Outstanding Chiroptical Properties of Conjugated Polygon-Shaped Macrocycles

C. Kress, M. Mayor*

University of Basel, Department of Chemistry,

St. Johanns-Ring 19, Basel, Switzerland

*E-mail: marcel.mayor@unibas.ch

The increasing interest in conjugated carbon-based macrocyclic structures, induced by their promising photophysical properties, is strongly coupled to the development of new synthetic strategies. Recently, we reported the use of pseudo-*meta*[2.2]paracyclophanes (PCPs) as corner units. Their geometry, given by the substituents angle, allows the straight-forward assembly of unstrained macrocyclic systems, while the efficient electronic conjugation and chiral information are maintained.[1]

The acetylene homocoupling of enantiopure dialkyne pseudo-*meta* PCP allowed to isolate four enantiopure polygon-shaped structures in high yields (see below). Unprecedented high molar circular dichroism values for all-carbon structures were found reaching up to 1307 $Lmol^{-1}cm^{-1}$.[1] In order to obtain bright circularly polarized emitters the 1,3-butadiyne linked library was heterocyclized to the 2,5-thienyl derivatives in high yields (see below).[2] The optical and chiroptical properties oft he two resulting libraries were analyzed and compared to each other. While the 1,3-butadiyne linked structures revealed through-space conjugation the 2,5-thienyl derivatives posses significantly higher quantum yields.[1,2]

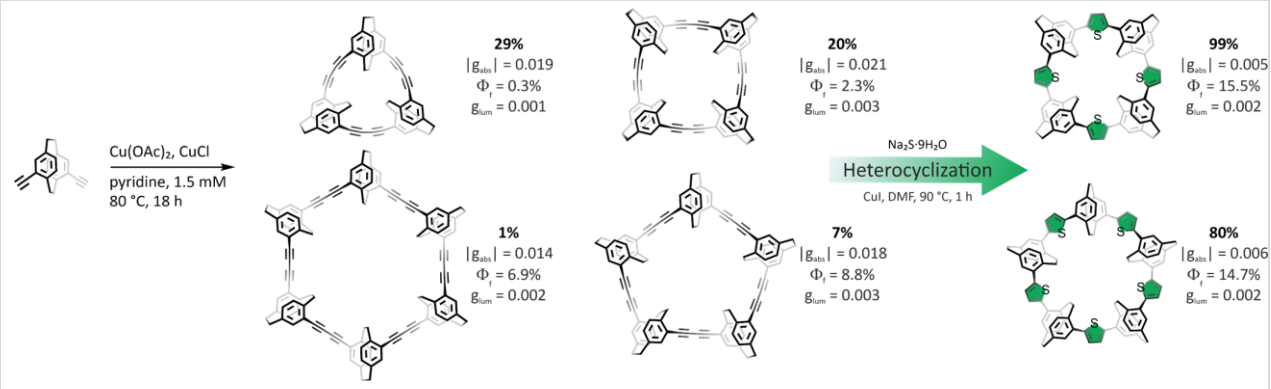

Figure 1: Synthesis and comparison of the polygon shaped 1,3-butadiyne and of the 2,5-thienyl linked pseudo-*meta* PCP macrocycles.

References:

[1] E. Sidler, P. Zwick, C. Kress, K. Reznikova, O. Fuhr, D. Fenske, M. Mayor, *Chem. Eur. J.* **2022**, e202201764.

[2] C. Kress, E. Sidler, P. Downey, P. Zwick, O. Fuhr, D. Fenske, S. Bernhard, M. Mayor, *Chem. Eur. J.* **2024**, e202303798.