Ab initio Calculation of the Molecular Structure and Vibration Frequencies of Carbonate Ions Coordinated to Calcium Ions in the Zeolite CaA by Hartree-Fock Methods

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The molecular structures and vibration frequencies of unidentate and bidentate coordinations of carbonate ions to calcium ions in the zeolite CaA have been investigated, using the Hartree-Fock method implementing 6-31 G and 6-311 G basis sets. From the calculations, for both coordinations the structures give rise to theoretical vibration frequencies corresponding well to the experimental results. Therefore the charge of the divalent calcium ion is distributed in the zeolitic structure, and not near the guest carbonate ion. Optimized structural parameters for the two coordinations have been given.

Key words: Carbonate; Calcium; Hartree-Fock Calculation; Vibration Frequencies; Molecular Charge.