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Raman spectroscopy of basic copper(II) and some complex copper(II) sulfate minerals: Implications for hydrogen bonding

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ABSTRACT

Raman spectroscopy has been applied to the study of basic Cu sulfates including antlerite, brochiantite, posnjakite, langite, and wroewulfeite and selected complex Cu sulfate minerals. Published X-ray diffraction data were used to estimate possible hydrogen bond distances for the basic Cu sulfate minerals. A Libowitzky empirical expression was used to predict hydroxyl-stretching frequencies and agreement with the observed values was excellent. This type of study was then extended to complex basic Cu sulfates: cyanotrichite, devilline, glaucocerinite, serpierite, and ktenasite. The position of the hydroxyl-stretching vibration was used to estimate the hydrogen bond distances between the OH and the SO_4 units. The variation in bandwidth of the OH-stretching bands provided an estimate of the variation in these hydrogen bond distances. By plotting the hydrogen bond O···O distance as a function of the position of the SO_4 symmetric stretching vibration, the position of the SO_4 symmetric stretching band was found to be dependent upon the hydrogen bond distance for both the basic Cu sulfates and the complex Cu sulfates.