

Simple, Ten-Membered Rings and the Effects of Aromatic Addition on the Bergman Cyclization

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Enediyne are molecules capable of undergoing the Bergman cyclization. During this cyclization, the enediyne transforms into an aromatic diradical (Figure 1). This highly reactive diradical will abstract hydrogen atoms from DNA, causing strand scission and cell death. Diradical products of the Bergman cyclization are currently under study as potential anti-cancer drugs.

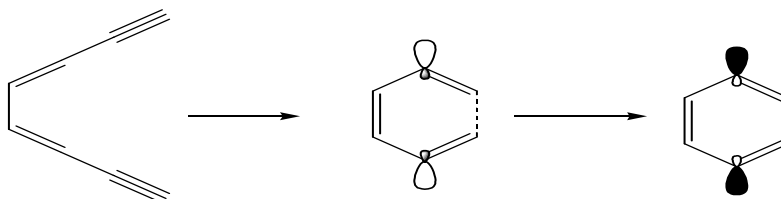


Figure 1 – The Bergman Cycle for a Simple Ten-Membered Ring

The aim of this project is to investigate how the energetics of the Bergman cyclization is affected as aromatic rings are added to the enediyne (Figure 2). These results will shed light on the relationship between structure and activity and eventually lead to improved cancer drugs.

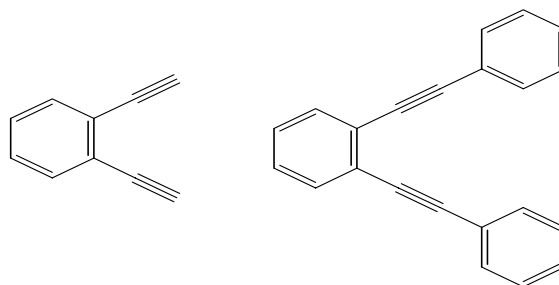


Figure 2 – Molecules under study.