This is a “preproof” accepted article for *Mineralogical Magazine*.
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10.1180/mgm.2025.23

Kantorite, $K_2NaMg(SO_4)_2F$, a new fumarolic mineral from the Tolbachik volcano, Kamchatka, Russia

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Abstract

The new mineral kantorite was found in the Arsenatnaya fumarole, Second scoria cone of the Northern Breakthrough of the Great Tolbachik Fissure Eruption, Tolbachik volcano, Kamchatka, Russia. The associated minerals are aphthitalite, langbeinite, arcanite, krasheninnikovite, vanthoffite, kononovite, wulffite, halite, sylvite, flinteite, fluoborite, chubarovite, johillerite, urusovite, zincite, tenorite, pseudobrookite, hematite, sanidine, and fluorophlogopite. Kantorite occurs as long-prismatic to acicular crystals up to 0.1 × 0.01 mm which form near-parallel and bush-like open-work clusters up to 0.2 mm across. It is transparent, colourless, with vitreous lustre. D_{calc} is 2.498 g cm^{-3}. Kantorite is optically biaxial (+), $\alpha = 1.447(2)$, $\beta = 1.449(2)$, $\gamma = 1.452(2)$ and $2V_{calc} = 79°$. The chemical composition (wt.%, electron microprobe data) is: Na_2O 9.80, K_2O 27.17, Rb_2O 0.12, MgO 12.02, CaO 0.09, SO_3 47.46, F 5.68, Cl 0.11, –O=(F,Cl) 2.42, total 100.03. The empirical formula calculated based on (O+F+Cl) = 9 *apfu* is $(K_{1.94}Na_{0.06})_{\Sigma 2.00}(Na_{1.00}Ca_{0.01})_{\Sigma 1.01}Mg_{1.00}(SO_{4.01})_{1.99}(F_{1.01}Cl_{0.01})_{\Sigma 1.02}$. The idealised formula is $K_2NaMg(SO_4)_2F$. Kantorite is orthorhombic, $Pna2_1$, $a = 6.9894(7)$, $b = 7.1378(7)$, $c = 17.925(2)$ Å, $V = 894.25(16)$ Å^3 and $Z = 4$. Strong reflections of the powder XRD pattern [d,Å(I)(hkl)] are: 8.99(91)(002), 4.83(57)(111), 4.498(43)(004), 3.588(47)(020), 3.511(74)(200), 3.270(43)(202), 2.926(100)(115), 2.805(44)(024), 2.768(53)(204) and 2.510(55)(220). The crystal structure was solved from single-crystal XRD data, $R_1 = 0.031$. The structure of kantorite is unique. It represents a quasi-framework in which the basic units are octahedra $[MgO_4F_2]$. They are linked *via* bridging F atoms to form infinite chains. These chains are encrusted by [SO_4] tetrahedra and assembled into the quasi-framework by alkali cations. The sulfate-encrusted chains of octahedra [MgO_4F_2] are topologically identical in the structures of kantorite and krasheninnikovite $KNa_2CaMg(SO_4)_3F$. The mineral is named in honour of the Russian mineralogist Boris Zinovievich Kantor (1930–2022).

Keywords: kantorite; new mineral; potassium sodium magnesium fluorosulfate; crystal structure; krasheninnikovite; fumarole sublimate; Tolbachik volcano.

Introduction

Anhydrous fluorosulfate minerals are few in number and very rare. Only seven natural hydrogen-free fluorosulfates without other species-defining anions were described to date: kogarkoite $Na_3(SO_4)F$ (Kogarko, 1961; Pabst and Sharp, 1973), grandreefite $Pb_2(SO_4)F_2$, pseudograndreefite $Pb_6(SO_4)F_{10}$ (Kampf *et al.*, 1989), thermessaite $K_2Al(SO_4)F_3$ (Demartin *et al.*, 2008), krasheninnikovite $KNa_2CaMg(SO_4)_3F$ (Pekov *et al.*, 2012), kononovite $NaMg(SO_4)F$ (Pekov *et al.*, 2015), and shuvalovite $K_2(Ca_2Na)(SO_4)_3F$ (Pekov *et al.*, 2016). The last three mineral species, anhydrous fluorosulfates with species-defining both alkali and alkali-earth cations, are known only in high-temperature sublimates of active fumaroles at the Tolbachik volcano (Kamchatka, Russia). In this article we describe the fourth of such minerals, kantorite $K_2NaMg(SO_4)_2F$.

Kantorite (Cyrillic: канторит) is named in honour of the Russian mineralogist Dr. Boris Zinovievich Kantor (1930–2022), a specialist in morphogenetic analysis of mineral crystals and aggregates (onthogeny of minerals). In particular, he made a significant contribution to the development of knowledge on the genesis of divergent crystals, spherulites of different types, and pseudo-stalactites (Kantor, 2003, 2021). Dr. Kantor was also a well-known mineral collector and made a great contribution to the popularization of mineralogical knowledge and mineral collecting among amateurs in Soviet Union and Russia in 1980s-2010s (Kantor, 1982, 1985, 1991, 2001, 2020).

