



## Article

# Rundqvistite-(Ce), $\text{Na}_3(\text{Sr}_3\text{Ce})(\text{Zn}_2\text{Si}_8\text{O}_{24})$ , a new mineral from the Darai-Pioz alkaline massif, Tien-Shan Mountains, Tajikistan: mineral description and crystal structure

Atali A. Agakhanov<sup>1</sup>, Maxwell C. Day<sup>2</sup>, Elena Sokolova<sup>3</sup>, Vladimir Yu. Karpenko<sup>1</sup>, Frank C. Hawthorne<sup>3</sup> , Leonid A. Pautov<sup>1,4</sup>, Anatoly V. Kasatkin<sup>1</sup> , Igor V. Pekov<sup>5</sup> and Vitaliya A. Agakhanova<sup>6</sup>

<sup>1</sup>Fersman Mineralogical Museum, Russian Academy of Sciences, Leninskyi Prospekt 18/2, 119071, Moscow, Russia; <sup>2</sup>Dipartimento di Geoscienze, Università degli Studi di Padova, Via Gradenigo 6, I-35131, Padova, Italy; <sup>3</sup>Department of Earth Sciences, University of Manitoba, Winnipeg, Manitoba, R3T 2N2, Canada; <sup>4</sup>South Urals Federal Research Center of Mineralogy and Geoecology UB RAS, 456317, Miass, Russia; <sup>5</sup>Faculty of Geology, Moscow State University, Vorobievsky Gory, 119991, Moscow, Russia; and <sup>6</sup>FSBI All-Russian Research Geological Oil Institute, Enthusiasts Highway 36, 105118, Moscow, Russia

### Abstract

Rundqvistite-(Ce), ideally  $\text{Na}_3(\text{Sr}_3\text{Ce})(\text{Zn}_2\text{Si}_8\text{O}_{24})$ , is a new mineral from the Darai-Pioz alkaline massif, Tien-Shan Mountains, Tajikistan. The mineral occurs as elongated grains up to 0.1 mm long and up to 0.03 mm thick embedded in quartz–pectolite aggregate in a silexite-like peralkaline pegmatite. Associated minerals are quartz, fluorite, pectolite, baratovite, aegirine, leucosphenite, neptunite, reedmergerite, orlovite, sokolovaite, mendeleevite-(Ce), odigitriaite, pekovite, zeravshanite, kirchhoffite and garmite. The mineral is colourless with a vitreous lustre and a white streak, brittle,  $D_{\text{meas.}}$  is 3.70(2) and  $D_{\text{calc.}}$  is 3.709 g/cm<sup>3</sup>. Rundqvistite-(Ce) is monoclinic, space group  $P2_1/c$ ,  $a = 5.1934(16)$ ,  $b = 7.8934(16)$ ,  $c = 26.011(5)$  Å,  $\beta = 90.02(3)^\circ$  and  $V = 1066.3(4)$  Å<sup>3</sup>. The chemical composition of rundqvistite-(Ce) is SiO<sub>2</sub> 40.17, La<sub>2</sub>O<sub>3</sub> 2.64, Ce<sub>2</sub>O<sub>3</sub> 7.55, Pr<sub>2</sub>O<sub>3</sub> 0.80, Nd<sub>2</sub>O<sub>3</sub> 2.43, Sm<sub>2</sub>O<sub>3</sub> 0.33, Eu<sub>2</sub>O<sub>3</sub> 0.09, Gd<sub>2</sub>O<sub>3</sub> 0.24, Tb<sub>2</sub>O<sub>3</sub> 0.18, Dy<sub>2</sub>O<sub>3</sub> 0.21, PbO 1.03, SrO 19.83, FeO 0.37, ZnO 13.08, CaO 2.55, Na<sub>2</sub>O 8.04, total 99.54 wt.%. The empirical formula calculated on 24 O apfu (atoms per formula unit) is  $\text{Na}_{3.10}\text{Sr}_{2.29}\text{Ca}_{0.54}\text{Pb}_{0.06}(\text{Ce}_{0.55}\text{La}_{0.19}\text{Nd}_{0.17}\text{Pr}_{0.06}\text{Sm}_{0.02}\text{Gd}_{0.02}\text{Eu}_{0.01}\text{Tb}_{0.01}\text{Dy}_{0.01})_{\Sigma 1.04}\text{Zn}_{1.92}\text{Fe}_{0.06}\text{Si}_{8.00}\text{O}_{24}$   $Z = 2$ . The structural formula based on refined site-occupancies is  $(\text{Na}_{2.94}\text{Sr}_{0.06})_{\Sigma 3.00}[(\text{Sr}_{2.23}\text{Ca}_{0.54}\text{Pb}_{0.06}\text{Na}_{0.13})_{\Sigma 2.96}\text{Ln}_{1.04}^{3+}]_{\Sigma 4.00}[(\text{Zn}_{1.92}\text{Fe}_{0.06})_{\Sigma 1.98}\text{Si}_8\text{O}_{24}]$ , where  $\text{Ln}_{1.04}^{3+} = (\text{Ce}_{0.55}\text{La}_{0.19}\text{Nd}_{0.17}\text{Pr}_{0.06}\text{Sm}_{0.02}\text{Gd}_{0.02}\text{Eu}_{0.01}\text{Tb}_{0.01}\text{Dy}_{0.01})_{\Sigma 1.04}$ . The crystal structure of rundqvistite-(Ce) was refined to  $R_1 = 2.76\%$  on the basis of 3184 unique reflections [ $F > 4\sigma(F)$ ]. In rundqvistite-(Ce), the main structural unit is a  $(\text{Zn}_2\text{Si}_8\text{O}_{24})^{12-}$  sheet parallel to (100). In the sheet, the Si and Zn tetrahedra form four-, five- and eight-membered rings. The interstitial cations at the Na and M(1–3) sites sum to  $[\text{Na}_3(\text{Sr}_3\text{Ce})]^{12-}$  apfu. The Na and M(1–3) polyhedra share common edges to form a layer. Rundqvistite-(Ce) is a structural analogue of vladkyinite, ideally  $\text{Na}_3\text{Sr}_4(\text{Fe}^{2+}\text{Fe}^{3+})\text{Si}_8\text{O}_{24}$ . Rundqvistite-(Ce) and vladkyinite are related by the following substitution:  $^{[8]}\text{Ce}^{3+} + ^{[4]}\text{Zn}^{2+} \leftrightarrow ^{[8]}\text{Sr}^{2+} + ^{[4]}\text{Fe}^{2+}\text{Fe}^{3+}$ . The mineral is named after Dmitry Vasilievich Rundqvist (1930–2022), a prominent Russian geologist and an expert on the geology of ore deposits, metallogeny and mineralogy of Precambrian rocks.

