Steric and Electronic Structure of Selenoanisole: A Quantum-Chemical Study

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Abstract - The potential functions of internal rotation around the C_{sp^2}–Se bond in selenoanisole were obtained by quantum-chemical calculations in the approximations HF/3-21G(*d*), HF/6-31G(*d*), MP2(*f*)/6-31G(*d*), and B3LYP/6-31G(*d*). The calculations were performed in the range of variation of the torsion angle φ (between the planes of the benzene ring and C_{sp^2}–Se–C_{sp^3} bonds) from 0° to 90° with 15° step. The energy minimum is in the region of the orthogonal conformation (φ 90°), and the energy maximum, in the region of the planar form (φ 0°). The rotation barriers (kJ mol^{-1}) are as follows: HF/3-21G(*d*), 9.20; HF/6-31G(*d*), 13.13; MP2(*f*)/6-31G(*d*), 10.25; and B3LYP/6-31G(*d*), 6.41. The geometric parameters, Koopmans ionization potentials, and dipole moments are given. The energies, degrees of hybridization, populations of the lone electron pairs of Se, energies of their interaction with the antibonding π* orbitals of the benzene ring, and electron density distributions were determined in terms of the natural bond orbital approach.