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Model Chemistries of Hydrazides VI. Semi Empirical Computations of Electronic Properties of Disubstituted six membered Aromatic Hydrazides

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ABSTRACT

The computational quantum chemical studies of disubstituted INH, a popular antitubercular drug are performed at SEMO level employing PM3 Hamiltonian in gas phase. Here the electronic structure, physicochemical and biochemical properties are computed using AMPAC 6.7 package for 11 disubstituted compounds of INH, containing F, I, NH_2, CF_3, CH_3, OH, NO_2 and OMe. The stabilities based total electronic energy substantially increases with either electron donating or withdrawing groups for all the compounds. The disubstituted trifluoro methane -INH has the minimum total energy (TE). The static dipole moment is highest (6.78) for dinitro INH while it is a minimum for diiodo compound (0.7) which is less than that for INH (1.1). The non-linear optical (NLO) properties of the substituted series of INH increase markedly. The hydrophobic character increases with number of fluorine atoms in fluoro methane group or from moving from F to I atoms. The change in the hydrophilic nature of INH to hydrophobic character with environment is useful to probe into drug metabolism.

Keywords: Disubstituted INH, PM_3-Hamiltonian, SEMO-level-CQC, AMPAC-package, magnetic properties, dipole, Polarizability, hyperpolarizability, NLO-material, hydrophobicity.