Both the new mineral and its name have been approved by the IMA Commission on New Minerals, Nomenclature and Classification (IMA CNMNC), IMA2024–042. The accepted symbol is Kao. The holotype material is deposited in the systematic collection of the Fersman Mineralogical Museum, Moscow with the catalogue number 98804.

Occurrence and general appearance

Kantorite occurs at the Arsenatnaya fumarole located at the summit of the Second scoria cone of the Northern Breakthrough of the Great Tolbachik Fissure Eruption (NB GTFE), Tolbachik volcano, Kamchatka peninsula, Far-Eastern Region, Russia. The Second scoria cone of the NB GTFE is a monogenetic volcano formed in 1975 and still demonstrates strong fumarolic activity. The fumaroles here belong to oxidizing type and some of them are very richly mineralised (Fedotov and Markhinin, 1983; Vergasova and Filatov, 2016; Pekov *et al*., 2020). Arsenatnaya is a large, active oxidizing-type fumarole. The temperature of gases, measured by us in the period 2012–2023, reaches 500°C. It is a greatly prolific mineral locality: more than 200 mineral species have been reliably identified here, including 72 new minerals. The general data on the Arsenatnaya fumarole and its mineral associations were reported by Pekov *et al*. (2018) and Shchipalkina *et al*. (2020).

Kantorite is one of the rarest minerals at the Arsenatnaya fumarole. It was found in only two specimens collected by us in July 2014 from a hot pocket located about 1 m below the day surface. The temperature measured when collected in this area using a chromel-alumel thermocouple was about 300°C. The minerals associated with kantorite are aphthitalite, langbeinite (including its Zn-bearing variety), arcanite, krasheninnikovite, vanthoffite, kononovite, wulffite, halite, sylvite, flinteite, fluoborite, chubarovite, johillerite, urusovite, zincite, tenorite, pseudobrookite, hematite, sanidine, and fluorophlogopite.

Kantorite occurs as long-prismatic to acicular crystals up to 0.1 mm long and up to 10 μm (typically up to 5 μm) thick, elongated along [100]. The main crystal faces, forming the prismatic zone, belong to the {0*kl*} zone; crystals are terminated by the pinacoid {100}. The crystals form near-parallel and bush-like open-work clusters up to 0.2 mm across, typically together with aphthitalite (Fig. 1), on the surface of basalt scoria altered by fumarolic gas.

We suggest that kantorite was formed as a result of the interaction between hot volcanic gas and basalt scoria at the temperatures not lower than 300ºC. Fumarolic gas is an obvious carrier of S, F, Na and K, whereas basalt can be a source of Mg which has low volatility in volcanic gases (Symonds and Reed, 1993).

Physical properties and optical data

Kantorite is transparent, colourless, with white streak and vitreous lustre. It is brittle. One direction of perfect cleavage was observed under both the optical microscope and the scanning electron microscope; based on the crystal structure data (see below), we suggest the (010) cleavage. The fracture is stepped. Density calculated using the empirical formula and unit-cell volume found from single-crystal X-ray diffraction (XRD) data is 2.498 g cm^{-3}.

Kantorite is optically biaxial (+), α = 1.447(2), β = 1.449(2), γ = 1.452(2) (589 nm). The angle 2*V* could not be measured due to small size of the crystals, their acicular habit and preferred orientation in immersion liquid prevented observation at the cross sections perpendicular to optical axes; 2*V* (calc.) = 79°. In transmitted plane-polarized light, kantorite is colourless and non-pleochroic.

Raman spectroscopy

The Raman spectrum of kantorite (Fig. 2a) was obtained using an EnSpectr R532 spectrometer with a green laser (532 nm) at room temperature. The output power of the laser beam was about 4 mW. The spectrum was processed using the EnSpectr expert mode program in the range 150 to 4000 cm^{-1} with a resolution of 6 cm^{-1}. The backscattered Raman signal was collected with a 40× PlanCN objective (numerical aperture 0.65). Signal acquisition time for a single scan was 1 s and the signal was averaged over 200 scans. The diameter of the focal spot on the sample was about 5 µm. The spectrum was obtained for randomly oriented crystal.

The main bands in the Raman spectrum of kantorite correspond to S–O vibrations in $(SO_4)^{2-}$ groups (assignments are according to Nakamoto, 1986, and Prieto-Taboada *et al*., 2019):

1) weak bands in the range 1050-1220 cm^{-1} correspond to ν_3 antisymmetric stretching vibrations;
2) strong band of ν_1 symmetric stretching vibrations near 1000 cm^{-1};
3) bands in the range 600-660 cm^{-1} are assigned to ν_4 symmetric stretching vibrations;
4) bands in the range 430-500 cm^{-1} belong to ν_2 antisymmetric bending vibrations.

