# Ulfanderssonite-(Ce), a new Cl-bearing *REE* silicate mineral species from the Malmkärra mine, Norberg, Sweden

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Abstract: Ulfanderssonite-(Ce) is a new mineral (IMA 2016-107) from the long-abandoned Malmkärra iron mine, one of the Bastnästype Fe-rare earth element (REE) deposits in the Bergslagen ore region, central Sweden. It is named for Ulf B. Andersson, a Swedish geologist and petrologist. In the type specimen, the mineral occurs with västmanlandite-(Ce), bastnäsite-(Ce), phlogopite, talc, magnetite, pyrite, fluorbritholite-(Ce) and scheelite. Ulfanderssonite-(Ce) forms pinkish, translucent subhedral grains, 100-300 µm, in aggregates up to 2 mm. Fracture is uneven, and there is an indistinct cleavage parallel (001). Mohs' hardness is 5-6,  $D_{\text{calc}} = 4.97 \text{ g cm}^{-3}$ . Optically, ulfanderssonite-(Ce) is nonpleochroic, biaxial negative, with  $2V_{\text{meas}} = 55^{\circ}$  and  $n_{\text{calc}} = 1.82$ . The ideal composition is Ce15CaMg2(SiO4)10(SiO3OH)(OH,F)5Cl3. Electron microprobe and LA-ICP-MS chemical analyses yielded (in wt%) La2O3 11.87, Ce2O3 30.98, Pr2O3 3.99, Nd2O3 17.14, Sm2O3 2.81, Eu2O3 0.18, Gd2O3 1.15, Dy2O3 0.30, Tb2O3 0.10, Y2O3 1.11, CaO 2.26, FeO 0.02, MgO 1.97, P<sub>2</sub>O<sub>5</sub> 0.08, SiO<sub>2</sub> 19.13, H<sub>2</sub>O<sub>calc</sub> 1.07, F 1.09, Cl 2.89, O=(F, Cl) -1.10, sum 97.04. The five strongest powder X-ray diffraction lines are  $[I(\%) d_{obs}(Å)(hkl)]$ : 100 2.948 (-421), 47 2.923 (204), 32 2.660 (-225), 26 3.524 (40-1), 25 1.7601 (6-23). Ulfanderssonite-(Ce) is monoclinic, Cm, with a = 14.1403(8), b = 10.7430(7), c = 15.498(1) Å,  $\beta = 106.615(6)^{\circ}$  and V = 2256.0(2) Å<sup>3</sup> for Z=2. The crystal structure has been solved by direct methods and refined to  $R_1 = 2.97\%$  for 5280 observed reflections. It consists of a regular alternation of two layers, designated A and B, along the c-axis: A (ca. 9 Å thickness), with composition [(Ce<sub>8</sub>Ca)  $MgSi_7O_{22}(OH,F)_4]^{8+}$ , and *B* (*ca*. 6.5 Å), with composition [Ce<sub>7</sub>MgSi<sub>4</sub>O<sub>21</sub>(OH,F)<sub>2</sub>Cl<sub>3</sub>]<sup>8-</sup>; the *A* layer is topologically and chemically closely related to cerite-(Ce). A FTIR spectrum shows strong absorption in the region 2850–3650 cm<sup>-1</sup>, related to the presence of O– H stretching bands. Ulfanderssonite-(Ce) is interpreted as a primary mineral at the deposit, along with the more common fluorbritholite-(Ce), formed by a magmatic-hydrothermal fluid with REE, Si, F and Cl ion complexes reacting with dolomite marble. The presence of ulfanderssonite-(Ce) is direct evidence of a Cl-rich mineral-forming aqueous solution, normally not reflected in the composition of skarn minerals in Bastnäs-type deposits.

Key-words: ulfanderssonite-(Ce); new mineral; *REE* silicate; chlorine; crystal structure; infrared spectra; Bastnäs-type deposits; Bergslagen; Sweden.

# 1. Introduction

The Bastnäs-type Fe–rare earth element (*REE*) deposits in Sweden (Geijer, 1961) are scattered along an eighty-km long zone – situated in the Bergslagen ore province – dominated by volcanic to subvolcanic and sedimentary Palaeoproterozoic (Svecofennian) rocks (or their metamorphic equivalents). The deposits, comprising *REE* silicates and fluorocarbonates in association with magnetite, Mg silicates and minor Cu–Mo–Bi–Co–Au minerals (Geijer, 1921, 1927; Holtstam & Ensterö, 2002; Holtstam & Andersson, 2007; Jonsson *et al.*, 2014), are metasomatic skarn mineralizations, formed by fluids rich in *REEs* and other metals that have reacted with carbonate layers in the volcano-sedimentary pile. From fluid-inclusion studies and stable-isotope data it is inferred that mineral-forming fluids were hot (initially  $\geq$ 400 °C), saline and essentially of magmatic origin (Holtstam *et al.*, 2014; Sahlström, 2014).

More than twenty *REE* minerals have been reported from the Bastnäs-type deposits (Holtstam & Andersson, 2007), and here we present the characterisation of a new species – ulfanderssonite-(Ce) – from the Malmkärra mine, recently approved by the Commission on New Minerals, Nomenclature and Classification (CNMNC) of the International Mineralogical Association (IMA no. 2016-107).

We named the mineral in honour of Ulf B. Andersson (b. 1960), a Swedish geologist–petrologist and an ardent investigator of Svecofennian rocks and ores, with more

than fifty peer-reviewed articles and book chapters published. He has contributed significantly to the understanding of the genesis of *REE* deposits of Bastnäs type. Dr. Andersson is presently active as specialist in geology at the Luossavaara-Kiirunavaara AB mining company.

The discovery sample was collected in 1986 from mine dumps by Dr. Per Nysten, and originally catalogued as cerite-(Ce) + allanite-(Ce) in the Mineralogical Museum of Uppsala University, under the number 318/77. A closer study by us revealed that it consisted of mainly västmanlandite-(Ce) and a previously unknown REE silicate mineral, physically resembling cerite-(Ce), but with a unique X-ray diffraction pattern, and with significant Cl contents. Ulfanderssonite-(Ce) corresponds to the unnamed "mineral E" of Holtstam & Andersson (2007), which is identical to UM2007-39 in the official list of valid unnamed mineral species (Smith & Nickel, 2007). Sahlström (2014) noted a Ca- and Cl-rich REE-silicate mineral intergrown with fluorbritholite-(Ce) from Malmkärra, but no more detailed information was provided by the author. In the Nya Bastnäs ore field, ca. 30 km to the SSW of the Malmkärra mine, rare microscopic mineral grains found in contact with cerite-(Ce) have a composition very similar to that of ulfanderssonite-(Ce), except that they have more Fe than Mg (Holtstam & Andersson, 2007) and thus may represent an unnamed Fe analogue of ulfanderssonite-(Ce). It is plausible that the "Cl- and Frich cerite-(Ce)" from the Crosetto talc mine (Germanasca valley, Torino Province, Italy; Piccoli et al., 2007), for which an infrared spectrum is available (Chukanov, 2014), is a closely related mineral.

