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Aiolosite, $Na_2(Na_2Bi)(SO_4)_3Cl$, a new sulfate isotypic to apatite from La Fossa Crater, Vulcano, Aeolian Islands, Italy

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ABSTRACT

Aiolosite, ideally $Na_4Bi(SO_4)_3Cl$, or better $Na_2(Na_2Bi)(SO_4)_3Cl$, is a new sulfate mineral isotypic to apatite. It was found in an active medium-temperature intracrater fumarole at La Fossa crater, Vulcano Island, Aeolian archipelago, Sicily, Italy. It occurs as acicular to slender prismatic crystals up to 0.5 mm long in an altered pyroclastic breccia, together with alunite, anhydrite, demicheleite-(Br), demicheleite-(Cl), bismuthinite, and panichiite. The symmetry is hexagonal (class $6/m$), space group $P6_3/m$, with $a = 9.626(3)$, $c = 6.880(3)$ Å, $V = 552.1(3)$ Å^3, $Z = 2$. The habit is prismatic, terminated by the pinacoid or, more rarely, by a bipyramid. Aiolosite is colorless to white, with white streak; the luster vitreous. It is non-fluorescent. The calculated density is 3.589 g/cm^3. The mineral is nonpleochroic, uniaxial (+), $n_\omega = 1.59(1)$, $n_\varepsilon = 1.60(1)$, mean $n_{obs} = 1.593$ (589 nm), $n_{calc} = 1.620$. The chemical analysis gave Na_2O 20.65, K_2O 0.96, Bi_2O_3 32.49, SO_3 41.27, Cl 4.02, Br 0.75, (H_2O 0.57 from structure refinement), –O = (Cl + Br) 0.98 wt%, total 99.73, corresponding to the empirical formula calculated on the basis of 13 anions: $Na_2(Na_{1.95}K_{0.12}Bi^{3+}_{0.83})_{\Sigma 2.90}S_{3.06}O_{12.08}[Cl_{0.67}Br_{0.06}(H_2O)_{0.19}]_{\Sigma 0.92}$. The crystal structure has been refined to a final R index of 0.048. One of the two independent Ca sites of apatite is exclusively occupied by Na, and the other one by statistically distributed Na and Bi. The SO_4^{2-} anion replaces the PO_4^{3-} anion of apatite; the chloride anion is located in the partially occupied (s.o.f. = 0.81) position at $x = 0$, $y = 0$, $z = 0$. Whenever the chloride position is vacant, the position at $x = 0$, $y = 0$, $z = 1/4$ is occupied by water (s.o.f. = 0.19). The strongest 6 lines in the X-ray powder diffraction pattern [d_{obs} (Å) (I) hkl] are: 2.853 (100) (121), 2.775 (85) (112), 3.432 (45) (002), 1.965 (35) (222), 2.306 (25) (310), 4.787 (20) (110). Both the mineral and the mineral name have been approved by the IMA CNMNC (No. 2008-015).

Keywords: Aiolosite, apatite structure, new mineral species, bismuth, sulfates, crystal structure, Vulcano Island, Aeolian Islands, Italy

INTRODUCTION

The new mineral aiolosite, $Na_2(Na_2Bi)(SO_4)_3Cl$, was discovered when investigating the fumaroles at La Fossa crater, Vulcano, Aeolian Islands, where a considerable number of new species have been observed in recent years [see for instance Garavelli et al. (1997, 2005), Campostrini et al. (2008), Demartin et al. (2008a, 2008b, 2008c, 2009a, 2009b, 2009c) and references therein]. Here, a description of the new species, as well as its properties and crystal structure, which is related to that of apatite, are reported.

The name of the mineral is from Aiolos (Aίολοσ, Latinized to Aeolus), the god ruler of the winds in Greek mythology. The Aeolian Islands (*Isole Eolie* in Italian) took their name from him. Both the mineral and the mineral name have been approved by the Commission on New Minerals, Nomenclature and Classification of the IMA (no. 2008-015). The holotype is deposited (no. 2008-3) in the Reference Collection of Dipartimento di Chimica Strutturale e Stereochimica Inorganica of Università degli Studi di Milano.

