The calculations were carried out on the HITAC M-200H computer at the Computer Center of the Institute for Molecular Science with the *Universal Crystallographic Computation Program System UNICS* III (Sakurai & Kobayashi, 1979).

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Structure of Disodium Guanosine 5′-Phosphate Heptahydrate

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Abstract

$C_{10}H_{12}N_5O_8P^{2-}.2Na^+.7H_2O$ is orthorhombic, $P2_12_12_1$, with $a = 22{\cdot}267$ (2), $b = 21{\cdot}360$ (2), $c = 9{\cdot}035$ (1) Å, $Z = 8$, $V = 4297$ (2) Å^3, $M_r = 533{\cdot}3$, $D_c = 1{\cdot}65$, $D_o = 1{\cdot}63$ Mg m^{-3}, λ(Cu $K\alpha_1$) = 1·54051 Å, $T = 299$ ($\pm$1) K, $F(000) = 2224$. The intensity data were collected on an automated diffractometer, and the structure was solved by direct methods. Block-diagonal least-squares refinement of the non-hydrogen atoms and placement of the H atoms from difference Fourier maps or at calculated positions resulted in an R of 0·056 for 3927 reflections. The two independent GMP molecules, fourteen water molecules and four Na^+ ions in the asymmetric unit form an intricate network of hydrogen and coordination bonds, but the packing scheme does not include base–base hydrogen bonds or the base stacking often observed in crystal structures of guanine compounds. The sodium coordination shells, which can be described as distorted octahedra, involve no direct interactions with the ionized phosphate groups.

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Introduction

Guanosine 5′-phosphate (GMP) is one of the four common nucleotides of ribonucleic acids and an important metabolite. Disodium GMP crystallizes as the heptahydrate, space group $P2_12_12_1$, with $Z = 8$. Another crystal form of this nucleotide was reported earlier which displayed a hair-like habit, the crystals being too fine for single-crystal work (Zimmerman, 1976). Fiber diffraction studies of bundles of these crystals indicated a stacked arrangement of the GMP monomers, held together in a tetrameric hydrogen-bonded array. A stacked helical arrangement of the monomers of the monosodium salt of GMP is believed to be responsible for the unique viscous gels observed when aqueous solutions of the disodium salt are acidified (Sasisekharan, Zimmerman & Davies, 1975). In addition, base stacking has been observed in a majority of the crystal structures of the ribose nucleosides and ribose and deoxyribose mononucleotides of guanine and the related base hypoxanthine reported to date (Nagashima, Wakabayashi, Matsuzaki & Iitaka, 1974; Young, Tollin & Wilson, 1974; Murayama, Nagashima & Shimizu, 1969; Thewalt, Bugg & Marsh, 1970; Munns & Tollin, 1970). We have found that in the crystals of disodium GMP heptahydrate the guanine bases are not stacked but are instead arranged in a 'herringbone' pattern primarily stabilized by coordination of N(7) of the bases to an Na^+ ion.

Experimental

Disodium GMP obtained from Sigma Chemical Company was crystallized from an aqueous ethanol solution in a thermal gradient. The crystallization apparatus was similar to one recently described (Watkin, 1972). A specimen 0·05 × 0·1 × 0·3 mm was selected for diffraction study. The space group and approximate cell dimensions were determined from precession and Weissenberg photographs. More accurate cell dimensions were obtained by least-squares refinement with the use of the observed setting angles for twelve Cu $K\alpha_1$ reflections in the range $100 < 2\theta < 116°$, measured with an Oak Ridge computer-controlled diffractometer (Busing, Ellison, Levy, King & Roseberry, 1968). The density of the crystals was measured by flotation in mixtures of chloroform and dibromomethane. Intensity data were collected on the diffractometer with Ni-filtered Cu $K\bar{\alpha}$ radiation using the θ–2θ scan technique. Of 4220 reflections with $2\theta < 132°$, 3931 were considered observed $[F_o > 3\sigma(F_o)]$. Each structure factor was assigned a variance $\sigma^2(I)$ based on counting statistics plus a term $(0{\cdot}04I)^2$, empirically derived during refinement. No absorption correction was

Table 1. *Positional and thermal parameters* ($\times 10^4$) *for non-hydrogen atoms*

The isotropic temperature factor is $\exp[-8\pi^2 U(\sin\theta/\lambda)^2]$; for those atoms refined anisotropically the values given are the arithmetic average of the principal components of the anisotropic temperature factors. Standard deviations in units of the last significant digits are given in parentheses.

