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Percleveite-(Ce) – a new lanthanide disilicate mineral from Bastnäs, Skinnskatteberg, Sweden

DAN HOLTSTAM[1], ROLF NORRESTAM[2] and ULF B. ANDERSSON[1]

[1]Research Division, Swedish Museum of Natural History, Box 50007, SE-104 05 Stockholm, Sweden
[2]Department of Structural Chemistry, Arrhenius Laboratory, Stockholm University, SE-106 91 Stockholm, Sweden

Abstract: Percleveite-(Ce), (Ce, La, Nd)$_2$Si$_2$O$_7$, is a new mineral species from the Bastnäs Fe-Cu-REE deposit, Skinnskatteberg, Västmanland, Sweden. It occurs closely associated with mainly cerite-(Ce), bastnäsite-(Ce) and quartz. The colour is greyish and the luster greasy to resinous. The anhedral crystals, up to 0.5 mm in size, are colourless in thin section and optically uniaxial (+). H ≈ 6. Cleavage is imperfect parallel to {001}. Electron-microprobe analyses give: La_2O_3 14.66, Ce_2O_3 31.36, Pr_2O_3 3.41, Nd_2O_3 12.97, Sm_2O_3 2.69, Gd_2O_3 2.26, Dy_2O_3 0.53, Ho_2O_3 0.07, Er_2O_3 0.21, Yb_2O_3 0.04, Y_2O_3 2.93, CaO 0.10, FeO 0.01, SiO_2 26.55, sum 97.79, yielding the empirical formula $(Ce_{0.87}La_{0.41}Nd_{0.35}Y_{0.12}Pr_{0.09}Sm_{0.07}Gd_{0.06}Dy_{0.01}Ca_{0.01})_{\Sigma=1.99}Si_{2.01}O_7$ based on 7 O atoms. The mineral is shown to be isostructural with the synthetic, low-temperature lanthanide disilicates (general formula $Ln_2Si_2O_7$) with tetragonal symmetry (space group $P4_1$). Unit-cell parameters are a = 6.7805(8) and c = 24.689(4) Å (refined from powder data) with Z = 8. The structure has been refined from single crystal data to a weighted Rw value of 0.036. All four symmetry independent Ln positions are slightly differently occupied by the lanthanide ions. Percleveite is formed at conditions with slightly higher SiO_2 activities, and lower concentrations of Ca and Mg, than conditions favourable for the crystallization of cerite-(Ce).

Key-words: percleveite-(Ce), new mineral, REE, disilicate, crystal structure, Bastnäs, Sweden.

Introduction

The Bastnäs deposit in the Skinnskatteberg district of Västmanland, Sweden (lat. 59°51'N, long. 15°35'E) is famous for its lanthanide minerals in particular. Here, Ce and La were extracted from cerite that was mined in the 19th century. The history of the Bastnäs mines, however, reaches 500 years back, when copper and iron initially were mined there. Chemical analyses of cerite (known as "Bastnäs tungsten" at the time) made by Hisinger & Berzelius (1804) revealed a new element, named cerium by them after the asteroid Ceres discovered shortly before. Later C.G. Mosander isolated lanthanum (first reported by Berzelius, 1840) from Bastnäs cerite. The Bastnäs deposit is the type locality for six minerals, including bastnäsite, (Ce, La, Nd)CO$_3$F, one of the industrially most important lanthanide or REE minerals in the world today. During a close examination of cerite specimens from this locality, another new mineral species, isomorphous to the synthetic tetragonal lanthanide disilicates, was discovered. There are a number of different structure types known among the compounds of the general formula $Ln_2Si_2O_7$, and the tetragonal polymorph, known to be stable at ambient P-T conditions, is designated type A (Felsche, 1973).

