

## Substituent Effect in the Mesoionic Ring on Optical and Electric Properties of Mesoionics Compounds

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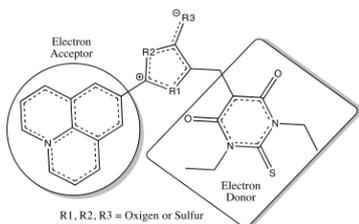
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### INTRODUCTION

Material science has given great attention to a new type of organic material class called mesoionic compounds. The interest in this type of materials is due to their photoluminescence, conductivity, low cost, faster optical response, greater versatility, ability to adjust their structure according to their nonlinear optical property and optical nonlinear susceptibility comparable to other conventional materials. In a previous paper, Simas *et al.*<sup>1</sup> reported a semi-empirical investigation for a series of mesoionic compounds varying the atoms in the mesoionic ring. Emphasis was dedicated to analyzing of the second hyperpolarizability results. The main goal of this work is to study the effect of substituents on the electric and optical properties of these molecular systems. To achieve this goal, we have used highly accurate *ab initio* and DFT methods.

### METHODS

The mesoionics rings studied in this work were generated from the variation of atoms O or S in positions R<sub>1</sub>, R<sub>2</sub> and R<sub>3</sub> of Figure 1. We have followed the same nomenclature adopted by Simas *et al.*<sup>1</sup>



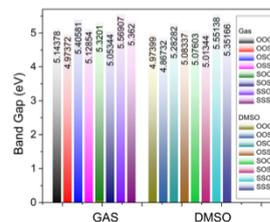
**Figure 1.** Structures of push-pull compounds with (a) mesoionic ring bridges generated from varying O and S atoms in R<sub>1</sub>, R<sub>2</sub> and R<sub>3</sub> positions.

For all compounds, the geometries were fully optimized at the MP2/6-31G(d) level of theory. Dipole moments, linear polarizabilities and first hyperpolarizabilities were calculated numerically using the Field Finite (FF) method at the MP2/6-31+G(d) level. Simulated absorption spectra were obtained at the TD-PBE1PBE/6-311+G(2d,p) level. All calculations were performed in gas phase and DMSO as solvent (implicit treatment).

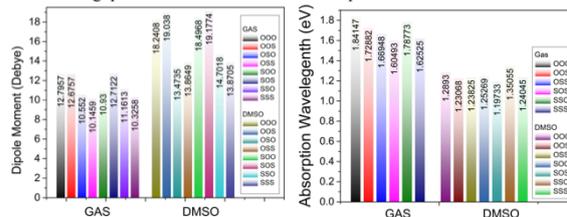
All calculations were performed using the G09 suite of programs.

### RESULTS AND DISCUSSION

Figures 1-3 show results for Band Gap, dipole moment and wavelength of maximum absorption for all mesoionic compounds calculated in gas phase and in solvent as a medium.



**Figure 2.** Band gaps values for all mesoionic compounds studied in this work..



**Figure 3.** Dipole moments (left) and wavelength of maximum absorption (right) of mesoionics Rings.

From these Figures, we can note a huge dependency of molecular properties as a function of the effect of the substituents in the mesoionic ring.

### CONCLUSIONS

In summary, a series of mesoionic compounds had their electronic properties calculated. MP2 and TD-DFT calculations revealed very interesting features of the new structures, allowing for a rational design of a candidate to be applied in nonlinear optics technologies.

### ACKNOWLEDGMENTS

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<sup>1</sup> SILVA, Andréa M. S. et al.; **J. Braz. Chem. Soc.**, São Paulo, v. 16, n. 3b, p. 583-588, June 2005.