

Crystal Structure, Vibration Study, and Calculated Frequencies by Density Functional Theory Method of Copper Phosphate Dihydrate

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Abstract : $\text{CuHPO}_3 \cdot 2\text{H}_2\text{O}$ was synthesized by the direct method. $\text{CuHPO}_3 \cdot 2\text{H}_2\text{O}$ crystallizes in the orthorhombic system, space group $\text{P2}_1\text{2}_1\text{2}_1$, $a = 6.7036(2) \text{ \AA}$, $b = 7.3671(4) \text{ \AA}$, $c = 8.9749(4) \text{ \AA}$, $Z = 4$, $V = 443.24(4) \text{ \AA}^3$. The crystal structure was refined to $R_1 = 0.0154$, $R_2 = 0.0380$ for 19018 reflections satisfying criterion $I \geq 2\sigma(I)$. The structural resolution shows the existence of chains of ions HPO_3^- linked together by hydrogen bonds. The crystalline structure is formed by chains consisting of $\text{Cu}[\text{O}_3(\text{H}_2\text{O})_3]$ deformed octahedral, which are connected to the vertices. The chains extend parallel to b and are mutually linked by PO_3 groups. The structure is closely related to that of $\text{CuSeO}_3 \cdot 2\text{H}_2\text{O}$ and $\text{CuTeO}_3 \cdot 2\text{H}_2\text{O}$. The experimental studies of the infrared and Raman spectra were used to confirm the presence of the phosphate ion and were compared in the (0-4000) cm^{-1} region with the theoretical results calculated by the density functional theory (DFT) method to provide reliable assignments of all observed bands in the experimental spectra.

Keywords : crystal structure, X-ray diffraction, vibration study, thermal behavior, density functional theory

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