Oxatriphyrins(2.1.1) incorporating an *ortho*-phenylene motif.

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Streszczenie

An understanding of fundamental aspects of archetypal organic structural motifs remains a key issue faced by the experimental and theoretical chemists. Two possible bonding modes for a disubstituted benzene ring, that is a meta and para, determines the π delocalization for oligomeric structures. When the less abundant *ortho*-substituted variant is introduced into a triphyrin(2.1.1) skeleton an aromatic molecule is obtained and the carbocyclic ring participates in the conjugation of the macrocycle. The two-electron reduction and introduction of boron(III) changes the aromatic character and results in an anti-aromatic structure which has been confirmed by single-crystal analysis and supported by theoretical calculations.

Słowa kluczowe

aromaticity, boron, density functional calculations, macrocycles, structure elucidation

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