pairing, involves O(1) and H(C9). However, at 2·69 Å this is too far beyond the combined van der Waals radii of H and O atoms to justify invoking any special dipolar interactions (Bolton, 1963; Eiland & Pepinsky, 1955).

Although the root causes for the choice of H-bonding mode in solid keto acids remain elusive, a reliable experimental method now exists for ascertaining this pattern in a given sample, short of X-ray structure determination (Vanderhoff, Lalancette & Thompson, 1990). The solid-state (KBr) infrared spectrum of (I) is normal, displaying C=O stretching absorptions at 1684 cm^{-1} (benzoyl) and 1709 cm^{-1} (carboxyl). The corresponding Raman frequencies are 1679 cm^{-1}, involving a difference of only 5 cm^{-1}, for the ketone and 1627 cm^{-1} for the carboxyl group. The frequency difference between infrared and Raman in the latter case, 82 cm^{-1}, is the largest we have observed, the average being about 51 cm^{-1} for the carboxyl dimers we have studied. This frequency difference is small (typically *ca* 4 cm^{-1}) for carboxyl groups which adopt catemeric hydrogen-bonding patterns and has been shown to be a reliable experimental predictor of H-bonding mode in solid-state keto carboxylic acids (Vanderhoff, Lalancette & Thompson, 1990).

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Structure of 5-Methylcytidine

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Abstract. 4-Amino-5-methyl-1-β-D-ribofuranosyl-2(1*H*)-pyrimidinone, $C_{10}H_{15}N_3O_5$, $M_r = 257{\cdot}2$, monoclinic, $P2_1$, $a = 5{\cdot}632\ (1)$, $b = 14{\cdot}636\ (3)$, $c = 13{\cdot}914\ (3)$ Å, $\beta = 90{\cdot}57\ (1)°$, $V = 1146{\cdot}9$ Å^3, $Z = 4$, $D_x = 1{\cdot}49$ Mg m^{-3}, λ(Cu $K\alpha$) = 1·5418 Å, $\mu = 0{\cdot}98$ mm^{-1}, $F(000) = 544$, $T = 295$ K, $R = 0{\cdot}036$ for 2025 unique observed reflections with $F \geq 3\sigma(F)$. The bond lengths, bond angles and conformation of the two independent molecules in the asymmetric unit are essentially similar. The cytosine bases are not protonated. Bases are in *anti* conformation, sugars show C(3′)-*endo* pucker (^3E) and *gg* conformation about the C(4′)—C(5′) bond for both molecules. The structure is stabilized by a number of hydrogen bonds between molecules *A* and molecules *B*. No base-stacking interactions were observed in the present structure. This is in agreement with the observation made in a comparison of methylated and unmethylated cytosine structures which showed that methylation at the 5 position of the cytosine base could result in reduced base-stacking interactions.

Introduction. Metabolite activities of 5-methylated cytosine bases with a key role in a variety of biochemical regulation processes have been discussed by Doerfler (1983, 1984), Razin & Riggs (1980), Rideout, Coetzee, Olumi & Jones (1990) and Ehrlich & Wang (1981). The structural and energetic alterations demonstrate that methylation of cytosine in the 5 position may be an important switch mechanism for influencing the B–Z equilibrium and DNA topology in general, thus potentially affecting DNA–

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protein interactions and gene regulation at the physiological levels of supercoiling (Zacharias, O'Connor & Larson, 1988). Considering the biological significance of the 5-methylation of a cytosine base, it is important to study the effect of methylation on the base and its surroundings at different levels of DNA organization. In this context we have already reported the crystal structure of 5-methylcytosine hydrochloride (Padmaja, Ramakumar & Viswamitra, 1987). In continuation of this work we now report the crystal structure of 5-methylcytidine. A comparison of 5-methylated cytosine structures has been made with their unmethylated analogues.

