

The Behavior of Benzo[*b*]tellurophene under Electron Impact as Compared with its Sulfur and Selenium Analogs

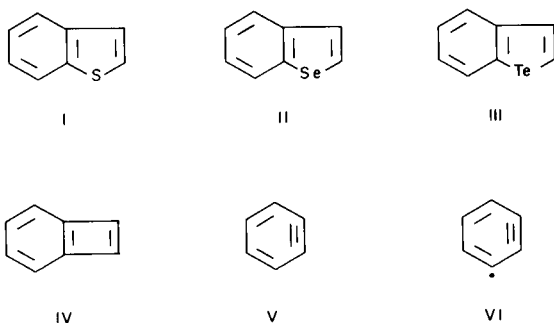
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Benzo[*b*]tellurophene (III) is the elusive isolog of benzo[*b*]thiophene (I) and benzo[*b*]selenophene (II) for which an accessible route was recently reported from one of our laboratories (1). It was of interest to compare the pattern of its fragmentation under electron impact with those recently reported by Porter (2) for compound I and by ourselves (3) for compound II. Such an investigation could be expected, firstly to give information on the



relative stability of the heterocyclic system III, and secondly to provide additional proof for the structures previously postulated for the main hydrocarbon fragments from I and II.

The mass spectrum of benzo[*b*]tellurophene (Fig. 1) is remarkably simple. The base peak corresponds to a detellurated species, probably benzocyclobutadiene (IV) ($m/e = 102$), which, as expected from earlier studies (3,1), loses ethylene to give the benzyne species V ($m/e = 76$) and its dehydrogenation product VI ($m/e = 75$). Another recognizable detellurated species is the ion VIII ($m/e = 63$) which, on the grounds of what had earlier been observed in the benzo[*b*]thiophene series (2), could be considered as arising from the bicyclic ion VII ($m/e = 89$) by loss of ethylene (here, the $m/e = 89$ peak is also present though less important). Direct extrusion of ethylene from III

leading to the bicyclic species IX, however slight, is distinctly recognizable by a series of small peaks corresponding to the most frequent isotopes of tellurium (especially $m/e = 206$ and $m/e = 204$, corresponding to ^{130}Te and ^{128}Te , respectively); the lower degree of stability of the tellurophene moiety in compound III as compared with the thiophene and selenophene moieties in I and II is evidenced by the much lesser prominence of the peak $M-C_2H_2$ here. All these fragmentation pathways were encountered in the mass spectra of benzo[*b*]thiophene and benzo[*b*]selenophene, and their presence here lends further support to the earlier postulated structures for the various fragments observed (3,1). Table I lists the metastable peaks observed for compound III.

TABLE I

Metastable Peaks

Transition	$m.^* \text{ calcd.}$	$m.^* \text{ found}$
$M(^{130}\text{Te}) \rightarrow \text{(IV)}$	45.3	broad peak from 45.3 to 47
$M(^{128}\text{Te}) \rightarrow \text{(IV)}$	45.7	
$M(^{126}\text{Te}) \rightarrow \text{(IV)}$	46.0	
$M(^{125}\text{Te}) \rightarrow \text{(IV)}$	46.2	
$\text{(IV)} \rightarrow \text{(V)}$	56.5	56.5
$\text{(V)} \rightarrow \text{(VI)}$	74	74

A feature of the electronolysis of benzo[*b*]tellurophene indicating that this heterocyclic system nevertheless enjoys a fair degree of stability, is the importance of the singly-charged molecular ions and the presence of doubly-charged ones, the most prominent of these peaks corresponding to the five most abundant isotopes (^{130}Te , ^{128}Te , ^{126}Te , ^{125}Te , and ^{124}Te). Table II records the peaks corresponding to the various tellurium-bearing ions which could be observed.

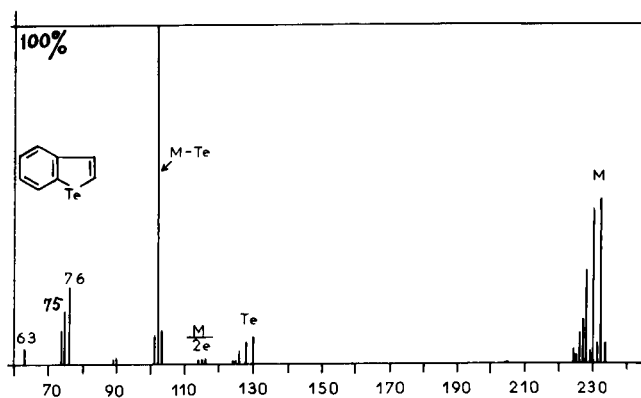
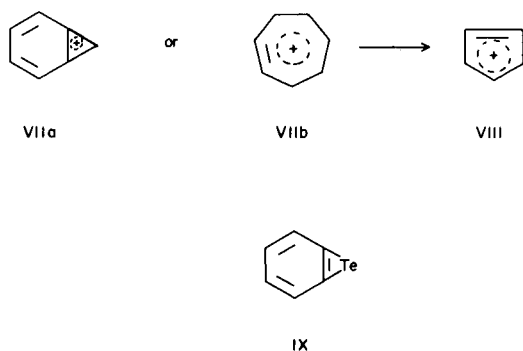


Figure 1.



The mass spectra were taken on an Atlas CH-4 spectrometer (70 eV) with direct introduction at 100°. We thank Mr. G. Bèrenger of the Department of Mass Spectrometry of this Institute (Director, Dr. B. Das) for his help.

TABLE II
Tellurium-containing Ions

M/e	% of base peak
233	6
232	49.3
231	6.7
230	46.5
229	4
228	28
227	13.3
226	9.33
225	2.6
224	4.2
206 (a)	~ 0.8
204 (a)	~ 0.5
130	7.35
128	6.7
126	4
125	~ 1
124	~ 1
116	2.65
115	2.5
114	1.9

(a) Corresponding to the species IX derived from ^{130}Te and ^{128}Te .

REFERENCES

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