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NOTE

Mass Spectra of Some 3-β-Bromoethyl-1,2-Benzisoxazoles

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Fragmentation pattern of some 3-β-bromothyl-1,2-benzisoxazole is studied.

Key Words: Mass Spectra, 3-β-Bromoethyl-1,2-Benzisoxazole.

The mass spectra of isoxazole[1], alkyl isoxazole[2], benzisoxazole[3] have been studied extensively. In connection with our earlier work an 3-β-bromoethyl-1,2-benzisoxazoles[4], the present paper deals with the primary fragmentation of some 3-β-bromoethyl-1,2-benzisoxazoles.

Mass spectra were taken on instrument VG 70–70 H. The 2-bromoethyl-1,2-benzisoxazoles were prepared by reported procedure[4].

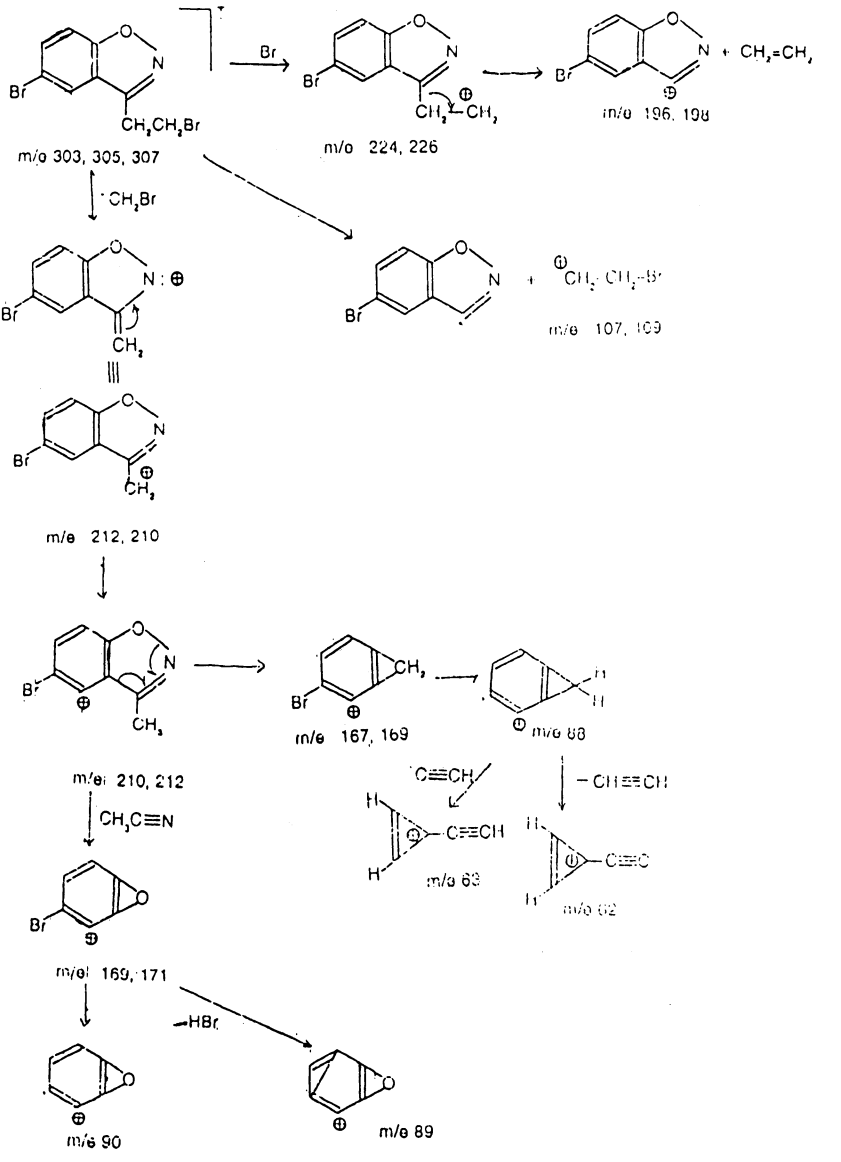
Isotope abundance of spectrum indicates the presence of two bromine atoms (M^+ 303, M^{+2} 305, M^{+4}4 307); peaks at m/e 226, 224 indicate that molecular ion loses bromine atom as radical; this corresponds to base peak (100%) and almost equal in intensity which is an indication of one more bromine atom; peak at m/e 198, 196 indicates elimination of ethylene from base peak.

