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Theoretical Degradation Study of Methomyl

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ABSTRACT

Quantum calculation methods have been used, that is packaged on two reliable well-known programs Hyperchem7.5 and Gaussian03W to achieve the theoretical calculations of degradation for Methomyl. Chemical reactivity and chemical interaction have been studied for pesticide molecules and the attached species (hydroxyl free radical), by calculating the surface potential energy, atomic charge, bond length, electrostatic potential and molecular orbital to estimate the highest probable active sites in pesticides to be degraded .Twenty one different chemical structures and four different probable transition state stabilities to get the first step have been studied through surface potential energy, zero point energy, and first negative frequency of vibration spectrum. Activation energy and rate constant of cleavage reaction step are calculated for all reaction components that is probable to be formed during the complete degradation into simple molecular structure. Thirty of different chemical reactions have been studied to estimate the reactions that have the highest probability to occur with lowest value of activation energy by comparing relatively to others competitive reactions, in order to estimate reasonable mechanisms of completely degraded. They found the first degradation step of methomyl is exothermic through O_8—N_{10} bond to give up two major components. The activation energy of first step is 109.648 kcal mol^{-1} and rate constant of first degraded step is 1.327 x 10^{11} s^{-1}. The enthalpy change value of overall reaction for methomyl degradation is equal to -1701.252 kcal mol^{-1}. Thirteen moles of hydroxyl radical needed to convert methomyl into simple moieties like CO_2, H_2CO_3, H_2O, H_2SO_4, HNO_3 and H_2.

Keywords: Methomyl, quantum calculation methods, degradation, computational chemistry, DFT, Ab-initio, semiemprical.
