

Multi-reference, Highly-Correlated Characterization of Furan

Lily Mawby and Carol Parish

*Department of Chemistry, Gottwald Center for the Sciences, University of Richmond,
Richmond, VA 23173*

This project concentrates on the characterization of the 2,5-Furan 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 also important for understanding the behavior of 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 C_{2v} symmetry. The geometry of the molecule was found by optimizing the molecule in both the singlet and triplet state using both single reference CCSD(T)/cc-pVTZ and multireference MR-CI. Using these geometries the change in energy for both adiabatic and vertical excitations can be found. Calculations were performed using the Gaussian, Q-Chem and Columbus software packages.