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Research Article

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Synthesis and characterization of *N*-allyl–*N*`-(4`-methylthiazol) -2ylthiourea

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Abstract

Thioure as typical join as either neutral (S, N- donor) ligand, or instead as bidentate ligands (typically S, N- bonded), Or monodentate (typically S-bonded) fashion. We have been successfully synthesized *N*-allyl -*N*'-(4`-methylthiazol) -2ylthiourea by reaction 2-amino-4-methylthiazol with allylisothiocyanate and well characterized by various analytical techniques, such as ^{1}H-^{13}C NMR, elemental analysis, IR and mass Spectra.

Keywords: Thioureas, thiazol, allylisothiocyanate.

1. Introduction

Thiourea derivativeshave many chemical and biological applications [1]. They have been used in antioxidant [2], anti-HIV [3], anti-cancer agents [4], rodenticide [5], anti-fungal agents [6], anti-inflammatory [7], anti-tubercular [8], anti-parasitic [9] and bacterial [10]. In past, thiourea derivatives were applied as organocatalysts and ligands in many asymmetric organic reaction [11]. They have been applied as chemical sensors for the detection of heavy metals [12] and in polymer synthesis [13]. Thiourea derivatives are used as agrochemicals such as herbicides [14], and insect growth regulator [15]. They have also wide applications in the chemical synthesis such as organic molecule and hetrocycles [16]. In this paper we report the synthesis andcharacterization of *N*-allyl -*N*'-(4'-methylthiazol) -2ylthiourea.

2. Experimental

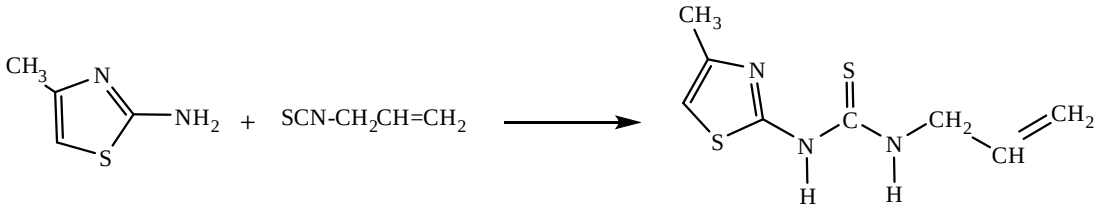
2. 1. Material and analytical equipment

All chemical used for the preparation of the compound were of analytical quality and were used without further purification DMSO-d_6 (Fluka) were used for NMR measurements. allylisothiocyanate and 2-methyl-4- methylthiazol was supplied by Aldrich Chemical Company.

^{1}H and ^{13}C NMR spectra were recoded at 25℃ with BRUKER 500 and 125 MHz. NMR apparatus with DMSO as solvent. Elemental analyses were carried out using a Perkin Elmer 2400 CHN Analyzer. Mass spectra were recorded on Shimadzu Qp. IR spectra (KBr) were recorded with a tometer (4000- 200 cm^{-1}).

2. 2. Preparation of *N*- allyl -*N*`-(4`-methylthiazol)-2ylthiourea

A solution of 2-amino-4-methylthiazol (0.01 mol) in warm ethanol 20 ml was added dropwise to a allyisothiocyanate (0.01 mol) under refluxed for 36 hours. The reaction product was filtered off. Washed with ethanol and recrystallized with ethanol afforded yallow crystals suitable for crystallography yield: 75% m.p:185℃. Yellow crystal. Anal. Calc. for $C_8H_{11}N_3S_2$ (213 g mol^{-1}): C, 44.96; H, 4.92; N, 19.36. Found: C,45.07; H, 5.16; N, 19.72.



3. Results and Discussion

3. 1. Infrared spectra

The infrared spectrum of *N*-allyl –*N*`-(4`-methylthiazol) -2ylthiourea measured in a KBr disc, shows two band at 3173 and 3022 cm^{-1}, assignable to (N1H) and (N2H) respectively [17, 18], the band at 1475 cm^{-1} for (CH_3), 823 cm^{-1} for (C=S), 1563, 1501, 1533 cm^{-1}forTz ring.

3. 2. NMR spectra

^{1}H NMR spectrum of the *N*-allyl –*N*`-(4`-methylthiazol) -2ylthiourea showed the presence (Fig. 1) δ 11.62 ppm for N1H, δ 10.85 ppm for N2H, δ 6.63 ppm for H(5) Tz, δ 2.2 ppm for (CH_3) Tz, 5.92,5.21, 4.20 ppm for proton of allyl. Show from ^{13}C NMR spectrum of the compound there are eight signs indicate the presence eight types of non-magnetically neutral carbon atoms in the molecule (Fig. 2) δ 179.10 ppm for C=S, δ 134.30; 146.00; 162.00 ppm for thiazol carbonatomes, 116.32; 106.50; 46,65 ppm for allyl carbon atoms.

