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**Key indicators**

Single-crystal X-ray study  
T = 105 K  
Mean  $\sigma(C-C)$  = 0.001 Å  
Disorder in solvent or counterion  
R factor = 0.034  
wR factor = 0.092  
Data-to-parameter ratio = 39.0

For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

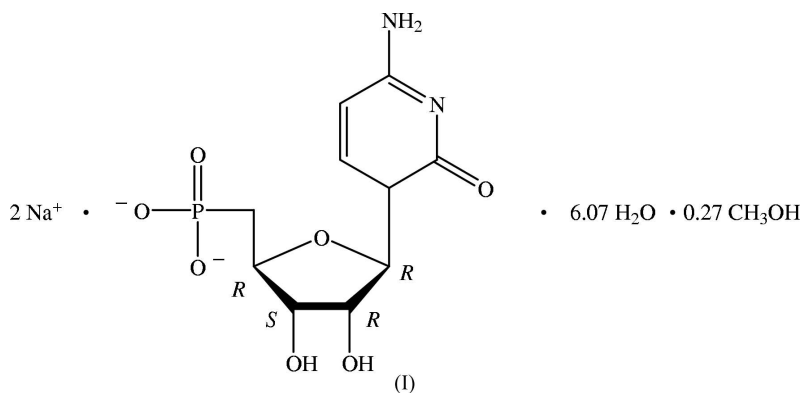
**Disodium cytidine-5'-monophosphate 6.07-hydrate methanol 0.27-solvate**

The crystal structure of the title complex,  $Na_2^+ \cdot C_9H_{12}N_3O_8P^- \cdot 6.07H_2O \cdot 0.27CH_4O$ , in space group  $P2_12_12_1$  is remarkably similar to the monoclinic  $P2_1$  structure of sodium cytidine-5'-monophosphate 6.5 hydrate [Borodi *et al.* (2001). *Acta Cryst. E57*, m514–m516].

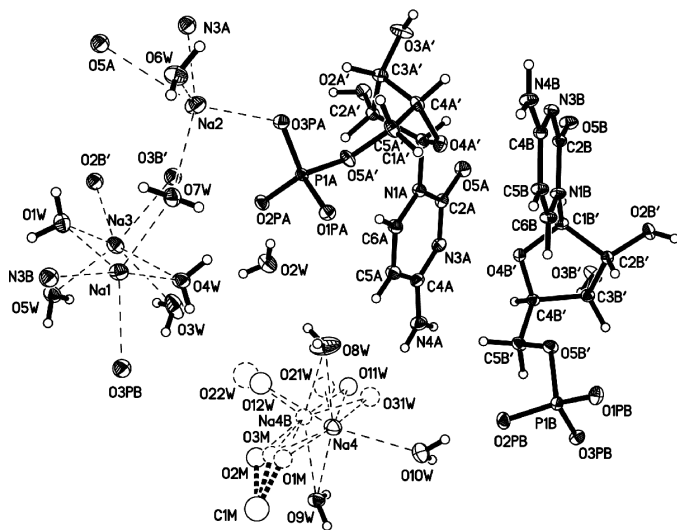
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**Comment**

The extent of molecular packing and complexing with nuclear proteins (histones) influences significantly the physical and chemical alterations of DNA induced by ionizing radiation (Becker & Sevilla, 1998; Weiland & Hüttermann, 2000). Model studies of crystalline 1:1 complexes of an amino acid and a nucleic acid constituent are useful for understanding mechanisms for charge transfers between the partners of the complex following the radiation-induced charge injection. For the purpose of electron paramagnetic resonance (EPR) studies of the radiation action on such systems, single crystals are the preferred type of sample. The crystal parameters of the cytidine-5'-monophosphate (CMP)–arginine complex have been reported (Bhat & Vijayan, 1973), but a full study has not been published. A preliminary study of crystals made for EPR studies revealed unit-cell parameters different from those previously published. Hence, a new structure analysis was undertaken.



When the structure was solved, it immediately became clear that the crystal did not contain arginine, but rather represented a new form of  $Na_2CMP$  hydrate, (I). The asymmetric unit of (I) shown in Fig. 1 contains two ribonucleotides ( $Z' = 2$ ), three ordered and one disordered sodium ion [ $Na4$  0.8958 (19),  $Na4B$  0.1042 (19)], as well as nine fully occupied water molecules and a number of lower occupancy water positions associated with the disordered sodium ion. There is also evidence for inclusion of methanol;  $C1M$  has an occupancy of 0.546 (9) and is within the right covalent distance


**Figure 1**

The asymmetric unit of (I). Displacement ellipsoids are drawn at the 50% probability level. H atoms are shown as spheres of arbitrary size. Ellipsoid or sphere style reflects occupancy, *i.e.* principal ellipsoids with no shaded segments 0.8958 (19), open circle 0.51–0.57 and dotted circle 0.10–0.29.

