High-Pressure Structural and Equation of State Study of Atacamite, a Copper Hydroxychloride Mineral

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We studied the effect of pressure on atacamite, Cu2Cl(OH)3, to 8.79 GPa using single-crystal X-ray diffraction. Atacamite, crystallizes in orthorhombic space group Pnma with a = 6.0323(1) Å, b = 6.8672(2) Å, c = 9.1207(5) Å, V= 377.018(8) Å^3, and Z = 4. The (OH)3Cl group forms a tetrahedron, O3Cl, with two H(2) atoms positioned inside its O(2)...C1 edges, and one H(1) just outside its O(1)...Cl edge [1]. The Cu atoms reside in distorted octahedral (4+2)-coordination sites: Cu(1) is bonded to four hydroxyl groups and two Cl atoms while Cu(2) is bonded to five hydroxyl groups and one Cl atom. These Cu-octahedra are edge-linked as in the spinel structure [1]. The structure is stable throughout the pressure range studied but there is a distinct change in the equation of sate of atacamite at 3.5 GPa reflected in the change of the isothermal bulk modulus, K, as a function of pressure (Fig. 1). A 3rd-order Birch-Murnaghan equation of state fit to the P-V data up to 3.44 GPa yielded K=79.8(9) GPa with a very low dK/dP = 0.5(5). Above 3.5 GPa, a 3rd-order Birch-Murnaghan equation of state fit to the data yielded K=74.0(5) GPa and dK/dP = 3.6(1). The structural changes that occur at 3.5 GPa will be discussed in detail in the presentation. [1] Parise and Hyde (1986) Acta Cryst, C42: 1277-1280

Fig. 1. Variation of the bulk modulus (K) with pressure in Atacamite

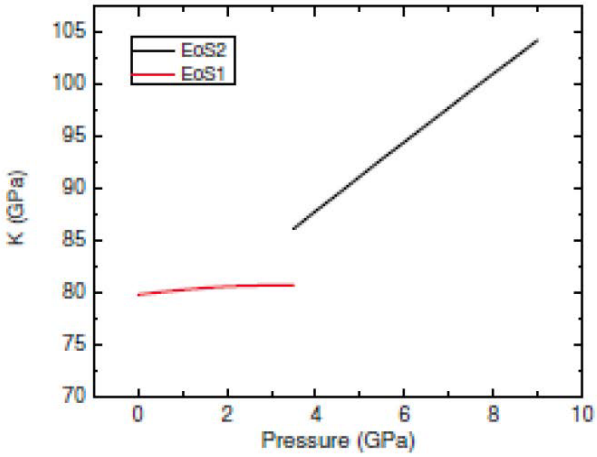

Figure 1.