

Demicheleite-(Cl), BiSCl, a new mineral from La Fossa crater, Vulcano, Aeolian Islands, Italy

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ABSTRACT

Demicheleite-(Cl), ideally BiSCl, is the chlorine analog of demicheleite-(Br) and is closely related to this species that occurs in the same locality. The mineral is the first natural bismuth sulfochloride discovered so far in a natural environment, and it is identical with the corresponding and already known synthetic compound. It was found in an active medium-temperature intracrater fumarole at La Fossa crater, Vulcano Island, Aeolian archipelago, Sicily, Italy. The mineral occurs as acicular to stout translucent crystals up to 0.25 mm long in an altered pyroclastic breccia, together with demicheleite-(Br), bismoclite, bismuthinite, godovikovite, panichiite, and three new minerals pending the IMA approval (IMA 2008-015, IMA 2008-039, and IMA 2008-057). The mineral is orthorhombic, space group *Pnam*, with $a = 7.7933(10)$, $b = 9.9293(12)$, and $c = 3.9880(4)$ Å, $V = 308.60(4)$ Å³ (from X-ray powder data), $Z = 4$. The crystal habit is prismatic with {110} as the dominant form, terminated by minor faces of another prism {011}, a pinacoid {010}, and a bipyramid {111}. The color is dark red to black; the luster submetallic. It is non-fluorescent. The tenacity is brittle. The cleavage and fracture were not observed. The calculated density is 5.934 g/cm³.

The chemical analysis obtained by WDS electron microprobe gave (wt%) Bi 72.74, Cl 11.42, Br 3.13, S 11.74, Se 0.01 wt%, total 99.04, corresponding to the empirical formula (based on 3 apfu): Bi_{0.97}(Cl_{0.90}Br_{0.11})_{Σ1.01}S_{1.02}.

The crystal structure has been refined to a final *R* index of 0.0218 and contains Bi in sevenfold coordination inside a monocapped trigonal prism. By base sharing, these polyhedra form rows extending along [001]. The rows are connected with symmetry-related rows by sharing S-S edges of the pyramidal caps; these pairs of rows are linked to the others by sharing Cl/Br atoms. The distribution of bond lengths is close to that of the synthetic counterparts BiSCl and BiSBr, with Bi-S distances of 2.601(2) and 2.709(1) Å, and Bi-Cl/Br distances of 2.937(1) and 3.388(1) Å.

The strongest 6 lines in the X-ray powder diffraction pattern [d_{obs} (Å) (*I*) (*hkl*)] are: 2.896 (100) (121), 4.174 (45) (120), 2.684 (42) (211), 2.784 (33) (201), 1.725 (30) (411), 2.543 (27) (031).

Both the mineral and the mineral name have been approved by the Commission on New Minerals, Nomenclature and Classification of the IMA (no. 2008-020).

Keywords: Demicheleite-(Cl), demicheleite-(Br), new mineral species, bismuth, sulfochlorides, crystal structure, Vulcano Island, Aeolian Islands, Italy