Aza-deficient porphyrin as a ligand.

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Streszczenie

Vacataporphyrin, a porphyrin devoid of one nitrogen atom is an annulene–porphyrin hybrid. Naming it in a different manner—butadieneporphyrin as one pyrrole unit is replaced with butadiene moiety, accents its carbaporphyrinoid nature. The molecule acts as a macrocyclic ligand which accommodates the following metal ions: cadmium(II), zinc(II), nickel(II) and palladium(II). The tripyrrin pincer of vacataporphyrin holds the metal close to the flexible butadiene fragment which may acquire different configurations depending on presence of light, acid concentration or axial ligand identity. The butadiene moiety of vacataporphyrin may be involved in a π-interaction with metal ions. A single example a σ palladium(II)–carbon bond has also been identified. Intricate multi-step structural changes have been spectroscopically detected for palladium(II) vacataporphyrin. A peculiar reversible switch between vacataporphyrin conformers characterized by Hückel or Möbius topology has been accompanied by a change of electronic structure revealed respectively by aromaticity or antiaromaticity.

Słowa kluczowe

Porphyrinoids, Annulene, Aromaticity, Conformation analysis, Nickel, Palladium, Cadmium, Zinc, Möbius antiaromaticity

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