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The Renaissance of 4,5-Diphenylphenanthrene

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The development of new topological molecular nanocarbons is important in advancing the understanding of the relationship between nonplanar aromatics and electronic topology, which is critical in the development of new organic materials.¹

Herein, we introduce 4,5-diarylphenanthrene² as a novel axially chiral, three-dimensional building block for the synthesis of a family of highly twisted and chiral carbocyclic macrocycles.³ These macrocycles with an approximately 90° twist angle were effectively synthesized through a quadruple Suzuki-Miyaura coupling of 4,5-diarylphenanthrene. By varying the cross-coupling partner as the spacer, a family of twisted macrocycles was obtained, allowing for a systematic study of the effect of the spacer on macrocycle shape and photophysical properties. For example, a unique macrocyclic aggregation-induced emission (AIE) emitter with double tetraphenylethylene units as the spacers was readily synthesized. Furthermore, attributed to its conformationally restricted twisted structure, a 3,6-disubstituted-1,8-naphthalimide-incorporated macrocycle showed remarkable solvatofluorochromism with high fluorescence quantum yields. The excellent conformational stability of these macrocycles further enabled complete enantiomeric resolution and characterization. The racemization barrier of the macrocycle was determined experimentally and supported by DFT calculations.



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