**Keywords:** rundqvistite-(Ce); new mineral; Darai-Pioz alkaline massif; Tien-Shan; Tajikistan; electron-microprobe analysis; vladkyinite; crystal structure; tetrahedral  $(\text{Zn}_2\text{Si}_8\text{O}_{24})$  sheet

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### Introduction

This paper reports the description and the crystal structure of rundqvistite-(Ce) [Russian Cyrillic: рундквистит-(Ce)], ideally  $\text{Na}_3(\text{Sr}_3\text{Ce})(\text{Zn}_2\text{Si}_8\text{O}_{24})$ , a new mineral from the Darai-Pioz alkaline massif, Tien-Shan Mountains, Central Tajikistan. Rundqvistite-(Ce) is a sheet zinco-silicate mineral. The mineral is named for Professor Dmitry Vasilievich Rundqvist (Russian Cyrillic: Дмитрий Васильевич Рундквист) (10.08.1930–15.01.2022), Academician of the Russian Academy of Sciences, a

prominent geologist and an expert on the geology of ore deposits, metallogeny and mineralogy of Precambrian rocks. In accord with Bayliss and Levinson (1988), the mineral is named rundqvistite-(Ce) as Ce is the dominant rare earth element.

The new mineral and its name (symbol Run-Ce) have been approved by the Commission on New Minerals, Nomenclature and Classification of the International Mineralogical Association (IMA2023–043, Agakhanov *et al.*, 2023). The holotype material is deposited in the systematic collection of the Fersman Mineralogical Museum of the Russian Academy of Sciences, Moscow, Russia, registration number 5999/1.

### Occurrence and associated minerals

Rundqvistite-(Ce) was found in the moraine of the Darai-Pioz glacier in the upper reaches of the Darai-Pioz River, Tien-Shan

**Corresponding author:** Elena Sokolova; Email: [Elena.sokolova@umanitoba.ca](mailto:Elena.sokolova@umanitoba.ca)

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mountains, near the junction of the Turkestan, Zeravshansky and Alaisky ranges (39°27'N 70°43'E). This area is in the Rasht (formerly Garm) district, Central Tajikistan. The alkaline Darai-Pioz massif belongs to the Upper Paleozoic Alaisky (Matchaisky) intrusive complex. Information on the geology of the Darai-Pioz massif can be found in Pautov *et al.* (2019, 2023) with reference to relevant earlier publications, and the genesis of these rocks was discussed by Pautov *et al.* (2022).

Rundqvistite-(Ce) was found in quartz–pectolite aggregate in a silexite-like peralkaline pegmatite. The following minor and accessory minerals are present: black crystals of aegirine, orange–brown semi-transparent lentic-like crystals of stillwellite-(Ce), aggregates of large white grains of microcline, large (up to 10 cm across) golden-brown tabular and lamellar crystals of polyolithionite, pink plates of sogdianite–sugilite, pale-yellow to orange aggregates and tabular crystals of reedmergnerite, grass-green or yellowish-green semi-transparent and transparent crystals of leucosphenite, and dark-green crystals of turkestanite. Rundqvistite-(Ce) occurs in fine-grained brown or greyish-brown aggregates of Mn-bearing pectolite, quartz, Sr-bearing fluorite, aegirine and a variety of rare minerals: baratovite, neptunite, orlovite, sokolovaita, mendeleevite-(Ce), odigitriaite, pekovite, zeravshanite, kirchhoffite and garnite.

### Physical properties

Rundqvistite-(Ce) occurs as elongated grains up to 0.1 mm long and up to 0.03 mm thick embedded in quartz–pectolite aggregate (Fig. 1). The mineral is transparent, colourless and has a white streak and a vitreous lustre. Rundqvistite-(Ce) does not fluoresce under cathode rays or ultraviolet light. The mineral is brittle, the fracture is uneven; no cleavage or parting were observed. The average micro-indentation hardness is  $VHN_{50} = 612$  (with range of 572–653). Measurements were done on the PMT-3 instrument, calibrated on NaCl at a loading of 50 g. Although micro-indentation and Mohs hardness are different hardness measurements (Broz *et al.*, 2006), the first representing the resistance to indentation and the second the resistance to scratching, the

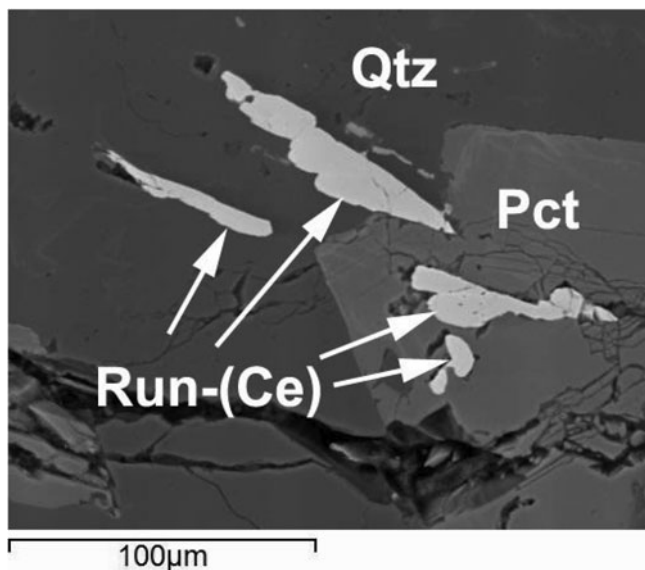
present value of micro-indentation hardness roughly corresponds to a Mohs hardness of  $\sim 5$ . The measured density by flotation in Clerici solution is  $3.70(2) \text{ g/cm}^3$ . The calculated density is  $3.709 \text{ g/cm}^3$ .

Rundqvistite-(Ce) is optically biaxial (–) with refractive indices ( $\lambda = 590 \text{ nm}$ )  $\alpha = 1.644(2)$ ,  $\beta = 1.659(2)$  and  $\gamma = 1.662(2)$ ;  $2V_{\text{calc.}} = 48^\circ$ . It is non-pleochroic. Dispersion is medium:  $r < v$ . The compatibility indices  $(1 - Kp/Kc) = 0.000$  (for  $D_{\text{meas.}}$ ) and  $0.002$  (for  $D_{\text{calc.}}$ ) are rated as superior (Mandarino, 1981).

### Chemical composition

The chemical composition of rundqvistite-(Ce) was determined using a JEOL Superprobe JCXA-733 electron microprobe with energy dispersive spectroscopy (EDS) (using an ultrathin ATW2 window and an INCA control system, Fersman Mineralogical Museum). Measurements were done using EDS with an accelerating voltage of 20 kV, a probe current of 2 nA and a beam diameter of 3  $\mu\text{m}$ . To avoid damage of the very thin (0.014 mm) rundqvistite-(Ce) flakes under the electron beam, we chose EDS as a less destructive method of chemical analysis due to the lower current (when compared to wavelength dispersive spectroscopy). The following standards were used: microcline USNM 143966 (Si), albite 107 (Na), SrTiO<sub>3</sub> (Sr), PbTiO<sub>3</sub> (Pb), ilmenite USNM 96189 (Fe), anorthite USNM 137041 (Ca), ZnS (Zn), LaPO<sub>4</sub> (La), CePO<sub>4</sub> (Ce), PrPO<sub>4</sub> (Pr), NdPO<sub>4</sub> (Nd), SmPO<sub>4</sub> (Sm), EuPO<sub>4</sub> (Eu), GdPO<sub>4</sub> (Gd), TbPO<sub>4</sub> (Tb) and DyPO<sub>4</sub> (Dy). Contents of other elements with atomic numbers > 8 are below the detection limits.

