

The Mass Spectrum of 5-Phenyl-1,3,4-oxathiazol-2-one

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IN the course of preparative work with trichloromethanesulphenyl chloride it was found that the reaction of either trichloromethanesulphenyl chloride or *N*-trichloromethanesulphenylbenzamide with benzamide in boiling dioxan

affords a product $C_8H_5NO_2S$ (m.p. 68.5—70°, b.p. 140—145°/10 mm. Hg)* the structure of which can be conveniently deduced by means of mass spectrometry.

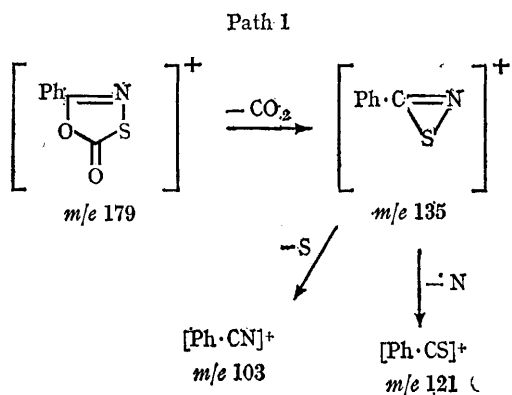
Apart from the usual aromatic fragmentation

* The details of our synthetic work with the 1,3,4-oxathiazol-2-ones will be included in a forthcoming publication.

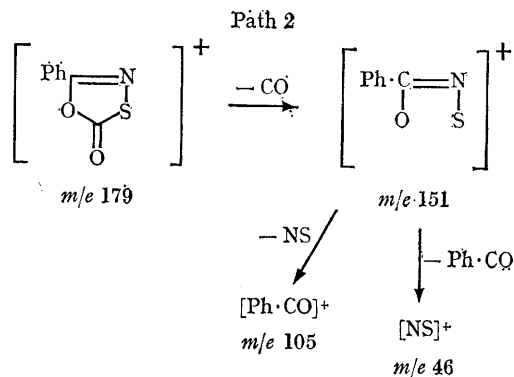
pattern the following peaks can be identified (the sulphur-containing fragments show the expected isotopic pattern due to ^{34}S):

| <i>m/e</i> | Formula | % |
|------------|---|-----|
| 179 | $[\text{C}_8\text{H}_8\text{NO}_2\text{S}]^+$ | 80 |
| 151 | $[\text{C}_7\text{H}_8\text{NOS}]^+$ | 3 |
| 135 | $[\text{C}_7\text{H}_8\text{NS}]^+$ | 31 |
| 121 | $[\text{C}_7\text{H}_8\text{S}]^+$ | 3 |
| 105 | $[\text{C}_7\text{H}_8\text{O}]^+$ | 100 |
| 103 | $[\text{C}_7\text{H}_8\text{N}]^+$ | 38 |
| 46 | $[\text{NS}]^+$ | 40 |
| 32 | $[\text{S}]^+$ | 22 |

It appears that the fragmentation mainly follows two paths, initiated by the loss of either CO_2 or CO (Paths 1 and 2).



Thus, the key fragment in Path 1 appears to be the ion $[\text{C}_7\text{H}_8\text{NS}]^+$ which probably must be formulated as 3-phenylthiazirine rather than benzonitrile sulphide. The preferred breakdown



of this species is by loss of sulphur yielding the rather stable benzonitrile ion $[\text{C}_7\text{H}_8\text{N}]^+$, while the loss of nitrogen with formation of the thiobenzoyl ion $[\text{C}_7\text{H}_8\text{S}]^+$ is a minor (somewhat unexpected) competing reaction.

The most interesting fragment due to Path 2 is the thionitrosyl ion $[\text{NS}]^+$ at m/e 46.

The mass spectrum was recorded on an Atlas CH 4 apparatus.

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