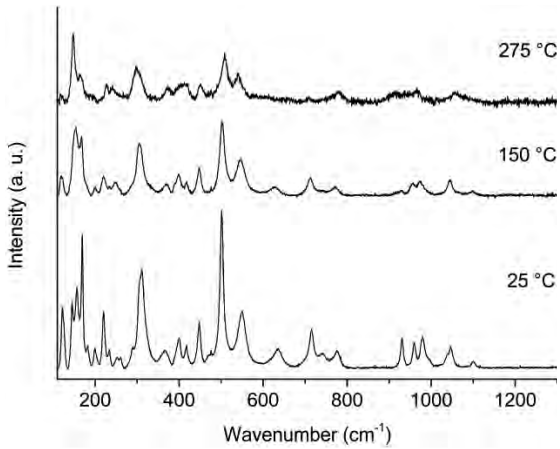

FIGURE 1. Unpolarized Raman spectra of a parthéite single crystal measured in the range of 110–1300 cm^{-1} at 25, 150, and 275 °C.

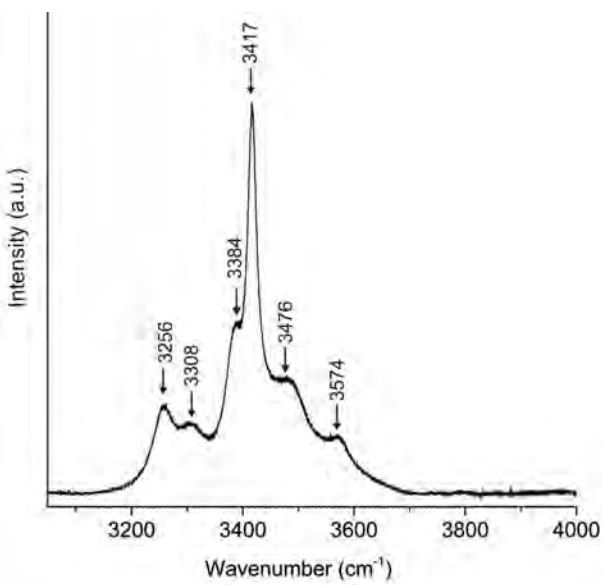

FIGURE 2. Raman spectrum of parthéite $Ca_2Al_4Si_4O_{15}(OH)_2{\cdot}4H_2O$ measured at room temperature in the range of 3000–4000 cm^{-1}.

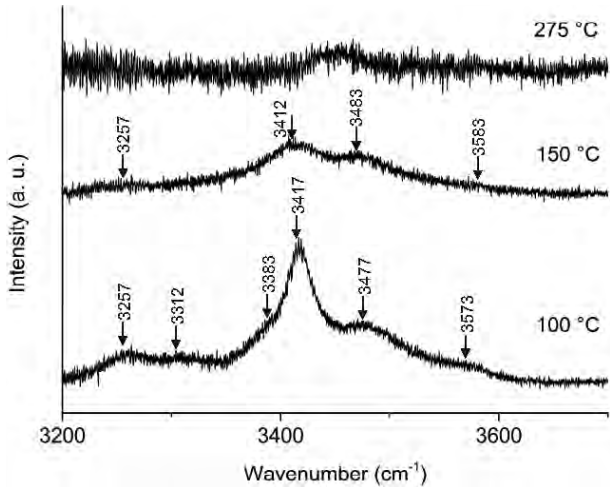

FIGURE 3. Raman spectra of parthéite measured in the range of 3200–3700 cm^{-1} at 100, 150, and 275 °C.

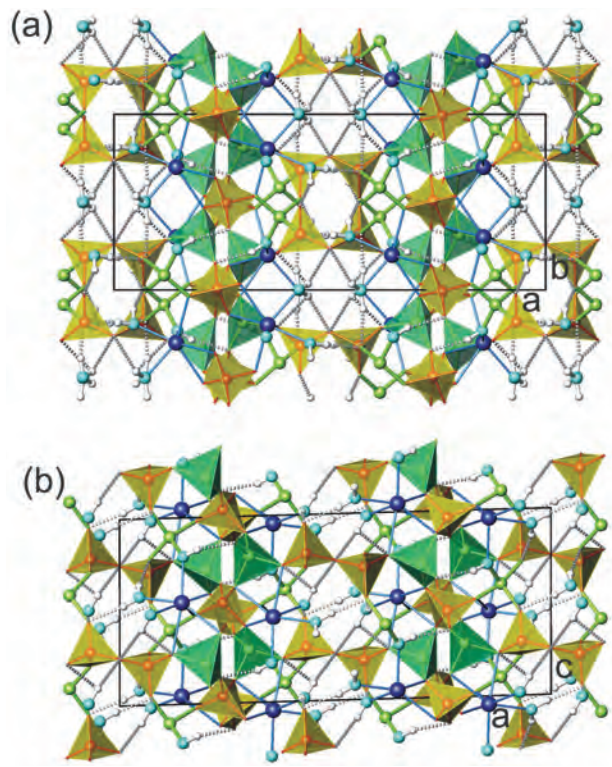

FIGURE 4. Crystal structure of parhéite $Ca_2Al_4Si_4O_{15}(OH)_2{\cdot}4H_2O$ at room temperature. Oxygen of H_2O and OH are shown as light blue spheres with attached small white spheres representing H. Hydrogen-bond acceptor interactions are shown by gray dashed connectors. Extraframework Ca is dark blue, SiO_4 tetrahedra are red with yellow faces. The $Al2O_4$ tetrahedron is green delimited by external faces, whereas, for better distinction, the $Al1O_4$ tetrahedron, terminated by the O9-H3 group, is only drawn with green spheres and bonds (without polyhedral faces). (**a**) Projection along the **c** axis showing the porous character of the structure, (**b**) projection along the **b** axis for better visibility of the hydrogen-bond system. (Color online.)

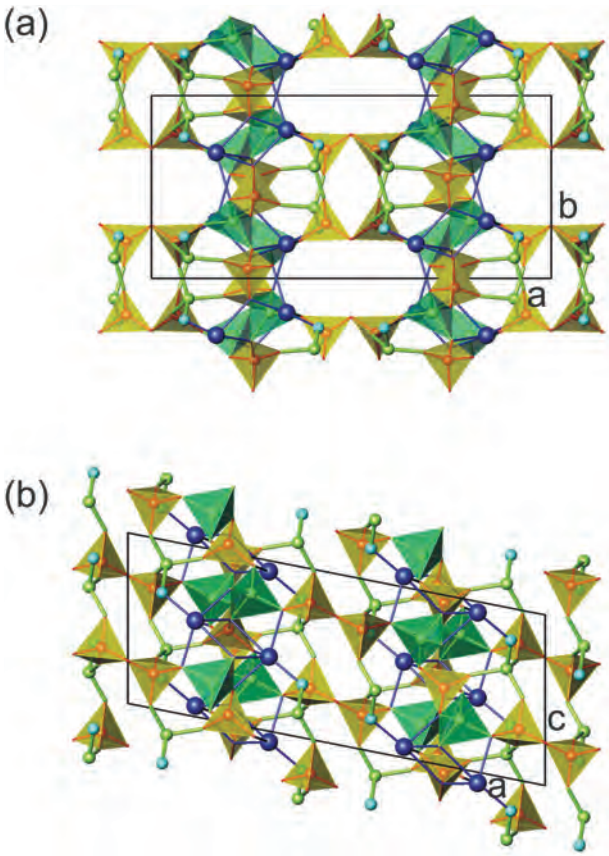

FIGURE 5. Distorted parthéite structure at 275 °C, $Ca_2Al_4Si_4O_{15}(OH)_2$, after all H_2O molecules have been expelled. Extraframework Ca is dark blue, SiO_4 tetrahedra are red with yellow faces. The $Al2O_4$ tetrahedron is green delimited by external faces, whereas, for better distinction, the $Al1O_4$ tetrahedron, terminated by the O9-H3 group, is only drawn with green spheres and bonds (without polyhedral faces). (**a**) Projection along the **c** axis showing the porous character of the structure, (**b**) projection along the **b** axis for better visibility of the Ca coordination. (Color online.)

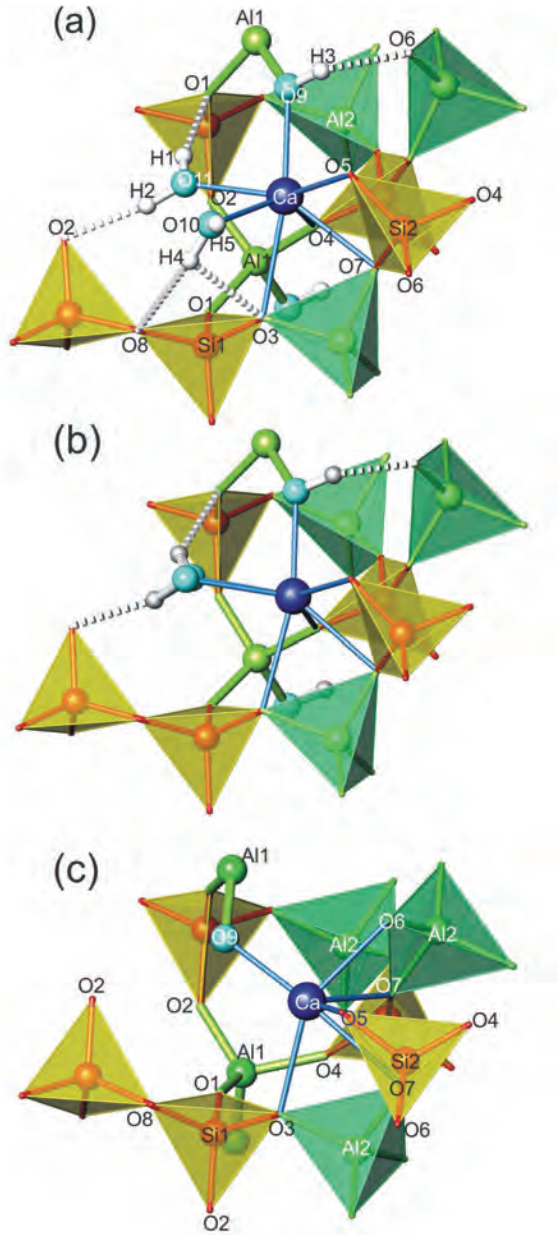

FIGURE 6. Decrease of the Ca coordination and hydrogen bonds in partheite structure at different temperatures. (**a**) Parthéite at room temperature with O10 and O11 fully occupied. The O10-H5···O2 hydrogen bond is not shown. The vector H5···O2 points toward the observer, approximately parallel to the **b** axis. (**b**) Parthéite at 150 °C: The H_2O molecule at O10 has been expelled, the H_2O molecule at O11 is disordered on a split position. Loss of H_2O at O10 reduces the Ca coordination from seven to six. (**c**) Parthéite at 275 °C: Both H_2O molecules are liberated. Ca is six-coordinated but has few new bonding partners compared to the coordination at 150 °C. (Color online.)

