

ABSTRACT

Complexes, metal-organic compounds and coordination polymers encompass an area of chemistry that has grown tremendously in the last decades, as indicated by not only a great number of research papers published but also the ever-expanding scope of the research and applications of this type of compounds.

The main scientific objective of this doctoral dissertation was the synthesis of new complexes of four N,O-donor ligands based on indole (indole-3-carboxylic acid, 5-methoxyindole-2-carboxylic acid) and 7-azaindole (7-azaindole-3-carboxylic acid, 7-azaindole-3-carboxaldehyde) with selected metal ions. The basic element was determination of crystal and molecular structures of the obtained complexes and of the two investigated ligands, elaboration of their detailed spectroscopic characteristics (FT-IR and FT-Raman) and study of biological activity of selected ligands and their complexes.

As a result of the conducted studies, single crystals of 7-azaindole-3-carboxylic acid and 7-azaindole-3-carboxaldehyde and ten new complexes were obtained for the first time. For six complexes, crystal and molecular structures were determined by X-ray analysis. A complete and detailed interpretation of the vibrational spectra using quantum chemistry methods (DFT) was elaborated for all compounds. For this purpose, calculations of molecular structures and vibrational spectra for the investigated systems were performed with the use of theoretical models that illustrate the structures present in the crystal lattices of these compounds and taking into account the intermolecular interactions. A detailed vibrational spectra interpretation was carried out based on the calculated potential energy distributions. The study also showed that the complexation of both examined 7-azaindole derivatives with Pt(II) and Pd(II) ions and of indole-3-carboxylic acid with Co(II) ions leads to an increase in biological activity of the obtained complexes compared to the free ligands. Particularly promising results have been obtained for the 7-azaindole-3-carbaldehyde complex with Pt(II) ions and for the coordination polymer of indole-3-carboxylic acid with Co(II) ions.

The obtained results are important for coordination chemistry, bioinorganic chemistry, vibrational spectroscopy and potentially medical chemistry. The research provides valuable information on interactions of indole and 7-azaindole with Pt(II), Pd(II), Cu(II), Co(II), Cd(II), Na(I) ions and the spectroscopic analysis performed can be useful for characterization of other structurally similar complexes.

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