	Molecule *A*				Molecule *B*			
	x	*y*	*z*	*U* (Å²)	*x*	*y*	*z*	*U* (Å²)
N(1)	4112 (2)	−627 (2)	3187 (5)	313 (10)	5924 (2)	6711 (2)	−1791 (5)	290 (9)
C(2)	3681 (2)	−286 (2)	2480 (6)	300 (11)	6312 (3)	6350 (3)	−2603 (6)	317 (11)
N(2)	3159 (2)	−590 (2)	2259 (8)	481 (31)	6847 (2)	6609 (2)	−2945 (7)	437 (29)
N(3)	3753 (2)	298 (2)	2046 (5)	300 (9)	6203 (2)	5768 (2)	−3014 (5)	279 (9)
C(4)	4305 (2)	516 (2)	2354 (6)	252 (10)	5643 (2)	5587 (2)	−2618 (6)	232 (10)
C(5)	4772 (2)	206 (3)	3033 (6)	301 (11)	5203 (2)	5925 (2)	−1887 (6)	268 (11)
C(6)	4689 (2)	−423 (3)	3487 (7)	326 (11)	5339 (2)	6543 (2)	−1406 (6)	295 (11)
O(6)	5046 (2)	−784 (2)	4103 (6)	492 (26)	5018 (2)	6919 (2)	−753 (6)	464 (25)
N(7)	5280 (2)	586 (2)	3121 (6)	359 (11)	4683 (2)	5577 (2)	−1756 (5)	329 (10)
C(8)	5111 (3)	1109 (3)	2497 (7)	331 (12)	4815 (3)	5041 (3)	−2366 (7)	321 (12)
N(9)	4528 (2)	1101 (2)	2041 (5)	276 (9)	5392 (2)	5013 (2)	−2910 (5)	262 (9)
C(1′)	4219 (2)	1620 (2)	1294 (6)	236 (10)	5673 (2)	4496 (2)	−3658 (6)	256 (10)
C(2′)	4190 (2)	2211 (2)	2236 (6)	246 (10)	5708 (2)	3895 (2)	−2740 (6)	253 (10)
O(2′)	3669 (2)	2185 (2)	3157 (4)	329 (19)	6230 (2)	3915 (2)	−1851 (5)	367 (21)
C(3′)	4191 (2)	2731 (2)	1076 (6)	255 (10)	5711 (2)	3396 (2)	−3934 (6)	283 (11)
O(3′)	3587 (2)	2802 (2)	565 (5)	311 (19)	6306 (2)	3336 (2)	−4449 (5)	447 (24)
C(4′)	4596 (2)	2454 (2)	−105 (6)	217 (9)	5298 (2)	3669 (2)	−5127 (6)	230 (10)
O(1′)	4556 (2)	1781 (2)	21 (4)	276 (8)	5321 (2)	4344 (2)	−4928 (4)	286 (8)
C(5′)	5246 (2)	2660 (2)	−78 (6)	281 (11)	4661 (2)	3449 (3)	−5104 (6)	298 (11)
O(5′)	5521 (2)	2544 (2)	1341 (4)	274 (7)	4392 (2)	3552 (2)	−3689 (4)	271 (7)
O(6′)	6360 (2)	3296 (2)	764 (4)	269 (7)	3546 (2)	2802 (2)	−4213 (4)	253 (7)
O(7′)	6552 (2)	2139 (2)	589 (4)	305 (8)	3379 (2)	3957 (2)	−4507 (5)	308 (8)
O(8′)	6366 (2)	2635 (2)	3083 (4)	324 (8)	3541 (2)	3496 (2)	−1948 (4)	283 (8)
P	6243·6 (5)	2656·8 (6)	1440·1 (1·4)	192 (2)	3672·1 (5)	3447·1 (6)	−3586·0 (1·5)	197 (2)

