

## NOTES

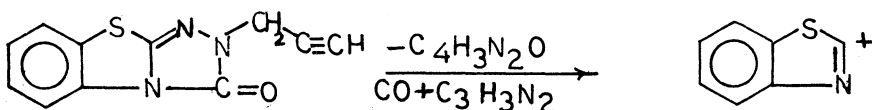
## Mass Spectral Fragmentation of 2N-Propargyl (1,2,4)- Triazolo (3,4-b)-Benzothiazol-3-One

MRS. M.V. DESHMUKH

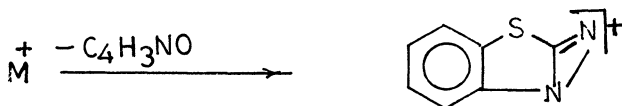
*Department of Chemistry,  
Science College, Nanded 431 602, India*

An interesting mass spectral fragmentation of 2N-propargyl (1,2,4)-triazolo (3,4-b)-benzothiazole is discussed. In one of the pathways retro Diels Alder fission is reported.

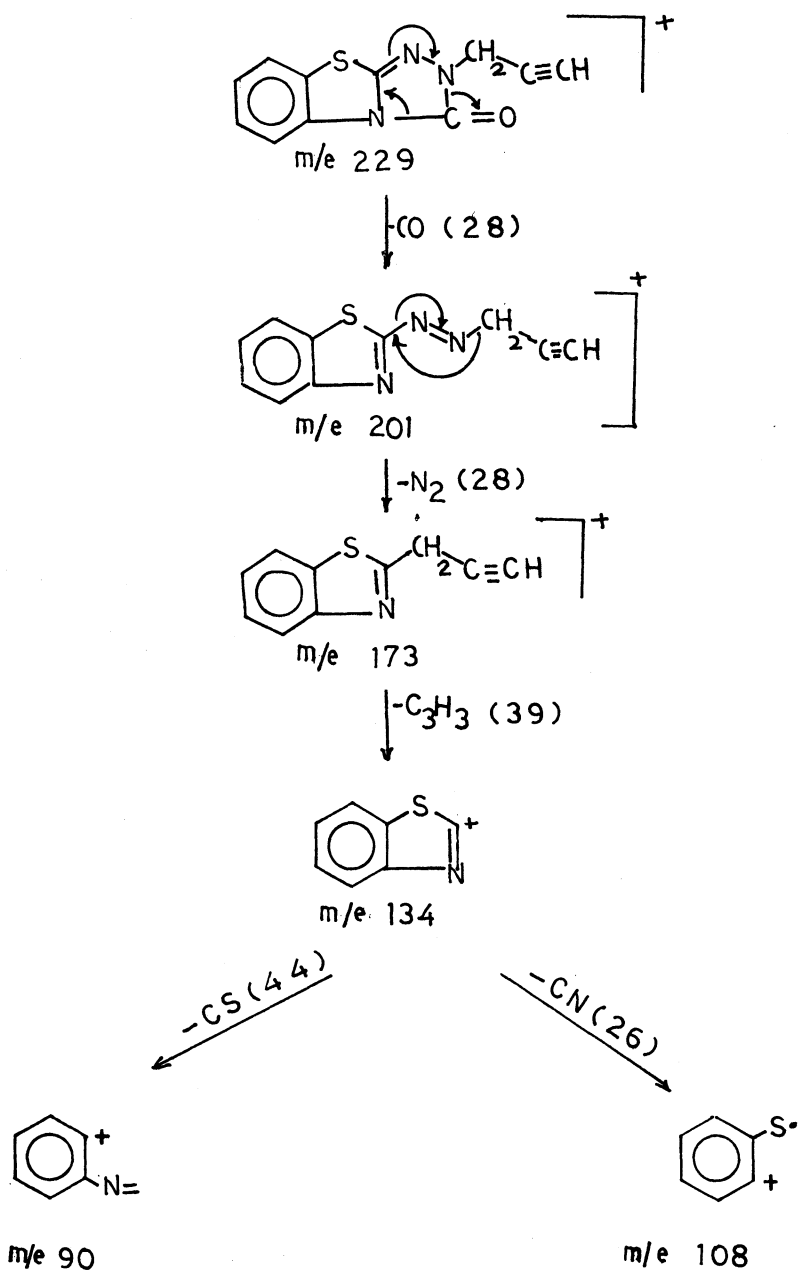
The mass spectral fragmentation of 2N-propargyl (1,2,4)-triazolo (3,4-b)-benzothiazol-3-one<sup>1</sup> is quite complex and does not follow the general pattern of fragmentation under electron impact as exhibited by simple (1,2,4)-triazolo (3,4-b)-benzothiazole<sup>2</sup>. The molecular ion peak is in 75% abundance. The elimination of -CN' or CS' in the first step appears to be logical which is also observed with simple triazole<sup>3</sup>. This process is found to be almost insignificant with the present compound. On the other hand loss of C<sub>4</sub>H<sub>3</sub>N<sub>2</sub>O involving the nitrogens at position 1 and 2 is reasonable. The propargyl substituent at 2N and C=O at 3 position yielded the peak m/e 134 which is very stable and is the base peak.



Loss of H-C=C- from molecular ion or from M-H ion is not observed. The second major fragmentation process is the formation of benzothiazoloazirine ion at m/e 148 from the molecular ion.

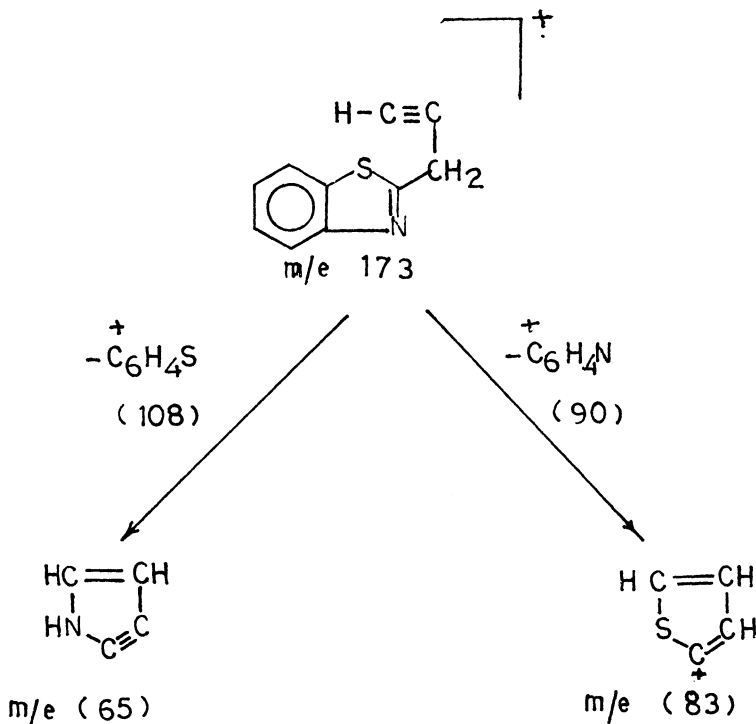


The peak at m/e 173 resulted from concentrated loss of C=O and N<sub>2</sub> by retro Diels Alder fission of the molecular ion together with the migration of propargyl group to the 2C. Subsequent elimination of propargyl ion yielded benzothiazole cation. The same on elimination of CN and CS gave m/e 108 and m/e 90 (Scheme I).



Scheme I

The ion  $m/e \ 170$  also can fission by another process leading to  $m/e \ 83$  and  $m/e \ 65$ . Scheme II.



Scheme II

### ACKNOWLEDGEMENT

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### REFERENCES

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