Okruschite, Ca₂Mn²⁺₅Be₄(AsO₄)₆(OH)₄ · 6H₂O, a new roscherite-group mineral from Sailauf, Bavaria, Germany

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Abstract: The new mineral okruschite (IMA No. 2013–097), the arsenate analogue of roscherite, was discovered in a hydrothermal vein cross-cutting rhyolite exposed in the Fuchs quarry, near Sailauf, Spessart Mountains, Bavaria, Germany. Associated minerals are braunite, Mn-bearing calcite and arseniosiderite. Okruschite forms tabular aggregates up to $0.15 \times 0.3 \times 0.3$ mm in size of curved and somewhat misaligned laths. It is white, semitransparent; lustre is vitreous. D_{meas} = 3.33(2), D_{calc} = 3.340 g/cm³. Okruschite is optically biaxial (–), $\alpha = 1.671(3)$, $\beta = 1.682(2)$, $\gamma = 1.687(3)$, $2V_{meas} = 65(5)^{\circ}$. The infrared spectrum is given. The chemical composition is (electron microprobe, B and Li by ICP MS, H₂O by gas chromatography of ignition products, wt. %): Li₂O 0.04, BeO 7.70, MgO 1.68, CaO 8.28, MnO 16.27, FeO 4.89, Al₂O₃ 0.22, As₂O₅ 51.11, H₂O 11.0, total 101.19. The empirical formula based on 34 O atoms is: Ca_{1.99}(Mn_{3.09}Fe_{0.92}Mg_{0.56}Al_{0.06}Li_{0.04})_{Σ 4.67}Be_{4.15}(AsO₄)_{5.99}(OH)_{3.64} · 6.40H₂O. The simplified formula is Ca₂Mn²⁺₅Be₄(AsO₄)₆(OH)₄ · 6H₂O. Okruschite is monoclinic, *C2/c*, *a* = 16.33(4), *b* = 12.03(3), *c* = 6.93(1) Å, β = 94.84(5)°, *V* = 1357(4) Å³, *Z* = 2. The strongest lines of the powder X-ray diffraction pattern [*d*, Å (*I*, %) (*hkl*)] are: 9.68 (39) (110), 4.95 (34) (310), 4.17 (34) (–311), 3.25 (100) (–202, 330), 3.11 (32) (–421), 2.841 (27) (240), 2.711 (26) (600), 1.726 (26) (461, –552, 004). Okruschite is named after Professor Martin Okrusch, from Germany. Type material is deposited in the collections of the Fersman Mineralogical Museum of the Russian Academy of Sciences, Moscow.

Key-words: okruschite; new mineral; roscherite group; rhyolite; beryllium arsenate; Fuchs quarry; Sailauf; Spessart.

Introduction

This paper describes the new mineral species okruschite discovered in the Fuchs quarry, at Hartkoppe Hill, near Sailauf community, 7 km NE of Hösbach, Spessart Mountains, Bavaria, Germany. The Fuchs quarry is known as the type locality of another arsenate mineral, sailaufite.

Okruschite is named in honour of the outstanding German scientist Professor Martin Okrusch (b. 1934), a specialist in mineralogy and petrology of magmatic and metamorphic rocks, as well as ore petrology and ore deposits. Martin Okrusch is the author of more than 200 publications, some of which are devoted to the Spessart Mountains. The mineral and its name have been approved by the IMA Commission on New Minerals, Nomenclature and Classification (IMA No. 2013–097).

Okruschite is the first arsenate member of the roscherite group, which to date comprised only phosphates (Atencio *et al.*, 2008).

The type material is deposited in the collection of the Fersman Mineralogical Museum of the Russian Academy of Sciences, Moscow, Russia, with catalogue number 94233.

Occurrence and general appearance

The Sailauf Mn–Fe–As vein mineralization is characterized by complex hydrothermal carbonate and oxide assemblages. The mineralization is hosted by a Permian rhyolite body approximately 400 m long and 200 m wide belonging to the Spessart district and structurally related to the Variscan unconformity that separates Permian sedimentary rocks from the underlying Variscan crystalline basement. The massive body of altered rhyolite is crosscut by five parallel, NW-striking fault systems which host discontinuously mineralized hydrothermal veins with thicknesses ranging from 1 to 25 cm (Fusswinkel *et al.*, 2013). Okruschite was found in one of these veins.