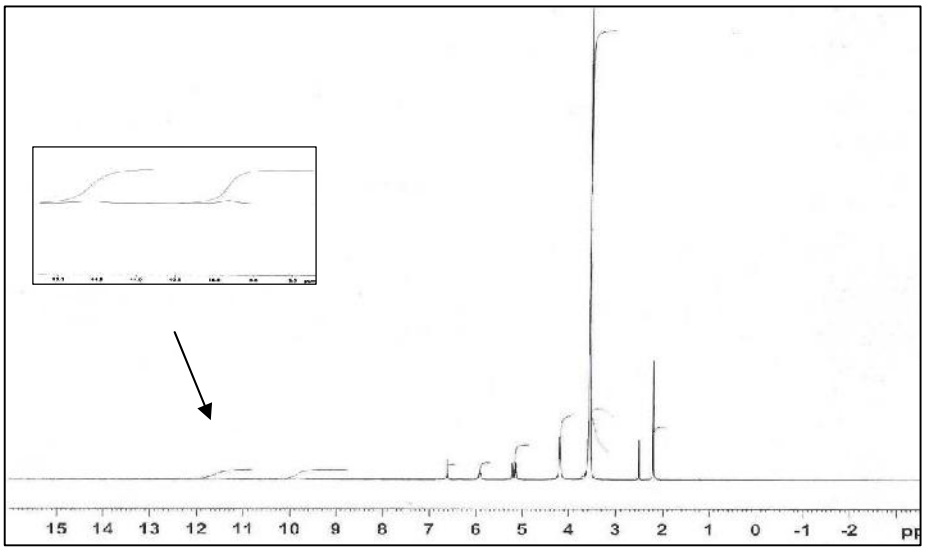


Fig. 1. ^{1}H NMR spectrum of in *N*-allyl –*N*`-(4`-methylthiazol) -2ylthiourea

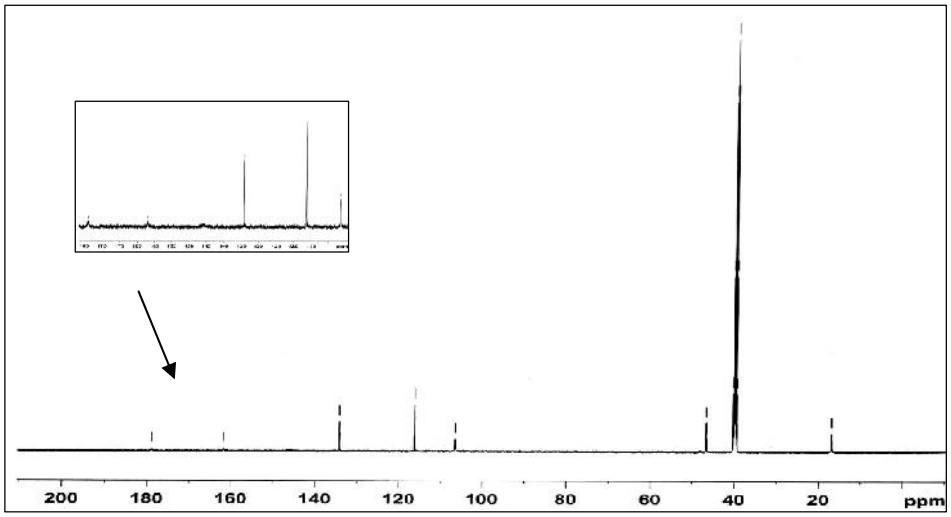


Fig. 2. ^{13}C NMR spectrum of in *N*-allyl –*N*`-(4`-methylthiazol) -2ylthiourea

3. 3. Mass spectra

The mass spectra of the *N*-allyl –*N*`-(4`-methylthiazol) -2ylthiourea, under EI condition (Figure 3) Showed the highest peak at m / z = 213 corresponds to the molecular of the compound . This molecular is undergo to different paths segmentation according to scheme 2 . The part (B`), (C), (D) forming from loses H_2S, allylimino, allyisothiocyanate from (A) respectively. Cation (E) forming where m / z = 198 from lose CH_3thiazole ring. Cation (F) forming where m / z = 72 from break bonds of C-N and C-S thiazole in the ring at once.

