

## Demicheleite, BiSBr, a new mineral from La Fossa crater, Vulcano, Aeolian Islands, Italy

FRANCESCO DEMARTIN,<sup>1</sup> CARLO MARIA GRAMACCIOLI,<sup>1,\*</sup> ITALO CAMPOSTRINI,<sup>1</sup>  
AND PAOLO ORLANDI<sup>2</sup>

<sup>1</sup>Dipartimento di Chimica Strutturale e Stereochimica Inorganica, Università degli Studi di Milano, via Venezian 21, I-20133 Milano, Italy

<sup>2</sup>Dipartimento di Scienze della Terra, Università degli Studi di Pisa, Via S. Maria 53, I-56126 Pisa, Italy

### ABSTRACT

Demicheleite, ideally BiSBr, is the first natural bismuth sulfohalogenide so far discovered. It is identical with the corresponding and analogous synthetic compound and is one of the very few minerals where bromine is an essential component. It was found in an active high-temperature fumarole at the rim of La Fossa crater, Vulcano Island, Aeolian archipelago, Sicily, Italy. The mineral occurs as prismatic translucent crystals up to 0.5 mm in size in an altered pyroclastic breccia, together with pseudocotunnite, bismoclite, bismuthinite, cotunnite, and challacolloite.

The mineral is orthorhombic, space group *Pnam*, with  $a = 8.0424(9)$ ,  $b = 9.8511(11)$ , and  $c = 4.0328(5)$  Å,  $V = 319.50(6)$  Å<sup>3</sup>,  $Z = 4$  (from single crystal); the habit is prismatic with {110} and {210} as prevailing forms, terminated by minor faces of another prism {011}, a pinacoid {010}, and a bipyramid {111}. The color is dark red to black; the streak is red; the luster submetallic. Non-fluorescent. Tenacity: brittle. Cleavage and fracture: not observed. The calculated density is 6.312 g/cm<sup>3</sup>.

The chemical analysis obtained by EDS microprobe gave (wt%) Bi 67.6(4), Br 17.4(7), Cl 4.1(4), I 0.6(1), S 10.1(1), total 99.8, corresponding to the empirical formula (based on 3 apfu):  $\text{Bi}_{0.99}\text{S}_{0.97}(\text{Br}_{0.67}\text{Cl}_{0.35}\text{I}_{0.02})_{\Sigma=1.04}$

The crystal structure has been refined to a final *R* index of 0.037 and contains Bi in sevenfold coordination at the center of a monocapped trigonal prism. By sharing the triangular bases, such polyhedra form rows extending along [001]. These rows are connected to symmetry-related rows by sharing S-S edges of the pyramidal caps; these double rows are connected to each other by sharing Br/Cl atoms. The bond lengths are close to those of the synthetic counterparts BiSBr and BiSCl, with Bi-S bonds 2.593(3) and 2.720(2) Å long and Bi-Br/Cl bonds 3.009(1) and 3.488(2) Å long.

The strongest 6 lines in the X-ray powder diffraction pattern [ $d_{\text{obs}}$ (Å) (*hkl*)] are: 4.220 (68) (120), 3.740 (62) (210), 2.909 (100) (121), 2.036 (47) (321), 1.865 (63) (022), and 1.774 (88) (411).

The mineral is named after Vincenzo de Michele (b. 1936), former curator of the Section of Mineralogy of the Museo di Storia Naturale, Milano, Italy. Both the mineral and the mineral name have been approved by the IMA Commission on New Minerals, Nomenclature and Classification (IMA 2007-022). The type specimen is deposited (no. 2007-1) in the Reference Collection of Dipartimento di Chimica Strutturale e Stereochimica Inorganica of Università degli Studi di Milano.

**Keywords:** Demicheleite, new mineral species, bismuth, sulfobromides, crystal structure, Vulcano Island, Aeolian Islands, Italy