Table 1 (*cont.*)

	x	y	z	U (Å^2)
Na(1)	6149·6 (1·0)	579·2 (1·0)	−5282 (3)	342 (11)
Na(2)	7000·2 (1·1)	1740·5 (1·3)	−3382 (3)	398 (12)
Na(3)	2869·0 (1·1)	4509·3 (1·1)	992 (3)	359 (11)
Na(4)	7138·6 (1·4)	3413·7 (1·7)	−2943 (5)	710 (21)
W(1)	6159 (2)	1671 (2)	−5001 (5)	362 (20)
W(2)	2997 (2)	3669 (2)	2681 (5)	375 (22)
W(3)	2416 (2)	3832 (2)	−933 (5)	375 (21)
W(4)	3077 (2)	5128 (2)	−3297 (6)	468 (26)
W(5)	2377 (2)	2499 (2)	−4908 (6)	436 (23)
W(6)	7308 (2)	2514 (2)	−1577 (5)	423 (23)
W(7)	3820 (2)	4455 (2)	−67 (5)	374 (21)
W(8)	6705 (2)	283 (2)	2430 (6)	489 (27)
W(9)	6314 (2)	1299 (2)	−1584 (6)	477 (25)
W(10)	7163 (2)	562 (2)	−4527 (6)	528 (28)
W(11)	7065 (3)	5127 (3)	−774 (9)	774 (42)
W(12)	2980 (3)	1151 (4)	3949 (12)	1168 (67)
W(13)	2569 (5)	1066 (5)	537 (10)	1569 (85)
W(14)	4129 (4)	4949 (4)	−5369 (9)	955 (54)

applied. No significant changes in two standard reflections were observed during the course of the data collection.

The structure was solved using the direct-methods program *MULTAN* (Germain, Main & Woolfson, 1971). Phase sets were generated using 412 $|E|$'s > 1·6. A Fourier synthesis calculated with the phase set having the highest combined figure of merit (CFM = 2·370, ABSFOM = 1·176, RESID = 33·9%) revealed the positions of 37 of the 48 non-hydrogen atoms of the GMP anions as well as several of the water molecules and Na^+ ions. The structure was completed from successive Fourier syntheses. The 66 non-hydrogen atoms in the asymmetric unit were refined by block-diagonal least-squares methods. Following initial isotropic refinement, those atoms with unusually high temperature factors were allowed to refine anisotropically. 44 of the total of 52 H atoms were included in the model during the final stages of refinement. Those H atoms whose positions could be calculated with confidence were placed at calculated positions which were updated after each round of refinement. The remainder of the H atoms were located from difference Fourier syntheses, except those of waters 11, 12, 13 and 14. All H atoms were arbitrarily assigned temperature factors approximately equivalent to those of the atoms to which they were bonded. Structure factors calculated with the H atoms alone were applied as a partial contribution during refinement of the non-hydrogen atoms. The quantity minimized during refinement was $\sum w(|F_o| - |F_c|)^2$ with $w = 1/\sigma^2(F_o)$. The final values of R, the weighted R $\{[\sum w(F_o - F_c)^2/\sum wF_o^2]^{1/2}\}$, and σ, the goodness of fit $\{[\sum w(F_o - F_c)^2/(n - p)]^{1/2}$, where n = 3927 reflections and p = 396 variables$\}$, were 0·056, 0·075 and 1·76, respectively. Four reflections were excluded from the final refinement because their weighted structure factor differences were greater than six times the standard deviation for an observation of unit weight. The average shift on the final cycle of refinement was 25% of the estimated standard deviation. All refinements were performed with the XRAY system (Stewart, Kruger, Ammon, Dickinson & Hall, 1972). The final atomic parameters are given in Table 1.*

Discussion

The two crystallographically independent GMP molecules in the asymmetric unit are quite similar and display no surprising conformational parameters (Fig. 1). Both ribose rings are in the 2′-*endo* conformation

* Lists of structure factors, anisotropic thermal parameters and H atom positional parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 36447 (27 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