The name of the mineral, percleveite-(Ce), has been chosen to honour the memory of Per Theodor Cleve (1840-1905), a professor of organic and inorganic chemistry at Uppsala University, and the discoverer of the elements holmium and thulium. ("Cleveite", also named after P.T. Cleve by Nordenskiöld (1878), is a REE-bearing variety of uraninite.) The mineral has been approved by the IMA Commission on New Minerals and Mineral Names. Holotype material is preserved at the Swedish Museum of Natural History, Stockholm, under the catalogue no. 19060375.

Geological environment

For a general overview of the volcanic paleoenvironments and ore deposits in the Bergslagen metallogenic province, se Allen *et al.* (1996) and references therein. In the area where the Bastnäs deposit is situated, known as the Riddarhyttan ore field (Geijer, 1923), the oldest bedrock is dominated by Palaeoproterozoic felsic metavolcanic rocks, and metacarbonate layers of varying thickness are common. Quite a number of iron oxide ores and base metal sulphide deposits are hosted in the supracrustal units. The metavolcanic rocks have often been hydrothermally modified at an

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[1]E-mail address: dan.holtstam@nrm.se

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Fig. 1. Photomicrograph of a thin section (transmitted light) with percleveite (**pc**), cerite (**ce**), quartz (**q**) and the unknown W-bearing silicate (**w**). The black arrow points to an area with fine-grained fluorocarbonates. The white scale bar corresponds to 0.5 mm. Sample #19060375.

early, volcanic stage and later became metamorphosed under amphibolite-facies conditions. The dominant country rock is a cordierite-bearing mica quartz schist, which is believed to be an alteration product of an alkali-rich quartz porphyry, also quite common in the area. The iron ore horizons are stratiform and thought to be of volcano-sedimentary origin, being deposited during quiet periods in the volcanic activity. The above units are intruded by two generations of granitoids. The older (1.90–1.85 Ga) intrusions range from tonalite to granite in composition and are normally foliated, whereas the younger (1.80–1.75 Ga) are essentially undeformed granites *sensu stricto*. The bedrock underwent ductile deformation in connection with the Svecofennian orogeny, while later movements have caused fracturing and faulting affecting all types of rock in the area (Geijer, 1923; Ambros, 1983).

Geijer (1921) described the mineral parageneses of the Bastnäs mineralization in some detail. Here quartz-banded hematite ore occurs in proximity with magnetite-skarn ore, the latter replacing a carbonate (mainly dolomitic) horizon. The cerite ore was worked in two small mines, Ceritgruvan and Sankt Göransgruvan, where it formed a restricted skarn zone (up to 0.6 m thick) composed mainly of cerite-(Ce), tremolitic amphibole, allanite-(Ce), bastnäsite-(Ce), törnebohmite-(Ce) and talc. Sulphide minerals, dominantly chalcopyrite, bismuthinite and molybdenite, are closely associated to the lanthanide minerals, and usually interstitial to them.

Geijer (1961) discussed the observations from Bastnäs and some other possibly related deposits in the Norberg district, Västmanland (for which he coined the term "Bastnäs-type deposits"), and concluded that the REE mineralizations to a large extent had formed epigenetically, through replacement of carbonate lenses associated to sedimentary Fe ores (*i.e.*, as metasomatic skarns). He also proposed a genetic link to the extensive metasomatic alteration that has affected the felsic volcanic successions, which resulted in a significant Mg enrichment of the surrounding rocks. In Geijer's opinion, the Mg metasomatism was largely driven by the emplacement of early orogenic granitoids. This concept is now largely obsolete (Trägårdh, 1988), and there is no particular evidence that the formation of the deposits is related to orogenic magmatic processes. The origin of the fluids responsible for the REE-Cu-Mo-Bi mineralization in the Bastnäs-type deposits still remains unknown.

Mineral association and physical description

The mineral has so far only been observed in a single specimen, and we would consider it very rare. We have no exact knowledge of its original position within the Bastnäs deposit, since it was found in an old museum specimen lacking any detailed locality information. The specimen consists of rich cerite ore with subordinate magnetite, chalcopyrite and green clinoamphibole crystals up to 10 mm in length. According to some energy-dispersion X-ray analyses performed, the amphibole's composition lies close to the borderline between tremolite and actinolite. Allanite-(Ce) and törnebohmite-(Ce) occur in microscopic amounts associated with the amphibole.

