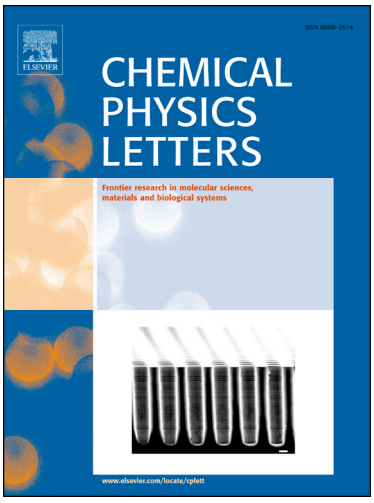

Research paper

Influence of intramolecular hydrogen bonding interaction on the molecular properties of N-*p*-tolyl-5-oxo pyrrolidine-3-carboxylic acid: a theoretical and experimental study

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Influence of intramolecular hydrogen bonding interaction on the molecular properties of N-*p*-tolyl-5-oxo pyrrolidine-3-carboxylic acid: a theoretical and experimental study

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Abstract

N-p-tolyl-5-oxo pyrrolidine-3-carboxylic acid (TOPCA) was synthesized by Michael addition-cyclo condensation. The molecular structure of TOPCA was optimized by B3LYP method with 6-311G(d,p) and aug-cc-pVDZ (Dunning) basis sets as well as CAM-B3LYP method with 6-311G(d,p) basis set. In addition, MEP, CHELPG and NBO analyses were carried out to understand the influence of hydrogen bonding interactions. The molecular structure of TOPCA is governed by intramolecular hydrogen bonding interactions (C-H…O) which influence charge transfer in TOPCA. The C-H…O interactions stimulate the emission property of TOPCA excited at 380 nm. Intramolecular H- bonding and charge transfer induce the second hyperpolarizability in TOPCA.

Keywords: Organic Crystals; Intramolecular Hydrogen bonding; Emission; Electrostatic Potential; CHELPG atomic Charges; Hyperpolarizability.

1. Introduction

Itaconic acid, a versatile reagent and an interesting compound is used in the synthesis of N-alkyl/aryl carboxypyrrolidones [1] and their polymers [2]. N-aryl carboxypyrrolidones are the products obtained from Michael-addition cyclo-condensation of itaconic acid with several aromatic amines have been used for various biomedical applications [3]. Pyrrolidone polymers have also been studied for optical wave guide applications [4]. Kitazawa et al. [5] exploited L-pyrrolidone-2-carboxylic acid for the tuneable UV generation at 266 nm. Organic molecules have been explored through quantum chemical calculations for the past few