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High-spin iron(III) tetramethylchiroporphyrins: structural, magnetic and H^1 NMR studies.

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The chloroiron(III) complex of αβαβ-tetramethylchiroporphyrin, FeCl(TMCP), was prepared, and its structure was determined by X-ray crystallography. Black crystals of FeCl(TMCP)·0.72CH_2Cl_2 form in the tetragonal space group $P4_32_12$ with $a = b$ = 13.245(1) Å and c = 26.355(5) Å at 130 K with Z = 4. The structure shows an unusual five-coordinate high-spin iron(III) center in a strongly ruffled and domed porphyrin, with short equatorial bond distances (Fe−N(av) = 2.034(9) Å), and the iron 0.64 Å out of the porphyrin mean plane toward the chlorine atom. The solid-state magnetic moment is 5.92 μ_B at 20 K, slightly decreasing to 5.68 μ_B at 300 K. In solution FeCl(TMCP) can be easily transformed to FeBr(TMCP) or FeOH(TMCP). The ^{1}H NMR spectra of the three species are consistent with their C_2 symmetry and $S = {}^5/_2$ spin state. The pyrrole proton resonances are shifted downfield to 80−100 ppm at 293 K, more than in the corresponding tetraaryl derivatives. The cyclopropyl protons on C_1, α to the porphyrin *meso* position, appear at ca. 160−200 ppm, in keeping with the nearly perpendicular orientation of the C_1−H bond with respect to the porphyrin mean plane. The temperature dependence of the ^{1}H NMR spectrum of FeCl(TMCP) suggests substantial zero-field splitting.

Adres publiczny

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