The holotype material, including a polished thin section, is deposited in the mineral collections of the Department of Geosciences, Swedish Museum of Natural History, under collection no. NRM 20010323.

# 2. Occurrence

The Malmkärra iron mine, Norberg District, Västmanland County, Sweden (lat. 60°3'34"N, long. 15°50'45"E, 200 m a.s.l.) is situated close to the tarn Stora Malmtjärnen. The ore deposit is hosted by a dolomitic marble layer, intercalated with felsic metavolcanic units. The carbonate layer appears to have its maximum thickness at this location due to folding. Local faulting in vertical movements has divided the deposit into separate ore bodies (Geijer, 1936). The underlying bed (footwall) consists of a plastically deformed mica-schist, dominated by quartz, muscovite and cordierite, with accessory tourmaline, magnetite and allanite-(Ce). In certain sections it grades into a Na-rich, better preserved metavolcanic rock. The magnetite-skarn ore has evidently replaced certain parts of the carbonate along its contact with the metavolcanic rock (Geijer, 1936; Holtstam *et al.*, 2014).

The mine demonstrably has a long history; the oldest written evidence is from the year 1664. Magnetite ore corresponding to more than 100 000 tons of iron in total was extracted over the years of production (Geijer & Magnusson, 1944). The *REE* mineralization was first noted by Geijer (1927), who described narrow bands of "cerite" and "orthite" between magnetite-skarn ore and dolomitic limestone with "ophicalcite", *i.e.* patches of Mg silicates (of the humite and serpentine groups) in recrystallized carbonate rock. The largest assemblage of *REE* minerals (a *circa* 0.5 m thick layer) was found at a depth of 205 m, close to an ore body known as *Lillgruvemalmen* at the bottom of the mine. Operations ceased in 1936, and the mine was thereafter flooded and forsaken.

Modern investigations of old collection material and dump samples show that the dominating REE minerals at Malmkärra are fluorbritholite-(Ce), västmanlandite-(Ce) and dollaseite-(Ce)-ferriallanite-(Ce) solid solutions, associated with minor dissakisite-(Ce), gadolinite-(Ce), gadolinite-(Nd), cerite-(Ce) and bastnäsite-(Ce) (Holtstam et al., 2005; Holtstam & Andersson, 2007; Škoda et al., 2016). Gadolinite-(Y) and magnesiorowlandite-(Y) are the rarest REE minerals found at the deposit. Magnesiorowlandite-(Y) was first identified at Malmkärra as the Mg analogue of rowlandite-(Y) ("mineral D" of Holtstam & Andersson, 2007 = UM2008-40 of Smith & Nickel, 2007), and later described as a new mineral species from Japan (Matsubara et al., 2014). Geijer (1936) reported that törnebohmite is quite frequent in the *REE* assemblages, but his observation has not been confirmed by present-day analytical methods; there is a suspicion that this claim comes from confusion with gadolinite varieties (in thin section also greenish and optically biaxial). The main skarn components beside the REE minerals are tremolite and phlogopite (F-bearing varieties), and magnetite, chondrodite, talc and fluorite; locally pyrite, chalcopyrite and molybdenite appear in the skarn masses (Geijer, 1936; Holtstam & Andersson, 2007).

# 3. Description

#### 3.1. Physical properties

The dominating minerals in the holotype specimen (Fig. 1) are västmanlandite-(Ce), ulfanderssonite-(Ce), bastnäsite-(Ce), phlogopite and talc. Fractured grains of magnetite ( $\leq 1$  mm), equant to skeletal in outline, occur in direct contact with both västmanlandite-(Ce) and ulfanderssonite-(Ce). Minor, scattered constituents are pyrite, fluor-britholite-(Ce) and scheelite. Ulfanderssonite-(Ce) occurs in granular aggregates up to two millimetres; individual grains are subhedral and measure 100–300 µm across. Alteration to bastnäsite-(Ce) and other, unidentified fluoro-carbonates locally occurs along grain boundaries and micro-cracks of the new mineral (Fig. 2).

The macroscopic colour of ulfanderssonite-(Ce) is flesh-pink to colourless-grey, with a white streak. The mineral is translucent (transparent in thin section), and it has a vitreous to greasy lustre. It is non-fluorescent under both short- and long-wave UV radiation. Hardness (Mohs) is between 5 and 6. Ulfanderssonite-(Ce) is brittle with an uneven fracture; cleavage is indistinct parallel to (001). The density could not be measured because of the small



Fig. 1. The type specimen with ulfanderssonite-(Ce) (pink areas). Associated minerals seen on the image are mainly västmanlandite-(Ce) and magnetite (brown to black). The specimen measures *ca*.  $7 \times 4.5$  cm. NRM catalogue no. 20010323. (Online version in colour.)

grain size and the presence of impurities in larger aggregates. The calculated value is  $4.972 \text{ g cm}^{-3}$ , using the empirical formula and unit-cell dimensions from single-crystal X-ray diffraction data (see below).

In thin section under the polarizing microscope, ulfanderssonite-(Ce) is nearly colourless, non-pleochroic and shows a slight undulatory extinction. The mineral is biaxial (–); the refractive indices are >1.8, which is higher than those of available immersion liquids ( $\bar{n}_{calc} = 1.82$  from the Gladstone–Dale relationship; Mandarino, 1981). The observed 2V is 55 ±5°, the dispersion is moderate, r > v.

#### 3.2. Mineral chemistry

Wave-length dispersion spot (n=10) analyses on two grains of ulfanderssonite-(Ce) were carried out using a Cameca SX50 electron microprobe (EMP) hosted by the Department of Earth Sciences, Uppsala University, at 20 kV and 20 nA. Data reduction was carried out using a Cameca version of the PAP (Pouchou & Pichoir, 1991) routine. The analytical results are given in Table 1, together with natural and synthetic standards used. Elements sought but not detected are Na, K, Sr, Ba, Al, Mn, Ti, Th and U. A complementary laser-ablation ICP-MS analysis was performed with a Finnigan MAT Element high-resolution ICP-MS equipped with a MAT UV Laser Probe operated at 266 nm in ca.  $200 \times 100 \,\mu\text{m}$ rasters, and using NIST 614, 612 and 610 glass standards complemented with fused NIST bedrock standards BCR-2, BIR-1 and RGM-1. Trace elements were analysed with Si as internal standard set to 19.13 wt% (cf. Table 1). The method is further described in detail by Holtstam *et al.* (2003) and Hode Vuorinen et al. (2005).