A detailed description of the interrupted framework of parthéite (Figs. 4 and 5), including secondary building units, has been given by Engel and Yvon (1984). Our structure refinement with five located H positions (Fig. 6) indicates that there are four strong hydrogen bonds with H···O acceptor distances below 2 Å: O9-H3···O6, O10-H5···O2, O11-H1···O1, and O11-H2···O2. Thus O2 with the lowest bvs, which is not an OH-group, acts as acceptor of two hydrogen bonds. The refined position of H4 has no bond acceptors within 2 Å. Within 2.6 Å, there are two potential acceptors (O3 and O8). This indicates that H4 is fixed by weak hydrogen bonds only. The potential hydrogen bond O10-H4···O8 is bent (156°) with an O10-O8 separation of 3.4 Å (Table 5). Actually O8 may accept two hydrogen bonds from H4 of adjacent H4-O10-H5 molecules (Fig. 4a). The alternative O10-H4···O3 hydrogen bond is even kinked (108°) but with a considerably shorter O10-O3 distance of 2.9 Å (Table 5). The increased U_{iso} displacement parameter of H4 (Table 3) is a factor of 3–5 times larger than U_{iso} of other H sites in parthéite. This suggests that H4 is disordered and an average position has been determined. Moreover, this is also evident from the large standard deviations associated with coordinates of this atom (Table 2a). The H4-O10-H5 angle of 115(5)° is within 2 e.s.d. values from the expected value of 104.5° for a H_2O molecule. In the H-corrected bvs calculations, we have added 0.1 v.u. to the bvs

of O3 and O8, respectively. Bond-valence sums of framework oxygen sites without hydrogen correction scatter between 1.78 and 2.01 v.u. (Table 4). After introducing the hydrogen correction the corresponding values are between 1.98 and 2.18 v.u.

H_2O at O10 is connected to Ca and plugs the elliptical channels parallel to **c**, confined by 10-membered rings of tetrahedra (Fig. 4). Hydrogen bonds fix O10 to opposite walls of the channel. In contrast to the position of O10, H_2O at O11, also with one bond to Ca, is positioned at a side pocket of the one-dimensional channels (Fig. 4a) and does not interfere with channel diffusion. In addition, H1 and H2 of the H_2O molecule at O11 form strong hydrogen bonds to O1 and O2, respectively. Another view of the hydrogen-bond system is shown in Figure 4b. Both H_2O molecules at O10 and O11 decorate the walls of a six-membered ring channel, running along **b**, formed by 4 × Si1 and 2 × Al1 with hydrogen bonds across the channel's transverse section.

The OH/H_2O-specific region of the powder IR spectrum of parthéite (Ivanov and Mozzherin 1982) is not easy to interpret. Their sample was probably contaminated by hydrocarbons as evidenced by strong absorptions at 2970 and 1500 cm^{-1}. Other observed bands characteristic of OH stretching modes are at 3300 (shoulder), 3420, and 3585 (shoulder) cm^{-1}. According to Libowitzky (1999) absorptions between 3300 and 3585 cm^{1} correspond to donor-acceptor (O···O) distances of ca. 2.8–3.2 Å, which agrees with the corresponding D-A distances in Table 5. Qualitatively, the high-frequency part of the IR spectrum shown by Sarp (1985) for parthéite from Turkey is very similar to that from Denezhkin Kamen (Ivanov and Mozzherin 1982). Sarp (1985) lists the following absorption bands (cm^{-1}): 2850 (w), 2920 (m), 3250 (w), 3304 (m), 3410 (vs), 3480 (sh), and 3580 (vs). Absorptions at 1650 and 1635 cm^{-1} were assigned to H_2O deformations. We interpret the bands at 2920 and 2850 cm^{-1} as hydrocarbon specific absorptions. Our room-temperature Raman spectrum (Fig. 2) displays bands (cm^{-1}) at 3256 (m), 3308 (m), 3384 (m shoulder), 3417 (vs), 3476 (m shoulder) and 3574 (m) cm^{-1}. Thus there is rather good agreement between Raman and IR data (Ivanov and Mozzherin 1982; Sarp 1985) for OH stretching signals. Due to the increased atomic vibrations with temperature the resolution of the Raman spectra at 150 and 275 °C (Figs. 1 and 3) strongly decreased. Major differences with temperature are noted below ca. 300 cm^{-1}, which is related to the coordination change of Ca upon dehydration.

Previous studies (e.g., Cruciani 2006; Wadoski et al. 2011 and references therein) have shown that dehydration of Ca-rich zeolites proceeds with only minor structural changes until the Ca-coordination decreases to six. Further dehydration leading to lower Ca-coordination may cause phase transitions, partial rupture of T-O-T bonds, or structural collapse (Alberti and Martucci 2011).

Our in situ dehydration experiments at elevated temperature and dry N_2 atmosphere showed that parthéite starts losing H_2O already at 100 °C. At this temperature the population of H_2O at O10 decreased to 0.88(1). The population was further lowered to 0.346(16) at 125 °C, and the unit-cell volume dropped from 1757.6(4) to 1742.6(7) $Å^3$ between 100 and 125 °C. At 150 °C, two H_2O pfu have been expelled and O10 became vacant. The Ca coordination decreased from seven to six (Table 6) accompanied by a shortening of the mean Ca-O distance from 2.461 to 2.425 Å (Table 6). In addition, the unit-cell volume reduced to 1733.1(10) $Å^3$ and H_2O at O11 became disordered over two positions (O11a and O11b), ca. 1 Å apart. From 150 to 225 °C, the O11 disorder increased while the unit-cell volume further decreased (Fig. 7). The decrease of the unit-cell volume (Fig. 7) after H_2O at O10 had already been expelled is rather unusual and one should instead expect "normal" thermal expansion. We assume that the structure at 150 °C was still too rigid to adapt to the new situation with 2 H_2O less in the structural channels. Thus upon increasing temperature (150–225 °C) the tetrahedral framework became more flexible (thermal motion) to adjust hysteresis-like to the less occupied channel system. Thus subsequent expansion led to slight reduction of porous space and not to increase of bulk volume. One indicator of the latter behavior is the decrease of the distance of the remote O7

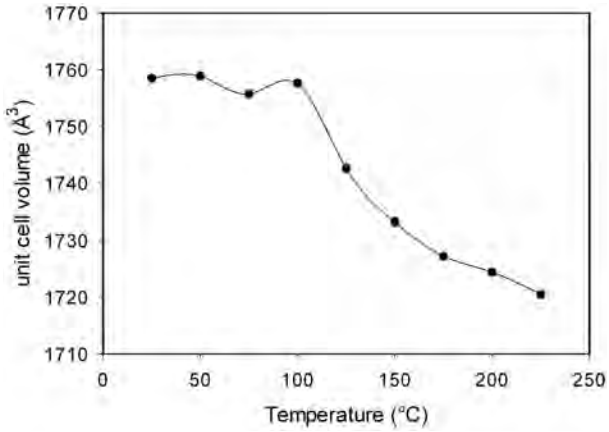

FIGURE 7. Development of unit-cell volume vs. temperature for in situ dehydration experiments of parthéite from $Ca_2Al_4Si_4O_{15}(OH)_2{\cdot}4H_2O$ (up to 100 °C) to $Ca_2Al_4Si_4O_{15}(OH)_2{\cdot}2H_2O$ (up to 225 °C). The size of the symbols approximately corresponds to e.s.d. values of volume.

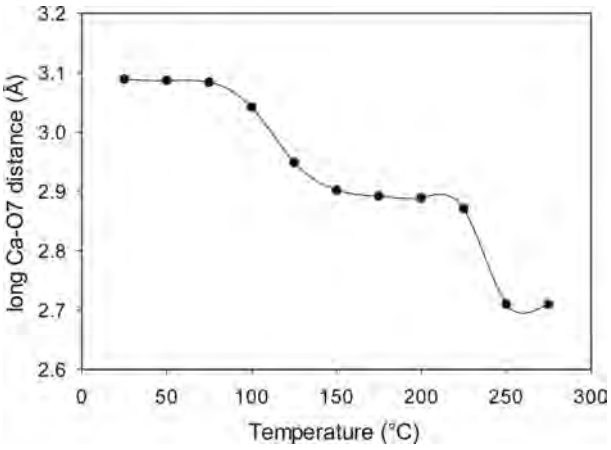

FIGURE 8. Development of the long Ca-O7′ distance vs. temperature for in situ dehydration experiments of parthéite from $Ca_2Al_4Si_4O_{15}(OH)_2{\cdot}4H_2O$ (up to 100 °C) to $Ca_2Al_4Si_4O_{15}(OH)_2{\cdot}2H_2O$ (up to 225 °C). The line largely follows the same trend as observed for the volume (Fig. 4). The size of the symbols approximately corresponds to e.s.d. values of Ca-O distances.

site to channel Ca (Fig. 8). This distance significantly decreases with temperature and largely follows the observed trend of the volume vs. temperature (Fig. 7). One may suggest that the framework structure compensates the loss of H_2O by offering an additional framework oxygen site (O7) as contributor to the Ca coordination.