Bands lower 300 cm^{-1} are mainly classified as bands corresponding to Mg–O, Mg–F, Na–O and K–O vibrations, as well as lattice modes.

The lack of bands higher than 1220 cm^{-1} indicates the absence of groups with O–H, C–H, C–O, N–H, N–O and B–O bonds in kantorite.

The Raman spectrum of krasheninnikovite $KNa_2CaMg(SO_4)_3F$ (Fig. 2b), the mineral related to kantorite (see below), was obtained under the same conditions. Both spectra are similar in general pattern, however, demonstrate significant individual features in the number and position of bands that helps distinguish these minerals from one another.

Chemical composition

The chemical composition of kantorite was studied by electron microprobe using a Jeol JSM-6480LV scanning electron microscope (SEM) equipped with an INCA-Wave 500 wavelength-dispersive spectrometer (Laboratory of Analytical Techniques of High Spatial Resolution, Dept.

of Petrology, Moscow State University), with an acceleration voltage of 15 kV and a beam current of 10 nA; the electron beam spot area was 3 μm^2.

The chemical data in wt.% are given in Table 1. Contents of other elements with atomic numbers > 6 are below detection limits.

The empirical formula calculated on the basis of (O+F+Cl) = 9 atoms per formula unit is $(K_{1.94}Na_{0.06})_{\Sigma 2.00}(Na_{1.00}Ca_{0.01})_{\Sigma 1.01}Mg_{1.00}(SO_{4.01})_{1.99}(F_{1.01}Cl_{0.01})_{\Sigma 1.02}$. The idealised formula is $K_2NaMg(SO_4)_2F$ which requires Na_2O 9.21, K_2O 27.98, MgO 11.97, SO_3 47.58, F 5.64, –O=F 2.38, total 100 wt.%.

The Gladstone–Dale compatibility index (Mandarino, 1981), $1 - (K_p/K_c) = 0.008$, is superior.

X-ray crystallography and crystal structure determination details

Powder XRD data for kantorite (Table 2) were collected in Debye-Scherrer geometry by means of a Rigaku RAXIS Rapid II diffractometer equipped with curved (semi-cylindrical) imaging plate detector (r = 127.4 mm), using Co*K*α radiation (λ = 1.79021 Å) generated by a rotating anode (40 kV, 15 μA) with microfocus optics; exposure time was set to 15 min. The image plate was calibrated against NIST Si standard. The image-to-profile data processing was performed using osc2xrd software (Britvin *et al*., 2017). Parameters of the orthorhombic unit cell refined from the powder data are: a = 7.008(2), b = 7.146(2), c = 17.961(4) Å and V = 899.5(7) Å^3.

Single-crystal XRD studies of kantorite were carried out at room temperature using a Rigaku-Oxford diffraction XtaLAB Synergy-S diffractometer equipped with a microfocus X-ray tube (Mo*K*α radiation) and HyPix-6000 hybrid photon counting detector. Data collection and reduction procedures were performed using CrysAlisPro, version 1.171.37.34 (Rigaku Oxford Diffraction). The crystal structure was solved and refined using SHELX-2018 software package (Sheldrick, 2015) incorporated into the Olex2 v.1.5 graphical user environment (Dolomanov et al., 2009). Data collection information and basic structure refinement details are presented in Table 3, coordinates and equivalent displacement parameters of atoms and bond-valence sums are given in Table 4, anisotropic displacement parameters in Table 5, and selected interatomic distances in Table 6. The detailed information on the data collection, reduction procedures, structure solution and refinement can be retrieved from the Crystallographic Information File (CIF) included in Supplementary materials.

We also had an attempt to refine the structure of kantorite in the centrosymmetric space group *Pbcn* which also gives reasonable results but with disordered Na site. However, the free refinement in the space group $Pna2_1$ shows that Na is perfectly ordered with site occupancy factor = 1. This is concordant with the bond-valence sum for Na = 1.00 (Table 4). Therefore, the data available imply that the centrosymmetric space group describes only a simplified, “averaged” structural model rather than a real one.

Discussion

The crystal structure of kantorite is unique. It represents a quasi-framework in which the basic units are octahedra [MgO_4F_2] (Table 6). These octahedra are linked *via* bridging F atoms to form infinite chains running along the **a**-axis (Fig. 3). The chains of octahedra are encrusted by [SO_4] tetrahedra *via* common corner-sharing oxygen atoms and assembled into the quasi-framework by alkali cations. The sulfate-encrusted chains of octahedra [MgO_4F_2] are topologically identical in the structures of kantorite and another fluorosulfate mineral, krasheninnikovite $KNa_2CaMg(SO_4)_3F$ (Pekov *et al.*, 2012), Fig. 4. This determines the similarity of unit-cell parameters of these minerals: the *a* and *c* orthorhombic unit cell parameters of kantorite are comparable to the *c* and *a* hexagonal unit cell parameters of krasheninnikovite, respectively (Table 7). However, both chemical and structural differences between kantorite and krasheninnikovite are significant. The latter contains “additional” sulfate groups which are not involved into the coordination of octahedral chains. These sulfate groups $(SO_4)^{2-}$ are charge-balanced by the introduction of Ca^{2+} cations into the structure of krasheninnikovite. The relationship between the formulae of both minerals can be schematically represented as follows:

$$\underset{\text{kantorite}}{K_2NaMg(SO_4)_2F} \xrightarrow{K\leftrightarrow Na + CaSO_4} \underset{\text{krasheninnikovite}}{KNa_2CaMg(SO_4)_3F}$$

