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Phenomenological modeling of the first hyperpolarizability of organic molecules applied in chalcone molecules

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Chalcone-derived molecules can be found in a large variety in Nature, especially in the vegetal plant kingdom. Chalcones can be also synthetized in order to obtain a molecule with some specific application. Chalcone reviews states that more than 92000 articles have been published in this subject.(1) For example, these molecules are used in electro-optic modulators and have also been shown in second harmonic generation of laser light.(2) Both examples are related to an intrinsic molecular photophysical parameter: the first-order molecular hyperpolarizability (β), which is associated to the scattering of the second harmonic of an incident light at a certain frequency. Until nowadays, the task of experimentally obtain the frequency dispersion of the first-order hyperpolarizability is time consuming and laborious and the experimental setup is not trivial, with the use of a sub-nanoseconds pulsed laser source and the second-harmonic signal acquisitioned by a photomultiplier. Therefore, in this work, we applied a well-known phenomenological modeling (3) of the first hyperpolarizability in five chalcone-based molecules dissolved in dichloromethane (DCM) which present three experimental linear absorption bands, implying a modeling of the frequency dispersion without any simplifications as usually done in works where the first hyperpolarizability is obtained only with incident light of 1064 nm wavelength. The modeling consists in the determination of β() through others photophysical parameters such as the transitions dipole moments, the central frequency and excited states width and the difference between permanent dipole moments of the molecular excited states, which were measured through one- and two-photon absorption spectra determination and fitting. Quantum chemical calculations (QCC), a widely used approach for such problem was used to analyze the correspondence of both methods. With QCC, the static first hyperpolarizability and its dispersion from 900 to 1200 nm was calculated. Finally, the values of the first hyperpolarizability in 1064 nm was also acquired with the hyper-Rayleigh scattering (HRS) experimental technique in order to confirm once more the validity of the phenomenological modeling in describe the dispersion of β.

Palavras-chave: First-order hyperpolarizability. Chacone molecule. Hypv.er-Rayleigh scattering.

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