Material of sufficient purity for direct analyses of volatile components could not be separated due to the alterations observed. The H<sub>2</sub>O concentration was calculated, in accordance with the crystal structure, on the basis of (OH) + F + Cl = 9 atoms per formula unit (*pfu*). No



Fig. 2. Scanning electron microscope picture (BSE mode) of polished section with ulfanderssonite-(Ce) (Ulf) and västmanlandite-(Ce) (Väs). Ulfanderssonite-(Ce) is partly altered to bastnäsite-(Ce) (Bas) and other fluoro-carbonates.

bands attributable to  $CO_3^{2-}$  groups were recorded in the Fourier transform infrared (FTIR) spectrum of the mineral (see below).

The empirical formula, calculated from the average composition (Table 1) on the basis of 29 cations *pfu*, is  $(Ce_{6.58}Nd_{3.55}La_{2.54}Pr_{0.84}Sm_{0.56}Y_{0.34}Gd_{0.22}Dy_{0.06}Eu_{0.04}Tb_{0.02}Ca_{1.41})_{\Sigma 16.16}Mg_{1.70}Fe_{0.01}Si_{11.11}P_{0.04}O_{43}(OH)_{4.16}F_{2.00}Cl_{2.84}$ . The simplified formula is  $Ce_{15}CaMg_2(SiO_4)_{10}$  (SiO<sub>3</sub>OH)(OH,F)<sub>5</sub>Cl<sub>3</sub>, which corresponds (in wt%, with OH:F=2:1) to 72.41% Ce<sub>2</sub>O<sub>3</sub>, 1.65% CaO, 2.37% MgO, 19.43% SiO<sub>2</sub>, 1.06% H<sub>2</sub>O, 1.12% F, 3.13% Cl and (F, Cl)=O -1.17, for a total sum of 100.00 wt%.

### 3.3. Powder diffraction data

A powder X-ray diffraction pattern was recorded with step (0.02°) scans in the 20-range 3 to 65° on an automated Philips PW1710 diffractometer using graphite-monochromatised CuK $\alpha$  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 silicon standard (NBS 640b). Indexed *d* values for reflections with  $20 \le 56^{\circ}$  and relative peak heights above background are given in Table 2. The monoclinic unit-cell parameters, obtained by least-squares refinement (Novak & Colville, 1989) are a = 14.140(2) Å, b = 10.740(2) Å, c = 15.506(2) Å,  $\beta = 106.64(2)^{\circ}$  and V = 2256.2(2) Å<sup>3</sup>.

# 3.4. Single-crystal data, structure solution and refinement

The X-ray intensity data were collected with an Oxford Diffraction X calibur 3 diffractometer (MoK $\alpha$  X-radiation,  $\lambda = 0.71073$  Å) fitted with a Sapphire 2 CCD detector (with 50 s exposure time per frame). Intensity integration and standard Lorentz-polarization corrections were done with the CrysAlis RED (Oxford Diffraction, 2006) software

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Table 1. Chemical analytical data for ulfanderssonite-(Ce) based on EMP point analyses and ICP-MS analysis (in wt% and ppm, respectively).

Table 2. X-ray powder diffraction data (Cu $K\alpha$  = 1.54178 Å; *d* in Å, main lines in bold) for ulfanderssonite-(Ce).

Constituent	Mean	Range	SD $(1\sigma)^*$	Probe standard
SiO <sub>2</sub>	19.13	18.47–19.47	0.30	Wollastonite
$P_2O_5$	0.08	0.00 - 0.28	0.09	Fluorapatite
FeO	0.02	0.00 - 0.08	0.03	Fe <sub>2</sub> O <sub>3</sub>
MgO	1.97	1.90-2.10	0.07	MgO
CaO	2.26	2.02-2.51	0.15	Wollastonite
$H_2O^a$	1.07	_		
F	1.09	0.93-1.25	0.12	LiF
Cl	2.89	2.85-2.97	0.04	KCl
$Y_2O_3$	1.11	0.82-1.45	0.19	$YPO_4$
$La_2O_3$	11.87	11.28-12.45	0.50	LaPO <sub>4</sub>
$Ce_2O_3$	30.98	29.66-31.83	0.62	CePO <sub>4</sub>
$Pr_2O_3$	3.99	3.78-4.20	0.14	PrPO <sub>4</sub>
$Nd_2O_3$	17.14	16.68-17.64	0.34	NdPO <sub>4</sub>
$Sm_2O_3$	2.81	2.60-3.13	0.18	SmPO <sub>4</sub>
$Eu_2O_3^{b}$	0.181		0.003	
$Gd_2O_3$	1.15	0.84-1.48	0.19	GdPO <sub>4</sub>
$Tb_2O_3^{b}$	0.096		0.002	
$Dy_2O_3$	0.30	0.22-0.42	0.06	DyPO <sub>4</sub>
O≡F	-0.46			
O=Cl	-0.64			
Total	97.04			
Trace elemen	nts (from	LA-ICP-MS)		
Но		225	5	
Er		350	6	
Tm		22	4	
Yb		104	3	
Lu		10	5	
Bi		28	2	
Cu		5.5	1.6	
W		3104	73	
U		67	2	
Th		1.3	0.4	

For the LA-ICP-measurement, SD is the analytical uncertainty in a single analysis.

<sup>a</sup> Calculated using OH + F + Cl = 9 apfu.

<sup>b</sup> From LA-ICP-MS.

package. The program ABSPACK of the CrysAlis RED package (Oxford Diffraction, 2006) was used for the multi-scan absorption correction.

Refinement of the single-crystal unit-cell dimensions gave the following parameters: a = 14.1403(8) Å, b = 10.7430(7) Å, c = 15.498(1) Å,  $\beta = 106.615(6)^{\circ}$  and V=2256.0(2)Å<sup>3</sup> for Z=2. Taking into account the results obtained by the analysis of reflection conditions (hkl: h+k=2n; hk0: h,k=2n; h00: h=2n; 0k0: k=2n), and the distribution of |E| values that strongly indicated the absence of an inversion centre ( $|E^2 - 1| = 0.789$ ), attempts to solve the crystal structure were made in the space group Cm. The positions of most of the atoms were determined by means of direct methods (the program SHELXS-97; Sheldrick, 2008). A least-squares refinement on  $F^2$  using these heavy-atom positions and isotropic temperature factors produced an R factor of 0.115. Three-dimensional difference-Fourier synthesis yielded the position of the remaining oxygen atoms. SHELXL-97 (Sheldrick, 2008)

