Table 1. *Final positional parameters* ($\times 10^4$, *for* Bi $\times 10^5$) *and isotropic thermal parameters* ($\times 10^3$, *for* Bi $\times 10^4$) *with e.s.d.'s in parentheses*

For Bi and Cl the equivalent isotropic thermal parameter is given $[U_{eq} = (U_{11}U_{22}U_{33})^{1/3}]$; for N and C atoms the isotropic thermal parameter is given.

	x	y	z	U_{eq}/U(Å^2)
Bi	54349 (4)	63800 (6)	41948 (5)	494 (4)
Cl(1)	5416 (5)	8677 (5)	4265 (6)	81 (5)
Cl(2)	6859 (4)	6332 (6)	5472 (6)	81 (4)
Cl(3)	4619 (4)	6235 (5)	5674 (5)	86 (3)
Cl(4)	3845 (4)	6400 (6)	2428 (5)	76 (4)
N	1857 (14)	5718 (20)	1430 (18)	94 (6)
C(1)	1879 (20)	4421 (31)	1592 (28)	126 (11)
C(2)	2010 (40)	3845 (43)	601 (49)	174 (21)
C(3)	1591 (45)	6303 (42)	2395 (56)	204 (26)
C(4)	838 (51)	6432 (42)	2369 (58)	182 (28)

Table 2. *Interatomic distances* (Å) *and angles* (°) *with e.s.d.'s in parentheses*

Bi–Cl(1)	2·559 (6)	Cl(1)–Bi–Cl(2)	90·9 (2)
Bi–Cl(2)	2·493 (6)	Cl(1)–Bi–Cl(3)	91·1 (2)
Bi–Cl(3)	2·688 (8)	Cl(1)–Bi–Cl(4)	90·2 (2)
Bi–Cl(4)	3·003 (6)	Cl(1)–Bi–Cl(3^i)	173·3 (2)
Bi–Cl(3^i)	2·919 (6)	Cl(1)–Bi–Cl(4^{ii})	91·9 (2)
Bi–Cl(4^{ii})	2·747 (7)	Cl(2)–Bi–Cl(3)	93·8 (2)
		Cl(2)–Bi–Cl(4)	172·1 (2)
N–Cl(4)	3·27 (2)	Cl(2)–Bi–Cl(3^i)	88·6 (2)
N–Cl(1^{iii})	3·26 (2)	Cl(2)–Bi–Cl(4^{ii})	90·4 (2)
		Cl(3)–Bi–Cl(4)	94·0 (2)
N C(1)	1·46 (4)	Cl(3)–Bi–Cl(3^i)	82·3 (2)
N–C(3)	1·61 (8)	Cl(3)–Bi–Cl(4^{ii})	174·8 (2)
C(1)–C(2)	1·54 (8)	Cl(4)–Bi–Cl(3^i)	91·1 (2)
C(3)–C(4)	1·24 (12)	Cl(4)–Bi–Cl(4^{ii})	81·7 (2)
		Cl(3^i)–Bi–Cl(4^{ii})	94·7 (2)
C(1)–N–C(3)	106 (3)		
N–C(1)–C(2)	107 (3)		
N–C(3)–C(4)	121 (6)		

Symmetry code: (i) $1-x, 1-y, 1-z$; (ii) $1-x, y, \frac{1}{2}-z$; (iii) $-\frac{1}{2}+x, \frac{3}{2}-y, -\frac{1}{2}+z$.

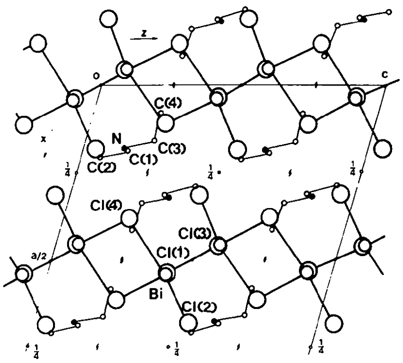

Fig. 1. Projection of the structure down **b**.

