Note added in proof

## The behaviour of thiamine under electron impact

## B. BLESSINGTON AND D. W. MATHIESON

## Postgraduate School of Pharmaceutical Chemistry, University of Bradford, Yorkshire, England

With a structure such as thiamine, which contains a quaternary nitrogen, it would appear that the effluent peak from the gas chromatograph column may represent a degradation product. Circumstantial evidence that this is so is provided by mass spectrometry.

When thiamine chloride is examined using the direct insertion probe of an MS902, the mass spectrum shown in Fig. 1 is obtained. Mass measurement of the undernoted ions shows them to possess the molecular formulae:

$$m/e 112 (C_5H_6NS); m/e 122 (C_6H_8N_3); m/e 143 (C_6H_9NOS).$$

This is consistent with the fragmentation shown below and metastable peaks are observed at  $m^* = 89.3$  (m/e 143 $\rightarrow$ 113) corresponding to loss of CH<sub>2</sub>O from the alcohol side chain and at  $m^* = 64.5$  (m/e 112 $\rightarrow$ 85 corresponding to loss of HCN from the thiazole ring).

When the "thiamine" peak from the gas chromatography column is examined, only the fragment ions ascribed to the thiazole half of the molecule can be detected, that of m/e 122 from the pyrimidine ring is absent.

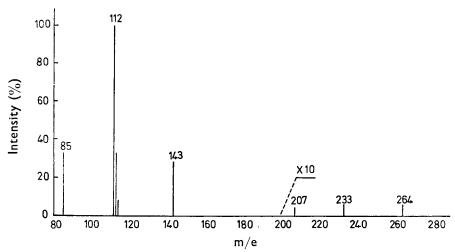


Fig. 1. Mass spectrum of thiamine chloride. Direct insertion probe: temperature 300°. Electron beam energy 70ev.