

MASS SPECTRA OF PARTIALLY METHYLATED  
2-ACETAMIDO-2-DEOXY SUGARS

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For the mass-spectrometric identification of partially methylated methyl glycosides of aminosugars we have obtained the mass spectra of a number of acetates of methyl esters of methyl N-acetyl-D-hexosaminides. The fragmentation of such compounds based on methyl 2-acetamido-2-deoxy- $\alpha$ -D-galactoside, with the exception of the 4-O-methyl and 3,4-di-O-methyl derivatives, has been studied previously by Heyns [1]. In the present communication we give the mass spectra of the acetates of methyl 2-acetamido-4-O-methyl- and 2-acetamido-3,4-di-O-methyl-2-deoxy- $\alpha$ -glucosides (I and II) (Fig. 1, a and b).

The peaks of the fragments  $C_6$  (containing the C-2 and C-3 atoms),  $C_5$  (C-2, C-3, and C-4), and  $C_6'$  in (I) and  $C_5$ ,  $C_6$ ,  $C_6'$ , and  $C_8$  (C-1 with OMe and the OMe substituent from C-3) in (II) and the approximate intensities of these peaks correspond to the values predicted by Heyns et al., [1] for the galactosides. However, in addition to this, in (I)  $D_2$  appears with  $m/e$  130 and  $D_3$  with  $m/e$  71, including C-6, C-5, and C-4, and in (II) the fragment  $A_5$  appears with  $m/e$  88 [2], which is characteristic only for a 3,4-di-O-methyl derivative.

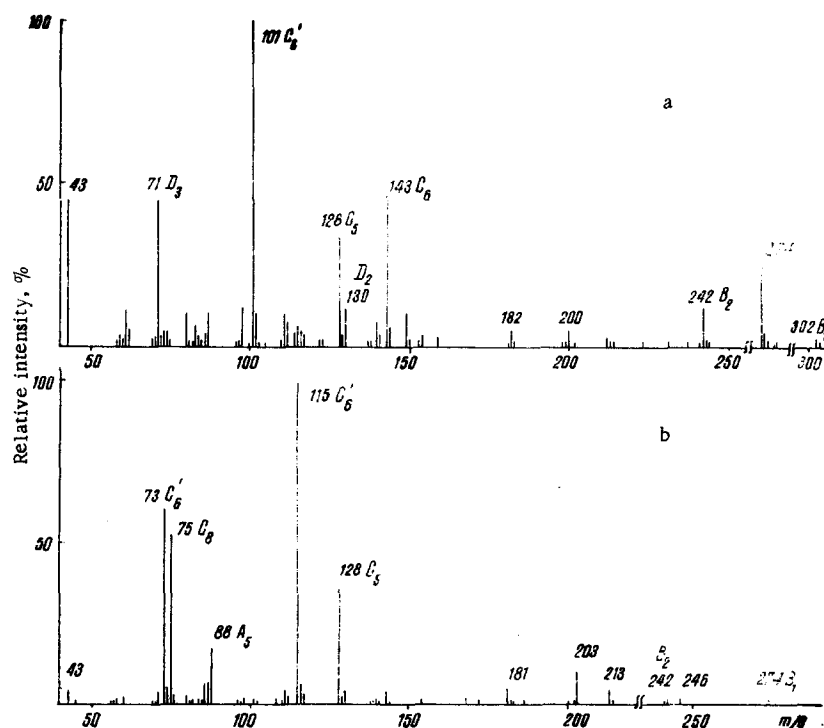


Fig. 1. Mass spectra of the acetates of methyl 2-acetamido-4-O-methyl-2-deoxy- $\alpha$ -D-glucoside (a) and of methyl 2-acetamido-3,4-di-O-methyl-2-deoxy- $\alpha$ -D-glucoside (b).

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Thus, the mass spectra of the acetates of partially-methylated methyl 2-acetamido-2-deoxyhexosides are characteristic, which permits their identification to be performed reliably.

The derivatives (I) and (II) were obtained as described by Jeanloz [3]. The mass spectra were taken in a MKh-1303 instrument at an electron energy of 70 eV.

#### LITERATURE CITED

1. K. Heyns, A. Kiessling, and D. Muller, *Carbohydrate Res.*, 4, 452 (1967).
2. K. Heyns and D. Muller, *Tetrahedron Lett.*, 449 (1966).
3. R. W. Jeanloz, *J. Amer. Chem. Soc.*, 74, 4597 (1952).