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MASS AND IR SPECTRAL STUDIES OF THE REACTION PRODUCT OF L-LEUCINE AND Se_4N_3Br

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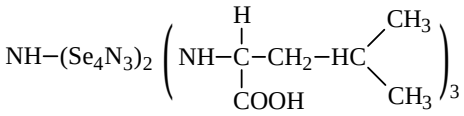
ABSTRACT

The reaction product of Se_4N_3Br with L-Leucine, an amino acid was synthesized in dichloroethane. The structure of the product is assigned on the basis of quantitative estimations, mol. wt., mass and IR spectrometric analysis as –



Key words: Se_4N_3Br, L-leucine.

INTRODUCTION

The adducts of Se_4N_3Cl with phenylhydrazine, urea and thio-urea have been reported[1,3], but the adducts of Se_4N_3Br with amino acids have not been synthesized till now. Therefore, it is intended to prepare the adducts of Se_4N_3Br with L-leucine and to investigate the reaction product, by mass and IR spectrometrically.

EXPERIMENTAL

Se_4N_3Br was prepared by the reaction of HBr on Se_4N_4, which was synthesized as reported[1-7] by the reaction of ammonia on Se_2Cl_2 at 0^oC. The adduct of Se_4N_3Br with L-Leucine was prepared by refluxing the equimular mixture of both in dichloroethane for 6-8 h. The product, obtained, was separated, washed with dichloro-ethane, alcohol and ether, dried and stored in a vacuum desiccator over fused calcium chloride. The mass and IR spectra of the product were recorded on Jeol SX-102 (FAB) and Perkin Elmer RX1 (450-4000 cm^{-1}) spectrometers, respectively.

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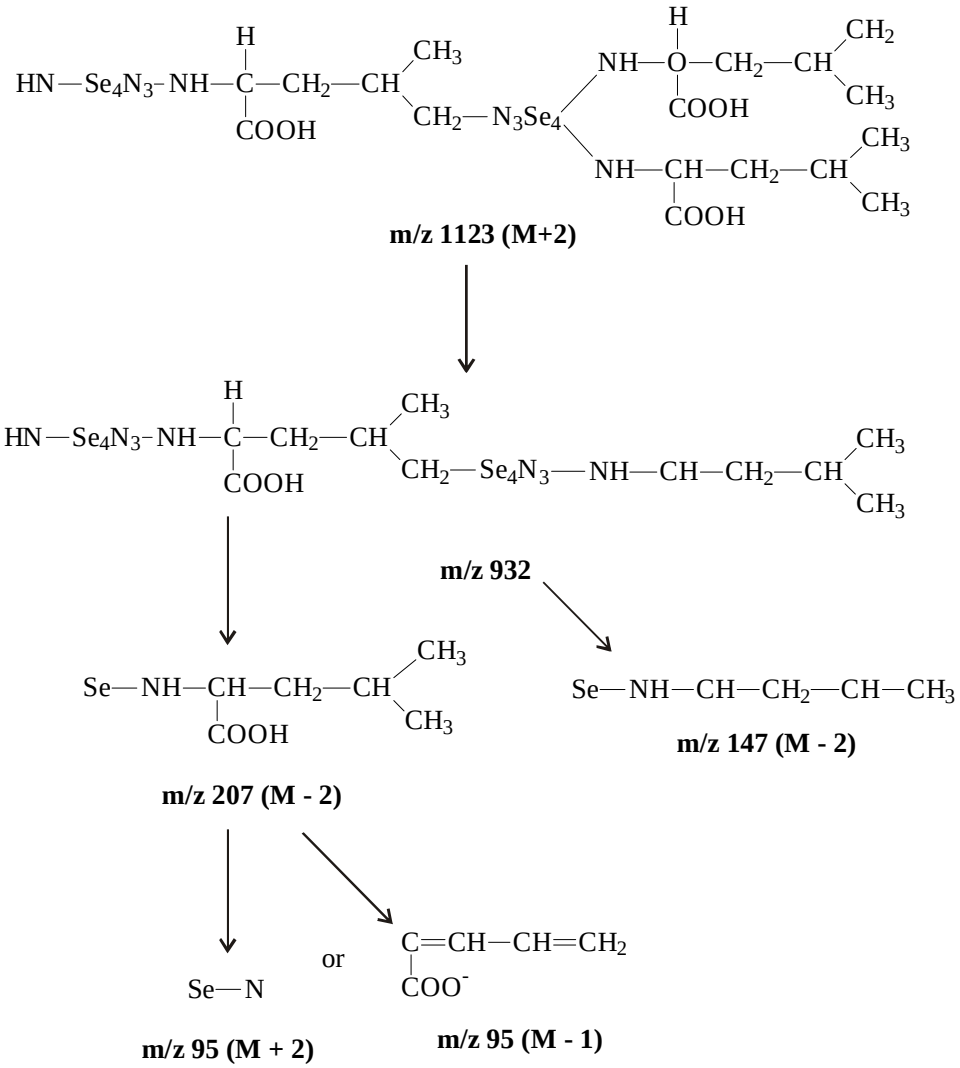
RESULTS AND DISCUSSION