Sarp et al. (1979) reported that the X-ray diffraction pattern of parthéite did not significantly change after 64 h heating at 150 °C. This can be explained by the fact that their X-ray pattern was recorded at ambient condition and a zeolite with intact framework structure will under moist ambient conditions rehydrate to its original composition. A first endothermic DTA signal and a corresponding DTG peak with a maximum at 230 °C have been noted by Ivanov and Mozzherin (1982). However, the onset of this dehydration is ca. 100 °C lower and may correspond to the loss of 2 H_2O pfu determined in this study. It should also be stressed again that our in situ dehydration has been performed under dry N_2 atmosphere but environmental conditions are not specified for the DTA and DTG experiments by Ivanov and Mozzherin (1982).

The H_2O I molecule with the weakest hydrogen bonds is H4-O10-H5. This molecule seems to be most favorable to escape at low temperature. The bands at 3476 and 3574 cm^{-1} of the room-temperature Raman spectrum (Fig. 2) are assigned to these soft hydrogen bonds based on donor (O10) acceptor distances (Libowitzky 1999). The sharp Raman band at 3417 cm^{-1} is assigned to the OH group and the broadened bands at 3256 and 3308 cm^{-1} correspond to H_2O II at O11 (Table 5). The shoulder at 3384 cm^{-1} (Fig. 2) remains unassigned. H4 of H_2O I is only fixed by a very weak hydrogen bond (Table 5) and if the hydrogen bond H5···O2 is broken the bvs of O2 reduces from 2.18 to 1.98 v.u. (Table 4). Thus, O2 retains an appropriate bvs even if H_2O at O10 is expelled. The expulsion of H4-O10-H5 was found in this study to be complete at 150 °C, decreasing the Ca coordination from seven to six. At 150 °C, the Raman spectrum (Fig. 3) of the range characteristic of OH stretching vibrations is only poorly resolved. Our structure data collected at the same temperature indicate (Tables 5 and 6) that according to donor-acceptor distances the strongest hydrogen bonds are formed by O9 (OH) followed by O11 as donor (H_2O II). Thus the broad shoulder in the Raman spectrum (Fig. 3) at 3483 cm^{-1} is assigned to H_2O II.

Sarp et al. (1979) report that the X-ray pattern became slightly modified after further dehydration 40 h at 300 °C and after 40 h at 350 °C a different pattern was recognized. Our in situ single-crystal dehydration experiments indicate that at 250 °C, the second H_2O molecules is released and that the tetrahedral framework strongly distorts and compacts by a volume decrease of ca. 8%. The associated distortions cause a strongly streaked diffraction pattern, thus significant reflection intensities were only monitored in the low-θ range. H completing the OH group with oxygen at O9 could not be resolved.

In addition, the asymmetric, strongly elongated shape of X-ray reflections prevents the reliable tracking of cell dimensions above 250 °C. Up to 375 °C, the space-group symmetry *C*2/*c* and the tetrahedral topology remained preserved. Ca nestles at the cavity wall and maintains sixfold coordination by five framework O atoms and the OH-group linked to Al1. The high-temperature structure is strongly distorted. Most significantly, β decreases from 91 to 79°, *b* increases from 8.7 to 9.4 Å, *c* decreases from 9.3 to 8.4 Å, and *a* from 21.5 to 20.8 Å, leading to a decline of volume from 1730 to 1600 $Å^3$.

The weakest connector in the framework of parthéite is the Al1 tetrahedron, which is linked to three Si tetrahedra and one terminate OH group at O9. At 275 °C Al1 strongly rotates, thus the hydrogen bond O9-H3···O6 becomes disconnected. The donor O9 to acceptor O6 distance increases from originally 2.8 (Table 5) to 3.6 Å. The new acceptor of the OH group at O9 becomes O2 with d(O9-O2) = 3.02(2) Å (Table 6). Thus, the O9-related poorly resolved Raman band (Fig. 3) shifts to higher frequency (Libowitzky 1999). O6 compensates for the lost bond valence from the hydrogen bond by formation of a new bond to Ca (Table 6, Fig. 6c) leading to strong bending of the Si2-O6-Al2 angle (Table 7) from 155° at 150 °C to 122° at 275 °C. On the other hand, readjustment of the Ca position leads to an increase of the Ca-O4 distance from 2.4 to 3.6 Å but simultaneously O7′ comes close (2.7 Å) to Ca. In spite of different bonding partners, Ca preserves its sixfold coordination (Table 6). Stepwise dehydration of parthéite did not cause significant change of average Si-O or Al-O bond distances (Table 7). Loss of hydrogen bonding (at 275 °C) and rotation of the Al1-tetrahedron can be clearly seen from modification of T-O-T angles: Si1-O1-Al1 increased from 138.46(12)° to 160.0(12)° and Si2-O4-Al1 from 129.57(12)° to 159.0(12)° (Table 7, Fig. 6).

After the heating excursion to 375 °C and subsequent equilibration for 48 h under ambient humidity, the crystal strongly swelled. However, neither a single crystal nor a powder diffraction-pattern could be monitored. This does not necessarily mean that parthéite turned X-ray amorphous. More probably upon rehydration the crystal disintegrated to a micro-aggregate whose powder pattern could not be detected due to the very small amount of material.

Heating 60 h at 400 °C led to destruction of the parthéite related high-temperature phase and the strongest reflections of anorthite appeared (Sarp et al. 1979). Ivanov and Mozzherin (1982) found additional DTA (endothermic) and DTG maxima at 400 and 600 °C. The onsets of the latter dehydration steps are, however, at least 100 and 150 °C lower.

The crystal structure of parthéite is unique for several reasons. (1) Essentially complete Si, Al order leads to an ordered arrangement of channel Ca and coordinating H_2O. Thus hydrogen positions could be straight forward extracted from routine single-crystal X-ray diffraction data. (2) Calcium does not plug the porous one-dimensional channels but occupies side pockets. (3) The interrupted tetrahedral framework with a terminate OH group linked to an Al tetrahedron has special flexibility (up to 400 °C) enabling to accomplish sixfold Ca coordination even if all H_2O molecules are expelled.

Acknowledgments

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Table 3a. (for deposit) Anisotropic displacement parameters (except hydrogen) for parthéite at RT.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Si1	0.0059(3)	0.0079(3)	0.0059(3)	0.0002(3)	0.0005(3)	0.0000(3)
Si2	0.0062(3)	0.0061(3)	0.0057(3)	-0.0003(3)	0.0007(3)	0.0009(3)
Al1	0.0072(4)	0.0079(4)	0.0058(4)	0.0013(3)	0.0010(3)	0.0005(3)
Al2	0.0068(4)	0.0064(4)	0.0055(3)	0.0004(3)	0.0001(3)	-0.0009(3)
Ca1	0.0126(3)	0.0107(3)	0.0105(3)	0.0002(2)	-0.0020(2)	-0.0031(2)
O1	0.0094(9)	0.0107(9)	0.0095(9)	-0.0017(7)	0.0044(8)	-0.0003(7)
O2	0.0106(9)	0.0117(9)	0.0076(9)	0.0008(7)	0.0004(8)	0.0026(7)
O3	0.0075(9)	0.0110(9)	0.0096(9)	0.0012(7)	0.0000(7)	-0.0020(7)
O4	0.0065(9)	0.0097(9)	0.0119(9)	-0.0005(7)	0.0037(7)	0.0004(7)
O5	0.0101(9)	0.0085(9)	0.0084(9)	-0.0011(7)	-0.0016(7)	0.0004(7)
O6	0.0139(10)	0.0090(9)	0.0099(9)	0.0045(7)	-0.0002(8)	0.0012(7)
O7	0.0112(9)	0.0089(9)	0.0053(8)	0.0003(7)	0.0023(7)	-0.0031(7)
O8	0.0046(12)	0.0088(12)	0.0112(12)	0.000	-0.0006(10)	0.000
O9	0.0123(10)	0.0139(10)	0.0114(9)	-0.0023(8)	0.0011(8)	-0.0051(8)
O10	0.0301(14)	0.0124(12)	0.0604(18)	0.0054(12)	0.0062(13)	0.0015(10)
O11	0.0145(11)	0.0264(12)	0.0231(12)	-0.0139(10)	0.0081(9)	-0.0073(9)

Table 3b. (for deposit) Anisotropic displacement parameters (except hydrogen) for parthéite at 150 °C.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Si1	0.0105(7)	0.0203(8)	0.0154(7)	-0.0012(7)	-0.0014(6)	0.0010(6)
Si2	0.0120(7)	0.0164(7)	0.0133(7)	-0.0006(6)	-0.0006(6)	0.0007(6)
Al1	0.0118(8)	0.0185(8)	0.0144(8)	0.0006(7)	-0.0006(7)	0.0007(7)
Al2	0.0142(8)	0.0156(8)	0.0119(8)	-0.0008(7)	-0.0013(6)	0.0000(7)
Ca1	0.0248(6)	0.0222(6)	0.0168(6)	0.0010(5)	-0.0038(5)	-0.0051(5)
O1	0.0141(19)	0.022(2)	0.025(2)	-0.0071(18)	0.0065(16)	-0.0023(16)
O2	0.022(2)	0.029(2)	0.0117(18)	0.0025(17)	-0.0016(16)	0.0065(17)
O3	0.0097(18)	0.025(2)	0.0186(18)	0.0004(17)	0.0000(15)	-0.0046(16)
O4	0.0111(18)	0.020(2)	0.0176(18)	-0.0005(16)	0.0045(15)	-0.0040(15)
O5	0.0163(19)	0.017(2)	0.0163(19)	-0.0031(15)	-0.0045(15)	0.0015(15)
O6	0.022(2)	0.0161(19)	0.0173(18)	0.0038(16)	0.0000(16)	0.0027(15)
O7	0.015(2)	0.0190(19)	0.0147(18)	0.0024(15)	-0.0005(15)	-0.0006(15)
O8	0.015(3)	0.019(3)	0.022(3)	0.000	-0.002(2)	0.000
O9	0.021(2)	0.033(3)	0.022(2)	-0.0036(18)	-0.0001(18)	-0.0074(18)
O11a	0.039(14)	0.15(5)	0.082(18)	0.04(2)	0.033(13)	0.037(19)
O11b	0.017(4)	0.065(8)	0.030(4)	-0.014(4)	0.008(3)	-0.008(4)

Table 4. (for deposit) Results of bond valence calculations for parthéite (RT), parameters from Brown and Altermatt (1985).

