Quantum Characterization of 3,5-didehydropyridine

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This project seeks to characterize the many valence states of 3,5-didehydropyridine, a diradical produced in low quantities in the oil shale extraction method. By analyzing the differences in properties between the stable pyridine molecule and its unstable diradical form, we can gain a greater understanding of diradical molecules. Additionally, the pyridine molecule is a major constituent of numerous enzymes and medicines. By gaining a more complete picture of the various energy states of this more reactive form of pyridine, we may be able to create new, useful pyridine based-materials in the future. The structures were optimized using multi-reference methods (CAS(8,8) MCSCF, MR-CI, and MRAQCC) due to the failure of single reference methods to accurately describe such complex systems. Calculations were done, and data were collected, using Columbus, Gaussian, and Molden. Preliminary data suggests the lowest lying state is a singlet, followed by a triplet, and then another singlet.