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Synthesis and Characterization of *N*- ethyl–*N*`(4`-methylthiazol) -2ylthiourea

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Abstract: ***An efficient synthesis of N- ethyl–N`(4`- methylthiazol) -2ylthiourea via the reaction of 2-amino- 4-methylthiazole and ethylisothiocyanate mild conditions has been developed. This reaction proceeded well at room temperature, to afford products in excellent yields. The compound was characterized by elemental analysis, ^{13}C- ^{1}H NMR, IR, electronic spectra and mass spectra.***

1. Introduction

Thiourea and it derivatives have long been attracting considerable attention due to their biological importance [1]. The facile synthesis of thioureas enabled the preparation of their numerous derivatives, most of which have been evaluated for their biological activities for example herbicidal, insecticidal [2], antiviral [3], antifungal [4], antibacterial [5].

The thiazol motif is an important building block [6], that is present in the structure of pharmacologically active substances and natural products [7]. Compounds containing thiazole rings have widespread biological applications as ani-inflammatory [8], antitumural [9], antiviral [10], antipiron [11],herbicidal,[12] .

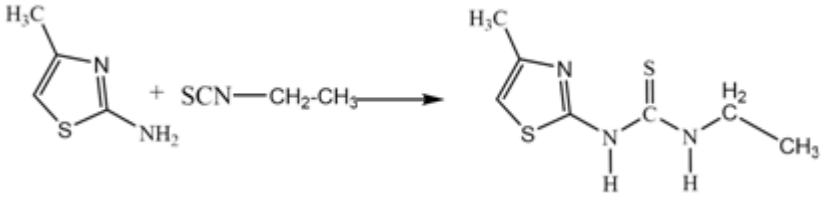
2. Experimental

2.1 Materials and instrumentation

2-amino-4-methylthiazole, ethylisothiocyanate and solvents were obtained from a commercial source and used without any further treatment. The (C, Hand N) elemental analysis was completed by using a Perkin–Elmer analyzer. JEOL ECA 500 MHz NMR spectrometer was used to measureNMR in deuterateddimethylsulfoxide and DMSO-d_6, using tetramethylsilane (TMS) as a reference. ThermoFisherNicoleteIS10 was used to measure Fourier-transform Infrared (FTIR) spectra applying KBr discs. ATI Unicam UV–vis. instrument was used to measure electronic spectra.

2.2 Preparation of - ethyl–*N*`(4`- methylthiazol) -2ylthiourea

1.14 gm (0.01 mol) of 2-amino-4-methylthaizole was dissolved in 20 ml of ethanol and stirred. 0.87 gm (0.01 mol) of ethylisothiocyanate was added to the solution and refluxed for 3 days. This produced a White precipitate that was separated and recrystallized by hot C_2H_5OH to obtain white crystals of - ethyl–*N*`(4`- methylthiazol) -2ylthiourea. Yield: 80%; m.p: 233℃. Anal. Calc. for $C_7H_{11}N_3S_2$ (201 g mol-1): C, 41.73; H, 4.97; N, 20.86; S, 31.79 Found: C,42.12; H, 5.05; N, 20.61; S, 31.38 .



3. Results and Discussion

3.1 Infrared spectra (IR)

The infrared spectrum of cpmpound measured in a KBr disc, shows two banbs at 3435 and 3177 cm^{-1} , assignable to υ(N1H) and υ(N2H) respectively [13,14]. The appearance of two bands for the NH groups of the thiourea part and the absence of a strong band in the 2500-2300 cm^{-1} region due to υ(S-H) [14, 15], is evidence for existence of the compound in the thione form in the solid state. The band at 823 $cm^{-1}\upsilon$ (C=S) , 1476.00 $cm^{-1}\upsilon$ (CH_3), 680 $cm^{-1}\upsilon$ (C-S-C), 1577; 1535; 1506 cm^{-1} (Tz ring).

3.2 Electronic spectra

The electronic spectra of the compound(Fig.1) was recorded in the DMF solvent. The spectrum of H_2EMT revealed asymmetric absorption pack is fascinated at 302 nm assigned to the n→ л*, л→ л* [16,17].

