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DETERMINATION OF MAGNESIUM WHITLOCKITE STRUCTURAL PROPERTIES: RIETVELD MODELING

Agnė Kizalaitė, Jonas Stadulis, Aleksej Žarkov

Institute of Chemistry, Vilnius University, Lithuania
agne.kizalaite@chgf.vu.lt

One of the major minerals in human body is magnesium whitlockite ($Ca_{18}Mg_2H_2(PO_4)_{14}$). This compound is one of the main components of the human hard tissue, constituting to approximately 20–35 wt%, and plays an important role in various bone formation processes [1]. Magnesium whitlockite is known for its excellent osteogenic capability as well as having an active role in natural bone healing processes, therefore it is a promising candidate for application in bone regenerative medicine and tissue engineering [2]. In recent years this compound has attracted a lot of attention and the scientific community however it is not yet widely researched.

In the present work, whitlockite powders were synthesised using hydrothermal synthesis method while using calcium hydrogen phosphate dihydrate and magnesium acetate tetrahydrate as starting materials. Synthesis was performed at a temperature of 160 °C for 3 h under hydrothermal conditions. Synthesized compounds were analyzed by X-ray diffraction (XRD) and the obtained data was used for Rietveld refinement. Whitlockite structure was modeled taking large number of crystallographic positions available for substitution into account. The simulation of the XRD data showed clear differences due to the presence of Mg^{2+} ions in crystalline structure. It also allowed us to obtain data about preferential sites of Ca^{2+}/Mg^{2+} substitutions.

Acknowledgements

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[1] H. Cheng, R. Chabok et al. Synergistic interplay between the two major bone minerals, hydroxyapatite and whitlockite nanoparticles, for osteogenic differentiation of mesenchymal stem cells, Acta Biomaterialia **69**, 342-351 (2018).

[2] H. L. Jang, G. Bin Zheng et al. s, In Vitro and In Vivo Evaluation of Whitlockite Biocompatibility: Comparative Study with Hydroxyapatite and β-Tricalcium Phosphate, Advanced Healthcare Material **5**, 128–136 (2015).