American Mineralogist, Volume 94, pages 352–358, 2009

High-pressure structural behavior of ingersonite, $Ca_3Mn^{2+}Sb_4^{5+}O_{14}$: An in-situ single-crystal X-ray study

Pier Francesco Zanazzi,[1,*] Laura Chelazzi,[2] Paola Bonazzi,[2] and Luca Bindi[3]

[1]Dipartimento di Scienze della Terra, Università di Perugia, Piazza dell'Università, I-06100 Perugia, Italy
[2]Dipartimento di Scienze della Terra, Università di Firenze, via La Pira 4, I-50121 Firenze, Italy
[3]Museo di Storia Naturale, sezione di Mineralogia, Università di Firenze, via La Pira 4, I-50121 Firenze, Italy

Abstract

An in-situ, high-pressure, single-crystal X-ray diffraction study has been carried out at room temperature up to 7.42 GPa on a crystal of ingersonite, ideally $Ca_3Mn^{2+}Sb_4^{5+}O_{14}$, from the type material. Ingersonite is isostructural with the synthetic weberite-3*T* polytype and related to the pyrochlore structure-type. Owing to the *P* range investigated and the quality of data, a second-order Birch-Murnaghan Equation of State (EoS) is the best approximation to describe the ingersonite volume evolution with *P*. The refined EoS parameters are V_0 = 810.6(1) Å^3 and K_0 = 154.5(2.4) GPa. The behavior of ingersonite with pressure is almost isotropic and the decrease of the unit-cell volume is mainly due to the kinking of the polyhedra rather than their volume decrease. The overall mean distances are quite constant, indicating virtually no compressibility of both the A and B polyhedra in the *P* range investigated. However, some geometrical changes in the pyrochlore-like AB_3 layer can be observed and compared with those observed in synthetic pyrochlore compounds. The largest change is observed for the *z* atomic coordinate of the O2 atom. Using an anion-centered polyhedral description, O2 is the only O atom that is asymmetrically located in an octahedral interstice, this feature being the most remarkable difference between the structure of ingersonite (i.e., weberite-3*T* type, space group $P3_121$) and that of zirconolite-3*T* (pyrochlore structure type, space group $P3_121$), where all the O atoms occupy the tetrahedral interstices of a cubic A_2B_2 array. With the increase of pressure, the O2 atom migrates from the A_4B_2 octahedral cavity toward the adjacent AB_3 tetrahedral cavity, suggesting that a transition from weberite-3*T* to zirconolite-3*T* structure type could occur at pressures higher than 11 GPa.

Keywords: Ingersonite, high pressure, compressibility, crystal structure, phase transition