Site	O1	O2	O3	O4	O5	O6	O7	O8	O9	O10	O11	Bvs*
Si1	1.03	1.01	1.02					0.96 2x ↓				4.02
Si2				1.00	0.98	1.06	1.00					4.04
Al1	0.80	0.77		0.74					0.74			3.05
Al2			0.76		0.76	0.81	0.77					3.10
Ca			0.18	0.25	0.24		0.24		0.33	0.29	0.37	1.90
H1	0.2										0.8	1
H2		0.2									0.8	1
H3						0.2			0.8			1
H4			0.1					0.1 2x ↓		0.8		1
H5		0.2								0.8		1
Bvs* without H	1.83	1.78	1.96	1.99	1.98	1.87	2.01	1.92	1.07			
Bvs* with H	2.03	2.18	2.06	1.99	1.98	2.07	1.99	2.12	1.87	1.89	1.97	

*bond valence sum

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_publ_contact_author_name        'Biljana Lazic'
_publ_contact_author_address
;Mineralogical Crystallography
Institute of Geological Sciences
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CH-3012 Bern
Switzerland
;
_publ_contact_author_email       biljana.lazic@krist.unibe.ch
loop_
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'Lazic, Biljana '
;Mineralogical Crystallography
Institute of Geological Sciences
University of Bern
Freiestr. 3
CH-3012 Bern
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;
'Armbruster, Thomas'
;Mineralogical Crystallography
Institute of Geological Sciences
University of Bern
Freiestr. 3
CH-3012 Bern
Switzerland
;
'Liebich, Bernard W.'
;Via Saleggi 9
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Switzerland
;
'Perfler, Lukas'
;Institute of Mineralogy and Petrography
University of Innsbruck
Innrain 52
6020 Innsbruck
Austria
;

#------------------------------------------------------------------------------#
#                    UNIT CELL INFORMATION                                     #
#------------------------------------------------------------------------------#

_chemical_formula_sum             'H2 Al4 Ca2 O17 Si4'
_chemical_formula_weight          574.43

_symmetry_cell_setting            monoclinic
_symmetry_space_group_name_H-M    'C 1 2/c 1'
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 'x, -y, z+1/2'
 'x+1/2, y+1/2, z'
 'x+1/2, -y+1/2, z+1/2'
 '-x, -y, -z'
 '-x, y, -z-1/2'
 '-x+1/2, -y+1/2, -z'
 '-x+1/2, y+1/2, -z-1/2'

_cell_length_a                    20.82(4)
_cell_length_b                    9.350(16)
_cell_length_c                    8.359(14)
_cell_angle_alpha                 90.000(0)
_cell_angle_beta                  78.86(2)
_cell_angle_gamma                 90.000(0)
_cell_volume                      1596.3(5)
_cell_formula_units_Z             4
_cell_measurement_temperature     586(2)
_cell_measurement_theta_min       1.99
_cell_measurement_theta_max       20.5

#-----------------------------------------------------------------------------#
#                    CRYSTAL INFORMATION                                      #
#-----------------------------------------------------------------------------#

_exptl_crystal_description        'plate'
_exptl_crystal_colour             'transparent'
_exptl_crystal_size_max           0.01
_exptl_crystal_size_mid           0.05
_exptl_crystal_size_min           0.1
_exptl_crystal_density_diffrn     2.382
_exptl_crystal_density_method     'not measured'
_exptl_crystal_F_000              1136
_exptl_absorpt_coefficient_mu     1.325
_exptl_absorpt_correction_type    'multi-scan'
_exptl_absorpt_correction_T_min   ?
_exptl_absorpt_correction_T_max   ?
_exptl_absorpt_process_details    SADABS

#-----------------------------------------------------------------------------#
#                    DATA COLLECTION                                          #
#-----------------------------------------------------------------------------#

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_diffrn_radiation_type            MoK\a
_diffrn_radiation_source          'fine-focus sealed tube'
_diffrn_radiation_monochromator   graphite
_diffrn_measurement_device_type   'Bruker Apex II Smart'
_diffrn_measurement_method        'phi-omega scans'
_diffrn_detector_area_resol_mean  ?
_diffrn_standards_number          ?
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_diffrn_standards_interval_count  ?
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_diffrn_reflns_number             3829
_diffrn_reflns_av_R_equivalents   0.2547
_diffrn_reflns_av_sigmaI/netI     0.1855
_diffrn_reflns_limit_h_min        -20
_diffrn_reflns_limit_h_max        20
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_diffrn_reflns_limit_k_max        9
_diffrn_reflns_limit_l_min        -8
_diffrn_reflns_limit_l_max        8
_diffrn_reflns_theta_min          1.99
_diffrn_reflns_theta_max          20.52
_reflns_number_total              807
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_reflns_threshold_expression      >2sigma(I)

#------------------------------------------------------------------------------#
#                    COMPUTER PROGRAMS USED                                    #
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_computing_data_reduction         ?
_computing_structure_solution           'SHELXS-97 (Sheldrick, 1990)'
_computing_structure_refinement         'SHELXL-97 (Sheldrick, 1997)'

#------------------------------------------------------------------------------#
#                    REFINEMENT INFORMATION                                    #
#------------------------------------------------------------------------------#

_refine_special_details
;
 Refinement of F^2^ against ALL reflections.  The weighted R-factor wR and
 goodness of fit S are based on F^2^, conventional R-factors R are based
 on F, with F set to zero for negative F^2^. The threshold expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is
 not relevant to the choice of reflections for refinement.  R-factors based
 on F^2^ are statistically about twice as large as those based on F, and R-
 factors based on ALL data will be even larger.
;

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_refine_ls_weighting_scheme       calc
_refine_ls_weighting_details
 'calc w=1/[\s^2^(Fo^2^)+(0.0867P)^2^+0.0000P] where P=(Fo^2^+2Fc^2^)/3'
_atom_sites_solution_primary      direct
_atom_sites_solution_secondary    difmap
_atom_sites_solution_hydrogens    geom
_refine_ls_hydrogen_treatment     mixed
_refine_ls_extinction_method      none
_refine_ls_number_reflns          807
_refine_ls_number_parameters      123
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_refine_ls_wR_factor_ref          0.1982
_refine_ls_wR_factor_gt           0.1488
_refine_ls_goodness_of_fit_ref    0.986
_refine_ls_restrained_S_all       0.986
_refine_ls_shift/su_max           0.000
_refine_ls_shift/su_mean          0.000

#-------------------------------------------------------------------------------#
#                    ATOMIC TYPES, COORDINATES AND THERMAL PARAMETERS           #
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Al Al 0.0645 0.0514 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
Ca Ca 0.2262 0.3064 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
O O 0.0106 0.006 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
Si Si 0.0817 0.0704 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

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Si2 Si 0.2415(3) 0.0525(6) 0.4526(7) 0.0394(17) Uani 1 1 d . . .
Al1 Al 0.0925(3) 0.1123(7) 0.6391(7) 0.0452(19) Uani 1 1 d . . .
Al2 Al 0.2041(3) 0.3130(7) 0.2866(7) 0.0419(18) Uani 1 1 d . . .
Ca1 Ca 0.3381(2) 0.1878(5) 0.0636(5) 0.0485(15) Uani 1 1 d . . .
O1 O 0.0697(8) 0.0570(16) 0.3036(19) 0.090(6) Uani 1 1 d . . .
O2 O 0.0539(6) 0.1847(13) 0.4903(14) 0.045(4) Uani 1 1 d . . .
O3 O 0.1291(6) 0.2954(14) 0.2252(15) 0.050(4) Uani 1 1 d . . .
O4 O 0.1760(6) -0.0984(14) 0.0659(16) 0.055(4) Uani 1 1 d . . .
O5 O 0.1968(6) 0.4310(13) 0.4506(14) 0.043(4) Uani 1 1 d . . .
O6 O 0.2525(6) 0.1574(13) 0.2924(14) 0.044(4) Uani 1 1 d . . .
O7 O 0.2539(6) 0.3842(13) 0.3906(13) 0.040(4) Uani 1 1 d . . .
O8 O 0.0000 0.2869(17) 0.2500 0.037(5) Uani 1 2 d S . .
O9 O 0.4178(7) 0.2720(16) 0.1886(15) 0.064(4) Uani 1 1 d . . .
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Si2 0.060(4) 0.033(4) 0.032(4) -0.005(3) -0.026(3) 0.002(3)
Al1 0.066(5) 0.047(4) 0.028(4) 0.000(3) -0.023(3) -0.003(4)
Al2 0.058(5) 0.044(4) 0.028(4) 0.002(3) -0.018(3) 0.001(3)
Ca1 0.064(3) 0.059(3) 0.029(3) -0.003(2) -0.023(2) -0.004(3)
O1 0.122(14) 0.065(12) 0.096(13) -0.041(10) -0.054(11) 0.023(10)
O2 0.063(10) 0.046(9) 0.030(8) 0.014(7) -0.015(7) -0.003(7)
O3 0.058(10) 0.068(10) 0.029(8) 0.007(8) -0.024(7) -0.004(8)
O4 0.050(10) 0.050(10) 0.068(11) 0.012(8) -0.023(9) -0.008(8)
O5 0.048(8) 0.049(9) 0.036(8) -0.001(7) -0.022(7) -0.004(7)
O6 0.066(9) 0.050(10) 0.025(8) 0.004(7) -0.026(7) -0.005(7)
O7 0.056(9) 0.044(9) 0.025(8) 0.004(7) -0.023(7) -0.006(7)
O8 0.056(13) 0.024(11) 0.032(11) 0.000 -0.013(10) 0.000
O9 0.077(11) 0.093(12) 0.026(8) -0.026(8) -0.023(8) 0.002(9)