Percleveite-(Ce) essentially forms anhedral grains up to 0.5 mm across, which can occur in aggregates several mm wide, and appears in close association with cerite-(Ce) and smaller amounts of bastnäsite-(Ce). Cerite and percleveite have occasionally been altered along grain boundaries, and the product assemblages consist of fine-grained fluorocarbonates. An unnamed silicate mineral with Ce, La, Nd, Fe, W and Mg as major metal components occurs as rare anhedral grains up to 300 µm in their greatest dimension (Fig. 1). It is optically biaxial and pleochroic in rust red to black. From textural relations it is clear that the mineral formed after cerite and perclevite. Minute grains of scheelite (containing about 1 mole% $CaMoO_4$ in solid solution) occur sparingly, usually in contact with the tungsten-bearing silicate. Quartz is, in relative terms, a later phase and appears in interstices and micro-cracks in the cerite-percleveite mass.

Percleveite-(Ce) has a yellowish gray to white megascopic colour, with a greasy to resinous luster and a white streak. The hardness is *ca.* 6 on Mohs's scale. Imperfect cleavage occurs parallel to {001}. The mineral is transparent and colourless in thin section, with low interference colours. Optically, percleveite is uniaxial positive with ω = 1.840(2) and ε = 1.846(2). There are no fluorescence effects seen under short-wave UV light. The density of the mineral has not been directly determined due to its close association with cerite, but a value of 5.21(1) g · cm^{-3} can be calculated from the unit-cell content.

Chemical composition

The chemical composition of the new mineral was determined using wavelength dispersion analyses on a

Table 1. Chemical composition of percleveite-(Ce) and associated cerite-(Ce).

	percleveite					cerite
					mean, *n* = 4	mean, *n* =5
La_2O_3	14.31	14.44	14.74	15.17	14.66	14.19
Ce_2O_3	30.73	31.10	31.46	32.13	31.36	31.48
Pr_2O_3	3.27	3.43	3.39	3.56	3.41	3.59
Nd_2O_3	12.20	12.99	12.90	13.78	12.97	14.40
Sm_2O_3	2.68	2.70	2.79	2.61	2.69	2.60
Gd_2O_3	2.36	2.35	2.30	2.02	2.26	1.79
Dy_2O_3	0.57	0.66	0.64	0.23	0.53	0.27
Ho_2O_3	0.06	0.06	0.04	0.11	0.07	0.05
Er_2O_3	0.27	0.22	0.29	0.06	0.21	0.11
Yb_2O_3	0.06	0.06	0.00	0.03	0.04	0.00
Y_2O_3	3.79	3.31	2.90	1.74	2.93	1.22
Fe_2O_3	0.01	0.00	0.02	0.00	0.01	0.71
MgO	0.00	0.00	0.00	0.00	0.00	1.63
Al_2O_3	0.00	0.00	0.00	0.00	0.00	0.00
SiO_2	26.40	26.85	26.19	26.74	26.55	21.24
CaO	0.09	0.09	0.08	0.14	0.10	1.89
F						1.13
Sum	96.80	98.26	97.74	98.32	97.79	96.30
O=F						-0.48
Total						95.82

n = number of analyses.

Cameca SX50 electron microprobe at GeoForschungsZentrum, Potsdam, Germany. The acceleration voltage was 20 kV, with a beam current of 40 nA and a 3 μm beam diameter. Standards used were pure synthetic REE phosphates (REE*L*β), YPO_4, (Y*L*α) Fe_2O_3 (Fe*K*α), wollastonite (Ca*K*α, Si*K*α) and LiF (F*K*α). Each peak was measured during 30 or 50 s (10 and 25 s for the background, respectively). Data reduction was made using a Cameca version of the PAP (Pouchou & Pichoir 1991) routine. Mn, Ti, Al, Mg, P, Ba, Sr, Na, Lu, Th, U were below the limit of detection (≤ 0.05 wt.%) in all points. F concentration values around 0.1 wt.% were obtained for percleveite-(Ce), but were not considered significant.

