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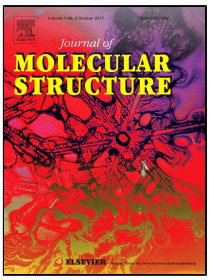

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Effect of Zinc Oxide on the Electronic Properties of Carbonated Hydroxyapatite

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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 $Ca_{10}(PO_4)_6(OH)_2.14H_2O$ is built then interacted with Zn with different schemes through 4 active sites namely O of (PO_4); O of OH; Ca of $Ca(OH)_2$ 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.