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Quantum Chemistry Calculations based on the Density Functional Theory on Diazinon Pesticides

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Abstract

In this research, to investigate the effect of organ phosphorus pesticides on serine amino acid, the quantum chemistry calculations based on the density functional theory on diazinon pesticides and its derivatives, as well as complexes of these derivatives with serine were also studied. The DFT quantum chemistry calculations were carried out using the B3LYP method and the 31-6G (d, p) basis set. Sustainable energy and dipole moment of the systems were measured. Enthalpy and Gibbs free energy of the diazinon complexes were all positive, indicating the endothermic and non-spontaneous nature of the formation of these complexes. The value of the band gap, which is calculated from the difference in the energy of the HOMO and LUMO orbitals, was close together in the diazinon complexes and about 5.7 electron volts. The dipole moment values of these complexes were in the range of 3.4 to 10.1 electron volts. Next, the quantum mechanical descriptors were examined and they were used in determining the best complexes. The lengths and angles of the bonds of compounds before and after the formation of the complex were calculated and compared and the change of angles and the general form of structures were separately evaluated. QTAIM data were

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