

“SYNTHESIS OF AN HETEROCYCLIC COMPOUND 2- AMINO THIAZOLE”

Dr. P.D. GOKULAN*¹, Dr. K.L. SENTHIL KUMAR*², M. ABIRAMI*³, M. ABISHEK*⁴, M. AKILA*⁵

¹Professor, Sri Vijay Vidyalaya College of Pharmacy, Tamil Nadu, India.

²Principal, Sri Vijay Vidyalaya College of Pharmacy, Tamil Nadu, India.

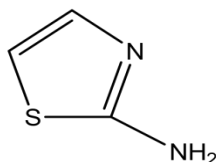
^{3,4,5}B. Pharm Students, Sri Vijay Vidyalaya College of Pharmacy, Tamil Nadu, India.

ABSTRACT- Heterocyclic compounds are very important in pharmaceutical chemistry, and thiazole derivatives are the most important of these. This dissertation presents a straightforward and dependable undergraduate methodology for synthesizing 2-aminothiazole within a regulated laboratory environment. We closely monitored the product's formation, fine-tuned the most important reaction conditions, and then quickly isolated and purified it. We used IR spectroscopy and physical constants to find out what the compound we made was and how pure it was. This study concentrates on the practical aspects of synthesizing heterocycles and establishes a foundation for further research and development of thiazole-derived applications. This method is a simple, cheap, and reliable way to make 2-aminothiazole. This means that it can be used in both labs and factories.

Key words: 2-Aminothiazole: Heterocyclic compound: Chemical synthesis: procedural method: IR Spectroscopy.

I. INTRODUCTION

Thiazole is a heterocyclic compound that has both a nitrogen atom and a sulfur atom in an aromatic five-membered ring. Most of the time, 2-aminothiazole and its derivatives are made by reacting with α -halogenocarbonyl compounds. Thiazoles are a very important group of natural and man-made substances [1]. Thiazole derivatives have a lot of different biological effects, including being cardiotoxic [2], fungicidal, sedative [3], anesthetic, bactericidal [4], and anti-inflammatory. Famotidine is a drug that is sold to treat peptic ulcers and gastroesophageal reflux. It has two thiazole nuclei. Thiazole derivatives are recognized for their significant antitumor and cytotoxic effects, with many derivatives engineered to target specific pathways. This thiazole compound is an example of one that has been tested in clinical trials and used to treat cancer [5]. Heterocyclic compounds are a big group of organic compounds in which one or more atoms in the ring are not carbon, like nitrogen, sulfur, or oxygen. These compounds are very important in organic and pharmaceutical chemistry because they have a lot of biological activities and are found in many natural and synthetic drugs. Thiazole and its derivatives are some of the most interesting heterocyclic systems because of their important chemical and pharmacological properties. Thiazole is a five-membered ring made up of sulfur and nitrogen atoms that are not the same type. Compounds with the thiazole nucleus have a wide range of biological effects, such as being antibacterial, antifungal, anti-inflammatory, and anticancer. 2-aminothiazole is one of these important derivatives. It is a useful intermediate in the making of many drugs and biologically active molecules. The Hantzsch thiazole method is the most common way to make 2-aminothiazole. It involves combining α -haloketones with thiourea in the right conditions. This method is preferred because it is easy to use, works well, and is good for making things in the lab. By changing the conditions of the reaction, you can get good yields and high purity of the product you want. This study concentrates on the synthesis of 2-aminothiazole employing a straightforward and effective undergraduate-level methodology. The focus is on optimizing reaction conditions, isolating and purifying the product, and characterizing the synthesized compound through physical properties and infrared spectroscopy. This work aims to provide practical exposure to heterocyclic synthesis while highlighting the importance of thiazole derivatives in pharmaceutical chemistry.