#-----------------------------------------------------------------------------#
#                    MOLECULAR GEOMETRY                                       #
#-----------------------------------------------------------------------------#

_geom_special_details
;
 All esds (except the esd in the dihedral angle between two l.s. planes)
 are estimated using the full covariance matrix.  The cell esds are taken
 into account individually in the estimation of esds in distances, angles
 and torsion angles; correlations between esds in cell parameters are only
 used when they are defined by crystal symmetry.  An approximate (isotropic)
 treatment of cell esds is used for estimating esds involving l.s. planes.
;

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Si1 O2 1.599(13) . ?
Si1 O8 1.638(9) . ?
Si1 O3 1.659(14) . ?
Si1 O1 3.050(17) 2 ?
Si1 Ca1 3.472(8) 7 ?
Si1 O4 3.690(14) 6_556 ?
Si1 O2 3.727(14) 2 ?
Si1 O4 3.922(15) . ?
Si1 O5 3.938(14) . ?
Si1 O6 3.971(15) . ?
Si1 O9 4.004(15) 8_456 ?
```

```
Si2 O4 1.564(14) 6_556 ?
Si2 O6 1.640(13) . ?
Si2 O5 1.651(13) 7_556 ?
Si2 O7 1.653(13) 4_545 ?
Si2 Ca1 3.266(8) 6_556 ?
Si2 O6 3.467(14) 7_556 ?
Si2 O6 3.495(14) 6_556 ?
Si2 O5 3.553(14) 4_545 ?
Si2 O5 3.660(14) . ?
Si2 O4 3.678(15) 4 ?
Si2 O3 3.700(14) 4_545 ?
Si2 O7 3.728(14) 7_556 ?
Al1 O1 1.695(16) 6_556 ?
Al1 O4 1.732(14) 6_556 ?
Al1 O2 1.742(13) . ?
Al1 O9 1.780(14) 7_556 ?
Al1 Ca1 3.626(8) 7_556 ?
Al1 O9 3.739(16) 8_456 ?
Al1 O1 3.741(19) 5_556 ?
Al1 O3 3.803(14) . ?
Al1 O5 3.841(14) . ?
Al1 O1 3.855(17) . ?
Al1 O2 3.962(14) 2_556 ?
Al1 O3 3.981(16) 6_556 ?
Al2 O3 1.742(14) . ?
Al2 O5 1.744(13) . ?
Al2 O7 1.766(13) . ?
Al2 O6 1.775(13) . ?
Al2 O4 3.048(15) 6_556 ?
Al2 O4 3.103(14) 4 ?
Al2 Ca1 3.214(8) 7 ?
Al2 Ca1 3.258(8) . ?
Al2 O6 3.375(14) 4 ?
Al2 O2 3.472(14) . ?
Al2 O5 3.716(14) 6_565 ?
Al2 O7 3.742(14) 7 ?
Ca1 O9 2.266(14) . ?
Ca1 O6 2.366(13) . ?
Ca1 O3 2.384(13) 7 ?
Ca1 O7 2.516(14) . ?
Ca1 O5 2.518(14) 4_545 ?
Ca1 O7 2.697(13) 7 ?
Ca1 Al2 3.214(8) 7 ?
Ca1 Si2 3.266(8) 6 ?
Ca1 Si1 3.472(8) 7 ?
Ca1 O1 3.535(18) 7 ?
Ca1 Al1 3.626(8) 7_556 ?
O1 Al1 1.695(16) 6 ?
O1 O8 2.58(2) . ?
O1 O3 2.58(2) . ?
O1 O2 2.694(19) . ?
O1 O4 2.70(2) . ?
O1 O9 2.86(2) 4_545 ?
O1 O1 2.87(3) 2 ?
O1 O2 2.899(19) 6 ?
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O1 O2 3.47(2) 2 ?
O1 Ca1 3.535(18) 7 ?
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O2 O3 2.663(16) . ?
O2 O4 2.850(17) 6_556 ?
O2 O9 2.885(17) 7_556 ?
O2 O1 2.899(19) 6_556 ?
O2 O9 3.021(18) 8_456 ?
O2 O1 3.47(2) 2 ?
O2 O5 3.725(17) . ?
O3 Ca1 2.384(13) 7 ?
O3 O8 2.657(13) . ?
O3 O7 2.720(18) . ?
O3 O5 2.858(18) . ?
O3 O6 3.022(19) . ?
O3 O5 3.543(17) 6_565 ?
O3 O4 3.678(18) 6_556 ?
O3 Si2 3.700(14) 4 ?
O4 Si2 1.564(14) 6 ?
O4 Al1 1.732(14) 6 ?
O4 O6 2.581(18) 6 ?
O4 O5 2.639(18) 4_545 ?
O4 O7 2.732(18) 7 ?
O4 O9 2.818(18) 4_545 ?
O4 O2 2.850(17) 6 ?
O4 Al2 3.048(15) 6 ?
O4 O6 3.085(18) 4_545 ?
O4 Al2 3.103(14) 4_545 ?
O4 O5 3.259(18) 6 ?
O5 Si2 1.651(13) 7_556 ?
O5 Ca1 2.518(14) 4 ?
O5 O7 2.601(17) 6_566 ?
O5 O4 2.639(18) 4 ?
O5 O6 2.700(17) 7_556 ?
O5 O7 2.903(16) . ?
O5 O6 2.982(18) 4 ?
O5 O6 3.007(18) . ?
O5 O4 3.259(18) 6_556 ?
O5 O3 3.543(17) 6_566 ?
O6 O4 2.581(18) 6_556 ?
O6 O7 2.612(17) . ?
O6 O7 2.678(18) 4_545 ?
O6 O5 2.700(17) 7_556 ?
O6 O5 2.982(18) 4_545 ?
O6 O4 3.085(18) 4 ?
O6 Al2 3.375(14) 4_545 ?
O7 Si2 1.653(13) 4 ?
O7 O5 2.601(17) 6_565 ?
O7 O6 2.678(18) 4 ?
O7 Ca1 2.697(13) 7 ?
O7 O4 2.732(18) 7 ?
O7 O7 3.13(2) 7 ?
O7 O4 3.326(17) 4 ?
O8 Si1 1.638(9) 2 ?
```

```
O8 O1 2.58(2) 2 ?
O8 O3 2.657(13) 2 ?
O8 O2 2.661(14) 2 ?
O8 O9 3.775(14) 8_456 ?
O8 O9 3.775(14) 7 ?
O8 Ca1 3.857(7) 8_456 ?
O8 Ca1 3.857(7) 7 ?
O9 Al1 1.780(14) 7_556 ?
O9 O4 2.818(18) 4 ?
O9 O1 2.86(2) 4 ?
O9 O2 2.885(17) 7_556 ?
O9 O2 3.021(18) 8 ?
O9 O1 3.56(2) 7 ?
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O2 Si1 O3 109.6(7) . . ?
O8 Si1 O3 107.3(7) . . ?
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O2 Si1 O1 91.0(6) . 2 ?
O8 Si1 O1 57.9(6) . 2 ?
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O2 Si1 Ca1 146.7(6) . 7 ?
O8 Si1 Ca1 90.7(3) . 7 ?
O3 Si1 Ca1 37.6(4) . 7 ?
O1 Si1 Ca1 122.2(4) 2 7 ?
O1 Si1 O4 95.5(7) . 6_556 ?
O2 Si1 O4 47.0(5) . 6_556 ?
O8 Si1 O4 154.7(4) . 6_556 ?
O3 Si1 O4 76.6(5) . 6_556 ?
O1 Si1 O4 123.8(4) 2 6_556 ?
Ca1 Si1 O4 105.1(3) 7 6_556 ?
O1 Si1 O2 68.3(6) . 2 ?
O2 Si1 O2 133.6(5) . 2 ?
O8 Si1 O2 39.0(4) . 2 ?
O3 Si1 O2 113.1(5) . 2 ?
O1 Si1 O2 45.5(3) 2 2 ?
Ca1 Si1 O2 78.8(3) 7 2 ?
O4 Si1 O2 162.7(3) 6_556 2 ?
O1 Si1 O4 31.0(6) . . ?
O2 Si1 O4 111.7(6) . . ?
```

