

Multireference Studies of Heteroaromatic Diradicals

Carol A. Parish

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

The ability to characterize open-shell radical species and the cyclization reactions that involve such molecules holds significant promise for advancing the fields of multireference theoretical chemistry, mechanistic organic chemistry, materials design and drug optimization. This talk will describe our recent work using highly correlated, multireference methods to characterize the geometries, ground states and excited states of the diradicals of benzene, thiophene, fulvene, pyrrole and furan.

.

.