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THE MASS SPECTROMETRIC FRAGMENTATION OF *N*-BENZYLACETAMIDE

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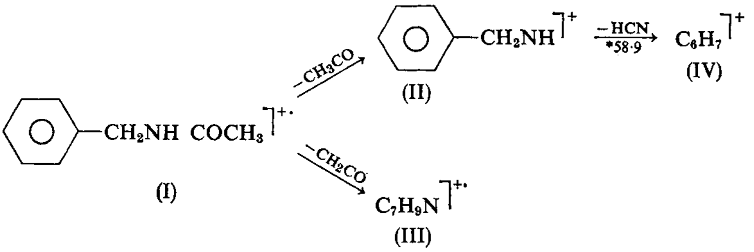
Abstract—The low energy mass spectra of *N*-benzylacetamide have been recorded. The major fragmentations of the molecular ion are similar to those observed in the acetanilide spectrum. In addition, the secondary dissociation of the $[C_6H_5CH_2NH]^+$ ion by loss of HCN is shown to occur with transfer of the -N—H hydrogen to the ring.

The recent interest shown in the mass spectra of acetanilide[1,2] has prompted us to investigate the mass spectrum of the *N*-benzylacetamide analogue (I).

At an electron energy of 14 eV, nominal, the major peaks present were: the molecular ion at *m/e* 149 (base peak) and peaks at *m/e* 106 $[M - CH_3CO]^+$ and *m/e* 107 $[M - CH_2CO]^{+\cdot}$ (Scheme 1). These fragmentations are similar to those found for acetanilide. Minor peaks (<0·5%) at *m/e* 92 $[M - 57]^{+\cdot}$ and *m/e* 91 $[M - 58]^+$ were also observed.



Scheme 1

Above electron energies of 18 eV the $[M - CH_3CO]^+$ ion undergoes a secondary decomposition involving loss of HCN (II → IV) with a metastable peak at 58·9 (calc. 58·88) to give the $C_6H_7]^+$ ion. The mass spectrum of the *N*-deuterated compound [*N* — [²H] — *N* — benzylacetamide] also shows a metastable corresponding to the loss of HCN from $C_6H_5CH_2ND]^+$ at *m/e* 59·8 (calc. 59·81). However, a metastable due to loss of DCN from the deuterated compound (calc. 58·32) was not observed, which indicates that the NH group hydrogen is not lost in the neutral species during this secondary decomposition.

EXPERIMENTAL

Spectra were measured with an AEI MS-12 mass spectrometer using an ion accelerating voltage of 8 kV and a direct insertion probe with a source temperature of 100 °C.

Benzylamine was acetylated using acetic anhydride at 5 °C to give *N*-benzylacetamide, which was recrystallised from water, m.p. 61 °C (Lit. 61 to 62 °C). The *N*-deuterated compound was prepared by successive recrystallisation of *N*-benzylacetamide from D_2O/K_2CO_3 solution.

REFERENCES

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