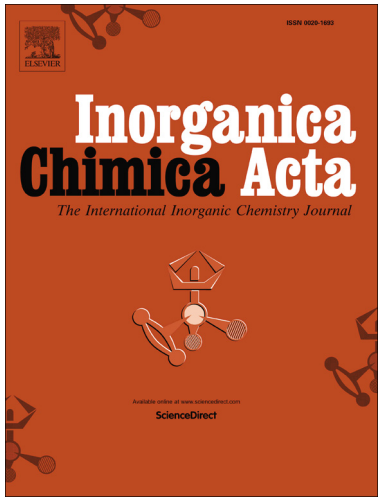

Research paper

Synthesis, characterization, solution equilibria, DFT study, DNA binding affinity and cytotoxic properties of a cobalt(II) complex with a 5-pyrazolone ligand

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Synthesis, characterization, solution equilibria, DFT study, DNA binding affinity and cytotoxic properties of a cobalt(II) complex with a 5-pyrazolone ligand

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Abstract

Our work describes the synthesis, the complexation and the characterization of a cobalt(II) complex with a 5-pyrazolone ligand carrying a thioamide group on N^1 position. The study of the complexation in solution allowed the determination of the stability constants of the complex and the distribution of the species involving Co(II) over the whole pH-range. The solid cobalt(II) complex has then been synthesized and fully characterized by infrared, electronic, EPR and mass spectrometries, in addition to magnetic and voltammetric measurements. The data clearly indicated an octahedral high spin Co(II) complex with two mononegative molecules of the N,S-ligand, and two water molecules, likely in a *cis* position because of the high anisotropy. DFT calculations performed on both the ligand and the complex structures allowed us to study the spectral features, and to propose the most fitting structures to the experimental data. The interaction of the 5-pyrazolone ligand and its Cobalt(II) complex with fish-sperm DNA has been studied by electronic spectrometry and cyclovoltammetry. Intercalation has been identified as a binding mode and the strength of the binding assessed. In order to explore eventual cytotoxic and/or cytostatic properties of our compounds, the ligand and the cobalt complex have been tested on PC-3 (human prostate carcinoma) and HT-29 (human colon carcinoma) using sulphorhodamine B (SRB) assay.

Keywords: Cobalt; pyrazolone; DNA-interactions; cytotoxicity; colon cancer, prostate cancer.

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