(about 1.4 Å) of the three electron-density peaks labelled O1M, O2M and O3M. The combined occupancy of these three O atoms is 1.0, so the positions are partly filled with water molecules. Sodium ions Na1 and Na2 are pentacoordinated, while Na3 and Na4 have six ligands forming distorted octahedra.

Na<sub>2</sub>CMP has previously been reported to crystallize as a 6.5-hydrate in the monoclinic space group *P*<sub>2</sub><sub>1</sub>, with *a* = 14.042 (2) Å, *b* = 8.924 (2) Å, *c* = 16.091 (3) Å, β = 94.430 (2)°, *V* = 2010.4 (7) Å<sup>3</sup> and *Z*' = 2 for (II) (Borodi *et al.*, 2001). The crystal packing patterns of (I) and (II) are compared in Fig. 2, where layers of CMP ions are seen edge-on, separated by layers of water molecules and sodium ions. It is very difficult to spot the origin of the space group difference between (I) and (II) from Fig. 2, but subtle modifications of the packing arrangements are evident from Fig. 3. The two modes of generating a CMP layer from two independent CMP ions with very similar geometries give rise to crystals with symmetry belonging to two different systems, orthorhombic for (I) and monoclinic for (II).

It is tempting to see the inclusion of a partial solvent methanol molecule in the structure of (I) as the factor that triggers the transition from space group *P*<sub>2</sub><sub>1</sub> for (II) to *P*<sub>2</sub><sub>1</sub><sub>2</sub><sub>1</sub> for (I), but this is not necessarily so. The water/sodium cavities of (I) and (II) are indeed remarkably similar, and methanol was also used for obtaining the crystals of (II). It may thus be that a low peak in the electron-density map of (II) corresponding to C1M in (I) was simply overlooked in the refinement.

The structure of (I) is closely related to the structure of the BaCMP hydrate in *P*<sub>2</sub><sub>1</sub><sub>2</sub> (Hogle & Sundaralingam, 1980). Orthorhombic space groups with cell dimensions close to those of (I) have also been observed for ten other hydrated complexes between alkali/alkaline-earth metals and 5'-ribo-

nucleotides in the Cambridge Structural Database (Version 5.26, November 2004; Allen, 2002), including sodium guanosine-5'-monophosphate heptahydrate (Barnes & Hawkinson, 1982) and strontium inosine-5'-monophosphate 6.5-hydrate (Brown & Bugg, 1980) in *P*<sub>2</sub><sub>1</sub><sub>2</sub><sub>1</sub> with *Z*' = 2.

## Experimental

Crystals of (I) were prepared by slowly diffusing methanol into an equimolar mixture of the disodium salt of 5'-CMP and L-arginine hydrochloride in water at about 310 K. Both compounds were obtained from Sigma-Aldrich.

### Crystal data

2Na<sup>+</sup>·C<sub>9</sub>H<sub>12</sub>N<sub>3</sub>O<sub>8</sub>P<sup>2-</sup>·6.07H<sub>2</sub>O·  
0.27CH<sub>3</sub>O  
*M<sub>r</sub>* = 482.25  
Orthorhombic, *P*<sub>2</sub><sub>1</sub><sub>2</sub><sub>1</sub>  
*a* = 8.9750 (1) Å  
*b* = 20.4196 (3) Å  
*c* = 21.9152 (4) Å  
*V* = 4016.31 (10) Å<sup>3</sup>  
*Z* = 8

*D<sub>x</sub>* = 1.595 Mg m<sup>-3</sup>  
Mo Kα radiation  
Cell parameters from 18 912  
reflections  
θ = 1.9–40.3°  
μ = 0.26 mm<sup>-1</sup>  
*T* = 105 (2) K  
Plate, colourless  
1.00 × 0.80 × 0.15 mm

### Data collection

Bruker SMART CCD  
diffractometer  
ω scans  
Absorption correction: multi-scan  
(SADABS; Sheldrick, 1996)  
*T*<sub>min</sub> = 0.782, *T*<sub>max</sub> = 0.962  
67 367 measured reflections

24 465 independent reflections  
23085 reflections with *I* > 2σ(*I*)  
*R*<sub>int</sub> = 0.026  
θ<sub>max</sub> = 40.3°  
*h* = -16 → 15  
*k* = -36 → 36  
*l* = -39 → 38

### Refinement

Refinement on *F*<sup>2</sup>  
*R* [*F*<sup>2</sup> > 2σ(*F*<sup>2</sup>)] = 0.034  
*wR* [*F*<sup>2</sup>] = 0.092  
*S* = 1.07  
24 465 reflections  
627 parameters  
H atoms treated by a mixture of  
independent and constrained  
refinement

