

Low-spin iron(III) chirophyrins: ^1H NMR studies of cyanide and substituted imidazole coordination.

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Streszczenie

Low-spin complexes of iron(III) chirophyrin, obtained from (1*R*)-*cis*-caronaldehyde acid methyl ester and pyrrole as the atropisomer, with R-imidazoles and cyanide have been studied by means of 1D and 2D ^1H NMR spectroscopy. A complete spectral assignment of resonances has been done on the basis of observed scalar, NOE, and EXSY correlations in 2D COSY and NOESY experiments. The chemical shift of β -H pyrrole resonances have been used as a sensitive probe of electronic state of iron(III) metal ion. Cyanide anion coordination both in methanol and methylene dichloride results in formation of bis(cyanide) low-spin complexes with the rare $(d_{xz}, d_{yz})^4 (d_{xy})^1$ electronic ground state, revealed by pyrrole β -H resonances at 11.12 and 10.56 ppm at 293 K, whereas imidazole and 1-methylimidazole produce the bis-ligated complexes with the $(d_{xy})^2 (d_{xz}, d_{yz})^3$ ground state. In case of sterically hindered imidazole derivatives, i.e., 2-methylimidazole and 1,2-dimethylimidazole, two rotational isomers have been observed at 293 K. Both electronic configurations contribute to the ground state of metal ion for the latter. The steric bulkiness of 2-methylimidazole (or 1,2-dimethylimidazole) is required to freeze a favorable configuration, even at room temperature, providing the perpendicular orientation of two imidazole planes which seems to be instrumental in the stabilization of the rare $(d_{xz}, d_{yz})^4 (d_{xy})^1$ electronic state.

Słowa kluczowe

Imidazoles, Ligands, Molecular structure, Pyrroles, Substituents

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