A total of four point analyses were performed on percleveite-(Ce) and the results are given in Table 1. The empirical chemical formula is $(Ce_{0.87}La_{0.41}Nd_{0.35}Y_{0.12}Pr_{0.09}Sm_{0.07}Gd_{0.06}Dy_{0.01}Ca_{0.01})_{\Sigma=2.00}Si_{2.01}O_7$, if calculated assuming seven O atoms per formula unit. The composition of a cerite-(Ce) grain in contact with percleveite (Table 1) was determined to $(Ce_{3.80}La_{1.72}Nd_{1.69}Pr_{0.43}Sm_{0.29}Y_{0.21}Gd_{0.20}Dy_{0.03}Er_{0.01}Ca_{0.66})_{\Sigma=9.04}(Mg_{0.80}Fe_{0.18})Si_{6.98}O_{24}[O_{1.52}(OH_{4.30})F_{1.18}]_{\Sigma=7.00}$ based on 17 cations.

X-ray diffraction analyses and atomic arrangement

Powder diffraction

Powder data were recorded with step (0.02°) scans in the 2θ-range 3 to 80° on an automated Philips PW1710 diffractometer using graphite-monochromatized Cu*K*α radiation (PW1830 generator operated at 40 kV and 40 mA). Peak positions were determined with the X'Pert Graphics & Identify program and corrected against an external Si standard (NBS 640b). Indexed *d* values for reflections with 2θ ≤ 62° and relative peak heights above background are given in Table 2. The pattern is similar to that reported for, *e.g.*, tetragonal $Nd_2Si_2O_7$ in the Powder Diffraction File (#22-1177). The unit-cell parameters of percleveite, refined from thirty-four reflections using a least-squares program (Novak & Colville, 1989), are a = 6.7805(8) Å, c = 24.689(4) Å, V = 1135.1(3) Å^3 and Z = 8.

Crystal structure determination

As the preliminary studies indicated that the new mineral is closely related to the synthetic type-A lanthanide disilicates with tetragonal crystal symmetry, a structure determination based on a single crystal X-ray diffraction experiment has been carried out to verify this observation. Data were recorded from a mineral fragment with dimensions 0.04 × 0.05 × 0.09 mm, selected from a mildly crushed subsample.

The diffraction data were collected with graphite monochromatized Mo*K*α radiation. The generator was operated at 50 kV and 35 mA, with a beam collimator diameter of 0.5 mm. Data were recorded under ambient conditions with an image plate detector system (Stoe IPDS) by oscillation covering a 200° angular (ϕ) range with a step size of 2.0°. Each image was exposed 6 minutes for a detector-to-crystal distance of 80 mm (corresponding to 2θ < 48.4°). The observed Laue symmetry and systematic extinctions among the reflections indicate the tetragonal space group symmetry $P4_1$ (or the enantiomeric $P4_3$). Data collection and reduction, including corrections for absorption (based on calculation of transmission factors from crystal shape and orientation), Lorentz and polarization effects were performed by using the program packages Stoe IPDS 2.87 and Stoe XRED 1.09. Further details on the

Table 2. Powder diffraction data for percleveite-(Ce).

