Fig. 1. Thermal ellipsoids (50% probability) for the atoms in the lower left corner of Fig. 2.

Fig. 2. The crystal structure of orthorhombic $AgN(CN)_2$.

difference between the two forms is that the threefold spiral parallel to the 3_1 axis in the trigonal form is replaced by a twofold spiral parallel to the 2_1 axis in the orthorhombic form. The distance parallel to the spiral axis corresponding to one monomeric unit is $c/3$ (7·621 Å) in the trigonal form and $a/2$ (8·066 Å) in the orthorhombic form. The former is slightly shorter owing to the greater tilt of the dicyanamide group in the threefold spiral. The shortest Ag···Ag distances, a (3·601 Å) in the trigonal form and b (3·612 Å) in the orthorhombic form, are approximately equal. The molecular volumes, 87·2 (1) Å³ in the orthorhombic form *vs* 85·6 (1) Å³ in the trigonal form, show that in spite of similarities in the bonding, the packing is significantly more efficient in the trigonal form.

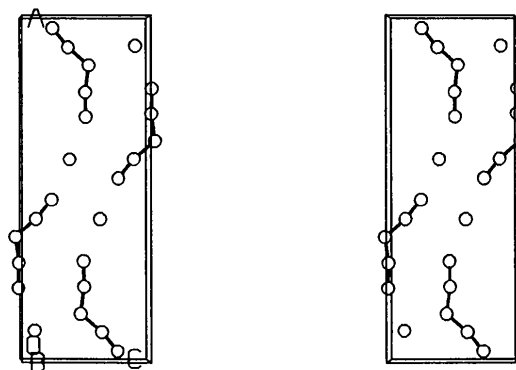The thermal ellipsoid of C1 (Fig. 1) looks strange; this is almost certainly a consequence of the poor quality of the crystal. If the refinement is carried out with all of the light atoms having isotropic temperature factors, convergence occurs with $R = 0·088$, $wR = 0·098$. Using Hamilton's (1965) test, $\mathscr{R}_{exp} = 1·03$ and $\mathscr{R}_{15,294,0·25} = 1·031$. Thus, the hypothesis that the temperature factors for the light atoms are isotropic can only be rejected at the 75% confidence level.

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Structure of Dipotassium Galactose 1-Phosphate Pentahydrate

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Abstract. $2K^+.C_6H_{11}O_9P^{2-}.5H_2O$, $M_r = 426·4$, monoclinic, $P2_1$, $a = 6·228$ (1), $b = 14·600$ (2), $c = 8·982$ (1) Å, $\beta = 102·01$ (1)°, $V = 798·4$ Å³, $Z = 2$, $D_m = 1·756$, $D_x = 1·773$ Mg m⁻³, $\lambda(Cu\ K\alpha) = 1·5418$ Å, $\mu = 7$ mm⁻¹, $F(000) = 444$, $T = 293$ K, $R = 0·033$, $wR = 0·035$ for 1549 unique reflections with $I > 3\sigma(I)$. The sugar ring adopts a $^4C_1$ conformation. The conformation about the exocyclic C5—C6 bond is *gauche–trans*. The phosphate group exists as a dianion with charges localized on O7 and O8 atoms.

One of the metal ions binds to the phosphate group directly. All the hydroxyl O atoms, except O4—H, are involved in hydrogen bonding with the water O atoms.

Introduction. Galactose 1-phosphate $(G\text{-}1\text{-}P^*)$ is converted to glucose 1-phosphate $(G\text{-}1\text{-}P)$ through a series of enzymatic reactions involving uridine triphosphate as a cofactor. $G\text{-}1\text{-}P^*$ differs from $G\text{-}1\text{-}P$ in its epimerization at the C4 atom of the sugar ring (Lehninger, 1970). The structure determination of $G\text{-}1\text{-}P^*$ was carried out to establish the conformational differences between these two molecules. We have reported earlier the structure of $G\text{-}1\text{-}P$ (Narendra, Seshadri & Viswamitra, 1984; Narenda & Viswamitra, 1984) as part of our studies on low-energy phosphates (Narendra, Seshadri & Viswamitra, 1985a,b).

