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Packing Interactions of 2,3,7,8,12,13,17,18-Octaethylporphyrinato(picrato)iron(III). Ratchadaporn Puntharod, Kenneth J. Haller, School of Chemistry, Inst. of Science, Suranaree Univ. of Technology, Nakhon Ratchasima 30000 Thailand.

The X-ray structure of 2,3,7,8,12,13,17,18-octaethylporphyrinato(picrato)iron(III), [Fe(OEP)(picrate)], is reported. The compound crystallizes in the monoclinic space group $C2/c$ with eight molecules per unit cell, thus one full molecule in the asymmetric unit. The five-coordinate Fe(III) atom is significantly displaced above the 4N-coordination plane towards the axially coordinated picrate ligand. The Fe–O distance and the Fe–O–C angle to the axial ligand are 1.935(4) Å and 125.9(4)°, respectively, both larger than the expected values, perhaps due to steric interactions between the 2,6 nitro substituents on the picrate and the plane of the porphyrin core. The nitro groups rotate relative to the picrate ligand such that they are parallel to, and in contact with the face of the porphyrin plane.

Crystal Data: $C_{42}H_{46}FeN_7O_7$, $Mr = 816.71$, monoclinic $C2/c$, $a = 26.400(2)$, $b = 13.781(2)$, $c = 25.413(2)$ Å, $\beta = 119.96(1)^\circ$, $V = 8010.2(2)$ Å³, $Z = 8$, $D_{Calc} = 1.354$ Mg m⁻³, $T = 298$ K, $\mu_{Mo} = 0.44$ mm⁻¹.