The data (10 point analyses) were reduced and corrected by the PAP method of Pouchou and Pichoir (1985). The chemical composition of rundqvistite-(Ce) is the mean of 10 determinations and is given in Table 1. The empirical formula calculated on 24 O apfu is  $\text{Na}_{3.10}\text{Sr}_{2.29}\text{Ca}_{0.54}\text{Pb}_{0.06}(\text{Ce}_{0.55}\text{La}_{0.19}\text{Nd}_{0.17}\text{Pr}_{0.06}\text{Sm}_{0.02}\text{Gd}_{0.02}\text{Eu}_{0.01}\text{Tb}_{0.01}\text{Dy}_{0.01})_{\Sigma 1.04}\text{Zn}_{1.92}\text{Fe}_{0.06}\text{Si}_{8.00}\text{O}_{24}$   $Z = 2$ . The structural formula based on refined site-occupancies (see below) is  $(\text{Na}_{2.94}\text{Sr}_{0.06})_{\Sigma 3.00}[(\text{Sr}_{2.23}\text{Ca}_{0.54}\text{Pb}_{0.06}\text{Na}_{0.13})_{\Sigma 2.96}\text{Ln}^{3+}]_{\Sigma 4.00}[(\text{Zn}_{1.92}\text{Fe}_{0.06})_{\Sigma 1.98}\text{Si}_8\text{O}_{24}]$ , where  $\text{Ln}^{3+}_{1.04} = (\text{Ce}_{0.55}\text{La}_{0.19}\text{Nd}_{0.17}\text{Pr}_{0.06}\text{Sm}_{0.02}\text{Gd}_{0.02}\text{Eu}_{0.01}\text{Tb}_{0.01}\text{Dy}_{0.01})_{\Sigma 1.04}$ . The simplified formula is  $(\text{Na},\text{Sr})_3(\text{Sr},\text{Ln}^{3+},\text{Ca})_4[(\text{Zn},\text{Fe})_2\text{Si}_8\text{O}_{24}]$  where Ce is the dominant lanthanoid ( $\text{Ln}^{3+}$ ). The ideal formula of rundqvistite-(Ce),  $\text{Na}_3(\text{Sr}_3\text{Ce})(\text{Zn}_2\text{Si}_8\text{O}_{24})$ , requires (wt.%): Na<sub>2</sub>O 7.68, SrO 25.66, Ce<sub>2</sub>O<sub>3</sub> 13.55, ZnO 13.44, SiO<sub>2</sub> 39.67, total 100.



**Figure 1.** Back-scattered electron image of a polished section of rundqvistite-(Ce) [Run-(Ce)] in association with pectolite [Pct] and quartz [Qtz].

**Table 1.** Chemical composition and unit formula\* for rundqvistite-(Ce).

Oxide	wt.%	Range		apfu
SiO <sub>2</sub>	40.17	39.67–40.71	Si	8.00
La <sub>2</sub> O <sub>3</sub>	2.64	1.15–4.15	La	0.19
Ce <sub>2</sub> O <sub>3</sub>	7.55	6.94–8.37	Ce	0.55
Pr <sub>2</sub> O <sub>3</sub>	0.80	0.32–1.15	Pr	0.06
Nd <sub>2</sub> O <sub>3</sub>	2.43	1.97–2.84	Nd	0.17
Sm <sub>2</sub> O <sub>3</sub>	0.33	0.00–0.74	Sm	0.02
Eu <sub>2</sub> O <sub>3</sub>	0.09	0.00–0.47	Eu	0.01
Gd <sub>2</sub> O <sub>3</sub>	0.24	0.00–0.58	Gd	0.02
Tb <sub>2</sub> O <sub>3</sub>	0.18	0.00–0.52	Tb	0.01
Dy <sub>2</sub> O <sub>3</sub>	0.21	0.00–0.70	Dy	0.01
PbO	1.03	0.19–1.11	Pb	0.06
SrO	19.83	18.73–21.66	Sr	2.29
FeO	0.37	0.01–0.54	Fe	0.06
ZnO	13.08	12.70–13.77	Zn	1.92
CaO	2.53	1.51–3.03	Ca	0.54
Na <sub>2</sub> O	8.04	7.41–8.43	Na	3.10
Total	99.54			

\*The empirical formula was calculated on 24 O apfu.

### Powder X-ray diffraction

Powder X-ray diffraction data were obtained using an RKU-86 camera, CrK $\alpha$  radiation and a V-filter (Table 2). Unit-cell parameters calculated from the powder-diffraction data are  $a = 5.196(1)$ ,  $b = 7.889(2)$ ,  $c = 26.012(9)$  Å,  $\beta = 90.04(4)^\circ$  and  $V = 1066.3(4)$  Å<sup>3</sup>.

### X-ray single-crystal data collection and structure refinement

X-ray single-crystal data for rundqvistite-(Ce) were collected from a twinned crystal with a Bruker APEX II ULTRA three-circle diffractometer with a rotating-anode generator (MoK $\alpha$ ), multilayer optics and an APEX II 4K CCD detector. The crystal of rundqvistite-(Ce) used for single-crystal X-ray diffraction measures  $0.014 \times 0.022 \times 0.034$  mm. The intensities of reflections with  $-7 \leq h \leq 7$ ,  $-11 \leq k \leq 11$  and  $-37 \leq l \leq 37$  were collected with a frame width of  $0.3^\circ$  and frame time of 26 s up to  $2\theta \leq 61.99^\circ$ , and an empirical absorption correction (SADABS, Sheldrick, 2015) was applied. The crystal structure was refined to  $R_1 = 2.76\%$  in space group  $P2_1/c$  using atom coordinates of vladkyinite, Na<sub>3</sub>Sr<sub>4</sub>(Fe<sup>2+</sup>Fe<sup>3+</sup>)Si<sub>8</sub>O<sub>24</sub> (Chakhmouradian et al., 2014), on the basis of 3184 unique reflections [ $F > 4\sigma(F)$ ] with the Bruker SHELXTL Version 2014/3 software (Sheldrick, 2015). The structure was refined as two components related by the

TWIN matrix  $(-1 \ 0 \ 0, 0 \ 1 \ 0, 0 \ 0 \ 1)$ ; the twin ratio being  $0.5153(12) : 0.4847(12)$ . Details of data collection and structure refinement are given in Table 3. The occupancies of five cation sites were refined with the following scattering curves: Na and M1 sites: Na; M(2,3) sites: Sr; and the T site: Zn. Refinement of the Na site-occupancy converged to an integer value (within 3 e.s.d.) and was subsequently fixed at full occupancy. Scattering curves for neutral atoms were taken from the *International Tables for Crystallography* (Wilson, 1992). Final atom coordinates and anisotropic displacement parameters are given in Table 4, selected interatomic distances and angles in Table 5, refined site-scattering values and assigned site-populations in Table 6 and bond-valence values in Table 7. A list of observed and calculated structure factors and a crystallography information file (cif) have been deposited with the Principal Editor of *Mineralogical Magazine* and are available as Supplementary Material (see below).

