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Better big or strained? Deformations of shape persistent arylene butadiynylene macrocycles

Autorzy

Marcin Małecki

Przemysław Dopieralski

Nurbey Gulia

Bartłomiej Pigulski

Tadeusz Lis

Sławomir Szafert

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Shape-persistent macrocycles have been of interest for many years to researchers due to their potential in synthesis and materials chemistry. They are regarded as reasonably rigid and in many cases they are able to spontaneously aggregate forming supramolecular assemblies. The dependence of a steric hindrance located on oxygen atoms in 2,6-bis-acetylenephenolates on the structure of macrocycles obtained from these precursors by Eglinton homocoupling has been investigated. A small library of crystal structures of arylene butadiynylene species has been obtained and analyzed in detail. Our results showed that regardless of the steric hindrance usually a wide range of macrocycles is formed (starting from tetramers) even though the smaller derivatives are significantly deviated from planarity, which might result from avoiding too much strain in these macrocyclic, cross-conjugated molecules.

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