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Research Article

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Synthesis and characterization of 1-(4-methylthiazol-2-yl)-3-propyl thiourea

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Abstract

A variety of thiourea and thiazole derivatives have several types of biological activates. An attractive feature of thioureas is their ready and synthesis change of the substitutes on nitrogen atoms and their physical and chemical properties. The compound was synthesized through the reaction of 2-amino-4-methylthiazol with propylisothiocyanate which was characterized by elemental analysis, ^{13}C- ^{1}H NMR, IR and mass spectra.

Keywords: thiourea, elemental analysis, ^{13}C- ^{1}H NMR, IR and mass spectra.

1. Introduction

Thiourea, having a large range amount of applications, are the related compounds of ureas in which oxygen has been taken place of sulfur. The properties of thiourea and urea have differed considerably because of the contradiction in electronegativity between oxygen and sulfur [1]. Thiourea has wide spectrum of biological activities for example herbicidal [2], insecticidal [3], antiviral [4], antifungal [5], antibacterial [6], antitubercular [7], and pharmacological properties [8], and act as antioxidants corrosion inhibitors, and as polymer components [9-11].

Thiazole and its derivatives are the main group of heterocyclic compounds, which have been found to possess useful bioactivity such as [12], anti-inflammatory, anti- microbial [13], anti- tumor, and anti- fungal properties[14]. In recent years, thiazole derivatives have attracted large attention because of their bioactivity and some applications in organic and medicinal chemistry[15-16].

This paper discussed below the structure of 1-(4-methylthiazol-2-yl)-3-propyl thiourea by spectroscopic analysis.

2. Experimental

Materials :

2-methyl-4 -methylthiazole and propylisothiocyanate was supplied by Aldrich Chemical Company. All solvents were spec-pure quality supplied by Fluka Chemical Company .

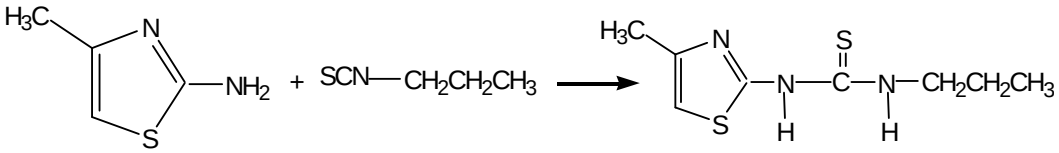
Equipments :

- Melting points were uncorrected and recorded on Reichert thermover apparatus.
- IR spectra were performed on a Perkin Elmer Infrared Spectrophotometer using KBr disk technique.

- ^{1}H, ^{13}C -NMR spectra were measured on BRUKER 500 and 125 MHz, NMR apparatus with DMSO as solvent.
- MS spectra were recorded on Shimadzu Qp .

Preparation of: 1-(4-methylthiazol-2-yl)-3-propyl thiourea:

A solution of an equal molar ratio of 2-methyl-4-methylthiazole and propylisothiocyanate in ethanol as a solvent was refluxed for 48 hours. The reaction result was filtered off then washed with ethanol and reccrystallized with ethanol afforded white crystals suitable for crystallography (Scheme 1).



Scheme 1. Synthesis of 1-(4-methylthiazol-2-yl)-3-propylthiourea.

Results and Discussion

The compound was prepared by boiling under reflux an equi molar ratio of 2-methyl-4-methylthiazole and propylisothiocyanate for 48 hrs in ethanol as a solvent. After the product reacted, it was filtererd off, washed with ethanol recrystallized white crystals suitable for crystallography (Scheme 1). Yield: 56%; m.p: 170℃. Yellow crystal. Anal. Calc. for $C_8H_{13}N_3S_2$ (215 g mol^{-1}): C, 44.65; H, 6.05; N, 19.53. Found: C,44.14; H, 6.25; N, 19.24.

Infrared spectra:

The IR spectral bands, useful for suggesting the bonding sites of 1- (4-methylthiazol-2-yl)-3 -propylthiourea . The infrared spectrum of compound considered in a KBr disc, shows two bands at 3480 and 3174 cm^{-1}, assignable to (N1H) and (N2H) respectively [17, 18], the band at 837cm^{-1} assignable to (C=S) , 1474cm^{-1} assignable to (CH_3), 707cm^{-1} for (C-S-C) Tz, 1575; 1531; 1505cm^{-1} for Tz ring.

NMR spectrum

^{1}H NMR spectrum of the compound (Figure 1) showed the presence δ 11.46 ppm for N1H, δ 9.87 ppm for N2H, δ 6.63 ppm for H(5) Tz, δ 2.50 ppm for (CH3) Tz, δ 3.49; 2.25; 1.55 ppm for proton of propyl. Moreover the ^{13}C NMR spectrum (Figure 2) δ 178 ppm for C=S, δ 161.21; 146.31; 129.80 ppm for thiazol carbons, δ 106; 18.52; 11.31ppm for propyl carbons.

