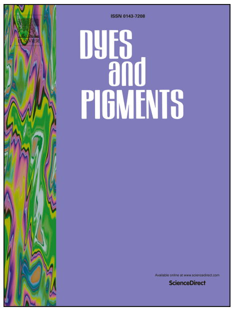

Optical tuning of tetrabenzo[8]circulene derivatives through pseudorotational conformational isomerization

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PII: S0143-7208(17)32272-6

DOI: 10.1016/j.dyepig.2018.01.013

Reference: DYPI 6487

To appear in: *Dyes and Pigments*

Received Date: 1 November 2017

Revised Date: 26 December 2017

Accepted Date: 10 January 2018

Please cite this article as: Baryshnikov GV, Valiev RR, Minaev BF, Ågren H, Optical tuning of tetrabenzo[8]circulene derivatives through pseudorotational conformational isomerization, *Dyes and Pigments* (2018), doi: 10.1016/j.dyepig.2018.01.013.

Optical tuning of tetrabenzo[8]circulene derivatives through pseudorotational conformational isomerization

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Abstract

In order to further search efficient [8]circulene materials for OLEDs application we have theoretically investigated the structure and electronic absorption spectra of functionalized tetrabenzo[8]circulenes with different substituents in the outer perimeter. These hydrocarbon materials complement the wide family of [8]circulenes which earlier have been demonstrated to possess promising emissive and exciplex-forming properties suitable for organic light emitting diodes. The hydrocarbon tetrabenzo[8]circulenes show saddle shape of the molecular skeleton which can exist in two different conformations with different curvatures of the macrocycle. The aromaticity, electronic structure and orbital pattern are found to be principally different for these two isomers, where the global minimum isomer is weakly antiaromatic and electronically less stable comparing with the non-aromatic local minimum structure. The absorption spectra are also very different: the global minimum structure is more active in the long-wavelength region while the local minimum isomer shows absorption only at short wavelengths. Our computational findings suggest a new concept for optical tuning of curved [8]circulenes through conformational isomerization and aromaticity control, thus through structural variations without changing the molecular composition. Based on this principle we have designed novel functionalized [8]circulenes with promising fluorescence activity.

Keywords: [8]circulene; conformational isomerization; pseudorotation; aromaticity; UV-Vis absorption.