### Site-population assignment

Silicon was assigned to four tetrahedrally coordinated Si sites, with  $\langle\langle\text{Si-O}\rangle\rangle = 1.632$  Å (Tables 4, 5). In accord with the refined site-scattering of 58.4 epfu (electrons per formula unit), all available Zn and Fe<sup>2+</sup> (Table 1) were assigned to the T site, with  $\langle\text{T-O}\rangle = 1.953$  Å (Tables 4–6). In accord with the structure-refinement results (see above), the Na site is occupied solely by

**Table 2.** Powder X-ray diffraction data for rundqvistite-(Ce).

<i>l</i>	<i>d</i> <sub>meas.</sub> (Å)	<i>d</i> <sub>calc.</sub> (Å)	<i>h</i>	<i>k</i>	<i>l</i>	<i>l</i>	<i>d</i> <sub>meas.</sub> (Å)	<i>d</i> <sub>calc.</sub> (Å)	<i>h</i>	<i>k</i>	<i>l</i>	<i>l</i>	<i>d</i> <sub>meas.</sub> (Å)	<i>d</i> <sub>calc.</sub> (Å)	<i>h</i>	<i>k</i>	<i>l</i>
10	7.57	7.553	0	1	$\bar{1}$	10	2.469	2.467	2	1	0	6	1.742	1.742	1	3	10
2	6.75	6.748	0	1	$\bar{2}$	15	2.439	2.439	0	3	$\bar{4}$	3	1.736	1.735	2	2	9
3	5.84	5.837	0	1	$\bar{3}$				0	3	4	4	1.693	1.694	0	1	$\bar{15}$
5	5.21	5.193	1	0	0	3	2.406	2.406	1	1	9		1.691	1.691	3	1	0
10	5.03	5.019	0	1	$\bar{4}$			2.405	1	1	9	6	1.678	1.677	3	1	2
6	4.83	4.823	1	0	2	5	2.397	2.399	1	2	7	3	1.671	1.673	3	0	4
<b>50</b>	<b>4.28</b>	4.280	1	1	$\bar{1}$	4	2.344	2.347	1	3	0				0	3	$\bar{12}$
		4.279	1	1	1	5	2.330	2.332	0	2	$\bar{9}$	3	1.665	1.666	2	2	10
3	4.11	4.116	1	1	$\bar{2}$			2.326	1	0	$\bar{10}$				1	3	11
		4.115	1	1	2			2.325	1	0	10	2	1.659	1.660	3	1	3
6	4.05	4.057	1	0	4	4	2.308	2.310	1	3	2				3	1	$\bar{3}$
3	3.95	3.947	0	2	0			2.307	2	1	$\bar{4}$	4	1.638	1.637	3	1	$\bar{4}$
3	3.89	3.880	1	1	$\bar{3}$			2.306	2	1	4			1.636	3	1	4
			1	1	3	2	2.128	2.127	1	2	9	3	1.628	1.629	2	1	$\bar{12}$
<b>33</b>	<b>3.616</b>	3.609	1	1	$\bar{4}$				1	2	$\bar{9}$			1.628	2	1	12
			1	1	4	5	2.103	2.104	2	2	3	5	1.604	1.604	1	4	8
<b>60</b>	<b>3.598</b>	3.592	0	2	$\bar{3}$	6	2.058	2.058	2	2	$\bar{4}$	5	1.593	1.593	0	3	$\bar{13}$
<b>42</b>	<b>3.336</b>	3.332	1	1	$\bar{5}$				2	2	4				1	3	$\bar{12}$
			1	1	5			2.055	2	1	7			1.592	1	3	12
		3.329	1	0	6	5	2.043	2.045	0	3	$\bar{8}$	6	1.583	1.582	3	2	1
		3.328	1	0	$\bar{6}$	3	2.026	2.028	2	0	8				3	2	$\bar{1}$
15	3.250	3.251	0	0	$\bar{8}$	3	1.971	1.973	0	4	0	4	1.555	1.555	1	4	9
<b>46</b>	<b>3.140</b>	3.144	0	2	$\bar{5}$	2	1.944	1.946	0	3	$\bar{9}$				1	4	$\bar{9}$
		3.142	1	2	0	2	1.938	1.939	1	1	$\bar{12}$	3	1.540	1.540	3	2	4
<b>100</b>	<b>2.952</b>	2.954	1	2	$\bar{3}$				1	1	12				3	2	$\bar{4}$
			1	2	3	3	1.922	1.924	0	4	$\bar{3}$	3	1.507	1.508	1	5	1
14	2.918	2.918	0	2	$\bar{6}$	3	1.893	1.890	1	2	$\bar{11}$			1.507	2	3	$\bar{10}$
<b>80</b>	<b>2.830</b>	2.830	1	2	$\bar{4}$			1.889	1	2	11			1.506	2	3	10
		2.829	1	2	4	4	1.856	1.858	0	0	$\bar{14}$	3	1.436	1.437	3	3	$\bar{2}$
<b>60</b>	<b>2.821</b>	2.823	1	1	$\bar{7}$	6	1.849	1.850	0	3	$\bar{10}$				3	3	2
		2.822	1	1	7			1.848	2	3	0	3	1.414	1.415	2	4	$\bar{8}$
17	2.706	2.705	0	2	$\bar{7}$	4	1.843	1.844	2	3	1				2	4	8
<b>23</b>	<b>2.593</b>	2.597	2	0	0	3	1.817	1.817	1	1	$\bar{13}$						
5	2.545	2.546	2	0	2	13	1.794	1.796	0	4	$\bar{6}$						
		2.545	1	2	$\bar{6}$	10	1.778	1.778	2	3	4						
		2.440	1	2	6	4	1.760	1.759	0	3	$\bar{11}$						

**Table 3.** Miscellaneous refinement data for rundqvistite-(Ce).

<b>Crystal data</b>	
<i>a</i> (Å)	5.1934(10)
<i>b</i>	7.8934(15)
<i>c</i>	26.011(5)
β (°)	90.02(3)
<i>V</i> (Å <sup>3</sup> )	1066.3(4)
Space group	<i>P</i> 2 <sub>1</sub> / <i>c</i>
<i>Z</i>	2
<b>Data collection</b>	
Reflections ( <i>I</i> > 10σ <i>I</i> )	9915
Absorption coefficient (mm <sup>-1</sup> )	11.37
<i>F</i> (000)	1121.9
<i>D</i> <sub>calc.</sub> (g/cm <sup>3</sup> )	3.709
Crystal size (mm)	0.014 × 0.022 × 0.034
Radiation/monochromator	MoKα/graphite
2θ-range (°)	61.99
Ratio of twin components*	0.5153(12): 0.4847(12)
<i>h</i>	-7 ≤ <i>h</i> ≤ 7
<i>k</i>	-11 ≤ <i>k</i> ≤ 11
<i>l</i>	-37 ≤ <i>l</i> ≤ 37
<i>R</i> (int) (%)	2.74
<i>R</i> (σ) (%)	2.08
Reflections collected	13543
Independent reflections	3403
<i>F</i> <sub>o</sub> > 4σ <i>F</i>	3184
<b>Refinement</b>	
Refinement method	Full-matrix least squares on <i>F</i> <sup>2</sup> , fixed weights proportional to 1/σ <i>F</i> <sup>2</sup>
Final <i>R</i> (obs) (%)	2.76
<i>F</i> <sub>o</sub> > 4σ <i>F</i>	3.13
<i>R</i> <sub>1</sub>	6.25
<i>wR</i> <sub>2</sub>	1.51, -1.50
Highest peak, deepest hole (e <sup>-</sup> Å <sup>-3</sup> )	1.080
Goodness of fit on <i>F</i> <sup>2</sup>	

\*Twin components are related by the transformation matrix (-100, 010, 001)