OCCURRENCE AND PHYSICAL PROPERTIES

Aiolosite occurs in a medium-temperature (250 °C) intracrater fumarole, as acicular to slender prismatic translucent crystals, up to 0.5 mm long, on altered pyroclastic breccia, together with alunite, anhydrite, bismuthinite, demicheleite-(Br), demicheleite-(Cl), and panichiite (Demartin et al. 2008c, 2009a, 2009c). The crystal habit is prismatic, terminated by the pinacoid or, more rarely, by a bipyramid (see Figs. 1a and 1b). The c:a ratio calculated from the unit-cell parameters is 0.7147. The mineral is colorless to white, the streak is white, and the luster is vitreous. We did not observe any fluorescence, either under SW or LW ultraviolet radiations. Tenacity is brittle. Cleavage and fracture were not observed. The calculated density is 3.589 g/cm^3 (from the empirical formula reported below and the unit-cell data). The mineral is nonpleochroic, uniaxial (+), $n_\omega = 1.59(1)$, $n_\varepsilon = 1.60(1)$, mean $n_{obs} = 1.593$ (589 nm) by immersion methods in bromoform and monochloronaphtalene, $n_{calc} = 1.620$ (Gladstone-Dale); $1 - (K_P/K_C) = -0.070$, fair (Mandarino 1981).

CHEMICAL DATA

Chemical analyses were carried out by means of a JEOL JSM 5500 LV scanning electron microscope, equipped with an IXRF EDS 2000 electron microprobe (EDS mode, 20 kV,

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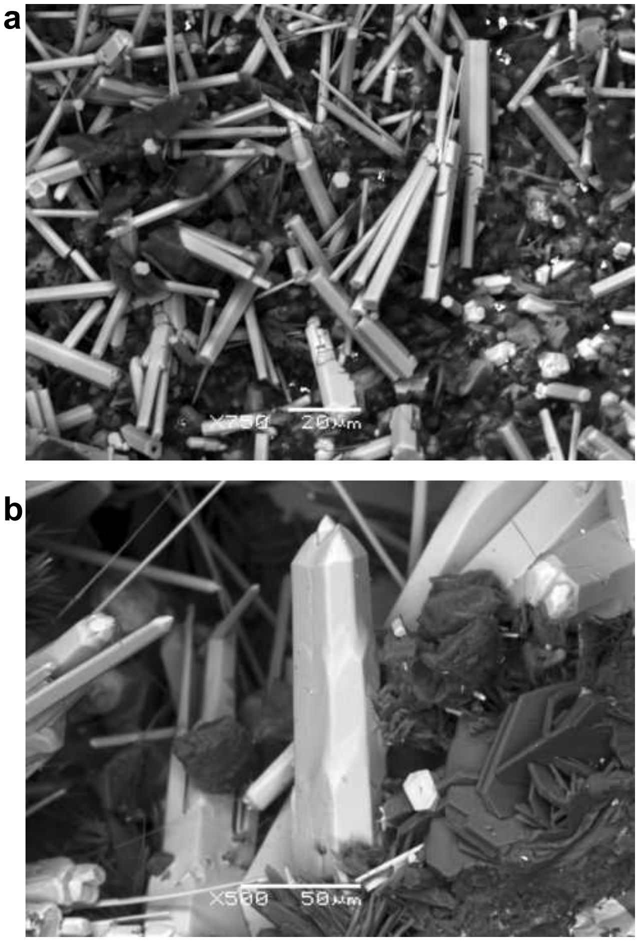

FIGURE 1. (**a–b**) Scanning electron microscope (SEM) images (BSE) of aiolosite.

10^{-11}A, 2 µm beam diameter). The mean analytical results are reported in Table 1; the empirical formula $Na_2(Na_{1.95}K_{0.12}Bi^{3+}_{0.83})_{\Sigma 2.90}S_{3.06}O_{12.08}[Cl_{0.67}Br_{0.06}(H_2O)_{0.19}]_{\Sigma 0.92}$ was calculated on the basis of a total of 13 anions, and considering the distribution of the cations in two different sites, similarly to all apatite-like compounds; the formula obtained from the structure refinement is: $Na_2(Na_{2.13}Bi^{3+}_{0.87})_{\Sigma 3.00}(SO_4)_3[Cl_{0.81}(H_2O)_{0.19}]_{\Sigma 1.00}$. Both these formulae satisfy the charge balance (the total charge of the cations is 25.3 vs. 25.3 e⁻ for the anions and 25.1 vs. 25.2 e⁻, respectively). The end-member formula can be written as $Na_2(Na_2Bi)(SO_4)_3Cl$, which requires: Na_2O 19.85, Bi_2O_3 37.30, SO_3 38.46, Cl 5.68, –O = Cl –1.28, total 100.00 wt%.

