

Protonation of 5,10,15,20-tetraphenylsapphyrin-identification of inverted and planar dicationic forms.

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Streszczenie

5,10,15,20-Tetraphenylsapphyrin (TPSH₃, I0) presents an unusual structural skeleton with an inverted pyrrole ring lying opposite to the bipyrrrolic unit. The acid–base chemistry of sapphyrin, involving hydrogen chloride, dichloroacetic acid or trifluoroacetic acid in chloroform, dichloromethane (293 and 203 K) and DMSO (293 K) has been followed by means of UV–VIS electronic and ¹H NMR spectroscopy. The protonation of TPSH₃ proceeds stepwise *via* a mono- and a variety of dicationic forms. The monoprotonated species (I1) preserves the inverted skeleton of I0. Two fundamental structures, inverted (I2) and expanded (P2), have been detected in the case of dications. The transformation of the macrocycle involves a reversible flip of a single pyrrole unit which relocates the 27-NH pyrrolic nitrogen between the periphery and the centre of macrocycle (I⇌P). The rearrangement is triggered by proton and/or anion addition and involves binding of anion(s) *via* a system of multiple NH-anion hydrogen bonds. The sequence of structural transformation is solvent dependent: I0 → I1 → P2 → I2 in dichloromethane (chloroform) but I0 → I1 → I2 → P2 in DMSO for all investigated acids.

Adres publiczny

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