

## **Spin-Flip Characterization of the Bergman Cyclization of the 5, 7 & 8 Member Systems**

*Salmika Gathoni Wairegi, Adam Luxon, Carol Parish*

*Department of Chemistry, University of Richmond, VA 23173*

The Bergman Cyclization is the process of enediyne cyclizing into the highly reactive diradical *p*-benzene. This benzene structure has a strong affinity to hydrogen, which breaks off from cell structures when in the presence of benzene. A more complete understanding of this structure in the Bergman Cyclization is crucial in the attempt to create more effective cancer treatments. The cyclization of the hexa-3-ene-1, 5-diyne system has been studied extensively, but the penta-1, 4-diyne anion, hepta-1, 6-diyne cation and octa-1, 7-diyne dication systems have not yet been studied. The Bergman cyclization of the penta-1, 4-diyne anion, hepta-1, 6-diyne cation and octa-1, 7-diyne dication systems were characterized using spin flip couple cluster (SF-CCSD) method. The activation barrier and energy of each reaction were calculated along with the adiabatic and vertical gaps for the singlet and triplet states.