

Pyridine-Fused Bis(azacorrole)s: Easily Accessible NIR III Absorbing Cation Radicals and Biradicaloids of Antiaromatic Ground State

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Streszczenie

A family of pyridine-fused bis(porphyrinoids) is obtained, including constitutionally isomeric bis(azacorrole)s, azacorrole-oxacorrole, as well as azacorrole-norcorrole heterodimers by two distinct synthetic approaches. Spectroscopic characteristics, corroborated by Density Functional Theory (DFT) calculations, indicate aromaticity of the bis(azacorrole) as well as azacorrole-oxacorrole products, while for the azacorrole-norcorrole heterodimers, the presence of both dia- and paratropic currents is detected. Electrochemical analyses indicate facile chemical access to cation radicals and dicationic species that have been characterized by electronic and electron spin resonance spectroscopy as well as by DFT calculations. Monocations give rise to the relatively strong absorption bands in the near infra red (NIR) region between 2400 and 3200 nm, while dications are characterized by a series of absorptions between 1000 and 2200 nm. Electron spin resonance (ESR) experiments indicate the presence of singlet-triplet spin equilibria for the dications. For the dication of bis(azacorrole) of the most planar structure, the singlet ground state is established, and low temperature nuclear magnetic resonance (NMR) as well as gauge-independent atomic orbital NMR calculations indicate its antiaromatic character.

Słowa kluczowe

antiaromaticity, aromaticity, biradicaloids, porphyrinoids, radicals

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