The reaction product is yellowish orange solid, soluble in benzene. On the basis of quantitative estimation, % found (Cal.) Se 56.248 (56.348), N 12.456 (12.489), C 19.223 (19.269), O 8.543 (8.564), H 3.292 (3.301) and molecular weight 1120.6 (1121.0) g/mol. the adduct has been assigned as HN- $(Se_4N_3)_2$-(NH-CH-COOH-CH_2-CH $(CH_3)_2)_3$, which is supported by the prominent mass line at m/z 1123 (M+2) in its mass spectrum (Fig. 1).

The other mass lines in the mass pattern may be explained by FAB fragmentation process as follow:



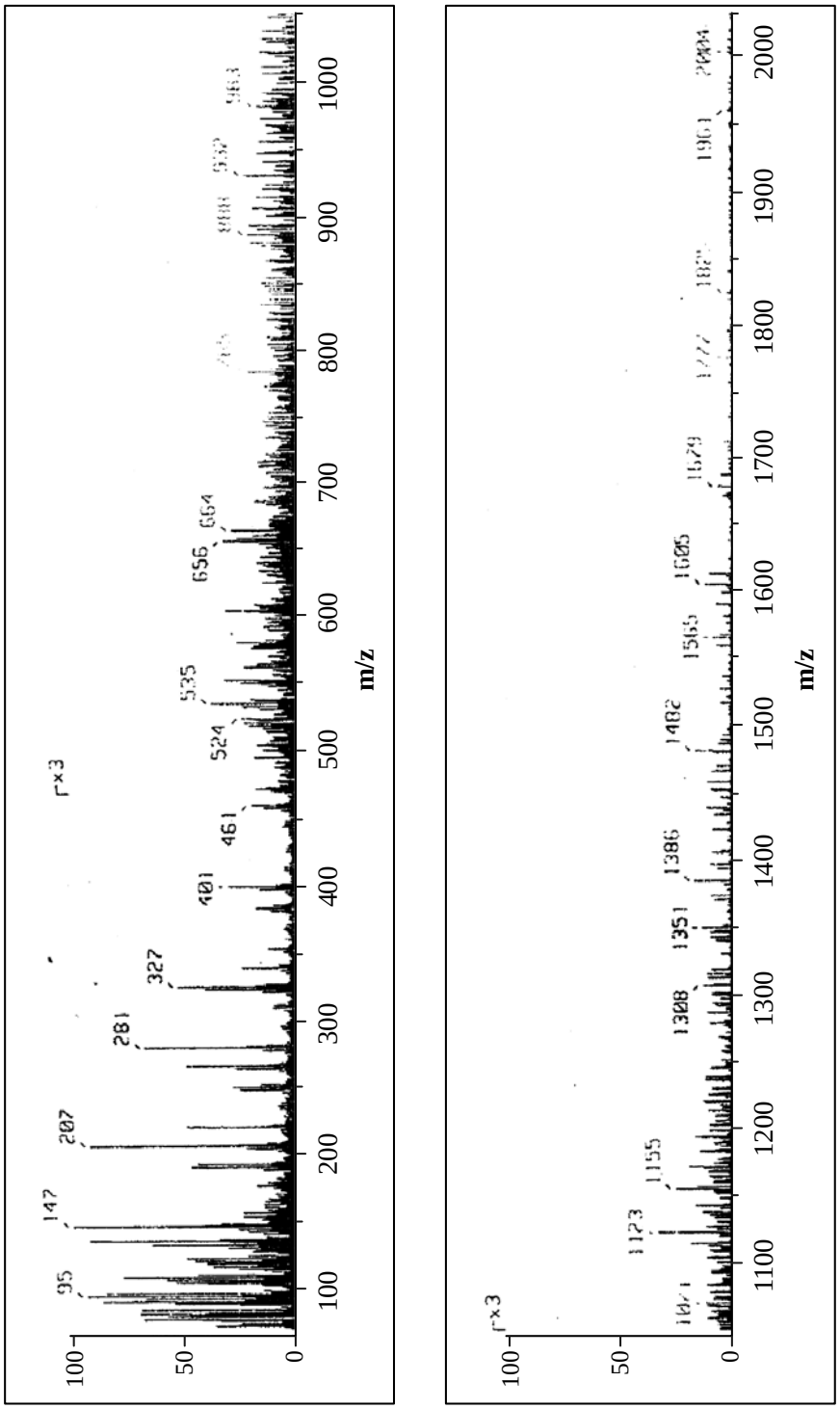
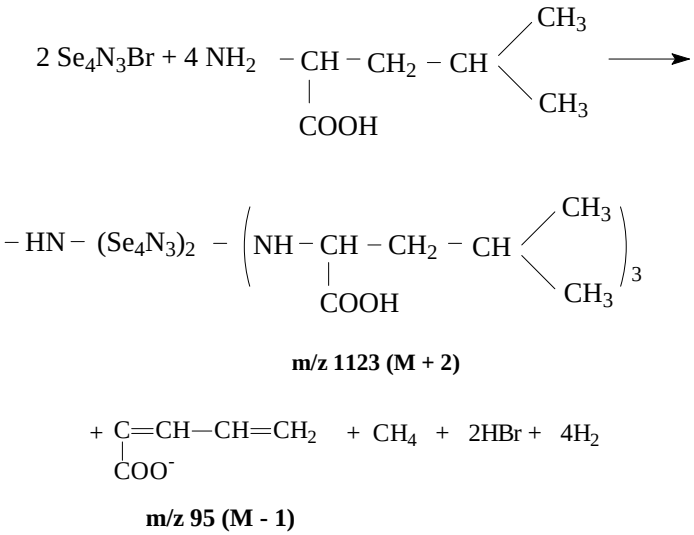


