Fundamental Characterization of 3,5-Didehydropyrazine

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My project focuses on the fundamental characterization of the diradical 3,5-didehydropyrazine. Since oil shale contains a high proportion of cyclic species and radical recombination reactions are significant in the combustion of oil shale, characterizing 3,5-didehydropyrazine provides valuable information to improving the productivity of oil shale.

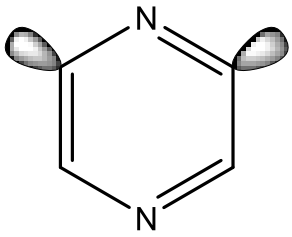

Figure 1. 3,5-Didehydropyrazine

In order to characterize this molecule, molecular orbitals were generated using ROHF/cc-pvDZ and assigned irreducible representation labels under C_{2v} symmetry. Active space orbitals symmetries were $11A_1$ (σ), $7B_2$ (σ^*), $5B_1$ ($6\pi^*$), $2A_2$ ($5\pi^*$), $3B_1$ ($4\pi^*$), $1A_2$ (3π), $2B_1$ (2π), and $4B_1$ (1π). Geometry optimizations were performed on both the ground and excited triplet states at the MCSCF, CISD, and AQCC levels of theory, using both cc-pvDZ and cc-pvTZ basis sets. The software packages used were Gaussian and Columbus. Small adiabatic gaps were observed between the ground state and the triplet excited state in the MRCI/cc-pvDZ. Also the results of the geometry optimization calculation showed the radical carbons moving closer to each other in the ground singlet state, while the excited triplet state shows the radical carbons moving away from each other.