Studies in Mass Spectrometry. Singly- and Doubly-charged Molecular Ions; Stability and Abundance

By E. S. WAIGHT

(Organic Chemistry Laboratories, Imperial College of Science and Technology, London, S.W.7)

Summary Attention is drawn to a doubly-charged molecular ion of higher abundance than that of the singlycharged ion.

SOLOMON and MANDELBAUM in a communication of the above title¹ have claimed the first example of a compound giving on electron impact a doubly-charged molecular ion of higher abundance than the singly-charged ion. In fact, a previous case has been reported.² 1-o-Nitrophenylanthra-9,10-quinone gives a doubly-charged molecular ion $(m/e \ 164.5)$ about three times as intense as the singly-charged ion $(m/e \ 329)$, (I), at an ionizing voltage of 70 ev. The weakness of the peak at $m/e \ 329$ may be attributed to the ready displacement of the o-nitro-group by electron-deficient oxygen to give the ion $m/e \ 283$, (II). It is conceivable that in the ion $m/e \ 164.5$ the two positive charges are located as far apart as possible, *i.e.* on the terminal

 $O_{2}N \xrightarrow{O_{+}} O_{+} \xrightarrow{O_{2}N} \overbrace{O}^{+} O_{+}$ $m/e 329 \qquad m/e 283$ (I)
(II)

benzene rings, rather than on the oxygen atoms, thus diminishing the probability of loss of the nitro-group.

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¹ M. Solomon and A. Mandelbaum, Chem. Comm., 1969, 890.

² E. S. Waight, "Some Newer Physical Methods in Structural Chemistry," ed. R. Bonnett and J. G. Davis, United Trade Press London, 1967, p. 67.