X-RAY DATA AND REFINEMENT OF THE STRUCTURE

X-ray powder diffraction data were obtained using a Gandolfi camera 114.6 mm in diameter, with Cu*K*α radiation (Table 2). A least-squares fit of these data provided the following hexagonal unit-cell parameters: $a = 9.602(1)$, $c = 6.863(1)$ Å, $V = 548.0(1)$ Å^3.

Single-crystal diffraction data were collected from a crystal fragment (0.10 × 0.02 × 0.02 mm) with Mo*K*α radiation ($\lambda = 0.71073$ Å), using a BRUKER Apex II diffractometer equipped with a 2K CCD detector. A one-minute frame-time and 0.3° frame width were used. A total of 6239 reflections, corresponding to a complete scanning of the reciprocal lattice up to $2\theta_{max} = 61.5°$, were measured; of these, 596 were unique. The unit-cell dimensions obtained from the single crystal were refined by least-squares from 1222 reflections with $I > 5\sigma(I)$; their values are given in Table 3, together with other details concerning the data collection and refinement. The diffraction data were reduced using the Bruker program SAINT, and were corrected for Lorentz, polarization, and background effects. No violations of the systematic absences of the space group $P6_3/m$ were observed. An absorption correction was applied (maximum and minimum transmission factors 0.746 and 0.345, respectively) using the SADABS program (Sheldrick 2000). The structure was solved by direct methods and refined using the SHELXL97 program (Sheldrick 1997) implemented in the WinGX suite (Farrugia 1999). The occupation parameters for the two metal sites as well as those of the halide ion and of the water molecule were refined; in view of steric requirements (see below), the sum of the halide and water occupancy was constrained to unity. Such parameters show the M1 site to be exclusively occupied by Na, whereas the M2 site contains Na and Bi statistically distributed. These results are in close agreement with the chemical analysis (see Table 1). Selected interatomic distances and angles for aiolosite are reported in Table 4. The final coordinates and displacement parameters of the atoms are reported in Table 5. The final *R* is 0.048 for 441 observed reflections [$I > 2\sigma(I)$]. Projections of the crystal structure are provided in Figures 2a and 2b.

TABLE 1. Chemical composition of aiolosite

Constituent	wt%	Range	Std. dev.	Probe standard
Na_2O	20.65	18.73–23.26	0.1	Omphacite
K_2O	0.96	0.22–1.93	0.2	K-feldspar
Bi_2O_3	32.49	30.52–35.74	0.1	Synthetic Bi_2Se_3
SO_3	41.27	37.84–44.03	0.1	Synthetic $CaSO_4$
Cl	4.02	3.20–4.68	0.1	Scapolite
Br	0.75	0.35–1.63	0.2	Synthetic TlBr
H_2O*	0.57			
–O=Cl	–0.98			
Total	99.73			

* From structure refinement.

TABLE 2. X-ray powder-diffraction data for aiolosite

I/I_o†	*hkl*	d_{obs} (Å)	d_{calc} (Å)*
20	110	4.787	4.801
5	111	3.923	3.934
45	002	3.432	3.431
100	121, $\bar{3}11$, $\bar{2}31$	2.853	2.858
85	112, 030	2.775	2.791
20	$\bar{1}32$, $\bar{3}22$	2.312	2.317
25	310, $\bar{1}40$	2.306	2.306
15	311, $\bar{1}41$, $\bar{4}31$	2.189	2.186
5	040, $\bar{4}40$	2.081	2.079
10	113, $\bar{1}23$	2.068	2.065
35	222, $\bar{2}42$	1.965	1.967
5	$\bar{2}50$, $\bar{5}30$, 520	1.909	1.908
15	123, $\bar{2}33$	1.851	1.849
15	231, $\bar{5}31$	1.836	1.838
5	$\bar{4}42$, 042	1.779	1.778
20	004	1.716	1.715
3	322, $\bar{5}32$	1.667	1.667
3	133, $\bar{3}43$	1.624	1.624
10	142, $\bar{4}52$	1.604	1.604
5	$\bar{2}60$, $\bar{6}40$	1.572	1.571
5	331, $\bar{3}61$	1.559	1.558
5	052, $\bar{5}52$	1.496	1.496
15	$\bar{6}11$, 151	1.459	1.459
5	242, $\bar{4}62$	1.429	1.428
1	314, $\bar{4}34$	1.377	1.376

* Calculated from the unit cell: $a = 9.602(1)$ $c = 6.863(1)$ Å, obtained from least-squares refinement from the above data using the program UNITCELL (Holland and Redfern 1997).

