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Preliminary communication

Electronic structure of cyclic hexoses

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We report herein the results of an approximate quantum-mechanical calculation of the electronic distribution in hexoses having pyranoid and furanoid rings. The charge distribution was calculated in order to ascertain the influence of electronic factors on the nucleophilic sensitivity of acyl groups in the reaction of ammonia with certain benzoylated monosaccharides.

Recently, Zhdanov *et al.*[1] calculated the electronic structure of some pentoses by applying the Del Re approximate method[2]. By following this method and solving the equation systems with a Mercury–Ferranti electronic computer, we have determined the effective charges on each atom of the hexoses (pyranoid and furanoid rings).

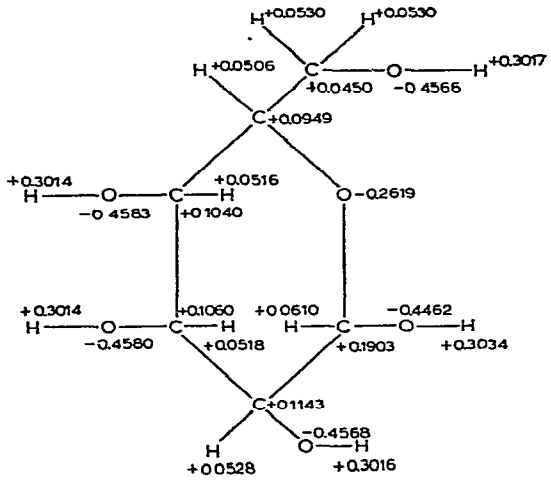
The resulting data are given as molecular diagrams **1** and **2**; the values are in agreement with those reported by Zhdanov *et al.*[1] for cyclic pentoses. Table I contains the data for C atoms.

TABLE I
LFFECTIVE CHARGE VALUES ON CARBON ATOMS OF CYCLIC PENTOSES AND HEXOSES

Compound	*C-1*	*C-2*	*C-3*	*C-4*	*C-5*	*C-6*
Furanoid pentose[a]	+0.1926	+0.1160	+0.1068	+0.0964	+0.0467	–
Pyranoid pentose[a]	+0.1929	+0.1162	+0.1079	+0.1069	+0.0362	–
Furanoid hexose	+0.1903	+0.1142	+0.1048	+0.0938	+0.1051	+0.0461
Pyranoid hexose	+0.1903	+0.1143	+0 1060.	+0.1040	+0.0949	+0.0450

[a] Data taken from Ref. 1.

The charge data reported herein allow a better explanation of the values reported for the O→N intramolecular migration of *O*-acyl groups in the methanolic ammonolysis of benzoylated monosaccharides[3,4], details of which will be published elsewhere.



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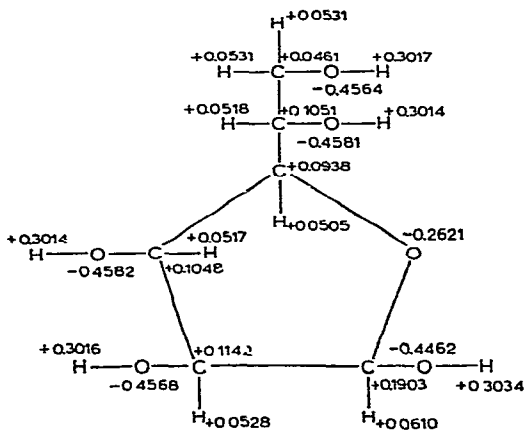

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