Kantorite and krasheninnikovite belong to different crystal systems and easily can be distinguished by powder X-ray diffraction patterns and optical data (Table 7).

Other chemically related hydrogen-free fluorosulfate minerals, kononovite $NaMg(SO_4)F$ (Pekov *et al.*, 2015) and shuvalovite $K_2(Ca_2Na)(SO_4)_3F$ (Pekov *et al.*, 2016), are quite different in terms of crystal structure from one another and from kantorite and krasheninnikovite. All four these fluorosulfates occur in the Arsenatnaya fumarole, of which kononovite, shuvalovite and kantorite are endemic minerals of this remarkable locality.

Acknowledgements

We are grateful to three anonymous referees for valuable comments. The study was conducted under the state assignment of Lomonosov Moscow State University (state task No. 121061600049-4). XRD investigation was carried out at the Research Centre for X-ray Diffraction Studies of St Petersburg University in accordance with the state task of the Russian Federation No. AAAA-A19-119091190094.

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Table 1. Chemical composition of kantorite.

Constituent	wt.%	Range	Standard deviation	Reference material
Na_2O	9.80	8.93 – 10.58	0.54	Albite
K_2O	27.17	26.36 – 28.47	0.81	Orthoclase
Rb_2O	0.12	0.00 – 0.31	0.12	$Rb_2Nb_4O_{11}$
MgO	12.02	10.90 – 13.28	0.92	MgF_2
CaO	0.09	0.00 – 0.30	0.09	$CaSiO_3$
SO_3	47.46	46.51 – 48.41	0.71	$SrSO_4$
F	5.68	5.12 – 6.51	0.53	MgF_2
Cl	0.11	0.00 – 0.39	0.11	Scapolite
–O=(F,Cl)	2.42			
Total	100.03			

Table 2. Powder X-ray diffraction data (*d* in Å) of kantorite.

I_{obs}	d_{obs}	I_{calc}*	d_{calc}**	*h k l*
91	**8.99**	98	8.963	002
23	6.67	20	6.631	011
57	**4.83**	55	4.811	111
43	**4.498**	55	4.481	004
7	4.390	5	4.362	112
47	**3.588**	60	3.569	020
74	**3.511**	67	3.495	200
30	3.332	4, 31	3.335, 3.316	114, 022
43	**3.270**	32	3.256	202
18	3.214	13	3.204	015
25	3.193	17	3.179	120
10	3.103	4	3.092	211
27	2.994	5, 1, 10	3.017, 2.996, 2.988	203, 122, 006
100	**2.926**	100	2.912	115
44	**2.805**	2, 47	2.806, 2.792	123, 024
53	**2.768**	51	2.756	204
12	2.577	3, 2, 9	2.593, 2.571, 2.564	124, 214, 116
55	**2.510**	9, 54	2.502, 2.497	205, 220
20	2.372	1, 12, 13	2.378, 2.362, 2.359	125, 215, 031
15	2.286	16, 4	2.279, 2.271	117, 206
12	2.220	8, 9	2.235, 2.210	131, 033
20	2.192	2, 8, 3	2.198, 2.184, 2.181	311, 132, 224
9	2.160	10, 1, 7	2.177, 2.164, 2.150	126, 216, 312
5	2.114	2	2.108	133
8	2.077	4	2.066	207
10	1.996	4, 8	1.994, 1.986	127, 314
18	1.961	5, 17	1.955, 1.939	231, 320
21	1.925	3, 23	1.921, 1.916	232, 226
7	1.906	3	1.906	322
6	1.896	6, 4	1.898, 1.884	028, 315
23	1.857	1, 22	1.855, 1.850	323, 119
9	1.797	1, 6, 8	1.798, 1.793, 1.789	136, 0.0.10, 324
7	1.720	11, 1, 1	1.724, 1.721, 1.714	235, 141, 325
5	1.693	1, 1, 2, 3	1.698, 1.690, 1.687, 1.682	142, 411, 1.1.10, 219
6	1.594	1, 1, 2, 1	1.604, 1.602, 1.589, 1.589	333, 0.2.10, 240, 0.1.11
6	1.567	2, 3, 1, 3	1.569, 1.565, 1.560, 1.560	420, 242, 334, 237
14	1.504	3, 15, 7	1.508, 1.498, 1.496	406, 244, 146
10	1.488	6, 8, 12	1.492, 1.481, 1.481	139, 424, 319
2	1.462	2	1.456	2.2.10
5	1.403	2, 1, 3	1.403, 1.399, 1.394	246, 239, 151
3	1.358	1, 1, 1	1.362, 1.356, 1.353	153, 512, 418
6	1.330	9, 3	1.329, 1.326	1.1.13, 055

*For the calculated pattern, only reflections with intensities ≥1 are given; **for the unit-cell parameters obtained from single-crystal data. The strongest reflections are marked in boldtype.