2-Amino thiazole

FIG 1: structure of 2-Amino thiazole

II. SYNTHESIS OF 1,3-THIAZOLE-2-AMINE:

i. CHEMICAL AND REAGENT:

Thiourea: 7.6g

Chloroacetaldehyde: 10 ml

Ethanol/water: 25 ml

NaHCO₃: 5 ml

Ethyl acetate: 30 ml

ii. EQUIPMENT AND INSTRUMENT:

Magnetic stirrer pH meter

Heating mantle

Conical flask

Beaker

III. SCHEME:

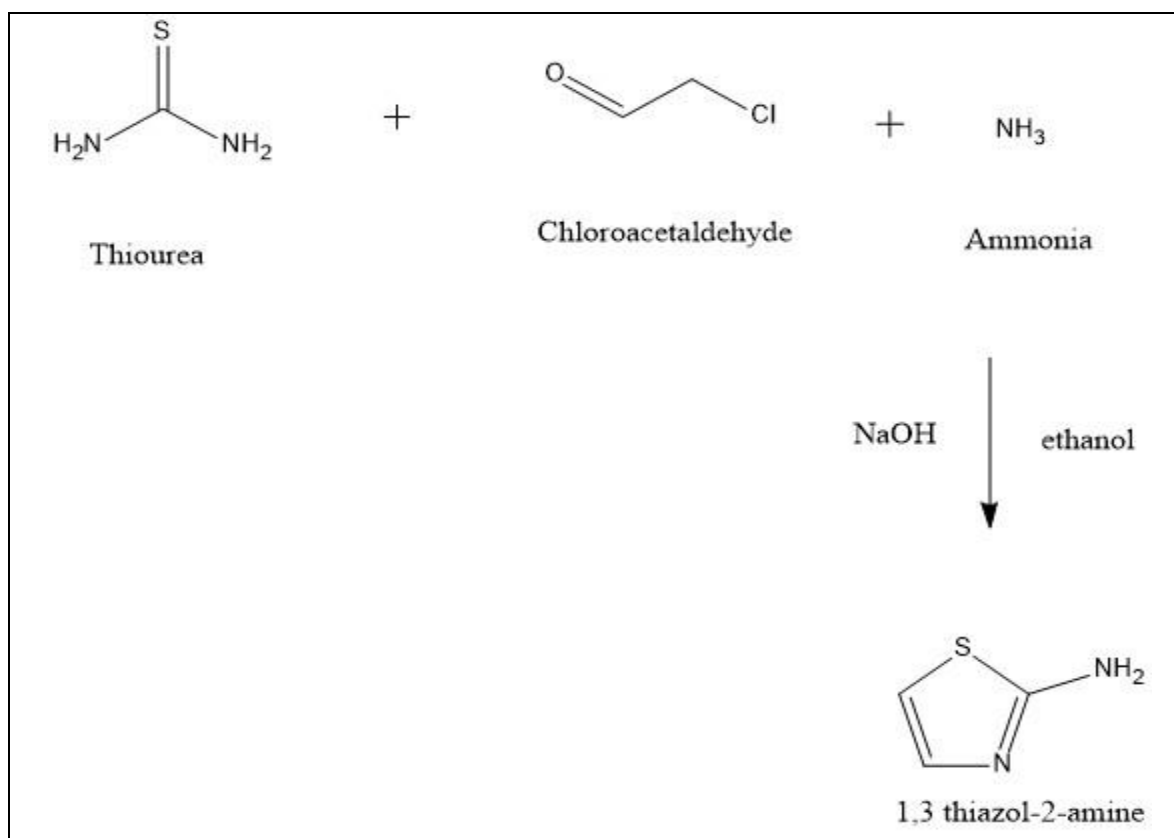


FIG 2: Scheme of the reaction

IV. PROCEDURE:

In the preparation of 1,3-thiazole-2-amine (2-aminothiazole), an accurately weighed amount of thiourea (7.6 g) was first dissolved in 25 mL of a 1:1 (v/v) ethanol-water solvent mixture in a conical flask. To this solution, 10 mL of chloroacetaldehyde was added slowly in a dropwise manner with constant stirring to ensure uniform mixing. The reaction mixture was then heated under reflux at a temperature of 70–80 °C for 2–3 hours with continuous agitation to promote cyclization and completion of the reaction. After reflux, the mixture was allowed to cool to room temperature and was gradually neutralized using sodium bicarbonate until a pH of 8–9 was attained, which facilitated the liberation of the amine product. The reaction mixture was then extracted with 30 mL of ethyl acetate, and the organic layer was separated and dried over anhydrous sodium sulfate. Finally, the dried extract was purified by recrystallization from 10 mL of ethanol, yielding pure 2-aminothiazole.

