opposite sides of the plane of the propyl chain. In SDPA, the plane defined by the side chain carbon atoms makes an angle of 70° with the adenine plane whereas in 3SDPA, it makes an angle of 96° and also contains 0(31). Thus the molecular conformation observed is determined more by packing considerations and ease of hydrogen bond formation than by intrinsic molecular properties.

Arpinocid crystallizes in the space group P1 with a = 7.967(2), b = 11.201 (4). The authors thank Prof. B. De Clercq for kindly supplying compound I and Drs G. V. Downing and I. Shinlai for a gift of Compound III. This work forms a part of the Ph.D. thesis of P. Thomas Luthiah. ("Crystallographic studies on some derivatives of nucleic acid and their complexes", Thesis, Univ. Calcutta, September 1983.)

As a part of structural studies on enamino-esters and ketones "enaminones" the crystal structure of the title compound of formula

\[ \text{HO}\text{CH}_2 \text{NH} \text{CH}_3 \]

has been determined from X-ray diffractometer data. A large number of substituted ethylenes are known where the C\(\text{C}\) bond is significantly longer than in ethylene and the deviation from the planarity is quite appreciable (Abrahamsson, Rehnberg, Liljefer & Sandstrom, 1974; Ammon & Wheeler, 1975; Ammon, 1976; Adhikesavatu & Venkatesan, 1981, 1982). The two main factors which determine the geometry of a push-pull system are conformation (push-pull effect) and steric strain in the planar state. In this paper we report our findings on the molecular geometry. Crystal are monoclinic, P2\(_1\), with a = 12.495 (4), b = 7.622 (2), c = 12.394 (3); \(\beta = 93.9^\circ\), \(V = 1715.6 \text{ A}^3\), Z = 2, \(D = 1.33 \text{ g cm}^{-3}\), \(D = 1.34 \text{ g cm}^{-3}\), \(\lambda (\text{MoK} \alpha) = 0.7106 \text{ Å}\), \(\mu (\text{MoK} \alpha) = 0.13 \text{ mm}^{-1}\), F(000) = 1308, T = 300 K. The structure was solved by direct methods and refined by full-matrix least squares to R = 0.052 for 1317 reflections with \(h0l\). Bond lengths and angles of the glucopyranose group are in good agreement with accepted values. As in other structure, one of the O-C bond is slightly longer than the other one, and that is due to the anomeric effect. Results of the X-Ray analysis confirm that there is extensive electron delocalization involving the donor (N-sugar ring) and acceptor (acetyl groups). Because of the delocalization, the acceptor part of the molecule assumes a carbonion-like structure. The acetyl groups adopt an EZ conformation.

03.5-9 STRUCTURE OF 2-((2,2-DIACETYLVINYL)AMINO)-2-DESOXY-0-GLUCOPYRANNOSE, C\(_{11}\)H\(_{19}\)NO\(_{5}\). By H. J. Díazán A. López-Castro & R. Marques. Depto. de Optica y Sección de Física del Depto. de Investigaciones Físicas y Químicas de la Universidad de Sevilla. Centro Coordinado del C.S.I.C., Sevilla, Spain.

The title compound has recently been synthesized in Organic Chemistry Dept. of Sevilla University. The compound of formula

\[ \text{HOH}_{2} \text{C} \text{OH} \text{N} \text{CH}_{3} \]

was obtained by cyclation of 3-phenyl-1,3 dihydro-1-methyl-4-(0-l-vynyltritol-1-yl)-2H-imidazole-2-thione, obtained by reaction of 1-aminol-1-desoxy-0-fructose and phenyl-isothiocyanate. Crystals are tetragonal, space group P\(_{4}\)\(_{2}\)2\(_{1}\) with 8 molecules in the unit cell of dimensions a = 11.255 (3), c = 24.825 (7) \text{ Å}, \(\gamma = 93.9^\circ\), \(\delta = 1.24 \text{ g cm}^{-3}\), \(\delta = 1.23\), \(\delta = 100\) \(^\circ\), \(\mu (\text{MoK} \alpha) = 0.23 \text{ mm}^{-1}\), F(000) = 1248. The structure has been solved by direct methods from 2033 dif.
fractometer-measurement intensities and refined by
full-matrix least-squares to \( R = 0.07 \). All the hy-
drogen atoms have been located as dominant peaks on
a difference electron density map and refined iso-
tropically. Bond lengths and angles agree well with
those of analogous compounds. The \( S = C(1) \), \( C(1)
- H(1) \) and \( C(1) - H(2) \) distances of 1.066(5),
1.334(7) and 1.321(7) indicate the effect of the
thiourea resonance system. The tetrahydrofurane ring
is in the envelope conformation, the best least-
squares fit was obtained with \( C(5) \) in the envelope
configuration.

3.5.12 LOW ENERGY PHOSPHATES: GLUCOSE 1-PHOSPHATE
HAS DIFFERENT CONFORMATIONS IN ITS POTASSIUM AND SODIUM
SALTS

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Glucose 1-phosphate plays an important role as a low
energy phosphate in glycolysis.

GI\( \text{PK}_2 \), crystallizes in the space group \( P\text{\bar{2}}_1 \), with \( a =
10.447(1); b = 9.019(3); c = 7.523(1) \). \( p = 110.44(1)^\circ \);
\( Z = 2; D_\text{m} = 1.85; D_\text{x} = 1.86 \text{ Mgm}^{-3} \). Cu\( \text{K} \) diffractometer
data were collected and final \( R \) for 1520 unique reflec-
tions is 0.075. GI\( \text{PK}_2 \), belongs to monochimic space

The conformation about the C(5)-C(6) exocyclic bond is
gauche-trans in GI\( \text{PK}_2 \), in contrast to gauche-gauche
observed in the crystal structures of GI\( \text{PK}_2 \), and G\( \text{P}_6 \)\( \text{Ba} \) (Katti, Seshadri and Viswamitra, Acta Cryst. (1982) \text{B38},
1136-1140).

The pyra~ose sugar ring in both the structures however,
has the \( C_3 \) chair conformation a geometry also found in
the low energy phosphate G\( \text{P}_6 \)\( \text{Ba} \). The phosphate ester bond
lengths in GI\( \text{PK}_2 \), and G\( \text{PK}_2 \), are 1.641(6) and 1.650(5) Å
respectively somewhat higher compared to the \( P = O \) bond
length of 1.612 Å found in the high energy phosphate,
monopotassium salt of phosphoenolpyruvate (Hosur and