Table 3. Crystal parameters, data collection and structure refinement details for kantorite

Crystal Data	
Chemical formula	$K_2NaMg(SO_4)_2F$
Crystal size (mm^3)	0.005 × 0.005 × 0.04
Crystal system, Space group	Orthorhombic, $Pna2_1$ (#33)
a, b, c (Å)	6.9894(7), 7.1378(7), 17.925(2)
V (Å^3)	894.25(16)
Z	4
Data collection and refinement	
Radiation	Mo$K\alpha$ (λ = 0.71073 Å)
Temperature (K)	293(2)
$2\Theta_{max}$ (°)	truncated at 56
No. of measured, independent and with $I > 2\sigma_I$ reflections	6210, 2004, 1568
h, k, l range	$-9 \rightarrow 8$, $-9 \rightarrow 9$, $-21 \rightarrow 23$
F(000)	664
μ (mm^{-1})	1.68
No. refined parameters	137
$R_{int.}$, R_σ	0.046, 0.048
Flack parameter	0.38(14)
R_1 [$F \geq 4\sigma(F)$], wR_2	0.031, 0.068
R_1, wR_2 for all reflections	0.049, 0.073
GoF	0.99
Data completeness	0.998
Residual density (Δe^-), min, max	–0.38, 0.42

Table 4. Fractional coordinates and equivalent displacement parameters (U_{eq}, Å^2) of atoms and bond-valence sums (BVS, v.u.) for kantorite[a].

Site	***x***	***y***	***z***	**U_{eq}**	**BVS**[b]
Na1	0.9311(3)	0.1912(3)	0.50768(19)	0.0319(6)	1.00
K1	0.2179(3)	1.0497(4)	0.83245(10)	0.0210(5)	1.04
K2	0.7849(3)	0.4470(4)	0.16720(10)	0.0220(5)	1.01
Mg1	0.5061(3)	0.7585(3)	0.4979(3)	0.0121(3)	2.07
S1	0.7573(2)	0.4870(4)	0.38283(13)	0.0115(6)	6.16
S2	0.2445(3)	1.0163(4)	0.61387(14)	0.0139(6)	5.92
O1	0.8075(9)	0.2918(9)	0.3935(4)	0.0312(14)	2.01
O2	0.6937(11)	0.5233(11)	0.3073(4)	0.0321(18)	1.99
O3	0.6018(8)	0.5350(6)	0.4349(4)	0.0175(12)	2.16
O4	0.9241(8)	0.6071(6)	0.3991(3)	0.0198(12)	2.09
O5	0.1916(8)	1.2114(8)	0.6009(4)	0.0266(13)	2.05
O6	0.0777(8)	0.8941(7)	0.5957(3)	0.0208(13)	2.05
O7	0.4071(9)	0.9713(6)	0.5627(3)	0.0171(13)	2.04
O8	0.3046(11)	0.9799(11)	0.6908(4)	0.0287(17)	1.92
F1	0.7604(5)	0.8785(3)	0.4997(5)	0.0160(5)	0.90

[a] Crystallographic tables were created using PublCIF software (Westrip, 2010).

[b] Bond-valence sums were calculated using ECoN21 software (Ilinca, 2022).

Table 5. Anisotropic displacement parameters (Å^2) of atoms for kantorite.

Atom	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Na1	0.0328(12)	0.0299(11)	0.0329(15)	0.0131(10)	–0.0036(11)	–0.0071(12)
K1	0.0211(9)	0.0212(12)	0.0207(11)	–0.0010(9)	0.0029(11)	–0.0025(10)
K2	0.0210(9)	0.0223(12)	0.0228(11)	–0.0013(10)	0.0025(12)	–0.0013(10)
Mg1	0.0086(6)	0.0100(6)	0.0176(7)	0.0008(5)	–0.0002(6)	–0.0012(7)
S1	0.0081(12)	0.0084(12)	0.0181(14)	0.0011(6)	0.0003(9)	–0.0021(10)
S2	0.0141(14)	0.0159(15)	0.0118(13)	–0.0003(6)	–0.0003(9)	–0.0023(10)
O1	0.031(3)	0.015(3)	0.048(4)	0.010(3)	–0.002(3)	–0.004(3)
O2	0.029(4)	0.049(5)	0.018(4)	–0.009(4)	0.002(3)	–0.002(3)
O3	0.012(3)	0.019(3)	0.022(3)	–0.005(2)	0.003(3)	–0.007(2)
O4	0.014(3)	0.020(2)	0.025(3)	–0.001(3)	0.002(3)	–0.004(2)
O5	0.024(3)	0.011(3)	0.045(4)	0.003(3)	0.001(3)	–0.002(3)
O6	0.015(3)	0.026(3)	0.021(3)	–0.012(3)	0.002(3)	–0.006(2)
O7	0.012(3)	0.015(3)	0.024(4)	0.003(2)	0.004(3)	–0.005(2)
O8	0.026(3)	0.046(5)	0.014(4)	0.003(4)	–0.009(3)	0.000(3)
F1	0.0062(11)	0.0137(10)	0.0281(14)	–0.0003(16)	0.0006(11)	–0.002(3)

