STRUCTURE AND CONFORMATION OF DISODIUM GUANOSINE-5′-PHOSPHATE HEPTAHYDRATE $C_{10}H_{13}N_5O_8PNa_2.7H_2O$

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ABSTRACT

Guanosine-5′-phosphate heptahydrate (5′-GMPNa$_2$.7H$_2$O) crystallises in the orthorhombic space group $P2_12_12_1$ with unit cell dimensions $a = 22{\cdot}259$ (4), $b = 21{\cdot}356$ (4), $c = 9{\cdot}040$ (2) Å and two molecules in the asymmetric unit. The current residual with the anisotropic temperature factors for the heavy atoms is 0·086. The conformation of the guanine base with respect to the sugar is *anti*. The furanose ring shows the usual C2′-*endo* puckering and *gg* conformation about the C4′-C5′ bond unlike the 5′-dGMPNa$_2$ which shows O1′-*endo*, *gt* conformation in its crystal structure. Also, the phosphate oxygens and O6 atom of the guanine base are not involved in the sodium coordination unlike in the 5′-dGMP.Na$_2$ structure. There is extensive overlap of the bases separated by 3·3 Å.

WE wish to report here the molecular structure of disodium guanosine-5′-phosphate heptahydrate (5′-GMPNa$_2$.7H$_2$O) (Fig. 1) as determined by a three dimensional X-ray analysis. This investigation was taken up to find out to what extent the geometry of ribonucleotides differs from that of deoxyribonucleotides[1–3]. The structure of 5′-dGMPNa$_2$ had been determined earlier[4,5].

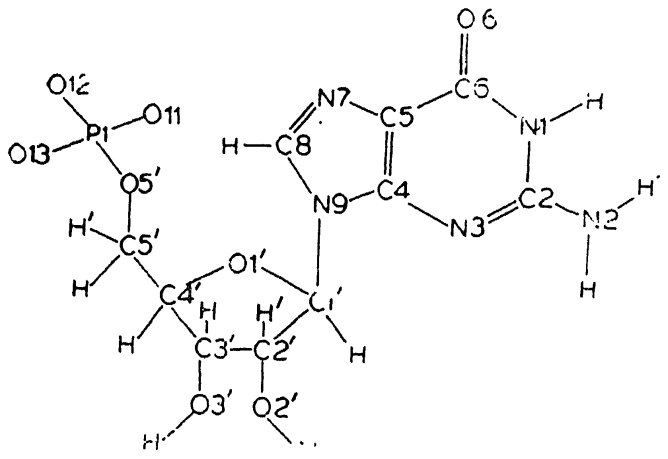

FIG. 1. Numbering of atoms in 5′-GMP.

Crystals of 5′-GMPNa$_2$ were grown by slow diffusion of alcohol into aqueous solutions of the compound. The crystals belong to orthorhombic space group $P2_12_12_1$ with unit cell dimensions, $a = 22{\cdot}259$ (4), $b = 21{\cdot}356$ (4), $c = 9{\cdot}040$ (2) Å. Density measurements indicated the presence of two nucleotide and 14 water molecules in the asymmetric unit of the cell. CuK_α intensity data consisting of 3925 unique reflections up to $\sin\theta/\lambda = 0{\cdot}59$ Å^{-1} were collected on a CAD-4 diffractometer. The structure was solved by a combination of direct methods and difference Fourier synthesis. The hydrogen atoms wherever possible were fixed from their expected geometry. The current residual after several cycles of block diagonal least square refinement with anisotropic temperature factors is 8·6% (Table I). Further refinement is in progress.

TABLE I

Positional parameters of the nonhydrogen atoms (e.s.d.s. given in the parentheses). All parameters and e.s.d.s. are multiplied by 10^4

Atoms	*x*	*y*	*z*
Molecule A			
P1	8757 (1)	2343 (1)	6434 (3)
O11	8451 (3)	2864 (3)	5591 (9)
O12	8630 (3)	2365 (3)	8114 (8)
O13	8633 (3)	1704 (3)	5784 (9)
O5′	9481 (3)	2454 (3)	6312 (8)
C5′	9750 (4)	2338 (5)	4886 (12)
C4′	10408 (5)	2547 (5)	4872 (12)
O1′	10446 (3)	3215 (3)	5028 (8)
C3′	10810 (4)	2267 (4)	6087 (12)
O3′	11409 (3)	2189 (4)	5549 (9)
C2′	10814 (4)	2783 (4)	7258 (11)
O2′	11331 (3)	2817 (3)	8166 (8)
C1′	10782 (4)	3390 (4)	6281 (12)
N9	10475 (4)	3900 (4)	7023 (10)
C8	9880 (5)	3884 (5)	7484 (15)
N7	9722 (4)	4419 (4)	8126 (12)
C6	10314 (5)	5416 (5)	8475 (14)
O6	9949 (4)	5791 (4)	9111 (12)
C5	10226 (5)	4798 (5)	8031 (13)
C4	10696 (5)	4483 (5)	7340 (11)
N3	11252 (4)	4698 (4)	7058 (11)
C2	11313 (5)	5277 (5)	7465 (13)
N2	11845 (5)	5594 (5)	7241 (13)
N1	10888 (4)	5637 (4)	8204 (10)