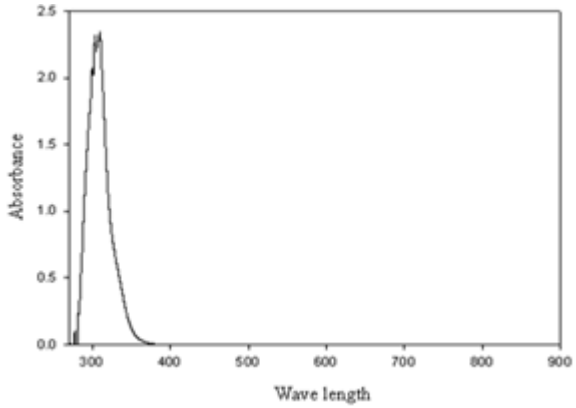


Figure 1: Electronic spectrum of *N*- ethyl–*N*`(4`-methylthiazol) -2ylthiourea

3.3 ^{1}H ^{13}C NMR

The^{1}H NMR spectrum of the *N*-ethlyl –*N*`-(4`-methylthiazol) -2ylthiourea showed(Fig.2) the presenceNMR δ= 1.16 ppm (CH_3), δ= 2.53 ppm (CH_2), δ= 2.23 ppm (CH_3), δ= 6.61 ppm (H-5), δ= 9.66 ppm (N2H), δ= 11.48 ppm (N1H).The^{13}C NMR spectrum of the compound(Fig.3) there are seven signs indicate the presence seven types of non-magnetically neutral carbon atoms in the moleculeδ= 14.30; 48.20 ppm (ethyl carbons), δ= 106.40 ; 145.90; 161.80 ppm (thiazol carbons), δ= 178.50 ppm (C=S), δ= 17.00 ppm (CH_3)

