Two 1,2,3,4-Thiatriazoles

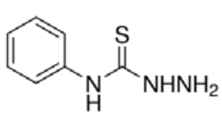
Abstract

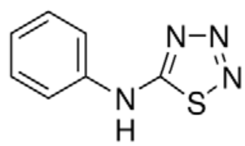
Thiatriazoles are considered mostly inorganic rings. They are not completely inorganic because they have a carbon in the ring structure. These thiatriazoles are interesting to study because they decompose into gas when they are heated. In this lab, two different 1,2,3,4-thiatriazoles were synthesized and characterized over one lab period.

Introduction

Explosive reactions are exothermic reactions that release a lot of heat. A commonly known explosive is dynamite. Alfred Nobel, the founder of the Nobel Prize, figured out how to mass produce dynamite in 1867 and also discovered a way to stabilize this reactive chemical. This discovery netted him enormous profits, and in his will he established the Nobel Prize which was to be awarded to people or organizations which promoted peace. Creating a prize committed to rewarding peace is in stark contrast to the destructive power of the chemical Nobel stabilized.

The decomposition of nitroglycerine is so favorable because forming the reaction products is highly favorable. Dynamite is commonly used for mining and road construction because it is powerful. While thiatriazoles are not dynamite, they are nitrogen and sulfur containing compounds which do a reasonable imitation of dynamite. In this report, two different 1,2,3,4-thiatriazoles were synthesized.



(s) + HCl(aq) + $NaNO_{2(aq)}$ →


(s) + H_2O + NaCl

Figure 2. Reaction for 5-anilino-1,2,3,4-thiatriazole

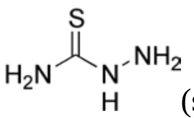
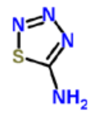
 (s) + $HCl_{(aa)}$ + $NaNO_{2(aq)}$ →  (s) + H_2O + NaCl

Figure 3. Reaction for 5-amino-1,2,3,4-thiatriazole

Thiatriazoles decompose when they are heated to high temperatures. Dynamite, however, does not need to be heated. Dynamite is extremely reactive and will if not stabilized, it can explode while being transported. The products of this laboratory experiment are likely going to react like dynamite.

Methods

5-anilino-1,2,3,4-thiatriazole (**1**)- 0.469 grams of 4-phenyl-3-thiosemicarbazide was added to 2.5 mL of HCl in a 25 mL Erlenmeyer flask. A small magnetic stir bar was added, and the suspension was cooled in an ice-bath with the temperature kept between 5℃ and 10℃. 0.210 grams of $NaNO_2$ were dissolved in 0.5 mL of water in a 25 mL beaker and 0.4 mL of this solution was added dropwise into the suspension of the 4-phenyl-3-thiosemicarbazide suspension over 10 minutes, with the stir bar on medium, to avoid causing the temperature to rise above 10℃. The reaction is exothermic so care must be taken to not allow the reaction to get too hot. The product was then isolated in a Hirsch funnel, using suction filtration. The product was then rinsed with 0.5 mL of ice cold water, three times.

5-amino-1,2,3,4-thiatriazole (**2**)- The procedure was repeated except with 0.275 grams of thiosemicarbazide being added to 1.0 mL of HCl. 0.212 grams of $NaNO_2$ were dissolved in 0.5 mL of water and 0.4 mL of the solution was added dropwise into the suspension of thiosemicarbazide.

Results

Products 1 and 2 both decomposed in the Mel-Temp apparatus, at 110℃ and 111℃ respectively. The IR and UV-Vis spectra are shown in figures and the peak assignment for the IR spectra is in the table.

<u>Discussion</u>

The temperature at which decomposition was expected to happen for both **1** and **2** was lower than the literature values.

5-anilino-1,2,3,4-thiatriazole		5-amino-1,2,3,4-thiatriazole	
Band position	Assignment	Band position	Assignment
3397	N-H	3256	NH_2
1614	C=N	1615	C=N
1601	Aromatic C=C		

Table 1.

While both products did decompose at high temperatures, **2** decomposed with an audible pop, whereas **1** did not. The IR spectrum for product 1 had peaks at 3397, 3328, 3244, 2935, 1614, 1601, 1566, 1455, 1293, 1197, 1095. The IR spectrum for product 2 had peaks at 3405, 3256, 3104, 1615, 1509, 1269, 1108, 684. The key peak assignment is in Table 1.

