CrystEngComm

PAPER

L-Phenylalanine L-phenylalaninium bromide – a new nonlinear optical material†

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Cite this: *CrystEngComm*, 2014, **16**, 7979

Received 5th April 2014,
Accepted 1st July 2014

DOI: 10.1039/c4ce00718b

www.rsc.org/crystengcomm

L-Phenylalanine L-phenylalaninium bromide (**LPLPB**), an amino acid non-centrosymmetric crystal having a large second harmonic generation (SHG) efficiency, being 4.5 times that of KH_2PO_4 (KDP), has been successfully grown using a slow evaporation method employing a temperature gradient technique. The structure of the grown crystal was solved and refined by single-crystal X-ray diffraction, and this demonstrates that it belongs to a monoclinic system with the space group $P2_1$. The confirmation of its functional groups was recorded using Fourier transform infrared spectroscopy. Thermogravimetric analysis (TGA) and differential scanning calorimetry (DSC) were used to study its thermal properties. The optical behaviour was examined and its optical constants were determined by UV-vis analysis. Dielectric spectroscopy reveals the dielectric nature of the grown crystal. The mechanical strength of the grown **LPLPB** was estimated by microhardness studies, and the Young's modulus of the grown **LPLPB** was calculated to be 3.310×10^{10} N m^{-2}.

1. Introduction

Nonlinear optical materials influence laser technology, optical communication and optical storage technology. New materials exhibiting nonlinear optical (NLO) effects have been explored for developing optical devices like optical modulators and frequency-doubling devices.[1] The combination of the high optical nonlinearity and chemical flexibility of organic materials with the good thermal stability and transmittance of inorganic and semiorganic materials has been proposed, attracting attention to the nonlinear optical field.[2] Even though many materials have nonlinear optical behaviour, amino acids have the maximum possibility of showing nonlinear optical properties.[3] They display specific features of interest such as (i) molecular chirality, which secures acentric crystallographic structures, (ii) absence of strongly conjugated bonds, which leads to wide transparency ranges in the visible and UV spectral regions, and (iii) zwitterionic nature of the molecule, which favours crystal hardness. Besides their technological applications they can also be used as a basis for synthesizing organic compounds and their derivatives.[2] The crystal structures of amino acids and their complexes have provided a thorough knowledge of the influence of their structure and molecular properties.[4] One such effort in developing a new amino acid crystal having appreciable optical nonlinearity and enhanced physical properties is **LPLPB**.

Among the amino acids, L-phenylalanine is an essential amino acid that is used by the body to build neurotransmitters. It is used in the manufacture of food and drinks and sold as a nutritional supplement for its reputed analgesic and antidepressant effects. It is a direct precursor to the neuromodulator phenylethylamine, a commonly used dietary supplement.[5]

A series of second-order NLO-active materials composed of L-phenylalanine have been synthesized, such as L-phenylalanine benzoic acid,[6] L-phenylalanine hydrochloride[7] and L-phenylalanine L-phenylalaninium nitrate.[8] The structure of several L-phenylalaninium compounds has also been reported already.[9–12] To the best of the authors' knowledge, studies on the growth and characterization of **LPLPB** have not been reported until now. Hence this paper reports the structure, synthesis, and solubility of **LPLPB** having large optical nonlinearity. Single-crystal X-ray diffraction (XRD) exhibits the lattice parameters, bond lengths and bond angles. Moreover, solid-state parameters like plasma energy, Fermi gap and polarizability were evaluated. The polarizability[12] was calculated by Penn analysis and Clausius–Mossotti theory

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† Electronic supplementary information (ESI) available. CCDC 873527. For ESI and crystallographic data in CIF or other electronic format see DOI: 10.1039/c4ce00718b