Aromatic and antiaromatic pathways in triphyrin(2.1.1) annelated with benzo[*b*]heterocycles.

Autorzy

Krzysztof Bartkowski

Maria Dimitrova

Piotr J. Chmielewski

Dage Sundholm

Miłosz Pawlicki

Rok wydania

2019

Czasopismo

Chemistry-A European Journal

Numer woluminu

25

Strony

15477-15482

DOI

10.1002/chem.201903863

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

Understanding of the aromatic properties and magnetically induced current densities of highly conjugated chromophores is important when designing molecules with strongly delocalized electronic structure. Linear extension of the triphyrin(2.1.1) skeleton with an annelated benzo[*b*]heterocycle fragment modifies the aromatic character by extending the electron delocalization pathway. Two-electron reduction leads to an antiaromatic triphyrin(2.1.1) ring and an aromatic benzo[*b*]heterocycle subunit. Current-density calculations provide detailed information about the observed pathways and their strengths.

Słowa kluczowe

acenes, antiaromaticity, aromaticity, chirality, triphyrin

Adres publiczny

http://dx.doi.org/10.1002/chem.201903863

Strona internetowa wydawcy

onlinelibrary.wiley.com