Na. The *M*1 site has a slightly higher refined site-occupancy and slightly longer mean bond-length: 23.62 epfu and 2.522 Å, (*i.e.* 11.81 epfu per one atom) than the *Na* site: 11.00 epfu and 2.447 Å. Hence we assign Na<sub>1.94</sub>Sr<sub>0.06</sub> apfu to the *M*1 site (Tables 4–6). Based on the refined site-scattering values and

observed bond-distances, we assign (Sr<sub>1.07</sub>Ca<sub>0.26</sub>Na<sub>0.04</sub>Pb<sub>0.02</sub>)Σ<sub>1.39</sub>Ln<sub>0.61</sub><sup>3+</sup> and (Sr<sub>1.16</sub>Ca<sub>0.28</sub>Na<sub>0.09</sub>Pb<sub>0.04</sub>)Σ<sub>1.57</sub>Ln<sub>0.43</sub><sup>3+</sup> apfu to the *M*2 and *M*3 sites, respectively (Tables 4–6). Sum of Ln<sub>0.61</sub><sup>3+</sup> and Ln<sub>0.43</sub><sup>3+</sup> apfu equals Ln<sub>1.04</sub><sup>3+</sup> = (Ce<sub>0.55</sub>La<sub>0.19</sub>Nd<sub>0.17</sub>Pr<sub>0.06</sub>Sm<sub>0.02</sub>Gd<sub>0.02</sub>Eu<sub>0.01</sub>Tb<sub>0.01</sub>Dy<sub>0.01</sub>) apfu, with an aggregate scattering of 60.93 epfu (Table 6). The bond-valence sums for the anions at the twelve O sites vary from 1.71 to 2.20 vu (valence unit) (Table 7), and hence they are O atoms.

## Description of the structure

The crystal structure contains 2 groups of cation sites: *Si* and *T* sites of the tetrahedral Si–Zn–O sheet and interstitial *Na* and *M*(1,2,3) sites. In the Si–Zn–O sheet, the *Si*(1–4) sites are occupied by Si, with <<Si–O>> = 1.632 Å and the *T* site is occupied mainly by Zn, ideally Zn<sub>2</sub> apfu (Tables 3, 4). The Zn atom is tetrahedrally coordinated by four O atoms. Zinc and Si tetrahedra form four-membered, five-membered and eight-membered rings in the ratio 1:4:1 (Fig. 2a). The ideal formula of the Si–Zn–O sheet is (Zn<sub>2</sub>Si<sub>8</sub>O<sub>24</sub>)<sup>12-</sup>. In the crystal structure of rundqvistite-(Ce), a sheet of Si and Zn tetrahedra parallel to (100) is the main structural unit.

The interstitial cations occur at the four cation sites situated at *x* ≈ 0.5, *i.e.* between two Si–Zn–O sheets at *x* ≈ 0 and *x* ≈ 1.0. The *Na* site is occupied by Na, giving Na<sub>1.0</sub> apfu, with <<sup>[6]</sup>Na–O> = 2.447 Å, and the Na-dominant *M*1 site ideally gives Na<sub>2</sub> apfu, with <<sup>[6]</sup>M1–O> = 2.522 Å (Tables 4–6). Hence the *Na* and *M*1 sites ideally give Na<sub>3</sub> apfu. The [8]-coordinated *M*2 and *M*3 sites, with <<sup>[8]</sup>M2–O> = 2.607 Å and <<sup>[8]</sup>M3–O> = 2.599 Å, respectively, give [(Sr<sub>2.23</sub>Ca<sub>0.54</sub>Pb<sub>0.06</sub>Na<sub>0.13</sub>)Σ<sub>2.96</sub>Ln<sub>1.04</sub>]Σ<sub>4.00</sub> apfu, ideally (Sr<sub>3</sub>Ce) apfu. Therefore, Na, *M*1, *M*2 and *M*3 interstitial cations sum to [Na<sub>3</sub>(Sr<sub>3</sub>Ce)]<sup>12+</sup> apfu. The [6]-coordinated Na and *M*1 polyhedra and [8]-coordinated *M*2 and *M*3 polyhedra share common edges to form a layer (Fig. 2b).

The layer of the [6]- and [8]-coordinated Na and *M*(1–3) polyhedra and the sheet of *Si*(1–4) and *T* tetrahedra connect via common vertices along **a**, forming a framework.

**Table 4.** Atom coordinates and anisotropic displacement parameters for rundqvistite-(Ce).

Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> <sup>11</sup>	<i>U</i> <sup>22</sup>	<i>U</i> <sup>33</sup>	<i>U</i> <sup>23</sup>	<i>U</i> <sup>13</sup>	<i>U</i> <sup>12</sup>	<i>U</i> <sub>eq</sub> (Å <sup>2</sup> )
Na	½	½	½	0.0140(11)	0.0392(15)	0.0211(11)	-0.0124(11)	0.0042(14)	-0.0078(17)	0.0248(6)
M1	0.4889(6)	0.4561(2)	0.63542(6)	0.0148(8)	0.0359(11)	0.0210(8)	0.0109(7)	0.0021(10)	0.0093(12)	0.0239(6)
M2	0.49551(8)	0.90166(3)	0.57079(2)	0.00874(13)	0.00780(13)	0.00950(14)	-0.00033(9)	0.0014(2)	-0.00004(15)	0.00868(9)
M3	0.50649(11)	0.58928(4)	0.77670(2)	0.00833(14)	0.00939(14)	0.00975(14)	-0.00058(10)	0.0016(2)	0.00072(17)	0.00916(9)
T	0.00295(11)	0.75458(5)	0.67557(2)	0.0107(2)	0.00782(19)	0.00889(19)	0.00026(12)	0.0013(3)	0.0000(3)	0.00915(13)
Si1	0.9417(2)	0.39125(14)	0.71493(4)	0.0081(6)	0.0083(5)	0.0096(4)	-0.0006(4)	0.0008(4)	-0.0003(4)	0.0087(2)
Si2	0.9570(2)	0.10531(13)	0.63427(4)	0.0075(6)	0.0089(4)	0.0086(4)	0.0001(3)	0.0007(4)	0.0008(4)	0.0083(2)
Si3	0.05202(19)	0.23168(13)	0.53130(4)	0.0084(5)	0.0071(4)	0.0083(5)	0.0001(4)	0.0012(4)	0.0003(3)	0.0079(2)
Si4	0.0323(2)	0.60214(12)	0.56797(4)	0.0070(5)	0.0073(4)	0.0093(4)	-0.0002(3)	0.0009(4)	0.0003(4)	0.0079(2)
O1	0.2493(6)	0.3915(4)	0.71938(12)	0.0106(14)	0.0207(16)	0.0168(15)	0.0005(13)	-0.0006(12)	-0.0025(13)	0.0160(6)
O2	0.8009(6)	0.5688(4)	0.70221(12)	0.0141(14)	0.0081(13)	0.0150(15)	0.0013(11)	0.0037(11)	-0.0004(11)	0.0124(6)
O3	0.7876(6)	0.3199(4)	0.76500(11)	0.0132(14)	0.0144(14)	0.0108(14)	0.0028(11)	0.0005(11)	0.0019(11)	0.0128(6)
O4	0.8418(6)	0.2647(4)	0.66758(12)	0.0143(13)	0.0140(15)	0.0121(14)	-0.0045(11)	0.0002(11)	0.0023(12)	0.0135(6)
O5	0.7400(6)	0.5835(4)	0.86127(12)	0.0088(14)	0.0190(16)	0.0185(15)	0.0004(12)	-0.0014(12)	-0.0022(13)	0.0154(6)
O6	0.7857(6)	-0.0559(4)	0.65204(12)	0.0122(14)	0.0101(14)	0.0180(15)	0.0035(11)	0.0008(12)	-0.0010(12)	0.0135(6)
O7	0.8637(5)	0.1409(4)	0.57391(12)	0.0131(12)	0.0142(13)	0.0074(12)	0.0026(11)	-0.0008(12)	-0.0038(10)	0.0116(5)
O8	0.2859(6)	0.1180(4)	0.51471(12)	0.0132(13)	0.0112(14)	0.0158(14)	0.0002(12)	0.0024(11)	0.0044(12)	0.0134(6)
O9	0.1537(6)	0.4105(4)	0.55763(12)	0.0158(14)	0.0066(13)	0.0153(14)	-0.0018(11)	-0.0009(11)	-0.0009(11)	0.0126(6)
O10	0.1393(6)	0.7125(4)	0.51710(11)	0.0111(13)	0.0141(14)	0.0087(13)	0.0018(11)	-0.0003(10)	0.0008(11)	0.0113(6)
O11	0.7274(5)	0.6082(4)	0.57056(11)	0.0092(12)	0.0146(14)	0.0130(14)	-0.0001(12)	0.0010(12)	-0.0001(11)	0.0123(6)
O12	0.1949(6)	0.6818(4)	0.61490(11)	0.0099(13)	0.0130(14)	0.0093(13)	-0.0029(11)	0.0013(11)	-0.0000(11)	0.0107(6)

