Japan Geoscience Union Meeting 2014
(28 April - 02 May 2014 at Pacifico YOKOHAMA, Kanagawa, Japan)

SMP47-12 Room:422 Time:May 1 12:00-12:15

Structure refinement of legrandite and paradamite : crystal chemistry and hydrogen bonds

JINNOUCHI, Satoshi[1*] ; YOSHIASA, Akira[1] ; SUGIYAMA, Kazumasa[2] ; ARIMA, Hiroshi[2] ; SHIMURA, Reiko[2] ; MIYAWAKI, Riturou[3]

[1]Graduate School of Science and Technology, Kumamoto University., [2]Institute for Materials Research, Tohoku University, [3]National Science Museum

Legrandite, $Zn_2AsO_4(OH)H_2O$ and paradamite, $Zn_2AsO_4(OH)$, are zinc arsenate minerals and have a color between pale yellow and yellowish brown. Related minerals of legrandite and paradamite are adamite, $Zn_2AsO_4(OH)$, and so on with different structures. We performed the structure refinement of legrandite and paradamite Oujela Mine, Mapimi, Durango, Mexico, by (RAPID) RIGAKU single-crystal structure analysis system. We determined the hydrogen position by difference Fourier method. We revealed the detail hydrogen bond using bond valence calculation and hydrogen positions and compared crystal structures of these. The structure of legrandite is constituted by two AsO_4 tetrahedrons, ZnO_6 octahedron and three ZnO_5 trigonal dipyramids that have large unique distortion. AsO_4 tetrahedron, ZnO_5 trigonal dipyramid and ZnO_6 octahedron constitutes the unique framework. The structure of paradamite is constituted by AsO_4 tetrahedron and two ZnO_5 trigonal dipyramid that have large unique distortion. In legrandite, 5 coordination of trigonal dipyrmids have a distance to be expected from ionic radii but interatomic distance of Zn(3)-O(1) has extraordinary distance. Two OH groups bond to Zn1 and Zn2, Zn3 and Zn4 make the $ZnO_3(H_2O)_2$ trigonal dipyramid that is bonded to two H_2O group in legrandite. In paradamite, Zn1 and Zn2 make $ZnO_3(OH)_2$ and $ZnO_4(OH)$ trigonal dipyramid. Hydrogen atoms make a lot of hydrogen bonding in legrandite and paradamite. Crystal structure of legrandite has a tunnel structure continuous that is only parallel to c axis and similar structure is observed in paradamite only parallel to a axis. There are path of proton-conduction in these direction and we conjecture that these proton-conductivity have large anisotropy of one dimension.

Keywords: structure refinement, legrandite, paradamite, crystal chemistry, hydrogen bonds