I(obs)	<i>I</i> (calc)	d(obs)	d(calc)	h	k	l
10	4	8.451	8.416	1	1	0
5	4	6.820	6.821	1	1	1
7	2	4.936	4.952	0	0	3
12	22	4.686	4.688	2	0	3
11	15	4.648	4.644	1	1	3
12	12	4.414	4.415	2	0	2
21	40	4.350	4.352	0	2	2
16	19	4.161	4.163	3	1	0
5	2	3.765	3.759	3	1	1
21	21	3.644	3.646	1	1	4
26	30	3.524	3.528	4	0	1
12	2	3.478	3.481	4	0	2
17	25	3.423	3.427	1	3	1
21	14	3.316	3.318	1	3	1
13	16	3.279	3.281	3	1	2
15	20	3.227	3.229	1	3	2
19	22	3.062	3.063	2	0	5
100	100	2.948	2.949	4	2	1
47	43	2.923	2.923	2	0	4
10	2	2.834	2.839	3	1	3
13	7	2.807	2.805	3	3	0
14	8	2.789	2.790	4	2	3
5	10	2.7447	2.7442	1	3	3
24	34	2.6826	2.6849	0	4	0
32	42	2.6604	2.6604	2	2	5
10	11	2.5676	2.5672	2	$\overline{2}$	4
7	10	2.4773	2.4760	0	0	6
2	1	2.3424	2.3407	1	3	5
13	21	2.2741	2.2736	3	3	3
11	11	2.2322	2.2342	6	0	4
4	1	2.1702	2.1702	5	3	3
15	8	2.1222	2.1215	1	5	0
10	16	2.0713	2.0717	5	3	1
16	20	1.9764	1.9762	1	1	7
15	16	1.9381	1.9381	2	0	8
11	13	1.8579	1.8570	0	0	8
25	30	1.7601	1.7600	6	$\overline{2}$	3
12	7	1.7413	1.7405	8	0	4
6	4	1.6500	1.6507	0	0	9

was used for the refinement of the structure. Site-scattering values were refined at the Ce positions and octahedral sites using scattering curves for neutral species (Wilson, 1992) as follows: Ce vs. Ca and Mg vs. Fe. The Si, Cl and O sites (refined as Si, Cl and O vs.  $\Box$ , respectively) were found fully occupied, and the occupancy factors were then fixed to 1.00. According to these occupancy refinements, a bond-valence analysis and crystal-chemical considerations, the F atoms substitute for most of the OH groups (see below).

Successive cycles were run introducing anisotropic temperature factors for all the atoms leading to  $R_1 = 2.97\%$  for 5280 observed reflections  $[F_o > 4\sigma(F_o)]$  and  $R_1 = 3.34\%$  for all 7704 independent reflections and 409 parameters. A careful inspection of the difference-Fourier maps did not reveal any H atoms. Experimental details are given in Table 3. Fractional atomic coordinates and isotropic displacement parameters are reported in Table 4. Bond distances are reported in Table 5. A table with

anisotropic displacement parameters (Table S1) and a CIFfile are freely available online as Supplementary Material linked to this article on the GSW website of the journal: http://eurjmin.geoscienceworld.org/.

#### 3.5. Description of the structure

The asymmetric unit of ulfanderssonite-(Ce) contains eleven REE (dominated by Ce, followed by Nd and La) or (REE,Ca) sites, two Mg sites (one of which contains minor Fe), seven Si sites, three Cl sites and 30 O sites, some of which are protonated and/or partly replaced by F (see below). The basic structural elements of ulfanderssonite-(Ce) (Fig. 3) are eleven distorted (REE,Ca)O<sub>7-9</sub>Cl<sub>0-2</sub> polyhedra, two regular MgO<sub>6</sub> octahedra and seven SiO<sub>4</sub> tetrahedra (one of which is protonated). Although strictly speaking not a layer topology, the crystal structure of the mineral can simply be described as a regular alternation of two kinds of layers along the *c*-axis: a first layer (labelled *A*), with thickness ~9.0 Å, with general composition  $[(Ce_8Ca)MgSi_7O_{22}(OH,F)_4]^{8+}$ , and a second layer (labelled *B*), ~6.5 Å thick, with general composition  $[Ce_7MgSi_4O_{21}(OH,F)_2Cl_3]^{8-}$ . The atoms of the *A* layer are: Ce1 to Ce6, Mg1, Si1 to Si5, and O1 to O17; the atoms of the B layer are: Ce7 to Ce11, Mg2, Si6 and Si7, O18 to O30, and C11 to C13. The REE-Cl bond distances in the B layer range between 2.850(5) and 3.289(5) Å.

The A layer is in structural terms identical to the atomic arrangement of cerite-(Ce), (Ce,Ca)<sub>9</sub>(Mg,Fe)(SiO<sub>4</sub>)<sub>3</sub>  $[SiO_3(OH)]_4(OH,F)_3$  (Moore & Shen, 1983), with the whitlockite-type structure. In contrast, the *B* layer (Fig. 4) has never been observed in the structure of any natural or synthetic compound, to the best of our knowledge. The bond-valence analysis of the structure, calculated according to Brese & O'Keeffe (1991) and with the site occupancy factors given in Table 4, is reported in Table 6. The analysis showed that O6, O13 (ligand of Si1), O14, O15, O28 and O30 are (OH,F) sites. The bond-valence sum for O15 (0.53 valence units, v.u.) appears rather low in comparison to the values calculated for the remaining (OH,F) sites (1.10, 0.86, 1.17, 1.21 and 1.06 v.u., respectively), and may indicate that part of the O15 site could host minor H<sub>2</sub>O not detectable by IR spectroscopy (see below). Although O17 has also a relatively low value (1.49 v.u.), it is bonded twice to Si1, which already has an OH ligand. The singly protonated Si1O<sub>4</sub> group is characterised by a Si1–OH13 bond distance of 1.710(3) A. This is similar to the Si3–OH10 bond distances of 1.69(2) Å in cerite-(La) (Pakhomovsky et al., 2002), 1.68(2) A in aluminocerite-(Ce) (Nestola et al., 2009) and 1.689(8)Å in synthetic cerite-like La<sub>9</sub>OMg[SiO<sub>4</sub>]<sub>6</sub> [SiO<sub>3</sub>(OH)] (Lipp & Schleid, 2008). All three distances are considerably longer than the average Si-OH bond length in minerals and inorganic compounds (1.643 A; Nyfeler & Armbruster, 1997), although they roughly fall within the observed range reported in the mentioned paper, 1.62–1.70 Å. In agreement with the finding of Nyfeler & Armbruster (1997) that the average distances of the nonhydroxylated Si-O bonds remain rather constant at 1.62 Å, the equivalent value in ulfanderssonite-(Ce) is 1.62 Å.

Table 3. Data and experimental details for the selected ulfanderssonite-(Ce) crystal.

