Quantum chemistry computations on chlorpyrifos pesticide based on Density Functional Theory

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Abstract

In this study, quantum chemistry computations based on Density Functional Theory (DFT) were performed using the B3LYP method and the basis set 31-6G(d,p) for examining the effect of organophosphate pesticides on Serine amino acid via hydrogen bonds in water. The interaction between 6 chlorpyrifos compounds and their derivatives led to the formation of 6 different complexes, and the stability energies of these systems were measured. The dipole moment values are close and approximately from 3.6 eV to 4.7 eV. The enthalpy and Gibbs free values are positive, indicating the endothermic and nonspontaneous nature of the formation process of these complexes. The band gaps, calculated from the energy difference of HOMO and LUMO orbitals, are close and about 5.1 eV. Given the close band gap of Serine amino acid, the formation of strong hydrogen bonds in all the complexes is likely. The quantum-mechanical descriptors of chlorpyrifos complexes were computed, examined, and used for determining the best complexes. The length and angles of the compound bonds before and after the formation of the complexes were computed and compared, and the changes in the angles and the general shape of the structures were studied individually. In the QTAIM data, the S1...H-O bonds in all the complexes and the intra-molecular hydrogen bond in the O...H-O Serine amino acid had an electrostatic nature. The C-H, N-H, P-O, and C-N bonds were of the covalent type.

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