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Chiral Resolution of Polar Subphthalocyanines – A Way to Control Self-Assembly in Liquid Crystals

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Materials containing bowl-shaped subphthalocyanine motifs (SubPc) (Figure 1) are emerging polar semiconductors used as acceptor materials in organic photovoltaic devices and can exhibit an anomalous photovoltaic effect due to polar order in their liquid-crystalline state.[1] Threefold substituted SubPcs are generated in a cyclocondensation reaction as a mixture of an enantiomer pair of C_3-symmetric compounds **1** and **2**, and of a C_1-symmetric enantiomer pair **3** and **4**. Enantiomers and regioisomers influence the details of their self-assembly,[1] therefore, separation and analysis of all four stereoisomers is essential.[2-3]

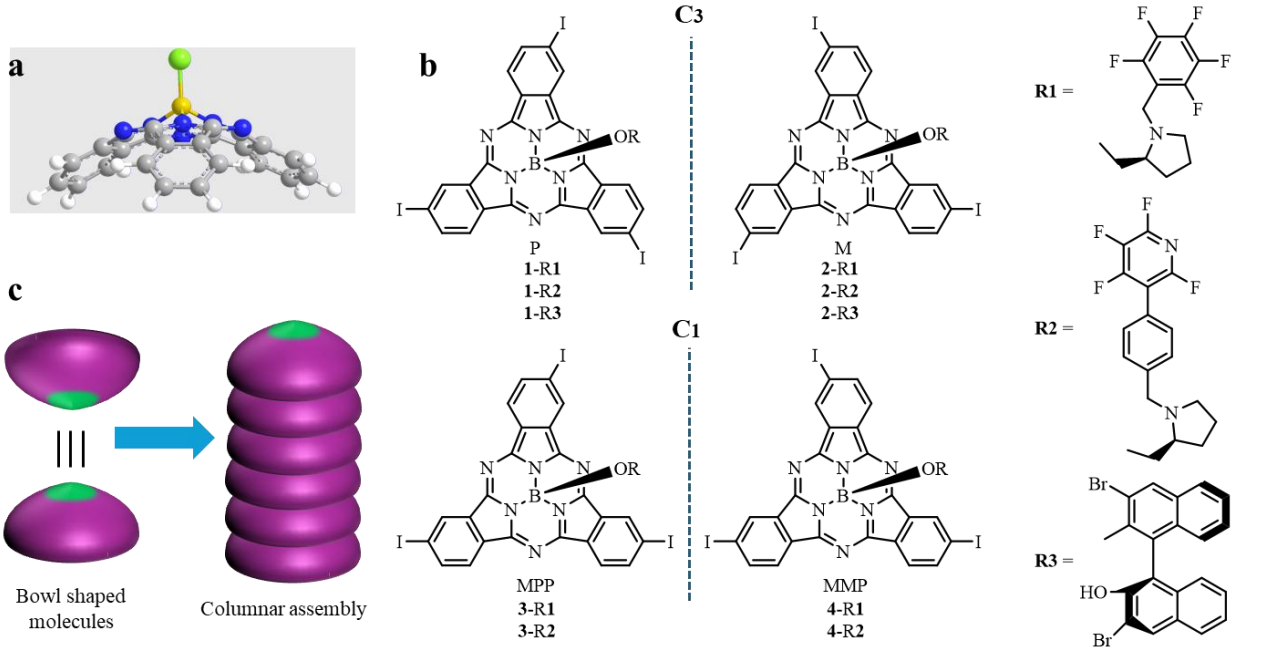

*Figure 1: Bowl-shaped SubPc (a); **C_1**- and **C_3**-symmetric regioisomers and their enantiomers with chiral auxiliaries* **R1**–**R3** *(b); and self-assembly into columnar structures (c).*

This study aims for the separation of regioisomers and enantiomers (SubPc **1**–**4**) with the help of rational designed chiral auxiliaries **R1**–**R2**. Therefore, we employ an *L*-proline-derived chiral auxiliaries with a pentafluorophenyl group (**R1**) and a fluoro-substituted pyridine (**R2**) proposed to allow for intramolecular interaction with the iodo-substituted aromatic units by halogen-bonding or π-π stacking. Auxiliary **R3** was successfully investigated for the separation of **C3** regioisomers.[2] Preliminary results show that diastereomers **1-R1**–**4-R1** reveal four signals in the HPLC eluogram hinting a successful chiral resolution.

References

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