† Determined densitometrically from a Gandolfi camera film.

RESULTS AND DISCUSSION

The structure analysis shows aiolosite to be isotypic to apatite (with $P6_3/m$ symmetry), where the cations are distributed over two independent sites M1 and M2 (Wyckoff notations 4*f* and 6*h*, respectively). This structural type is particularly widespread both in nature and in synthetic compounds. All these substances derive from the ideal apatite-(CaF) formula $Ca_5(PO_4)_3F$ by replacing the Ca^{2+} ion with other cations such as Pb^{2+}, Na^+, REE^{3+}, Sr^{2+}; the P atom in the phosphate group is usually replaced by other small tetrahedrally coordinated atoms such as As, V, S, or Si; and F is replaced by Cl, OH, or both. In some cases, such as hedyphane $Ca_2Pb_3(AsO_4)_3Cl$ or phosphohedyphane, the $P6_3/m$ symmetry is maintained (Rouse et al. 1984; Kampf et al. 2006), whereas in others the symmetry is lowered due to partial ordering of the different cations. For instance, ordering in the M2 sites leads to different subgroups of $P6_3/m$, such as $P6_3$ in fluorcaphite $(Ca,Sr,Na,Ce)_5(PO_4)_3F$ (Khomyakov et al. 1996, 1997; Rastsvetaeva and Khomyakov 1996), or $P3$ in deloneite-(Ce) $Na(Ca,Sr)_3Ce(PO_4)_3(F,OH)$ (Rastsvetaeva and Khomyakov 1996; Khomyakov et al. 1997).

The alternation of different kinds of atoms in the M2 sites, which transforms the sixfold symmetry axis into a $\overline{6}$ axis or a threefold axis, is favored by a marked difference between the atoms in question (e.g., in the ionic radii): for instance, if one atom is appreciably "bigger" than another, a model having two "big" atoms close to each other is energetically less favored than an "ordered" structure showing an alternating distribution. On the other hand, the entropy relative to an entirely "disordered" distribution (which would maintain the $P6_3/m$ symmetry of the apatite structure) is higher. On these grounds, considering the relationships between entropy and free energy, as for most cases of order-disorder, temperature also becomes very important in determining the distribution in the M2 sites and, consequently, the symmetry and the structural type. In some cases, the symmetry lowering is even more marked, as for instance for the low-temperature modification of caracolite $Na_2(NaPb_2)(SO_4)_3Cl$ (Schneider 1969) that displays monoclinic $P2_1/m$ symmetry, whereas the high-temperature modification shows $P6_3/m$ symmetry.

For aiolosite, the $P6_3/m$ symmetry is maintained, in agreement with the above criteria, due to the close similarity in the ionic radii of Na^+ and Bi^{3+} (Shannon 1976). The reason why Bi exclusively prefers the M2 site instead of M1 can be mainly ascribed to a Coulombic effect, in view of the higher charge of Bi^{3+} relative to Na^+, since the average <M2-O> distance (2.516 Å) is shorter than <M1-O> (2.617 Å). A similar effect also occurs for Ca in cesanite $Na_2(NaCa_2)(SO_4)_3OH$, which was described to show $P6_3/m$ symmetry by Tazzoli (1983) and instead $P\overline{6}$ symmetry by Piotrowski et al. (2002). For hedyphane, where the formal charges of Ca^{2+} and Pb^{2+} are instead the same, the exclusive presence of Pb in the M2 site is probably due to the presence of a stereoactive lone pair of electrons characteristic of the Pb^{2+} ion in many compounds (Moore et al. 1982).

The average of the S-O bond lengths in the sulfate group (1.459 Å) is identical with the corresponding average found in synthetic cesanite by Piotrowski et al. (2002). A similar comparison with high caracolite, another sulfate with the apatite structure, might be interesting, but it is not currently useful due to the low accuracy of the presently available data (Schneider 1969).