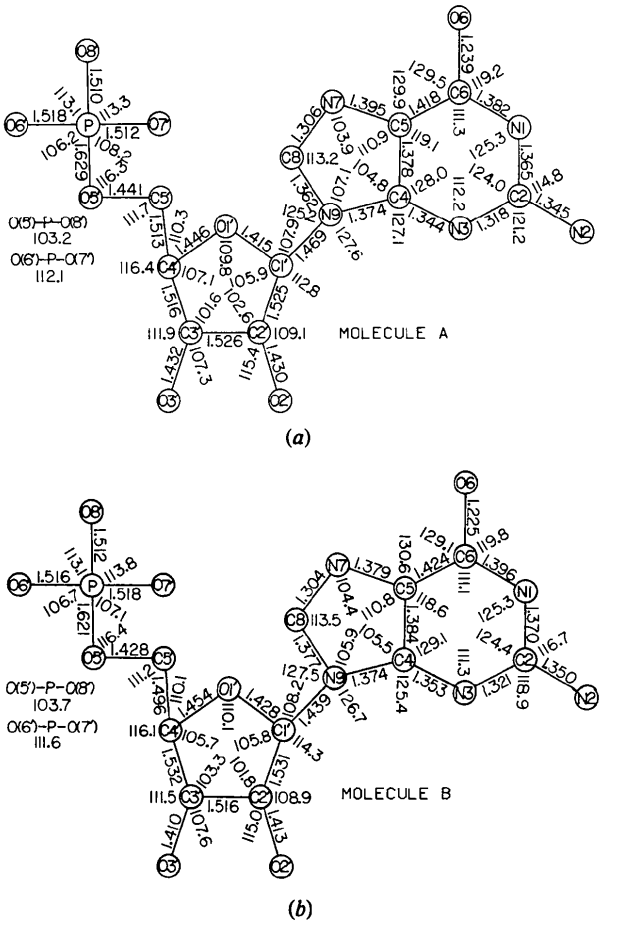

Fig. 1. Bond distances (Å) and angles (°) for (*a*) molecule *A* and (*b*) molecule *B*. The average standard deviation in the bond lengths and bond angles is 0·007 Å and 0·5°, respectively.

Table 2. *Torsion angles and ribose pseudo-rotation parameters for molecules A and B* (°)

		A	*B*
χ	O(1′)–C(1′)–N(9)–C(8)	55·5 (7)	57·4 (7)
τ_0	C(4′)–O(1′)–C(1′)–C(2′)	−15·8 (5)	−18·4 (5)
τ_1	O(1′)–C(1′)–C(2′)–C(3′)	32·0 (5)	33·5 (5)
τ_2	C(1′)–C(2′)–C(3′)–C(4′)	−34·9 (5)	−35·2 (5)
τ_3	C(2′)–C(3′)–C(4′)–O(1′)	26·6 (5)	25·4 (5)
τ_4	C(3′)–C(4′)–O(1′)–C(1′)	−7·2 (5)	−4·4 (5)
φ	P–O(5′)–C(5′)–C(4′)	171·9 (3)	169·8 (3)
ψ	O(5′)–C(5′)–C(4′)–C(3′)	55·5 (6)	55·1 (6)
ψ'	C(5′)–C(4′)–C(3′)–O(3′)	148·4 (4)	147·8 (5)
Ribose pseudorotation parameters			
P	Phase angle from ^3_2T	173·5	169·7
τ_m	Magnitude of pucker	35·2	35·7
	Conformational descriptor	$^2T_3$	$^2T_3$

and the *anti* conformation relative to the bases. The conformation about the exocyclic C(4′)–C(5′) sugar bond in both molecules is *gauche*$^+$. The relevant torsion angles and ribose conformational descriptors are given in Table 2.

Fig. 2 is a stereoview of the packing, showing the alternating layers of solvent and nucleotide molecules. Despite the high degree of hydration in this crystal, there is no apparent disorder of the non-hydrogen solvent atoms. Table 3 is a list of the hydrogen bonds present in the structure. It should be noted that difficulty in the placement of some of the water H atoms results in ambiguities in the assignment of donor and acceptor status in the last several hydrogen bonds listed. The two GMP molecules, fourteen water molecules and four Na^+ ions in the asymmetric unit form an intricate network of hydrogen and coordination bonds (Table 4). There are no base–base hydrogen bonds in the structure; such bonds are important in the description of the spontaneously formed helix of the gel of the monosodium salt and of the packing in the hair-like crystals of the disodium salt (Sasisekharan *et al.*, 1975; Zimmerman, 1976). The atoms involved in base pairing in double-stranded polynucleotides, N(1), N(2) and O(6), are in this case hydrogen bonded to a phosphate oxygen and waters, respectively. The pseudo-twofold symmetry resulting from this hydrogen-bonding pattern and the above mentioned N(7)–Na^+ coordination is shown in Fig. 3. The view of Fig. 3 is down the *a* axis; the pseudo-twofold axis is normal to the plane of the figure at the position of Na(1). Fig. 4 shows the relation of the pseudo-twofold axes to the crystallographic symmetry operations and the resulting pseudo-twofold screw axis.

