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Symesite, $Pb_{10}(SO_4)O_7Cl_4(H_2O)$, a new PbO-related sheet mineral: Description and crystal structure

MARK D. WELCH,[1,*] MARK A. COOPER,[2] FRANK C. HAWTHORNE,[2] AND ALAN J. CRIDDLE[1]

[1] Department of Mineralogy, The Natural History Museum, Cromwell Road, London, SW7 5BD, U.K.
[2] Department of Geological Sciences, University of Manitoba, Winnipeg, Manitoba, R3T 2N2, Canada

ABSTRACT

Symesite, $Pb_{10}(SO_4)O_7Cl_4(H_2O)$, is a Pb sheet mineral found in the oxidized zone of a Carboniferous Mn-Pb-Cu deposit at Merehead Quarry, Somerset. It occurs as pink crystal blebs up to 2 mm long and as pink crystalline aggregates up to 1 cm in diameter, and is associated with cerussite, hydrocerussite, paralaurionite, blixite, chloroxiphite, pyrolusite, coronadite, hematite, parkinsonite, and mereheadite. Crystals of symesite are blocky, translucent pink with a vitreous luster and a white streak. Mohs hardness is 4, $D_{meas} = 7.3(2)$ g/cm^3 and there is a perfect cleavage parallel to {001}; the refractive indices exceed 2. Electron-microprobe analysis gave the following composition (wt%): PbO 90.66, SO_3 3.15, Cl 5.83 (O = Cl 1.32), sum 98.32, giving the anhydrous formula $Pb_{10.31}S_{1.00}O_{11.22}Cl_{4.18}$; solution of the crystal structure gave the ideal formula $Pb_{10}(SO_4)O_7Cl_4(H_2O)$. The six strongest peaks in the X-ray powder-diffraction pattern [*d* in Å, (*I*), (*hkl*)] are: 2.911 (10)(414, $3\bar{2}3$), 3.286 (9)(004), 2.955 (9)($41\bar{2}$), 2.793 (8)($7\bar{1}1$, 131), 6.573 (4)(002), 3.768 (4)(412, $3\bar{2}1$). The structure of symesite was solved by direct methods and refined to an *R* index of 4.0%. Symesite is triclinic, space group $B\bar{1}$, $a = 19.727(2)$, $b = 8.796(1)$, $c = 13.631(2)$ Å, $\alpha = 82.21(1)$, $\beta = 78.08(1)$, $\gamma = 100.04(1)°$, $V = 2242.4(5)$ Å^3, $Z = 4$. The structural unit of symesite is a $[Pb_{10}(SO_4)O_7]^{4+}$ single sheet; adjacent sheets are linked by layers of Cl. One-eleventh of the Pb atoms are replaced by S, with the addition of an apical oxygen to form an SO_4 tetrahedron and a compensating O vacancy within the PbO sheet. The distribution of Pb and SO_4 groups is highly ordered and defines a 22 cation-site superstructure motif within the PbO sheet. Eight of eleven interlayer anion sites are occupied by Cl, two are occupied by O of H_2O groups, and one site is vacant. Incident bond-valence sums at O atoms indicate that hydrogen bonds occur between the H_2O group and the apical oxygen of the SO_4 group, providing additional linkage between adjacent PbO sheets. The structure of symesite is closely related to those of tetragonal PbO and the family of PbO-related sheet minerals that includes nadorite, thorikosite, mereheadite, parkinsonite, and kombatite. There are ten non-equivalent Pb sites with coordination numbers of five, seven, or eight; these polyhedra are variants of the $Pb[O_4Cl_4]$ square-antiprism that is characteristic of these minerals.