

Abstract Submitted
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Nonlinear optical properties of polychlorotriphenylmethyl radicals: a computational study CLAUDIA CARDOSO, BRUCE FORBES MILNE, FERNANDO NOGUEIRA, Centro de Física Computacional, Faculdade de Ciências e Tecnologia, Universidade de Coimbra — The special interest in molecular design for the development of novel second-order nonlinear optical (SONLO) materials is driven by their potential applications in new optoelectronic technologies. Various strategies are currently employed to enhance the molecular SONLO activity, and studies revealed that species having open-shell electronic states exhibit larger β values than analogous closed-shell systems. Their open-shell electronic structure leads to accessible low-lying charge transfer electronic states which enhance the β values with respect to their closed-shell counterparts. We present the results of a Density Functional Theory calculations of a series of substituted polychlorinated triphenylmethyl radicals. This family of radicals has been measured by Ratera et al using Hyper-Rayleigh Scattering and showed to have enhanced β values. The present study compares results obtained within LDA and several hybrid functionals, namely long-range corrected functionals. The effect of solvents was also considered through the use of the polarizable continuum model.

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