**Table 5.** Selected interatomic distances (Å) and angles (°) for rundqvistite-(Ce).

Na–O11 ×2	2.343(3)	M1–O12	2.406(4)	T–O2a	1.932(3)	Si1–O4–Si2	137.4(2)
Na–O9 ×2	2.446(3)	M1–O11	2.413(4)	T–O12	1.953(3)	Si2–O7–Si3g	122.4(2)
Na–O10 ×2	2.553(3)	M1–O4	2.518(4)	T–O3b	1.959(3)	Si3–O9–Si4	136.3(2)
<Na–O>	2.447	M1–O2	2.536(4)	T–O6c	1.971(3)	Si3f–O10–Si4	122.4(2)
		M1–O1	2.565(4)	<T–O>	1.953		
		M1–O9	2.693(4)				
		<M1–O>	2.522				
M2–O8d	2.496(3)	M3–O2	2.474(3)	Si4–O11a	1.586(3)		
M2–O8e	2.502(3)	M3–O5	2.512(3)	Si4–O12	1.612(3)		
M2–O5b	2.585(3)	M3–O1	2.538(3)	Si4–O9	1.661(3)		
M2–O12	2.602(3)	M3–O3	2.597(3)	Si4–O10	1.679(3)		
M2–O11	2.611(3)	M3–O3b	2.612(3)	<Si4–O>	1.635		
M2–O6d	2.617(3)	M3–O6b	2.656(3)				
M2–O7d	2.689(3)	M3–O4b	2.700(3)				
M2–O10	2.757(3)	M3–O1b	2.704(3)				
<M2–O>	2.607	<M3–O>	2.599				
Si1–O1g	1.602(3)	Si2–O5h	1.587(4)	Si3–O8	1.571(3)		
Si1–O2	1.615(3)	Si2–O6	1.620(3)	Si3–O7a	1.643(3)		
Si1–O3	1.629(3)	Si2–O4	1.641(3)	Si3–O9	1.655(3)		
Si1–O4	1.668(3)	Si2–O7	1.667(3)	Si3–O10f	1.663(3)		
<Si1–O>	1.629	<Si2–O>	1.629	<Si3–O>	1.633		

Symmetry operators: a:  $x-1, y, z$ ; b:  $-x+1, y+1/2, -z+3/2$ ; c:  $x-1, y+1, z$ ; d:  $x, y+1, z$ ; e:  $-x+1, -y+1, -z+1$ ; f:  $-x, -y+1, -z+1$ ; g:  $x+1, y, z$ ; h:  $-x+2, y-1/2, -z+3/2$ .

**Table 6.** Refined site-scattering and assigned site-populations for rundqvistite-(Ce).

Site	Refined site-scattering (epfu)	Assigned site-population (apfu)	Calculated site-scattering (epfu)	<Cation–O> <sub>obs.</sub> (Å)	Ideal composition (apfu)
<sup>[6]</sup> Na*	11.0	Na <sub>1.0</sub>	11.0	2.447	Na
<sup>[6]</sup> M1	23.62(2)	Na <sub>1.94</sub> Sr <sub>0.06</sub>	23.62	2.522	Na <sub>2</sub>
ΣNaM1	34.62	Na <sub>2.94</sub> Sr <sub>0.06</sub>	34.62		Na <sub>3</sub>
<sup>[8]</sup> M2**	87.0(2)	(Sr <sub>1.07</sub> Ca <sub>0.26</sub> Na <sub>0.04</sub> Pb <sub>0.02</sub> )Σ <sub>1.39</sub> Ln <sub>0.61</sub> <sup>3+</sup>	83.68	2.607	
<sup>[8]</sup> M3	83.6(2)	(Sr <sub>1.16</sub> Ca <sub>0.28</sub> Na <sub>0.09</sub> Pb <sub>0.04</sub> )Σ <sub>1.57</sub> Ln <sub>0.43</sub> <sup>3+</sup>	80.15	2.599	
ΣM(2,3)	170.6	(Sr <sub>2.23</sub> Ca <sub>0.54</sub> Pb <sub>0.06</sub> Na <sub>0.13</sub> )Σ <sub>2.96</sub> Ln <sub>1.04</sub> <sup>3+</sup>	163.83		(Sr <sub>3</sub> Ce)
Zn–Si–O-sheet					
<sup>[4]</sup> T	58.4(2)	Zn <sub>1.92</sub> Fe <sub>0.06</sub> <sup>2+</sup>	59.16	1.954	Zn <sub>2</sub>
<sup>[4]</sup> Si(1–4)		Si <sub>8</sub>		1.632	Si <sub>8</sub>
O(1–12)		O <sub>24</sub>			O <sub>24</sub>
Total		(Zn <sub>1.92</sub> Fe <sub>0.06</sub> <sup>2+</sup> )Si <sub>8</sub> O <sub>24</sub>			(Zn <sub>2</sub> Si <sub>8</sub> O <sub>24</sub> )

