

# SESSION I: SPEAKER ABSTRACTS

# Understanding the Effect of Conformational Dynamics on Alkyne-metathesis Cage Forming Processes

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Dynamic covalent chemistry (DCC) has proven to be a versatile platform for the synthesis of complex molecular architectures. Key to the success of DCC is the reversible formation of bonds that allow for the system to reach a thermodynamically favored product distribution. We have recently taken advantage of this platform for the synthesis of kinetically trapped tetrahedral cages *via* alkyne metathesis. These studies have inspired us to further investigate the effect of precursor conformation and preorganization on the overall product distribution of cage formation *via* alkyne metathesis. In preliminary computational studies, we have observed that substitution of the starting material significantly effects the favored conformation of the precursor to productive (bowl) or unproductive (chair) conformers. Given that both of these precursors afford cage in nearly quantitative yield, we sought to investigate whether enhancing these conformational differences would result in altered product distributions that are dependent on the precursor structure. To test this hypothesis, we prepared a series of extended cage precursors and subjected them to alkyne metathesis conditions. The results of these experiments indicate that by extending the size of the precursor, the effect of precursor substitution leads to a more significant difference in the metathesis product distribution. Computational and spectroscopic experiments are currently being pursued to further understand the conformational dynamics of these extended cage precursors.