Fig. 5 shows the Na^+-ion coordination. Each of the four Na^+ ions is coordinated to six ligands. The coordination shells about Na^+ ions 1 and 3 are fairly regular octahedra while those about Na^+ ions 2 and 4 are more distorted. The mechanisms by which metal

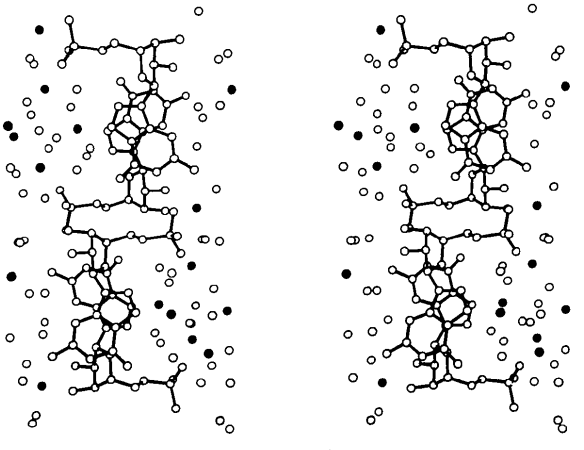

Fig. 2. Stereoview of packing interactions. The view is down the *c* axis. The Na^+ ions are shown as shaded ellipsoids. The thermal ellipsoids are drawn at the 50% probability level. Illustrations were prepared with the aid of the computer program *ORTEP* (Johnson, 1965).

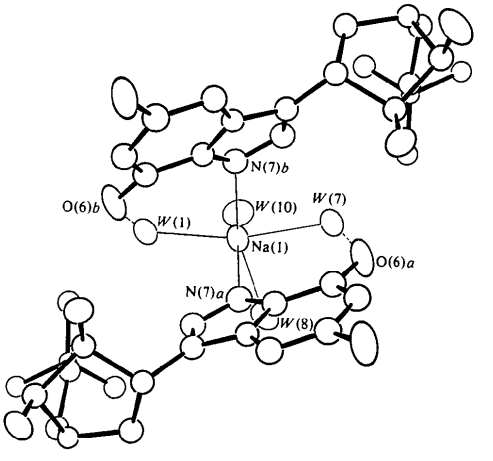

Fig. 3. View of near-symmetric coordination of Na(1). The view is down the *a* axis. The thin solid lines indicate sodium coordination; the dotted lines indicate hydrogen bonds. The thermal ellipsoids are drawn at the 50% probability level.

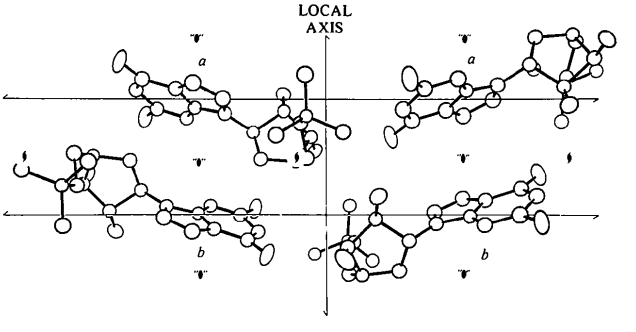

Fig. 4. Relation of pseudosymmetry elements to crystallographic symmetry axes. The view is along the *a* axis. The crystallographic symmetry elements are indicated by standard symbols. Pseudo-twofold axes are indicated by symbols in quotes; the pseudo-twofold screw axis, labelled LOCAL AXIS, is generated by operation on the pseudo-twofold axes of the crystal symmetry elements.

