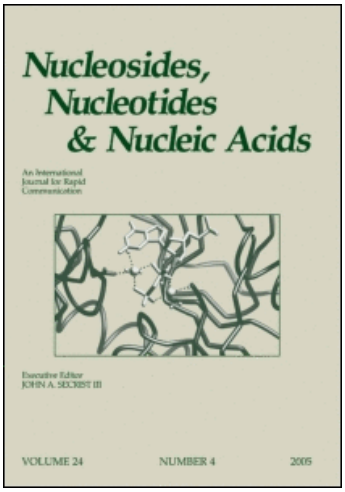

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On the Conformation of UDPG, a Sugar Nucleotide

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ON THE CONFORMATION OF UDPG, A SUGAR NUCLEOTIDE

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ABSTRACT: UDPG [uridine 5'-(∝-D-glucopyranosyl pyrophosphate)] has a folded conformation in solution in which the glucose and uracil rings lie, approximately, in the same plane with the 2"- & 3"- hydroxyl groups facing the 5- & 6- hydrogens of the uracil ring.

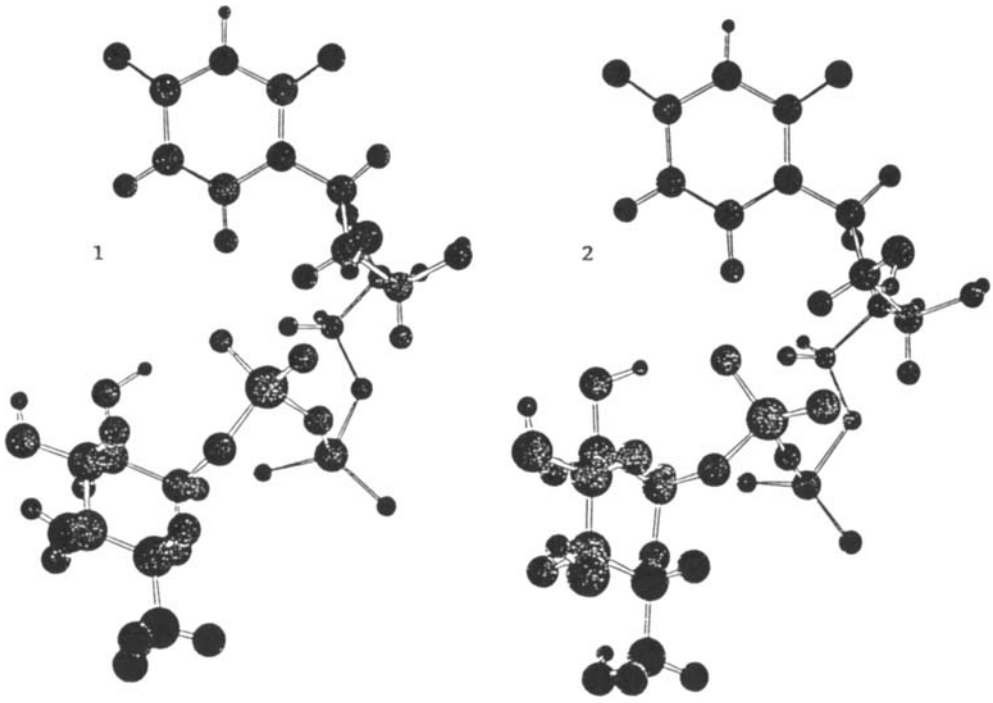
Sugar nucleotides were discovered about 50 years ago but the conformation of these molecules in solution is unclear. Although an x-ray crystal structure of UDPG shows an extended conformation[1], there is considerable evidence for a folded structure of some kind [2-4].

We present here evidence for a definite conformation of UDPG based on differential reactivity of its hydroxyl groups toward acylation and on calculations of minimum energy structures.

UDPG reacted with a number of anhydrides to give products monoacylated at the 2'- & 3'- positions (ribose). Under more vigorous conditions, the glucose residue was also acylated, but preferentially at the 6"- & 4"- positions; the 2"- & 3"- positions were relatively unreactive although the usual reactivity order is 2"-, 3"- > 4"-.[5]

This diminished reactivity of the 2"- & 3"- hydroxyl groups in UDPG is consistent with a folded conformation in which these hydroxyl groups are partially protected from reaction by the uracil ring. The glucose and uracil rings lie in the same plane (approximately) with the 2"- & 3"- hydroxyl groups facing the 5- & 6- hydrogens of the uracil ring.

Energy minimization calculations both semi-empirical (MOPAC AM1) and *ab initio* at the 631 G basis level lead to the same type of structure (Figs. 1, 2). The solvation energy as calculated by the Onsager reaction field model is very small and thus the structure is almost independent of the dielectric constant of the solvent. Protonation of the two negative charges of the pyrophosphate linkage leads to a more extended structure.



Figures 1 & 2: Minimum energy structures using the 631G basis by Gaussian 94 (Fig. 1) and by the AM1 Hamiltonian (MOPAC). (Fig. 2). The glucose portion is $^4C_1$ and the uridine portion anti. The torsional angles are: 631G/AM1: C3'-C4'-C5'-05' = -61.4/-57.0, C4'-C5'-05'-P = 126.0/155.3, C5'-05'-P-0_{pp} = -53.1/-77.1, 05'-P-0_{pp}-P = 98.2/81.7, P-0_{pp}-P-01" = 70.0/70.6, 0_{pp}-P-01"-C1" = -37.2/-64.4.

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