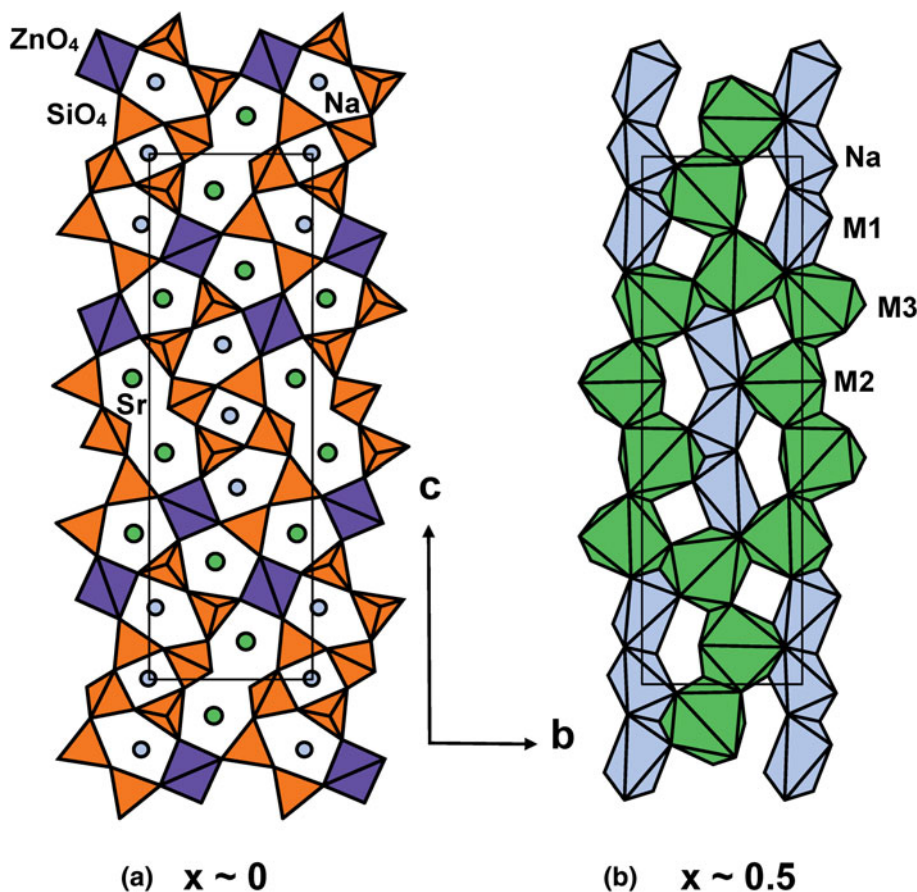
\*Site-scattering was refined, converted to an integer and then fixed at the last stages of the refinement;

\*\* $Ln_{1.04}^{3+} = Ce_{0.55}La_{0.19}Nd_{0.17}Pr_{0.06}Sm_{0.02}Gd_{0.02}Eu_{0.01}Tb_{0.01}Dy_{0.01}$  (60.93 epfu);  $f_{av} = 58.59$  el.

**Table 7.** Bond-valence\* values for rundqvistite-(Ce).

	Si1	Si2	Si3	Si4	T	Na	M1	M2	M3	Σ
O1	1.05						0.14		0.31	1.71
									0.21	
O2	1.02				0.49		0.15		0.37	2.03
O3	0.98				0.44				0.27	1.95
									0.26	
O4	0.89	0.95					0.15		0.21	2.20
<sup>[3]</sup> O5		1.10						0.28	0.33	1.71
O6		1.01			0.43			0.26	0.23	1.90
<sup>[3]</sup> O7		0.89	0.95					0.21		2.05
<sup>[3]</sup> O8			1.15					0.36		1.86
								0.35		
O9			0.92	0.90		0.17 <sup>×2</sup> ↓	0.11			2.10
O10			0.90	0.86		0.14 <sup>×2</sup> ↓		0.13		1.99
O11				1.10		0.21 <sup>×2</sup> ↓	0.18	0.27		1.76
O12				1.05	0.46		0.18	0.27		1.96
Total	3.94	3.95	3.92	3.89	1.82	1.04	0.91	2.30	2.19	
Aggregate charge	4.00	4.00	4.00	4.00	2.00	1.00	1.03	2.29	2.17	

\*Bond-valence parameters (vu) are from Brown (1981); bond-valence contributions calculated from Zn (T), Na (Na, M1) and (Sr + Ce<sup>3+</sup>) (M2, M3); coordination numbers are shown for non-[4]-coordinated anions.



**Figure 2.** Crystal structure of rundqvistite-(Ce): (a) the  $(\text{Zn}_2\text{Si}_8\text{O}_{24})^{12-}$  sheet of  $\text{SiO}_4$  and  $\text{ZnO}_4$  tetrahedra at  $x \approx 0$ , Na and Sr atoms above the sheet are shown as blue and green spheres; (b) the layer of Na-dominant Na and M1 octahedra and [8]-coordinated Sr-dominant M(2,3) polyhedra at  $x \approx 0.5$ ; Na-dominant octahedra are blue, Sr-dominant polyhedra are green. Drawn with *Atoms 6.4* software (Dowty, 2016).

We write the ideal structural formula of rundqvistite-(Ce) as the sum of the interstitial cations and the Si–Zn–O sheet:  $\text{Na}_3(\text{Sr}_3\text{Ce}) + (\text{Zn}_2\text{Si}_8\text{O}_{24}) = \text{Na}_3(\text{Sr}_3\text{Ce})(\text{Zn}_2\text{Si}_8\text{O}_{24})$  for  $Z = 2$ .

### Relation to other species

Rundqvistite-(Ce), ideally  $\text{Na}_3(\text{Sr}_3\text{Ce})(\text{Zn}_2\text{Si}_8\text{O}_{24})$ , is a structural analogue of vladyskinite, ideally  $\text{Na}_3\text{Sr}_4(\text{Fe}^{2+}\text{Fe}^{3+})\text{Si}_8\text{O}_{24}$  (Chakhmouradian *et al.*, 2014). Rundqvistite-(Ce) and vladyskinite are related by the following substitution:  $^{[8]}\text{Ce}^{3+} + ^{[4]}\text{Zn}^{2+} \leftrightarrow ^{[8]}\text{Sr}^{2+} + ^{[4]}\text{Fe}^{2+}\text{Fe}^{3+}$ . Table 8 lists comparative data for rundqvistite-(Ce) and vladyskinite.