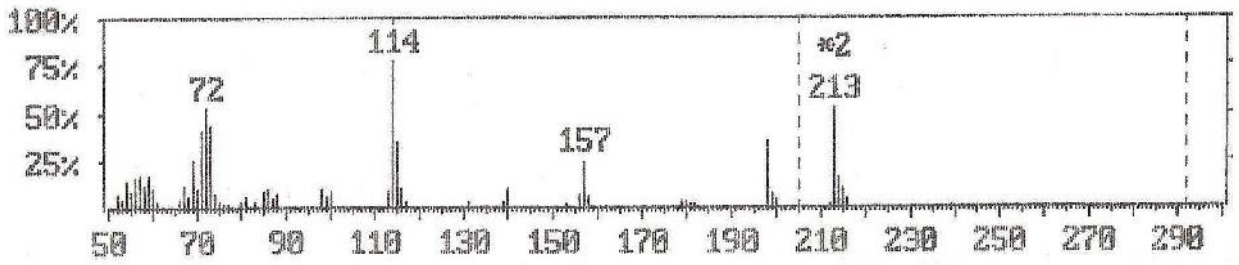
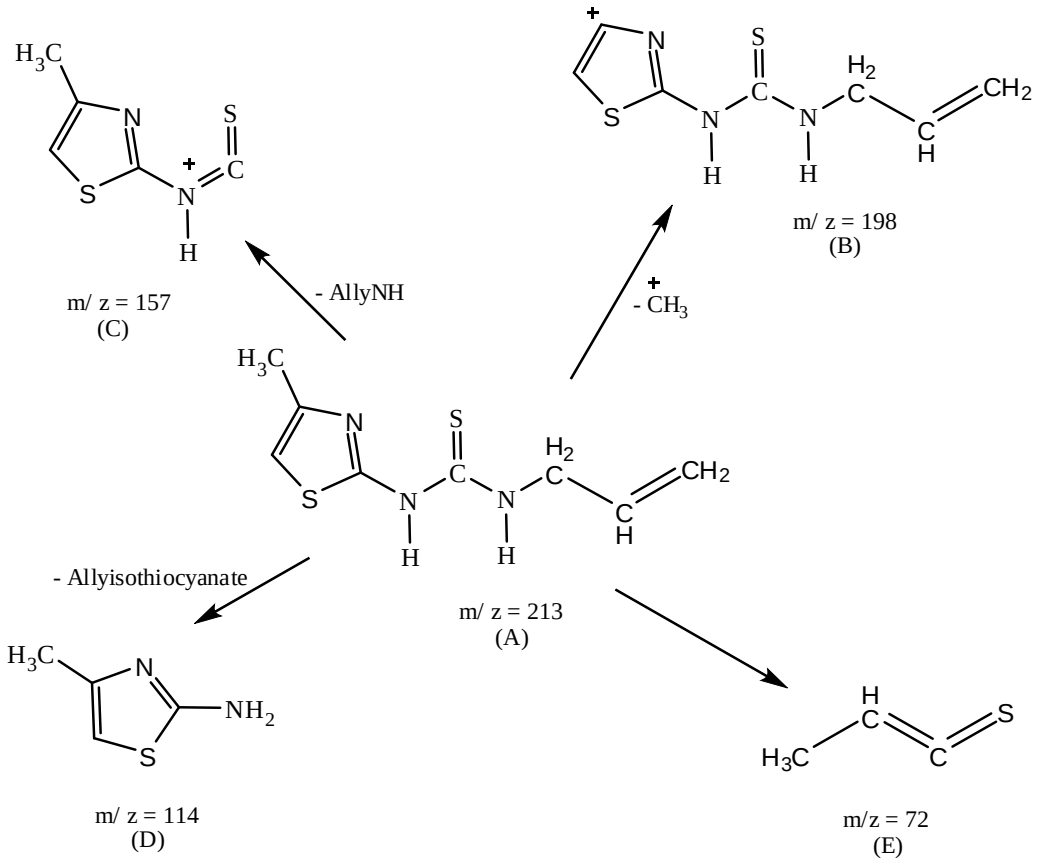


Fig. 3. Electronic impact mass spectrum of *N*-allyl –*N*`-(4`-methylthiazol) -2ylthiourea



Scheme I: Fragmentation pathway of *N*-allyl –*N*`-(4`-methylthiazol) -2ylthiourea

4. Conclusion

In conclusion, we report that *N*-allyl –*N*`-(4`-methylthiazol) -2ylthiourea can be prepared by treating easily available 2-amino-4-methylthiazol with allyisothiocyanate. The reaction provides products in good yields at room temperature with the advantage of operational simplicity. The structures of *N*-allyl –*N*`-(4`-methylthiazol) -2ylthiourea were characterized by elemental analysis, ^{1}H- ^{13}C NMR, IR and mass Spectra.

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