Table 6. Selected bond lengths (Å) in the structure of kantorite*

Bond	**Length**	**Bond**	**Length**
Na1–O1	2.335(7)	Mg1–O3	2.066(6)
Na1–O3	2.394(6)	Mg1–O4	2.095(7)
Na1–O5	2.475(6)	Mg1–O6	2.123(6)
Na1–O5	2.465(6)	Mg1–O7	2.034(6)
Na1–O6	2.835(6)	<Mg1–O>	2.080
Na1–O7	2.609(5)	Mg1–F1	1.973(4)
<Na1–O>	2.519	Mg1–F1	1.977(4)
Na1–F1	2.535(4)		
		S1–O1	1.449(6)
K1–O1	2.678(7)	S1–O2	1.448(8)
K1–O2	2.918(8)	S1–O3	1.473(7)
K1–O2	3.142(8)	S1–O4	1.476(6)
K1–O3	2.894(6)	<S1–O>	1.462
K1–O4	2.803(6)		
K1–O4	2.900(5)	S2–O5	1.460(6)
K1–O8	2.657(7)	S2–O6	1.493(6)
<K1–O>	2.856	S2–O7	1.495(6)
K1–F1	3.046(8)	S2–O8	1.465(7)
		<S2–O>	1.478
K2–O2	2.647(7)		
K2–O5	2.717(6)		
K2–O6	2.914(6)		
K2–O6	2.865(6)		
K2–O7	2.859(7)		
K2–O8	3.140(8)		
K2–O8	2.909(7)		
<K2–O>	2.864		
K2–F1	3.058(8)		

*Average *atom*-oxygen bond lengths were calculated separately from *atom*-fluorine bond lengths, as oxygen and fluorine represent the different chemical elements.

Table 7. Comparative data for kantorite and krasheninnkiovite.

Mineral	Kantorite	Krasheninnikovite
Ideal formula	$K_2NaMg(SO_4)_2F$	$KNa_2CaMg(SO_4)_3F$
Crystal system	Orthorhombic	Hexagonal
Space group	$Pna2_1$	$P6_3/mcm$
Unit cell data:		
a, Å	6.9874(7)	16.6682(2)
b, Å	7.1378(7)	
c, Å	17.925(2)	6.9007(1)
V, $Å^3$	894.25(16)	1660.36(4)
Z	4	6
Strong lines of the powder X-ray diffraction pattern: *d*, Å – *I*, %	8.99 – 91	4.286 – 22
	4.83 – 57	3.613 – 24
	4.498 – 43	3.571 – 17
	3.588 – 47	3.467 – 42
	3.511 – 74	3.454 – 43
	3.270 – 43	3.153 – 100
	2.926 – 100	3.116 – 22
	2.805 – 44	2.660 – 39
	2.768 – 53	2.085 – 17
	2.510 – 55	
D(calc.), g cm^{-3}	2.50	2.67
Optical data	Biaxial (+)	Uniaxial (–)
	α = 1.447(2)	ω = 1.500(2)
	β = 1.449(2)	ε = 1.492(2)
	γ = 1.452(2)	
Source	this work	Pekov *et al*., 2012

