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Conformational flexibility of nickel(II) benziporphyrins.

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^{1}H NMR spectra of three paramagnetic Ni(II) complexes of benziporphyrins have been investigated in a broad temperature range. For the *m*- and *p*-benziporphyrin complexes, the line widths of certain signals exhibit an unusual temperature dependence characteristic of a dynamic process. This behavior is interpreted in terms of an equilibrium in which one of the forms is present at a very small concentration and cannot be observed directly. For the benziporphodimethene complex, the two exchanging forms are present at comparable concentrations and can yield separate signals in the slow exchange limit. To account for the observed exchange process, a mechanism is proposed involving the motion of the phenylene moiety. This hypothesis is further explored with DFT modeling, which indicates that the postulated conformers are thermally accessible.

Adres publiczny

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