

Ruthenium(II) Polypyridine Complexes: Photophysics and Electrochemistry

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Abstract: Since the report in 1972 by Gafney and Adamson [1] of the electron-transfer quenching of the triplet charge-transfer excited state of $[\text{Ru}(\text{bpy})_3]^{2+}$, the interest in the study of the photochemistry of ruthenium polypyridine complexes has increased. Luminescent properties of Ru(II) polypyridine complexes are related to their lowest excited states energy, as well as the orbital nature of these states. The energy of the excited states depends on the field-strength of the ligands, the redox properties of the metal and the ligands, and other intrinsic properties of the ligands [2]. Thus, luminescent characteristics of the complexes can be controlled by choice of the ligands. In the present work, the effect of different ligands on the structural, electronic and spectroscopic properties of $[\text{Ru}(\text{bpy})_2\text{L}]^{2+}$ complexes (where L = phen: 1,10-phenanthroline, hat: 1,4,5,8,9,12-hexaazatriphenylene, dppz: dipyrindo[3,2-a:2',3'-c]phenazine, bpz: 2,2'-bipyrazine, and tap: 1,4,5,8-tetraazaphenanthrene) in gas phase and water solvent have been investigated by means of combined DFT/TD-DFT calculations. CDA and EDA analysis showed the complexes with L = bpy, phen and dppz are the ones with a stronger Ru-L bond and also the ligands that present stronger π -acceptor character, while the others are stronger σ -donors. The absorption spectra of the complexes were obtained and they all exhibit MLCT absorption bands between 350-450 nm and LC transitions in the ultraviolet region. However, the MLCT bands in the complexes with L = bpy, phen and dppz are red-shifted in comparison with the other ones and, in general, water also induces a red-shift of the spectral bands. Characterization of the first excited states of the complexes is in progress, as well as their emission spectra.

Key-words: ruthenium, polypyridine, photophysics, photochemistry, luminescence.

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References:

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