Poster Presentation

MS74.P17

Structure refinements of kottogite and symplesite solid-solution

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Kottogite and symplesite are zinc and ferrous arsenate minerals, respectively. These minerals make the Zn3-x,Fex(AsO4)2 • 8H2O solid-solution and belongs to the vivianite group of minerals with the chemical formula M3(TO4)2 • 8H2O. The structure of vivianite and symplesite were determined firstly by Mori and Ito, (1950). The structure of kottigite was refined by Hill, (1979). The strucrure of Zn1.63Fe1.37(AsO4)2 • 8H2O solid-solution crystallize in space group C2/m with a= 10.342(1), b= 13.484(2), c= 4.7756(5), β =105. 306(4), and Z=2. We performed the structure refinements of (Zn,Fe)3(AsO4)2 • 8H2O solid-solutions, Ojuela mine, Mapimi Durango, Mexico and Kiura mine, Ohita, Japan by RIGAKU single-crystal structure analysis system RAPID. The R and S values are around 0.03 and 1.08. We determined detail atomic coordinate and hydrogen atom positions. The hydrogen bonds were revealed based on hydrogen positions and bond valence caluculations. The octahedral edge-shareing M2O6(H2O)4 dimers and insular MO2(H2O)4 octahedra are linked by AsO4 terahedra. Two H2O group bonds to (Zn,Fe). Four hydrogen atoms are in the normal hydrogen bonds. Hydrogen atom positions have a tunnel structure and there is a path of proton-conduction and we conjecture that proton conductivity has large anisotropy of one direction. The related minerals, such as paradamite, legrandite and warikahnite have tunnel structure similar to vivianite group.

[1] H. Mori and T. Ito, Acta Crystallographica, 1950, 3, 1-6, [2] R.J. Hill, American Mineral. 1979, 64, 376-382

Keywords: (Zn,Fe)3(AsO4)2 • 8H2O, single crystal diffraction, hydrogen bonds in minerals