Experimental. Crystals were grown by diffusion of acetone into an aqueous solution of the compound obtained from Sigma Chemicals. They were found to dissolve in the surrounding mother liquor at the time of mounting them for diffraction experiments. Therefore, a slightly larger crystal $0.4 \times 0.4 \times 0.6$ mm, was used to compensate for the diminution in crystal size. Hence, the absorption was higher than that usually detected for crystals containing light atoms alone. Density measured by flotation in acetone/bromoform suggested one molecule of $G\text{-}1\text{-}P^*$ with five water molecules in the asymmetric unit. Unit-cell parameters were refined using 25 accurately determined reflections $(16 < \theta < 48°)$ on a CAD-4 diffractometer. Intensity data were collected using Cu $K\alpha$ radiation, $\omega\text{--}2\theta$ scan, to $(\sin\theta)/\lambda$ of 0.58 Å^{-1}. The data were corrected for Lorentz and polarization effects. An empirical absorption correction (North, Phillips & Mathews, 1968) was applied, transmission factors varied from 0.75 to 0.99. 1922 reflections were measured for $0 \le h \le 7$, $0 \le k \le 17$, $-10 \le l \le 10$ of which 1549 were uniquely observed with $I > 3\sigma(I)$. Two reflections $(22\bar{1}$ and $23\bar{1})$ monitored periodically during the data collection showed less than 2% variation, indicating crystal stability. The structure was solved using the *RANTAN* option in *MULTAN*80 (Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1980). An E map computed with the best set of phases (CFOM = 2.89) revealed the positions of the K$^+$ ions and the phosphate group. The remaining non-H atoms of the molecule along with the water O atoms were located from successive difference Fourier maps. Full-matrix refinement on F with anisotropic temperature factors reduced R to 0.062. 16 of the 21 H atoms were located from a difference Fourier map computed at this stage and were refined isotropically. The refinement of the structure converged at $R = 0.033$

Table 1. *Fractional atomic coordinates and equivalent isotropic temperature factors*

$$B_{eq} = (4/3)[a^2\beta_{11} + b^2\beta_{22} + c^2\beta_{33} + (2ab\cos\gamma)\beta_{12} + (2ac\cos\beta)\beta_{13} + (2bc\cos\alpha)\beta_{23}].$$

	x	y	z	$B_{eq}(\text{Å}^2)$
K1	0.1558 (2)	0.16542	0.7293 (1)	2.51 (2)
K2	0.8142 (2)	0.0989 (8)	0.2904 (1)	2.31 (2)
P1	0.3603 (2)	0.3892 (9)	0.9674 (1)	1.27 (2)
C1	0.5682 (7)	0.4093 (3)	0.7442 (4)	1.45 (8)
C2	0.7445 (7)	0.3504 (3)	0.6961 (5)	1.47 (8)
C3	0.6540 (7)	0.2950 (3)	0.5528 (5)	1.48 (8)
C4	0.5191 (7)	0.3541 (3)	0.4293 (5)	1.57 (8)
C5	0.3460 (7)	0.4054 (3)	0.4921 (4)	1.47 (8)
C6	0.2132 (7)	0.4696 (3)	0.3760 (5)	1.83 (8)
O1	0.4199 (5)	0.3553 (2)	0.8079 (3)	1.49 (5)
O2	0.8369 (5)	0.2872 (3)	0.8118 (4)	2.11 (6)
O3	0.8317 (5)	0.2513 (2)	0.5000 (4)	2.25 (6)
O4	0.6610 (5)	0.4167 (2)	0.3731 (3)	2.14 (6)
O5	0.4513 (5)	0.4612 (2)	0.6198 (3)	1.56 (6)
O6	0.0457 (5)	0.5144 (3)	0.4331 (4)	2.45 (7)
O7	0.2176 (5)	0.3137 (2)	1.0045 (3)	1.84 (6)
O8	0.5781 (5)	0.3992 (2)	1.0806 (3)	1.85 (6)
O9	0.2422 (5)	0.4814 (2)	0.9364 (4)	2.16 (6)
OW1	0.3808 (6)	0.1597 (3)	0.1651 (4)	2.93 (8)
OW2	0.5748 (6)	0.1267 (3)	0.8492 (5)	3.54 (9)
OW3	0.1246 (6)	0.0383 (3)	0.9561 (4)	2.52 (7)
OW4	0.9096 (6)	0.2739 (3)	0.1908 (4)	3.11 (8)
OW5	0.2738 (6)	0.1236 (3)	0.4437 (5)	3.35 (8)

