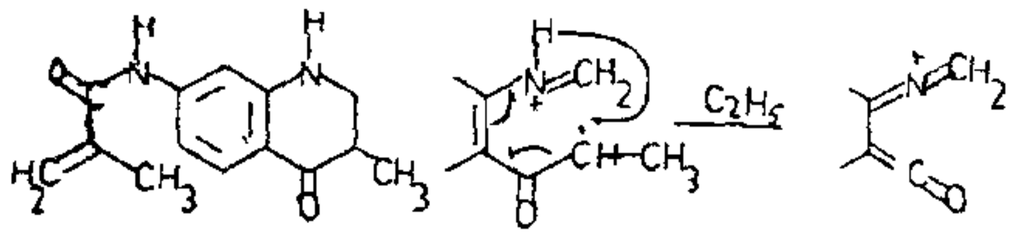
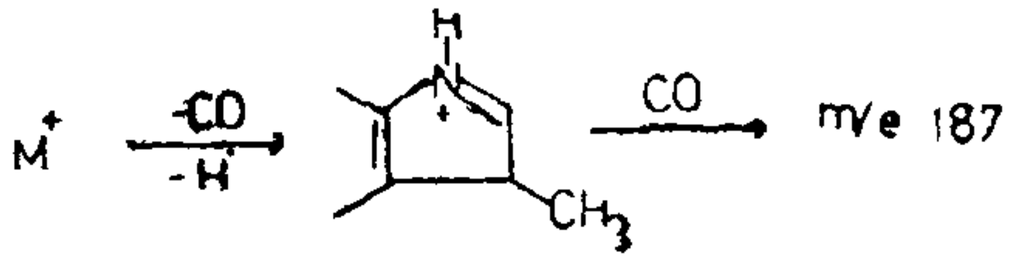
MASS SPECTRAL FRAGMENTATION PATTERN OF SOME COMPOUNDS OBTAINED BY REACTION OF PHENYLENEDIAMINES WITH ACRYLIC ACIDS

IN a previous communication[1] we have reported the formation of some new nitrogen heterocycles obtained by the reaction of phenylenediamines with acrylic and methylacrylic acids in the presence of PPA. The structures of these compounds were assigned on the basis of their spectral analytical evidence. Their mass spectra apart from giving the molecular weights present some interesting fragmentation patterns which are discussed here.

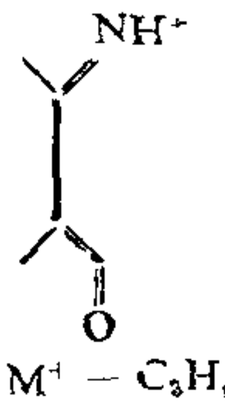
The mass spectrum of I, (M 244) shows a peak at m/e 229 ($M-CH_3$) and at m/e 201 due to loss of carbon monoxide. Further, I undergbes α cleavage as shown followed by loss of C_2H_5 to give a fragment corresponding to m/e 215 which loses CO to give the peak at m/e 187.



Alternatively, the fragmentation could occur as follows.



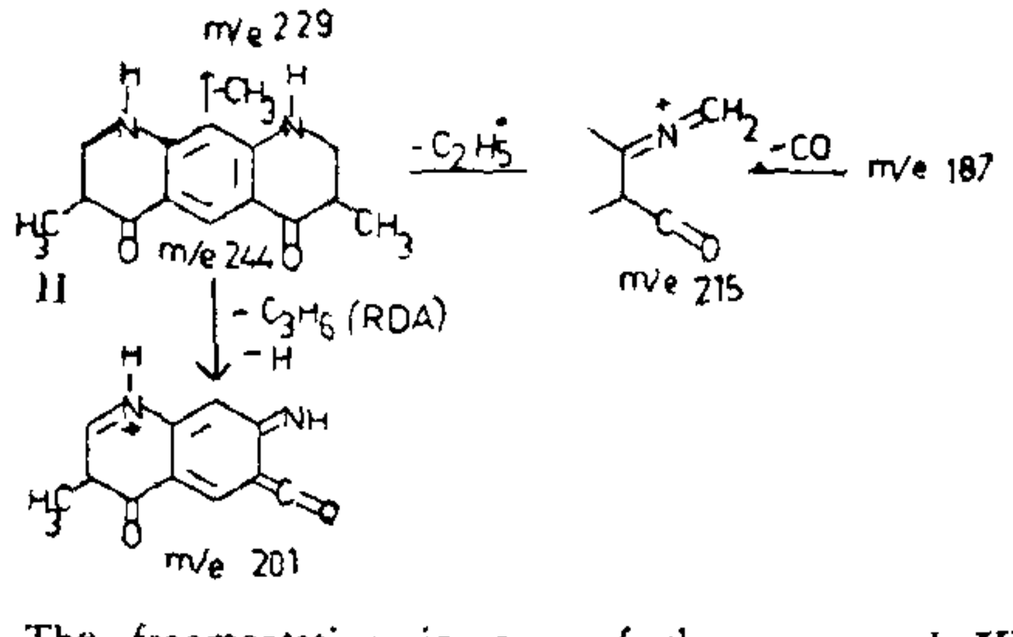
A retro Diels Alder reaction possibly occurs giving NH^+ which by loss of H° accounts for the peak at