The list of associated minerals in order of their crystallization sequence (*i.e.*, in the direction from hosting rhyolite to the central part of the vein) is: braunite (a thin layer, in some samples it is absent) \rightarrow Mn-bearing calcite of the first generation (a layer up to several mm thick) \rightarrow arseniosiderite covering walls of cavities \rightarrow Mn-bearing calcite of the second generation and okruschite (both form isolated imperfect crystals consisting of disordered blocks) \rightarrow late arseniosiderite growing on okruschite crystals. Some small cavities in the rhyolite contain bertrandite.

Okruschite forms separate imperfect blocky thick-tabular crystals up to $0.15 \times 0.3 \times 0.3$ mm in size, consisting of curved and differently oriented laths up to 5×150 µm (Figs. 1 and 2). The major crystal forms is {010}, the subordinate forms are {100}, {001} and, probably, {110}.



Fig. 1. Crystal of okruschite (white) with arseniosiderite. View width is 1 mm. Photograph: M. Burkhardt (Online version in colour).



Fig. 2. Split crystal of okruschite in association with arseniosiderite. SEM image. Micrograph: S. Diller.

Physical properties

Okruschite is brittle, with Mohs hardness of $3\frac{1}{2}$. Cleavage is distinct on (010). Parting is observed on (100), along borders of blocks. Density measured by flotation in heavy liquids is 3.33(2) g/cm³. Density calculated from the empirical formula is 3.340 g/cm³.

Crystals of okruschite are white, semitransparent, with a vitreous lustre. Okruschite is optically biaxial (–), $\alpha = 1.671(3)$, $\beta = 1.682(2)$, $\gamma = 1.687(3)$, $2V_{\text{meas}} = 65(5)^{\circ}$, $2V_{\text{calc}} = 68^{\circ}$. The dispersion of the optical axes is weak, r > v. The orientation is: X = b.

Infrared spectroscopy

Absorption bands in the IR spectrum of a powdered sample of okruschite (Fig. 3) and their assignments are $(cm^{-1};$ s – strong band, sh – shoulder): 3510, 3400sh, 3360, 3282s, 2960sh (O-H stretching vibrations), 1661 (bending vibrations of H_2O molecules), 982, 900sh, 855sh, 843s (stretching vibrations of AsO_4^{3-} anions), 798s, 769, 736, 680s, 635sh (Be–O stretching vibrations of BeO₄ tetrahedra, possibly combined with $M \cdot \cdot \cdot O$ -H bending vibrations where M = Mn, Fe, Mg), 555, 450, 370 (stretching vibrations of (Mn,Fe,Mg)O₆ octahedra, possibly combined with librational vibrations of H₂O molecules). Bands in the range $635-800 \text{ cm}^{-1}$ are assigned to Be–O stretching bands by analogy with IR spectra of phosphate members of the roscherite group (Fig. 4). Bands of B- or C-bearing groups are absent in the IR spectrum of okruschite. The IR spectrum of okruschite is unique and is considered to be a good diagnostic tool for the mineral.

Chemical data

Five chemical point analyses for major elements were carried out in the Institute of Experimental Mineralogy, Russian Academy of Sciences (Chernogolovka, Russia)



Fig. 3. The IR spectrum of okruschite.



Fig. 4. The IR spectra of phosphate members of the roscherite group; ruifrancoite (1), greifensteinite (2), atencioite (3) and footemineite (4) (after Atencio *et al.*, 2008).

using a Tescan VEGA-II XMU scanning electron microscope (EDS mode, 20 kV, 510–520 pA, 160–180 nm beam diameter; K.V. Van analyst). Chemical tests with potassium ferro- and ferricyanides, with subsequent centrifugal separation of the precipitate, showed that most iron is divalent, whereas Fe^{3+} is present in only trace amounts.

Lithium and beryllium were analyzed by ICP MS method using a Thermo Fisher Scientific X Series II instrument (Institute of Geochemistry and Analytical Chemistry, Russian Academy of Sciences, Moscow). A hand-picked sample was dissolved in a mixture of concentrated aqueous HCl, HF and HNO₃ solutions. After total evaporation, 5 cm³ of 0.5 M nitric acid was added, and the solution analysed by measuring the intensities of the lines corresponding to m/e = 7 for Li and 9 for Be.

The H_2O content was determined by gas chromatography of products of the mineral ignition at 1200°C. CO_2 was not analyzed because of the absence of absorption bands corresponding to vibrations of C–O bonds in the IR spectrum.