and $wR = 0.035$ with unit weights. Maximum Δ/σ for non-H atoms is 0.08 and residual electron density in the final difference Fourier map is within ± 0.034 e Å^{-3}. All calculations were performed using *SDP Structure Determination Package* (Enraf–Nonius, 1979) on a PDP/11 computer. The scattering factors for all the atoms were taken from *SDP*.

Discussion. The final positional parameters of the non-H atoms are given in Table 1.† The molecular geometry is listed in Table 2. Fig. 1 shows the numbering scheme in $G\text{-}1\text{-}P^*$, Fig. 2 the K$^+$ coordination and Fig. 3 the molecular packing.

The bond lengths and angles in the galactose ring are close to those found in $G\text{-}1\text{-}P$ Na$_2$ (Narendra, Seshadri & Viswamitra, 1984) and $G\text{-}1\text{-}P$ K$_2$ (Narendra & Viswamitra, 1984) and agree quite well with the average values for such structures. The sugar ring adopts a $^4C_1$ conformation. The displacements of the atoms C1 and C4 from the best least-squares plane through C2—C3–C5—O5 are -0.624 and 0.663 Å respectively.

Each hydroxyl group in the sugar ring is *gauche* with respect to its adajcent hydroxyl group. The conformation about the C5—C6 exocyclic bond is *gauche–trans* [O6—C6—C5—O5 = -62.6 (5) and

† Lists of structure factors, anisotropic thermal parameters, H-atom parameters and least-squares planes have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 52950 (13 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

O6—C6—C5—C4 = 177·5 (4)°] as in *G*-1-*P* K$_2$ but different from in *G*-1-*P* Na$_2$, where it is *gauche-gauche*. The Cremer–Pople (1975) puckering parameters are Q = 0·551 Å, θ = 7·13 and φ = 161·20°. The value of φ is higher than that observed for *G*-1-*P* K$_2$ (Q = 0·553 Å, θ = 6·5 and φ = 100°).

The phosphate group exists as a dianion in this structure. The two negative charges in the structure
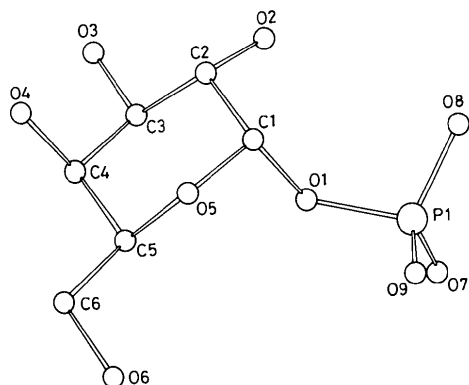

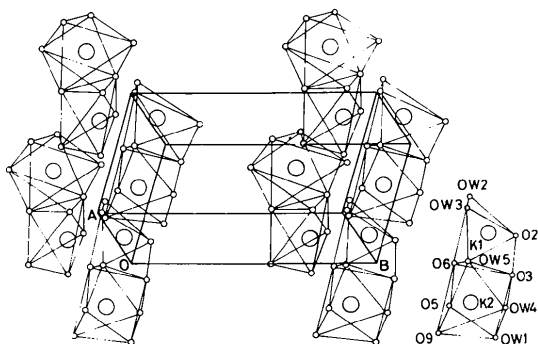Fig. 1. Numbering in galactose 1-phosphate (*G*-1-*P**).