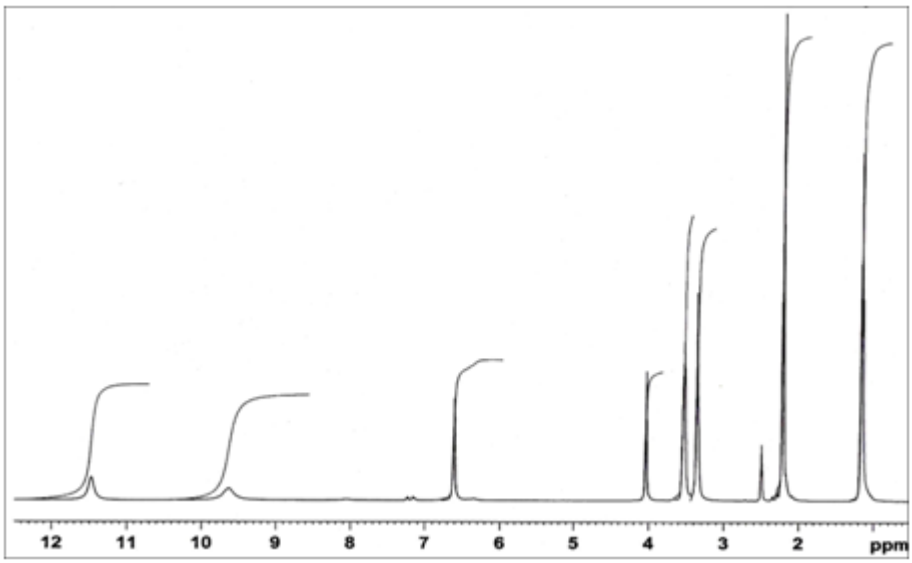


Figure 2: ^{1}H NMR spectrum of *N*- ethyl–*N*`(4`- methylthiazol) -2ylthiourea

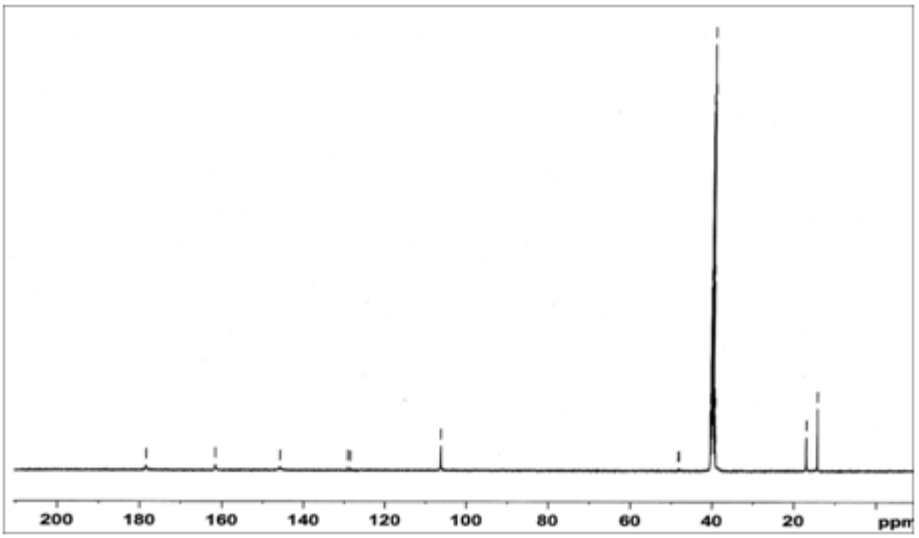


Figure 3: ^{13}C NMR spectrum of *N*- ethyl–*N*`(4`- methylthiazol) -2ylthiourea

3.4 Mass spectra

The mass spectra of the *N*-ethyl –*N*`-(4`-methylthiazol) -2ylthiourea, under EI condition (Figure 4) Showed the highest peak at m / z = 201 corresponds to the molecular of the compoundcorresponding to a molecular weight of the compound. The molecular compound A loses H_2S forming B(Scheme.1), loses $EtNH_2$ forming C, loses EtSCN forming D,…and E.

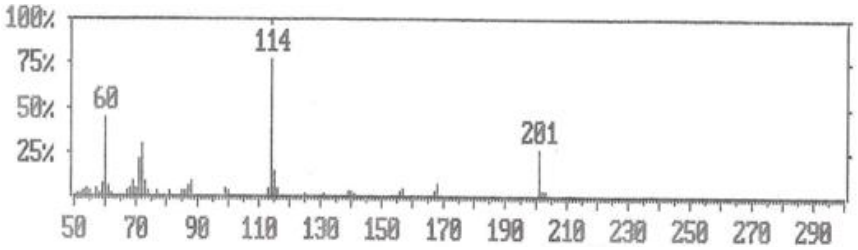
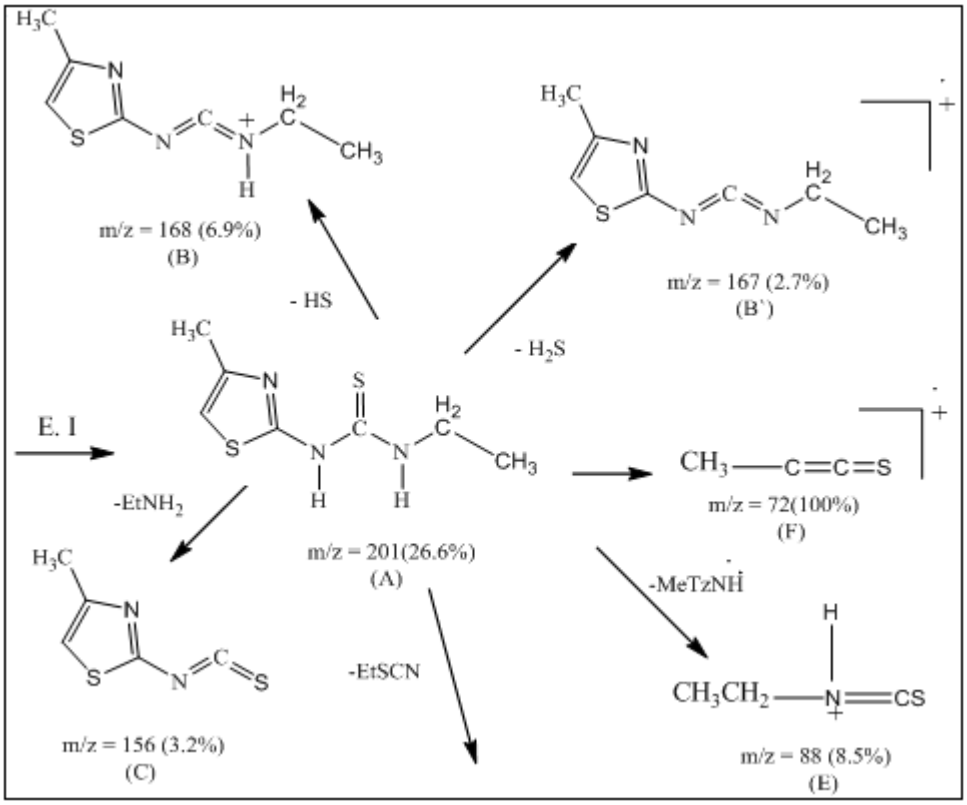


Figure 4: Electronic impact massspectrum of *N*- ethyl–*N*`(4`- methylthiazol) -2ylthiourea



Scheme 1: Fragmentation pathways of *N*- ethyl–*N*`(4`- methylthiazol) -2ylthiourea

4. Conclusion

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

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