Energetics of the Bergman Cyclization in Enediyne Tautomers

Sarah Booth, Maximilian Macaluso, Matthew G. Fanelli, and Carol A. Parish
Department of Chemistry, University of Richmond
Richmond, Virginia, 23173

The goal of this project was to examine the energetics of the Bergman Cyclization of Enediyne molecules. Enediyne molecules are organic molecules that are most known for their powerful ability to undergo the Bergman Cyclization reaction. These reactions typically produce molecules containing a benzene diradical structure. Due to the aromatic resonance of the benzene molecule and the reactivity of the diradicals, this molecule is both stable and very reactive; a unique characteristic of enediynes. This ability both to react with DNA and still remain relatively stable renders enediyne molecules a prudent choice for cancer treatment. This project aims to investigate the structure and energy of the three stages of the Bergman cyclization: the reactant, the transition state and the product (states referred to as the reactive intermediates). All three of these stages have a specific geometrical structure and potential energy that corresponds to a specific point on the potential energy surface. Quantum mechanics was used to create a potential energy surface and locate the energy coordinates of these structures. This project was completed using conformational analysis using B3LYP density functional theory and 6-311++G** basis set for all calculations.