

**P 30. STATIC LINEAR POLARIZABILITY AND FIRST HYPERPOLARIZABILITY  
VALUES OF ACETYLENIC LINKAGE HAVING DONOR-ACCEPTOR GROUPS**

Mehmet Taser<sup>1</sup>, Mustafa Karakaya<sup>2</sup>, Yusuf Ceylan<sup>1</sup>, Nuretdin Eren<sup>1</sup>, Mehmet Hakan Colpan<sup>1</sup>, Aysun Gozutok<sup>1</sup>, Asli Karakas<sup>1</sup>

<sup>1</sup>*Selcuk University, Faculty of Sciences, Department of Physics, Campus, Konya, Turkey*

<sup>2</sup>*Department of Energy Systems, Faculty of Engineering & Architecture, Sinop University, Sinop 57000, Turkey*

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

**ABSTRACT:** A potential nonlinear optical (NLO) compound acetylenic linkage having donor-acceptor groups has been designed. The NLO properties are expected and can be more or less accurately predicted due to the assembly of the title molecule and theoretical computations of dispersion-free dipole polarizability and first hyperpolarizability. These parameters determined by means of density functional theory (DFT) have been used to reveal the relationship of linear and NLO properties with the molecular structure. The computation results with non-zero values on static first hyperpolarizability indicate that the investigated molecule might possess microscopic second-order NLO behaviour.

*Keywords: Density Functional Theory, Linear Polarizability, Second-order Hyperpolarizability, Acetylenic Linkage, Optical Nonlinearity.*