π-Extended Hexapyrrolylbenzenes: Exploring Charge-Transfer Phenomena in Donor-Acceptor Propellers

Autorzy

Daniel Matuszczyk

Yu Jin Lee

Seongsoo Kang

Piotr J. Chmielewski

Joanna Cybińska

Dongho Kim

Marcin Stępień

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Streszczenie

A family of propeller-shaped donor-acceptor hexapyrrolylbenzenes (HPBs) were designed and synthesized by sequential nucleophilic substitution of hexafluorobenzene with π-extended pyrroles. In particular, four hybrids were obtained, containing various combinations of electron-rich and electron-poor acenaphthylene-fused pyrroles. Additionally, to probe the efficiency of *ortho* transfer interactions, a system was designed containing unique donor and acceptor subunits spatially separated with four unfunctionalized pyrroles. DFT calculations showed propeller-shaped geometries of all HPB molecules and separation of frontier molecular orbitals between donor and acceptor subunits. Steady-state and time-resolved photophysical measurements revealed charge-transfer (CT) character of the emission with strong positive dependence on solvent polarity. The principal CT pathway involves *ortho*-positioned pairs of donors and acceptors and requires bending of the acceptor in the excited state.

Słowa kluczowe

chromophores, charge transfer, computational chemistry, nucleophilic aromatic substitution, pyrroles

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