```
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O3 Si1 O4 79.6(5) . . ?
O1 Si1 O4 98.6(4) 2 . ?
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O2 Si1 O4 93.4(3) 2 . ?
O1 Si1 O5 129.7(7) . . ?
O2 Si1 O5 70.6(5) . . ?
O8 Si1 O5 117.1(6) . . ?
O3 Si1 O5 39.4(5) . . ?
O1 Si1 O5 158.4(4) 2 . ?
Ca1 Si1 O5 77.1(2) 7 . ?
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O1 Si1 O6 85.1(7) . . ?
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O4 Si1 O6 39.2(3) 6_556 . ?
O2 Si1 O6 139.4(3) 2 . ?
O4 Si1 O6 54.4(3) . . ?
O5 Si1 O6 44.7(3) . . ?
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O6 Si2 O5 110.2(7) . 7_556 ?
O4 Si2 O7 116.2(7) 6_556 4_545 ?
O6 Si2 O7 108.8(7) . 4_545 ?
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O4 Si2 Ca1 122.0(6) 6_556 6_556 ?
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O5 Si2 Ca1 49.2(5) 7_556 6_556 ?
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Ca1 Si2 O6 105.5(3) 6_556 7_556 ?
O4 Si2 O6 81.3(6) 6_556 6_556 ?
O6 Si2 O6 168.1(7) . 6_556 ?
O5 Si2 O6 58.4(5) 7_556 6_556 ?
O7 Si2 O6 73.3(5) 4_545 6_556 ?
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O6 Si2 O6 85.64(19) 7_556 6_556 ?
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O6 Si2 O5 56.5(5) . 4_545 ?
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O7 Si2 O5 53.8(5) 4_545 4_545 ?
Ca1 Si2 O5 85.4(3) 6_556 4_545 ?
O6 Si2 O5 141.6(3) 7_556 4_545 ?
O6 Si2 O5 121.5(3) 6_556 4_545 ?
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O6 Si2 O5 54.1(5) . . ?
O5 Si2 O5 97.7(5) 7_556 . ?
O7 Si2 O5 156.6(5) 4_545 . ?
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Si2 O5 O6 34.8(4) 7_556 7_556 ?
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Al2 O5 O7 34.4(4) . . ?
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Ca1 O5 O4 154.2(5) 4 6_556 ?
O7 O5 O4 122.0(5) 6_566 6_556 ?
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O6 O5 O4 48.4(4) . 6_556 ?
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Al2 O5 O3 158.4(7) . 6_566 ?
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O7 O5 O3 49.7(4) 6_566 6_566 ?
O4 O5 O3 112.2(5) 4 6_566 ?
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# The following lines are used to test the character set of files sent by
# network email or other means. They are not part of the CIF data set
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# END of CIF
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##LOCALITY= Denezhkin Kamen, Urals, Russia
##CHEMISTRY= Ca2Al4Si4O15(OH)2 ◊ 4H2O
unoriented sample, background corrected

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473.8200,	684.6510

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475.7100,	913.3430
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476.6550,	847.0630
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478.0730,	698.4570
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479.9620,	740.7730
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487.9950,	1123.710
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489.8850,	1396.280
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491.3020,	1711.800
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493.6650,	2394.910
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494.6100,	2900.130
495.0820,	3171.300
495.5550,	3410.350
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496.9720,	4331.370
497.4450,	4806.290
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_publ_contact_author_address
;Mineralogical Crystallography
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CH-3012 Bern
Switzerland
;
_publ_contact_author_email       biljana.lazic@krist.unibe.ch
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'Lazic, Biljana '
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CH-3012 Bern
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'Armbruster, Thomas'
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;
'Perfler, Lukas'
;Institute  of Mineralogy and Petrography
University of Innsbruck
Innrain 52
6020 Innsbruck
Austria
;

#-------------------------------------------------------------------------------#
#                    UNIT CELL INFORMATION                                      #
#-------------------------------------------------------------------------------#

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#                    REFINEMENT INFORMATION                                 #
#---------------------------------------------------------------------------#

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 Refinement of F^2^ against ALL reflections.  The weighted R-factor wR and
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 F^2^ > 2\s(F^2^) is used only for calculating R-factors(gt) etc. and is
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 on F^2^ are statistically about twice as large as those based on F, and R-
 factors based on ALL data will be even larger.
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Al2 Al 0.19875(7) 0.31896(18) 0.28582(15) 0.0139(4) Uani 1 1 d . . .
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O2 O 0.07327(16) 0.1748(4) 0.4609(3) 0.0208(9) Uani 1 1 d . . .
O3 O 0.12215(15) 0.2932(4) 0.2225(3) 0.0178(8) Uani 1 1 d . . .
O4 O 0.17264(15) 0.0304(4) 0.0293(3) 0.0161(8) Uani 1 1 d . . .
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O9 O 0.35323(18) 0.2632(5) 0.2884(4) 0.0256(14) Uani 1.000(11) 1 d D . .
O11A O 0.0402(12) 0.333(9) -0.078(3) 0.092(17) Uani 0.27(3) 1 d P . .
```

```
O11B O 0.4544(4) 0.2796(18) 0.0813(8) 0.037(4) Uani 0.73(3) 1 d PD . .
H1 H 0.492(2) 0.266(11) 0.033(8) 0.050 Uiso 0.73(3) 1 d PD . .
H2 H 0.467(4) 0.368(6) 0.132(8) 0.050 Uiso 0.73(3) 1 d PD . .
H3 H 0.3168(18) 0.224(7) 0.330(6) 0.05(2) Uiso 1 1 d D . .

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 _atom_site_aniso_U_22
 _atom_site_aniso_U_33
 _atom_site_aniso_U_23
 _atom_site_aniso_U_13
 _atom_site_aniso_U_12
Si1 0.0105(7) 0.0203(8) 0.0154(7) -0.0012(7) -0.0014(6) 0.0010(6)
Si2 0.0120(7) 0.0164(7) 0.0133(7) -0.0006(6) -0.0006(6) 0.0007(6)
Al1 0.0118(8) 0.0185(8) 0.0144(8) 0.0006(7) -0.0006(7) 0.0007(7)
Al2 0.0142(8) 0.0156(8) 0.0119(8) -0.0008(7) -0.0013(6) 0.0000(7)
Ca1 0.0248(6) 0.0222(6) 0.0168(6) 0.0010(5) -0.0038(5) -0.0051(5)
O1 0.0141(19) 0.022(2) 0.025(2) -0.0071(18) 0.0065(16) -0.0023(16)
O2 0.022(2) 0.029(2) 0.0117(18) 0.0025(17) -0.0016(16) 0.0065(17)
O3 0.0097(18) 0.025(2) 0.0186(18) 0.0004(17) 0.0000(15) -0.0046(16)
O4 0.0111(18) 0.020(2) 0.0176(18) -0.0005(16) 0.0045(15) -0.0040(15)
O5 0.0163(19) 0.017(2) 0.0163(19) -0.0031(15) -0.0045(15) 0.0015(15)
O6 0.022(2) 0.0161(19) 0.0173(18) 0.0038(16) 0.0000(16) 0.0027(15)
O7 0.015(2) 0.0190(19) 0.0147(18) 0.0024(15) -0.0005(15) -0.0006(15)
O8 0.015(3) 0.019(3) 0.022(3) 0.000 -0.002(2) 0.000
O9 0.021(2) 0.033(3) 0.022(2) -0.0036(18) -0.0001(18) -0.0074(18)
O11A 0.039(14) 0.15(5) 0.082(18) 0.04(2) 0.033(13) 0.037(19)
O11B 0.017(4) 0.065(8) 0.030(4) -0.014(4) 0.008(3) -0.008(4)

#-----------------------------------------------------------------------------#
#                    MOLECULAR GEOMETRY                                       #
#-----------------------------------------------------------------------------#

_geom_special_details
;
 All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes)
 are estimated using the full covariance matrix.  The cell s.u.'s are taken
 into account individually in the estimation of s.u.'s in distances, angles
 and torsion angles; correlations between s.u.'s in cell parameters are only
 used when they are defined by crystal symmetry.  An approximate (isotropic)
 treatment of cell s.u.'s is used for estimating s.u.'s involving l.s. planes.
;

loop_
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 _geom_bond_atom_site_label_2
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 _geom_bond_site_symmetry_2
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Si1 O2 1.616(3) . ?
Si1 O8 1.635(3) . ?
Si1 O3 1.637(4) . ?
Si2 O6 1.594(4) . ?
```

```
Si2 O7 1.627(4) 8_546 ?
Si2 O4 1.628(3) 2 ?
Si2 O5 1.634(3) 7_556 ?
Si2 Ca1 3.1543(19) 2 ?
Si2 Ca1 3.266(2) 8_546 ?
Al1 O1 1.722(4) 2 ?
Al1 O2 1.726(4) . ?
Al1 O9 1.762(4) 7_556 ?
Al1 O4 1.777(4) 2 ?
Al1 Ca1 3.640(2) 8_546 ?
Al2 O6 1.735(4) . ?
Al2 O3 1.754(4) . ?
Al2 O5 1.761(4) . ?
Al2 O7 1.761(3) . ?
Al2 Ca1 3.241(2) 7 ?
Ca1 O11B 2.309(7) . ?
Ca1 O9 2.317(4) . ?
Ca1 O11A 2.37(2) 7 ?
Ca1 O4 2.400(4) 7 ?
Ca1 O5 2.470(4) 8_546 ?
Ca1 O7 2.501(3) 7 ?
Ca1 O3 2.549(3) 7 ?
Ca1 O7 2.902(4) . ?
Ca1 Si2 3.1543(19) 2_554 ?
Ca1 Al2 3.241(2) 7 ?
Ca1 Si2 3.266(2) 8_556 ?
Ca1 Al1 3.640(2) 8_556 ?
Ca1 H3 2.78(5) . ?
O1 Al1 1.722(4) 2_554 ?
O3 Ca1 2.548(3) 7 ?
O4 Si2 1.628(3) 2_554 ?
O4 Al1 1.777(4) 2_554 ?
O4 Ca1 2.400(4) 7 ?
O5 Si2 1.634(3) 7_556 ?
O5 Ca1 2.470(4) 8_556 ?
O7 Si2 1.627(4) 8_556 ?
O7 Ca1 2.501(3) 7 ?
O8 Si1 1.635(3) 6_556 ?
O9 Al1 1.762(4) 7_556 ?
O9 H3 0.95(2) . ?
O11A O11B 0.98(7) 7 ?
O11A Ca1 2.37(2) 7 ?
O11B O11A 0.98(7) 7 ?
O11B H1 0.94(2) . ?
O11B H2 0.94(2) . ?

