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Preparation and Physicochemical Properties of [6]Helicenes Fluorinated at Terminal Rings.

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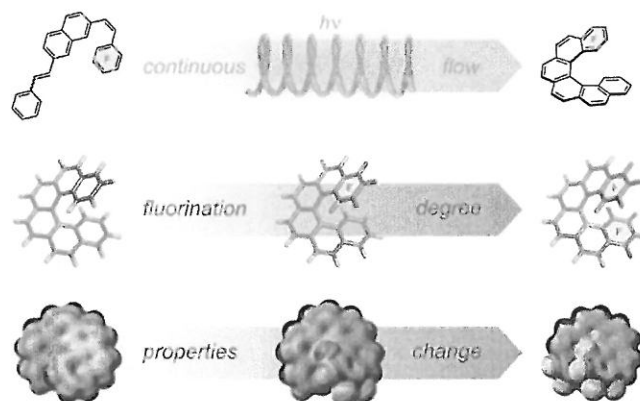
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The introduction of fluorine substituents into helicene skeleton is a promising strategy for tuning of properties required for their further applications. The fluorine substitution can affect C-H/ π interactions, which prevail in molecular assembly in the solid state, or can modulate the HOMO-LUMO gap. Generally, the fluorine substitution can induce changes in crystal structures, in physical properties of compounds and also in chemical reactivity.

Two fluorinated helicenes, tetrafluoro[6]helicene and octafluoro[6]helicene were prepared photochemically and their physicochemical and optical properties were investigated (Fig. 1). A separation of racemic tetrafluoro[6]helicene into individual enantiomers (*P* and *M*) was performed and the racemization barrier was determined. Crystal structures of major synthetic products including individual enantiomers of tetrafluoro[6]helicene were determined showing the replacement of $\pi\cdots\pi$ and CH $\cdots\pi$ interactions by CH \cdots F interactions with increasing fluorine substitution. DFT calculation were performed to get an insight into the charge distribution and HOMO-LUMO gap.

Fig. 1



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