

Electron impact induced fragmentations of 5-phenylamino-1,2,3,4-thiatriazole by mass spectrometry

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ABSTRACT

5-Phenylamino-1,2,3,4-thiatriazole has been characterised by Mass Spectrometry. The study of the principal mode of fragmentations subsequent to electron impact of thiatriazole using low resolution has been recorded as below.

Key words: Electron impact induced fragmentation, mass spectrometry.

INTRODUCTION

We have synthesised about twenty 5-Arylamino-1,2,3,4-thiatriazoles by method of Lieber *et al.* and used by Wahab & Rao, their Structures were determined by using various spectroscopy especially M/S. The beauty of mass spectra of 5-Phenylamino- 1,2,3,4-thiatriazole is the molecular ion does not form the base peak. These thiatriazoles were screened by various biological activities such as Agro chemicals antitubercular and anticancer few compounds have shown the good activity against mycobactirium tuberculosis strain H37 Ra Lavenstein Jensen medium.

EXPERIMENTAL

5-Phenylamino-1,2,3,4-thiatriazole was synthesised by the diazotized cyclization of 4-phenyl-3-thiosemicarbazide in presence of NaNO₂ / HCl maintained the temperature in between 0 to -

4°C (Ref. 1) Mass spectra of 5- Phenylamino-1,2,3,4-thiatriazole were recorded on AE₁ Mass spectrometer using a heated inlet system, ionization energy 70 ev, inlet-temperature 150°C.

RESULTS AND DISCUSSION

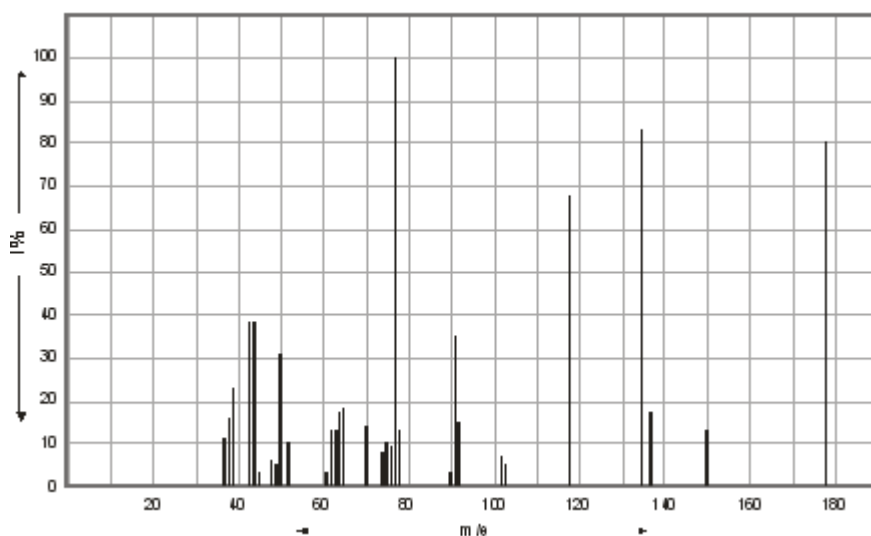
The mass spectra 5-Phenylamino-1,2,3,4-thiatriazole (A) has been recorded on AE-MS 9 Mass Spectrometer using a heated inlet system. Ionization energy of 70ev, inlet temperature of 150°C, accurate mass measurement were used to determine the nature of various peaks in the spectra²⁻⁸.

The mass spectra of 5-Phenylamino-1,2,3,4-thiatriazole has been recorded (Fig. 1 and data 2 and the electron impact induced fragmentations have been show in data 3 & 4, eg.

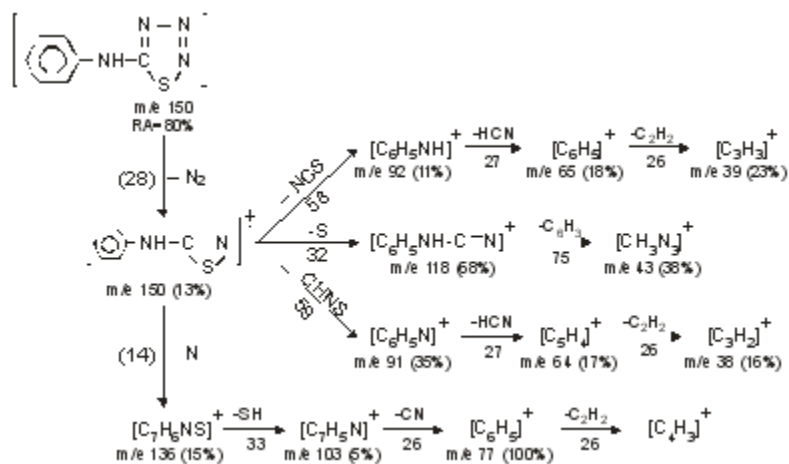
The low resolution mass spectra of

M/e	37	38	39	43	44	45	48	49	50
I%	11	16	23	38	38	3	6	5	31
M/e	51	52	61	62	63	64	65	70	74
I%	78	10	3	13	13	17	18	14	8
M/e	75	76	77	78	90	91	92	103	102
I%	10	9	100	13	3	35	15	5	7
M/e	118	119	135	136	137	150	178		
I%	68	6	83	15	17	13	80		