*w* = 1/[σ<sup>2</sup>(*F<sub>o</sub>*<sup>2</sup>) + (0.0485*P*)<sup>2</sup>  
+ 0.6755*P*]  
where *P* = (*F<sub>o</sub>*<sup>2</sup> + 2*F<sub>c</sub>*<sup>2</sup>)/3  
(Δ/σ)<sub>max</sub> = 0.007  
Δρ<sub>max</sub> = 0.90 e Å<sup>-3</sup>  
Δρ<sub>min</sub> = -0.42 e Å<sup>-3</sup>  
Absolute structure: Flack (1983),  
10733 Friedel pairs  
Flack parameter = 0.01 (3)

**Table 1**

Selected bond lengths (Å).

Na1—O3PB <sup>i</sup>	2.3252 (7)	Na4—O3M	2.340 (4)
Na1—N3B <sup>ii</sup>	2.5201 (8)	Na4—O8W	2.3374 (11)
Na1—O1W	2.3655 (9)	Na4—O9W	2.4415 (9)
Na1—O4W	2.3824 (8)	Na4—O10W	2.4241 (11)
Na1—O7W	2.3583 (9)	Na4—O11W	2.4716 (18)
Na2—N3A <sup>iii</sup>	2.3852 (9)	Na4—O21W	2.394 (3)
Na2—O5A <sup>iii</sup>	2.8008 (9)	Na4—O31W	2.310 (7)
Na2—O3PA	2.3621 (8)	Na4—O12W	2.619 (6)
Na2—O6W	2.3950 (10)	Na4B—O1M	2.629 (6)
Na2—O7W	2.3430 (9)	Na4B—O2M	2.260 (5)
Na3—O3B <sup>iii</sup>	2.3093 (8)	Na4B—O3M	2.359 (6)
Na3—O2B <sup>iii</sup>	2.3955 (8)	Na4B—O8W	2.383 (4)
Na3—O1W	2.3573 (9)	Na4B—O9W	2.464 (4)
Na3—O3W	2.7470 (13)	Na4B—O11W	2.288 (5)
Na3—O4W	2.4488 (9)	Na4B—O31W	2.400 (8)
Na3—O5W	2.3832 (9)	Na4B—O22W	2.424 (5)
Na4—O1M	2.451 (3)	Na4—Na4B	0.921 (4)
Na4—O2M	2.4351 (19)		

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

**Table 2**  
Hydrogen-bonding geometry (Å, °).

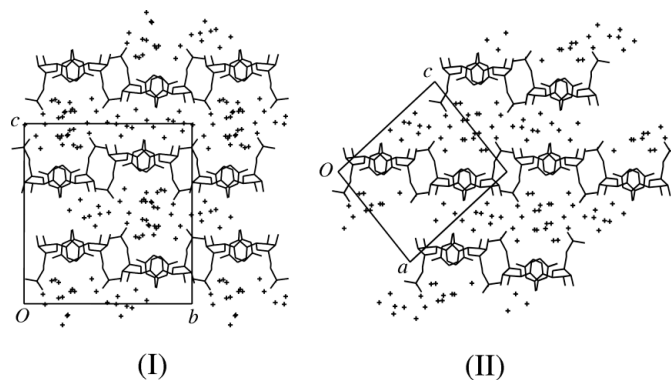
<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
N4A—H41A...O3PA <sup>iv</sup>	0.88	2.18	3.0107 (11)	158
N4A—H42A...O11W	0.88	2.04	2.862 (2)	156
O2A'—H2A'...O3PB <sup>iii</sup>	0.89 (2)	1.76 (2)	2.6480 (10)	170.5 (19)
O3A'—H3A'...O1PB <sup>v</sup>	0.77 (2)	1.86 (2)	2.6147 (10)	167 (2)
N4B—H41B...O3PB <sup>v</sup>	0.88	1.98	2.8360 (10)	163
N4B—H42B...O2W <sup>vi</sup>	0.88	2.08	2.9224 (11)	161
O2B'—H2B'...O3PA <sup>vii</sup>	0.83 (2)	1.83 (2)	2.6439 (9)	166 (2)
O3B'—H3B'...O2PA <sup>iv</sup>	0.79 (2)	1.82 (2)	2.5920 (9)	164 (2)
O1W—H11W...O5A <sup>viii</sup>	0.82 (2)	2.07 (2)	2.8264 (11)	151.3 (19)
O1W—H12W...O6W <sup>ix</sup>	0.86 (2)	2.03 (2)	2.8412 (13)	161 (2)
O2W—H21W...O3W	0.72 (2)	2.07 (2)	2.7826 (12)	176 (2)
O2W—H22W...O2PA	0.82 (2)	1.89 (2)	2.6934 (10)	167 (2)
O3W—H31W...O1PA <sup>x</sup>	0.82 (2)	1.87 (2)	2.6645 (11)	165 (3)
O3W—H32W...O10W <sup>i</sup>	0.81 (2)	2.04 (2)	2.8325 (15)	169 (3)
O4W—H41W...O2PA	0.836 (19)	2.044 (19)	2.8723 (9)	171 (2)
O4W—H42W...O2PB <sup>i</sup>	0.751 (19)	2.155 (19)	2.8577 (10)	156 (2)
O5W—H51W...O3A <sup>viii</sup>	0.828 (19)	2.07 (2)	2.8559 (10)	159 (2)
O5W—H52W...O1PA <sup>x</sup>	0.870 (19)	1.86 (2)	2.7257 (10)	171 (2)
O6W—H61W...O5A <sup>ii</sup>	0.81 (2)	2.05 (2)	2.8281 (11)	162 (2)
O6W—H62W...O5B <sup>v</sup>	0.88 (2)	1.94 (2)	2.7887 (12)	163 (2)
O7W—H71W...O5B <sup>ii</sup>	0.85 (2)	1.81 (2)	2.6429 (10)	166 (2)
O7W—H72W...O5W <sup>vi</sup>	0.78 (2)	2.05 (2)	2.7938 (12)	157 (2)
O8W—H81W...O9W <sup>vii</sup>	0.85 (3)	1.99 (4)	2.8146 (13)	164 (3)
O8W—H82W...O2W	0.77 (3)	2.14 (4)	2.8850 (15)	163 (3)
O9W—H91W...O1PA <sup>i</sup>	0.765 (19)	2.028 (19)	2.7824 (10)	169 (2)
O9W—H92W...O1PB <sup>x</sup>	0.895 (19)	2.026 (19)	2.8789 (10)	158.7 (19)
O10W—H13W...O3A <sup>iv</sup>	0.63 (2)	2.43 (2)	2.9984 (13)	153 (3)
O10W—H14W...O2PB	0.90 (2)	1.82 (2)	2.7066 (11)	169 (2)