Experimental. Crystals were obtained from an aqueous solution of the title compound (Sigma Chemicals) by direct evaporation. Cell dimensions were obtained from 23 accurately determined reflections, $6{\cdot}0 \le \theta \le 26{\cdot}3°$, on an Enraf–Nonius CAD-4 diffractometer. Intensity data were collected up to $(\sin\theta)/\lambda = 0{\cdot}588$ Å^{-1}, with ω–2θ scans using Ni-filtered Cu $K\alpha$ radiation, from a crystal of size $0{\cdot}6 \times 0{\cdot}3 \times 0{\cdot}16$ mm; index range: $-6 \le h \le 6$, $0 \le k \le 17$, $0 \le l \le 16$; three reflections ($05\bar{6}$, $\bar{1}30$ and 113) monitored preiodically showed no evidence of crystal decay; Lorentz and polarization corrections were applied, but the data were not corrected for absorption. Of the 2409 reflections measured, 2025 were considered observed [$F \ge 3\sigma(F)$]. Structure solution by direct methods using *MULTAN*11/82 (Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1982). Though the absolute configuration was not determined, and enantiomorph corresponding to the D-sugar has been chosen to facilitate the comparison with other reported structures of nucleosides and nucleotides, which contain the sugar in the biologically important D form. 24 of the 30 expected H atoms could be located from difference electron density maps computed at different stages of full-matrix least-squares refinement on F using *SHELX*400 (enhanced version of *SHELX*76; Sheldrick, 1976). Of the remaining six H atoms, three could be fixed geometrically and were later varied in the last stages of refinement. The refinement was carried out with the y coordinate of the O(2) atom of molecule A fixed, which defines the origin. Non-H atoms were refined anisotropically and H atoms isotropically. The number of parameters refined was 432. The final discrepancy indices were $R = 0{\cdot}036$, $wR = 0{\cdot}037$ and $S = 1{\cdot}59$ with individual weights, $w \propto 1/[\sigma^2(F) + 0{\cdot}001(F^2)]$; $(\Delta/\sigma)_{max} = 0{\cdot}2$ and the heights in the final $\Delta\rho$ map were within $+0{\cdot}23$ and $-0{\cdot}29$ e Å^{-3}. The atomic scattering factors were as supplied in *SHELX*76. The structure was solved using *SDP* (Enraf–Nonius, 1979) on a PDP11/44 computer.

The program *TRACER*II (Lawton, 1973) showed that, at a tolerance factor of 1·0, the present structure could possibly be described in an orthorhombic space group. The coordinates of molecule A as described in $P2_1$ were then suitably converted to $P2_12_12_1$ and a least-squares refinement was carried out. The R factor, after a few cycles of refinement, converged to as high a value as 31·5% and some of the bond lengths were unreasonable. This indicates that the structure is better described in $P2_1$ with two molecules in the asymmetric unit than in $P2_12_12_1$. No physical measurements were made to check that the chosen space group was polar.

Discussion. The final fractional coordinates and isotropic temperature factors and bond lengths and selected torsion angles of the non-H atoms of molecules A and B are listed in Tables 1 and 2, respectively.* The molecular conformation along with the atomic numbering scheme for both the molecules is shown in Fig. 1. Fig. 2 shows the hydrogen-bonding pattern in the crystal structure of the title compound. The conformations of the two molecules in the asymmetric unit are essentially the same, except for differences in torsion angles involving the base atoms (Table 2). The bases of both independent molecules are unprotonated and show an *anti* conformation with respect to the sugar ring [C(2)—N(1)—C(1′)—O(4′): $\chi = -169{\cdot}7\,(2)°$ for A and $-168{\cdot}8\,(2)°$ for B]. The furanose sugar ring shows C(3′)-*endo* conformation (^3E), with the C(3′) atom displaced by $-0{\cdot}546\,(3)$ Å in A and $-0{\cdot}522\,(3)$ Å in B from the best least-squares plane formed by the rest of the atoms of the ring. The pseudorotation parameters (Altona & Sundaralingam, 1972) P and τ_m are 17·4°, 36·0° for molecule A and 17·0°, 34·4° for molecule B, respectively.

