American Mineralogist, Volume 97, pages 143–149, 2012

Single-crystal Raman spectroscopy of natural paulmooreite $Pb_2As_2O_5$ in comparison with the synthesized analog

Silmarilly Bahfenne,[1] Llew Rintoul,[1] Jörgen Langhof,[2] and Ray L. Frost[1,*]

[1]Chemistry Discipline, Faculty of Science and Technology, Queensland University of Technology, GPO Box 2434, Brisbane Queensland 4001, Australia
[2]Department of Mineralogy, Swedish Museum of Natural History, Box 50007, SE-104 05 Stockholm, Sweden

Abstract

The single-crystal Raman spectra of the natural mineral paulmooreite $Pb_2As_2O_5$ from the Långban, Filipstad district, Värmland province, Sweden, are presented for the first time. It is a monoclinic mineral containing an isolated $[As_2O_5]^{4-}$ dimer. Unpolarized single-crystal spectra of the natural and synthetic samples compare favorably with each other and are characterized by strong bands around 186 and 140 cm^{-1} and three medium bands at 800–700 cm^{-1}. Band assignments were made based on band symmetry and spectral comparison between experimental band positions and those resulting from Hartree-Fock calculation of an isolated $[As_2O_5]^{4-}$ anion complex. Spectral comparison was also made with lead arsenites such as synthetic $PbAs_2O_4$ and $Pb_2(AsO_2)_3Cl$ and natural finnemanite to determine the contribution of the terminal and bridging O in paulmooreite. Bands at 760–733 cm^{-1} were assigned to terminal As-O vibrations, whereas stretches of the bridging O occur at 562 and 503 cm^{-1}. The single-crystal spectra showed good mode separation, allowing bands to be assigned a symmetry species of A_g or B_g.

Keywords: Paulmooreite, finnemanite, single-crystal Raman spectroscopy, $PbAs_2O_4$, $Pb_2(AsO_2)_3Cl$