TABLE I (*Contd.*)

Atoms	*x*	*y*	*z*
Molecule B			
P2	6329 (1)	3443 (1)	8590 (3)
O21	6618 (3)	3951 (3)	9480 (9)
O22	6468 (3)	3497 (3)	6915 (8)
O23	6454 (3)	2802 (3)	9191 (8)
O5′	5612 (3)	3552 (3)	8699 (8)
C5′	5336 (5)	3433 (5)	10115 (12)
C4′	4703 (4)	3674 (4)	10114 (12)
O1′	4679 (3)	4341 (3)	9940 (8)
C3′	4284 (5)	3386 (5)	8915 (13)
O3′	3693 (3)	3338 (4)	9468 (10)
C2′	4298 (5)	3904 (4)	7739 (12)
O2′	3766 (3)	3904 (4)	6835 (9)
C1′	4320 (4)	4492 (4)	8683 (12)
N9	4605 (4)	5012 (4)	7895 (11)
C8	5189 (5)	5033 (5)	7349 (14)
N7	5318 (4)	5572 (4)	6752 (11)
C6	4655 (5)	6554 (5)	6413 (14)
O6	4977 (4)	6924 (4)	5752 (11)
C5	4799 (5)	5918 (4)	6889 (13)
C4	4355 (4)	5578 (5)	7625 (11)
N3	3795 (4)	5771 (4)	7999 (10)
C2	3680 (6)	6342 (5)	7606 (13)
N2	3145 (4)	6605 (5)	7946 (13)
N1	4066 (4)	6715 (4)	6785 (10)
Na1	8848 (2)	4425 (2)	9718 (5)
Na2	3003 (2)	1740 (2)	8376 (5)
Na3	2131 (2)	496 (2)	6009 (5)
Na4	2858 (2)	3426 (3)	7921 (8)
W1	6174 (4)	4445 (4)	5066 (10)
W2	1990 (4)	1340 (4)	7683 (9)
W3	7587 (3)	3818 (4)	5929 (10)
W4	7620 (3)	2501 (4)	9903 (10)
W5	2695 (4)	2517 (4)	6544 (9)
W6	2830 (4)	552 (4)	9514 (11)
W7	8849 (3)	3323 (4)	9988 (10)
W8	9135 (7)	5052 (7)	5369 (18)
W9	8299 (4)	4720 (4)	7417 (11)
W10	2036 (6)	3838 (8)	9050 (22)
W11	3685 (4)	1301 (4)	6604 (10)
W12	3077 (4)	121 (4)	6707 (11)
W13	2059 (5)	4881 (6)	814 (14)
W14	2408 (7)	3975 (7)	5592 (16)

Both the nucleotide molecules in the asymmetric unit have identical conformational features. The orientation of the guanine base with respect to the ribose sugar is *anti*, with $\chi_{CN} = 53{\cdot}6°$ (·9°) and 55·7° (·9°) for molecules A and B respectively. The C2′ atom is displaced from the plane of the rest of the atoms on the same side of C5′ atom by 0·50 and 0·57 Å (·01) for molecules A and B respectively. The furanose ring conformation is, therefore, C2′-*endo*. The conformation about the C4′–C5′ bond is the common *gauche-gauche* with $\Phi_{OO} = -66{\cdot}9°$ (Mol. A); $-63{\cdot}6°$ (Mol. B); $\Phi_{OC} = 54{\cdot}0°$ (Mol. A); 59·4° (Mol. B) (e.s.d. = 0·9°). Thus, 5′-GMP has the usual *anti*, C2′-*endo*, *gg* nucleotide conformations unlike 5′-dGMP which shows unusual *anti*, O1′-*endo*, *gt* conformations (Fig. 2).

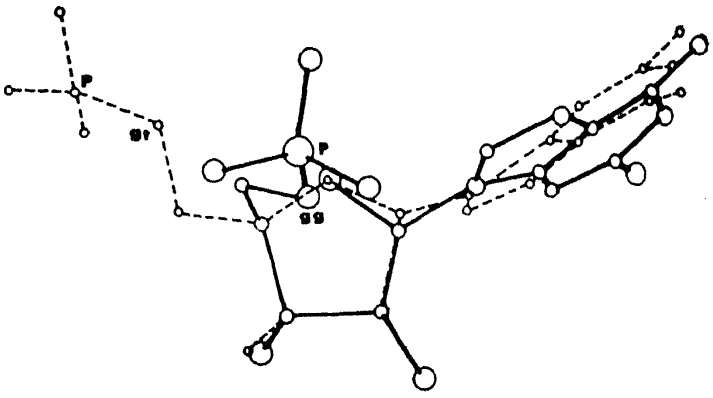

FIG. 2. 5′-GMP structure (dark lines) is superposed over the 5′-dGMP structure (dotted lines). The view is down the perpendicular to the plane of C2′–C3′–C4′ atoms. The *gg* and *gt* conformational differences can be clearly seen.

