Crystal chemistry of conichalcite and adelite group minerals: hydrogen atom position and structural deformation

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CaCu(AsO4)(OH) conichalcite belongs to the conichalcite-adelite group. Crystal structure refinements were performed using the single-crystal X-ray diffraction methods. Hydrogen atom positions were determined by the deference-Fourier and bond-valence-sum methods. Structural deformations in the structure are caused by hydrogen bond and Jahn-Teller effect. The structure includes liner CuO6 octahedral chains along the b-axis, which is much like CuO6 octahedral chains of spin-Peierls material CuGeO3. It may be observed spin-Peierls transition at lower temperature in conichalcite. The possibility of magnetic transitions and structural deformations in conichalcite and isomorphous minerals will be discussed.