d(obs)	*d*(calc)	*h*	*k*	*l*	*I* (%)
6.18	6.17	0	0	4	3
5.95	5.94	1	0	2	2
5.238	5.234	1	0	3	3
4.796	4.796	1	1	0	7
4.465	4.470	1	1	2	11
4.140	4.143	1	1	3	14
3.990	3.991	1	0	5	4
3.518	3.518	1	0	6	9
3.436	3.440	1	1	5	14
3.391	3.391	2	0	0	14
3.360	3.360	2	0	1	16
3.271	3.270	2	0	2	31
3.135	3.135	2	0	3	27
3.121	3.123	1	1	6	24
3.084	3.086	0	0	8	100
3.011	3.011	2	1	1	18
2.972	2.972	2	0	4	6
2.940	2.946	2	1	2	15
2.846	2.846	2	1	3	22
2.796	2.795	2	0	5	14
2.720	2.722	2	1	4	4
2.615	2.617	2	0	6	6
2.583	2.584	2	1	5	7
2.381	2.381	1	1	9	8
2.283	2.282	2	0	8	6
2.251	2.251	3	0	1	8
2.195	2.195	1	1	10	3
2.178	2.180	3	0	3	4
2.134	2.133	2	0	9	11
2.122	2.123	3	0	4	14
2.071	2.072	2	2	6	6
2.056	2.056	3	0	5	16
2.034	2.034	2	1	9	19
2.026	2.026	3	1	4	12
1.996	1.996	2	0	10	7
1.982	1.983	2	2	7	7
1.914	1.915	2	1	10	6
1.873	1.871	2	0	11	6
1.858	1.860	2	3	2	5
1.804	1.804	1	2	11	10
1.763	1.765	1	1	13	4
1.743	1.745	3	0	9	3
1.711	1.711	2	3	6	5
1.655	1.655	1	1	14	8
1.641	1.641	4	1	1	4
1.631	1.631	1	4	2	3
1.613	1.613	1	4	3	4
1.587	1.585	3	3	2	4
1.559	1.561	1	4	5	6
1.523	1.521	3	0	12	3
1.492	1.491	1	4	7	4

Table 3. Experimental details of the crystal structure refinement of percleveite-(Ce)

Space group	$P4_1$
Unit-cell dimensions	$a = 6.7805(8)$ Å $c = 24.689(5)$ Å $V = 1135.1(3)$ Å^3
Formula units/unit cell	$Z = 8$
Density (calculated)	5.20(1) g · cm^{-3}
Radiation	Mo$K\alpha$
Wavelength	0.71073 Å
Temperature	293(2) K
Intensity data collection	
θ_{max}	24.2°
Internal *R*	0.11
Collected reflections	7281
Independent reflections	1812
Observed reflections	1103
Criterion for significance	$I \geq 2\sigma$
Absorption correction	Analytical
Linear abs. coefficient	16.5 mm^{-1}
Structure refinement	Full matrix least squares
No. of refined parameters	112
R for observed reflections	0.047
wR for observed reflections	0.034
R for all unique reflections	0.035
Max. of $\mid \Delta \mid \sigma$	0.0001
Max. and min. of $\Delta\rho$	4.8 and -8.1 e/Å^3

refinement procedure are given in Table 3. A list of observed and calculated structure factors can be obtained in electronic form from the authors or through the E.J.M. Editorial Office in Paris.

A structural model was derived from the data given for the assumed isotypic structure of $Pr_2Si_2O_7$ (Felsche, 1971). The unit-cell parameters obtained from powder data were considered the most accurate and used in the following. The structural model was refined by least squares methods using the program package JANA2000 (Petricek & Dusek, 2000). In the refinements, neutral atomic scattering factors taken from Ibers & Hamilton (1974) were used. The four symmetry independent lanthanide positions were assumed to be fully occupied by a mixture of La and Ho. La and Ho were selected as their atomic numbers differ by 10, while they still have similar shapes of the scattering factor curves as a function of $\sin\theta/\lambda$. The composition at each position was varied throughout the refinements. With G as the fraction of La, the effective atomic number Z_{eff} at each lanthanide position can be estimated as $Z_{eff} = 67 - 10 \times G$. In the final refinement cycles all lanthanide ions were allowed to vibrate anisotropically, while the silicon and the oxygen atoms were kept isotropic to reduce the number of parameters to obtain a reasonable overdetermination ratio (Table 3). The obtained atom coordinates and bond distances are listed in Tables 4 and 5, respectively.

