

Carbonyl rhenium(I) complexes with triimine ligands in the aspect of structural and luminescence studies

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Rhenium was discovered in 1925 by Walter Noddack, Ida Tacke and Otto Berg. Since then, this metal has come a long way from newly discovered element to very important part of modern technology. Also, coordination compounds with rhenium(I) as central ion have gained much significance. The complex $[\text{Re}(\text{CO})_3\text{Cl}(\text{phen})]$ was the first carbonyl compound with transition metal that showed luminescence at room temperature solution. Since this groundbreaking work of Wrighton and Morse published in 1974, many more photoluminescent tricarbonyl rhenium(I) compounds with diimine ligands based on 1,10-phenanthroline (R-phen) and 2,2'-bipyridine (R-bpy) cores were synthesized and thoroughly investigated. These compounds have been at the center of scientific attention mostly because of their possible applications in solar energy conversion devices, luminescent sensors, photosensitization of organic substrates, organic, light-emitting diodes (OLED) and other domains, such as catalysis or medical chemistry.

Within this dissertation I have studied how the structural modifications of 2,2':6',2''-terpyridine (*terpy*), 2,6-dithiazolylpyridine (*dtpy*) and 2,6-dipyrazinylpyridine (*dppy*) influence optical, thermal, electrochemical and electroluminescent properties of carbonyl rhenium(I) coordination compounds. My inspiration to undertake this research were the results of experimental and theoretical studies by Wang et al, and also by Velmurugan and Venuvanalingam. Those studies were dealing with the possibility to enhance emissive properties of $[\text{Re}(\text{CO})_3\text{Cl}(\text{terpy})]$ complex by introducing structural modifications to terpyridine ligand, as well as possible use of this type of compounds in OLED technology. In comparison to thoroughly researched complexes of $[\text{Re}(\text{CO})_3\text{Cl}(\text{R-bpy})]$ and $[\text{Re}(\text{CO})_3\text{Cl}(\text{R-phen})]$ type, those with 2,2':6',2''-terpyridine derivatives were poorly described in literature. What is more, coordination properties of 2,6-dithiazolylpyridine and 2,6-dipyrazinylpyridine (ligands designed as 2,2':6',2''-terpyridine analogues) towards $\{\text{Re}(\text{CO})_3\}$ group have been studied for the first time within this dissertation.

As a result of my research, I have obtained and characterized 45 new rhenium(I) coordination compounds, in which 22 were based on *terpy*, 14 on *dtpy* and 9 on *dppy* skeleton. Basing on my results I have determined the impact of triimine ligand skeleton and also electron donating/electron accepting properties of ligand substituents on optical, thermal and electrochemical properties of tricarbonyl rhenium(I) complexes. I also formulated series of relationships between the structure of organic ligand and selected functional parameters of rhenium(I) carbonyls. This issue is important in the context of rational design and synthesis of new coordination compounds with desirable functional parameters. Furthermore, I conducted initial assessment of the studied compounds for use in OLED technology. For 39 obtained carbonyls electroluminescent diodes (OLED) in the guest-host configuration or with neat coordination compound as an active layer were manufactured.