World Academy of Science, Engineering and Technology
International Journal of Chemical and Molecular Engineering
Vol:17, No:02, 2023

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

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Abstract : $CuHPO_3.2H_2O$ was synthesized by the direct method. $CuHPO_3.2H_2O$ crystallizes in the orthorhombic system, space group $P2_12_12_1$, a = 6.7036 (2) Å, b = 7.3671 (4) Å, c = 8.9749 (4) Å, Z = 4, V = 443.24 (4) $Å^3$. 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 $Cu[O_3(H_2O)_3]$ 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 $CuSeO_3.2H_2O$ and $CuTeO_3.2H_2O$. 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
Conference Title : ICCEC 2023 : International Conference on Chemical Engineering and Chemistry
Conference Location : Jeddah, Saudi Arabia
Conference Dates : February 20-21, 2023