Analytical data are given in Table 1. The contents of other elements with atomic numbers > 8 are below detection limits. The empirical formula (based on 34 O *apfu*, H

Table 1. Chemical composition (wt. %) of okruschite.

Constituent	Average content	Range	Standard deviation	Probe standard
Li ₂ O	0.04			
BeO	7.70			
MgO	1.68	1.31-1.97	0.24	Diopside
CaO	8.28	8.05-8.66	0.25	Wollastonite
MnO	16.27	16.03-16.42	0.13	MnTiO ₃
FeO*	4.89	4.68-5.16	0.18	Fe
Al_2O_3	0.22	0-0.43	0.17	Al_2O_3
As_2O_5	51.11	50.35-52.06	0.74	Scorodite
H ₂ O	11 ± 1			
Total	101.19			

*On the basis of the results of chemical tests, all iron is considered as Fe^{2+} .

apportioned between OH and H₂O according to charge balance, under the assumption that other H-bearing groups are absent) is Ca_{1.99}(Mn_{3.09}Fe_{0.92}Mg_{0.56}Al_{0.06}Li_{0.04}) \sum 4.67 Be_{4.15}(AsO₄)_{5.99}(OH)_{3.64} · 6.40H₂O. The simplified formula is Ca₂Mn²⁺₅Be₄(AsO₄)₆(OH)₄ · 6H₂O, which requires BeO 7.14, CaO 8.01, MnO 25.33, As₂O₅ 49.23, H₂O 10.29, total 100.00 wt%.

The Gladstone-Dale compatibility index is: $1-(K_p/K_c) = -0.024$ ("excellent").

X-ray diffraction data

The single-crystal X-ray diffraction study of okruschite was carried out using an Xcalibur S diffractometer equipped with a CCD detector. The monoclinic unit cell with following parameters was found: a = 16.32(3), b = 12.04(2), c = 6.92(1) Å, $\beta = 94.8(1)^{\circ}$, V = 1355(3) Å³.

Powder X-ray diffraction data for okruschite (Table 2) were collected by means of Agilent Technologies SuperNova single-crystal diffractometer equipped with Atlas CCD detector (X-Ray Diffraction Resource Center, St. Petersburg State University) using microfocused mono-chromated Cu*K* α radiation (50 kV, 0.8 mA, the distance between sample and detector was 55 mm). The series of simple scans was obtained in ω operating in CrysAlisPro program complex (Agilent Technologies, Version 1.171.36.20). Diffraction peaks are well indexed with a monoclinic unit cell, space group *C*2/*c*, by analogy with phosphate members of the roscherite group. The refined unit-cell parameters are: a = 16.33(4), b = 12.03(3), c = 6.93(1) Å, $\beta = 94.84(5)^\circ$, V = 1357(4) Å³, Z = 2.

The crystal structure of okruschite could not be solved because of the poor quality of single crystals, consisting of curved and differently oriented blocks (Figs. 1 and 2). However unit-cell parameters obtained for a single crystal, as well as powder X-ray diffraction data and the stoichiometry of okruschite clearly indicate that this mineral is isostructural with monoclinic members of the roscherite group.

Discussion

Okruschite is the first arsenate representative of the roscherite group, whereas the other members of this group are phosphates (Table 3). Roscherite-group minerals can be subdivided into two subgroups different in symmetry. Most of them belong to the roscherite subgroup. They are monoclinic, space group C2/c (Fanfani *et al.*, 1975; Clark *et al.*, 1983; Leavens *et al.* 1990; Chukanov *et al.*, 2002, 2007; Rastsvetaeva *et al.*, 2002, 2005, 2009; Barinova *et al.*, 2004; Atencio *et al.*, 2007). Their crystal structure is based on a three-dimensional heteropolyhedral framework formed by PO₄ and BeO₄ tetrahedra, and octahedra centred with Mg, Mn, Fe, Al, Zn. The framework contains cavities occupied by Ca atoms with coordination number 7 and H₂O molecules forming free vertices of the

Table 2. Powder X-ray diffraction data for okruschite.