Fig. 1: Mass spectrum of Adduct

From this mass spectrum, it is proved that Se_4N_3Br and L-Leucine has reacted in 1 : 3 ratio according the following reaction.



Scheme 1

The formation of the product is also confirmed by the vibration observed in its IR spectrum (Fig. 2, Table 1) compared to that of Se_4N_3Br.

Table 1: I.R. Spectral Data of the adduct

S. No.	Vibrations cm^{-1}		Bands assigned (c)	Force constant K × N. (d)
	Ligand (a)	Product (b)		
1	670.2	543.3	Se-N	2.075
2	761.2	579.8	Se-N	2.363
3	929.8	647.5	Se-N	2.9471
4	1043.8	729.8	Se-N	3.744
5	1215.5	761.5	Se-N	4.077
6	1422.0	803.1 (s)	Se-N	4.534

Cont…

S. No.	Vibrations cm^{-1}		Bands assigned (c)	Force constant K × N. (d)
	Ligand (a)	Product (b)		
7	1520.0	944.6 (s)	Se-N	6.2735
8	1652.1	940.7 (s)	Se-N	6.22182
9	2360.9	1105.6 (s)	C-O	4.955
10	3020.5	1212.1 (s)	CH_3	0.8012
11	3417.8	1400.9 (s)	CH_3	1.070
12	3620.8	1524.6	C-C	8.241
13	3684.9	1577.3 (b,d)	Se-N	17.49
14		1703.0 (b,d)	COOH	11.756
15		1956.0 (b,w)	Se-N	26.90
16		2339.5	Se=N	38.4823
17		2362.2	Se=N	39.2327
18		3160.9 (b)	N-H	5.449

