Protonated N-confused porphyrin dimer: formation, structure, and guest binding.

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Streszczenie

The protonation of 3,3′-bis(*meso*-tetratolyl-2-aza-21-carbaporphyrin) with various acids was studied. The stepwise formation of mono-, di-, and tetracationic species was shown on the basis of UV–vis–near-IR and low-temperature ^{1}H NMR. Upon going from di- to tetraprotonated form, the bis(porphyrinoid) skeleton changes its conformation from cisoid to bent-transoid, which was found by single-crystal X-ray analyses, 2D NMR, and density functional theory (DFT) calculations. The formation of cation–anion complexes was established in both the solid state and solution. The substitution of anions was studied by spectrophotometric and ^{1}H NMR titrations. A pronounced decrease of the HOMO–LUMO gap in the tetraprotonated species was shown by cyclovoltametry and time-dependent DFT calculations.

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