On looking at the atomic displacement parameters (ADPs), a notably high value of U_{33} is observed for O2 (Table 5). However

TABLE 3. Single-crystal data and refinement parameters for aiolosite

Crystal system	hexagonal
Space group	$P6_3/m$ (no.176)
a (Å)	9.626(2)
c (Å)	6.880(3)
V (Å^3)	552.1(3)
Z	2
Radiation	Mo$K\alpha$
μ (cm^{-1})	14.90
D_{calc} (g/cm^3)	3.589
Measured reflections	6239
Independent reflections	596
Observed reflections [$I > 2\sigma(I)$]	441
Parameters refined	44
Final R and $wR2$*	0.0480 0.1095
S	1.080

* $w = 1/[\sigma^2(F_o^2) + (0.0487k)^2 + 4.100k]$, where $k = (F_o^2 + 2F_c^2)/3$.

TABLE 4. Selected interatomic distances (Å) and angles (°)

M1-O1 ×3	2.469(5)	S-O1	1.460(6)
M1-O2 ×3	2.568(6)	S-O2	1.458(7)
M1-O3 ×3	2.815(8)	S-O3 ×2	1.460(5)
<M1-O>	2.617	<S-O>	1.459
M2-O1	2.814(7)	O1-S-O2	112.0(4)
M2-O2	2.351(7)	O1-S-O3 ×2	111.9(3)
M2-O3 ×2	2.440(6)	O2-S-O3 ×2	107.1(4)
M2-O3 ×2	2.562(7)	O3-S-O3	106.5(6)
M2-OW	2.444(1)	<O-S-O>	109.4
<M2-O>	2.516		

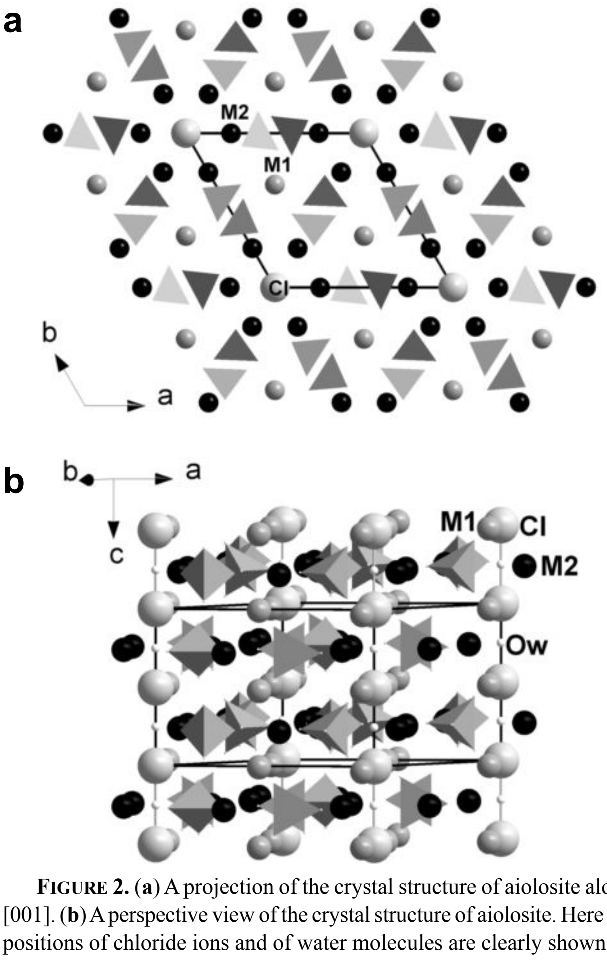

FIGURE 2. (**a**) A projection of the crystal structure of aiolosite along [001]. (**b**) A perspective view of the crystal structure of aiolosite. Here the positions of chloride ions and of water molecules are clearly shown.

