Optik
Available online 20 October 2021, 168196
In Press, Journal Pre-proof

All optical switching and the optical nonlinear properties of 4-(benzothiazolyldiazenyl)-3-chlorophenyl 4-(nonylthio)benzoate (EB-3Cl)

Uhood J. Al-Hamdani [a], Qusay M.A. Hassan [b] ✉, C.A. Emshary [b], H.A. Sultan [b], Adil Muala Dhumad [a], Afrah A. Al-Jaber [a]

https://doi.org/10.1016/j.ijleo.2021.168196

Abstract

Chemical computational calculations are carried out to investigate the molecular structure of 4-(benzothiazolyldiazenyl)-3-chlorophenyl 4-(nonylthio)benzoate (EB-3Cl) via the density functional theory (DFT) method. The B3LYP method is used to optimize the geometrical structure of the EB-3Cl compound with 6-31 G(d,p) basis set level. HOMO-LUMO energies and some nonlinear optical (NLO) properties are calculated via the same method used in geometry optimization. The results show that the synthesized compound has good optical properties. Good agreement correlations of experimental and theoretical findings are found. The index of nonlinear refraction (INR) of EB-3Cl is determined via two methods, the diffraction ring pattern (DRP) and the Z-scan. High INR value of 5.92 $\times 10^{-7}$ cm^2/W is obtained via the first method. Optical limiting (OLg), of the synthesized compound is studied with OLg threshold value of 8 mW is obtained. All optical switching technique is tested in the prepared compound with good results are obtained and DRPs are simulated numerically based on the Fresnel-Kirchhoff integral.

Keywords

DRPs; Z-scan; INR; OLg; Fresnel-Kirchhoff integral