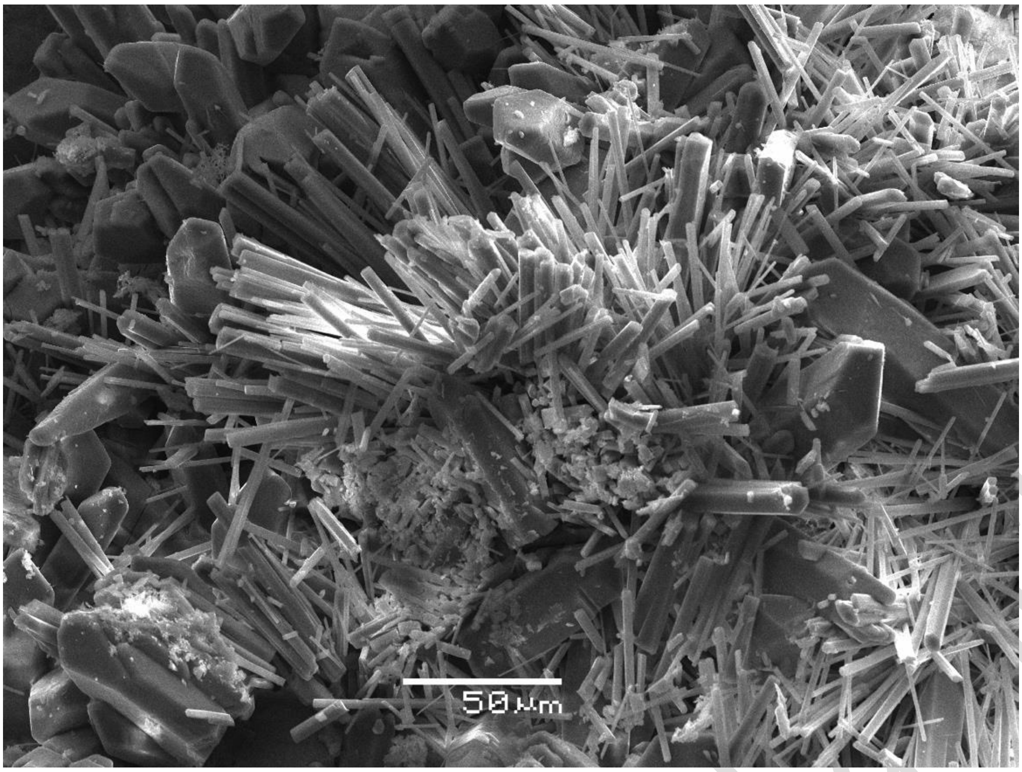
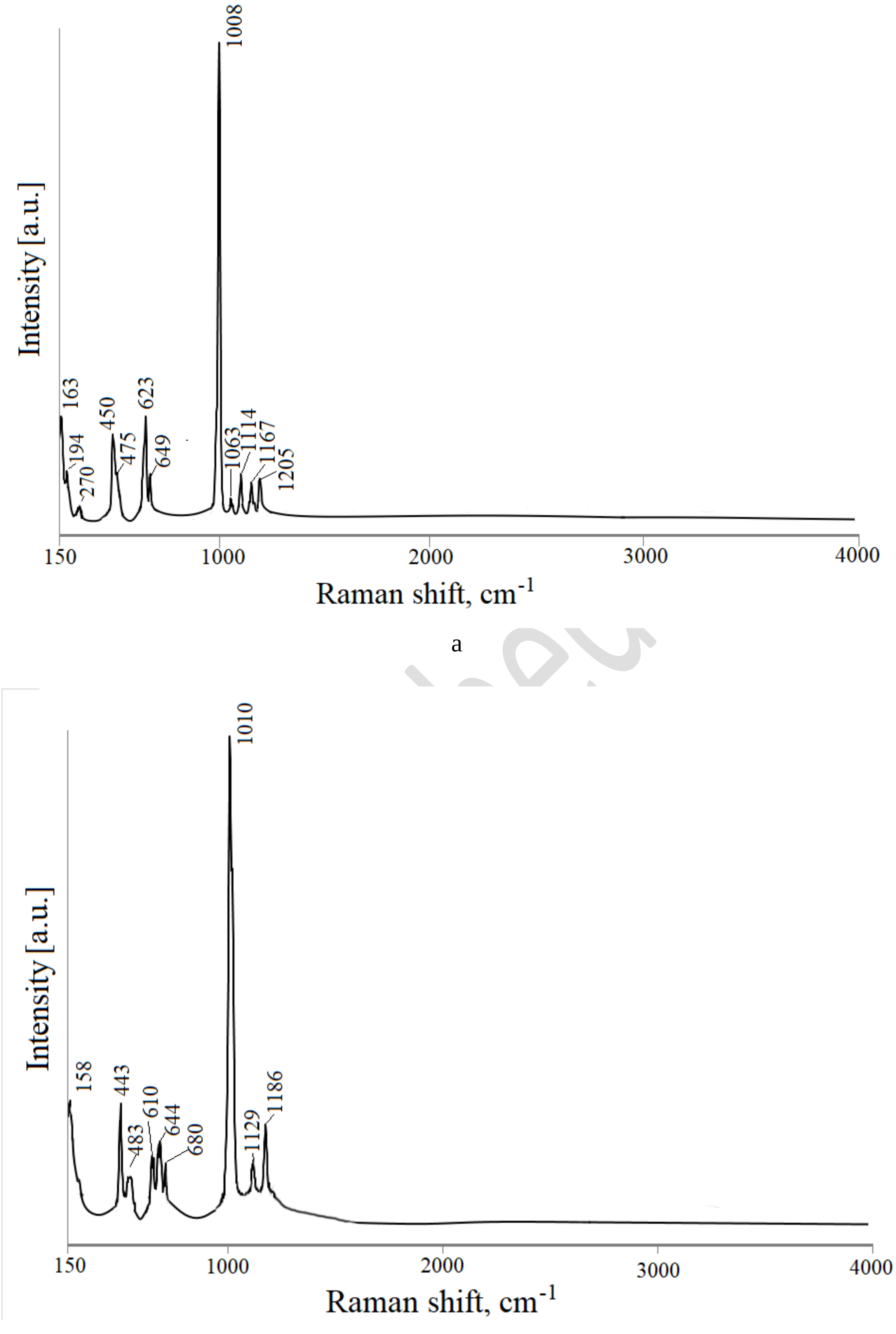