TABLE 5. Atomic coordinates and displacement parameters ($U_{eq}/U_{i,j}$) for aiolosite

Atom	Wyckoff notation	Site occupancy	*x*	*y*	*z*	U_{eq}
M1	4*f*	Na 1.00	1/3	2/3	0.0067(6)	0.0206(8)
M2	6*h*	Na 0.712(8) Bi 0.288(8)	0.2534(1)	0.9990(1)	1/4	0.0331(4)
S	6*h*		0.4029(2)	0.3742(2)	1/4	0.0201(5)
O1	6*h*		0.3320(8)	0.4775(8)	1/4	0.036(1)
O2	6*h*		0.5776(8)	0.4664(9)	1/4	0.058(2)
O3	12*i*		0.3543(9)	0.2695(7)	0.0800(9)	0.064(2)
OW	2*a*	0.19(2)	0	0	1/4	0.08(3)
Cl	2*b*	0.81(2)	0	0	0	0.087(4)

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
M1	0.0213(11)	0.0213(11)	0.0193(18)	0	0	0.0107(5)
M2	0.0339(6)	0.0225(5)	0.0425(7)	0	0	0.0137(4)
S	0.0195(9)	0.0187(9)	0.0219(9)	0	0	0.0095(7)
O1	0.048(4)	0.044(4)	0.032(3)	0	0	0.036(3)
O2	0.022(3)	0.032(4)	0.114(8)	0	0	0.010(3)
O3	0.105(5)	0.061(4)	0.053(4)	−0.033(3)	−0.046(4)	0.060(4)
Cl	0.050(3)	0.050(3)	0.162(11)	0	0	0.025(1)

such a particular value is not unique because the corresponding root mean-square displacements, R, for O2 and O3 are similar and are about twice as large as those of O1 [R_{max}/R_{min} = 5.23 and 5.84 vs. 2.63, respectively]. The difference between the value of U_{33} for O2 and that for O3 arises because the largest mean-square displacement of the former is aligned along the *z* axis. The behavior with respect to O1 is however physically significant and a similar situation was observed for cesanite by Tazzoli (1983). An exhaustive explanation of such a phenomenon can be only achieved by complex lattice-dynamical calculations (Gramaccioli 2002); however, for disordered compounds those are much beyond the usual practice.

The chloride anion is located in the partially occupied Wyckoff position 2*b* at $x = 0$, $y = 0$, $z = 0$, (s.o.f. = 0.81 from structure refinement, in agreement with charge balance). The shortest contacts of this anion with its surroundings are two symmetry-equivalent Cl···M2 distances, 2.989(1) Å long. Due to steric requirements (the 2*a* and 2*b* positions are too close to each other to be occupied at the same time), and to the reluctance of such structures to form "true" vacancies, whenever the halide position is vacant, the Wyckoff position 2*a* at $x = 0$, $y = 0$, $z = 1/4$ is occupied (s.o.f. = 0.19) by water (not by OH^- ions, due to charge-balance requirements). The occupation of different sites by the "larger" chloride ions and water is in agreement with the results observed for the other minerals isotypic to apatite, the chloride ion always being at the 2*b* position and the OH^- or the F^- anions at 2*a*.

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REFERENCES CITED

Campostrini, I., Demartin, F., Gramaccioli, C.M., and Orlandi, P. (2008) Hephaistosite, $TlPb_2Cl_5$, a new thallium mineral species from La Fossa crater, Vulcano, Aeolian Islands, Italy. Canadian Mineralogist, 46, 701–708.

Demartin, F., Gramaccioli, C.M., Campostrini, I., and Orlandi, P. (2008a) Knasibfite, $K_3Na_4[SiF_6]_3[BF_4]$, a new hexafluorosilicate-tetrafluoroborate from La Fossa crater, Vulcano, Aeolian Islands, Italy. Canadian Mineralogist, 46, 447–453.

——— (2008b) Thermessaite $K_2[AlF_3|SO_4]$, a new ino-aluminofluoride-sulfate from La Fossa crater, Vulcano, Aeolian Islands, Italy. Canadian Mineralogist, 46, 693–700.

——— (2008c) Demicheleite, BiSBr, a new mineral from La Fossa crater, Vulcano, Aeolian Islands, Italy. American Mineralogist, 93, 1603–1607.

Demartin, F., Campostrini, I., and Gramaccioli, C.M. (2009a) Panichiite, natural ammonium hexachlorostannate, $(NH_4)_2SnCl_6$, from La Fossa crater, Vulcano, Aeolian Islands, Italy. Canadian Mineralogist, 47, 367–372.

Demartin, F., Gramaccioli, C.M., and Campostrini, I. (2009b) Steropesite Tl_3BiCl_6, a new thallium bismuth chloride from La Fossa crater, Vulcano, Aeolian Islands, Italy. Canadian Mineralogist, 47, 373–380.