I _{rel}	$d_{\rm meas}$, Å	$d_{ m calc}, { m \AA}^*$	hkl
39	9.68	9.68	110
18	6.04	6.02	020
13	5.54	5.49	-201
34	4.95	4.94	310
17	4.48	4.53	021
34	4.17	4.17	-311
20	3.46	3.45	002
13	3.38	3.38	401
100	3.25	3.27, 3.23	-202, 330
32	3.11	3.11	-421
23	2.955	2.949, 2.948	-511, 421
27	2.841	2.823	240
26	2.711	2.711	600
2	2.612	2.608	-132
3	2.535	2.527	402
6	2.475	2.472	620
6	2.434	2.424	-531
15	2.285	2.281	710
2	2.247	2.248, 2.243	441, 151
2	2.133	2.118, 2.117	-223, -351
3	2.065	2.049	602
7	1.989	1.979, 1.978	-712, 532
2	1.950	1.949, 1.949	152, 260
10	1.816	1.819, 1.818	-802, 821
24	1.781	1.788, 1.787, 1.787	-642, 513, 910
26	1.726	1.726, 1.725, 1.724	461, -552, 004
22	1.687	1.690, 1.690, 1.685, 1.685, 1.623	802, -713, 840, 732, 114
9	1.651	1.653, 1.650, 1.648, 1.648, 1.648	552, -224, 533, -751, 930
8	1.629	1.631, 1.627, 1.626, 1.626	-931, 822, 443, 10.0.0
3	1.560	1.564, 1.563 1.558, 1.557, 1.557	-643, 353, -10.2.1, -842, 713
9	1.511	1.513, 1.512	-604, 063
7	1.476	1.480, 1.475, 1.474, 1.473, 1.472	280, -10.2.2, 842, 571, 263
10	1.388	1.392, 1.391, 1.390, 1.389, 1.387, 1.387	463, -481, -933, 154, 11.3.0, 10.2.2
4	1.359	1.358, 1.357, 1.357, 1.356, 1.356 1.356	-734, 913, -10.4.2, 115, -315
7	1.352	1.355, 1.353, 1.352, 1.352, 1.351, 1.351	12.0.0, 282, -663, -644, -12.0.1, -373
2	1.316	1.319, 1.319, 1.316, 1.316, 1.315	373, -12.2.1, 843, 680, 753

*Calculated with unit-cell parameters obtained from single-crystal X-ray diffraction data.

Ca-centred polyhedra. The general crystal-chemical formula of monoclinic roscherite-group minerals may be written as $Ca_2D_2M_4Be_4(PO_4)_6(OH)_4X_2 \cdot 4H_2O$, where D and M are octahedrally coordinated cations Mg, Mn^{2+} , Fe^{2+} , Fe^{3+} , Al, Zn, and $X = OH^{-}$ or H_2O . As a rule, the D site is predominantly vacant: its occupancy usually varies within the limits 1/3 to 1/2. In the framework, two Po₄ tetrahedra and two BeO₄ tetrahedra form four-membered ring. Those rings are connected via additional Po₄ tetrahedra forming chains parallel to [100]. The D octahedra, connected via common X vertices, form chains running perpendicular to the 2-fold axis, *i.e.*, along the short period $c \sim 7$ Å. These chains link pairs of edge-connected M octahedra into columns stretched along [110]. Tetrahedral and octahedral constructions are linked via P–O–M(D) and Be–OH–M bridges forming three-dimensional heteropolyhedral framework.

The X site, common to two D octahedra and one $CaO_4(H_2O)_2X$ polyhedron, lies on the 2-fold axis. Its composition depends on that of the D site, as shown in the

example of roscherite in Table 4. Statistically, the most probable case is when one of two adjacent *D* sites is occupied and the other is vacant. As a result, the probability of the presence of oxygen in the *X* site is low. Minerals belonging to this subgroup are distinguished from one another by the predominant *M* cation. In roscherite $M = \text{Mn}^{2+}$, in zanazziite M = Mg, in greifensteinite $M = \text{Fe}^{2+}$, in ruifrancoite $M = \text{Fe}^{3+}$, and in guimarãesite M = Zn (Table 3).

Another subgroup, which can be named the atencioite subgroup, includes triclinic members of the roscherite group (Fanfani *et al.*, 1977; Leavens *et al.*, 1990; Taucher *et al.*, 1992; Rastsvetaeva *et al.*, 2004, 2007; Chukanov *et al.*, 2006; Atencio *et al.*, 2008). The crystal structures of these minerals are topologically similar to those of their monoclinic analogues, but symmetry lowering results in the subdivision of D and M sites into pairs of non-equivalent sites, which may be differently occupied. Therefore, the general formula for minerals of the atencioite subgroup may be written as $Ca_2D(1)D(2)M(1)_2M(2)_2Be_4(PO_4)_6(OH)_4X_2$.

