

Cyclic metalloporphyrin trimers: ^1H NMR identification of trimeric heterometallic (iron(III), gallium(III), manganese(III)), 2-hydroxy-5,10,15,20-tetraphenylporphyrins and X-ray crystal structure of the Iron(III) 2-hydroxy-5,10,15,20,-tetra-*p*-tolylporphyr.

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Streszczenie

Oligomerization of a mixture of monomeric iron(III) 2-hydroxy-5,10,15,20-tetraphenylporphyrin, $(2\text{-OH-TPP})\text{Fe}^{\text{III}}\text{Cl}$, manganese(III) 2-hydroxy-5,10,15,20-tetraphenylporphyrin, $(2\text{-OH-TPP})\text{Mn}^{\text{III}}\text{Cl}$, and gallium(III) 2-hydroxy-5,10,15,20-tetraphenylporphyrin, $(2\text{-OH-TPP})\text{Ga}^{\text{III}}\text{Cl}$, complexes affords the series of heterometallic cyclic trimeric species of the general formula $\{[(2\text{-O-TPP})\text{Ga}^{\text{III}}]_n[(2\text{-O-TPP})\text{Fe}^{\text{III}}]_{3-n}\}$, $\{[(2\text{-O-TPP})\text{Ga}^{\text{III}}]_n[(2\text{-O-TPP})\text{Mn}^{\text{III}}]_{3-n}\}$, and $\{[(2\text{-O-TPP})\text{Fe}^{\text{III}}]_n[(2\text{-O-TPP})\text{Mn}^{\text{III}}]_{3-n}\}$ ($n = 0-3$). The ^1H NMR spectroscopic and mass spectrometric investigations indicate that these compounds have a head-to-tail cyclic trimeric structure. In the ^1H NMR spectra the interactions between paramagnetic, weakly coupled centers are reflected by marked variations of chemical shifts and line widths of pyrrole resonances. The characteristic upfield positions of the 3-H pyrrole resonances are diagnostic for the trimeric motifs. The structure of the prototypical molecule, $[(2\text{-O-TTP})\text{Fe}^{\text{III}}]_3$, has been determined by X-ray crystallography. $[(2\text{-O-TTP})\text{Fe}^{\text{III}}]_3 \cdot 3n\text{-octane}$ crystallizes in the monoclinic space group $P2_1/n$ with $a = 16.729(6)$ Å, $b = 43.671(13)$ Å, $c = 19.564(7)$ Å, $\beta = 105.83(3)^\circ$, and $Z = 4$ at 130 K. The refinement of 1612 parameters and 5072 reflections yields $R_1 = 0.089$ and $wR_2 = 0.1848$. The trimeric iron(III) complex has a head-to-tail cyclic arrangement with the pyrrolic alkoxide groups forming bridges from one macrocycle to the metal in adjacent macrocycle. The three iron(III) porphyrin subunits are not equivalent but have typical geometry for high-spin five-coordinate iron(III) porphyrin complexes. The porphyrin skeleton of $[(2\text{-O-TTP})\text{Fe}^{\text{III}}]_3$ is expected to be representative of the structures of the homometallic and heterometallic trimeric complexes of 2-hydroxytetraarylporphyrin with M(III) ions.

Słowa kluczowe

Mixtures, Transition metals, Metals, Pyrroles, macrocycles

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