

## Syntheses of Organic 3D Cages via Alkyne Metathesis

Anna Yang, Semin Lee, Timothy Money Penny, Jeffrey S. Moore

Dynamic covalent chemistry (DCC) is a useful method to obtain thermodynamic products in high yields from simple monomeric building blocks. Among various DCC methods, alkyne metathesis provides structurally rigid linear acetylene linkages with good chemical stability. Utilizing ditopic building blocks in alkyne metathesis, two-dimensional (2D) macrocycles of various sizes and shapes have been achieved. We recently expanded the scope of alkyne metathesis towards synthesizing shape persistent three-dimensional (3D) architectures. A rigid tritopic building block (**A**) was synthesized as a means to target a tetrahedron. The building block was expected to adopt a fully alternating up-down conformation to favorably direct the formation of tetrahedral (**Td**) cage. This building block provided the targeted **Td-A** cage in high yields within 2 hours. The highly symmetric tetrahedral structure of **Td-A** was confirmed by X-ray crystallography. In addition, **Td-B** was prepared with alkoxy side groups for improved solubilities in organic solvents. In order to exploit the dynamic nature of alkyne metathesis, scrambling reaction between **Td-A** and **Td-B** was performed. Surprisingly, this reaction did not provide any scrambled products, which suggested that the tetrahedral cages were thermodynamic and kinetic products. Further systematic studies on intermediates and different cage forming reaction conditions will be discussed. We anticipate that these studies will provide further insights to approaching rational design rules and strategies on our path towards more complex 3D cages.