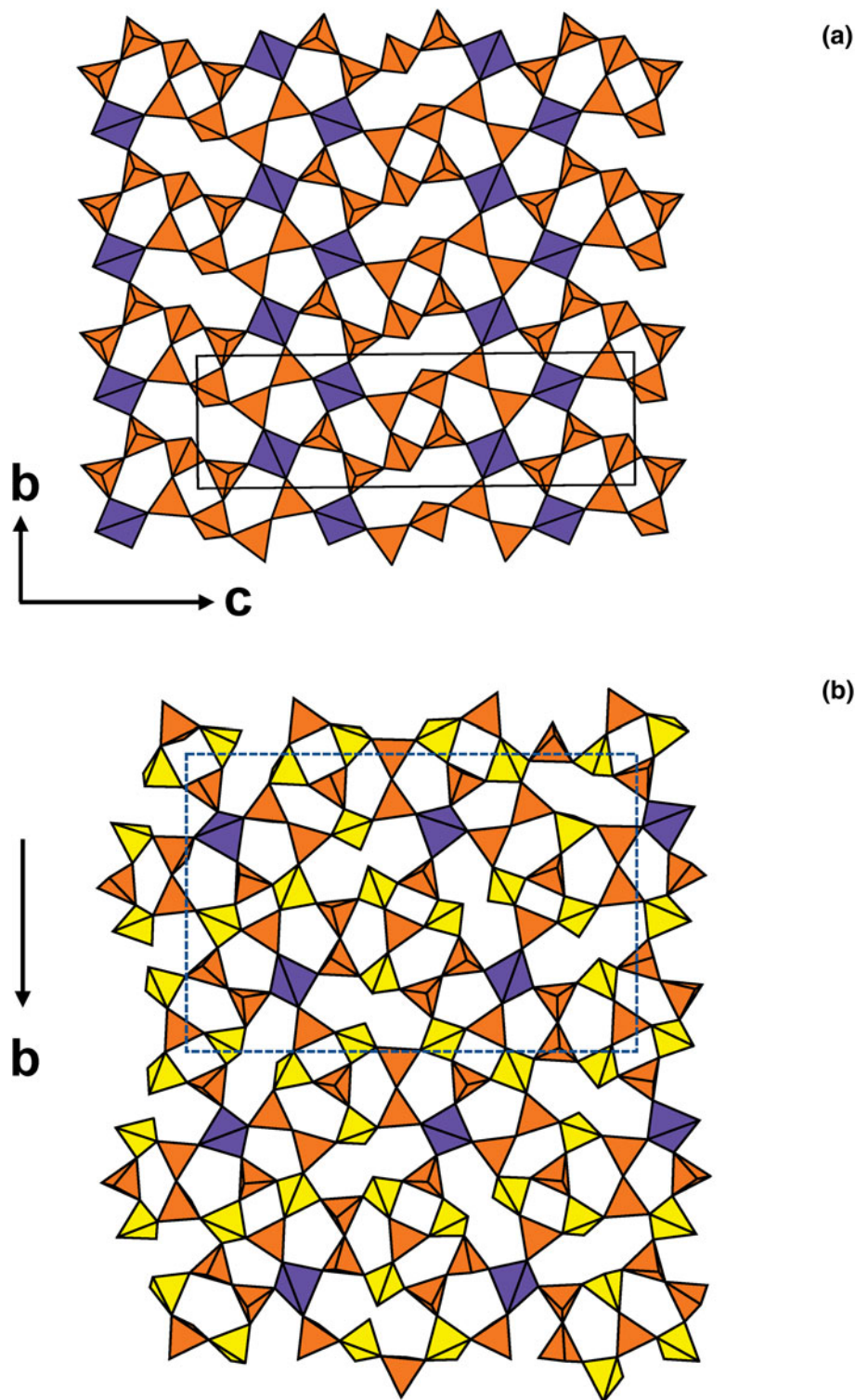
There is an interesting relation between rundqvistite-(Ce) and samfowlerite, ideally  $\text{Ca}_{14}\text{Mn}_3\text{Zn}_2(\text{Zn},\text{Be})_2\text{Be}_6(\text{SiO}_4)_6(\text{Si}_2\text{O}_7)_4(\text{OH},\text{F})_6$  (Rouse *et al.*, 1994). Samfowlerite is monoclinic,  $P2_1/c$ ,  $a = 9.068(2)$ ,  $b = 17.992(2)$ ,  $c = 14.586(2)$  Å,  $\beta = 104.86(1)^\circ$ ,  $V = 2312(4)$  Å<sup>3</sup> and  $Z = 2$ . Rouse *et al.* (1994) described a sheet of “vertex-sharing  $\text{TO}_4$  tetrahedra ( $T = \text{Si}, \text{Be}, \text{Zn}$ )” which form 4-, 5- and 8-membered rings. Hawthorne *et al.* (2019) compared topologies of tetrahedral sheets in vladyskinite and samfowlerite and wrote the ideal formula of samfowlerite as follows:  $\text{Ca}_{14}\text{Mn}_3[(\text{Be}_7\text{Zn})\text{Zn}_2\text{Si}_{14}\text{O}_{52}(\text{OH})_6]$ ; composition of the Si–Be–Zn–O–OH sheet is given in square brackets. In samfowlerite, there are two sites that contain Zn: the Zn1 site is occupied solely by Zn giving  $\text{Zn}_2$  apfu and the Zn2 site is occupied by  $\text{Be} > \text{Zn}$  giving  $(\text{Be}_{1.25}\text{Zn}_{0.75})$ , ideally  $\text{Be}_2$  apfu. Rouse *et al.* (1994) noted that “substitution of Be for Zn at the Zn2 site suggests that the space group  $P2_1/c$  is only that of an average structure, and that the true structure is of lower symmetry, with ordering of Zn

and Be on separate sites.” Here we can write the ideal composition of the Si–Be–Zn–O–OH sheet as  $[\text{Be}_8\text{Zn}_2\text{Si}_{14}\text{O}_{52}(\text{OH})_6]^{34-}$ . The  $(\text{Zn}_2\text{Si}_8\text{O}_{24})^{12-}$  sheet in rundqvistite-(Ce) and  $[\text{Be}_8\text{Zn}_2\text{Si}_{14}\text{O}_{52}$

**Table 8.** Comparison of rundqvistite-(Ce) and vladyskinite.

Mineral	Rundqvistite-(Ce)*	Vladyskinite**
Ideal formula	$\text{Na}_3(\text{Sr}_3\text{Ce})(\text{Zn}_2\text{Si}_8\text{O}_{24})$	$\text{Na}_3\text{Sr}_4(\text{Fe}^{2+}\text{Fe}^{3+})\text{Si}_8\text{O}_{24}$
Space group	$P2_1/c$	$P2_1/c$
$a$ (Å)	5.1934(10)	5.21381(13)
$b$ (Å)	7.8934(15)	7.9143(2)
$c$ (Å)	26.011(5)	26.0888(7)
$\beta$ (°)	90.02(3)	90.3556(7)
$V$ (Å <sup>3</sup> )	1066.3(4)	1076.50(5)
$Z$	2	2
$D_{\text{calc.}}$ (g cm <sup>-3</sup> )	3.709	3.51
$D_{\text{meas.}}$ (g cm <sup>-3</sup> )	3.70	not measured
Strongest reflections in the X-ray powder diffraction data, $d/\text{Å}$ ( $l$ )	2.952(100) 2.830(80) 3.598(60) 2.821(60) 4.28(50) 3.140(46) 3.336(42) 3.616(33) 2.593(23)	2.957(100) 2.826(100) 3.612(58) 3.146(37) 2.470(32) 4.290(30) 3.339(30) 2.604(28) 2.437(25)
Optical class, sign	biaxial (–)	biaxial (–)
$\alpha$	1.644	1.624
$\beta$	1.659	1.652
$\gamma$	1.662	1.657
$2V_{\text{calc}}$ (°)	48	45

\*This work; \*\*Chakhmouradian *et al.* (2014).



**Figure 3.** The sheets of 4-, 5- and 8-membered rings of tetrahedra in (a) rundqvistite-(Ce), projection on the (100) plane and (b) samfowlerite, projection on the (102) plane. Si tetrahedra are orange, Zn and Zn-dominant tetrahedra are purple, Be and Be-dominant tetrahedra are yellow. The unit cell of rundqvistite-(Ce) and the repeat of the samfowlerite sheet are shown in thin solid lines and dashed lines, respectively.

$(\text{OH})_6]^{34-}$  sheet in samfowlerite are shown in Fig. 3a,b. The two sheets have three common elements: Si, Zn and O.

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**Competing interests.** The authors declare none.

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