Mineral	Unit-cell parameters	Crystal-chemical formulae for structurally studied samples	References		
Monoclinic members: roscherite subgroup (space group C2/c)					
Zanazziite	a = 15.874 Å, $b = 11.854$ Å, $c = 6.605$ Å, $\beta = 95.21^{\circ}$	$\begin{array}{c} Ca_2[Mg_{0.61}Fe_{0.40}\Box_{0.99}] \\ [Mg_{2.38}Fe^{2+}{}_{1.08}Al_{0.31}Mn_{0.23}Fe^{3+}{}_{0.10}] Be_4(PO_4)_6(OH)_6 \cdot \\ 4H_2O \end{array}$	Leavens et al., 1990		
Zanazziite (Fe- rich)	a = 15.876 Å, b = 11.860 Å, $c = 6.607 \text{ Å}, \beta = 95.49^{\circ}$	$\begin{array}{l} Ca_{2}[Mg_{0.65}Fe^{2+}_{0.35}\Box_{1.00}] [Mg_{1.90}Fe_{1.25}Al_{0.50}Mn_{0.35}] \\ Be_{4}(PO_{4})_{6}(OH,H_{2}O)_{6} \cdot 4H_{2}O \end{array}$	Rastsvetaeva et al., 2009		
Greifen- steinite	$a = 15.903 \text{ Å}, b = 11.885 \text{ Å}, c = 6.677 \text{ Å}, \beta = 94.68^{\circ}$	$\begin{array}{c} Ca_{2}[Mn^{2+}_{0.7}\square_{1.3}] [(Fe^{2+}, Fe^{3+})_{3.2} Mg_{0.4}Al_{0.4}] \\ Be_{4}(PO_{4})_{6}(OH)_{4} \cdot 6H_{2}O \end{array}$	Chukanov <i>et al.</i> , 2002; Rastsvetaeva <i>et al.</i> , 2002		
Greifen- steinite (Zn-bearing)	a = 15.941 Å, $b = 11.877$ Å, $c = 6.625$ Å, $\beta = 95.09^{\circ}$	$\begin{array}{l} Ca_2[Mn^{2+}{}_{0.68}\square_{1.32}][(Fe^{2+},Fe^{3+})_{2.35}\\ Zn_{0.72}Mn_{0.46}Al_{0.28}Mg_{0.19}] \ Be_4(PO_4)_6(OH)_4(OH,H_2O)_2\\ \cdot \ 4H_2O \end{array}$	Barinova et al., 2004		
Roscherite ¹	a = 15.935 Å, b = 11.963 Å, $c = 6.664 \text{ Å}, \beta = 94.77^{\circ}$	$Ca_{2}[Al_{0.46}Fe_{0.30}Mg_{0.17}\Box_{1.07}] [Mn_{2.56}Fe_{1.44}]$	Rastsvetaeva et al., 2005		
Guimarãesite	a = 15.98 Å, $b = 11.84$ Å, $c = 6.63Å, \beta = 95.15^{\circ}$	$Be_4(PO_4)_6(OH)_4 \cdot 6H_2O$ Ca ₂ [\Box ,Mg,Fe,Al] ₂ [Zn,Mg,Mn] ₄ Be ₄ (PO ₄) ₆ (OH) ₄ · 6H ₂ O	Chukanov et al., 2007		
Ruifrancoite	a = 15.911 Å, $b = 11.894$ Å, $c = 6.625$ Å, $\beta = 94.5^{\circ}$	$Ca_2(\Box, Mn^{2+})_2(Fe^{3+}, Mg, Mn)_4$ $Be_4(PO_4)_6(OH)_4(OH H_2O)_2 \cdot 4H_2O$	Atencio et al., 2007		
Okruschite	a = 16.32 Å, $b = 12.04$ Å, $c = 6.92Å, \beta = 94.8^{\circ}$	$\begin{array}{c} \text{Ca}_{2}(\Box,\text{Mn}^{2+})_{2}(\text{Mn}^{2+},\text{Fe}^{2+},\text{Mg})_{4} \text{ Be}_{4}(\text{AsO}_{4})_{6}(\text{OH})_{4} \\ \text{6H}_{2}\text{O} \end{array}$	This work		
Triclinic membe	ers: atencioite subgroup (space group	P_1)			
Atencioite	$a = 9.883 \text{ Å}, b = 9.879 \text{ Å}, c = 6.668 \text{ Å}, \alpha = 86.93^{\circ}, \beta = 85.60^{\circ}, \gamma = 73.53^{\circ}$	$\begin{array}{l} Ca_{2}[Fe^{2+}{}_{0.5}Mn_{0.2}Al_{0.1}\square_{0.2}][Mg_{0.2}\square_{0.8}]\\ [Mg_{1.1}Fe^{3+}{}_{0.5}Fe^{2+}{}_{0.4}][Fe^{2+}{}_{1.1}Mg_{0.9}]\\ Be_{4}(PO_{4})_{6}(OH)_{4}(OH, H_{2}O)_{2} \cdot 4H_{2}O \end{array}$	Chukanov <i>et al.</i> , 2006; Rastsvetaeva <i>et al.</i> , 2004		
"Triclinic roscherite" ²	a = 9.992 Å, $b = 9.924$ Å, $c = 6.741$ Å, $\alpha = 87.25^{\circ}$, $\beta = 86.02^{\circ}$, $\gamma = 73.85^{\circ}$	$\begin{array}{c} Ca_{2}[\Box_{1,00}][Fe^{3+}_{0,42}Al_{0,13} \\ Mn^{3+}_{0,12}[\Box_{0,33}][Mn^{2+}_{1,96}Ca_{0,02}Mg_{0,02}] \\ [Mn^{2+}_{1,96}Qa_{0,02}Mg_{0,02}]Be_{4}(PO_{4})_{6}(OH)_{4} \cdot 6H_{2}O \end{array}$	Fanfani et al., 1977		
Footemineite	$a = 10.014 \text{ Å}, b = 9.972 \text{ Å}, c = 6.788(2) \text{ Å}, \alpha = 87.44^{\circ}, \beta = 85.34^{\circ}, \gamma = 73.84^{\circ}$	$\begin{array}{c} Ca_{2}[(Mn,Fe)_{0.9} \square_{0.1}][Mg_{0.1} \square_{0.9}][Mn_{2}]\\ [Mn_{2}]Be_{4}(PO_{4})_{6}(OH)_{4}(H_{2}O)_{6} \end{array}$	Atencio <i>et al.</i> , 2008; Rastsvetaeva <i>et al.</i> , 2007		

