

Helically-Locked Tethered Twistacenes

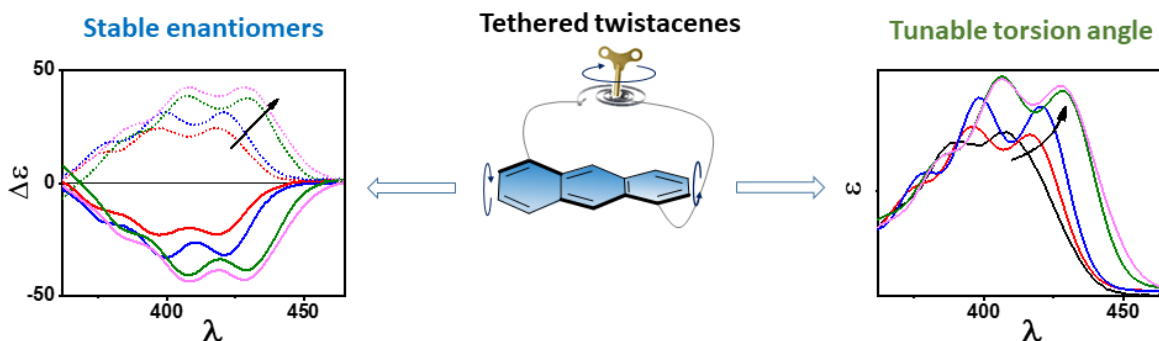
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Acenes, which can be viewed as one-dimensional graphene nanoribbons, are an important class of organic electronic materials. Twisting linear acenes out of planarity affects their electronic and optical properties, and induces axial chirality. However, it is difficult to isolate the effect of twisting from the varying substituents surrounding the acene core. Additionally, many twistacenes (twisted acenes) readily racemize in solution.^[1] We envisaged that the dynamic conformation flipping of acene backbone could be locked by molecular tethering, such as was previously applied to achieve bending in larger polyaromatic systems.^[2]

Here we present a new series of twistacenes having an anthracene backbone diagonally tethered by *n*-alkyl bridge of different lengths, which induce a backbone twist of various angles.^[3] This allows us to systematically monitor the effect of twisting on electronic, optical and chiroptical properties. We find that absorption is bathochromically shifted with increasing twist, while fluorescence quantum efficiency drops dramatically. Enantiomerically pure twistacenes display strong chiroptical properties with no racemization even upon prolonged heating, rendering them as attractive candidates for axially-chiral building units of π -conjugated backbones.^[4]

In addition, we present here a first experimental investigation of charge delocalization in any PAH as a result of twist.^[5] Our results, establishes that twisting in PAH backbone should not be neglected, rather should be explored, because it evolves certain fundamentally important bright aspects that could upgrade the current ongoing research in the area involving π -conjugated systems.^[6]



Schematic representation of tethered twisted acenes (center). Arrows indicate increasing Cotton effect in ECD spectra (left) and bathochromic shift in absorption spectra (right) upon increasing anthracene twist.

References

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