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Structure of the Monosodium Salt of D-Glucose 6-Hydrogenphosphate

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Abstract. $Na^+.C_6H_{12}O_9P^-$, $M_r = 282·1$, monoclinic, $P2_1$, $a = 5·762$ (1), $b = 7·163$ (2), $c = 12·313$ (1) Å, $\beta = 99·97$ (1)°, $U = 500·5$ Å^3, $Z = 2$, $D_m = 1·86$, $D_x = 1·87$ Mg m^{-3}, Cu $K\alpha$, $\lambda = 1·5418$ Å, $\mu = 3·3$ mm^{-1}, $F(000) = 292$, $T = 300$ K, final R for 922 observed reflections is 0·042. The phosphate ester bond, P—O(6), is 1·575 (5) Å, slightly shorter than the P~O bond in monopotassium phosphoenolpyruvate [1·612 (6) Å] [Hosur & Viswamitra (1981). *Acta Cryst.* B**37**, 839–843]. The pyranose sugar ring takes a $^4C_1$ chair conformation. The conformation about the exocyclic C(5)—C(6) bond is *gauche–trans*. The endocyclic C—O bonds in the glucose ring are nearly equal with C(5)—O(5) = 1·435 (8) and C(1)—O(5) = 1·436 (9) Å. The sodium ion has seven near neighbours within a distance of 2·9 Å. The crystal structure is stabilized by hydrogen bonds between the O atoms of symmetry-related molecules.

0108-2701/85/111621-04$01.50

Introduction. Glucose 6-phosphate (G6P) is an intermediate in glycolysis. Its free energy of hydrolysis is small, $-13{\cdot}8\ \text{kJ mol}^{-1}$, compared to that of 'high-energy' phosphates such as phosphoenolpyruvate ($-61{\cdot}9\ \text{kJ mol}^{-1}$) (Lehninger, 1973). We report here the structure of G6PNa as obtained from X-ray diffraction studies. This investigation follows our earlier studies on the glucose 6-phosphate and glucose 1-phosphate anions (Katti, Seshadri & Viswamitra, 1982; Narendra, Seshadri & Viswamitra, 1984; Narendra & Viswamitra, 1984).

Experimental. Crystals grown from aqueous solutions of the compound by diffusion of acetone. Density measured using acetone and bromoform mixtures. Unit-cell dimensions and space group from rotation and Weissenberg photographs. Cell parameters refined by least-squares calculations from 23 high-angle reflections collected on a CAD-4 diffractometer. Cu $K\alpha$ intensity data collected up to $\sin\theta/\lambda = 0{\cdot}62\ \text{Å}^{-1}$ using crystal $0{\cdot}1 \times 0{\cdot}3 \times 0{\cdot}4$ mm, ω–2θ scan mode. 1017 out of 1297 reflections considered observed $[F > 3\sigma(F)]$; 922 unique, $R_{\text{int}} = 0{\cdot}041$. Three strong reflections monitored periodically during data collection showed crystal stable to X-rays. Max. and min. intensities recorded for reflections 012, 013 and 120 are 73 011 and 68 247, 15 676 and 15 157 and 25 732 and 24 179 respectively. h,k,l range 0–7, 0–8, −15–15; Lorentz and polarization corrections applied. Structure solved by direct methods (Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1980). Phosphate group located in first E map. Remaining non-H atoms located from successive difference Fourier maps; block-diagonal least-squares refinement (Shiono, 1965) with anisotropic thermal parameters; all H atoms obtained from difference Fourier map. Refinement, including H with isotropic thermal parameters, reduced R to 4·2%; $\sum w(|F_o| - |F_c|)^2$ minimized, $w = 1{\cdot}0$, $S = 1{\cdot}19$. Scattering factors for non-H atoms from Cromer & Waber (1965), for H atoms from Stewart, Davidson & Simpson (1965). Δ/σ for non-H atoms $>1{\cdot}0$ only for $B(2,2)$ of C(6) ($= 1{\cdot}39$); Δ/σ max. for H 1·64; min. and max. residual electron density in final difference Fourier map $-0{\cdot}42$ and $0{\cdot}76\ \text{e Å}^{-3}$.

