

SESSION II: SPEAKER ABSTRACTS

Efficient Synthesis of an Aromatic Möbius Annulene via Alkyne Metathesis

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We have synthesized a novel Möbius annulene using alkyne metathesis. Cyclotrimerization of a writhe-bearing monomer renders the Möbius annulene more kinetically accessible than a synthetic strategy requiring the introduction of a twist in the macrocyclization step. In this way, 2,2'-bis-propynyl-[5]helicene (**1**) serves as an excellent precursor for cyclooligomerization through alkyne metathesis. Cyclic trimer (**2**) was obtained with high efficiency. While the *PPP/MMM* C_3 symmetric enantiomeric pair was predicted to be more thermodynamically stable than the C_2 symmetric *PPM/MMP* pair by DFT, we observe exclusive formation of the kinetic product **2**. DFT calculations of various transition states provide insight into the kinetic driving force of the reaction. The two-fold symmetry of the product was confirmed by ^1H and ^{13}C NMR and single crystal X-ray diffraction. UV-Vis and excitation-emission spectra are very similar between the monomeric precursor and the trimeric product. Computational (ACID current and EDDDB) evidence shows weak conjugation between the alkynyl units and the adjacent aryl units. Together, these data suggest that the macrocycle displays $[4n+2]$ aromaticity isolated in the helicene subunits rather than $[4n]$ electron global aromaticity.

