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The vibrational features of hydroxylapatite and type A carbonated apatite: A first principle contribution

Gianfranco Ulian,[1] Giovanni Valdrè,[1,*] Marta Corno,[2] and Piero Ugliengo[2]

[1]Dipartimento di Scienze della Terra e Geologico-Ambientali, Centro di Ricerche Interdisciplinari di Biomineralogia, Cristallografia e Biomateriali, Università di Bologna "Alma Mater Studiorum" Piazza di Porta San Donato 1, Bologna, Italy
[2]Dipartimento di Chimica, NIS Centre of Excellence and INSTM (Materials Science and Technology) National Consortium, UdR Torino, Via P. Giuria 7, Torino, Italy

Abstract

In this work, the vibrational spectra of hexagonal hydroxylapatite OHAp (space group $P6_3$) and type A carbonated apatite [$Ca_{10}(PO_4)_6(CO_3)$, space group $P1$] have been calculated with an ab initio approach by the density function method using the hybrid B3LYP functional and an all-electron polarized double-ζ quality Gaussian-type basis set using the CRYSTAL09 computer program. The effect on the vibrational properties due to improving the Ca pseudopotential, usually adopted in previous studies on hydroxylapatite, toward the present all-electron basis set has also been briefly addressed. The anharmonic correction for hydroxyl groups in OHAp has also been considered. The results of the modeling are in good agreement with the available FTIR and Raman data presented in the literature and can be useful to experimental researchers to assign unequivocally the bands in infrared and Raman spectra to specific fundamental vibrational modes.

Keywords: Hydroxylapatite, type A carbonated apatite, IR, vibrational properties, ab initio quantum mechanics, DFT