——— (2009c) Demicheleite-(Cl), BiSCl, a new mineral from La Fossa crater, Vulcano, Aeolian Islands, Italy. American Mineralogist, 94, 1045–1048.

Farrugia, L.J. (1999) WinGX suite for small-molecule single-crystal crystallography. Journal of Applied Crystallography, 32, 837–838.

Garavelli, A., Laviano, R., and Vurro, F. (1997) Sublimate deposition from hydrothermal fluids at the Fossa crater, Vulcano, Italy. European Journal of Mineralogy, 9, 423–432.

Garavelli, A., Mozgova, N.N., Orlandi, P., Bonaccorsi, E., Pinto, D., Moëlo, Y., and Borodaev, Yu.S. (2005) Rare sulfosalts from Vulcano, Aeolian Islands, Italy. VI. Vurroite $Pb_{20}Sn_2(Bi,As)_{22}S_{54}Cl_6$, a new mineral species. Canadian Mineralogist, 43, 703–711.

Gramaccioli, C.M. (2002) Lattice dynamics: Theory and application to minerals. In C.M. Gramaccioli, Ed., Energy Modelling in Minerals, 4, p. 245–270. EMU Notes in Mineralogy, Eötvös University Press, Budapest.

Holland T.J.B. and Redfern S.A.T. (1997) Unit cell refinement from powder diffraction data; the use of regression diagnostics. Mineralogical Magazine, 61, 65–77.

Kampf, A.R., Steele, I.M., and Jenkins, R.A. (2006) Phosphohedyphane, $Ca_2Pb_3(PO_4)_3Cl$, the phosphate analog of hedyphane: Description and crystal structure. American Mineralogist, 91, 1909–1917.

Khomyakov, A.P., Lisitsin, D.V., Kulikova, I.M., and Rastsvetaeva, R.K. (1996) Deloneite-(Ce), $NaCa_2SrCe(PO_4)_3F$, a new mineral with a belovite-like structure. Zapiski Vserossiskogo Mineralogicheskogo Obshchetstva, 125, 83–94 (in Russian, English abstract).

Khomyakov, A.P., Kulikova, I.M., and Rastsvetaeva, R.K. (1997) Fluorcaphite $Ca(Sr,Na,Ca)(Ca, Sr, Ce)_3(PO_4)_3F$, a new mineral with the apatite structural motif. Zapiski Vserossiskogo Mineralogicheskogo Obshchetstva, 126, 87–97 (in Russian, English abstract).

Mandarino, J.A. (1981) The Gladstone-Dale relationship. IV. The compatibility index and its application. Canadian Mineralogist, 19, 441–450.

Moore, P.B., Araki, T., and Ghose, S. (1982) Hyalotekite, a complex lead borosilicate: its crystal structure and the lone-pair effect of Pb(II). American Mineralogist, 67, 1012–1020.

Piotrowski, A., Kahlenberg, V., Fischer, R.X., Lee, Y., and Parise, J.B. (2002) The crystal structures of cesanite and its synthetic analogue—A comparison. American Mineralogist, 87, 715–720.

Rastsvetaeva, R.K. and Khomyakov A.P. (1996) Crystal structure of deloneite-(Ce), the highly ordered Ca analog of belovite. Doklady Akademii Nauk, 349, 354–357 (in Russian).

Rouse, R.C., Dunn, P.J., and Peacor, D.R. (1984) Hedyphane from Franklin, New Jersey and Långban, Sweden: Cation ordering in an arsenate apatite. American Mineralogist, 89, 920–927.

Schneider, W. (1969) Bestimmung einer Überstruktur am Caracolit. Neues Jahrbuch für Mineralogie, Monatshefte, 58–64.

Shannon, R.D. (1976) Revised effective ionic radii and systematic studies of interatomic distances in halides and chalcogenides. Acta Crystallographica, A32, 751–767.

Sheldrick, G.M. (1997) SHELXL97 Program for Crystal Structure Refinement. University of Göttingen, Germany.

——— (2000) SADABS Area-Detector Absorption Correction Program. Bruker AXS Inc., Madison, Wisconsin.

Tazzoli, V. (1983) The crystal structure of cesanite, $Ca_{1+x}Na_{4-x}(SO_4)_3(OH)_x\cdot(1-x)H_2O$, a sulfate isotypic to apatite. Mineralogical Magazine, 47, 59–63.

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