Table 3. *Distances and angles in the hydrogen bonds and close contacts, D—H···A*

The donor atom belongs to the basic set listed in Table 1 and the acceptor atom is related to this set by the symmetry operations of the space group and/or translations. The code used (shown as a suffix to the atom label) is as follows:

(1)	x,	y,	z	(7)	$-\frac{1}{2}+x$,	$\frac{1}{2}-y$,	$-z$
(2)	x,	y,	$1+z$	(8)	$1-x$,	$\frac{1}{2}+y$,	$\frac{1}{2}-z$
(3)	x,	y,	$-1+z$	(9)	$1-x$,	$\frac{1}{2}+y$,	$-\frac{1}{2}-z$
(4)	$\frac{1}{2}-x$,	$1-y$,	$\frac{1}{2}+z$	(10)	$1-x$,	$-\frac{1}{2}+y$,	$\frac{1}{2}-z$
(5)	$\frac{1}{2}+x$,	$\frac{1}{2}-y$,	$-z$	(11)	$1-x$,	$-\frac{1}{2}+y$,	$-\frac{1}{2}-z$
(6)	$\frac{1}{2}+x$,	$\frac{1}{2}-y$,	$-1-z$				

Donor (*D*) Acceptor (*A*)	Distance (Å) *D*—*A*	H—*A*	*D*—H···*A* angle (°)
N(1)*a*···O(6′)*a* 10	2·702 (6)	1·9*	166*
N(1)*b*···O(6′)*b* 9	2·765 (6)	1·9	170
N(2)*a*···*W*(11) 7	2·953 (9)	2·1	167
N(2)*b*···W(13) 9	2·919 (12)	2·2	148
O(3′)*a*···O(8′)*b* 1	2·713 (6)	2·0	175
O(2′)*a*···O(6′)*b* 2	2·730 (6)	1·8	167
O(3′)*b*···O(8′)*a* 3	2·690 (6)	2·0	171
O(2′)*b*···O(6′)*a* 1	2·723 (6)	1·9	158
W(1)···O(8′)*a* 3	2·730 (6)	2·0	169
W(1)···O(6)*b* 11	2·759 (6)	1·9	177
W(2)···O(3′)*a* 1	2·968 (6)	2·3	156
W(2)···O(7′)*b* 2	2·749 (6)	1·8	153
W(3)···O(8′)*b* 1	2·761 (6)	1·9	160
W(3)···O(7′)*a* 7	2·947 (6)	2·0	155
W(4)···*W*(9) 9	2·849 (7)	2·1	142
W(4)···O(7′)*b* 1	2·811 (6)	1·8	174
W(5)···O(8′)*a* 7	2·806 (6)	2·0	150
W(5)···O(6′)*b* 1	2·752 (6)	2·0	161
W(6)···O(7′)*a* 1	2·703 (6)	2·0	170
W(6)···O(3′)*a* 5	3·066 (6)	2·3	154
W(7)···O(6)*a* 8	2·718 (6)	1·8	174
W(7)···O(8′)*b* 1	2·733 (6)	2·0	155
W(8)···*W*(14) 11	2·725 (10)	1·9	163
W(8)···*W*(3) 5	2·814 (7)	2·0	171
W(9)···O(7′)*a* 1	2·711 (6)	1·8	161
W(9)···*W*(4) 11	2·849 (7)		
W(10)···O(7′)*b* 6	3·025 (6)	2·2	164
W(10)···*W*(4) 11	2·767 (8)	2·0	160
W(11)···*W*(12) 8	2·740 (12)		
W(11)···N(3)*b* 1	3·105 (10)		
W(12)···O(2′)*a* 1	2·782 (9)		
W(12)···N(3)*a* 1	3·038 (10)		
W(13)···*W*(11) 7	2·793 (12)	1·9	167
W(14)···O(7′)*b* 1	2·808 (9)		
W(14)···O(1′)*b* 1	2·979 (9)		

* Hydrogen atoms were not refined. Therefore these values have no e.s.d.'s.

ions interact with nucleotides have recently been reviewed by Sternglanz, Subramanian, Lacey & Bugg (1976) in their paper reporting the structure of barium adenosine 5′-monophosphate heptahydrate. In that structure the barium ion was found to be completely hydrated, forming an outer-sphere complex with the nucleotide. In the present structure, two of the Na^+ ions are completely hydrated (2 and 3) and the other two (1 and 4) form inner-sphere complexes with N(7)*a* and N(7)*b* and with O(2′)*b* and O(3′)*b*, respectively. Na(1) is 0·94 and 0·67 Å, respectively, from the least-squares planes of the purine rings of molecules *A* and *B*. The equations of the planes, calculated by a locally written program, are $0{\cdot}3422x + 0{\cdot}3541y + 0{\cdot}8704z = 9{\cdot}7689$ and $0{\cdot}3134x - 0{\cdot}3294y - 0{\cdot}8907z = 0{\cdot}7574$. There is no direct Na^+-ion coordination to phosphate O atoms.

