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Spectral, structural and theoretical studies of α–methyl *trans* cinnamaldehyde semicarbazone

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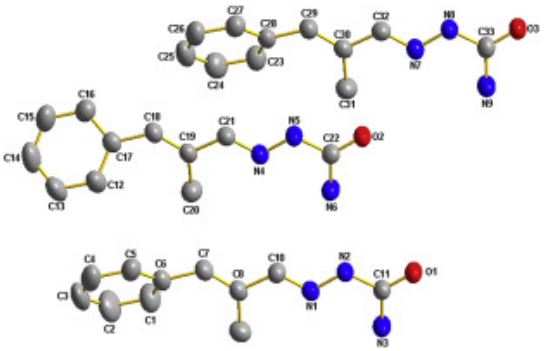
Abstract

A novel semicarbazone, α–methyl *trans* cinnamaldehyde semicarbazone has been synthesized and characterized by elemental analysis, FT-IR, FT-Raman, NMR and UV-Visible spectral techniques. The single crystal X-ray diffraction study of the isolated crystals of the compound reveals that the compound crystallizes in triclinic $P\bar{1}$ space group with cell dimensions a=7.1821(4)Å, b=14.9090(13)Å, c=16.1096(11)Å, α=84.496(4)°, β=79.046(3)° and γ=80.758(3)°. The thermal stability of the compound was investigated by thermogravimetry. The DFT calculations of the title compound were performed by B3LYP 6–31++G (d,p) level of theory by using Gaussian 09 programme.

Graphical abstract

α-Methyl *trans* cinnamaldehyde semicarbazone was synthesized and characterized. Asymmetric unit consists of three molecules of the title compound (showing atom numbering scheme and hydrogen atoms are omitted for clarity) is shown.



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Introduction

Semicarbazones are extremely gifted compounds from the view point of coordination chemistry, having the general formula $R^1R^2C{=}N\text{-}NH\text{–}(CO)\text{—}NH_2$, and are the condensation products of semicarbazides with suitable aldehydes or ketones. Semicarbazones exist predominantly in the amido form in the solid state, and exhibit amido–iminol tautomerism in solution due to the interaction of solvent molecules (Scheme 1). These compounds sometimes exhibit ring-chain tautomerism [1]. Literature reports show that semicarbazones and their metal complexes show wide therapeutic applications with less toxicity compared to their sulfur analogues [[2], [3], [4], [5]]. In recent times there are many reports that semicarbazones show pronounced *in vitro* antiproliferative activity, reasonable cytotoxic activity and outstanding antibacterial and antifungal properties and their complexes show enhanced activity compared to corresponding semicarbazones [6,7].

Cinnamaldehyde is a natural flavonoid and its derivatives have potential antifungal activity against diverse class of pathogenic fungi [[8], [9], [10], [11]]. Because of its slow reactivity with amines, α–substituted cinnamaldehydes are well known as less skin sensitizer and thus α-methylcinnamaldehyde is a derivative which is expected to be more effective due to its increased hydrophobicity [12]. α–Methyl *trans* cinnamaldehyde is a less irritating derivative due to its less minimum inhibitory concentration (MIC) and skin sensitivity compared to cinnamaldehyde [13]. In recent years, DFT has been extensively used to study the structures and spectral features of several semicarbazones and some of their metal complexes [[14], [15], [16], [17], [18], [19]]. In the present investigation, we have synthesized and characterized α–methyl *trans* cinnamaldehyde semicarbazone (ACS). The single crystals of the synthesized ACS were structurally analyzed. The experimental values of ACS were compared with theoretical calculations. The present study intends to investigate various spectral, structural and theoretical facets of ACS.

Section snippets

Materials

Semicarbazide hydrochloride (Sigma-Aldrich, ≥ 99%), anhydrous sodium acetate (Merck, AR), and α–methyl *trans* cinnamaldehyde (Sigma-Aldrich, ≥ 98%) were used as received. The solvents used for the synthesis of title compound were distilled water and ethanol.…

Synthesis of α–methyl trans cinnamaldehyde semicarbazone ($C_{11}H_{13}N_3O$)

ACS was synthesized from semicarbazide hydrochloride, sodium acetate and α–methyl *trans* cinnamaldehyde. Semicarbazide hydrochloride (0.1115 g, 1 mmol) dissolved in 15 mL distilled water and sodium acetate (0.1230 g, 1.5 mmol) in 10 mL…

Elemental analysis

The percentage of carbon, hydrogen and nitrogen present in the compound were calculated and compared with the experimental values. It is clear that the experimental values are in good agreement with the theoretical values and this agreement confirms the stoichiometry of the synthesized compound. The observed (calculated) % of C, H and N are C: 65.21 (64.95), H: 7.24 (6.40) and N: 21.03 (20.67).…

Single crystal X-ray diffraction study

The photograph of the grown crystals of ACS is shown in Fig. 1. The compound crystallizes in triclinic …

Conclusion

A novel semicarbazone, α–methyl *trans* cinnamaldehyde semicarbazone was synthesized and characterized by elemental analysis, FT-IR, FT-Raman, NMR, electronic spectral and single crystal X-ray diffraction studies. The DFT calculations of ACS were carried out by B3LYP 6–31++G (d,p) level of theory by using Gaussian 09 programme. The FT-IR and single crystal X-ray diffraction studies reveal that the compound exist in amido form in solid state. The single crystal X–ray diffraction study of the grown …

Acknowledgements

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Research data for this article

Cambridge Crystallographic Data Center

Crystallographic data

Data associated with the article:

CCDC 1872001: Experimental Crystal Structure Determination

Further information on research data

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2022, Materials Today: Proceedings

Citation Excerpt :

…Semicarbazones fall into the class of organic molecules (General Structure: R-C = NNHCONH2) that have attracted growing interest among the researchers due to their versatile use in industry. These are important compounds for researchers because of their excellent coordination behavior, analytical applications [2–4] and antibacterial activities [5,6]. Semicarbazones and their derivatives have been used in synthetic chemistry, medicinal chemistry, polymers [7–8] and herbicides.…

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…Some herbal extracts have been shown to be helpful in controlling coccidiosis (Peek and Landman, 2011). Cinnamaldehyde (CINN), a component of cinnamon oil, is a flavonoid (Saritha et al., 2019). CINN is added to drinks, chewing gums, and sweets as a spice to flavor them.…

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…Based on this perspective, the hyperpolarizability of the compound was calculated using the same basis set and NLO activity was experimentally determined using urea as reference. The theoretical and structural studies of a semicarbazone derivative of alpha methyl trans cinnamaldehyde was earlier reported from our laboratory [18]. In continuation of our investigation on structure-activity relationship of semicarbazones and thiosemicarbazones, herein we report the structural studies of a related thiosemicarbazone.…

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