There are four crystallographically independent sodium ions in the structure. Na1 coordinates with water oxygen and imino nitrogen atoms of the base. Na2 and Na3 are completely surrounded by water oxygens. Na4 has four water oxygen and two ribose oxygen atoms as its neighbours as shown in Fig. 3. The phosphate oxygens and O6 atom of the guanine base are not involved in the sodium coordination unlike in the 5′-dGMP.Na$_2$ structure. Also, each of the sodium ion has six near neighbours in contrast to the 5′-dGMP.Na$_2$ structure where one of the sodiums is five coordinated. There is an extensive overlap of the bases separated by a distance of 3·3 Å. When this investigation was in progress a short report of 5′-GMP.Na$_2$ structure with closely similar results

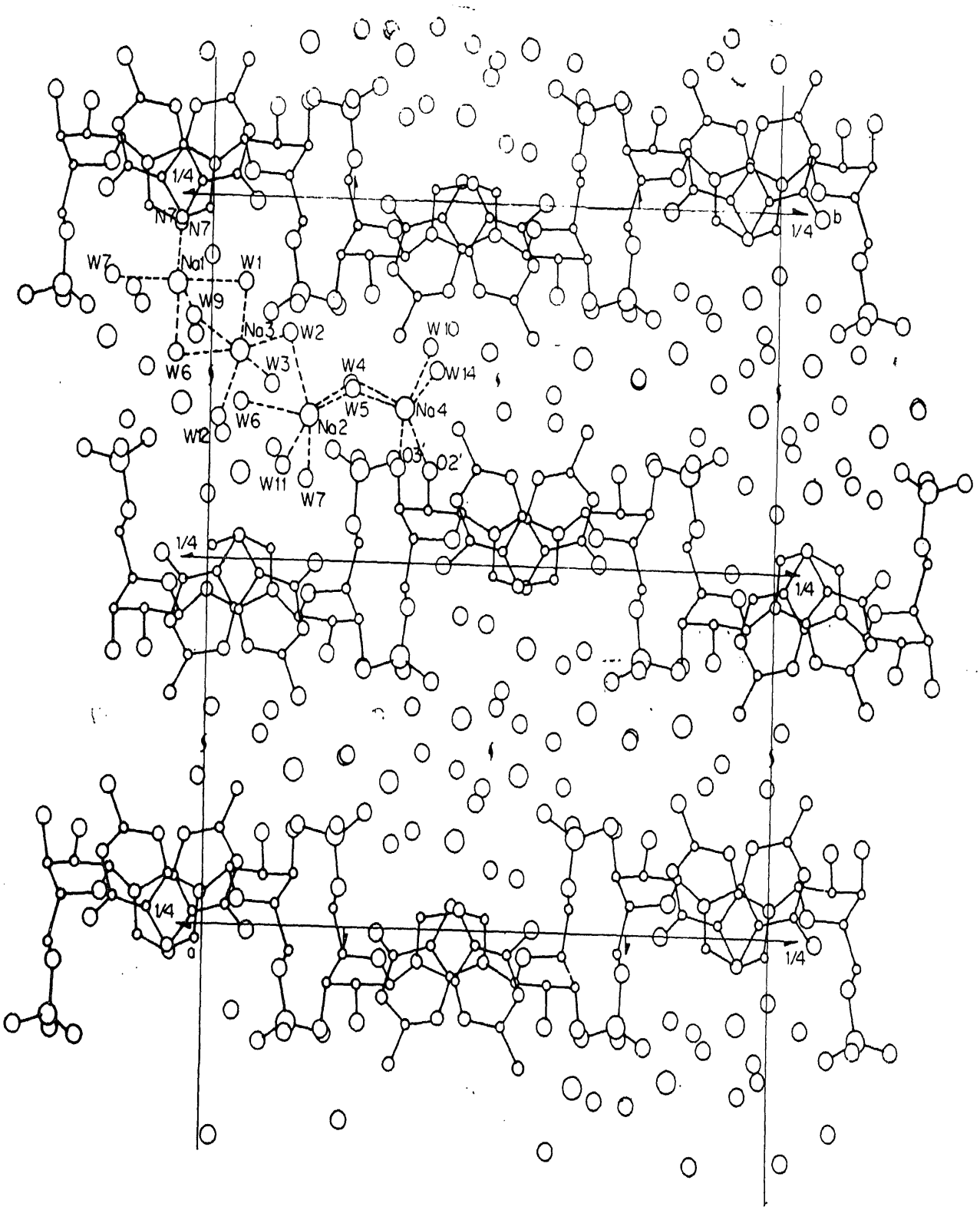

FIG. 3. Packing of 5'-GMP molecules in the unit cell viewed down *c*-axis. Sodium coordination is shown in dotted lines.

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