

Analyzing Tautomeric Triggers of the Bergman Cyclization Using Quantum Mechanical Methods

Quincy McKoy and Carol Parish

Chemistry Department, University of Richmond, Richmond, VA

Under the influence of heat or light, enediyne are converted to para-benzenes by the Bergman cyclization reaction. The purpose for studying this cyclization reaction is the potential the corresponding diradical molecules have for cancer drugs. Unfortunately, an efficient manner for catalyzing the Bergman cyclization only in the presence of a cancer cell is still unknown. A possible trigger for the reaction is via enol-keto tautomerization. In this tautomerization reaction, we are studying the energy required to move a hydrogen atom and a pair of electrons to convert from an enol to a keto form of the molecule. To calculate the energy barriers and activation energies, the B3LYP functional and 6-31G* basis set was used. This study will allow us to determine the energy necessary for tautomerization in various enediyne tautomers.