Peak at m/e 212 and 210 is formed with the loss of CH_2Br from molecular ion, which on hydrogen transfer to methylene group undergoes loss of neutral molecule methyl cyanide to give peaks at m/e 171, 169. The same fragment (m/e 212, 210) also loses cyanic acid and gives the ion at m/e 169, 167 which further loses bromine as radical and gives the fragment ion at m/e 88. The decomposition of even electron ion to yield an odd electron ion to yield an odd electron ion and radical is unusual but due to the presence of bromine strongly electron attracting atom it gives odd electron ion and radical[5] **(Scheme-1).**

Peak at m/e 109, 107 corresponds to $^+CH_2CH_2Br$. Peak at m/e 63 and m/e 38 corresponds to cyclopropyl acetylenic cation and cyclopropyl cation respectively. Peak at m/e 89 is due to loss of HBr for m/e 169, 171.

The mass spectrum of 5,7-dichloro-3-β-bromoethyl-1,2-benzisoxazole, **(Scheme-2)** is very similar to that of **I**. Isotope abundance of spectrum II indicates the presence of two chlorine atom and one bromine atom.

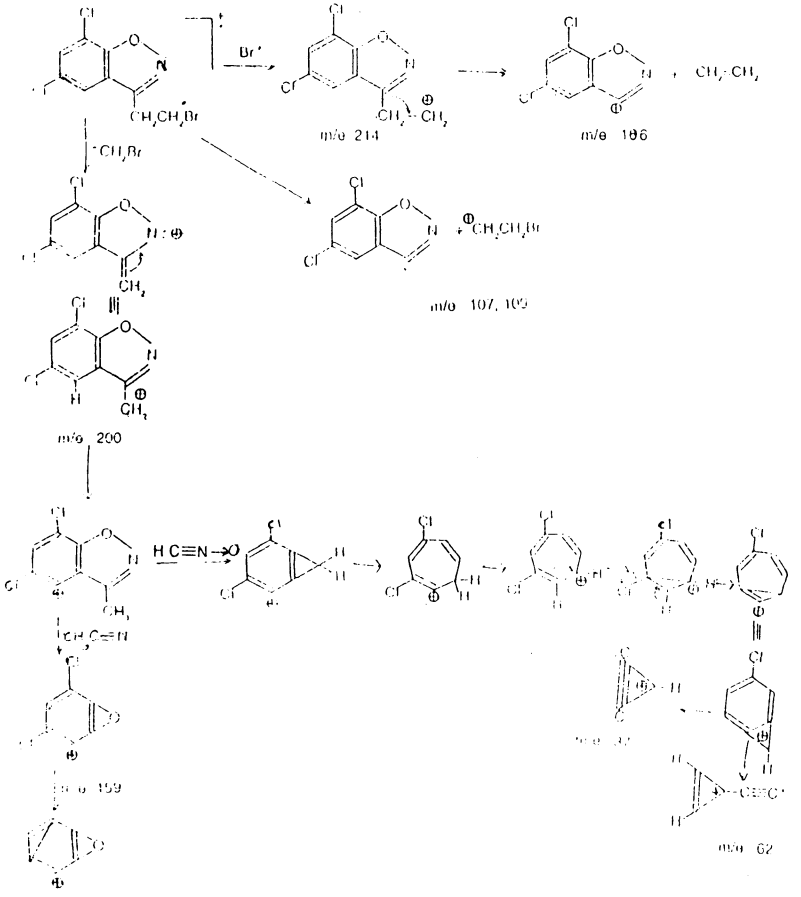
Peak at m/e 214 is the base peak formed after losing bromine radical from molecular ion, which subsequently undergoes elimination of ethane to give



Scheme-1. Mass fragmentation pattern of 5-bromo 3-β-bromo ethyl-1,2-benzisoxazole

isoxazole fragment. Molecular ion also undergoes elimination of CH_2Br to give a stable fragment ion at m/e 200 which undergoes elimination of cyanic acid to give peak at m/e 158.

