XIX SBQT
Simpósio Brasileiro de Química Teórica 2017
12 a 17/Nov, 2017, Águas de Lindóia/SP, Brasil

# Molecular Modeling of Azo-Enaminone Derivatives in Solvent Medium: Investigation of the Nonlinear Optical Properties

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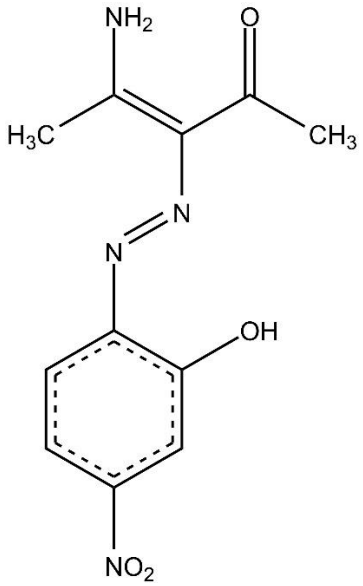
**Abstract:** Azo dyes are the most fundamental and representative class of commercial synthetic organic dyes [1]. These dyes have the azo group −N=N− in its molecular structures and are well-known by its applications like pigments, photoelectronics, optical storage technology, analytical chemistry and printing systems. In this work, we investigate the solvent effects in the nonlinear optical properties of the azo-enaminone derivative shown in the Figure below. We performed quantum chemical calculations and molecular dynamics simulations with different models considering the polarization for solute due to the presence of the solvent. Namely, the tetrahydrofuran, ethanol, water and dimethyl sulfoxide were included using both the implicit and explicit solvation models. Molecular Dynamics (MD) simulations, using the GROMCAS software were carried out with the azo-enaminone in aqueous solution. Quantum Chemical calculations using Gaussian 09 [2] package were performed to access the nonlinear optical properties, with the solvent described by both polarizable continuum model (PCM), [3] and point charges model [4]. Our results were compared to reported work of Machado, D.F.S. et al [5], which solvent medium was included only by PCM model.



**Key-words**: Azo-enaminone, PCM, Molecular Dynamics.
**Support:** D.A.S.F. gratefully acknowledges the financial support from CNPq, grants 304020/2016-8 and 407682/2013-9, and FAP-DF grants 0193.001.062/2015 and 193.001.284/2016.

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