Table 3. Comparative crystal-chemical characteristics of roscherite-group minerals.

¹Data for the first find of roscherite.

²The "triclinic roscherite" is the same as footmineite. The supposition that Fe is trivalent was not confirmed (Atencio *et al.*, 2008). Unit-cell parameters are given in unified orientations.

4H₂O. As compared with monoclinic analogues, in these minerals the number of independent sites for phosphorus increases from 2 to 3, for beryllium from 1 to 2, for OH groups on the *M*–OH–Be bridges from 1 to 2, and for H₂O molecules coordinating Ca from 1 to 2. The D(1) and, especially, D(2) sites preserve the tendency to be vacant, with their total occupancy amounting to no more than $\frac{1}{2}$ (Table 3).

Table 4. Possible local situations at the junction of two *D* octahedra (after Chukanov *et al.*, 2006).

2D	X
	H ₂ O
$Mg + \Box$	OH
$Al + \Box$	OH
Mg + Mg	0
Al + Mg	0
Al + Al	0

Okruschite is a representative of the roscherite subgroup. It is isostructural with zanazziite, greifensteinite, ruifrancoite, guimarãesite and roscherite, being the arsenate analogue of the latter (Table 5). The substitution of PO_4 for AsO₄ results in the increase of unit-cell dimensions, density and refractive indices.

All finds of roscherite-group minerals are in hydrothermal assemblages related to acid magmatic rocks. Okruschite is not an exception. Its formation is obviously connected with late derivatives of rhyolite magma. Rhyolite is considered to be the source of Be for okruschite. Be-enriched rhyolites are widespread, commonly in the same districts as hydrothermal Be deposits (Levinson, 1962; Shawe, 1966; Kovalenko & Yarmolyuk, 1995; Barton & Young, 2002). In rhyolite-hosted hydrothermal veins at Sailauf, arsenate minerals are present as late vug fillings and are intergrown with late-stage carbonates and/or native arsenic. The textural features suggest significant mobility of As in the hydrothermal fluids during late-stage, low-temperature fluid-mineral reactions (Fusswinkel *et al.*, 2012). Another

