

**Summary of doctoral thesis: "Transition metal complexes of 2,3,5,6-tetrakis(2-pyridyl)pyrazine - structural, spectroscopic, and magnetic studies."**

The research subject of my thesis concerns mono- and polynuclear transition metal coordination compounds incorporating 2,3,5,6-tetrakis(2-pyridyl)pyrazine (*tppz*) and halide or pseudohalide ligands. The main goal of this work was to synthesize new coordination compounds with promising photoluminescent, catalytic and magnetic properties. In the first part of my thesis based on the literature data, I showed that transition metal compounds containing *tppz* may be functional materials in many fields, such as molecular magnetism, catalysis and photoluminescence. Compared to the related complexes incorporating 2,2';6',2''-terpyridine derivatives, however, the number of transition metal coordination compounds of *tppz* is still limited. Therefore, the results of these studies also allow us to understand factors which determine the type of binding modes of *tppz* as well as allow us to predict the structure and properties of new coordination compounds with 2,3,5,6-tetrakis(2-pyridyl)pyrazine in future.

As a result of my studies, I have obtained 21 new coordination compounds, among which there are compounds of Mn(II), Co(II), Cd(II), Ni(II), Re(IV) and Re(III). For all the examined systems, X-ray structural analysis was performed in order to determine coordination modes of *tppz* and inorganic ions. It is worth mentioning that I have synthesized a completely new type of coordination polymers ( $[\text{Cd}(\text{NCS})_2(\mu\text{-tppz})]_n$  or  $[\text{Co}(\mu\text{-1,3-NCS})(\text{NCS})(\text{tppz})]_n$ ) with Cd ions linked by *tppz* and single, thiocyanate anion, respectively.

Most importantly, my research confirmed that the complexes incorporating *tppz* are promising inorganic materials due to their catalytic, spectroscopic and magnetic properties. Magnetic susceptibility measurements of the complexes of general formula  $[\text{M}(\text{tppz})_2\text{X}_n]$  (where X = dca, tcm,  $[\text{Co}(\text{NCS})_4]^{2-}$  or  $[\text{Co}(\text{NCO})_4]^{2-}$ , n = 1 lub 2) revealed the occurrence of an incomplete spin crossover behavior  $1/2$  (LS)  $\leftrightarrow$   $3/2$  (HS). On the other hand, the isomorphous coordination polymers  $[\text{M}^{\text{II}}(\mu\text{-1,3-NCS})(\text{NCS})(\text{tppz})]_n$  (where  $\text{M}^{\text{II}} = \text{Co}(\text{II})$  or  $\text{Ni}(\text{II})$ ), which are made up of zigzag chains of cobalt(II) and nickel(II) bridged by single end-to-end thiocyanate groups, exhibited intrachain ferromagnetic interactions. Measurements of temperature-dependent magnetic susceptibility for  $[\text{H}_2\text{tppz}][\text{ReCl}_4]$  revealed that the Re(IV) centers are magnetically isolated. In turn, the magnetic susceptibility of  $[\text{ReCl}_3(\text{tppz})] \cdot \text{CH}_3\text{CN}$  can be attributed to the second-order Zeeman effect between the non-magnetic ground state ( $M_J = 0$ ) and higher energy levels ( $M_J \neq 0$ ). The compounds  $[\text{Mn}(\text{NO}_3)_2(\text{tppz})(\text{H}_2\text{O})]$  and  $[\text{Mn}(\text{N}_3)(\text{NO}_3)(\text{tppz})(\text{H}_2\text{O})]$  turned out to be effective and selective catalysts in oxidation reactions of alcohol to aldehydes/ketones and oxidation reactions of sulfides to sulfoxides. All the obtained Cd(II) compounds were emissive in solid state. Most importantly, the ladder-like coordination polymer  $[\text{Cd}_2(\mu\text{-1,3-NCS})_2(\text{NO}_3)_2(\mu\text{-tppz})]_n$  exhibited long lifetime photoluminescence at room temperature with large separation between excitation and emission luminescence, which indicates phosphorescence nature of the emission.