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

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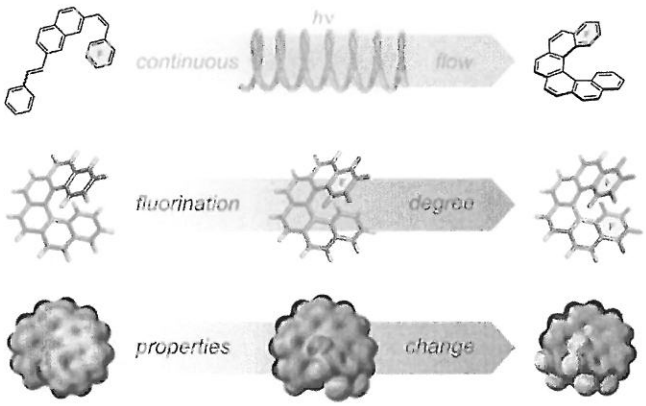
The introduction of fluorine substituents into helicene skeleton is a promising strategy for tuning of properties required for their further applications. The fluorine substitution can affect C-H/π interactions, which prevail in molecular assembly in the solid state, or can modulate the HOMO-LUMO gap. 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 π···π and CH···π interactions by CH···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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