2-Hydroxy-3,5-dinitrobenzoate: A Novel μ_2-Bridging Ligand

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μ_2-(2-Hydroxy-3,5-dinitrobenzoato)(octaethylporphinato)Fe(III) dimer was synthesized as part of our studies of malaria pigment model systems[1-3]. The asymmetric bridging ligand coordinates one Fe(III)OEP moiety through the phenylato-oxygen atom and the second Fe(III)OEP through one oxygen atom of the *trans*-NO_2 group. The complex crystallizes in the triclinic space group $P\bar{1}$ with one molecule in the unit cell ($Z' = 0.5$). The bridging ligand is statistically disordered, while the centrosymmetrically-related Fe(III)OEP moieties are ordered. The average Fe—N distance, 2.050 Å, the Fe—O(phenolate) distance, 1.909 Å, and the Fe displacement from the 24-atom porphyrin plane, 0.464 Å, are similar to those found in the related Fe(III)(OEP)picrate[3] complex showing a five-coordinate square-pyramidal geometry in the high-spin ferric state. The bridging ligand with its abundance of O atoms engages in extensive C—H···O hydrogen bonding as established by the crystal structure and IR shifts of spectral bands.

Crystal data: dark-purple block shaped crystals; $C_{79}H_{90}N_{10}O_7Fe$, M_w = 1403.31; a = 12.8776(6), b = 13.0097(6), c = 13.1232(6)Å, α = 96.894(2), β = 109.182(2), γ = 113.718(1)°, V = 1818.46(15) Å^3; T = 296.2 K; μ = 0.46 mm^{-1}, d_{calc} = 1.281 Mg m^{-3}; θ_{max} = 25.35°, 6645 unique data, 4307 > 2σ(I), R_1 = 0.054, wR_2 = 0.114, *gof* = 1.025; ρ_{max} = 0.26 e Å^{-3}.

References:

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