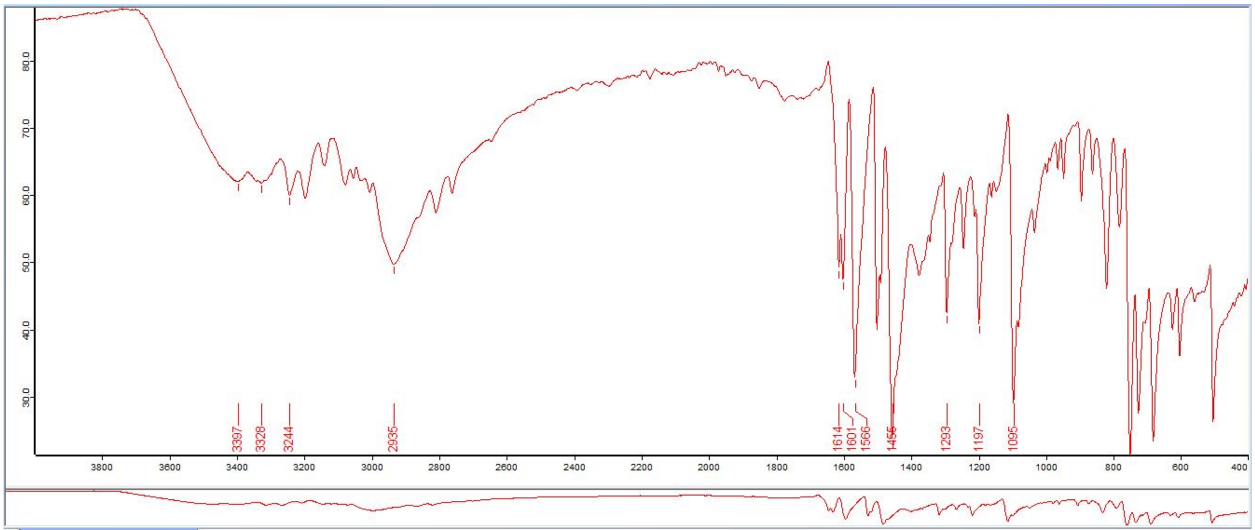


Figure 4.

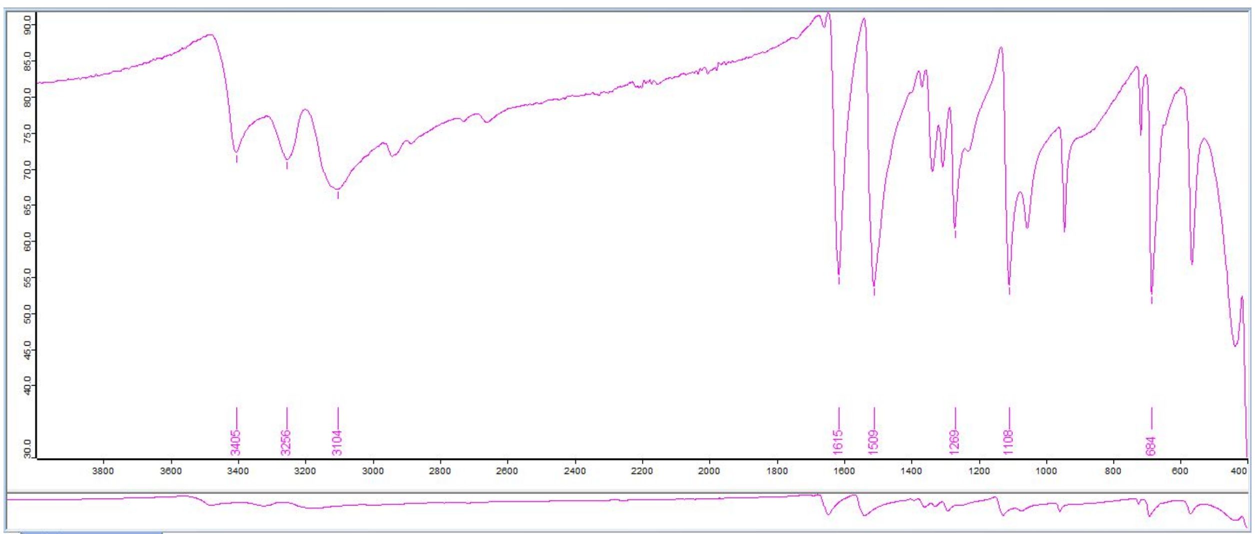


Figure 5.

