



Octulene: a hyperbolic molecular belt that binds chloride anions.

Autorzy

Marcin A. Majewski

Yongseok Hong

Tadeusz Lis

Janusz Gregoliński

Piotr J. Chmielewski

Joanna Cybińska

Dongho Kim

Marcin Stępień

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Streszczenie

Octulene, the higher homologue of kekulene and septulene, was synthesized using the fold-in method. This new hydrocarbon macrocycle contains a large 24-membered inner circuit, which is peripherally fused to 24 benzene rings. Such an arrangement produces considerable hyperbolic distortion of the π -conjugated surface. The consequences of distortion in octulene were explored using photophysical methods, which revealed a reduced electronic band gap and greater flexibility of the π system. Octulene contains a functional cavity with a diameter larger than 5.5 Å that is capable of efficiently binding the chloride anion in a nonpolar solvent ($K_a = 2.2(4) \times 10^4 \text{ m}^{-1}$, 1 % dichloromethane (DCM) in benzene). The octulene-chloride interaction is stabilized by eight weak C(sp²)H...Cl bonds, providing the first example of a hydrocarbon-based anion receptor.

Słowa kluczowe

anion binding, aromaticity, hydrocarbons, organic synthesis, photophysics

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