Crystal data	
Formula	$Ce_{15}CaMg_2(SiO_4)_{10}$
	(SiO <sub>3</sub> OH)(OH,F) <sub>5</sub> Cl <sub>3</sub>
Crystal size (mm)	$0.045 \times 0.055 \times 0.060$
Form. colour	Block, pink
Crystal system	Monoclinic
Space group	Cm
a(A)	14.1403(8)
$b(\dot{A})$	10.7430(7)
$c(\dot{A})$	15.498(1)
β(°)	106.615(6)
$V(A^3)$	2256.0(2)
Ζ	2
Data collection	
Instrument	Oxford Diffraction Xcalibur 3
Radiation type	$M_0 K_{\alpha} (\lambda = 0.71073 \text{ Å})$
Temperature (K)	298(3)
Detector-to-sample	5
distance (cm)	5
Number of frames	7526
Measuring time (s)	50
Maximum covered $2\theta$ (°)	66.00
Absorption correction	Multi-scan (ABSPACK:
	Oxford Diffraction, 2006)
Collected reflections	13 800
Unique reflections	7704
Reflections with $F_{0} > 4\sigma(F_{0})$	5280
R <sub>int</sub>	0.0436
$R_{\sigma}$	0.0663
Range of $h, k, l$	$-21 \le h \le 20, -16 \le k \le 16,$ $-23 \le l \le 23$
Refinement	
Refinement	Full-matrix least squares on $F^2$
Final R1 $[F_{\circ} > 4\sigma(F_{\circ})]$	0.0297
Final R1 (all data)	0.0334
Flack x parameter	-0.10(3)
GoF	1.018
Number of least-squares	409
parameters	
$\Delta \rho_{\rm min} (e {\rm \AA}^{-3})$	2.29 (0.12 Å from Cl3)
$\Delta \rho_{\rm max} \ ({\rm e}  {\rm \AA}^{-3})$	-2.08 (0.61 Å from Cl3)

In the Strunz mineral classification (Strunz & Nickel, 2001), ulfanderssonite-(Ce) is a neso-silicate with additional cations, mostly with six- and higher coordination (group 9.AG).

#### **3.6. Infrared spectroscopy**

An unpolarised single-crystal FTIR-spectrum in the range  $600-5000 \text{ cm}^{-1}$  was collected at a spectral resolution of  $2 \text{ cm}^{-1}$  from a 26 µm thick polished random section of a single crystal with a Bruker Vertex 70 spectrometer attached to a Bruker Hyperion2000 IR-microscope. The recorded spectrum was fitted in the range 2000–3800 cm<sup>-1</sup> using the Jandel 4.12 software assuming Gaussian peak shapes (Fig. 5). The spectrum shows strong absorption

Site	s.o.f.	x	У	Ζ	$U_{ m eq}$
Ce1	Ce <sub>1.00</sub>	0.48575(5)	0.19529(8)	0.71950(4)	0.01401(17)
Ce2	Ce <sub>1.00</sub>	0.44630(5)	0.19049(7)	0.45272(4)	0.00992(15)
Ce3	$Ce_{0.750(7)}Ca_{0.250}$	0.55958(10)	1/2	0.38449(9)	0.0112(4)
Ce4	$Ce_{0.819(7)}Ca_{0.181}$	0.37061(10)	1/2	0.78961(8)	0.0142(4)
Ce5	$Ce_{0.790(7)}Ca_{0.210}$	0.29108(7)	1/2	0.35528(6)	0.0104(3)
Ce6	Ce <sub>1.00</sub>	0.21659(10)	0.24881(11)	0.58549(7)	0.01470(10)
Ce7	$Ce_{1,00}$	0.11059(5)	0.21239(7)	0.14663(4)	0.01080(15)
Ce8	$Ce_{1,00}$	0.32210(5)	0.28790(9)	0.02188(4)	0.01194(16)
Ce9	$Ce_{0,804(7)}Ca_{0,196}$	0.43753(10)	0	0.92541(8)	0.0143(4)
Ce10	$Ce_{0.850(7)}Ca_{0.150}$	-0.00413(9)	1/2	0.24545(7)	0.0120(4)
Ce11	$Ce_{1,00}$	0.65186(7)	1/2	0.88431(6)	0.01353(16)
Mg1	$Mg_{1.00}$	0.6599(6)	0	0.8719(5)	0.0155(14)
Mg2	$Mg_{0.87(2)}Fe_{0.13}$	0.2681(4)	0	0.2971(4)	0.0110(14)
Sil	20.07(2) 0.15	0.4736(5)	1/2	0.5903(4)	0.0147(7)
Si2		0.2597(3)	0.2424(4)	0.8050(3)	0.0137(8)
Si3		0.1703(3)	0.2547(4)	0.3640(3)	0.0126(8)
Si4		0.6135(5)	0	0.6413(4)	0.0152(11)
Si5		0.3135(4)	0	0.5322(3)	0.0108(10)
Si6		0.5495(3)	0.2647(4)	0.9322(3)	0.0135(8)
Si7		0.3801(3)	0.2017(1) 0.2605(4)	0.2374(3)	0.0133(0) 0.0112(8)
C11		0.3430(4)	0	0.2571(5) 0.0650(3)	0.0205(10)
C12		0.0882(4)	1/2	0.0000(3)	0.0209(10) 0.0259(12)
C12		0.0002(4)	1/2	0.0076(9)	0.0237(12) 0.073(7)
01		0.4033(13) 0.2803(7)	0.2841(8)	0.0970(9) 0.4245(5)	0.073(7)
$\Omega^2$		0.2803(7)	0.2041(0)	0.4245(5) 0.4334(6)	0.0119(17)
02		0.1039(7)	0.2403(9)	0.4334(0) 0.7571(5)	0.014(2)
03		0.1474(7) 0.5001(7)	0.2032(8) 0.3669(10)	0.7371(3) 0.8527(6)	0.0120(18) 0.022(2)
04		0.3091(7) 0.7252(11)	0.5009(10)	0.6576(0)	0.022(2)
05		0.7552(11) 0.4032(12)	0	0.0370(9) 0.7634(8)	0.025(5)
010		0.4032(13)	0 1255(11)	0.7034(8)	0.030(3)
07		0.3719(8) 0.5835(12)	-0.1255(11)	0.3909(0) 0.7365(8)	0.020(2) 0.027(4)
00		0.3833(12)	0 1207(10)	0.7303(8)	0.027(4)
09		0.3595(8)	0.1507(10)	0.3823(6)	0.021(2)
010		0.4144(8)	0.3628(9)	0.3180(6)	0.021(2)
011		0.3248(8)	0.2672(10)	0.7343(7)	0.022(2)
012		0.1978(11)	0	0.5168(8)	0.021(3)
OHI3		0.397(2)	<sup>2</sup> /2	0.6469(16)	0.022(3)
OH14		0.0264(9)	1/2	0.4102(8)	0.014(3)
OHIS		0.2226(8)	1/2	0.4857(7)	0.025(2)
016		0.4555(8)	<sup>1</sup> /2	0.481/(7)	0.024(2)
01/		0.4266(6)	0.3/52(6)	0.6201(5)	0.0263(17)
018		0.5559(9)	0.1326(10)	0.8818(6)	0.024(2)
019		0.3776(8)	0.1290(10)	0.2912(6)	0.024(2)
020		0.1389(8)	0.3719(11)	0.2945(6)	0.026(2)
021		0.1575(9)	0.1275(11)	0.3053(6)	0.033(3)
022		0.4847(8)	0.2387(9)	0.9989(6)	0.016(2)
023		0.6550(8)	0.3025(8)	0.9985(6)	0.013(2)
024		0.2710(7)	0.3733(9)	0.8625(6)	0.018(2)
025		0.2721(7)	0.2978(8)	0.1667(5)	0.0116(19)
026		0.2960(8)	0.1376(9)	0.8848(6)	0.019(2)
027		0.4575(7)	0.2324(10)	0.1781(6)	0.0168(19)
OH28		0.1830(10)	0	0.1638(8)	0.017(3)
O29		0.3387(11)	0	0.4375(8)	0.027(4)
OH30		0.7377(12)	0	0.0071(9)	0.023(3)