Peak at m/e 109, 107 corresponds to $^{+}CH_2CH_2Br$ fragments which are almost equal in intensity. Peaks at m/e 62 and at m/e 37 are due to cyclopropyl acetylenic fragment ion and cyclopropyl cation.

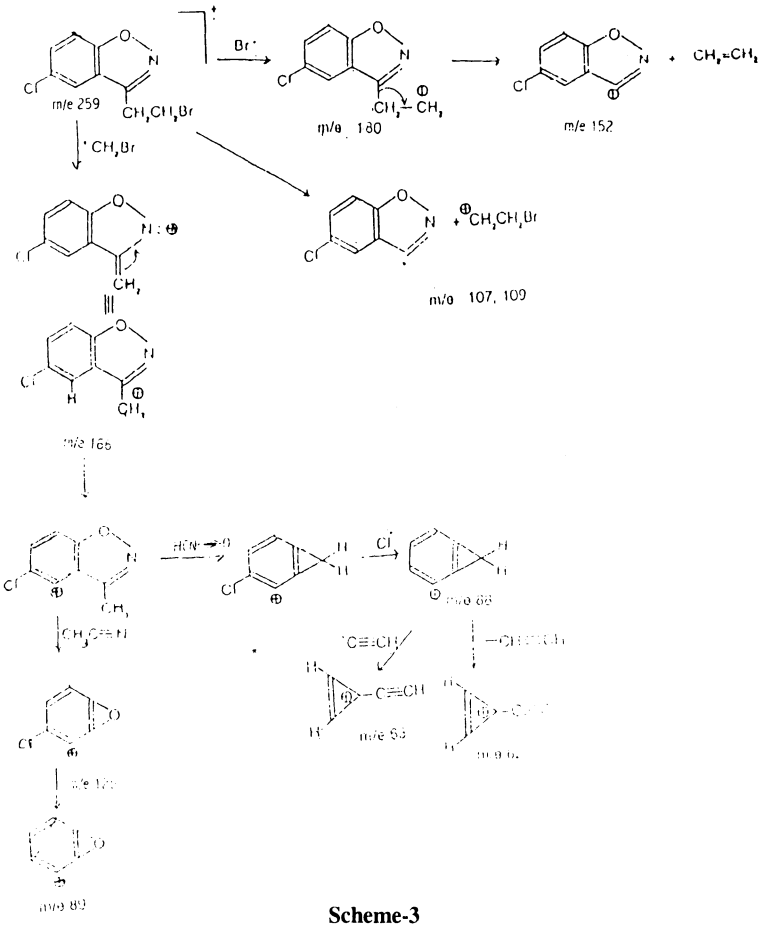


Scheme-2. Mass Fragmentation pattern of 5-7-dichloro 3-β-bromo ethyl 1,2-benzisoxazole.

The mass spectrum of 5-chloro 3-β-bromo ethyl 1,2-benzisoxazole **(Scheme-3)** also shows the same fragmentation pathway as discussed earlier for I and II.

MASS SPECTRA OF ISOXAZOLES

Sr.No.	Isoxazole	m/e
1.	5 bromo-3-β bromoethyl 1,2 benzisoxazole	303 (M^+), 305 (M + 2) 307 (M + 4), 224 (100%), 226 (95%), 212 (13%), 210 (12.8%), 198 (12%), 196 (9–8%), 167 (9.5%), 109 (41%), 107 (25%), 88 (18%), 63 (78%), 62 (42%), 38 (22%)
2.	5,7 dichloro 3-β bromo ethyl 1,2 benzisoxazole	295 (M^+), 214 (100%) 216 (67%), 200 (10%), 187 (10%), 158 (13%), 109 (50%), 107 (48%), 88 (39%), 62 (31%), 37 (10%)
3.	5 chloro 3-β bromo ethyl 1,2 benzisoxazole	259 (M^+), 180 (100%), 182, 166 (25%), 152 (15%), 139 (25%), 109 (42%), 107 (50%), 88 (25%), 63 (49%), 62 (31%), 37 (81%)



Scheme-3

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