Discussion. Final positional parameters for the atoms are given in Table 1.* Bond lengths and angles are listed in Table 2. The *ORTEP* (Johnson, 1965) diagram of the molecule with the numbering scheme is shown in Fig. 1, which also shows the sodium coordination polyhedron. The packing arrangement is shown in Fig. 2.

Table 1. *Fractional coordinates* ($\times 10^4$; *for* H $\times 10^3$) *with equivalent isotropic temperature factors for non-hydrogen atoms,* B_{iso} *for* H *atoms, with e.s.d.'s in parentheses*

$$B_{\text{eq}} = \tfrac{4}{3}\textstyle\sum_i\sum_j \beta_{ij}\mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	$B_{\text{eq}}/B_{\text{iso}}$
P	−5041 (3)	8247	1007 (1)	1·38 (3)
O(7)	−3443 (8)	7700 (8)	128 (4)	2·17 (11)
O(8)	−7529 (7)	7685 (7)	615 (3)	1·71 (10)
O(9)	−4528 (8)	10268 (7)	1288 (4)	1·76 (10)
O(6)	−4098 (8)	7074 (8)	2074 (4)	2·05 (11)
C(1)	322 (10)	2587 (10)	2502 (5)	1·59 (13)
C(2)	2896 (10)	2795 (10)	3070 (5)	1·57 (14)
C(3)	2877 (10)	3931 (10)	4099 (5)	1·50 (14)
C(4)	1645 (10)	5798 (10)	3850 (5)	1·54 (14)
C(5)	−753 (10)	5566 (10)	3117 (5)	1·46 (13)
C(6)	−1766 (10)	7394 (10)	2682 (5)	2·16 (16)
O(1)	92 (8)	1525 (8)	1559 (4)	2·08 (11)
O(2)	3958 (9)	1045 (8)	3333 (4)	2·40 (12)
O(3)	5252 (8)	4231 (8)	4646 (3)	2·16 (11)
O(4)	1288 (8)	6670 (8)	4832 (4)	2·00 (11)
O(5)	−540 (8)	4422 (8)	2182 (3)	1·78 (10)
Na	−10186 (5)	9922 (5)	−345 (2)	2·40 (6)
H(1)	−44 (12)	189 (10)	296 (5)	2·5 (15)
H(2)	364 (10)	334 (9)	258 (4)	0·1 (11)
H(3)	214 (11)	307 (10)	466 (4)	1·7 (13)
H(4)	222 (14)	677 (12)	352 (6)	3·2 (18)
H(5)	−179 (11)	491 (10)	353 (5)	0·9 (13)
H(6)	−164 (11)	812 (10)	336 (4)	0·8 (12)
H′(6)	−126 (14)	797 (13)	250 (6)	4·2 (18)
O(1)H	−107 (15)	250 (14)	122 (6)	10·9 (41)
O(2)H	411 (16)	63 (14)	286 (7)	4·5 (22)
O(3)H	551 (13)	465 (11)	542 (5)	2·4 (16)
O(4)H	228 (12)	722 (10)	511 (5)	1·3 (14)
O(7)H	−404 (23)	666 (21)	−31 (9)	3·8 (20)

Table 2. *Bond lengths* (Å), *bond angles* (°) *and sodium coordination distances* (Å)

P–O(7)	1·587 (5)	C(2)–O(2)	1·408 (9)
P–O(8)	1·487 (4)	C(3)–C(4)	1·520 (10)
P–O(9)	1·506 (5)	C(3)–O(3)	1·433 (7)
P–O(6)	1·575 (5)	C(4)–C(5)	1·523 (8)
C(1)–O(1)	1·375 (8)	C(4)–O(4)	1·408 (8)
C(1)–O(5)	1·436 (9)	C(5)–C(6)	1·494 (10)
C(1)–C(2)	1·533 (8)	C(5)–O(5)	1·435 (8)
C(2)–C(3)	1·507 (9)	C(6)–O(6)	1·439 (8)