Structure characteristics

The general features of the structure of percleveite-(Ce) are the same as those observed in the isostructural lanthanide disilicates of the larger lanthanide ions La^{3+}, Ce^{3+}, Nd^{3+}, Pr^{3+}, and Sm^{3+} (*e.g.*, Felsche & Hirsiger, 1969; Felsche, 1971). The basic structure type is that of the pyrophosphate β-$Ca_2P_2O_7$.

The crystal structure is composed of eclipsed $[Si_2O_7]^{6-}$ dimers linked through Ln^{3+} cations (Fig. 2). The four symmetry independent lanthanide atoms have slightly different oxygen coordinations. Within 3.0 Å the *Ln*1 position is 7-coordinated, *Ln*2 is 9-coordinated, *Ln*3 is 7-coor-

Table 4. Fractional atom coordinates for percleveite-(Ce)

Atom	*x*/*a*	*y*/*b*	*z*/*c*	U_{eq}/U_{iso}	*G*
*Ln*1	0.7706(2)	0.2953(2)	0	0.0150(6)	0.82(5)
*Ln*2	0.5228(2)	0.1679(2)	0.14732(10)	0.0111(6)	0.83(5)
*Ln*3	0.3428(2)	0.9189(2)	0.00098(11)	0.0136(6)	0.94(4)
*Ln*4	0.1252(2)	0.7615(2)	0.13878(8)	0.0122(6)	0.86(5)
Si1	0.8568(11)	0.7645(10)	0.0144(2)	0.008(2)	
Si2	0.6039(10)	0.6957(11)	0.1128(3)	0.0061(18)	
Si3	0.2682(11)	0.3810(12)	0.0220(3)	0.0112(18)	
Si4	0.0154(10)	0.2892(10)	0.1207(3)	0.0064(19)	
O1	0.893(2)	0.609(2)	-0.0340(6)	0.012(4)	
O2	0.725(2)	0.945(2)	-0.0096(6)	0.014(4)	
O3	0.047(2)	0.843(2)	0.0451(6)	0.004(4)	
O4	0.729(2)	0.623(2)	0.0581(5)	0.008(3)	
O5	0.493(2)	0.516(2)	0.1382(8)	0.019(4)	
O6	0.443(2)	0.856(2)	0.0939(6)	0.012(4)	
O7	0.753(2)	0.814(2)	0.1542(6)	0.005(4)	
O8	0.335(2)	0.573(2)	-0.0089(6)	0.008(4)	
O9	0.450(2)	0.234(2)	0.0391(7)	0.009(4)	
O10	0.132(2)	0.244(2)	-0.0190(6)	0.011(4)	
O11	0.128(2)	0.429(2)	0.0762(7)	0.015(4)	
O12	0.981(2)	0.448(2)	0.1666(7)	0.023(5)	
O13	0.158(2)	0.124(2)	0.1442(7)	0.013(4)	
O14	0.822(2)	0.208(2)	0.0925(6)	0.014(4)	

G is the fraction of La obtained if the *Ln* positions are considered as mixtures of La and Ho.

Table 5. Selected bond distances (Å) in percleveite-(Ce).

*Ln*1–	O14	2.38(2)	Si1–	O3	1.59(2)
	O7	2.40(2)		O1	1.61(2)
	O2	2.41(2)		O2	1.63(2)
	O9	2.42(2)		O4	1.68(2)
	O1	2.43(2)			
	O10	2.52(2)	Si2–	O5	1.56(2)
	O4	2.66(2)		O6	1.61(2)
				O7	1.64(2)
*Ln*2–	O5	2.38(2)		O4	1.67(2)
	O14	2.45(2)			
	O13	2.49(2)	Si3–	O8	1.57(2)
	O6	2.55(2)		O9	1.64(2)
	O10	2.61(2)		O10	1.66(2)
	O8	2.66(2)		O11	1.67(2)
	O1	2.67(2)			
	O9	2.76(2)	Si4–	O12	1.58(3)
	O7	2.87(2)		O14	1.58(2)
				O13	1.59(2)
*Ln*3–	O12	2.30(2)		O11	1.64(3)
	O3	2.34(2)			
	O8	2.36(2)			
	O6	2.43(2)			
	O9	2.44(2)			
	O2	2.61(2)			
	O10	2.68(2)			
*Ln*4–	O3	2.44(2)			
	O12	2.44(2)			
	O13	2.47(2)			
	O6	2.50(2)			
	O2	2.56(2)			
	O7	2.58(2)			
	O11	2.74(2)			
	O1	2.77(2)			

