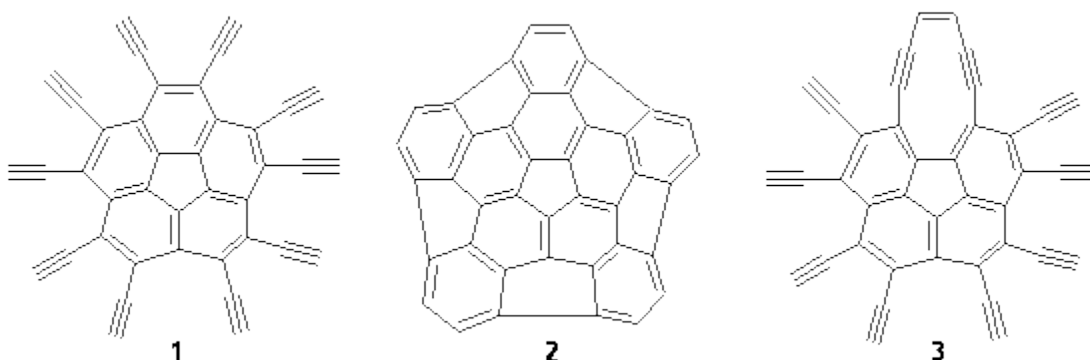
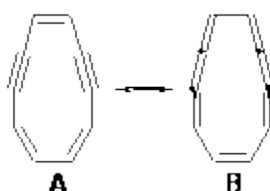


BERGMAN CYCLIZATION AND [10] ANNULENES

In their continuing efforts to build novel aromatic systems, Siegel and Baldrige report the preparation of the decapropyl analogue of the per-ethynylated corannulene **1**.¹ They were hoping that this might cyclize to the bowl **2**. It is however stable up to 100 °C, however, the analogue **3** was obtained in the initial preparation of decapropyl-**1**.



The B3LYP/cc-pVDZ optimized structures of **1** and **3** are shown in Figure 1. **1** is bowl-shaped, reflecting the property of corannulene, but interestingly **3** is planar. The geometry of the {10}annulene is interesting as it is more consistent with the alkynyl resonance form **B**.



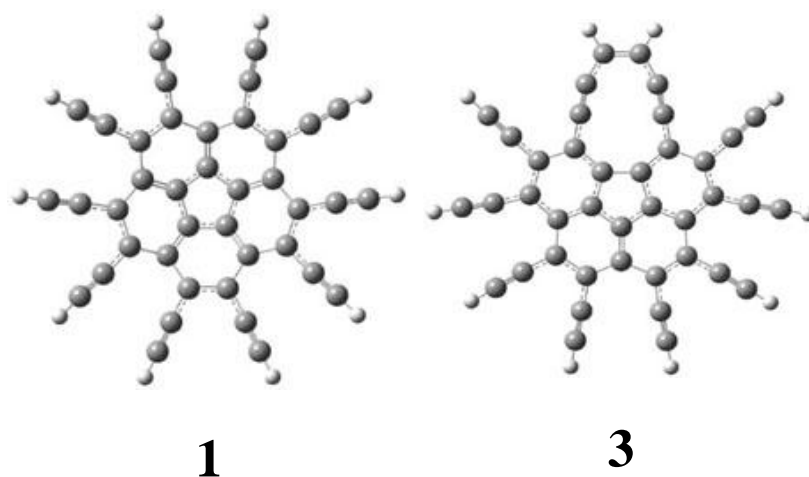
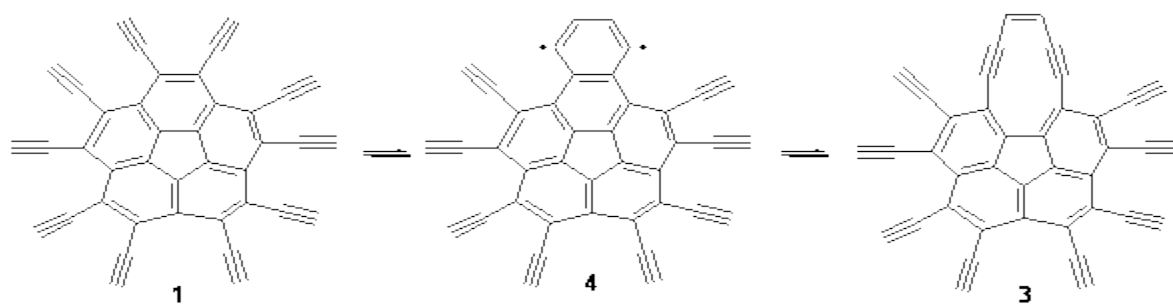


Figure 1. B3LYP/cc-pVDZ optimized structures of **1** and **3**.¹

Siegel and Baldrige speculate that the conversion of **1** \rightarrow **3** occurs by first undergoing the Bergman cyclization to give **4**, which then opens to give **3**.

Unfortunately, they did not compute the activation barrier for this process. They do suggest that further cyclization to give the hoped for **2** might be precluded by the long distances between radical center and neighboring alkynes in **4**, but the radicals are too protected to allowing trapping by the solvent, allowing for the formation of **3**.



Source: <http://comporgchem.com/blog/?p=44>