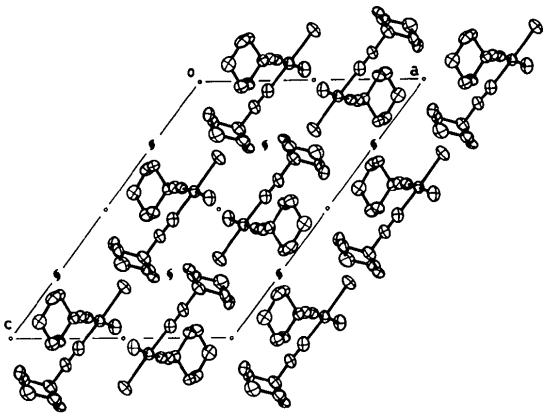

Fig. 2. Projection of the crystal structure of $PdCl_2(C_6H_{11}NC)_2$ along **b**.

other isocyanide group C(8)—N(2), on the other hand, adopts the equatorial position and the dihedral angle between the plane through C(10), C(11), C(13) and C(14) and the coordination plane is 36·5 (2)°. Each cyclohexane ring is in the chair conformation. The ring bond lengths and angles are normal.

The molecular arrangement in the crystal viewed along **b** is illustrated in Fig. 2. The crystal is built up of discrete molecules of $PdCl_2(C_6H_{11}NC)_2$, with the adjacent molecules held together by van der Waals forces. There are no abnormally short distances.

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5-Iodo-2′-deoxycytidine

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Abstract. $C_9H_{12}IN_3O_4$, monoclinic, $P2_1$, a = 12·743 (10), b = 4·750 (5), c = 9·963 (8) Å, β = 97·70 (10)°, U = 597·6 Å^3, Z = 2, D_x = 1·962 Mg m^{-3}. Diffractometer data, Mo $K\alpha$ radiation. Final R = 0·061 for 1313 unique reflexions. The molecule is in the *anti* conformation and the C(5′)—O(5′) bond is in the *gauche-trans* conformation. The sugar pucker is C(3′)-*exo*—C(4′)-*endo* relative to the mean plane of the ring.

Introduction. Crystals were obtained by slow evaporation of an aqueous solution of 5-iodo-2′-deoxycytidine (Fig. 1). The intensities of 1712 unique reflexions in the range up to $2\theta = 55°$ were measured on a Stoe two-circle diffractometer with graphite-monochromated Mo $K\alpha$ radiation. Of these, 1313 with $F_o > 5\sigma(F_o)$ were used for the structure analysis. Data were collected from a crystal mounted about **b**. Lorentz, polarization and absorption corrections were applied.

The structure was determined by the heavy-atom method. Full-matrix least-squares refinement of positional and isotropic thermal parameters and inter-layer scale factors was made, and then the H-atom positions were calculated on the basis of the chemical structure and H-bonding scheme suggested by the interatomic distances and angles. With fixed H-atom coordinates and temperature factors, refinement of the positional parameters of the non-H atoms, the anisotropic thermal parameters of the I atom and the isotropic thermal

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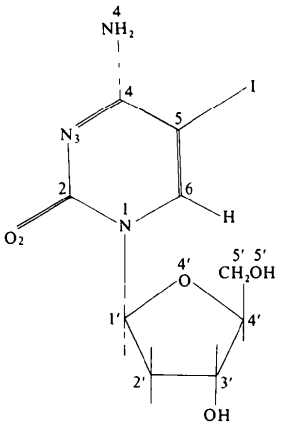

Fig. 1. 5-Iodo-2′-deoxycytidine, showing atom numbering.

Table 1. *Positional parameters* ($\times 10^4$) *and isotropic thermal parameters* ($\times 10^3$) *of the non-*H *atoms with e.s.d.'s in parentheses*