The structure is stabilized by a number of hydrogen bonds between molecules A and B. The details of the possible hydrogen-bond geometry are shown in Fig. 2. It is interesting to note that the atoms are pairwise hydrogen bonded to each other between various translated and symmetry-related molecules A and B. The possible hydrogen bonds are: O(2)A···H—O(5′)B [2·647 (3) Å, 176 (5)°], O(2)B···O(5′)A [2·634 (3) Å], N(4)A—H···O(5′)B [2·971 (4) Å, 159 (5)°], N(4)B—H···O(5′)A [2·938 (4) Å, 167 (4)°], O(2′)A—H···O(3′)B [2·944 (4) Å, 143 (4)°], O(2′)B···O(3′)A [2·944 (3) Å], O(3′)B—H···N(3)A

* Lists of observed and calculated structure factors, H-atom parameters, bond angles, anisotropic thermal parameters and possible H bonds have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 53708 (19 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 1. *Final fractional coordinates and equivalent isotropic temperature factors for non-*H *atoms, with e.s.d.'s in parentheses*

$$U_{eq} = (1/3)\sum_i \sum_j U_{ij} a_i^* a_j^* \mathbf{a}_i . \mathbf{a}_j .$$

	x	y	z	U_{eq}(Å^2)
Molecule *A*				
N(1)	0·9506 (4)	0·2370 (2)	0·0890 (1)	0·030 (1)
C(2)	0·7739 (4)	0·2302 (2)	0·0199 (2)	0·031 (1)
N(3)	0·6612 (4)	0·1484 (2)	0·0067 (2)	0·035 (1)
C(4)	0·7310 (5)	0·0764 (2)	0·0566 (2)	0·031 (1)
C(5)	0·9316 (5)	0·0778 (3)	0·1214 (2)	0·032 (1)
C(6)	1·0310 (5)	0·1603 (2)	0·1354 (2)	0·032 (1)
O(2)	0·7237 (4)	0·2996	−0·0284 (1)	0·041 (1)
N(4)	0·6044 (5)	−0·0012 (2)	0·0453 (2)	0·044 (1)
C(7)	1·0272 (6)	−0·0079 (3)	0·1669 (3)	0·045 (1)
O(4′)	1·2651 (3)	0·3187 (2)	0·1607 (1)	0·032 (1)
C(1′)	1·0628 (4)	0·3283 (2)	0·1003 (2)	0·028 (1)
C(2′)	0·8938 (4)	0·3976 (2)	0·1476 (2)	0·029 (1)
C(3′)	0·9768 (4)	0·3927 (2)	0·2526 (2)	0·026 (1)
C(4′)	1·2420 (4)	0·3753 (2)	0·2448 (2)	0·027 (1)
C(5′)	1·3507 (5)	0·3288 (3)	0·3319 (2)	0·039 (1)
O(5′)	1·2210 (4)	0·2523 (2)	0·3630 (2)	0·047 (1)
O(2′)	0·9228 (4)	0·4851 (2)	0·1063 (1)	0·042 (1)
O(3′)	0·9246 (3)	0·4737 (2)	0·3042 (1)	0·035 (1)
Molecule *B*				
N(1)	0·5961 (3)	0·3307 (2)	0·5827 (1)	0·027 (1)
C(2)	0·7656 (4)	0·3436 (2)	0·5122 (2)	0·027 (1)
N(3)	0·8446 (4)	0·4299 (2)	0·4950 (2)	0·031 (1)
C(4)	0·7601 (4)	0·5001 (2)	0·5449 (2)	0·029 (1)
C(5)	0·5659 (4)	0·4904 (2)	0·6106 (2)	0·030 (1)
C(6)	0·4967 (4)	0·4042 (2)	0·6276 (2)	0·030 (1)
O(2)	0·8382 (3)	0·2759 (2)	0·4674 (1)	0·036 (1)
N(4)	0·8578 (4)	0·5819 (2)	0·5303 (2)	0·037 (1)
C(7)	0·4508 (6)	0·5714 (3)	0·6579 (2)	0·044 (1)
O(4′)	0·3174 (3)	0·2368 (2)	0·6592 (1)	0·031 (1)
C(1′)	0·5194 (4)	0·2351 (2)	0·6000 (2)	0·025 (1)
C(2′)	0·7141 (4)	0·1799 (2)	0·6510 (2)	0·027 (1)
C(3′)	0·6338 (4)	0·1845 (2)	0·7553 (2)	0·025 (1)
C(4′)	0·3638 (4)	0·1874 (2)	0·7477 (2)	0·027 (1)
C(5′)	0·2431 (4)	0·2347 (3)	0·8306 (2)	0·036 (1)
O(5′)	0·3499 (4)	0·3193 (2)	0·8566 (2)	0·043 (1)
O(2′)	0·7074 (4)	0·0895 (2)	0·6139 (1)	0·039 (1)
O(3′)	0·7215 (4)	0·1099 (2)	0·8097 (1)	0·037 (1)

