

RESEARCH ARTICLE



# Synthesis, single-crystal X-ray diffraction, NLO and DFT studies of centrosymmetric 4-amino-3,5-dimethyl-1H-pyrazolium citrate monohydrate salt

B. Radhika<sup>a</sup>, J. Prashanth<sup>b</sup>, Srinivas Basavoju<sup>c</sup>, S. Jyothi<sup>a</sup> and B. Venkatram Reddy<sup>a,b</sup>

<sup>a</sup>Department of Chemistry, Kakatiya University, Warangal, India; <sup>b</sup>Department of Physics, Kakatiya University, Warangal, India; <sup>c</sup>Department of Chemistry, National Institute of Technology, Warangal, India

## ABSTRACT

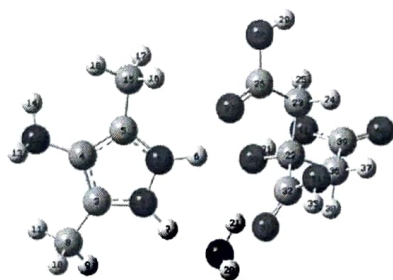
An organic salt compound 4-amino-3,5-dimethyl-1H-pyrazole (ADMP) has been combined with citric acid and crystallised at room temperature, forming a new molecular salt 4-amino-3,5-dimethyl-1H-pyrazolium citrate (ADMPCA) as a monohydrate. The compound was then structurally characterised by single-crystal X-ray diffraction (XRD), spectral analysis of FTIR, NMR and UV, and thermal studies. The structural analysis has shown that the ADMP molecules participate in the dominant hydrogen-bonding patterns forming a ladder-like structure *via* charge-assisted N<sup>+</sup>–H...O, O–H...O and N–H...O hydrogen bonds. The Hirshfeld surface analysis has been performed to understand the importance of intermolecular interactions in the stability of the salt structure. Theoretical studies were performed employing the DFT/B3LYP/6-311++G(d,p) level of theory to investigate Non-linear optical (NLO) behaviour, first-order hyperpolarisability, dipole moment and polarisability. The molecular properties, such as natural charge analysis and MESP analysis, were also explored in the present study.

## ARTICLE HISTORY

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## KEYWORDS

4-amino-3,5-dimethyl-1H-pyrazolium citrate monohydrate salt; XRD; DFT; Hirshfeld surface analysis; NLO



- Synthesized ADMPCA crystal
- DFT/B3LYP/6-311++G(d,p) method
- Characterized by XRD, FTIR, NMR, UV spectra and thermal studies

### Results

- Observed dominant hydrogen bondings and established by thermal analysis
- Computed structure parameters agreed well with the experimental counter parts
- NLO behavior is studied and verified with NBO analysis.
- Observed the presence of chromophore COO<sup>-</sup> unit from UV spectral analysis

## Introduction

Exploring novel organic compounds that exhibit physical properties of interest by investigating the intermolecular interactions is one of the main objectives of solid-state

chemistry and crystal engineering due to their potential applications in non-linear optics (NLO). Extensive research has been carried in the NLO field due to their requirement in technology in everyday life. Hence the

CONTACT B. Venkatram Reddy bvreddy67@yahoo.com

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