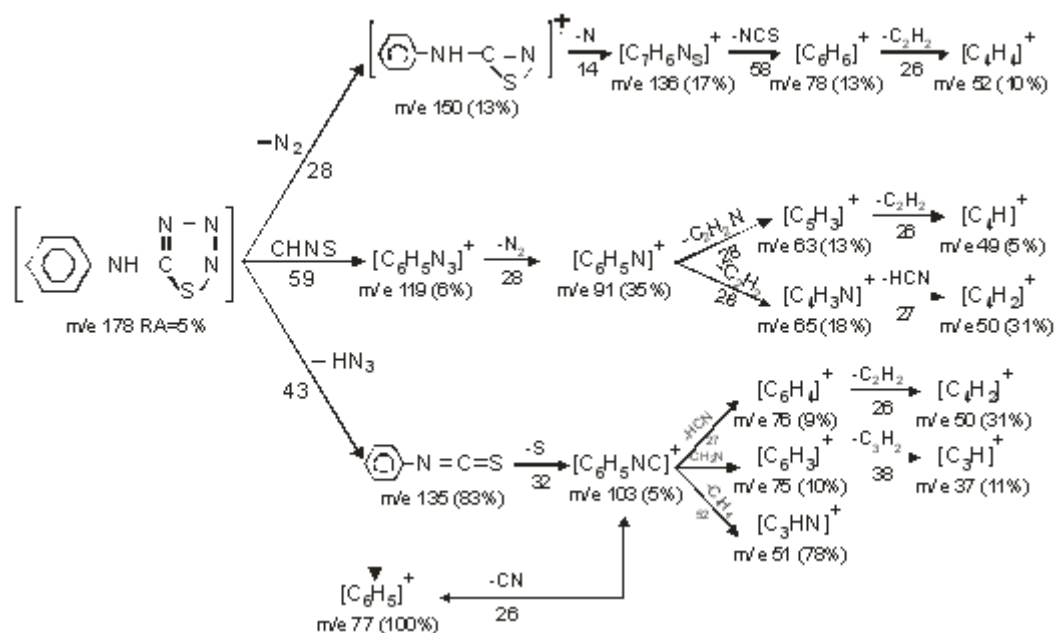
Data 1: Mass spectral data of 5-Phenylamino-1,2,3,4-thiaziazole



Data 2: Mass spectral graph of 5-Phenylamino-1,2,3,4-thiaziazole



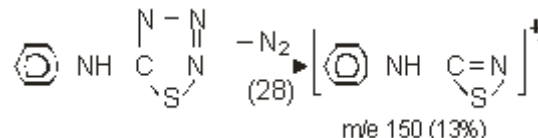
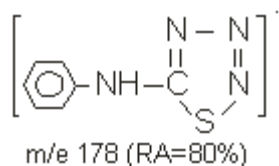
Data 3: Electron Impact Induced Fragmentations of 5-Phenylamino-1,2,3,4-thiaziazole



Data 4: Electron Impact Induced Fragmentations of 5-Phenylamino-1,2,3,4-thiaziazole

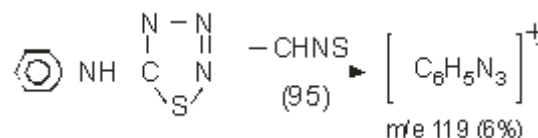
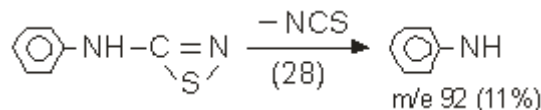
5- Phenylamino-1,2,3,4-thiaziazole indicated that the molecular ions does not form the base peak. The intensity is 80%.

1. It has been found the N₂ lost from the molecular ion gives prominent ion m/e 150 (13%).



2. Loss of NCS radical from (I) gives phenylamino m/e 91 (11%)

3. Elimination of CHNS fragment from (A) gives (C₆H₅N₃) m/e 119 (6%).



4. Ejection of Nitrogen fragment yield C₇H₅NS (m/e 150, 135), which losses sulphhydryl

radicals to give C₆H₅NHCN (m/e, 118, 68%).