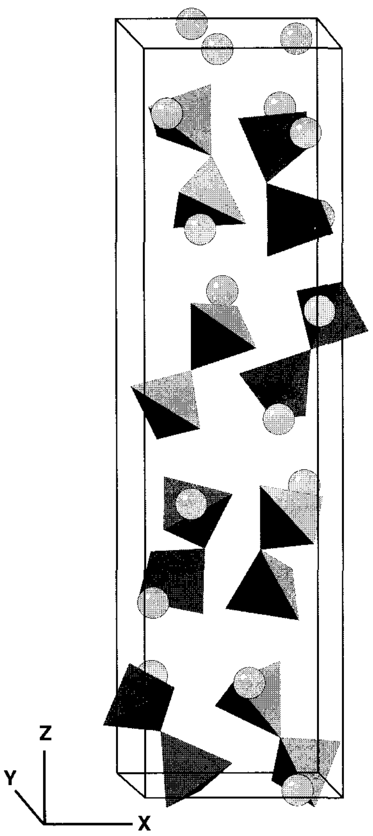

Fig. 2. Crystal structure of percleveite-(Ce) with the unit cell indicated. The spheres show the positions of the mixed lanthanide (Ce, La *etc.*) positions.

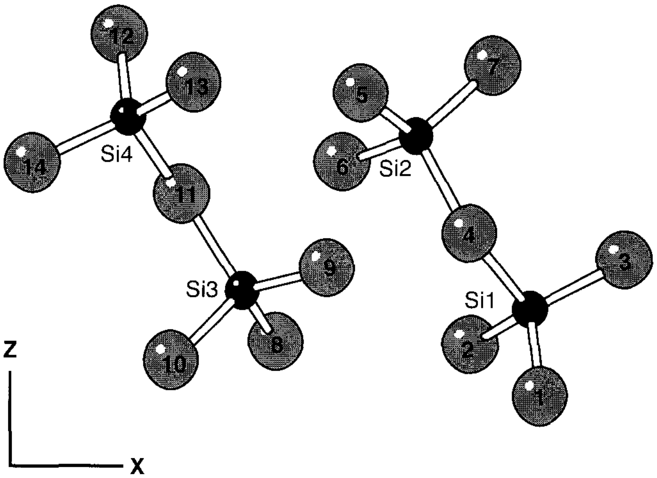

Fig. 3. The two eclipsed disilicate groups of the percleveite-(Ce) structure. The numbers given on the oxygen ligands correspond to the labeling used in Tables 4 and 5.

dinated and *Ln*4 is 8-coordinated. The difference in coordination numbers is reflected also in the average *Ln*–O distances, which are 2.46, 2.60, 2.45 and 2.56 Å, respectively. The 7-, 8- and 9-coordination polyhedra might be regarded as substantially distorted mono-, di- and tricapped trigonal prisms. The compositions vary slightly at each lanthanide position. Thus, the effective atomic numbers Z_{eff} at the *Ln*1, *Ln*2, *Ln*3, and *Ln*4 positions, when estimated as described above, become 58.8(5), 58.7(5), 57.6(4) and 58.4(5), respectively. It could be noted that La, Ce, Pr and Nd have atomic numbers 57, 58, 59 and 60, respectively. An estimate of the average atomic number from the chemical analyses gives 57.5, in good agreement with the value 58.4 calculated from the average numbers obtained in the structure refinement.