V. IR SPECTROSCOPY:

GRAPH 1

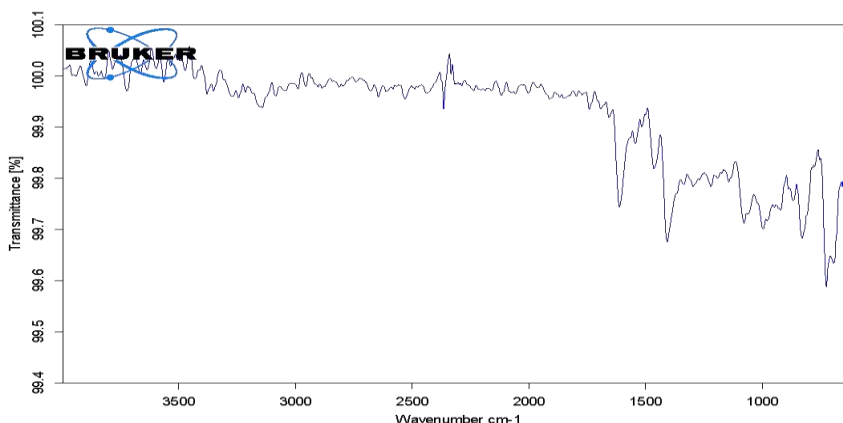


FIG 3: FT-IR Spectroscopy of 1,3-thiazol-2-amine

GRAPH 2

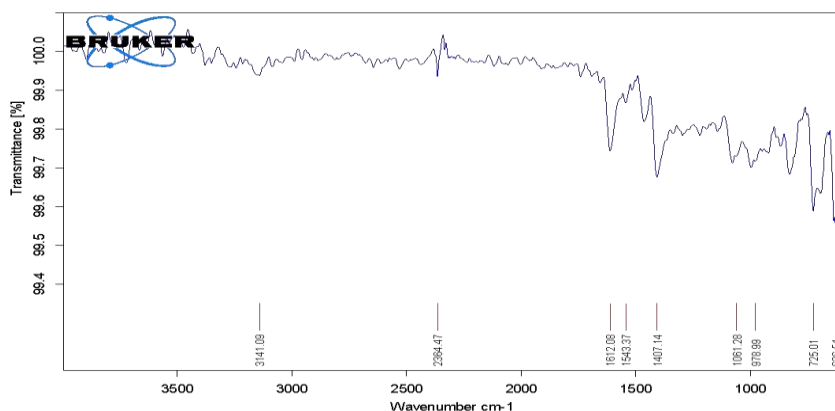


FIG 4: FT-IR Spectroscopy of 1,3-thiazol-2-amine with peak lines

VI. RESULT:

The IR spectra of the compound that was made were recorded, and the characteristic absorption bands were seen in the areas that matched the different functional groups. Absorption bands were seen in Figure 06 at the following wavelengths: 3400–3300 cm^{-1} , 2920–2850 cm^{-1} , 1650–1600 cm^{-1} , 1500–1450 cm^{-1} , 1350–1300 cm^{-1} , 1200–1050 cm^{-1} , and 900–700 cm^{-1} .

Figure 07 also had characteristic absorption bands at about 3380 cm^{-1} , 3050 cm^{-1} , 2925 cm^{-1} , 1635 cm^{-1} , 1530 cm^{-1} , 1380 cm^{-1} , 1120 cm^{-1} , and 760–680 cm^{-1} .