O(7)–P–O(8)	110·6 (3)	O(2)–C(2)–C(3)	110·7 (5)
O(7)–P–O(9)	106·3 (3)	C(2)–C(3)–C(4)	112·1 (5)
O(7)–P–O(6)	106·3 (3)	C(2)–C(3)–O(3)	109·3 (5)
O(8)–P–O(9)	118·4 (3)	O(3)–C(3)–C(4)	109·7 (5)
O(8)–P–O(6)	107·4 (3)	C(3)–C(4)–C(5)	111·6 (5)
O(9)–P–O(6)	107·1 (3)	C(3)–C(4)–O(4)	110·5 (5)
P–O(6)–C(6)	120·3 (4)	O(4)–C(4)–C(5)	107·7 (5)
O(1)–C(1)–C(2)	112·5 (5)	C(4)–C(5)–C(6)	112·0 (5)
C(2)–C(1)–O(5)	107·3 (5)	C(4)–C(5)–O(5)	110·0 (5)
O(1)–C(1)–O(5)	107·2 (5)	O(5)–C(5)–C(6)	107·2 (5)
C(1)–C(2)–C(3)	106·7 (5)	C(5)–C(6)–O(6)	108·6 (5)
C(1)–C(2)–O(2)	111·4 (5)	C(1)–O(5)–C(5)	112·1 (5)

Na–O(1^{iv})	2·59 (1)	Na–O(7^{ii})	2·87 (1)
Na–O(1^{ii})	2·86 (1)	Na–O(8^{i})	2·38 (1)
Na–O(5^{ii})	2·40 (1)	Na–O(8^{iii})	2·37 (1)
Na–O(7^{v})	2·60 (1)		

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

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* Lists of structure amplitudes, anisotropic thermal parameters, torsion angles, H-bond distances and angles and mean-plane calculations have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 42385 (14 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Phosphate group. The phosphate group carries a single negative charge, as the compound is a monosodium salt. The H atom attached to the phosphate group was clearly located near O(7). Since the other two terminal P—O bonds are nearly equal [P—O(8) = 1·487 (4); P—O(9) = 1·506 (5) Å], the single negative charge on the phosphate group is likely to be distributed between O(8) and O(9). The phosphate ester bond P—O(6) is 1·575 (5) Å, which is slightly shorter than the high-energy P ~ O bond in the structure of monopotassium phosphoenolpyruvate (Hosur & Viswamitra, 1981).

Glucose ring. The pyranose ring has the $^4C_1$ chair conformation (Fig. 1) with C(4) and C(1) displaced from the C(2)—C(3)—C(5)—O(5) plane by 0·608 (6) and −0·759 (6) Å. The Cremer & Pople (1975) puckering parameters are $Q = 0{\cdot}595\,(3)$ Å, $\theta = 10{\cdot}8\,(3)$ and $\varphi = 62{\cdot}2\,(15)°$. The distortion from the perfect-chair form is towards the $B_{1,4}$ geometry. The two endocyclic C—O bonds, C(5)—O(5) and C(1)—O(5), are almost equal [1·435 (8); 1·436 (9) Å] in contrast to that found in G6PBa (Katti *et al.*, 1982). The C(1)—O(1) distance (Table 2) follows the usual trend of being shorter than the other exocyclic C—O(H) distances. The torsion angles O(6)—C(6)—C(5)—O(5) and O(6)—C(6)—C(5)—C(4) are 63·7 (6) and −175·5 (5)° respectively. The conformation about the C(5)—C(6) bond is therefore *gauche–trans* in significant contrast to the *gauche–gauche* geometry (−70·3, 48·6°) found in G6PBa (Katti *et al.*, 1982).

