P 29. THE INVESTIGATION OF FIRST HYPERPOLARIZABILITIES OF BENZALDEHYDE-4-NITRO PHENYL HYDRAZONE DERIVATIVE

Aysenur Ordukaya[1], Mustafa Karakaya[2], Yusuf Ceylan[1], Nuretdin Eren[1], Mehmet Taser[1], Aysun Gozutok[1], Asli Karakas[1]

[1]Selcuk University, Faculty of Sciences, Department of Physics, Campus, Konya, Turkey
[2]Department of Energy Systems, Faculty of Engineering & Architecture, Sinop University, Sinop 57000, Turkey

E-mail: akarakas@selcuk.edu.tr, mkarakayafizik@hotmail.com

ABSTRACT: To investigate microscopic second-order nonlinear optical (NLO) behaviour of benzaldehyde-4-nitro phenyl hydrazone derivative with donor substituent chlorine, we have computed electric dipole moment and static first hyperpolarizability values using ab-initio quantum mechanical procedure (finite field). Theoretical calculations offer a quick and inexpensive way of predicting the NLO responses of the materials especially during the design of new materials. According to the results of finite field computations, the investigated compound exhibits non-zero quadratic hyperpolarizability tensor components, implying microscopic NLO phenomena.

Keywords: Nonlinear Optics, Electric Dipole Moment, First Hyperpolarizability, Ab-Initio, Finite Field.