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Chiral Conjugated Corrals

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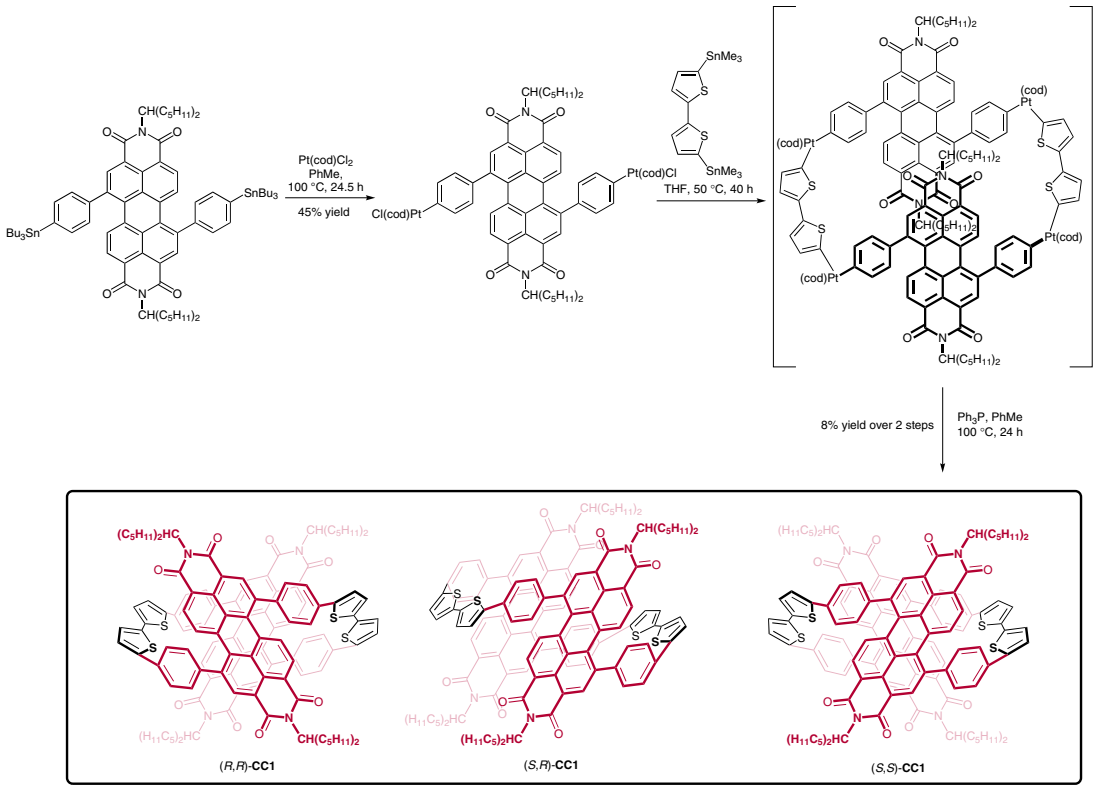
Hand Specific Rings



Significance: The first conjugated macrocycle containing alternating aromatic subunits –A–B–A–B– pattern was synthesized and studied in detail. Here, the diphenyl perlyene diimides serve as electron donors and the bithiophenes serve as electron acceptors. The new macrocycle has interesting structures and exists in dynamic equilibrium between the chiral and achiral forms. The unique electronic structure gives rise to an absorption spanning the entire visible light spectrum.

Comment: The three isomers (two enantiomers and one *meso* isomer) of macrocycle **CC1** were isolated by HPLC on a chiral column. Enantiomers (*R*,*R*)-**CC1** and (*S*,*S*)-**CC1** interconvert at room temperature through the intermediacy of the *meso* isomer (*S*,*R*)-**CC1**. Due to the branched undecyl side chains and the molecular dynamics, crystals of **CC1** could not be obtained. DFT calculations showed that the frontier orbitals participate in intramolecular charge transfer.

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