	x	*y*	*z*	*U* (Å²)
I	3929 (1)	5000	803 (1)	*
N(1)	1809 (7)	8673 (27)	3268 (9)	24 (2)
C(2)	778 (9)	7995 (34)	2645 (11)	31 (2)
O(2)	17 (8)	9006 (24)	3104 (9)	39 (2)
N(3)	699 (7)	6346 (29)	1548 (9)	28 (2)
C(4)	1536 (7)	5373 (33)	1048 (9)	24 (2)
N(4)	1395 (9)	3482 (34)	23 (11)	41 (3)
C(5)	2588 (8)	6285 (34)	1627 (11)	27 (2)
C(6)	2668 (8)	7848 (31)	2730 (10)	26 (2)
C(1′)	1846 (7)	10489 (30)	4516 (9)	26 (2)
O(4′)	2919 (6)	11165 (22)	4924 (7)	26 (2)
C(2′)	1438 (10)	8893 (33)	5690 (12)	32 (2)
C(3′)	2225 (8)	9702 (38)	6892 (10)	28 (2)
O(3′)	2022 (7)	12350 (25)	7445 (8)	35 (2)
C(4′)	3261 (7)	9906 (41)	6253 (9)	26 (2)
C(5′)	3846 (11)	7357 (43)	6133 (15)	42 (2)
O(5′)	4748 (9)	7776 (30)	5470 (11)	53 (3)

* Anisotropic temperature factors for I ($\times 10^4$):

U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
279 (4)	749 (24)	448 (4)	−284 (6)	89 (3)	50 (6)

$$T = \exp[-2\pi^2(U_{11}a^{*2}h^2 + \cdots + 2U_{12}a^*b^*hk + \cdots)].$$

parameters of the other atoms was continued. After refinement, R was 0·061, and there were no shifts $>0{\cdot}01\sigma$. Positional and thermal parameters are given in Table 1.*

After the structure was determined it was pointed out to us that a preliminary account of a structure determination of 5-iodo-2′-deoxycytidine had been given by Ambady, Phillips & Kartha (1973).

* A list of structure factors has been deposited with the British Library Lending Division as Supplementary Publication No. SUP 36089 (9 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Discussion. The nucleoside is in the *anti* conformation, like the majority of pyrimidine nucleosides and nucleotides. The pyrimidine base is essentially planar (Table 2). The sugar ring has a C(3′)-*exo*–C(4′)-*endo* pucker relative to the mean plane of the ring, which differs from that reported by Ambady *et al.* (1973). The pseudorotation parameters of the sugar ring (Altona & Sundaralingam, 1972) are $P = 205°$ and $\psi_m = 38°$. This is a less-favoured type of pucker amongst nucleosides and nucleotides but, interestingly, is also observed in deoxycytidine 5′-monophosphate (Viswamitra, Reddy, Lin & Sundaralingam, 1971), which has a pseudorotation phase angle $P = 213{\cdot}6°$ and also has a similar glycosidic torsion angle of 182·1°. The pucker is also not very different from the C(3′)-*exo*–C(2′)-*endo* pucker observed in deoxyadenosine (Watson, Sutor & Tollin, 1965) and thymidine (Young, Tollin & Wilson, 1969), which have pseudorotation phase angles of 194·3 and 187·5° respectively. All these are closer to the favoured C(2′)-*endo* pucker ($P = 162°$) than the favoured C(3′)-*endo* pucker ($P = 18°$). The C(5′)–O(5′) bond is in the *gauche-trans* orientation relative to C(4′)–O(4′) and C(4′)–C(3′), which is less-favoured than the *gauche-gauche* conformation in nucleosides and nucleotides. The corresponding conformational parameters of 5-iodocytidine (Radwan & Wilson, 1979) are *anti*, C(3′)-*endo*–C(2′)-*exo*, *gauche-gauche*. The parameters of other cytosine-containing nucleosides and nucleotides have been summarized by Young & Wilson (1975). They all have the *anti* and *gauche-*

Table 2. *Deviations* (Å) *of atoms from least-squares planes, and torsion angles* (°)

E.s.d.'s are *ca* 0·01 Å and 1·0°. The atoms marked with daggers were used to calculate the mean planes. X, Y and Z are coordinates, in Å, relative to **a**, **b** and **c***.

