

Simulation of Regioselectivity in the Electrophilic Substitution of Imidazoles

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Both Molecular Mechanics (MM2) and Quantum Mechanics (Semi-empirical method) are employed to provide a useful insight into the site of chlorination of 4(5)-nitroimidazole. The features of the MM2 force-field allows calculation of the energies of 4-nitroimidazole in comparison with 5-nitroimidazole, in spite of the tendency of *N*-unsubstituted imidazoles to undergo tautomerism. Charges on the atoms in 4(5)-nitroimidazole obtained from Extended Hückel calculations show excellent correlation with the greater stability of the 5-chloro-4-nitroimidazole obtained by MM2 calculations. Execution of the General Atomic and Molecular Electronic Structure System (GAMESS) Interface provides predicted infra red spectrum of the proposed compound.