Quantum Characterization of 3,5-didehydropyridine

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Abstract

Pyridine is a well-studied molecule in experimental and computational chemistry because of its contributions to drug synthesis. Pyridine is used to create antimicrobial drugs such as sulfapyridine and antihistaminic drugs such as pyrilamine. It is used in "in vitro" synthesis of DNA as well. In this project, diradical pyridine isomer 3,5-didehydropyridine was characterized through a series of geometry optimizations and single-point calculations. The molecular orbitals were generated using a ROHF/cc-pvdz geometry optimization with the Gaussian09 software. Each orbital was assigned an irreducible representation under C_{2v} point group symmetry, in order to create COLUMBUS input files. A complete active space with 8 electrons in 8 orbitals (CAS(8,8)) was included for the molecule's specific π and π* orbitals and σ and σ* orbitals. Geometry optimizations and single point calculations were conducted for both the lowest lying singlet and triplet states using COLUMBUS software. Energies and geometries were gathered using MCSCF, MRCI, and AQCC methods with both cc-pvDZ and cc-pvTZ basis sets. Using the results from these methods, the singlet-triplet adiabatic and vertical gaps were calculated.