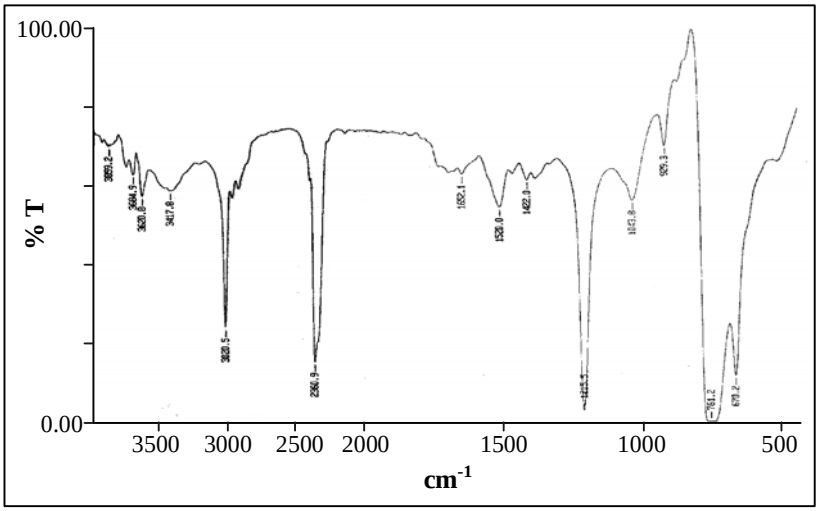


Fig. 2(a): IR Spectrum of Ligand (Se_4N_3Br)

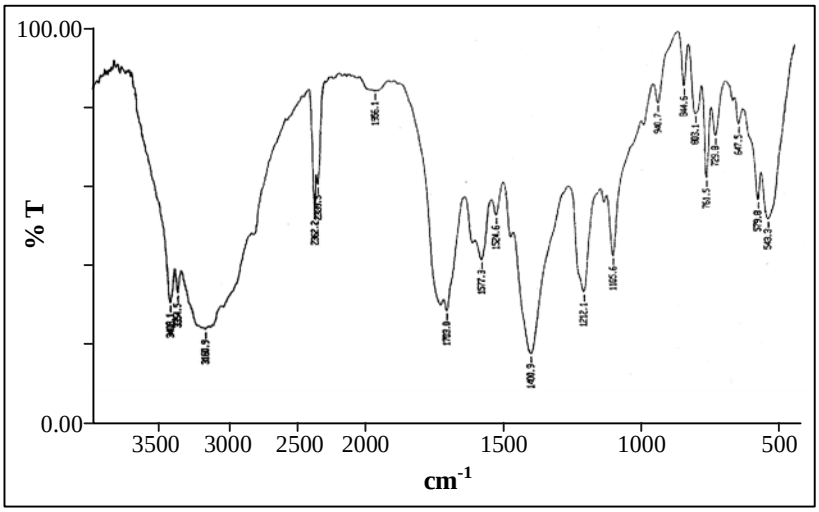
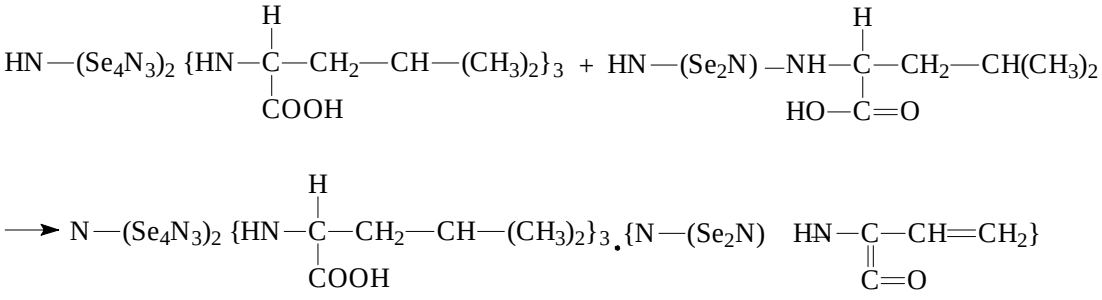