(1) Pyrimidine ring

$$0{\cdot}4709X + 3{\cdot}8688Y - 5{\cdot}7661Z = 1{\cdot}5844$$

N(1)†	−0·029	C(6)†	0·003
C(2)†	0·021	C(1′)	−0·045
N(3)†	0·013	O(2)	0·111
C(4)†	−0·037	N(4)	−0·186
C(5)†	0·030	I	0·072

(2) Sugar ring

$$-3{\cdot}4751X + 4{\cdot}4179Y + 2{\cdot}7940Z = 5{\cdot}1988$$

C(1′)†	0·053	O(4′)†	0·095
C(2′)†	−0·180	O(3′)	1·636
C(3′)†	0·239	O(5′)	−1·887
C(4′)†	−0·207	C(5′)	−1·575

O(4′)–C(1′)–N(1)–C(2)	185
O(4′)–C(1′)–N(1)–C(6)	2
O(5′)–C(5′)–C(4′)–C(3′)	177
O(5′)–C(5′)–C(4′)–O(4′)	58

Table 3. *Bond lengths* (Å) *for the non*-H *atoms*

I–C(5)	2·08 (1)	N(1)–C(1′)	1·51 (2)
C(5)–C(4)	1·45 (1)	C(1′)–O(4′)	1·41 (1)
C(4)–N(4)	1·35 (2)	C(4′)–C(4′)	1·46 (1)
C(4)–N(3)	1·32 (1)	C(4′)–C(5′)	1·44 (3)
N(3)–C(2)	1·34 (2)	C(5′)–O(5′)	1·41 (2)
C(2)–O(2)	1·22 (2)	C(4′)–C(3′)	1·54 (1)
C(2)–N(1)	1·41 (1)	C(3′)–O(3′)	1·41 (2)
N(1)–C(6)	1·34 (1)	C(3′)–C(2′)	1·51 (2)
C(6)–C(5)	1·32 (2)	C(2′)–C(1′)	1·54 (2)

Table 4. *Bond angles* (°) *for the non*-H *atoms*

I–C(5)–C(4)	121 (1)	C(1′)–N(1)–C(6)	124 (1)
I–C(5)–C(6)	121 (1)	N(1)–C(1′)–O(4′)	107 (1)
C(5)–C(4)–N(4)	121 (1)	N(1)–C(1′)–C(2′)	112 (1)
C(5)–C(4)–N(3)	120 (1)	C(1′)–O(4′)–C(4′)	109 (1)
N(4)–C(4)–N(3)	119 (1)	O(4′)–C(4′)–C(5′)	111 (1)
C(4)–N(3)–C(2)	122 (1)	O(4′)–C(4′)–C(3′)	103 (1)
N(3)–C(2)–O(2)	124 (1)	C(4′)–C(5′)–O(5′)	113 (2)
N(3)–C(2)–N(1)	117 (1)	C(5′)–C(4′)–C(3′)	118 (2)
O(2)–C(2)–N(1)	119 (1)	C(4′)–C(3′)–O(3′)	108 (1)
C(2)–N(1)–C(6)	121 (1)	C(4′)–C(3′)–C(2′)	102 (1)
C(2)–N(1)–C(1′)	115 (1)	O(3′)–C(3′)–C(2′)	114 (1)
N(1)–C(6)–C(5)	121 (1)	C(3′)–C(2′)–C(1′)	103 (1)
C(6)–C(5)–C(4)	118 (1)	C(2′)–C(1′)–O(4′)	108 (1)

Table 5. *Hydrogen-bond lengths* (Å) *and angles* (°)

O(5′)–H···O(5′^{i})	2·66 (1)	O(3′)–H···O(2′^{iii})	2·70 (1)
N(4)–H···O(3′^{ii})	2·82 (1)	N(4)–H···N(3^{iv})	3·06 (1)
C(5′)–O(5′)–O(5′)	123 (1)	C(3′)–O(3′)–O(2)	114 (1)
C(4)–N(4)–O(3′)	142 (1)	C(4)–N(4)–N(3)	128 (1)

Symmetry code: (i) $1-x, -\frac{1}{2}+y, 1-z$; (ii) $x, -1+y, -1+z$; (iii) $-x, \frac{1}{2}+y, 1-z$; (iv) $-x, -\frac{1}{2}+y, -z$.

gauche conformation and either a C(2′)-*endo*–C(3′)-*exo* or a C(3′)-*endo*–C(2′)-*exo* pucker.

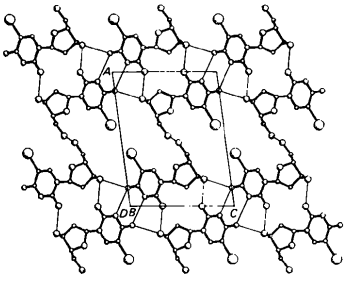

Fig. 2. A projection of the structure viewed along **b**. The thin lines represent hydrogen bonds.

Bond lengths and angles (Tables 3 and 4) in the present structure are in good agreement with those in related structures. The molecules are linked together by H bonds (Table 5 and Fig. 2), the ones between atoms O(5′) forming a zig-zag arrangement about the *b* axis. The I atoms do not appear to be involved in intermolecular bonding.

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