Table 2. *Bond lengths* (Å) *and selected torsion angles* (°), *with e.s.d.'s in parentheses*

	Molecule *A*	Molecule *B*		Molecule *A*	Molecule *B*
N(1)—C(2)	1·380 (3)	1·389 (3)	C(1′)—C(2′)	1·543 (4)	1·531 (4)
N(1)—C(6)	1·370 (4)	1·367 (4)	C(1′)—O(4′)	1·416 (3)	1·411 (3)
N(1)—C(1′)	1·486 (4)	1·485 (4)	C(2′)—C(3′)	1·531 (4)	1·526 (4)
C(2)—N(3)	1·367 (4)	1·361 (4)	C(2′)—O(2′)	1·414 (4)	1·421 (4)
C(2)—O(2)	1·249 (3)	1·242 (4)	C(3′)—C(4′)	1·520 (3)	1·524 (3)
N(3)—C(4)	1·320 (4)	1·331 (4)	C(3′)—O(3′)	1·418 (4)	1·415 (3)
C(4)—C(5)	1·439 (4)	1·439 (4)	C(4′)—C(5′)	1·514 (4)	1·512 (4)
C(4)—N(4)	1·349 (4)	1·334 (4)	C(4′)—O(4′)	1·441 (4)	1·450 (3)
C(5)—C(6)	1·344 (5)	1·342 (4)	C(5′)—O(5′)	1·407 (5)	1·422 (5)
C(5)—C(7)	1·502 (6)	1·506 (5)			

	Molecule *A*	Molecule *B*
C(6)—N(1)—C(2)—N(3)	7·8 (4)	5·6 (4)
C(6)—N(1)—C(1′)—O(4′)	3·2 (3)	6·7 (3)
C(2)—N(1)—C(1′)—O(4′)	−169·7 (2)	−168·8 (2)
N(1)—C(2)—N(3)—C(4)	−3·4 (4)	−0·1 (4)
C(2)—N(3)—C(4)—C(5)	−3·7 (4)	−7·0 (4)
N(3)—C(4)—C(5)—C(6)	6·3 (5)	8·4 (4)
C(4)—C(5)—C(6)—N(1)	−1·8 (4)	−2·7 (4)
O(4′)—C(1′)—C(2′)—C(3′)	−21·9 (3)	−21·0 (3)
C(1′)—C(2′)—C(3′)—C(4′)	33·6 (2)	32·2 (3)
C(2′)—C(3′)—C(4′)—O(4′)	−34·4 (3)	−32·7 (3)
C(3′)—C(4′)—O(4′)—C(1′)	21·2 (3)	20·0 (3)
O(4′)—C(4′)—C(5′)—O(5′)	−69·8 (3)	−70·9 (3)
C(3′)—C(4′)—C(5′)—O(5′)	47·7 (4)	46·0 (3)

[2·822 (3) Å, 170 (4)°] and O(3′)*A*···N(3)*B* [2·772 (3) Å] (*A* and *B* represent atoms belonging to molecules *A* and *B*, respectively).

To study the effects on the base-stacking interactions of protonation at N(3) and methylation at the 5 position of the cytosine base, a comparison (Table 3) of the unmethylated and methylated cytosine structures has been made. The analysis indicates that unprotonated unmethylated cytosine structures generally show considerable stacking by ring–ring overlap of the bases, as compared to the protonated unmethylated cytosine structures. In contrast, the methylated cytosine structures generally show no ring–ring overlap interactions even though the bases are not protonated at N(3). It is seen that methylated cytosine structures show reduced base-stacking interactions irrespective of the base being unprotonated or protonated (as in the structure of 5-methylcytosine hydrochloride).

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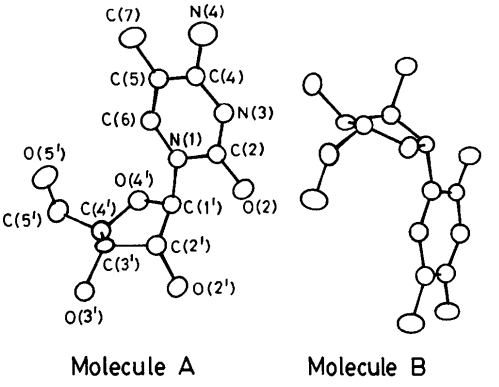

Fig. 1. Molecular conformation and atomic numbering scheme.

