

O 67. AB-INITIO COMPUTATIONS ON ELECTRIC DIPOLE MOMENT, DIPOLE POLARIZABILITY AND VERTICAL TRANSITION WAVELENGTHS OF ISOPROPYL-4-(4-METHOXYPHENYL METHYLAMINO) BENZOATE

Berna Betül Terlemez¹, Mustafa Karakaya², Aysun Gozutok¹, Yusuf Ceylan¹, Nuretdin Eren¹, Mehmet Taser¹, Mehmet Hakan Colpan¹, Asli Karakas¹

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 provide an insight into the linear optical behaviour of isopropyl-4-(4-methoxyphenyl methylamino) benzoate; the electric dipole moment and static linear polarizability values have been theoretically investigated by means of finite field (FF) method. The ab-initio calculated non-zero electric dipole moment value shows that the title compound might have dispersion-free dipole polarizability with non-zero value obtained by the numerical derivative of the electric dipole moment according to the applied field strength. The electronic transition wavelengths of the lowest lying transitions have been also calculated for the examined molecule.

Keywords: Electric dipole moment, Static Linear Polarizability, One-photon Absorption, Ab-initio, Finite Field