Fig. 2(b): IR Spectrum of Adduct

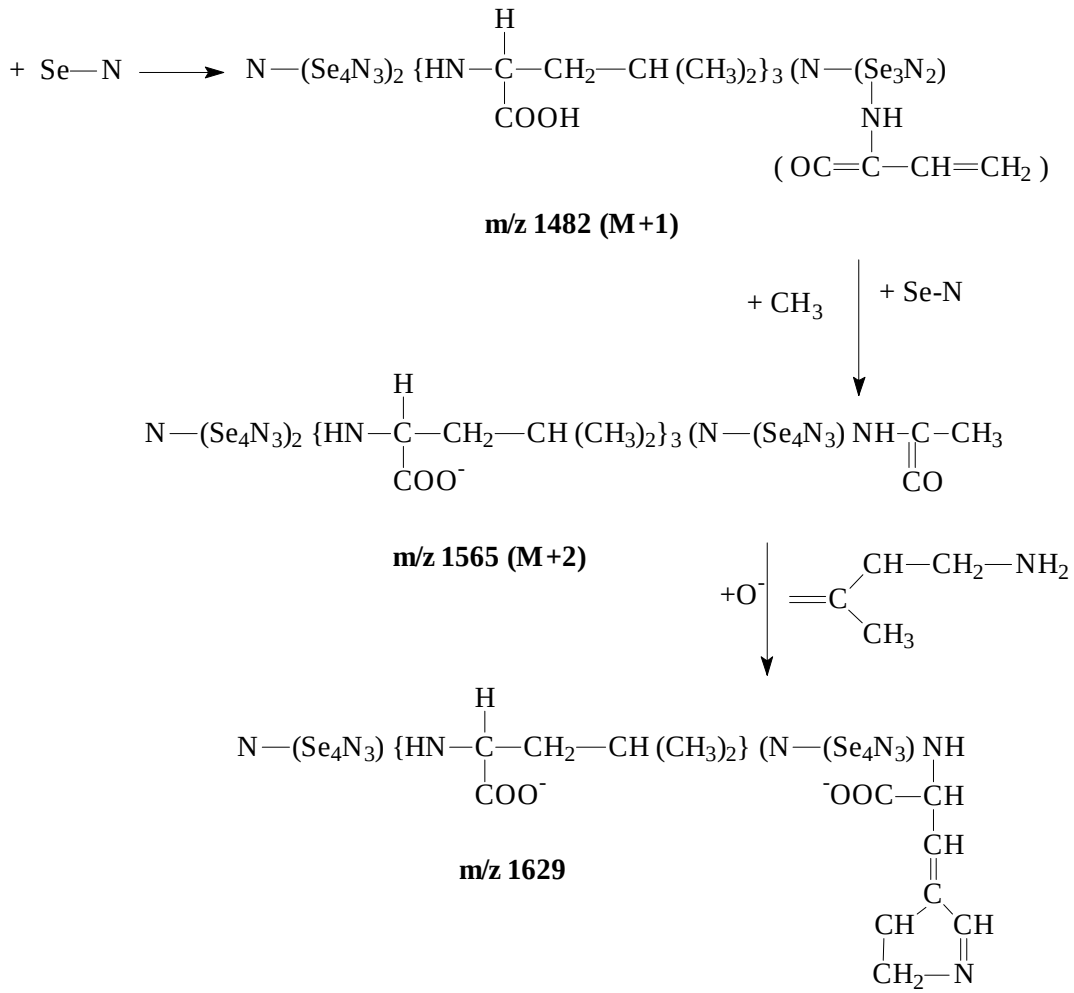
The appearance of other mass lines at m/z 1386, 1482, 1507 and 1629 in its mass pattern may be impounded on the basis of recombination of Leucine phosphazanide and other fragments formed as follows:

The vibrations appeared in I.R. spectrum (Fig. 2, Table 1) at 543.3 cm^{-1}, 579.8 cm^{-1}, 647.5 cm^{-1}, 729.8 cm^{-1}, 761.5 cm^{-1}, 803.1 cm^{-1}, 944.6 cm^{-1}, 940.7 cm^{-1} are for the Se-N bands while the vibration 1105.6 cm^{-1} for C-O band and 1212.1 cm^{-1}, 1400.9 cm^{-1} for CH_3 group, 1524.6 cm^{-1} for C-C band and 1703.0 cm^{-1} for COOH group, 3160.9 cm^{-1} for C-H band and 3354.5 cm^{-1}, 3408.1 cm^{-1} for N-H band, of the L. Leucine amino acid, showing its presence and linkage in the adduct alongwith $Se_4N_3^-$ion.

The results revealed that Se_4N_3Br has reacted with L-Leucine an amino acid with formation of adduct and eliminating HBr during their reaction as mentioned Scheme 1.



m/z 1386 (M - 2)



Scheme 1

The presence of Se – N and Se = N bands in Se_4N_3 ring is also inferred by the values of force constants (Table 1), calculated from the frequencies appear in its I.R. spectrum.

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