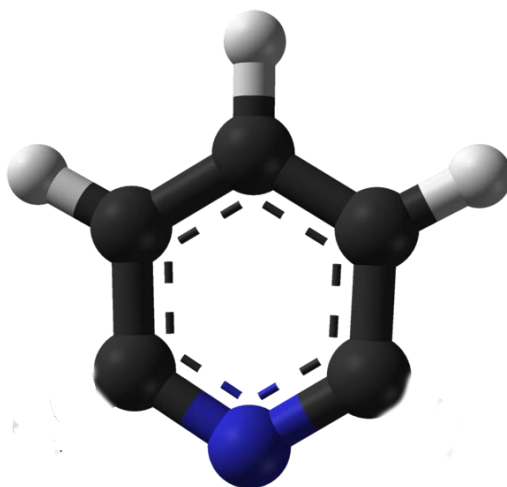


Theoretical Characterization of the Pyridine Diradical

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Diradicals are reactive and short-lived. As a result, they are difficult to study experimentally and a challenge to modern electronic structure methods. But they can be analyzed theoretically using highly correlated, multi-reference methods. We hypothesize that pyridine diradicals are formed during the high temperature pyrolysis and decomposition of the asphaltenes contained in oil shale. This project focused on one of the C_{2v} isomers of didehydropyridine formed by loss of two hydrogens adjacent to the nitrogen atom.



The molecular orbitals of didehydropyridine were analyzed and labeled according to the irreducible representations under C_{2v} symmetry. These MOs were then used to performed SCF, MCSCF, and MR-CI calculations using the Columbus quantum chemical software package. Geometry optimizations were performed on the singlet A1 and triplet B2 states using the cc-pvdz basis set. These results will be presented.