Characterizing 2,5-Didehydrofuran with Quantum Mechanics

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This project concentrates on the characterization of the 2,5-Didehydrofuran diradical. This is a species likely to be formed during the high temperature decomposition of the asphaltenes found in oil shale. The study of diradicals is important for understanding the behavior of potential anti-cancer drugs. Proper characterization of the structures and excitation energies may allow better control of the Bergman cyclization responsible for the active form of enediyne pro-drugs. The molecular orbitals of diradical furan were analyzed and irreducible representations labeled under C2v symmetry. The geometry of the molecule was found by optimizing the molecule in both the singlet and triplet states using both single reference CCSD(T)/cc-pVTZ and multi-reference MCSCF, CISD and AQCC. Using these geometries the change in energy for both adiabatic and vertical excitations were found. Calculations were performed using the Gaussian, Q-Chem and COLUMBUS software packages.