Mineral	Okruschite	Roscherite	
Formula	$\begin{array}{c} Ca_{2}Mn^{2+}{}_{5}Be_{4} \\ (AsO_{4})_{6}(OH)_{4} \\ \cdot \ 6H_{2}O \end{array}$	$Ca_2Mn^{2+}{}_5Be_4$ (PO ₄) ₆ (OH) ₄ · 6H ₂ O	
Space group	C2/c	C2/c	
a, Å	16.32	15.935	
b, Å	12.04	11.963	
<i>c</i> , Å	6.92	6.664	
β,°	94.8	94.77	
$V, Å^3$	1355	1265.9	
Ζ	2	2	
Strong lines of the	9.678 (39)	9.51 (90)	
powder X-ray	4.953 (34)	5.95 (100)	
diffraction pattern:	4.170 (34)	4.84 (40)	
d, Å (I, %)	3.248 (100)	3.17 (80)	
	3.109 (32)	3.08 (20)	
	2.842 (27)	2.788 (60)	
	2.711 (26)	2.644 (40)	
	1.726 (26)		
Strong bands in the IR	3510	3455	
absorption spectrum,	3360	3340	
cm ⁻¹	3282	1660	
	1661	1082	
	982	1031	
	900	812	
	843	720	
	798	612	
	680	562	
	450	523	
	370		
Optical data:			
α	1.671	1.624–1.636	
β	1.682	1.639–1.644	
γ	1.687	1.643-1.651	
Optical sign; 2V, °	-	-	
Density, g/cm ³	3.325 (meas)	2.90-2.97 (meas)	
X 1 1 1	3.34 (calc)	2.94-2.97 (calc)	
Mons nardness	3 ¹ /2	4½-5 L: II (1050)	
Kelerences	1 nis work	Eindberg (1958); Feklichev (1989); Rastsvetaeva <i>et al.</i> (2005); our data for the IR spectrum.	

Table 5. Comparative data for okruschite and roscherite.

beryllium arsenate, bergslagite, CaBe(AsO₄)(OH), has been described in hydrothermal veins hosted by the rhyolite body at Sailauf (Kolitsch, 1996).

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References

Atencio, D., Chukanov, N.V., Coutinho, J.M.V., Menezes Filho, L.A.D., Dubinchuk, V.T., Möckel, S. (2007): Ruifrancoite, a new Fe³⁺-dominant monoclinic member of the roscherite group, from Galiléia, Minas Gerais, Brazil. *Can. Mineral.*, **45**, 1263–1273.

