Geometric and electronic structure of paramagnetic tetraarylporphyrin complexes of chromium.

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Rok wydania

1992

Czasopismo

Inorganic Chemistry

Numer woluminu

31

Strony

1148-1151

DOI

10.1021/ic00033a007

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

(TPP)Crm(OPh)(THF) (TPP is the dianion on mesotetraphenylporphyrin; THF is tetrahydrofuran) crystallizes in the triclinic space group Pi with a = 9.583 (5) A, b = 11.473 (7) A, c = 11.504 (6) A, a = 63.90 (4)°, ß = 91.04 (4)°, y = 77.29 (4)°, and Z = 1 at 130 K. Refinement of 151 parameters and 2125 reflections yields R = 0.082, = 0.076. The structure consists of a six-coordinate chromium located at the center of the planar porphyrin with axial phenoxide (Cr-O distance 1.943 (10) A) and THF (Cr-O distance 2.069 (10) A) ligands which are disordered about the chromium. The 2H NMR spectra of deuterated-pyrrole

Cr(III) and Cr(II) complexes have been examined in solution, and the hyperfme shifts are interpreted in terms of their electronicstructures. Axial ligand resonances have also been observed for (TPP-d8)Cr!II(OPh-</5)(THF). The reaction of fert-butyl hydroperoxide with (TPP)CrmCl has been monitored by 2H NMR and electronic spectroscopy. An unstable isoporphyrin complexis formed.

Adres publiczny

https://doi.org/10.1021/ic00033a007

Strona internetowa wydawcy

https://www.acs.org/content/acs/en.html