Table 4. Atom sites, site-occupancy-factors (s.o.f.), atom coordinates and isotropic displacement factors in the structure of ulfanderssonite-(Ce).

between ~2850 and ~3650 cm<sup>-1</sup>, with broad band features at ~2850 and ~3250 cm<sup>-1</sup>, and relatively sharp bands at 3400, 3510 and 3635 cm<sup>-1</sup>, caused by O–H stretching vibrations. As stated in the previous section, the crystal structure of ulfanderssonite-(Ce) displays six distinct OH sites with potential hydrogen bonds charac-

terised by O···O distances ranging from 2.619 Å to 3.223 Å. Based on the calibration of O···O distances vs. O–H stretching mode frequencies by Libowitzky (1999), OHbands in ulfanderssonite-(Ce) spectra are predicted to occur between 2846 and 3588 cm<sup>-1</sup>, which is in very good agreement with the experimental data. The broad low-

Table 5. Selected bond distances (in  $\text{\AA}$ ) in the structure of ulfanderssonite-(Ce).

Ce1–O9	2.453(9)	Ce9–OH6	2.416(12)
Ce1–O3	2.448(10)	Ce9–O26 (×2)	2.422(11)
Ce1-011	2.476(12)	Ce9–O18 (×2)	2.436(12)
Ce1-017	2.464(7)	Ce9–O22 (×2)	2.808(10)
Ce1-08	2.485(9)	Ce9–Cl1	2.850(5)
Ce1-018	2.518(9)	Ce9–Cl2	2.949(5)
Cel-O6	2.585(11)	<ce9–o></ce9–o>	2.62
Cel-O4	2.717(10)		
Cel-O7	2.722(11)	Ce10–O20 (×2)	2.384(11)
<ce1–o></ce1–o>	2.54	Ce10–O19 ( $\times 2$ )	2.428(11)
		Ce10–OH14	2.465(12)
Ce2–O7	2.460(9)	Ce10 $-027 (\times 2)$	2.700(10)
Ce2–O2	2.447(11)	Ce10–Cl2	2.882(6)
Ce2–O1	2.475(10)	Cel0–Cl1	3.006(5)
Ce2-019	2.501(9)	<ce10–o></ce10–o>	2.60
Ce2–O29	2.521(9)		
Ce2–OH14	2.516(8)	Cell-O26 ( $\times$ 2)	2.515(10)
Ce2-09	2.714(10)	$Cell=O23 (\times 2)$	2.754(9)
Ce2-O10	2.729(9)	Cell $-O3$ (×2)	2.930(8)
<ce2–o></ce2–o>	2.55	Cell-Cll	3.289(5)
<b>a a a i i</b>		<cell-o></cell-o>	2.81
Ce3-016	2.389(11)		
Ce3-012	2.395(12)	Mg1–O8	2.067(14)
$Ce3-O10 (\times 2)$	2.498(10)	Mg1–OH30	2.070(15)
$Ce_{3}-O_{21}(\times 2)$	2.504(12)	$MgI-O18 (\times 2)$	2.084(13)
$Ce3-O2 (\times 2)$	2.713(10)	MgI-O24 (×2)	2.114(12)
<ce3-0></ce3-0>	2.53	<mg1–o></mg1–o>	2.09
Ce4–O5	2.369(14)	Mg2–OH28	2.072(12)
Ce4–O4 (×2)	2.395(10)	Mg2–O19 (×2)	2.099(12)
Ce4–O24 (×2)	2.454(10)	Mg2–O21 (×2)	2.109(13)
Ce4–O11 $(\times 2)$	2.663(11)	Mg2–O29	2.119(13)
<ce4–o></ce4–o>	2.48	<mg1–o></mg1–o>	2.10
Ce5–OH15	2.478(11)	Si1–O17 (×2)	1.621(8)
Ce5–O10 (×2)	2.475(11)	Si1-016	1.629(12)
Ce5–O20 (×2)	2.501(11)	Si1-OH13	1.710(3)
Ce5-016	2.576(11)	<si1–o></si1–o>	1.65
Ce5–O1 (×2)	2.578(8)		
<ce5–o></ce5–o>	2.52	Si2–O3	1.606(10)
		Si2-011	1.642(13)
Ce6-011	2.384(10)	Si2026	1.643(10)
Ce609	2.399(11)	Si2024	1.648(10)
Ce6–O2	2.441(8)	<si2–o></si2–o>	1.63
Ce6–O7	2.473(11)		
Ce6-O12	2.861(5)	Si3–O1	1.601(10)
Ce6–O5	2.904(5)	Si3-O21	1.623(12)
Ce6-O1	2.910(9)	Si3–O2	1.625(12)
<ce6–o></ce6–o>	2.62	Si3-O20	1.633(11)
		<si3–o></si3–o>	1.62
Ce7025	2.398(10)	Si4–07 (×2)	1.585(11)
Ce7-027	2.425(10)	Si4-08	1.647(17)
Ce7–OH28	2.484(5)	Si4–O5	1.666(17)
Ce7-O21	2.527(10)	<si4–o></si4–o>	1.62
Ce7-O22	2.521(9)		-
Ce7-O23	2.553(10)	Si5012	1.584(15)
Ce7-O20	2.796(10)	Si5-O29	1.606(15)
Ce7–Cl3	3.034(12)	Si5–O9 (×2)	1.646(11)
Ce7–Cl2	3.1622(13)	<si5–o></si5–o>	1.62
<ce7–o></ce7–o>	2.66		
		Si6-O22	1.589(12)
Ce8–O22	2.483(11)	Si6-O23	1.603(10)
Ce8–O23	2.483(10)	Si6-04	1.628(10)

Table 5. (continued).