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 _geom_angle_atom_site_label_2
 _geom_angle_atom_site_label_3
 _geom_angle
 _geom_angle_site_symmetry_1
 _geom_angle_site_symmetry_3
 _geom_angle_publ_flag
O1 Si1 O2 111.6(2) . . ?
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O1 Si1 O8 109.6(2) . . ?
O2 Si1 O8 107.25(15) . . ?
O1 Si1 O3 109.13(19) . . ?
O2 Si1 O3 110.63(19) . . ?
O8 Si1 O3 108.54(19) . . ?
O6 Si2 O7 112.09(18) . 8_546 ?
O6 Si2 O4 110.26(19) . 2 ?
O7 Si2 O4 107.33(19) 8_546 2 ?
O6 Si2 O5 112.19(19) . 7_556 ?
O7 Si2 O5 102.18(18) 8_546 7_556 ?
O4 Si2 O5 112.47(18) 2 7_556 ?
O6 Si2 Ca1 132.47(14) . 2 ?
O7 Si2 Ca1 51.83(12) 8_546 2 ?
O4 Si2 Ca1 117.22(14) 2 2 ?
O5 Si2 Ca1 50.79(12) 7_556 2 ?
O6 Si2 Ca1 126.16(14) . 8_546 ?
O7 Si2 Ca1 62.61(13) 8_546 8_546 ?
O4 Si2 Ca1 44.73(12) 2 8_546 ?
O5 Si2 Ca1 121.40(14) 7_556 8_546 ?
Ca1 Si2 Ca1 88.76(5) 2 8_546 ?
O1 Al1 O2 113.94(18) 2 . ?
O1 Al1 O9 105.12(19) 2 7_556 ?
O2 Al1 O9 109.2(2) . 7_556 ?
O1 Al1 O4 108.32(18) 2 2 ?
O2 Al1 O4 108.62(17) . 2 ?
O9 Al1 O4 111.68(18) 7_556 2 ?
O1 Al1 Ca1 81.28(13) 2 8_546 ?
O2 Al1 Ca1 101.80(13) . 8_546 ?
O9 Al1 Ca1 141.75(15) 7_556 8_546 ?
O4 Al1 Ca1 34.61(12) 2 8_546 ?
O6 Al2 O3 116.26(18) . . ?
O6 Al2 O5 107.00(17) . . ?
O3 Al2 O5 112.87(18) . . ?
O6 Al2 O7 106.99(17) . . ?
O3 Al2 O7 100.44(16) . . ?
O5 Al2 O7 113.21(17) . . ?
O6 Al2 Ca1 117.07(13) . 7 ?
O3 Al2 Ca1 51.45(11) . 7 ?
O5 Al2 Ca1 135.63(13) . 7 ?
O7 Al2 Ca1 49.90(11) . 7 ?
O11B Ca1 O9 78.8(2) . . ?
O11B Ca1 O11A 24.2(16) . 7 ?
O9 Ca1 O11A 84.4(10) . 7 ?
O11B Ca1 O4 90.2(4) . 7 ?
O9 Ca1 O4 95.33(13) . 7 ?
O11A Ca1 O4 113.3(18) 7 7 ?
O11B Ca1 O5 132.6(4) . 8_546 ?
O9 Ca1 O5 90.23(13) . 8_546 ?
O11A Ca1 O5 109.7(18) 7 8_546 ?
O4 Ca1 O5 136.97(12) 7 8_546 ?
O11B Ca1 O7 150.2(2) . 7 ?
O9 Ca1 O7 130.74(13) . 7 ?
O11A Ca1 O7 140.9(15) 7 7 ?
O4 Ca1 O7 83.66(12) 7 7 ?
O5 Ca1 O7 61.39(11) 8_546 7 ?

```
O11B Ca1 O3 85.5(2) . 7 ?
O9 Ca1 O3 162.86(13) . 7 ?
O11A Ca1 O3 84.0(7) 7 7 ?
O4 Ca1 O3 77.77(12) 7 7 ?
O5 Ca1 O3 105.57(11) 8_546 7 ?
O7 Ca1 O3 64.69(11) 7 7 ?
O11B Ca1 O7 131.9(3) . . ?
O9 Ca1 O7 70.14(12) . . ?
O11A Ca1 O7 151.3(16) 7 . ?
O4 Ca1 O7 58.36(10) 7 . ?
O5 Ca1 O7 84.15(11) 8_546 . ?
O7 Ca1 O7 67.76(12) 7 . ?
O3 Ca1 O7 117.26(10) 7 . ?
O11B Ca1 Si2 156.3(4) . 2_554 ?
O9 Ca1 Si2 110.50(11) . 2_554 ?
O11A Ca1 Si2 133(2) 7 2_554 ?
O4 Ca1 Si2 109.85(9) 7 2_554 ?
O5 Ca1 Si2 30.83(8) 8_546 2_554 ?
O7 Ca1 Si2 30.77(8) 7 2_554 ?
O3 Ca1 Si2 86.63(8) 7 2_554 ?
O7 Ca1 Si2 71.20(8) . 2_554 ?
O11B Ca1 Al2 117.8(2) . 7 ?
O9 Ca1 Al2 160.17(11) . 7 ?
O11A Ca1 Al2 115.2(9) 7 7 ?
O4 Ca1 Al2 74.85(9) 7 7 ?
O5 Ca1 Al2 85.83(8) 8_546 7 ?
O7 Ca1 Al2 32.60(8) 7 7 ?
O3 Ca1 Al2 32.57(8) 7 7 ?
O7 Ca1 Al2 90.11(7) . 7 ?
Si2 Ca1 Al2 59.07(4) 2_554 7 ?
O11B Ca1 Si2 111.9(4) . 8_556 ?
O9 Ca1 Si2 81.92(11) . 8_556 ?
O11A Ca1 Si2 136(2) 7 8_556 ?
O4 Ca1 Si2 28.50(8) 7 8_556 ?
O5 Ca1 Si2 111.85(9) 8_546 8_556 ?
O7 Ca1 Si2 74.21(9) 7 8_556 ?
O3 Ca1 Si2 97.84(9) 7 8_556 ?
O7 Ca1 Si2 29.86(7) . 8_556 ?
Si2 Ca1 Si2 91.24(5) 2_554 8_556 ?
Al2 Ca1 Si2 81.55(4) 7 8_556 ?
O11B Ca1 Al1 67.9(4) . 8_556 ?
O9 Ca1 Al1 100.75(11) . 8_556 ?
O11A Ca1 Al1 89.5(17) 7 8_556 ?
O4 Ca1 Al1 24.86(8) 7 8_556 ?
O5 Ca1 Al1 158.82(9) 8_546 8_556 ?
O7 Ca1 Al1 98.15(9) 7 8_556 ?
O3 Ca1 Al1 66.56(9) 7 8_556 ?
O7 Ca1 Al1 82.68(7) . 8_556 ?
Si2 Ca1 Al1 128.23(5) 2_554 8_556 ?
Al2 Ca1 Al1 77.70(4) 7 8_556 ?
Si2 Ca1 Al1 52.95(4) 8_556 8_556 ?
O11B Ca1 H3 96.9(9) . . ?
O9 Ca1 H3 18.7(8) . . ?
O11A Ca1 H3 99.1(13) 7 . ?
O4 Ca1 H3 99.9(13) 7 . ?
```

```
O5 Ca1 H3 74.5(10) 8_546 . ?
O7 Ca1 H3 112.9(9) 7 . ?
O3 Ca1 H3 176.7(12) 7 . ?
O7 Ca1 H3 59.4(12) . . ?
Si2 Ca1 H3 92.0(9) 2_554 . ?
Al2 Ca1 H3 144.7(9) 7 . ?
Si2 Ca1 H3 79.2(13) 8_556 . ?
Al1 Ca1 H3 112.2(12) 8_556 . ?
Si1 O1 Al1 141.1(2) . 2_554 ?
Si1 O2 Al1 144.3(2) . . ?
Si1 O3 Al2 129.3(2) . . ?
Si1 O3 Ca1 121.79(17) . 7 ?
Al2 O3 Ca1 95.99(14) . 7 ?
Si2 O4 Al1 130.9(2) 2_554 2_554 ?
Si2 O4 Ca1 106.77(16) 2_554 7 ?
Al1 O4 Ca1 120.53(17) 2_554 7 ?
Si2 O5 Al2 127.3(2) 7_556 . ?
Si2 O5 Ca1 98.38(16) 7_556 8_556 ?
Al2 O5 Ca1 134.25(18) . 8_556 ?
Si2 O6 Al2 155.5(2) . . ?
Si2 O7 Al2 137.1(2) 8_556 . ?
Si2 O7 Ca1 97.40(15) 8_556 7 ?
Al2 O7 Ca1 97.50(15) . 7 ?
Si2 O7 Ca1 87.53(14) 8_556 . ?
Al2 O7 Ca1 122.75(16) . . ?
Ca1 O7 Ca1 112.24(12) 7 . ?
Si1 O8 Si1 128.9(3) . 6_556 ?
Al1 O9 Ca1 135.1(2) 7_556 . ?
Al1 O9 H3 110(4) 7_556 . ?
Ca1 O9 H3 110(4) . . ?
O11B O11A Ca1 74.3(16) 7 7 ?
O11A O11B Ca1 82(2) 7 . ?
O11A O11B H1 76(6) 7 . ?
Ca1 O11B H1 136(5) . . ?
O11A O11B H2 143(6) 7 . ?
Ca1 O11B H2 124(5) . . ?
H1 O11B H2 96(7) . . ?

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 _geom_hbond_atom_site_label_H
 _geom_hbond_atom_site_label_A
 _geom_hbond_distance_DH
 _geom_hbond_distance_HA
 _geom_hbond_distance_DA
 _geom_hbond_angle_DHA
 _geom_hbond_site_symmetry_A
O11B H2 O1  0.94(2) 2.09(6) 2.859(12) 138(7) 8_556
O11B H1 O2  0.94(2) 1.95(4) 2.839(8) 156(8) 4_554
O9 H3 O6  0.95(2) 1.88(3) 2.802(5) 163(5) .

_diffrn_measured_fraction_theta_max    0.995
_diffrn_reflns_theta_full              28.45
_diffrn_measured_fraction_theta_full   0.995
_refine_diff_density_max    0.759
```

```
_refine_diff_density_min   -0.558
_refine_diff_density_rms    0.153

# The following lines are used to test the character set of files sent by
# network email or other means. They are not part of the CIF data set
# abcdefghijklmnopqrstuvwxyzABCDEFGHIJKLMNOPQRSTUVWXYZ0123456789
# !@#$%^&*()_+{}:"~<>?|\-=[];'`,./

# END of CIF
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_publ_requested_journal          'American Mineralogist'
_publ_contact_author_name        'Biljana Lazic'
_publ_contact_author_address
;Mineralogical Crystallography
Institute of Geological Sciences
University of Bern
Freiestr. 3
CH-3012 Bern
Switzerland
;
_publ_contact_author_email       biljana.lazic@krist.unibe.ch
loop_
_publ_author_name
_publ_author_address
'Lazic, Biljana'
;Mineralogical Crystallography
Institute of Geological Sciences
University of Bern
Freiestr. 3
CH-3012 Bern
Switzerland
;
'Armbruster, Thomas'
;Mineralogical Crystallography
Institute of Geological Sciences
University of Bern
Freiestr. 3
CH-3012 Bern
Switzerland
;
'Liebich, Bernard W.'
;Via Saleggi 9
6612 Ascona
Switzerland
;
'Perfler, Lukas'
;Institute of Mineralogy and Petrography
University of Innsbruck
Innrain 52
6020 Innsbruck
Austria
;
data_partheite_rt

_chemical_formula_sum                    'H10 Al4 Ca2 O21 Si4'
_chemical_formula_weight                 646.52

#-------------------------------------------------------------------------------#
#                    UNIT CELL INFORMATION                                      #
#-------------------------------------------------------------------------------#

_symmetry_cell_setting                   monoclinic
_symmetry_space_group_name_H-M           'C 1 2/c 1'
loop_
```

```
    _symmetry_equiv_pos_as_xyz
'x, y, z'
'x, -y, z+1/2'
'x+1/2, y+1/2, z'
'x+1/2, -y+1/2, z+1/2'
'-x, -y, -z'
'-x, y, -z-1/2'
'-x+1/2, -y+1/2, -z'
'-x+1/2, y+1/2, -z-1/2'

_cell_length_a                          21.5474(4)
_cell_length_b                          8.75638(15)
_cell_length_c                          9.30578(16)
_cell_angle_alpha                       90
_cell_angle_beta                        91.5524(18)
_cell_angle_gamma                       90
_cell_volume                            1755.15(5)
_cell_formula_units_Z                   4
_cell_measurement_temperature           293(2)
_cell_measurement_theta_min             1.8871
_cell_measurement_theta_max             29.7259

#-----------------------------------------------------------------------------#
#                    CRYSTAL INFORMATION                                      #
#-----------------------------------------------------------------------------#

