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Ruthenium(II) and Iron(II) Complexes bearing low band-gap thiophenic ligands as possible NLO switches

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Over the past decade, there was growth of interest in discovering new conducting molecules due to their potential applications in electrochromic devices, sensors, OLED's and more recently molecular switches. Non-Linear Optics (NLO) phenomenons, namely Second-Harmonic Generation (SHG), is one of the recently topics in molecular switching [1]. In this case, a molecule possessing high hyperpolarizability (β) can be electrochemically changed in order to reduce drastically its β value and therefore act as a switch, upon a redox process.

Monocyclopentadienyliron (II) and ruthenium (II) complexes, combined with thiophene ligands possessing nitrile or acetylide linkages are known to have enhanced β values and have been widely studied for NLO [2]. Regarding the switching properties, oxidation in the transition metal, from M (II) to M (III) (M=Fe, Ru), can drastically reduce the NLO properties of these molecules and therefore it provides a way to electrochemically switch from an "*on*" form to an "*off*" form.

In this communication, monocyclopentadienyliron (II) and ruthenium (II) complexes bearing thiophene ligands (Figure 1) with low band-gaps will be electrochemically tested as possible molecules for NLO switching. The electrochemical results will be correlated with spectroscopic data and the NLO properties predicted by DFT calculations, in order to anticipate the potentialities of the new compounds as molecular switches.

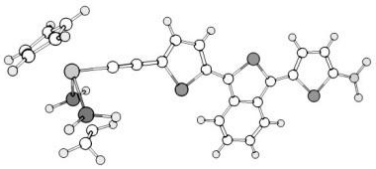

Figure 1 – Elucidating picture of the studied ruthenium complexes

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