The Si atoms are tetrahedrally coordinated by oxygen atoms to form discrete disilicate groups (Fig. 3). The two non-linear $[Si_2O_7]^{6-}$ groups have apparently conformations close to that of the eclipsed *syn* (C_{2v}) form. The deviations of observed Si_2O_7 conformations from those of the three ideal conformations; the eclipsed *syn*, the staggered and the eclipsed *anti* forms (having C_{2v}, Cs and C_{2v} point symmetries, respectively) can be numerically described with the conformational parameter $T = |360 - 1/3\ \Sigma\tau_j|$ (Frank *et al.*, 2002). Here τ_j ($j = 1, 2, \ldots, 6$) are the six O–Si–O_b–Si torsion angles of the disilicate bridge Si–O_b–Si (given as positive numbers by utilising the τ periodicity 360°). The T value for the three above mentioned ideal conformations would be 0, 60 and 120°, respectively. In the present case the T values of the two disilicate groups become 8(2)° and 15(2)° close to the value 0° of the eclipsed *syn* form, but still indicating significant distortions. The Si1–O4–Si2 and Si3–O11–Si4 bridging angles at the disilicate bridges are 128(1)° and 134(1)°, respectively. The bond distances of the Si–O bonds to the bridging O atoms are elongated and range from 1.64 to 1.68 Å. The non-bridging Si–O bond lengths have an average of 1.60 Å.

Discussion

Percleveite is the first pure lanthanide silicate mineral, with major Ce and La, ever found. A few Y- or Sc-dominated disilicates with the monoclinic C-type structure are, however, known (*e.g.*, keiviite-(Y), thortveitite). In the chemical-structural classification system, percleveite is a sorosilicate belonging to the subdivision 9.BC. (Si_2O_7 groups without non-tetrahedral anions, cations in octahedral or greater coordination; Strunz & Nickel, 2001).

At present there are no well-defined constraints on the *P-T-t* conditions on the formation of this unique lanthanide silicate. The polymorphic transformations known for the synthetic equivalents have little relevance in geothermometry as they occur at conditions hardly attained in crustal rocks. The pure tetragonal Ce disilicate undergoes a transition at 1274°C to a monoclinic phase with the G-type structure, which melts congruently at 1770°C (Tas & Akinc, 1994).

Although cerite-(Ce) is an exceedingly rare mineral, with less than ten localities known world-wide (see Förster, 2000, for an overview), is was locally a rock-forming component at Bastnäs. The paragenesis of the cerite-percleveite assemblage must therefore represent unique conditions, in view of its rarity. In the Bastnäs deposit, the textural relations clearly suggest that cerite-(Ce) is the primary lanthanide mineral, which formed earlier than, *e.g.* bastnäsite and allanite (Geijer, 1921). In the present investigation we have found no textural evidence for percleveite-(Ce) being secondary in relation to cerite-(Ce).

Cerite is a nesosilicate with a crystal structure based on that of whitlockite (Moore & Shen, 1983), and the absence of SiO_4 polymerization suggests that it forms from silica-undersaturated fluids. Cerite is sometimes reported to occur with quartz, but the assemblages described in the references cited above are clearly not representing equilibrium conditions. Ca is present (in a range corresponding to 1.3 to 8.2 wt.% CaO) in all available analyses of cerite (Glass *et al.*, 1958; Förster, 2000; Holtstam & Andersson, unpubl.), and this element is likely to play a crucial role in the stabilisation of the mineral as it partly occupies a unique cation site in the structure (confirmed by crystallographic work on the recently described species cerite-(La); Pakhomovsky *et al.*, 2002). Local fluctuations in the availability of SiO_2 and to some extent CaO and MgO, have thus probably been critical to the crystallization of percleveite-(Ce), as opposed to cerite-(Ce). Percleveite-(Ce) is furthermore the only (Ce,La)-mineral at Bastnäs that contains no volatiles (*i.e.* hydrogen or fluorine) in its nominal formula. These small-scale variations might reflect conditions prevailing when the REE-bearing fluid of unknown origin interacted with the original carbonate rock.

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