American Mineralogist, Volume 98, pages 242–247, 2013

Quadratite, $AgCdAsS_3$: Chemical composition, crystal structure, and OD character

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Abstract

A re-investigation of the crystal structure of quadratite, ideally $AgCdAsS_3$, was undertaken using a single crystal from the type locality, Lengenbach, Binntal, Switzerland. The average of five electron microprobe analyses led to the empirical formula $(Ag_{0.994}Cd_{0.738}Pb_{0.231}Cu_{0.006}Tl_{0.005}Mn_{0.003}Fe_{0.004}Zn_{0.002}Cr_{0.001})_{\Sigma=1.984}(As_{0.955}Sb_{0.003})_{\Sigma=0.958}S_{3.058}$. A single-crystal structure refinement ($R1 = 4.84\%$ for 558 observed reflections) shows that quadratite crystallizes in the space group $P4_322$ and exhibits an atomic arrangement similar to that of the recently approved new mineral manganoquadratite, $AgMnAsS_3$. Like manganoquadratite, quadratite adopts a galena-derivative framework, with metal atoms occupying all the available octahedral interstices, although only M1 and M2 cations, occupied mainly by Cd, adopt a fairly regular octahedral coordination; the M3 cation, occupied by Ag, is located outside the center cavity in a square-pyramidal coordination, whereas Pb at the split position M3′ coordinates six S atoms. Arsenic also adopts a 3 + 3 asymmetrical coordination, thus forming the AsS_3 pyramidal groups that typically occur in sulfosalts.

The structure can be also described as a stacking of BAB slabs [A: $(Cd,Ag)CdS_2$ atomic plane; B: $(Ag,Pb)AsS_2$ atomic plane] along [001]. The rectangular unit cell of these slabs is oriented diagonally to the **a** axes of quadratite and consecutive slabs are related via interlayer twofold rotation operations parallel either to [100] or to [010]. This ambiguity leads to an OD structure with various possible stacking sequences, from which the tetragonal space group $P4_322$ was observed.

Keywords: Quadratite, Cd-sulfosalts, crystal structure, chemical composition, OD character, Lengenbach