- Atencio, D., Matioli, P.A., Smith, J.B., Chukanov, N.V., Coutinho, J.M.V., Rastsvetaeva, R.K., Möckel, S. (2008): Footemineite, the Mn-analog of atencioite, from the Foote mine, Kings Mountain, Cleveland County, North Carolina, USA, and its relationship with other roscherite-group minerals. *Am. Mineral.*, **93**, 1–6.
- Barinova, A.V., Rastsvetaeva, R.K., Chukanov, N.V., Pietraszko, A. (2004): Refinement of the crystal structure of Zn-containing greifensteinite. *Crystallogr. Rep.*, **49**, 942–945.
- Barton, M.D. & Young, S. (2002): Non-pegmatitic deposits of beryllium: mineralogy, geology, phase equilibria and origin. *Rev. Mineral. Geochem.*, **50**, 591–691.
- Chukanov, N.V., Möckel, S., Rastsvetaeva, R.K., Zadov, A.E. (2002): Greifensteinite, Ca₂Be₄(Fe²⁺,Mn)₅(PO₄)₆ · 6H₂O a new mineral from Greifenstein, Saxony. *Zapiski Rossiiskogo Mineralogicheskogo Obshchestva*, **131**(4), 47–52. (in Russian)
- Chukanov, N.V., Rastsvetaeva, R.K., Möckel, S., Zadov, A.E., Levitskaya, L.A. (2006): The roscherite group and its new representative member atencioite Ca₂Fe²⁺ □Mg₂Fe²⁺₂Be₄(PO₄)₆ (OH)₄ · 6H₂O. *New Data on Minerals*, **41**, 18–25.
- Chukanov, N.V., Atencio, D., Zadov, A.E., Menezes Filho, L.A.D., Coutinho, J.M.V. (2007): Guimarãesite, a new Zn-dominant monoclinic roscherite-group mineral from Itinga, Minas Gerais, Brazil. *New Data on Minerals*, **42**, 11–15.
- Clark, A.M., Fejer, E.E., Couper, A.G., von Knorring, O., Turner, R.W., Barstow, R.W. (1983): Iron-rich roscherite from Gunnislake, Cornwall. *Mineral. Mag.*, 47, 81–83.
- Fanfani, L., Nunzi, A., Zanazzi, P.F., Zanzari, A.R. (1975): The crystal structure of roscherite. *Tschermaks Mineralogische und Petrographische Mitteilungen*, 22, 266–277.
- Fanfani, L., Zanazzi, P.F., Zanzari, A.R. (1977): The crystal structure of triclinic roscherite. *Tschermaks Mineralogische und Petrographische Mitteilungen*, 24, 169–178.
- Feklichev, V.G. (1989): Diagnostic Constants of Minerals. Nedra, Moscow (in Russian).
- Fusswinkel, T., Wenzel, T., Wagner, H., Wälle, M., Lorenz, J. (2012): Arsenic distribution in an unconformity related hydrothermal vein system. *Goldschmidt 2012 Conference Abstracts*. *Mineralogical Magazine*, **76**, 877.
- Fusswinkel, T., Wagner, T., Wenzel, T., Wälle, M., Lorenz, J. (2013): Evolution of unconformity-related Mn–Fe–As vein mineralization, Sailauf (Germany): insight from major and trace elements in oxide and carbonate minerals. *Ore Geol. Rev.*, **50**, 28–51.
- Kolitsch, U. (1996): Bergslagit aus dem Rhyolith-Steinbruch bei Sailauf im Spessart. *Mineral. Welt*, 7(5), 45–46.
- Kovalenko, V.I. & Yarmolyuk, V.V. (1995): Endogenous rare metal ore formations and rare metal metallogeny of Mongolia. *Econ. Geol.*, **90**, 520–529.
- Leavens, P.B., White, J.S., Nelen, Y.A. (1990): Zanazziite, a new mineral from Minas Gerais, Brazil. *Mineral. Rec.*, 21, 413–417.
- Levinson, A.A. (1962): Beryllium-fluorine mineralization at Aguachile mountain, Coahuila, Mexico. Am. Mineral., 47, 67–74.
- Lindberg, M.L. (1958): The beryllium content of roscherite from the Sapucaia Pegmatite Mine, Minas Gerais, Brazil, and from other localities. *Am. Mineral.*, **43**, 824–838.
- Rastsvetaeva, R.K., Gurbanova, O.A., Chukanov, N.V. (2002): Crystal structure of greifensteinite Ca₂Be₄(Fe²⁺, Mn)₅(PO₄)₆(OH)₄ · 6H₂O. *Doklady Chem.*, **383**, 78–81.

- Rastsvetaeva, R.K., Barinova, A.V., Chukanov, N.V., Pietrashko, A. (2004): Crystal structure of a magnesium-rich triclinic analogue of greifensteinite. *Doklady Chem.*, **398**, 191–195.
- Rastsvetaeva, R.K., Barinova, A.V., Chukanov, N.V., Verin, I.A. (2005): Crystal structure of roscherite. *Doklady Chem.*, 403, 160–163.
- Rastsvetaeva, R.K., Chukanov, N.V., Verin, I.A., Atencio, D. (2007): The crystal structure of footemineite. *Doklady Earth Sci.*, **416**, 1053–1056.
- Rastsvetaeva, R.K., Rozenberg, K.A., Chukanov, N.V., Möckel, S. (2009): The crystal structure of iron-rich variety of zanazziite belonging to heteropolyhedral framework roscherite-group beryllophosphates. *Crystallogr. Rep.*, 54, 568–571.
- Shawe, D.R. (1966): Arizona-New Mexico and Nevada-Utah beryllium belts. United States Geological Survey Professional Paper, 550, C206–C213.
- Taucher, J., Walter, F., Postl, W. (1992): Mineralparagenesen in Pegmatiten der Koralpe. Teil 1: Die Lithium-Lagerstätte am Brandrücken, Weinebene, Koralpe, Kärnten. Die Minerale des feinkörnigen Spodumenpegmatits (MH-Pegmatit). *Matrixx, Mineralogische Nachrichten aus Österreich*, 1, 23–72. (in German)

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