Table 4. *Sodium coordination (distances in* Å)

The symmetry operations are as defined in Table 3.

Na(1)···*W*(1) 1	2·346 (5)	Na(3)···*W*(2) 1	2·373 (5)
···*W*(7) 11	2·423 (5)	···*W*(3) 1	2·476 (5)
···*W*(8) 3	2·491 (6)	···*W*(4) 4	2·334 (5)
···*W*(10) 1	2·358 (5)	···*W*(7) 1	2·328 (5)
···N(7)*a* 3	2·415 (6)	···*W*(8) 8	2·379 (6)
···N(7)*b* 11	2·613 (5)	···*W*(10) 9	2·611 (6)
Na(2)···*W*(1) 1	2·382 (5)	Na(4)···*W*(5) 6	2·803 (6)
···*W*(2) 5	2·468 (5)	···*W*(6) 1	2·315 (6)
···*W*(5) 6	2·393 (6)	···*W*(12) 5	2·281 (9)
···*W*(6) 1	2·421 (5)	···*W*(13) 5	2·623 (11)
···*W*(9) 1	2·422 (6)	···O(2′)*b* 1	2·492 (5)
···*W*(10) 1	2·746 (6)	···O(3′)*b* 1	2·305 (6)

From the preponderance of purine structures involving a stacked arrangement of the aromatic bases, it is reasonable to conclude that such base stacking is highly favored in achieving an energy minimum in the molecular packing of guanine nucleosides and nucleotides. More generally, any molecule with a sufficiently large and dominant planar substituent would tend to pack with the aromatic portions stacked. The packing scheme achieved by disodium GMP heptahydrate is indicative of alternative interactions possible with this nucleotide. Similar interactions with solvent and cations were observed in the structure of monosodium inosine 5′-phosphate hexahydrate (Rao & Sundaralingam, 1969), suggesting the importance of the degree of hydration in determining the mode of packing. Such interactions with solvent and cations must be considered in a complete description of polynucleotide structures in aqueous environments.

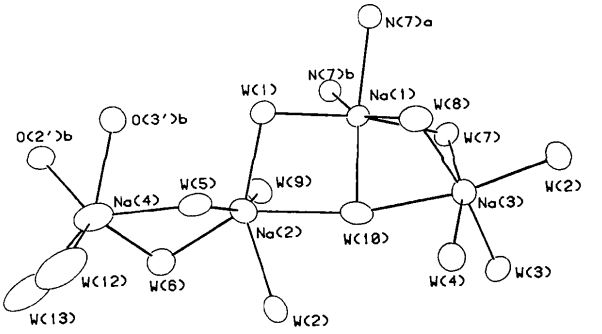

Fig. 5. Na^+-ion coordination polyhedra. The bonds indicate coordination interactions. The polyhedra interactions are: Na(1) and Na(3) share a face composed of *W*(7), *W*(8) and *W*(10); Na(1) and Na(2) share an edge, *W*(1) and *W*(10); Na(2) and Na(4) share an edge, *W*(5) and *W*(6); Na(2) and Na(3) share an apex, *W*(2). Coordination distances are listed in Table 4.

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Note added in proof: While this paper was in the press, the structure of disodium GMP heptahydrate was published by Katti, Seshadri & Viswamitra (1981). The two structures are identical, with cell constants, positional parameters and derived quantities varying by generally no more than one to two times the estimated standard deviations. Though Katti *et al.* describe the base rings as being 'stacked' because of the extensive overlap, we prefer to reserve that term for instances in which the planes of the aromatic rings are nearer to parallel. In the present structure there is a 38° angle between the planes of the bases of molecules *A* and *B*.

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