



SANTIAGO DE COMPOSTELA 2011

Ninth triennial congress of the
**WORLD ASSOCIATION
OF THEORETICAL AND
COMPUTATIONAL
CHEMISTS**

Santiago de Compostela (Spain)
17-22 July, 2011



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posters

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MONO AND BINUCLEAR COMPLEXES FOR NONLINEAR
OPTICAL SWITCHING: A DFT STUDY

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The search for materials exhibiting switchable second-order nonlinear optical (SONLO) properties has attracted a great deal of attention owing to their potential application as key nanoscale components for digital processing and data storage. Our research in organometallic complexes with SONLO properties resulted in the development of some new promising thienyl-acetylide η^5 -monocyclopentadienyliron(II) and ruthenium(II) complexes [1,2]. These compounds present typical *push-pull* architecture (crucial for maximizing the molecular quadratic hyperpolarizability, β), where an electron donor is linked to an electron acceptor group by a conjugated π system. Changing the donor/acceptor abilities of any of these end-groups, by redox means for example, gives the chance to control the magnitude of β value, and hence obtain a SONLO switch.

In this presentation, we show the application of Density Functional Theory (DFT) in the prediction of SONLO switching properties of mono and bimetallic complexes bearing two organometallic fragments, η^5 -monocyclopentadienyliron(II) and η^5 -monocyclopentadienylnickel(II) moieties, in different formal oxidation states. The obtained hyperpolarizabilities will be correlated with structural and electronic data. Results show that redox changes provide a feasible way to obtain good SONLO switches.

References:

- [1] – M. Helena Garcia, P. Florindo, Nova Science Publishers, Inc., New York, (in press)
[2] – Paulo J. Mendes, J. P. Prates Ramalho, A. J. Palace Carvalho, J. Mol. Struct.: THEOCHEM, 900 (2009) 110-117