These absorption peaks show that the compound has N–H, aromatic C–H, aliphatic C–H, C=N, C–N, and aromatic ring vibrations.

TABLE 1

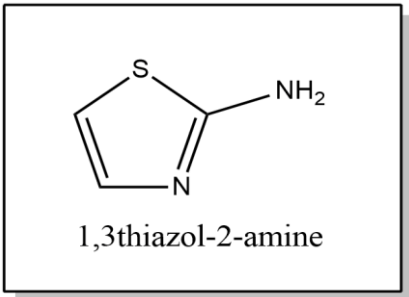
Structure	 <p>1,3thiazol-2-amine</p>
Molecular formula	$\text{C}_3\text{H}_4\text{N}_2\text{S}$
Chemical Name	2-Aminothiazole
Yield	60% – 85%
Melting point	155 °C – 158 °C
Molecular weight	100.14 g/mol

TABLE 2

S. No	Wavenumber (cm^{-1})	Intensity	Functional Group / Assignment
1	~3400–3300	Weak–Broad	O–H / N–H stretching

2	~2920-2850	Weak	C-H stretching (aliphatic)
3	~1650-1600	Medium	C=C / C=N stretching
4	~1500-1450	Medium	Aromatic C=C stretching
5	~1350-1300	Medium	C-N stretching
6	~1200-1050	Strong	C-O / C-N stretching
7	~900-700	Strong	Aromatic C-H bending

TABLE 3

S. No	Wavenumber (cm ⁻¹)	Intensity	Functional Group / Assignment
1	~3380	Weak	N-H stretching
2	~3050	Weak	Aromatic C-H stretching
3	~2925	Weak	Aliphatic C-H stretching
4	~1635	Medium	C=N stretching
5	~1530	Medium	Aromatic ring vibration
6	~1380	Medium	C-N stretching
7	~1120	Strong	C-N / C-O stretching
8	~760-680	Strong	Aromatic C-H out-of-plane bending

VII. DISCUSSION

The absorption band seen in Figure 06 at 3400–3300 cm⁻¹ and in Figure 07 at ~3380 cm⁻¹ is due to N-H stretching vibrations, which means that there are nitrogen-containing functional groups present. The weak bands between 2920 and 2850 cm⁻¹ and around 2925 cm⁻¹ are caused by aliphatic C-H stretching. The band near 3050 cm⁻¹ shows that aromatic C-H stretching is going on.

The medium-intensity absorption bands at ~1635 cm⁻¹ and in the range of 1650–1600 cm⁻¹ are due to C=N stretching vibrations, which suggest that the structure is either heterocyclic or unsaturated. The bands seen between 1500 and 1450 cm⁻¹ and around 1530 cm⁻¹ are due to aromatic C=C vibrations, which proves that the compound is aromatic.

The C-N stretching vibrations cause the absorption peaks around 1350–1300 cm⁻¹ and ~1380 cm⁻¹. The strong bands between 1200 and 1050 cm⁻¹ and ~1120 cm⁻¹ are caused by C-N or C-O stretching vibrations. The strong absorption bands between 900 and 700 cm⁻¹ and 760 and 680 cm⁻¹ are due to aromatic C-H out-of-plane bending vibrations.

Overall, the IR spectral features that were seen match up with the expected functional groups of the compound that was made. The IR spectral data show that the compound was made correctly and that its structure is still intact.

VIII. CONCLUSION:

The traditional cyclization method used a thioamide and an α -haloketone to make 2-aminothiazole, an important heterocyclic molecule. It was easy, fast, and very reproducible to make things in a lab using this method. The reaction happened in a mild way, and the product that was needed was made with good purity and a good yield. Recrystallization was used to purify the chemical that was made, and then it was characterized using standard analytical methods. Infrared spectroscopy was very useful for confirming the molecular structure of the compound. The fact that there were clear absorption bands for the amino group, thiazole ring, and other important functional groups showed that 2-aminothiazole was made correctly. The IR spectrum data that was recorded matched up well with what other researchers have found.

REFERENCE

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