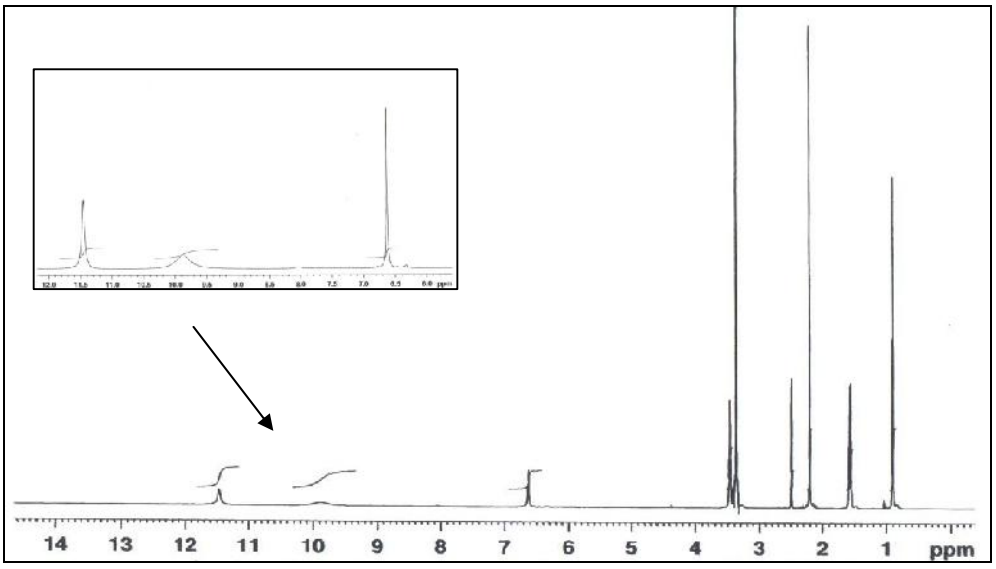


Fig. 1. ^{1}H NMR spectrum of 1-(4-methylthiazol-2-yl)-3 -propyl thiourea

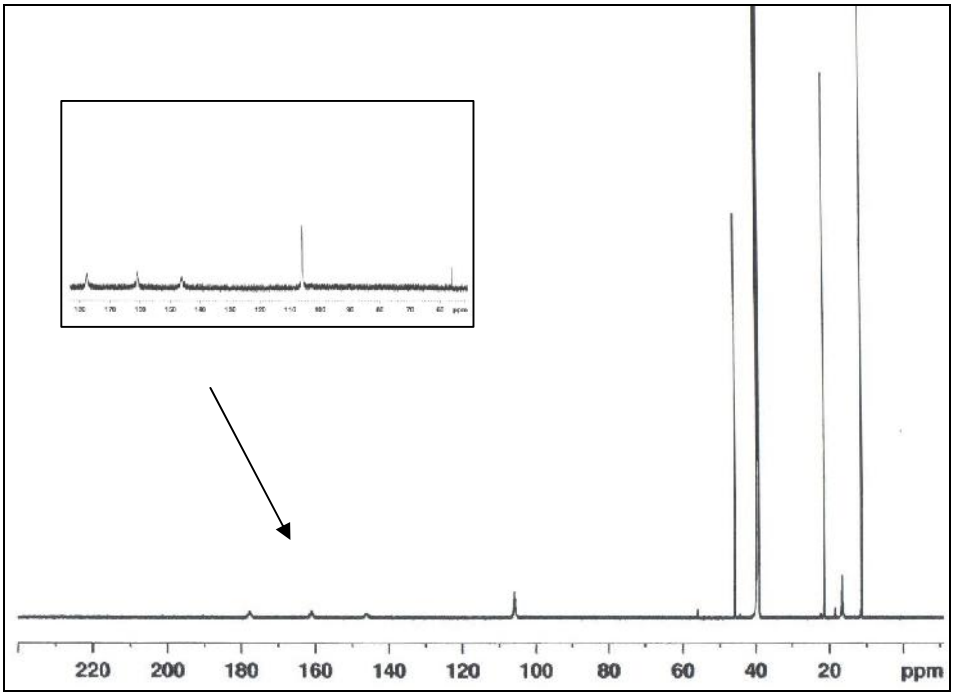


Fig. 2. ^{13}C NMR spectrum of 1-(4-methylthiazol-2-yl)-3 -propyl thiourea

Mass spectra

Figure 3, (Scheme 2) the mass spectram of 1-(4-methylthiazol-2-yl)-3 -propyl thiourea is an descriptive example for a compound under electron impact condition with its fragmentation pattern. The spectrum shows first peak at m/z 215 corresponding to a molecular weight of the molecular of the 1-(4-methylthiazol-2-yl)-3-propyl thiourea . The molecular A (Scheme 2) loses $2CH_3^+$ forming B, lose $^+NH_2$-$CH_2CH_2CH_3$ forming C, lose propylisothiocyanate forming E, …E‘, D and F.

