

A Mechanism for Annealing Bicyclic Polyynyl Rings into Fullerenes

Alexis Achey, Jeff Schriber, Carol A. Parish

Department of Chemistry, Gottwald Center for the Sciences, University of Richmond,
Richmond, VA 23173

Buckminster Fullerene (Buckyballs) molecules are spherical ball shaped structures made up of interlocking twenty hexagons and twelve pentagons, similar to the pattern of a soccer ball. This project utilized quantum mechanical methods to evaluate a mechanism, proposed by Hunter, for the formation of Buckminster Fullerene molecules by annealing together bicyclic polyynyl precursors¹.

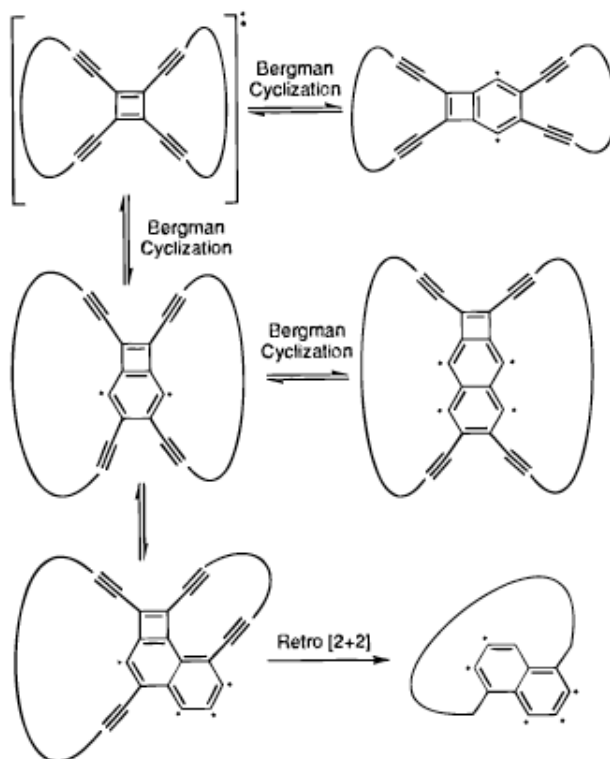


Figure 1: Mechanism proposed by Hunter et al. in ref 1 to initiate the annealing of bicyclic polyynyl rings into fullerenes.²

Calculations were performed using the Q-Chem software package. Preliminary scans of the potential energy surface were done using a computationally efficient density functional theory (DFT) approach with a standard basis set (UB3LYP/6-31G**). Energies and structures of various reactants, transition states and diradical intermediates were then refined using single- and multi-reference wavefunction methods.

¹ Hunter, J. M.; Fye, J. L.; Roskamp, E. J.; Jarrold, M. F. *J. Phys. Chem.* 1994, 98, 1810 - 1818.

² Goroff, N. S.; *Acc. Chem. Res.* 1996, 29, 77 - 83.