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## Study of Potential Switchable SONLO Ruthenium Complexes Using the TD-DFT Approach

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Molecular second-order nonlinear optical (SONLO) organometallic materials continue to attract considerable interest on account of the promise they hold for applications in optical devices technology. Recently, the SONLO response of different metal complexes has been modulated by means of reversible redox active moieties able to act as efficient switches [1]. As a result, a new promising approach has emerged that is the concept of redox-switchable SONLO properties. This makes possible to achieve a switch in the SONLO response between two forms ('on' and 'off') since that the two molecular forms have great difference in the magnitude of the corresponding first hyperpolarizabilities. To date, the majority of the studies in this field were made on iron or ruthenium derivatives having a traditional dipolar donor- $\pi$ -system-acceptor (D- $\pi$ -A) structure with benzene-based backbone as organic spacer [2]. Due to their interesting electronic properties, thiophene-based derivatives are good candidates for SONLO purposes. Thus, the presence of redox-active metal centres together with a thiophene-based conjugated framework provides good opportunities for modulation of molecular NLO responses, and is hence a primary justification for the study of these systems. The time-dependent density functional theory (TD-DFT) method, since it provides a good molecular orbital description of processes involving electronic transitions, has been increasingly used to accurately calculate first hyperpolarizabilities of organometallic complexes. Thus, it can play a role in the study of complexes with potential modulation of their SONLO properties.

In this work we report a preliminary TD-DFT study on  $\eta^5$ -monocyclopentadienylruthenium complexes with substituted thiophene-based ligands in order to give a first insight on the potential use of these systems as switchable SONLO materials.

### References

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