

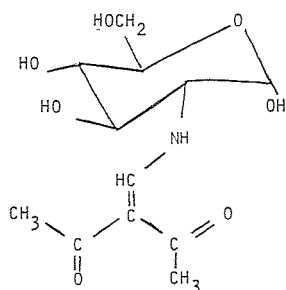
opposite sides of the plane of the propyl chain. In SDPA, the plane defined by the side chain carbon atoms makes an angle of 70° with the adenine plane where as in RSDPA, it makes an angle of 86° and also contains O(3'). Thus the molecular conformation observed is determined more by packing considerations and ease of hydrogen bond formation than by intrinsic molecular properties.

Arprinocid crystallizes in the space group $P1$ with $a = 7.967(2)$, $b = 11.251(4)$, $c = 7.484(2)$ Å and $\alpha = 93.03(2)$, $\beta = 111.36(2)$, $\gamma = 72.58(3)$ and $z = 2$. The structure was solved direct method and refined to $R = 0.105$. Each molecule participates in two types of A:A pairing simultaneously-through pairs of N(6)-H...N(1) and N(6)-H...N(7) hydrogen bonds about the two inversion centres.

The authors thank Prof. E. De Clercq for kindly supplying compound I and Drs G.V. Downing and I. Shinkai for a gift of Compound III. This work forms a part of the Ph.D. thesis of P. Thomas Muthiah. ("Crystallographic studies on some derivatives of nucleic acid bases and their complexes", Thesis, Univ. Calcutta, September 1983).

03.5-9 STRUCTURE OF 2-((2,2-DIACETYLVINYL)AMINO)-2-DESOXY- α -D-GLUCOPYRANNOSE, $C_{12}H_{19}NO_7$. By M. J. Diáñez, A. López-Castro & R. Marquez. 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.

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

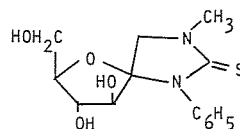


has been determined from X-Ray diffractometer data. A large number of substituted ethylenes are known where the C=C bond is significantly longer than in ethylene and the deviation from the planarity is quite appreciable (Abrahamsson, Rehnberg, Liljefors & Sandstrom. 1974; Ammon & Wheeler, 1975; Ammon, 1976; Adhikesavatu

& Venkatesan, 1981, 1982). The two main factors which determine the geometry of a push-pull system are conjugation (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 $a = 12.495(4)$, $b = 4.632(2)$, $c = 12.394(3)$, $\beta = 93.9^\circ(1)$, $V = 715.6$ Å³, $Z = 2$, $D_m = 1.33$ Mg m⁻³, $D_x = 1.34$ Mg m⁻³, $\lambda(\text{MoK}\alpha) = 0.7106$ Å, $\mu(\text{MoK}\alpha) = 0.13$ mm⁻¹, $F(000) = 308$, $T = 300^\circ\text{K}$. The structure was solved by direct methods and refined by full-matrix least squares to $R = 0.052$ for 1317 reflections with $1/2\sigma(I_o)$. 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.

03.5-10 THE CRYSTAL AND MOLECULAR STRUCTURE OF (2R,3R,4S)-6-PHENYL-3,4-DIHYDROXY-2-HYDROMETHYL-8-METHYL-7-THIOXO-1-OXA-6,8-DIAZASPIRO-(4,4)-NONANE. By E. Moreno, A. López-Castro & R. Marquez. 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



was obtained by cyclation of 3-phenyl-1,3-dihydro-1-methyl-4-(D-lyxotetritol-1-yl)-2H-imidazole-2-thione, obtained by reaction of 1-amino-1-desoxy-D-fructose and phenyl-isothiocyanate. Crystals are tetragonal, space group $P4_12_1$ with 8 molecules in the unit cell of dimensions $a = b = 11.255(3)$, $c = 24.829(7)$ Å, $V = 3145.2$ Å³, $D_x = 1.24$ Mg m⁻³, $D_m = 1.23$, $T = 300$ °K, $\mu(\text{MoK}\alpha) = 0.23$ mm⁻¹, $F(000) = 1248$. The structure has been solved by direct methods from 2033 dif-