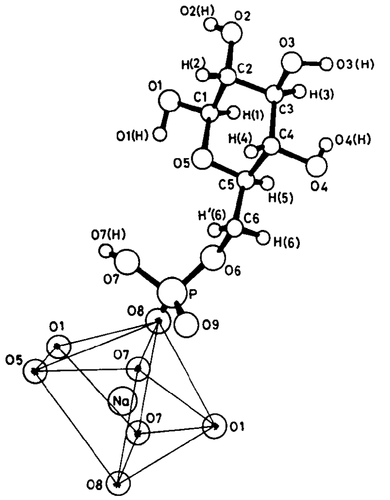

Fig. 1. The structure of the molecule, also showing the sodium coordination polyhedron.

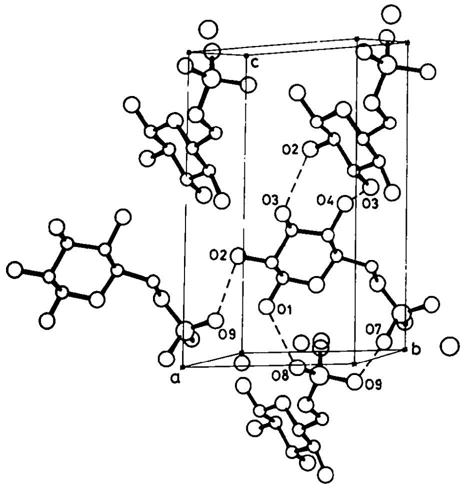

Fig. 2. The packing arrangement in the unit cell viewed approximately along **c**. Dashed lines indicate hydrogen bonds.

Sodium coordination. The Na^+ ion is surrounded by seven ligand O atoms within a distance of 2·9 Å (Table 2). Of these, four are phosphate O and the other three are sugar O atoms. The phosphate ester oxygen O(6) and also O(9) of the phosphate group are not involved in metal-ion binding (see Fig. 1).

*Molecular packing and hydrogen bonding.** The hydroxyls O(2) and O(3) take part in hydrogen bonds both as acceptors and as donors. The hydroxyls O(1), O(4) and O(7) act only as donors in the formation of hydrogen bonds. There is neither intramolecular hydrogen bonding nor the involvement of the ring O(5) and the phosphate ester O(6) in hydrogen-bond formation, unlike the situation in the structure of G6PBa (Katti *et al.*, 1982). The packing arrangement as viewed approximately along **c** shows the hydrogen bonds clearly (Fig. 2). The molecules related by the twofold screw axis are linked to each other through O(1)···O(8), O(3)···O(2), O(4)···O(3) and O(7)···O(9) hydrogen bonds.

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* See deposition footnote.

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Structure of N^6-Methyl-2′-deoxyadenosine

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Abstract. $C_{10}H_{15}N_5O_3$, $M_r = 265{\cdot}3$, orthorhombic, $P2_12_12_1$, $a = 10{\cdot}246\ (1)$, $b = 22{\cdot}686\ (2)$, $c = 5{\cdot}233\ (1)$ Å, $V = 1216{\cdot}4\ (2)$ Å^3, $Z = 4$, $D_x = 1{\cdot}448$ Mg m^{-3}, Mo $K\alpha$, $\lambda = 0{\cdot}7107$ Å, $\mu = 0{\cdot}12$ mm^{-1}, $F(000) = 560$, room temperature, final $R = 0{\cdot}037$ for 1490 observed reflections. The molecule has a C(1′)-*exo*—C(2′)-*endo* (${}^2_1T$) sugar associated with an *anti* base: O(4′)—C(1′)—N(9)—C(8) = 67·2 (3)°. The conformation about the C(4′)—C(5′) bond is *gauche–trans*; C(3′)—C(4′)—C(5′)—O(5′) = −170·7 (2)°. The orientation of the methyl substituent at N(6) is *anti* with respect to the purine ring. C(1′) is appreciably displaced from the imidazole ring [0·254 (2) Å]. There is an intermolecular short contact between C(8)—H and N(3).

