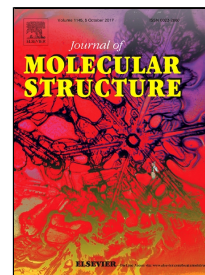


Accepted Manuscript

Effect of Zinc Oxide on the Electronic Properties of Carbonated Hydroxyapatite

Ahmed Refaat, Rasha A. Youness, Mohammed A. Taha, Medhat Ibrahim



PII: S0022-2860(17)30873-6
DOI: 10.1016/j.molstruc.2017.06.091
Reference: MOLSTR 23977
To appear in: *Journal of Molecular Structure*
Received Date: 26 May 2017
Revised Date: 19 June 2017
Accepted Date: 19 June 2017

Please cite this article as: Ahmed Refaat, Rasha A. Youness, Mohammed A. Taha, Medhat Ibrahim, Effect of Zinc Oxide on the Electronic Properties of Carbonated Hydroxyapatite, *Journal of Molecular Structure* (2017), doi: 10.1016/j.molstruc.2017.06.091

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.

Effect of Zinc Oxide on the Electronic Properties of Carbonated Hydroxyapatite

Ahmed Refaat¹, Rasha A. Youness¹, Mohammed A. Taha², Medhat Ibrahim*¹

¹*Spectroscopy Department, National Research Centre, El-Bohouh Str., 12622, Dokki, Giza, Egypt.*

²*Solid-State Physics Department, National Research Centre, El-Bohouh Str., 12622, Dokki, Giza, Egypt.*

Email: medahmed6@yahoo.com

Zinc oxide (ZnO)-doped carbonate substituted hydroxyapatite (CHA) was successfully prepared with different ZnO contents up to 3 wt% and then samples were subjected to study with Fourier transform infrared (FTIR) spectroscopy. FTIR indicated that the interaction is physical and consequently molecular modeling is consulted to understand the effect of ZnO upon CHA. A model molecule of $\text{Ca}_{10}(\text{PO}_4)_6(\text{OH})_2 \cdot 14\text{H}_2\text{O}$ is built then interacted with Zn with different schemes through 4 active sites namely O of (PO_4) ; O of OH; Ca of $\text{Ca}(\text{OH})_2$ and P of (PO_4) . For each interaction, two possibilities were tried; one through oxygen and the other through zinc of ZnO. The interaction of ZnO with CHA resulted in changes in the physical properties such as the final heat of formation, ionization potential, and even molecular dimensions. This may be due to the change in the electronic distribution which in turn changes the total dipole moment and hence the reactivity that could also affect the physical properties.

Download English Version:

<https://daneshyari.com/en/article/5161006>

Download Persian Version:

<https://daneshyari.com/article/5161006>

[Daneshyari.com](https://daneshyari.com)