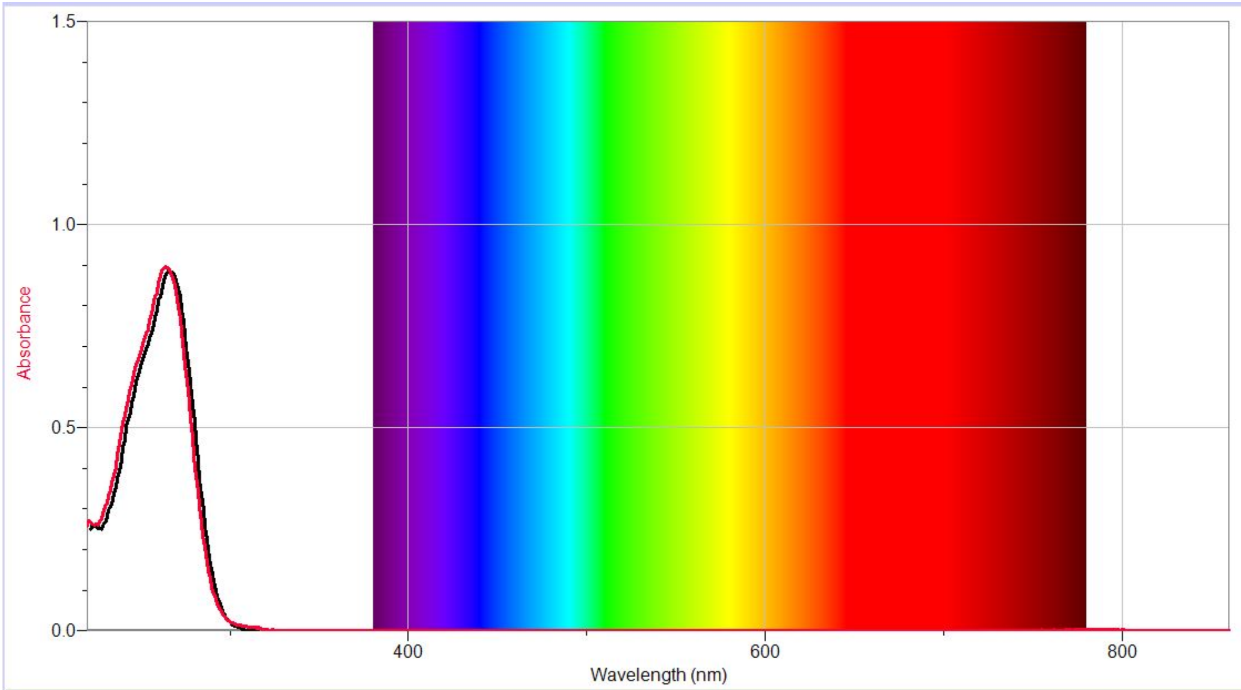


Figure 6.

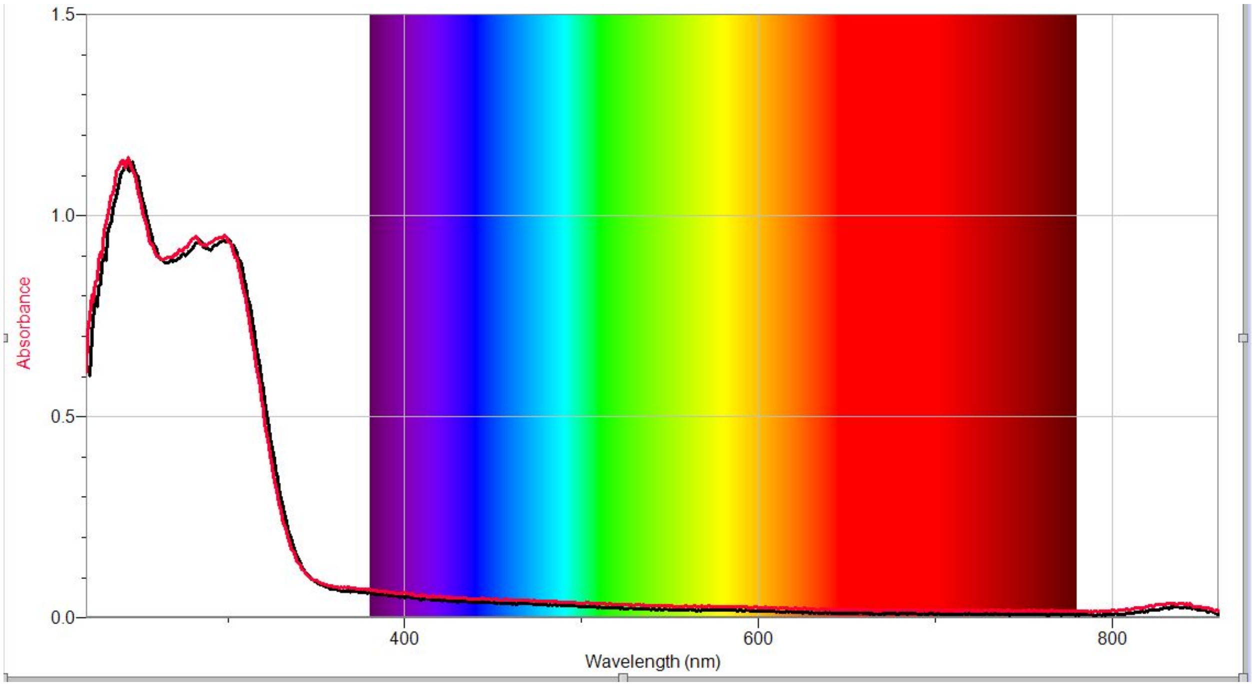


Figure 7.

<u>Conclusion</u>

The two different 1,2,3,4-thiatriazoles were synthesized and they bubbled and decomposed when they were heated.

References

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