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DFT Studies on Thiophene Acetylide Ru (II) Complexes for NLO Purposes: Tuning their Electronic Properties

Tiago J. L. Silva, Paulo J. Mendes, A. J. Palace Carvalho, J. P. Prates Ramalho

Centro de Química de Évora, Departamento de Química da Universidade de Évora, Rua Romão Ramalho 59, 7002-554 Évora, Portugal

Organometallic complexes have been widely used as building blocks for second-order non-linear optical (SONLO) materials, particularly η^5 -monocyclopentadienyls, as they can act as a good electron or releasing groups when bonded to highly polarisable chromophores such as thiophene based organic frameworks.^[1]

Density Functional Theory (DFT) methods, especially Time Dependent methods (TD-DFT), have been successfully used for understanding the electronic factors behind the SONLO phenomenon. Recently, our studies shown that not only the η^5 -monocyclopentadienyliron(II) organometallic fragment plays a determinant role in order to obtain large second-order non linear optical responses but additionally electronic properties of the substituents on the thiophene moiety are also important.^[2] In this communication we present a TD-DFT study on the effect of different thiophene acetylide derivatives on the first hyperpolarizability, β , in the parent η^5 -monocyclopentadienylruthenium(II) complexes in order to confirm the ability of these thiophene ligands as polarisable chromophores when interacting with a good electron-donor organometallic fragment such as the η^5 -monocyclopentadienylruthenium(II) group. We also studied the solvation effect, using the self-consistent reaction field approach (SCRF), on the electronic properties and first hyperpolarizabilities for the complex for which the higher value of static quadratic hyperpolarizability was obtained.

References:

- [1] Garcia, M. H.; Mendes, P. J.; Robalo, M. P.; Romão Dias, A.; Campo, J.; Wenseleers, W.; Goovaerts, E.; *Journal of Organometallic Chemistry* 692 (2007) 3027.
[2] Mendes, P.; Carvalho, A.; Ramalho, J. P.; *Journal of Molecular Structure: THEOCHEM* 900 (2009) 110.

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