**Polypyridyl Ru(II) Complexes and their Template Effect in the Condensation Reaction of Ethyleneglycol with 1,10-Phenanthroline-5,6-dione**

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Date of Submission: 2012/02/14

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Degree: M.Sc. Language: Farsi

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**Abstract**

In this thesis, three mononuclear polypyridyl complexes of Ru(II), [Ru(phen-diox)3](PF6)2, [Ru(phen-diox)2(DMF)2](PF6)2 and [Ru(phen-diox)2(H2O)2](PF6)2 have been prepared and characterized by elemental analysis, FT-IR and UV-Vis spectroscopies. [Ru(phen-diox)3](PF6)2 has been purified by column chromatography with Alumina as stationary phase. Orange crystals of [Ru(phen-diox)3](PF6)2 were grown by ether diffusion into an actonitrile solution of the complex. Solid state structure of [Ru(phen-diox)3](PF6)2 was determined by single crystal X-ray crystallography. In the complex, Ru(II) is six-coordinate and the phen-diox ligand is coordinated as a bidentate chelate, with two Npyridyl atoms. Single crystal X-ray crystallography of [Ru(phen-diox)3](PF6)2 shows a distorted octahedral geometry around Ru(II). Electronic spectrum of the complex was taken in actonitrile. For the complex, the intense absorption bands seen in the UV region are assigned to ligand-centered transitions and an absorption band seen in the visible region is assigned to MLCT transition. The FT-IR spectrum of the compound shows a sharp and strong absorption band at 842 cm-1 for the υ(P-F). The electrochemical studies of the complex indicate a metal-base reduction at the positive potentials and ligand-base reduction at the negative potentials. Also, the fluorescence spectra of the complex show high intensity emission in the visible region. There is a very good agreement between experimental elemental analysis and calculated results. [Ru(phen-diox)2(DMF)2](PF6)2 has been purified by column chromatography. Alumina has been used as stationary phase. Brown crystals of [Ru(phen-diox)2(DMF)2](PF6)2 were grown by ether diffusion method. Electronic spectrum of the complex was taken in actonitrile. For the complex, the intense absorption bands seen in the UV region are assigned to ligand-centered transitions and an absorption band seen in the visible region is assigned to MLCT transition. The FT-IR spectrum of the compound shows a sharp and strong absorption band at 843 cm-1 for the υ(P-F). The electrochemical studies of the complex indicate a metal-base reduction at the positive potentials and ligand-base reduction at the negative potentials. Also, the fluorescence spectra of the complex show high intensity emission in the visible region. There is a very good agreement between experimental elemental analysis and calculated results. [Ru(phen-diox)2(H2O)2](PF6)2 has been purified by column chromatography with Alumina as stationary phase. Brown crystals of [Ru(phen-diox)2(H2O)2](PF6)2 were grown by acetone diffusion into an aqueous solution of the complex. Electronic spectrum of the complex was taken in actonitrile. The intense absorption bands seen in the UV region are assigned to ligand-centered transitions and an absorption band seen in the visible region is assigned to MLCT transition. The FT-IR spectrum of [Ru(phen-diox)2(H2O)2](PF6)2 shows a sharp and strong absorption band at 845 cm-1 for the υ(P-F). Also, the fluorescence spectra of the complex show high intensity emission in the visible region. There is a very good agreement between experimental elemental analysis and calculated results. [Ru(phen-dione)3](BF4)2 and [Ru(phen-dione)2(H2O)2](BF4)2 have a template effect for condensation reaction ethyleneglycol with the coordinate phen-dione ligands. Also, HOMO and LUMO orbitals of [Ru(phen-diox)3](PF6)2 were determined by computational methods using Gaussian 03 and Gaussian 09 softwares performed by DFT calculations using GEN level of theory. There is a very good agreement between experimental and calculated results.

**Keywords:**

Ru(II) complexes, Polypyridyl ligands, 1,10-Phenanthroline-5,6-dione, Crystal structure, Cyclic voltammetry, Fluorescence spectrum.