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

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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) Å³, 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 bipyramidal {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/cm³.

The chemical analysis obtained by EDS microprobe gave (wt%) Bi 67.6(4), Br 17.4(7), Cl 4.0328(5) Å, 2.720(2) Å long and Bi-Br/Cl bonds 3.009(1) and 3.488(2) Å long. The bond lengths are close to those of the synthetic counterparts BiSBr and BiSCl, with Bi-S bonds 3.740 (62) (210), 2.909 (100) (121), 2.036 (47) (321), 1.865 (63) (022), and 1.774 (88) (411).

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_{obs}(Å) (I 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 Stereochemia Inorganica of Università degli Studi di Milano.

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

INTRODUCTION

The fumaroles at La Fossa crater, Vulcano, Aeolian Islands, have long been the object of mineralogical investigation. By the end of the nineteenth century, two new species, hieratite (Cossa 1881–1882, 1882, 1884) and cannizzarite (Zambonini et al. 1924) had been discovered. After a long period of reduced activity, in 1988–1990 these fumaroles have notably increased their temperature. Therefore, in recent years a renewed interest in the rare minerals occurring in this environment has arisen, leading to the discovery of additional lead-bismuth sulfosalts, including new species such as mozgovaite PbBi4(S,Se)2Cl6 (Vurro et al. 1999) and vurroite Pb20Sn3(Bi,As)22S22Cl6 (Garavelli et al. 2005, and references therein). Moreover, four new complex fluorides, barberiite, NH4BF4 (Garavelli and Vurro 1994), demartinite K2SiF6 (Gramaccioli and Campostrini 2007), IMA 2006-42 K2Na4(SiF6)2BF4, and IMA 2007-030 K2AlF6SO4 were discovered, as well as two new thallium chlorides, lafossaite Tl(Cl,Br) (Roberts et al. 2006) and hephaistosite TlPbCl4 (Campostrini et al. 2008). Here we report the discovery of another new mineral, demicheleite, ideally BiSBr, which also occurs in a high-temperature fumarole (~450 oC) at the rim of the crater. A picture of the fumarole field with indications is reported in Borodaev et al. (2000).

Occurrence and physical properties

Demicheleite forms well-shaped red to black translucent crystals up to 0.5 mm long on altered pyroclastic breccia, together with pseudocotunnite, bismoclite, bismuthinite, cotunnite and...