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FT-IR and FT-Raman spectra of 5-chlorocytosine: solid state simulation and tautomerism. Effect of the chlorine substitution in the Watson-Crick base pair 5-chlorodeoxycytidine-deoxyguanosine

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Abstract

The laser Raman and IR spectra of 5-chlorocytosine have been recorded and accurately assigned in the solid state using Density functional calculations (DFT) together with the linear scaling equation procedure (LSE) and the solid state simulation of the crystal unit cell through a tetramer form. These results remarkably improve those reported previously by other authors. Several new scaling equations were proposed to be used in related molecules. The six main tautomers of the biomolecule 5-chlorocytosine were determined and optimized at the MP2 and CCSD levels, using different basis sets. The relative stabilities were compared with those obtained in cytosine and their 5-halo derivatives. Several relationships between energies, geometric parameters and NBO atomic charges were established. The effect of the chlorine substitution in the fifth position was evaluated through the stability of the Watson-Crick (WC) base pair of 5-chlorodeoxycytidine with deoxyguanosine, and through their vibrational spectra.

Keywords: 5-chlorocytosine, 5-chlorodeoxycytidine, scaling, IR, Raman, tautomer