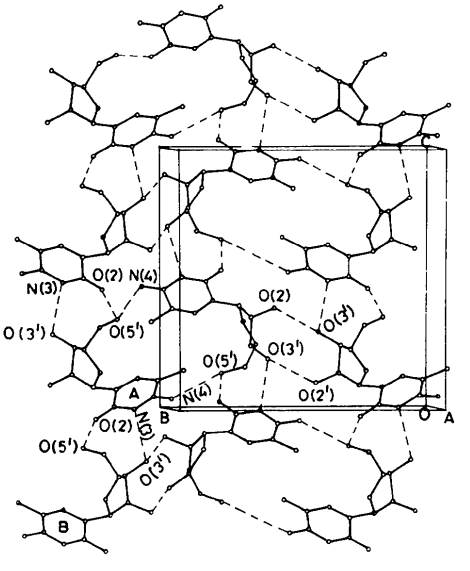

Fig. 2. Crystal packing showing the hydrogen-bonding pattern.

Table 3. *Comparison between unmethylated and methylated cytosine structures*

Compound	Whether protonated	Whether stacking by ring–ring overlap present	Reference
Unmethylated compounds			
Cytosine	No	Yes	(*a*)
Cytosine.H_2O	No	No	(*b*)
Cytosine.HCl	Yes	Yes, charge on N(3) delocalized by a strong N(3)—H···Cl hydrogen bond	(*c*)
Cytidine	No	No, O(4′) stacks on base ring	(*d*)
2′-Deoxycytidine.HCl	Yes	Yes, very little overlap exists	(*e*)
5′-dCMP*.H_2O	Yes	No	(*f*)
5′-dCMP* Na_2.7H_2O	No	Yes	(*g*)
5′-dCMP* Na_2.11H_2O	No	Yes	(*h*)
Methylated compounds			
5-Methylcytosine.0·5H_2O	No	No	(*i*)
5-Methylcytosine.HCl	Yes	No	(*j*)
5-Methyl-2-thiocytosine.0·5H_2O	No	No	(*k*)
5-Methylcytidine	No	No	Present work
5-Methyl-2′-dCMP.2H_2O	Yes	No	(*l*)

References: (*a*) Barker & Marsh (1964); (*b*) Jeffrey & Kinoshita (1963); (*c*) Mandel (1977); (*d*) Furberg, Peterson & Rømming (1965); (*e*) Subramanian & Hunt (1970); (*f*) Viswamitra, Swaminatha Reddy, Lin & Sundaralingam (1971); (*g*) Pandit, Seshadri & Viswamitra (1983); (*h*) Viswamitra & Pandit (1983); (*i*) Grainger & Bailey (1981); (*j*) Padmaja, Ramakumar & Viswamitra (1987); (*k*) Ravichandran, Chacko, Ponnuswamy & Trotter (1985); (*l*) Lalitha, Ramakumar & Viswamitra (1989).

* dCMP = deoxycytidine monophosphate.

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Structure of 3-Methoxytyramine Hydrochloride

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Abstract. 2-(4-Hydroxy-3-methoxyphenyl)ethylammonium chloride, $C_9H_{14}NO_2^+.Cl^-$, $M_r = 203{\cdot}67$, orthorhombic, $P2_12_12_1$, $a = 10{\cdot}586\ (2)$, $b = 17{\cdot}885\ (2)$, $c = 5{\cdot}190\ (2)$ Å, $V = 982{\cdot}6\ (4)$ Å^3, $Z = 4$, $D_x = 1{\cdot}377$ Mg m^{-3}, λ(Mo $K\alpha$) = 0·71069 Å, $\mu = 0{\cdot}354$ mm^{-1}, $F(000) = 432$, $T = 296$ K. The final values for R and wR were 0·037 and 0·039, respectively, for 1053 observed reflections. The amino side chain is in the fully extended *trans* conformation and lies in the same plane as the phenyl ring. There is a hydrogen-bonding network involving the *p*-hydroxyl group, the protonated amino group and the Cl^- ions.

Introduction. The crystal structure of catecholamines, such as dopamine (Bergin & Carlström, 1968; Giesecke, 1980), adrenaline (Andersen, 1975*a*),

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