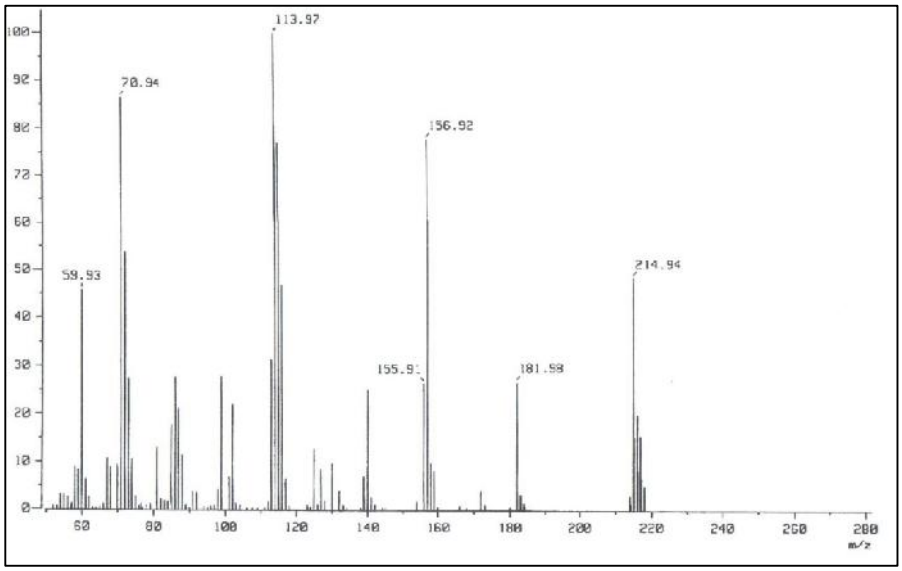
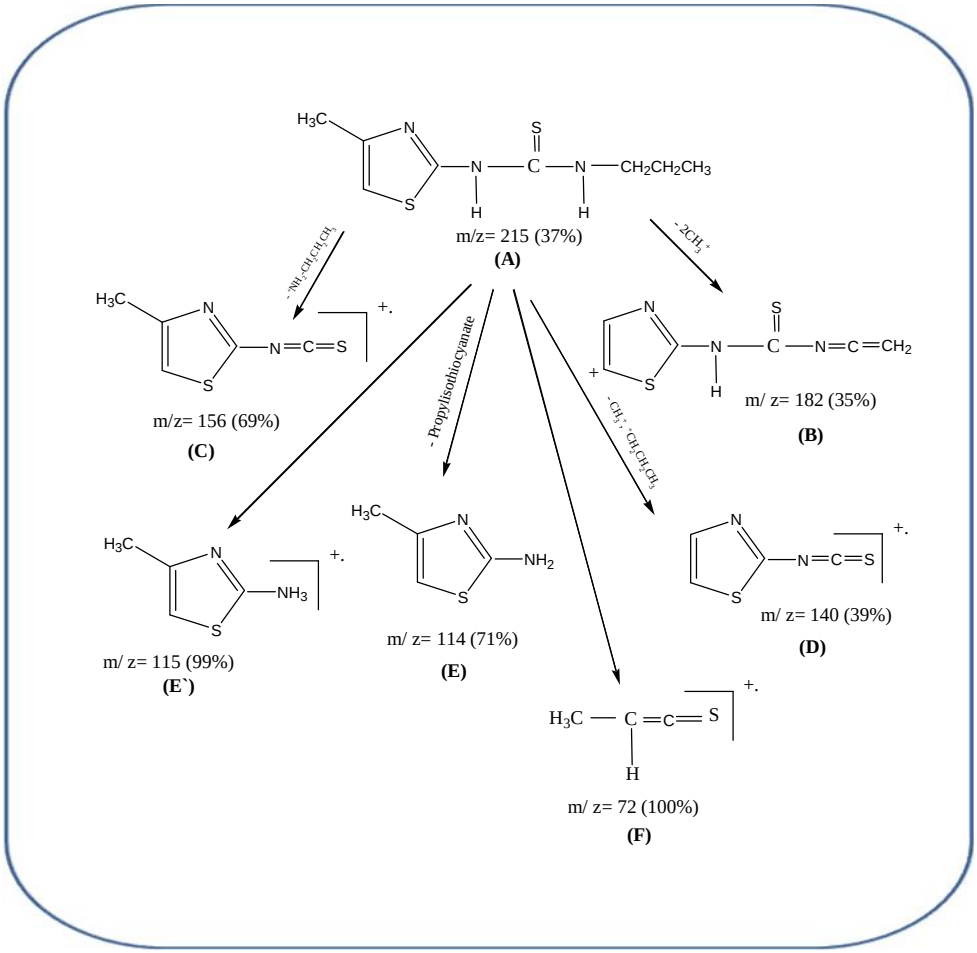


Fig. 3. Electronic impact mass spectrum of 1-(4-methylthiazol-2-yl)-3-propyl



Scheme 2. Fragmentation pathways of 1-(4-methylthiazol-2-yl)-3-propylthiourea.

Acknowledgments

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