Cyclopropyl Disrotary Ring Opening Reactions

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This study examines the cyclopropyl disrotary ring opening reactions shown in Figure 1.

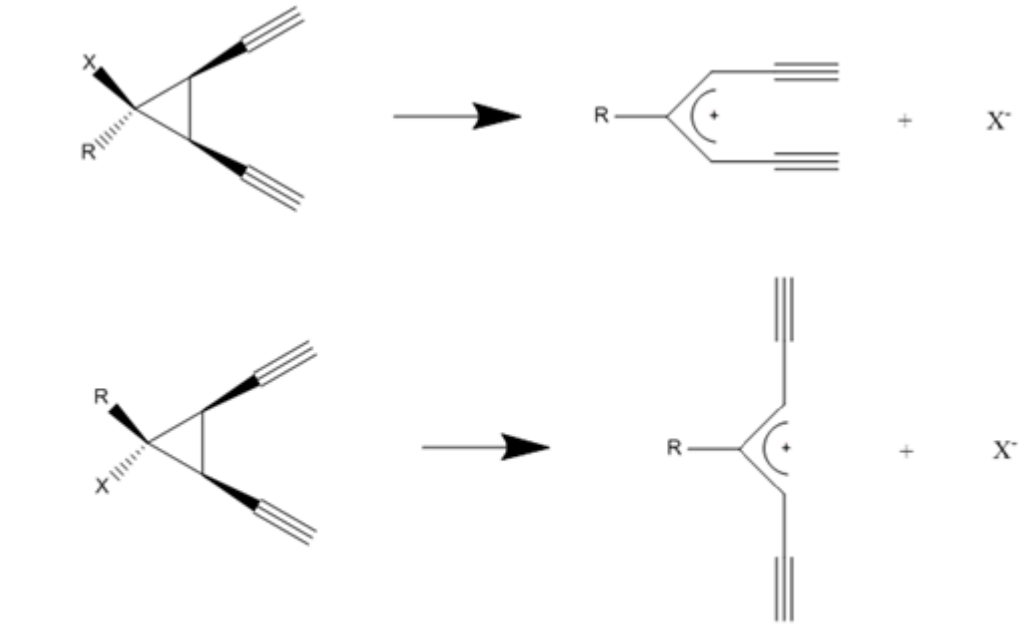

Figure 1. Cyclopropyl disrotary ring opening reactions

The product formed whenever the ring opens is dependent upon the stereochemistry of the molecule. The first product is likely to undergo Bergman cyclization, while the second is highly unlikely to result in such a reaction. Multiple leaving groups (represented in the diagram above as "X") were studied in order to determine the effect of the leaving group on the reaction. Two different R-groups were also tested, as well. Geometry optimizations using BLYP, B3LYP, MPWB1K, M06-2X, and MN12-SX geometry optimizations were performed with 6-31G* and 6-311++G** basis sets, and single-point QCISD/6-311++G** calculations were performed on the B3LYP/6-311++G** optimized structures. After gas-phase optimizations, single-point solvent-phase calculations were performed on the optimized structures. The reaction energies and barrier heights were compared between the two reactions in both gas phase and solvent phase, which helped determine the differences between the two reactions and the effects of a solvent on both reactions. The geometries of the molecules were also analyzed and compared.