Symmetry codes: (i)  $x - \frac{1}{2}, \frac{3}{2} - y, 1 - z$ ; (ii)  $\frac{3}{2} - x, 1 - y, z - \frac{1}{2}$ ; (iii)  $1 - x, y - \frac{1}{2}, \frac{3}{2} - z$ ; (iv)  $1 - x, \frac{1}{2} + y, \frac{3}{2} - z$ ; (v)  $2 - x, y - \frac{1}{2}, \frac{3}{2} - z$ ; (vi)  $1 + x, y, z$ ; (vii)  $2 - x, \frac{1}{2} + y, \frac{3}{2} - z$ ; (viii)  $\frac{1}{2} - x, 1 - y, z - \frac{1}{2}$ ; (ix)  $x - \frac{1}{2}, \frac{1}{2} - y, 1 - z$ ; (x)  $x - 1, y, z$ ; (xi)  $\frac{1}{2} + x, \frac{3}{2} - y, 1 - z$ .

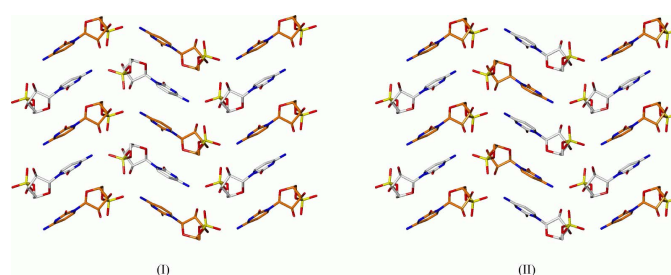
The non-H atoms were refined anisotropically, except those with occupancy less than 0.6 which were refined isotropically. Positional parameters were refined for H atoms bonded to O atoms. Other H atoms were positioned with idealized geometry and fixed C—H (0.95–1.00 Å) and N—H distances, and refined as riding with  $U_{iso}(H) = 1.2U_{eq}$  or  $1.5U_{eq}$  (water) of the carrier atom.

Data collection: SMART (Bruker, 2001); cell refinement: SAINT (Bruker, 2001); data reduction: SAINT; program(s) used to solve structure: SHELXTL (Bruker, 2001); program(s) used to refine structure: SHELXTL; molecular graphics: SHELXTL; software used to prepare material for publication: SHELXTL.

The purchase of the Bruker SMART CCD diffractometer was made possible through support from the Research Council of Norway (NFR)



**Figure 2**  
The molecular packing and unit cells of (I) and (II), viewed along the *a* and *b* axes, respectively. H atoms have been omitted for clarity.



**Figure 3**  
Layers of cytidine-5'-monophosphate anions in (I) and (II). C atoms have been drawn in different colours (white and orange) for the two independent ions in the asymmetric unit.

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