MOLECULAR PHYSICS e2022797
https://doi.org/10.1080/00268976.2021.2022797

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RESEARCH ARTICLE



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

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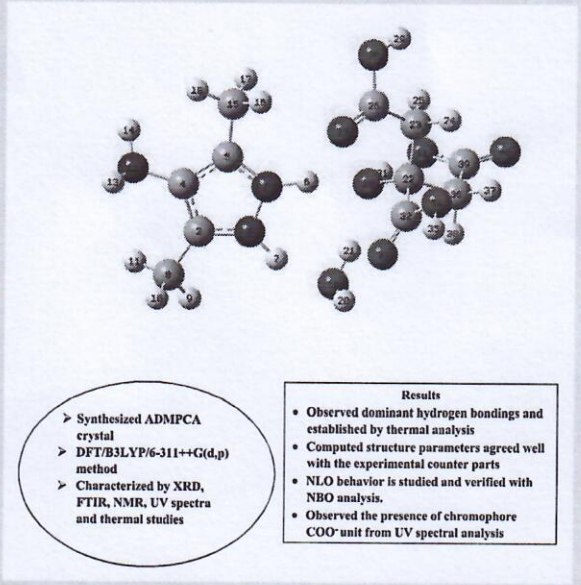
**ABSTRACT**

An organic salt compound 4-amino-3,5-dimethyl-1*H*-pyrazole (ADMP) has been combined with citric acid and crystallised at room temperature, forming a new molecular salt 4-amino-3,5-dimethyl-1*H*-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 $N^+$–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**
Received 26 September 2021
Accepted 17 December 2021

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

## 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

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Supplemental data for this article can be accessed here. https://doi.org/10.1080/00268976.2021.2022797