Introduction. As part of a series of crystallographic investigations of nucleic-acid constituents the X-ray analysis of the title compound was carried out.

Experimental. Crystals grown from methanol/hexane solution by vapor diffusion. D_m not measured. Colorless plate, 0·08 × 0·35 × 0·35 mm. Rigaku AFC-5 diffractometer, graphite-monochromated Mo $K\alpha$ radiation. Lattice parameters refined by least-squares method (25 reflections, $30 < 2\theta < 37°$). ω scan ($2\theta \le 30°$), ω–2θ scan ($2\theta > 30°$), $2\theta_{\max} = 55°$; h 0 to 13, k 0 to 29, l 0 to 6. Three standard reflections: no variation. 1649 unique reflections, 1490 with $I \ge 0{\cdot}75\sigma(I)$ considered observed. No absorption correction. Structure solved by *MULTAN*78 (Main, Hull, Lessinger, Germain, Declercq & Woolfson, 1978), H atoms located from difference map. Block-diagonal least-squares refinement. Anisotropic temperature factors for non-H atoms, isotropic for H atoms. No correction for secondary extinction. $\sum w\Delta^2$ minimized, $\Delta = |F_o| - |F_c|$, $w = 1/\sigma^2(F_o)$ for $|F_c| \ge 3\sigma(F_o)$, $w = 0$ for $|F_c| < 3\sigma(F_o)$ or $|\Delta| \ge 3\sigma(F_o)$, $\sigma(F_o) = [\sigma_1{}^2(F_o) + 0{\cdot}00040|F_o|^2]^{1/2}$, $\sigma_1(F_o)$ = e.s.d. based on counting errors (Grant, Killean & Lawrence, 1969). $R = 0{\cdot}037$, $wR = 0{\cdot}042$, $S = 1{\cdot}07$. $(\Delta/\sigma)_{\max} = 0{\cdot}1$, $(\Delta\rho)_{\max} = 0{\cdot}4$ e Å^{-3}. Atomic scattering factors from *International Tables for X-ray Crystallography* (1974). Calculations performed on a FACOM-M34OR computer.

Discussion. Final atomic parameters are in Table 1.* Bond distances and angles are listed in Table 2. A perspective view of the molecule is shown in Fig. 1.

The deoxyribose ring is puckered in a C(1′)-*exo*–C(2′)-*endo* (${}^2_1T$) twist form. The pseudorotation coordinates of the five-membered ring (Sato, 1983) are $\Pi = 34{\cdot}5\ (2)°$ and $\Phi = 237{\cdot}9\ (4)°$. The conformation about the glycosidic bond is *anti*. This structure involves a short sugar–base contact between C(2′) and C(8) [3·090 (3) Å]. The conformation about the C(4′)—C(5′) bond is *gauche–trans:* C(5′)—O(5′) is *gauche* to C(4′)—O(4′) and *trans* to C(4′)—C(3′). As in other N^6-alkylated adenines (*e.g.* Takeda, Ohashi, Sasada & Kakudo, 1976), the orientation of the methyl substituent at N(6) is *anti* with respect to the purine ring, torsion angle C(5)—C(6)—N(6)—C(10) being −169·7 (2)°.

Compared with the bond distances and angles of the unsubstituted adenine base (Taylor & Kennard, 1982), those of the present structure are quite normal except for the exocyclic bond angles involving N(6): the angle N(1)—C(6)—N(6) is 1·8° larger than the standard value probably owing to a steric hindrance of the methyl group. The purine ring is slightly buckled: the N(1), C(2), N(3) and C(6) atoms are displaced by 0·025 (2), −0·025 (2), −0·024 (2) and 0·075 (2) Å, respectively, from the mean plane of the imidazole ring,

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* Lists of structure factors, anisotropic temperature factors and H-atom coordinates have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 42344 (13 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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