Theoretical Studies using NDDO Semi Empirical Methods to Study Electronic Structure of Some Schiff Bases

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ABSTRACT

Schiff bases are aldehydes and ketones like compounds in which the carbonyl group is replaced by an imine or azomethine group. They have numerous analytical, industrial and biological importance. Substantial experimental data is available for these compounds but theoretical perspectives have not been comprehensively investigated yet.

Objective: This fact led us to conduct a theoretical exploration of the electronic structure of these compounds.

Introduction: Semi Empirical methods are widely employed to get rapid insights into the electronic structures of small to medium sized chemical systems. Properties like total energy, FMOs predictions, spectroscopic calculations (including vibrations, NMR, and UV-Vis etc.), and thermodynamic properties can be simulated rapidly by employing semi empirical methods.

Methodology: Modern semi empirical models are based on the Neglect of Diatomic Differential Overlap (NDDO) method in which the overlap matrix S is replaced by the unit matrix. Existing semi empirical models differ by the further approximations that are made when evaluating one-and two-electron integrals and by the parameterization philosophy.

Conclusion: In this work we have reported AM1 (Austin Model 1) calculations of eightschiff bases. Calculated chemical properties e.g. geometry optimization, total energy, vibrations and IR spectrum, population analysis, dipole moments and some thermodynamic properties are reported. The geometry of all title compounds were optimized using AM1 and PM3 Hamiltonian employed by GAMESS software package, images were rendered using Chem-Craft molecular visualization software. Results showed that these NDDO methods can be effectively employed on similar systems to get faster theoretical insights.

Keyword: Parameterization, Hamiltonian