

### **Abstract of doctoral thesis**

"Mono- and binuclear complexes of ruthenium, osmium and iridium with cyclometalating pyrene and terpyridine ligands"

The presented doctoral dissertation is devoted to fundamental research in the field of synthesis and comprehensive characterization of new, double NCN-cyclometalating ligands based on pyrene structure and tridentate ligands which are derivatives of 2,2':6',2''-terpyridine and its analogs. These ligands in the next stages of the research were used in obtaining of new designed mono- and binuclear complexes of ruthenium, osmium and iridium with the general chemical formula  $[(NNN)M(NCN\text{-pyrene}\text{-}NCN)M(NNN)]^n$  and  $[(NNN)M(NCN\text{-pyrene}\text{-}NCN)]^m$ . The current state of knowledge in the field of that kind of compounds is just five scientific papers published by the team from the Chinese Academy of Sciences under the leadership of Professor Yu-Wu Zhong, where the ruthenium was the only one used. Furthermore, NCN-cyclometalating pyrene ligands have been described in the literature insignificantly. That makes the field of science definitely requires the development and undertaking of in-depth research that will allow a better understanding of the relation between structure and properties. As in the case of ligands, the purpose of the work is also the characterization of the target complexes, including the examination of thermal stability and optical properties. In addition, at the stage of planning the structures of synthesized ligands and complexes, as well as the analysis of their properties, they were supported by computational methods based on the DFT (density functional theory) and TD-DFT (time-dependent density functional theory) methods.

In the area of the NCN-cyclometalating pyrene ligands, pyrene derivatives containing at positions 1,3,6 and 8 pyridyl, pyrazolyl, triazolyl and tetrazolyl substituents were obtained. The results of the research have shown that structural changes within pyrene systems do not affect their optical properties, which has also been proved by quantum chemical calculations; frontier orbitals are mainly located on the pyrene, the contribution of substituent orbitals increases in the following order: pyridyl, triazolyl, tetrazolyl, pyrazolyl. This is due to the geometry of the molecule, as indicated by the change in the angle between the pyrene and the substituent, which decreases exactly in the same series.

In the field of research dedicated to derivatives of 4'-phenyl-2,2':6',2''-terpyridine, compounds containing fluoroene, anthracene, carbazole, triazole and tetrazole motifs were obtained based on coupling and cycloaddition reactions. Based on the physicochemical and theoretical studies, the nature of the terpyridine ligand was recognized which was crucial in the next stage of research devoted to complexes.

Complexes of ruthenium, osmium and iridium were obtained and thoroughly examined. Differences and similarities of the properties between mononuclear and binuclear compounds of ruthenium and osmium were presented. Furthermore, the effect of the absence of symmetry on the properties of the ruthenium complexes was also checked. The next part was the investigation of the influence of coordinated metal, i.e. ruthenium, osmium and iridium on the properties of complexes built of the same ligands. Studies have also been conducted in the field of mononuclear osmium complexes in order to determine the effect of heteroaryl groups in the bridging ligand on the properties of the target compounds.