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Crystal Chemistry of Wulfenite ($PbMoO_4$) and Wolframite ($(Fe,Mn)WO_4$)

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Summary

In this study, the crystal structure and chemistry of a selection of wulfenite ($PbMoO_4$) and wolframite ($(Fe,Mn)WO_4$) samples from various worldwide localities are examined. These minerals have the same general formula, ABO_4, where A is a divalent metal cation (e.g. Mn^{2+}, Fe^{2+}, Pb^{2+}, etc.) and B is a highly charged cation (W^{6+} or Mo^{6+}). These minerals crystallize in two different space groups; (1) wulfenite crystallizes in the tetragonal scheelite-type structure (space group $I4_1/a$, formula units, Z, = 4), whereas (2) wolframite crystallizes in the monoclinic wolframite-type structure (space group $P2/c$, Z = 2). The space group symmetry and cell dimensions are largely dictated by the ionic radius of the A site cation. In general, when the A cation radius is >0.90Å the crystal will form the tetragonal scheelite-type structure, whereas an A cation radius <0.90Å will favor the monoclinic wolframite-type structure. X-ray diffraction analyses of these minerals have long been a challenge because they are composed of heavy atoms (Pb, Mo, and W) which dominate in scattering X-rays. This makes it challenging to precisely determine the atomic coordinates of oxygen, being a much lighter element with a weaker atomic scattering power. Therefore, in an effort to overcome the aforementioned obstacle, and to acquire accurate structural data for these minerals, this study uses synchrotron high resolution powder X-ray diffraction (HRPXRD).

The natural wulfenite specimens analyzed so far in this study from various worldwide localities are very pure in composition, with all specimens being represented by the formula: $Pb_{0.99\text{-}1.00}Mo_{0.99\text{-}1.00}O_4$. Trace amounts of V^{5+}, Cr^{6+}, W^{6+}, and S^{6+} were detected with the electron probe microanalyzer (EPMA). So far, synchrotron high-resolution powder X-ray diffraction (HRPXRD) has been performed on wulfenite samples from Laurion, Greece, and from Red Cloud Mine, Arizona. The cell parameters and bond distances were computed in the program GSAS, and are comparable to literature values. Currently, more X-ray data is being gathered on wulfenite and wolframite samples in an effort to better understand relationships between composition and structure.