World Academy of Science, Engineering and Technology
International Journal of Chemical and Materials Engineering
Vol:9, No:02, 2015

Electron Density Analysis and Nonlinear Optical Properties of Zwitterionic Compound

Authors : A. Chouaih, N. Benhalima, N. Boukabcha, R. Rahmani, F. Hamzaoui

Abstract : Zwitterionic compounds have received the interest of chemists and physicists due to their applications as nonlinear optical materials. Recently, zwitterionic compounds exhibiting high nonlinear optical activity have been investigated. In this context, the molecular electron charge density distribution of the title compound is described accurately using the multipolar model of Hansen and Coppens. The net atomic charge and the molecular dipole moment have been determined in order to understand the nature of inter- and intramolecular charge transfer. The study reveals the nature of intermolecular interactions including charge transfer and hydrogen bonds in the title compound. In this crystal, the molecules form dimers via intermolecular hydrogen bonds. The dimers are further linked by C–H…O hydrogen bonds into chains along the c crystallographic axis. This study has also allowed us to determine various nonlinear optical properties such as molecular electrostatic potential, polarizability, and hyperpolarizability of the title compound.

Keywords : organic compounds, polarizability, hyperpolarizability, dipole moment
Conference Title : ICSSC 2015 : International Conference on Solid State Chemistry
Conference Location : Barcelona, Spain
Conference Dates : February 26-27, 2015

Open Science Index, Chemical and Materials Engineering Vol:9, No:02, 2015 publications.waset.org/abstracts/26077.pdf