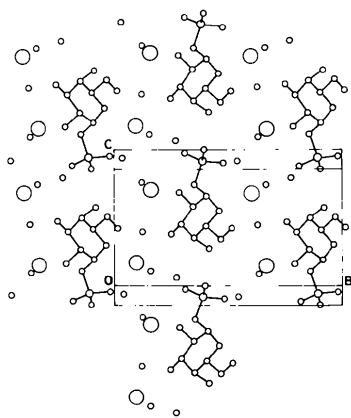Fig. 2. Sharing of potassium polyhedra in *G*-1-*P**.

Fig. 3. Packing of *G*-1-*P** in monoclinic lattice viewed down *a* axis.

might be distributed between O7 and O8 phosphate O atoms as indicated by their bond lengths [P—O7 1·496 (3) and P—O8 1·523 (3) Å]. The phosphate ester bond is 1·630 (3) Å, comparable to the values in other sugar phosphates (Narendra, Seshadri & Viswamitra, 1984, 1985*a,b*).

There are two crystallography independent K$^+$ ions in the asymmetric unit. K1 and K2 have six and seven neighbours respectively as shown in Fig. 2, at distances ranging from 2·63 to 2·93 Å (Table 2). Six- and sevenfold coordination for potassium has been reported for *F*-6-*P* K$_2$ (Narendra, Seshadri & Viswamitra, 1985*a*). In the present structure there is

Table 2. *Molecular geometry; bond distances* (Å), *bond angles* (°), *torsion angles* (°), K$^+$ *ion coordination and hydrogen-bond distances* (Å) *and angles* (°)

E.s.d.'s are given in parentheses.

P—O1	1·630 (3)	C2—O2	1·420 (5)
P—O7	1·496 (3)	C3—C4	1·515 (6)
P—O8	1·523 (3)	C3—O3	1·441 (6)
P—O9	1·532 (3)	C4—C5	1·515 (6)
C1—C2	1·526 (6)	C4—O4	1·434 (6)
C1—O1	1·423 (5)	C5—C6	1·513 (6)
C1—O5	1·419 (5)	C5—O5	1·447 (5)
C2—C3	1·526 (6)	C6—O6	1·414 (6)

O1—P—O7	103·1 (2)	C2—C3—C4	111·5 (4)
O1—P—O8	106·4 (2)	C2—C3—O3	109·8 (3)
O1—P—O9	107·2 (4)	C4—C3—O3	111·1 (4)
O7—P—O8	114·2 (2)	C3—C4—C5	109·8 (4)
O7—P—O9	113·7 (2)	C3—C4—O4	109·4 (3)
O8—P—O9	111·1 (3)	C5—C4—O4	110·8 (4)
C2—C1—O1	111·5 (3)	C4—C5—C6	112·3 (4)
C2—C1—O5	111·1 (3)	C4—C5—O5	109·4 (3)
O1—C1—O5	110·1 (3)	C6—C5—O5	106·8 (3)
C1—C2—C3	112·1 (3)	C5—C6—O6	112·0 (4)
C1—C2—O2	111·4 (3)	P—O1—C1	118·0 (2)
C3—C2—O2	107·1 (4)	C1—O5—C5	113·4 (*')

O7—P—O1—C1	− 175·9 (3)	O2—C2—C3—O3	− 65·8 (4)
O8—P—O1—C1	− 55·5 (3)	C2—C3—C4—C5	− 52·4 (5)
O9—P—O1—C1	63·8 (3)	C2—C3—C4—O4	69·3 (4)
O1—C1—C2—C3	73·2 (4)	O3—C3—C4—C5	− 175·2 (3)
O1—C1—C2—O2	− 46·9 (4)	O3—C3—C4—O4	− 53·4 (5)
O5—C1—C2—C3	− 50·0 (5)	C3—C4—C5—C6	177·0 (4)
O5—C1—C2—O2	− 170·1 (3)	C3—C4—C5—O5	58·5 (4)
C2—C1—O1—P1	132·7 (3)	O4—C4—C5—C6	56·1 (5)
O5—C1—O1—P1	− 103·6 (3)	O4—C4—C5—O5	− 62·4 (4)
C2—C1—O5—C5	58·3 (4)	C4—C5—C6—O6	177·5 (4)
O1—C1—O5—C5	− 65·7 (4)	O5—C5—C6—O6	− 62·6 (5)
C1—C2—C3—C4	48·2 (5)	C4—C5—O5—C1	− 63·1 (4)
C1—C2—C3—O3	171·7 (3)	C6—C5—O5—C1	175·1 (3)
O2—C2—C3—C4	170·8 (3)		