_exptl_crystal_size_max                 0.0762
_exptl_crystal_size_mid                 0.0296
_exptl_crystal_size_min                 0.0199
_exptl_crystal_density_diffrn           2.447
_exptl_crystal_density_method           'not measured'
_exptl_crystal_F_000                    1304
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    _exptl_crystal_face_index_k
    _exptl_crystal_face_index_l
    _exptl_crystal_face_perp_dist
0 0 1 0.0378
0 0 -1 0.0378
1 0 0 0.01
-1 0 0 0.01
-1 -1 0 0.01
1 1 0 0.01

_exptl_absorpt_coefficient_mu           1.236
_exptl_absorpt_correction_type          multi-scan
_exptl_absorpt_process_details
;
        CrysAlisPro, Agilent Technologies,
        Version 1.171.35.10 (release 06-04-2011 CrysAlis171 .NET)
        (compiled Apr  6 2011,09:17:13)
        Empirical absorption correction using spherical harmonics,
 implemented in SCALE3 ABSPACK scaling algorithm.
;
_exptl_absorpt_correction_T_min         0.99033
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_exptl_absorpt_correction_T_max         1

#----------------------------------------------------------------------------#
#                    DATA COLLECTION                                         #
#----------------------------------------------------------------------------#

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_diffrn_radiation_wavelength            0.71073
_diffrn_radiation_type                  MoK\a
_diffrn_radiation_monochromator         graphite
_diffrn_detector_area_resol_mean        16.0965
_diffrn_orient_matrix_ub_11             0.0057791
_diffrn_orient_matrix_ub_12             0.0105423
_diffrn_orient_matrix_ub_13             -0.0740279
_diffrn_orient_matrix_ub_21             0.0049326
_diffrn_orient_matrix_ub_22             0.0790635
_diffrn_orient_matrix_ub_23             0.0123083
_diffrn_orient_matrix_ub_31             0.0320409
_diffrn_orient_matrix_ub_32             -0.014069
_diffrn_orient_matrix_ub_33             0.0135584
_diffrn_measurement_device_type
                                       'SuperNova, Single source at offset), Eos'
_diffrn_measurement_method              'phi-omega scans'
_diffrn_reflns_av_R_equivalents         0.0489
_diffrn_reflns_av_unetI/netI            0.0495
_diffrn_reflns_number                   10172
_diffrn_reflns_limit_h_min              -29
_diffrn_reflns_limit_h_max              29
_diffrn_reflns_limit_k_min              -12
_diffrn_reflns_limit_k_max              12
_diffrn_reflns_limit_l_min              -12
_diffrn_reflns_limit_l_max              12
_diffrn_reflns_theta_min                1.89
_diffrn_reflns_theta_max                29.79
_diffrn_reflns_theta_full               29.79
_diffrn_measured_fraction_theta_full
                                        0.946
_diffrn_measured_fraction_theta_max
                                        0.946
_reflns_number_total                    2375
_reflns_number_gt                       1897
_reflns_threshold_expression            >2sigma(I)

#----------------------------------------------------------------------------#
#                    COMPUTER PROGRAMS USED                                  #
#----------------------------------------------------------------------------#

_computing_data_collection
;
        CrysAlisPro, Agilent Technologies,
        Version 1.171.35.10 (release 06-04-2011 CrysAlis171 .NET)
        (compiled Apr  6 2011,09:17:13)
;
_computing_cell_refinement
;
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        CrysAlisPro, Agilent Technologies,
        Version 1.171.35.10 (release 06-04-2011 CrysAlis171 .NET)
        (compiled Apr  6 2011,09:17:13)
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_computing_data_reduction
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        CrysAlisPro, Agilent Technologies,
        Version 1.171.35.10 (release 06-04-2011 CrysAlis171 .NET)
        (compiled Apr  6 2011,09:17:13)
;
_computing_structure_solution           'SHELXS-97 (Sheldrick, 1990)'
_computing_structure_refinement         'SHELXL-97 (Sheldrick, 1997)'

#------------------------------------------------------------------------------#
#                    STRUCTURE SOLUTION
#------------------------------------------------------------------------------#

_atom_sites_solution_primary            direct
_atom_sites_solution_secondary          difmap
_atom_sites_solution_hydrogens          geom

#------------------------------------------------------------------------------#
#                    REFINEMENT INFORMATION                                    #
#------------------------------------------------------------------------------#

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;
 Refinement of F^2^ against ALL reflections.  The weighted R-factor wR and
 goodness of fit S are based on F^2^, conventional R-factors R are based
 on F, with F set to zero for negative F^2^. The threshold expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is
 not relevant to the choice of reflections for refinement.  R-factors based
 on F^2^ are statistically about twice as large as those based on F, and R-
 factors based on ALL data will be even larger.
;
_refine_ls_structure_factor_coef        Fsqd
_refine_ls_matrix_type                  full
_refine_ls_weighting_scheme             calc
_refine_ls_weighting_details
         'calc w=1/[\s^2^(Fo^2^)+(0.0250P)^2^+3.5267P] where P=(Fo^2^+2Fc^2^)/3'
_refine_ls_hydrogen_treatment           mixed
_refine_ls_extinction_method            none
_refine_ls_number_reflns                2375
_refine_ls_number_parameters            162
_refine_ls_number_restraints            5
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_refine_ls_R_factor_gt                  0.0346
_refine_ls_wR_factor_ref                0.0732
_refine_ls_wR_factor_gt                 0.0683
_refine_ls_goodness_of_fit_ref          1.039
_refine_ls_restrained_S_all             1.04
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_refine_ls_shift/su_mean                0
_refine_diff_density_max                0.51
_refine_diff_density_min                -0.397
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_refine_diff_density_rms               0.107

#-----------------------------------------------------------------------------#
#                    ATOMIC TYPES, COORDINATES AND THERMAL PARAMETERS         #
#-----------------------------------------------------------------------------#

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    _atom_type_scat_dispersion_real
    _atom_type_scat_dispersion_imag
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O7 O 0.23371(8) 0.3601(2) 0.12194(18) 0.0084(4) Uani 1 1 d . . .
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O11 0.0145(11) 0.0265(12) 0.0231(12) -0.0139(10) 0.0081(9) -0.0073(9)


#-----------------------------------------------------------------------------#
#                    MOLECULAR GEOMETRY                                       #
#-----------------------------------------------------------------------------#

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 All esds (except the esd in the dihedral angle between two l.s. planes)
 are estimated using the full covariance matrix.  The cell esds are taken
 into account individually in the estimation of esds in distances, angles
 and torsion angles; correlations between esds in cell parameters are only
 used when they are defined by crystal symmetry.  An approximate (isotropic)
 treatment of cell esds is used for estimating esds involving l.s. planes.
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Si2 O5 1.6333(18) 7_556 ?
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