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NOTES

The Mass Spectra of Some of Substituted Tetrahydroquinoxaline Compounds

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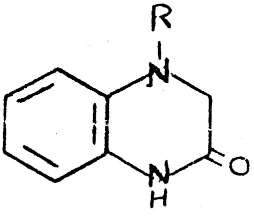
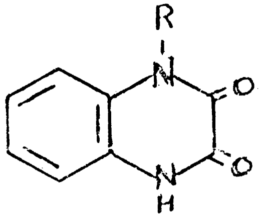
In the present notes, the authors have described the electron impact mass spectra of the N-substituted tetrahydroquinoxaline compounds.

The mass spectra of some heterocyclic compounds containing two nitrogen atoms have been reported[1,2] but little has appeared concerning quinoxaline compounds. Lately the mass spectra of some quinoxaline derivatives have been reported[3-5] but no detailed record of the mass spectral fragmentation of this useful class of compounds has been reported so far. In present communication we have investigated the electron impact mass spectra of the N-substituted derivative of 2-oxo (1–3) and 2,3-dioxotetrahydroquinoxaline (4–6). All compounds display an intense molecular ion signal. The fragmentation pattern of all the oxo compounds is almost identical and it is true in case of dioxo compounds. A notable feature in the spectrum is the observation of peak at m/e 149 (62.50) which appear to have resulted from m/e 176 by the loss of HCN. This feature is common to other dioxoquinoxaline derivatives which has not been observed in mono-oxo-quinoxaline derivatives. The relative abundance of some of the significant ions in mass spectra of these compounds is given in Table 1.



1. $R=CH_2COOCH_3$
2. $R=CH_2COOH$
3. $R=CH_3$



4. $R=CH_2COOCH_3$
5. $R=CH_2COOH$
6. $R=CH_3$

TABLE 1
RELATIVE ABUNDANCE (% BASE PEAK) OF IMPORTANT FRAGMENT IN THE 70-eV EI MASS SPECTRA OF COMPOUNDS 1–6

Type of ion	1	2	3	4	5	6
$[M]^+$	220(82.50)	206(68.55)	162(100)	234(85)	220(25)	176(100)
a	191(46.89)	176(62.89)	148(42)	206(68.00)	176(34)	160(29)
b	161(100)	161(65.40)	147(43)	202(61.70)	161(82.95)	148(84.21)
c	146(65.07)	146(95.59)	146(49)	175(63.82)	149(62.50)	147(84.21)
d	133(90.81)	134(67.29)	133(90.47)	162(61.70)	147(64.77)	134(77.63)
e	119(65.62)	133(67.29)	119(52.53)	147(97.87)	146(73.86)	130(71.05)
f	118(61.25)	131(100)	118(55.05)	134(56.73)	135(76.13)	118(88.15)
g	92(51.25)	118(81.76)	105(37.14)	119(100)	133(100)	104(60.52)
h	91(58.87)	104(38.36)	104(36.00)	104(47.87)	119(67.04)	93(76.31)
i	77(49.37)	91(58.49)	92(60.47)	92(65.24)	105(59.09)	69(97.36)
j	65(65.62)	77(56.60)	65(52.85)	77(73.75)	91(68.18)	64(93.42)
–	–	65(76.10)	–	64(73.04)	64(98.86)	–
Base peak	161[a]	131[b]	169[c]	119[d]	135[e]	176[f]

[a] $[C_9H_9N_2O]^+$ [b] $[C_8H_7N_2]^+$ [c] $[C_9H_{10}N_2O]^+$ [d] $[C_7H_7N_2]^+$ [e] $[C_7H_5N_2O]^+$
[f] $[C_9H_8N_2O_2]^+$

Mass spectra were recorded on an AEI-MS-30 instrument equipped with a direct ionizing voltage inlet system at 70 CV, on ion source temperature of 250° at 1 to 2×10^{-6} torr. Compounds 1–6 have been synthesized previously.

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