Figure 1. Clusters of long-prismatic to acicular crystals of kantorite associated with pyramidal-prismatic (resembling typical quartz crystals in shape) aphthitalite crystals. SEM image, second-electron mode.



a

b

Figure 2. The Raman spectra of kantorite (a) and krasheninnikovite (b).

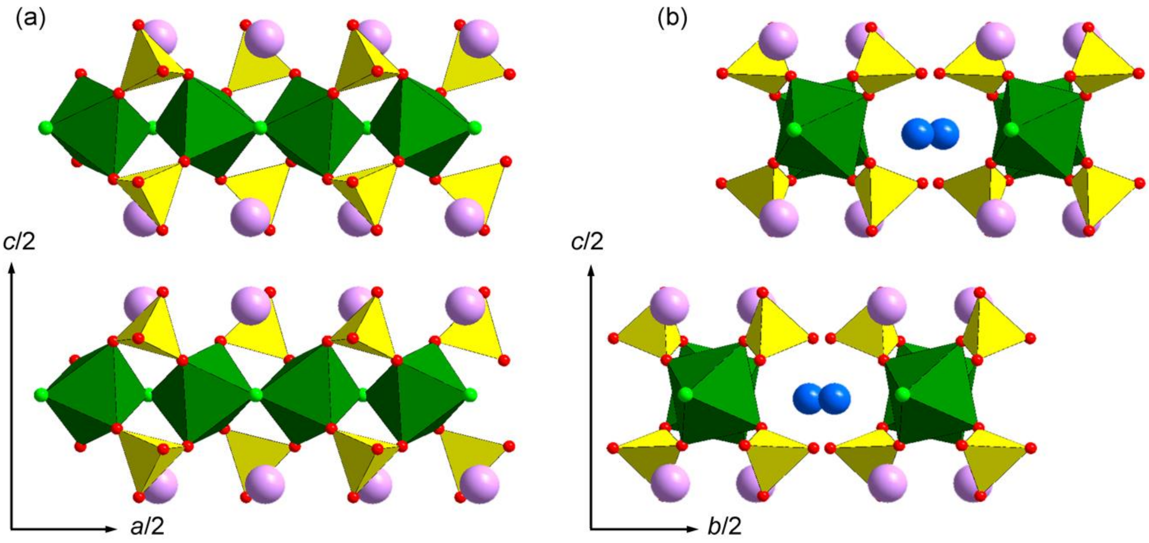


Figure 3. Crystal structure of kantorite. Octahedra [MgO_4F_2] are linked by bridging F atoms to form infinite chains running along the *a* axis, in two projections. The octahedral chains are encrusted by [SO_4] tetrahedra *via* common corner-sharing oxygen atoms, and connected by alkali cations to form a quasi-framework. Legend: green octahedra = [MgO_4F_2]; yellow tetrahedra = [SO_4]; red balls = oxygen; green balls = fluorine; blue balls = sodium; purple balls = potassium.

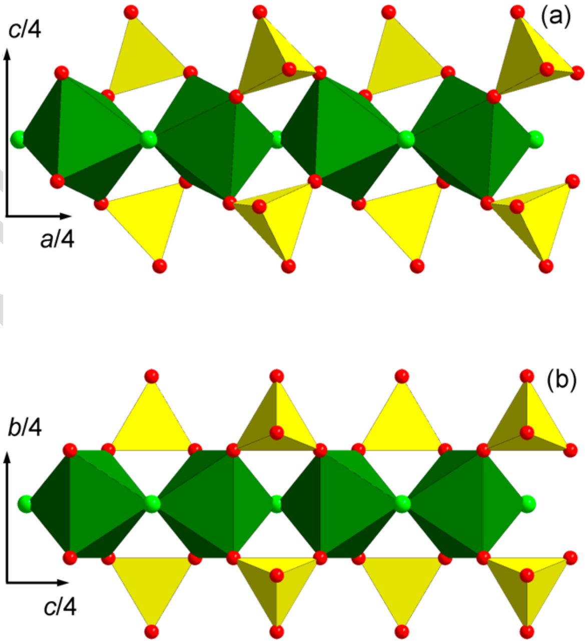


Figure 4. The basic common structural units of (a) kantorite and (b) krasheninnikovite: infinite chains of octahedra [MgO_4F_2] encrusted by sulfate tetrahedra. The occurrence of these chains determines the similarity of unit-cell parameters of both minerals (see Table 7). For legend see Figure 3.