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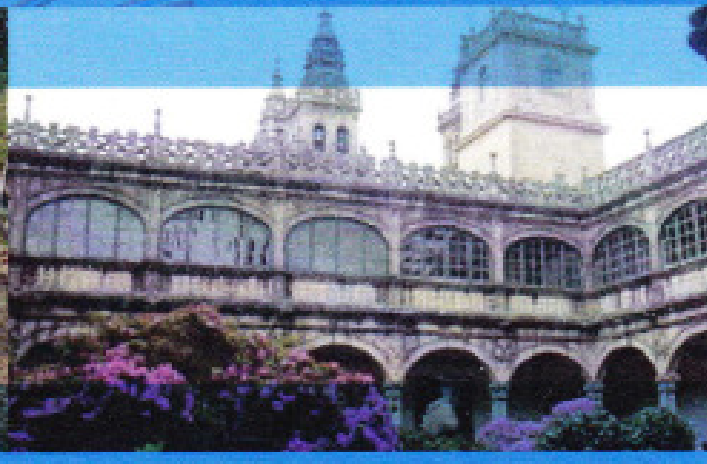

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DFT STUDIES ON THE NLO PROPERTIES OF RUTHENIUM (II) THIENYL COMPLEXES

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The limitations of semiconductor-based electronic devices have inspired many researchers to develop new molecular photonic materials. Non-linear optical (NLO) phenomena can be used for electro-optic signalling and data processing. Molecular organotransition metal complexes have been extensively investigated for second-order NLO (SONLO) purposes, such as Second Harmonic Generation (SHG), due to fast and large NLO response, structural diversity and architectural flexibility allowing molecular design and engineering [1]. η^5-Monocyclopentadienylmetal complexes of group VIII containing aromatic organic chromophores have proven to be promising molecules for SONLO applications. Among these organic chromophores, thiophene rings have shown to be very versatile due to low band-gap energies and intense electronic transitions [2,3].

In this communication, we present Density Functional Theory (DFT) and Time Dependent DFT (TD-DFT) studies on the elongation of the π electronic system in a series of new thiophene based η^5-monocyclopentadienylruthenium (II) complexes of general formula [RuCp(P_P)-C≡C-{SC_4H_2}$_n$-CHO] (where Cp = η^5-monocyclopentadienyl; P_P = $H_2P(CH_2)_2PH_2$; n =1-3). Calculated structural and electronic data, namely β and UV-Vis spectra, will be correlated with experimental values in order to evaluate the accuracy of the B3LYP functional in the estimation of the SONLO properties of this type of complexes.

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