Structural characterization and DFT calculation of the Fe-C coordinating bond in bis (*tert*-butyl isocyanide) iron (II) phthalocyanine.

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Rok wydania

2013

Czasopismo

Journal of Porphyrins and Phthalocyanines

Numer woluminu

17

Strony

742-749

DOI

10.1142/S1088424613500181

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

Bis(*tert*-butyl isocyanide) iron(II) phthalocyanine complex in the crystalline form was obtained by a direct reaction of β-FePc with *tert*-butyl isocyanide. This complex crystallizes in the centrosymmetric space group P 2_1/c of the monoclinic system. The Fe(II) cation is equatorially ligated by the four N-isoindole atoms of Pc^{2-} macrocycle and axially by the C atom of *tert*-butyl isocyanide on both sides of a planar FePcmolecule. Gas-phase conformation of the bis(*tert*-butyl isocyanide) iron(II) phthalocyanine molecule obtained by molecular orbital calculations shows a similar conformation as in the crystal. In both phases (solid and gas) a similar correlation between the equatorial Fe–N and axial Fe–Cbonds are observed. Steric hindrance of the *tert*-butyl isocyanide molecules ligated to Fe in axial positions of planar FePc leads to the lowering of the π–π interaction between the π-clouds of Pc macrorings and makes the crystals of the bis(*tert*-butyl isocyanide) iron(II) phthalocyanine complex better soluble in the most organic solvents than the parent FePc compound. EPR and magnetic susceptibility measurements clearly show that ligation of the intermediate spin FePc by *tert*-butyl isocyanide leads to the change of the ground state from S = 1 (for FePc, $e_g^3b_{2g}^2a_{1g}^1$) to S = 0 yielding the low-spin complex ($((CH_3)_3C\text{-}N{\equiv}C)_2FePc$, $e_g^4b_{2g}^2$). The calculated three-dimensional MESP maps are helpful for understanding of the interaction between the FePc and *tert*-butyl isocyanide molecules forming bis(*tert*-butyl isocyanide) iron(II) phthalocyanine complex.

Słowa kluczowe

iron phthalocyanine, tetra-butyl isocyanide, crystal structure, DFT, spectroscopy

Adres publiczny

http://dx.doi.org/10.1142/S1088424613500181