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 cycliclization of 4phenyl-3-thiosemicarbazide in presence of NaNO₂ / HCI maintained the temperature in between 0 to - 4°C (Ref. 1) Mass spectra of 5- Phenylamino-1,2,3,4-thiatriazole were recorded on AE_1 Mass spectrometer using a heated inlet system, ionization energy 70 ev, inlet-temperature 150°C.

RESULTS AND DISCUSSION

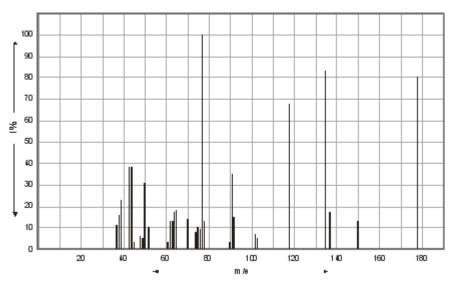
The mass spectra 5-Phenylamino-1,2,3,4thiatriazole (A) has been recorded on AE-MS 9 Mass Spectrometer using a heated inlet system. Ionization energy of 70ev, inlet temperature of 150°C, accurate mass measurement were used to determine the nature of various peaks in the spectra²⁻⁸.

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.

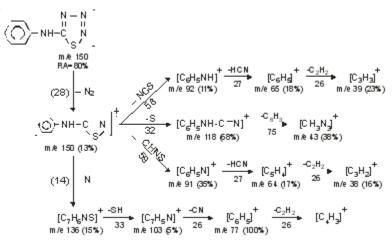
The low resolution mass spectra of

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 I%	118 68	119 6	135 83	136 15	137 17	150 13	178 80		

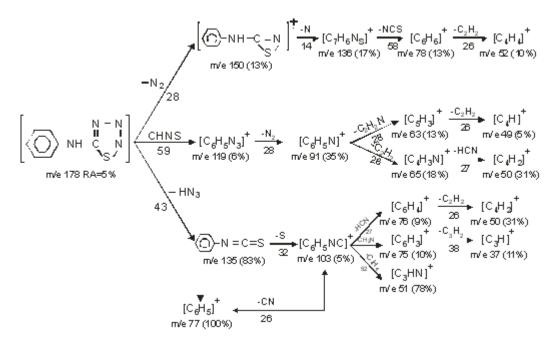
Data 1: Mass spectral data of 5-Phenylamino-1,2,3,4-thiatriazole



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



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

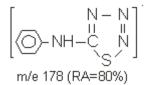


Data 4: Electron Impact Induced Fragmentations of 5-Phenylamino-1,2,3,4-thiatriazole

1.

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

It has been found the N_2 lost from the molecular ion gives prominent ion m/e 150 (13%).



2.

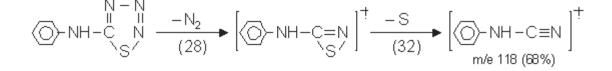
Loss of NCS radical from (I) gives 3. phenylamino m/e 91 (11%)

$$\bigcirc$$
-NH-C=N
S' (28)
m/e 92 (11%)

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

- - Elimination of CHNS fragment from (A) gives $(C_6H_5N_3)$ m/e 119 (6%).

radicals to give C_6H_5 NHCN (m/e, 118, 68%).



5. Ejection of CHNS and Nitrogen (i) yield C_7H_6NS (m/e 136, 15%) which losses

mercapto (SH) and cyanide radicals yield $C_7 H_6 N$ (m/e 103%, 5%) and $C_6 H_5$ (m/e 77, 100%).

6. Ejection of CHNS and Nitrogen molecule give $[C_6H_5N]^+$ m/e 91, 35%.

$$(\bigcirc -NH-C \underset{S'}{\overset{N}{\longrightarrow}} \xrightarrow{-CHNS} \begin{bmatrix} C_6H_5N_3 \end{bmatrix} \xrightarrow{-N_2} \begin{bmatrix} C_6H_5N \\ m/e \ 192 \ (6\%) \end{bmatrix} \xrightarrow{m/e \ 91 \ (35\%)}$$

 Elimination of HN₃ molecular give the phenyl isothnocyanate (m/e 135, 8.3%) ion radical which losses sulphur fragment to give phenylisocynamide [C $_{6}H_{5}NC$]. It losses [CN} gives [C $_{6}H_{5}$], (m/e 77, 100%).

$$\bigcirc -NH - C \underset{S'}{\overset{N}{\longrightarrow}} \xrightarrow{-HN_3} [\bigcirc -N = C = S] \xrightarrow{-S} [C_6H_5NC] \xrightarrow{-CN} [26] \xrightarrow{-CN} [135 (83\%)] \xrightarrow{-N} [135 (83\%)] \xrightarrow{-N} [C_6H_5NC] \xrightarrow{-CN} [26] \xrightarrow{-$$

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