Quantum Mechanical Studies of Aromatic Substituted Enediynes

Heather Hollis and Carol Parish
Department of Chemistry, University of Richmond

An enediyne moiety undergoes a Bergman cyclization to become a parabenzyne diradical. This diradical then abstracts two hydrogen atoms from its environment, forming benzene. In the body, these molecules abstract hydrogen from DNA, causing the cell to denature. The enediyne moiety is therefore a powerful anti-cancer agent, but is also unspecific. This study seeks to understand the structural factors that affect the Bergman cyclization by focusing on aromatic substitutions at the ene moiety. The energetics of the molecules were determined computationally with the *GAUSSIAN03* program using the pure BLYP and the hybrid B3LYP functionals with the basis set 6-311G**. Structures and energies of uncyclized reactants, transition states and singlet and triplet diradical intermediates were found. The energies of various substituted enediynes were compared.