Ce8–O25	2.540(10)	Si6018	1.635(12)
Ce8–OH30	2.552(7)	<si6-o></si6-o>	1.61
Ce8–O24	2.539(9)		
Ce8026	2.609(9)	Si7-010	1.630(10)
Ce8–O27	2.690(9)	Si7-019	1.646(11)
Ce8–Cl3	3.037(10)	Si7-O27	1.647(11)
Ce8–Cl1	3.1603(13)	Si7-O25	1.654(10)
<ce8–o></ce8–o>	2.68	<si7-o></si7-o>	1.64

energy band at  $\sim 2850 \,\mathrm{cm}^{-1}$  most likely represents O-H stretching in O15-H...O5. The O-H stretching bands in the range 3100-3400 cm<sup>-1</sup> may be assigned to O13-H.O3 and O13–H···O12 modes. The bands at 3510 and  $3635 \text{ cm}^{-1}$ may be due to O15-H…O17 stretching. As more than one type of cation occupy the Ce5 site, different short-range arrangements of cations will occur around the OH15 group, which will give rise to absorption at different energies. The absence of absorption bands close to  $1600 \text{ cm}^{-1}$ , which are typically attributable to H<sub>2</sub>O bending modes, demonstrates, in agreement with the results of our structure refinements, that H<sub>2</sub>O molecules are not present in any significant amounts in the structure of ulfanderssonite-(Ce). In addition to the bands caused by O-H stretching in hydroxyl groups, the FTIR spectrum shows very intense absorption due to SiO<sub>4</sub> modes in the range  $800-1050 \text{ cm}^{-1}$ . Absorption bands at 2140 and  $\sim$ 2330 cm<sup>-1</sup> are tentatively assigned to lattice combination modes.

Ulfanderssonite-(Ce) bears resemblance with the spectrum of the "Cl- and F-rich cerite-(Ce)" from the Crosetto mine, which shows absorption bands at 3356, 3457, 3490 and  $3545 \text{ cm}^{-1}$  (Chukanov, 2014).

# 4. Discussion

#### 4.1. Crystal-chemical aspects

The refined total composition for ulfanderssonite-(Ce) based on the single-crystal XRD data (Table 4) is Ce<sub>15.00</sub>Ca<sub>1.00</sub>Mg<sub>1.87</sub>Fe<sub>0.13</sub>Si<sub>11</sub>O<sub>43</sub>(OH,F)<sub>6</sub>Cl<sub>3</sub>. Compared to the empirical formula obtained from the EMP data (Table 1), it is clear that the Fe content is slightly higher. This can be explained by some chemical heterogeneity in the sample (laser ablation ICP-MS analysis of different portions of ulfanderssonite-(Ce) showed up to 0.2 wt% FeO) or that a fraction of some other heavy scattering species occurs at the Mg2 site. Of the metals occurring in elevated amounts in the Bastnäs-type deposits, only W was found above the trace level, 3104 ppm (Table 1), in ulfanderssonite-(Ce). Overall, the mean electron number calculated from the X-ray formula, 1062  $e^{-}$ , is in very good agreement with that obtained from EMP data, 1070  $e^{-}$ . We have no specific explanation for the relatively low totals of the chemical analyses (Table 1), although partial sample degradation under the electron beam was observed.

Chondrite-normalized *REE* data (Fig. 6) for ulfanderssonite-(Ce) indicate a good capability of the mineral to host the middle *REE*, relative to västmanlandite-(Ce), and



Fig. 3. The ulfanderssonite-(Ce) crystal structure viewed along the monoclinic *b*-axis. The SiO<sub>4</sub> tetrahedra and MgO<sub>6</sub> octahedra are depicted in blue and green, respectively. The (*REE*,Ca), Cl and O atoms are drawn as yellow, orange and red spheres, respectively. The structure can be simply described as a regular alternation of two kinds of layers along the *c*-axis: a first layer (labelled *A*), ~9.0 Å thick, with general composition  $[(Ce_8Ca)_{\Sigma9}MgSi_7O_{22}(OH,F)_4]^{8+}$ , and a second layer (labelled *B*), ~6.5 Å thick, with general composition  $[Ce_7MgSi_4O_{21} (OH,F)_2Cl_3]^{8-}$ . (Online version in colour.)

the pattern is very similar to that of coexisting fluorbritholite-(Ce). The relative enrichment of Nd, Sm and Gd in particular is probably related both to crystalchemical factors (a similar behaviour is consistently observed for cerite-(Ce); Holtstam & Andersson, 2007) and the geochemical character of the Malmkärra deposit (Holtstam *et al.*, 2014). Although the Ca contents are low compared to *REE*, and the Ca atoms are distributed over several *REE*-dominated sites, this element is essential to the structure to keep overall electro-neutrality.

Alongside the minor variations in cation composition, there is some evidence for minor F–OH exchange in the ulfanderssonite-(Ce) structure as well. The F–Cl or Cl–OH exchange is probably limited. This is related to differences in ionic size, Cl<sup>–</sup> is large (radius 1.81 Å; Shannon, 1976) relative to OH<sup>–</sup> (1.38 Å) and F<sup>–</sup> (1.31 Å).

# 4.2. Formation of the mineral

Cerite-(Ce) and fluorbritholite-(Ce) are, according to textural observations and mass balance calculations (Holtstam & Andersson, 2007), considered to be primary *REE* minerals in the Bastnäs-type deposits, formed from acidic *REE*- and Si-rich aqueous fluids reacting with preexisting carbonate (dolomitic) rock. A similar opensystem mechanism of formation can be envisaged for ulfanderssonite-(Ce), abbreviated as Ulf in the formulae below [for simplicity, ideal composition of reactants and products is assumed, and ion complexes of *REE* are given as  $Ce^{3+}(aq)$  nominally]:

$$15Ce^{3+} + 11SiO_4^{4-} + 2F^- + 3Cl^- + 6H^+ + 2CaMg(CO_3)_2(s) \rightarrow Ulf(s) + Ca^{2+} + 4CO_2 + H_2O.$$
dolomite
(1)

Following this, västmanlandite-(Ce) and the minor magnetite formed from a Fe-rich solution (*cf.* Holtstam & Andersson, 2007), partly at the expense of ulfandersson-ite-(Ce).

At some stage, presumably at lower temperatures and higher pH, destabilization and partial alteration of ulfanderssonite-(Ce) occurred via a replacement reaction,



Fig. 4. The B layer of the ulfanderssonite-(Ce) crystal structure viewed along the c-axis. Symbols as in Fig. 3. (Online version in colour.)

involving an F- and CO<sub>2</sub>-rich fluid, of the type:

where the molar volume difference between the solid phases is less than 4%.