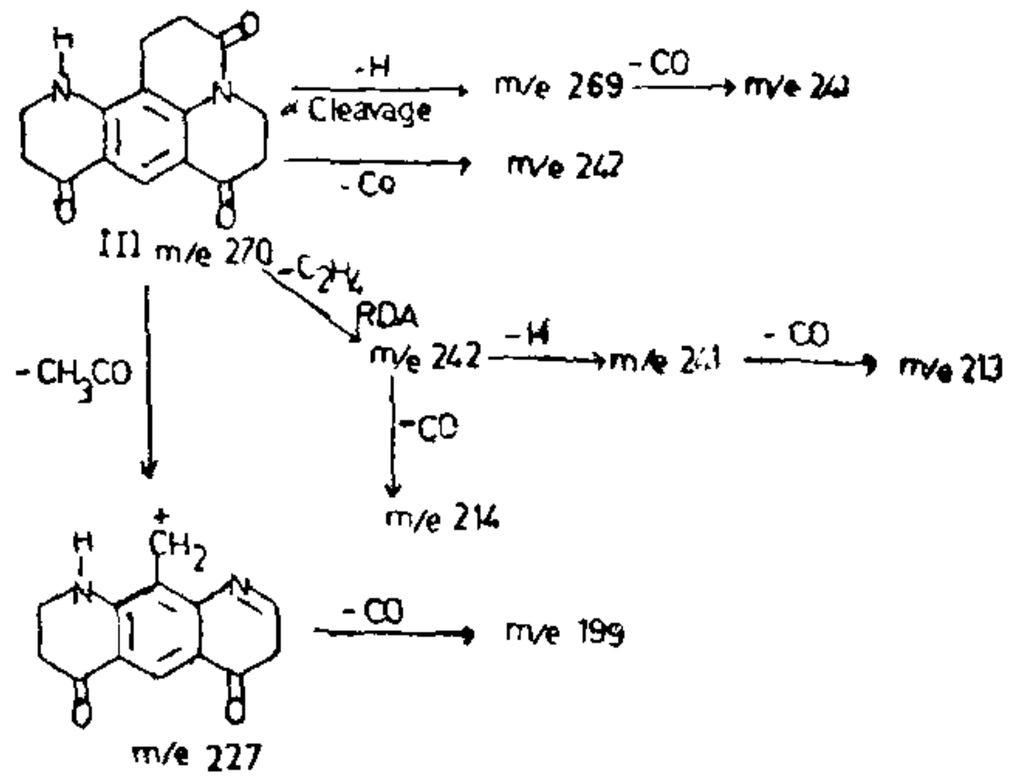
$M^+ - C_3H_5$

m/e 201 which on loss of CO gives the peak at m/e 172 and loss of $CH_2^\bullet$ gives m/e 187. The peak at m/e 69 corresponds to the fragment $CH_3-\underset{\underset{CH_2}{\|}}{C}-CO$ which eliminates CO to give the C_3H_5 peak (m/e 41).

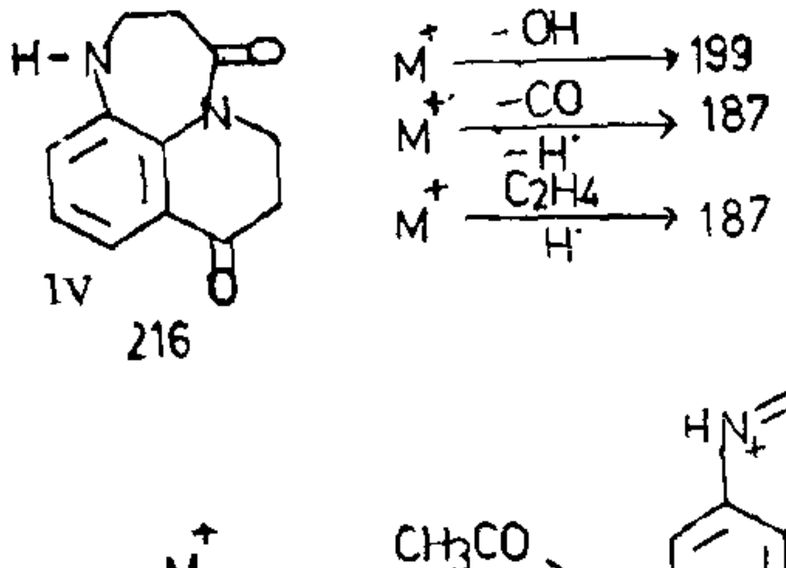
The appearance of the various peaks in the mass spectrum of II could be rationalised by the following fragmentation pattern,

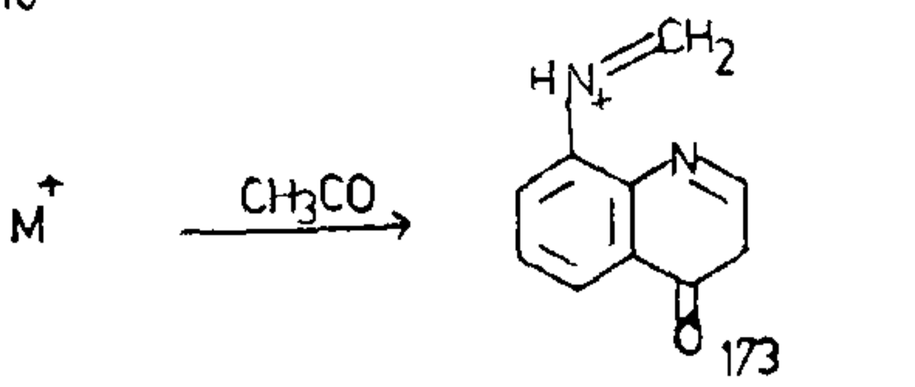


The fragmentation in case of the compound III could be explained as indicated below :



In the case of the compound IV the following fragmentation scheme could be envisaged.





Thanks are due to Professor H. Budzikiewicz, W. Germany, for the mass spectra.

Institute of Science, J. R. MERCHANT.
Bombay 400 032,
January 20, 1978.

1. Merchant, J. R. and Chothia, D. S., *Indian J. Chem.*, 1975, **13**, 814.