Title of the thesis: **"Design of Luminescent Polypyridyl-Imidazole Based Ruthenium Complexes and Implication of Machine Learning and Artificial Intelligent Tools to Analyse Their Stimuli-Responsive Behaviours"**

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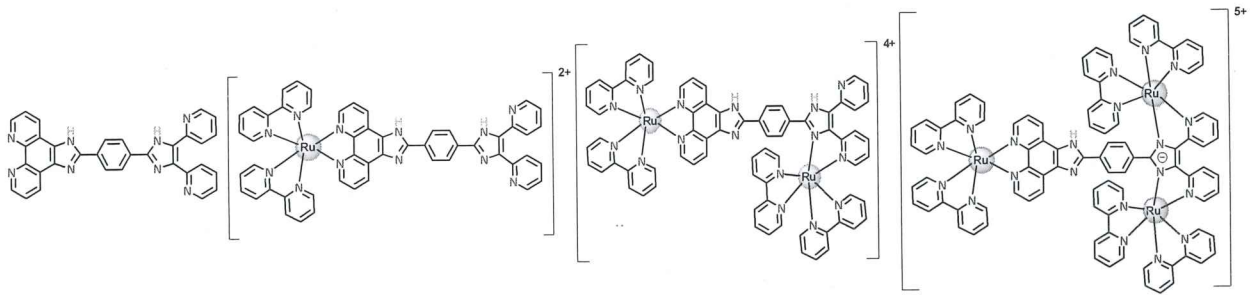
Abstract

This thesis deals with synthesis, characterization, exploration of photo-redox behaviors and implication of machine learning and artificial intelligent tools to analyze the stimuli-response behaviors of a wide range of Ru(II) complexes based on polypyridyl-imidazole ligands. Following synthesis, all the complexes were thoroughly characterized by standard analytical tools and spectroscopic techniques. Absorption and luminescence spectral characteristics as well as electrochemical behaviour of the complexes were thoroughly investigated. Titration experiments were executed upon addition of varying range of analytes (such as anions and cations) and the binding constant and detection limit of the complexes were determined via the use of titration data in both aqueous and organic media. Temperature dependent emission spectral measurements were executed to acquire knowledge about deactivation dynamics of the complexes. pH-induced modulation of the absorption and emission as well as electrochemical properties were thoroughly investigated and associated pK_a values of the complexes were determined. The absorption, emission spectral as well as the electrochemical responses of the complex upon the influence of external stimuli were utilised to fabricate multiple Boolean (BL) and Fuzzy logic (FL) operations. Finally, artificial intelligence assisted machine learning {Decision Tree Regression (DTR), Support Vector Regression (SVR) and Linear Regression (LR)} and deep learning techniques {Artificial Neural Networks (ANNs) and Adaptive Neuro-Fuzzy Inference System (ANFIS)} were employed to fully understand as well as to forecast the complete stimuli-responsive behaviors of the complexes. DFT and TD-DFT studies were also carried out to understand the electronic structures of the complexes and for appropriate assignment of the spectral bands.
The thesis is comprised of 7 chapters and consists of 222 pages.



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