# 4.3. The role of chlorine

The Cl-contents for most *REE* minerals in the Bastnästype deposits are generally low with exceptionally up to a maximum of 0.3 wt% for fluorbritholite-(Ce) from Malmkärra (Holtstam & Andersson, 2007). Analyses of västmanlandite-(Ce) and fluorbritholite-(Ce) (as an inclusion in ulfanderssonite-(Ce)) in the holotype specimen yielded very little Cl (0–0.05 wt%), even though fluorbritholite-(Ce) has the crystallochemically very flexible apatite structure. In other potential hosts from these deposits, such as tremolite, Cl is close to or below the detection limit (0.01–0.1 wt%).

These results are somewhat unexpected in the light of modern research results that indicate that  $Cl^-$  is the most effective transporting ligand of  $REE^{3+}$  in hydrothermal

solutions (Migdisov & Williams-Jones, 2014; Migdisov *et al.*, 2016). This is probably also true for the genesis of Bastnäs-type deposits, although anion complexes of  $F^-$  and  $(SiO_4)^{4-}$  also likely played a role (Holtstam *et al.*, 2014). The relatively high Cl concentration in fluid inclusions of bastnäsite from some of the localities, corresponding to 6–29 wt% CaCl<sub>2</sub> equivalent (Holtstam *et al.*, 2014), is direct evidence for a high chloride activity in the mineral-forming fluids. Moderately saline fluid inclusions also occur in fluorite and tremolite associated with *REE* mineral assemblages (Holtstam *et al.*, 2014).

It is somewhat enigmatic why ulfanderssonite-(Ce) is relatively rare in this environment, because the essential components seem to be ubiquitous in the fluid–rock system. It is actually the presence of Cl<sup>-</sup> that allows ulfanderssonite-(Ce) to form, instead of more common components of the *REE*-rich skarn assemblages, in the Bastnäs-type deposits. It is the only silicate mineral containing essential *REE*, Mg and Cl, hitherto globally known. Minerals combining *REE* and Cl are very rare at all (and mostly belonging to alkaline and agpaitic systems), compared to the number of existing *REE*-F compounds in nature. From inspection of reaction (1) above it becomes clear that the relative activity ratio HCl/HF in the reacting fluid is crucial, and it is largely controlled by three factors

Si6 Si7 20	$\begin{array}{c} 1.96\\ 2.17\\ 2.16\\ 1.03\\ 1.72\\ 1.10\\ 1.10\\ 2.25\\ 2.17\\ 1.10\\ 2.25\\ 2.17\\ 1.12\\ 2.26\\ 1.94\\ 1.17\\ 0.26\\ 1.81\\ 1.17\\ 0.98\\ 2.17\\ 0.98\\ 1.93\\ 0.98\\ 1.93\\ 2.01\\ 1.14\\ 1.16\\ 2.08\\ 1.02\\ 2.18\\ 1.06\\ 1.12\\ 2.18\\ 1.02\\$	orizontally and
Si5	4.22	a factor 2 h
Si2 Si3 Si4	$\begin{array}{c} 1.11 \\ 1.10 \\ 1.04 \\ 1.06 \\ 1.06 \\ 1.06 \\ 1.05 \\ 1.05 \\ 0.98 \\ 0.99 \\ 0.99 \\ 0.99 \\ 1.05 \\ 1.$	ust be multiplied by
Sil	0.83 1.03 ×1 1.03 ×1 3.96	e value m
Mg2	24 0.34 × 0.33 × 0.37 0.37 0.32 2.03	an that th
Mg1	21 0.36 0.35 × 0.32 × 0.36 0.36	and ↓ me
Ce11	0.13 × 0.51 × 0.51 × 0.51 × 0.51 × 0.51 × 0.051 × 0.051 × 0.013 × 0.01	mbols →
Ce10	$\begin{array}{c} 0.41 \\ 0.45 \\ 0.51 \\ 2 \\ 0.26 \\ 0.36 \\ 0.36 \\ 3.39 \end{array}$	4. The sy
Ce9	0.46 0.44 ×2 0.44 ×2 0.16 ×2 0.45 ×2 0.30 3.25	ı in Table
Ce8	$\begin{array}{c} 0.42\\ 0.42\\ 0.36\\ 0.36\\ 0.36\\ 0.38\\ 2.88\\ 2.88\\ 2.88\end{array}$	ctors giver
Ce7	→ 0.18 0.37 0.38 0.38 0.34 0.49 0.38 0.49 0.49 0.49 0.49 0.40 0.42 0.40 0.42 0.40 0.42 0.26 3.15	cupancy fa
Ce6	$\begin{array}{c} 10.13 \\ 0.47 \\ 0.13 \\ -2.43 \\ 0.15 \\ -2.47 \\ 0.07 \\ -2.47 \\ 2.47 \end{array}$	he site-occ
Ce5	0.29 × 0.29 × 0.39 × 0.30 × 0.30 × 0.30 × 0.30 0.30 × 0.30 2.37	ted with t
Ce4	24 0.53 × 0.53 × 0.24 × 0.42 × 2.83	ere calcula
Ce3	0.20 × 0.36 × 0.48 0.48 0.35 × 2.78	e sums we
Ce2	$\begin{array}{c} 0.43 \\ 0.46 \\ 0.46 \\ 0.21 \\ 0.21 \\ 0.238 \\ 0.38 \\ 0.38 \\ 0.38 \\ 2.92 \\ 0.38 \\ 2.92 \end{array}$	nd valence
Ce1	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	<i>Note</i> : The bo

vertically, respectively.

Table 6. Bond-valence sums for the structure of ulfanderssonite-(Ce).



Fig. 5. Room-temperature single-crystal FTIR spectrum (red line) of ulfanderssonite-(Ce). Absorption bands due to Si–O fundamental modes in the range  $800-1050 \text{ cm}^{-1}$  are truncated due to excessive absorption caused by their high absorption coefficients. Results of spectrum deconvolution in the range  $2000-3800 \text{ cm}^{-1}$  are shown by fitted bands (thin black lines) and resulting total absorption (thin blue line). A low-amplitude pattern clearly visible below *ca.*  $2100 \text{ cm}^{-1}$  is due to interference effects caused by perfectly polished parallel surfaces of the thin absorber. (Online version in colour.)



Fig. 6. Normalized *REE* patterns for coexisting minerals in the type specimen, using the chondrite abundance-values of Boynton (1984). Elemental analyses are from Table 1 and from EMP analyses of the coexisting minerals (Holtstam & Andersson, 2007).

(*cf.* Zhu & Sverjensky, 1991): temperature, pH and pressure (*i.e.*, if boiling conditions are attained or not) of the hydrothermal fluid.

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