Effect of Molecular Conformation on the Physical Properties of Three-dimensional Biradicaloids

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The marriage of a biradicaloid heptazethrene structure with helicenes leads to novel three-dimensional helically chiral biradicaloids, namely Helical Heptazethrenes (HHZ). This fusion results in a unique combination of physical properties of both classes of molecules. Our molecular design includes a straightforward synthesis, as well as an optimized strategy to separate the emerging stereoisomers. The outer edges of the helicene units of the enantiomers (*M**,*M**-HHZ) face in the same direction, while a continuous helical structure is formed in the *meso*-compound (*P,M*-HHZ). In this context, the effect of molecular conformation on the singlet–triplet energy gap, biradical character and chiroptical properties was investigated in particular.

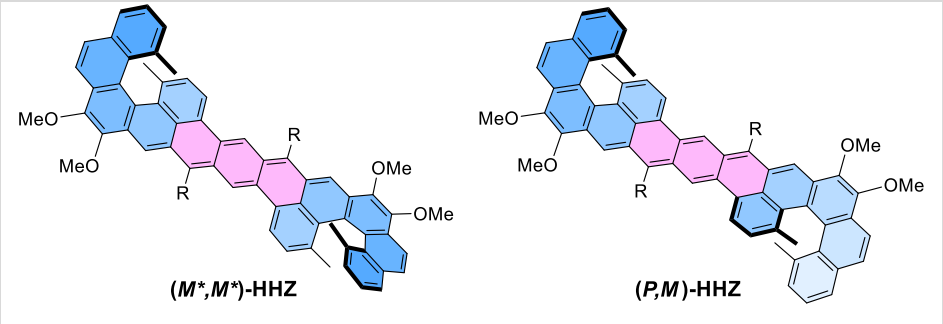

Figure 1: Emerging conformational diastereomers as result of the unique combination of biradicaloid heptazethrene and three-dimensional helicene structures.

References:

[1] P. Ravat, *et al.*, *Angew. Chem. Int. Ed.* **2016**, *55*, 1183-1186.
[2] Z. Sun *et al.*, *Angew. Chem. Int. Ed.* **2013**, *60*, 18229-18236.