EGU22-9288
https://doi.org/10.5194/egusphere-egu22-9288
EGU General Assembly 2022

Hydroxyl group of libethenite $Cu_2(OH)PO_4$ – olivenite $Cu_2(OH)AsO_4$ solid solution series - vibrational spectroscopic study

Edyta Waluś and Maciej Manecki
Faculty of Geology, Geophysics and Environmental Protection, AGH University of Science and Technology, al. Mickiewicza 30, 30-059 Kraków, Poland

Libethenite and olivenite present itself as a particularly interesting candidates for a photocatalyst due to its unique structure. One of the features of copper hydroxy- phosphates and -arseniates is the presence of bridging hydroxyl (OH) groups shared between neighboring Cu atoms. In materials used in photoelectrochemical applications, the role of surface OH groups and OH-related defects is often variable and depends on the material system and reaction of interest. For instance, OH groups can improve photocatalytic activity by forming OH radicals or act as an important intermediate in the catalytic reaction. As such, the presence of the OH group inherent in the crystal structure of the material may lead to potentially interesting behavior. Seven compounds of the libethenite $Cu_2(OH)PO_4$ – olivenite $Cu_2(OH)AsO_4$ solid solution series were synthesized at 70 °C from aqueous solutions and characterized using XRD, SEM–EDS and FTIR and Raman. The substitution effect of $[PO4]^{3-}$ anions by $[AsO4]^{3-}$ on systematic changes in lattice parameters and spectral properties has been explained based on correlation between chemical composition and the peak positions. The substitution results in systematic linear increase in unit cell parameters and unit cell volume. Isomorphic substitutions are apparent in IR and Raman as a change in the position and intensity of bands derived from phosphates, arsenates and hydroxyl ions. Isomorphic substitutions of As for P in the solid solution series change the bond length and geometry. Investigation into materials that contain intrinsic OH groups may lead to better understanding of these processes and impact for photocatalytic properties. These studies will help determine the potential of libethenite $Cu_2(OH)PO_4$ – olivenite $Cu_2(OH)AsO_4$ isomorphic series as photocatalysts.