Quantum Characterization of 3,5-didehydropyridine

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This project seeks to characterize the lowest energy singlet and triplet states of 3,5-didehydropyridine, a diradical produced in low quantities in the oil shale extraction method. By analyzing the differences in properties between closed-shell pyridine and its open-shell 3,5-didehydro-diradical, we can gain a greater understanding of the reactivity and bonding in diradicals. Initially, the molecular orbitals of 3,5-didehydropyridine were assigned to irreducible representations under the C_{2V} symmetry group. An active space of 8 orbitals and 8 electrons was utilized (CAS(8,8)). Active orbitals included the $\pi_1(b_1)$, π_2 (b_1), π_3 (a_2), σ_1 (a_1), σ^*_2 (b_2), π^*_4 (b_1), π^*_5 (a_2), and π^*_6 (b_1). The structures were optimized using multi-reference methods (MCSCF, MR-CI, and MRAQCC) which are required in order to accurately describe such complex systems. Calculations were done, and data were collected, using Columbus, Gaussian, and Molden. Data suggests the lowest lying state is a singlet, followed by a triplet, and then another singlet.