		Translation		
		Symmetry	*a*	*b*	*c*
K1—O*W*2	2·667 (4)	1	0	0	0
K1—O*W*3	2·785 (4)	1	0	0	0
K1—O6	2·785 (3)	2	0	− 1	1
K1—O3	2·861 (3)	1	− 1	0	0
K1—O*W*5	2·875 (4)	1	0	0	0
K1—O2	2·882 (4)	1	− 1	0	0
K2—O9	2·632 (3)	2	1	− 1	1
K2—O6	2·748 (4)	2	1	− 1	1
K2—O*W*4	2·811 (4)	1	0	0	0
K2—O5	2·826 (3)	2	1	− 1	1
K2—O*W*1	2·842 (4)	1	0	0	0
K2—O3	2·901 (4)	1	0	0	0
K2—O*W*5	2·929 (4)	1	1	0	0

Table 2 (cont.)

X—H···Y	X—H	X···Y	H···Y	X—H···Y	Symmetry	Translation		
OW1—H1W1···O7	0·76	2·750 (5)	2·01	165	1	0	0	−1
OW1—H2W1···OW3	0·99	2·822 (5)	1·84	168	1	0	0	−1
O2—HO2···O7	0·82	2·658 (3)	1·97	142	1	1	0	0
O6—HO6···O4	0·78	2·745 (5)	1·97	175	1	−1	0	0.
O3···OW4		2·935 (5)			1	0	0	0
O7···OW4		2·855 (5)			1	−1	0	1

a direct interaction between the phosphate group and the K^+ ion (Fig. 2), a feature also observed in the crystal structures of G-1-P K_2 (Narendra, Seshadri & Viswamitra, 1984), ADP K_2 (Katti & Viswamitra, 1979) and PEP K (Katti & Viswamitra, 1981). Interestingly, the O5, O6 and O9 atoms of the same molecule bind to the K^+ ion while in G-1-P K_2, O9 belongs to another molecule related by space-group symmetry. In G-1-P Na_2 the O5 and O6 atoms of the same molecule also bind to the Na^+ ion. However, the additional link with the phosphate O atom of the same molecule does not exist because of the smaller ionic radius of Na^+ (0·98 Å) compared to K^+ (1·33 Å). The two coordination polyhedra share a face formed by OW5, O6 and O3 atoms and their arrangement in the monoclinic lattice is shown in Fig. 2.

There is extensive hydrogen bonding summarized in Table 2. All the hydroxyl O atoms except O4—H are involved in hydrogen bonding with the water O atoms. The G-1-P* molecules are linked to form an infinite chain along the a axis through the intermolecular hydrogen bond between O2 and O7 atoms.

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Structure of
Poly[-μ-(2,2'-dithiodibenzoato-O^1,O^2:O^3:O^4)-hexamethylenetetraminiocobalt(II)-]*

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Abstract. [Co($C_6H_{13}N_4$)($C_{14}H_8O_4S_2$)], $M_r = 504·46$, triclinic, $P\bar{1}$, $a = 11·074$ (3), $b = 12·000$ (4), $c = 9·585$ (3) Å, $\alpha = 117·40$ (2), $\beta = 70·41$ (2), $\gamma = 116·65$ (2)°, $V = 997·3$ (6) Å^3, $Z = 2$, $D_x = 1·68$, $D_m = 1·68$ Mg m^{-3}, λ(Mo $K\alpha$) = 0·71069 Å, $\mu = 1·09$ mm^{-1}, $F(000) = 520$, $T = 296$ K. The structure was solved by the heavy-atom method and refined to $R = 0·067$ and $wR = 0·063$ for 3632 unique observed reflections. The single Co in the unit cell occupies

* Hexamethylenetetramine is 1,3,5,7-tetraazatricyclo[3.3.1.1^{3,7}]-decane.