

Table 4. Possible hydrogen bonds involving the two non-equivalent H atoms

Transformation (on last atom)	O...O (Å)	∠C—O...O (°)
C(2)—O(1)—H...O(2)	$x + 1, y, z$	113 (1)
C(2)—O(1)—H...O(2)	$x + 1, \frac{1}{2} - y, z - \frac{1}{2}$	117 (1)
C(4)—O(2)—H...O(1)	$x - 1, y, z$	111 (1)
C(4)—O(2)—H...O(1)	$x - 1, \frac{1}{2} - y, z + \frac{1}{2}$	134 (1)

Froehlich & Eichhorn, 1978) where hydrogen bonding between the amine and X groups in adjacent molecules gives rise to a Pt—Pt separation of 3.4 Å. Such short distances are usually not observed in *trans* compounds. In this structure, the shortest Pt—Pt distance is mainly determined by I—I contacts, the sum of the van der Waals radii being 4.3 Å.

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The Structure of the Monobarium Salt of Glucose 6-Phosphate Heptahydrate

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Abstract

$C_6H_{11}O_9P^{2-} \cdot Ba^{2+} \cdot 7H_2O$, $M_r = 521.5$, is monoclinic, space group $P2_1$, $a = 11.881$ (4), $b = 8.616$ (5), $c = 8.350$ (4) Å, $\beta = 102.95$ (3)°, $Z = 2$, $U = 833.0$ Å³, $d_m = 2.09$, $d_c = 2.08$ Mg m⁻³, $F(000) = 516$. Mo $K\alpha$ ($\mu = 0.034$ mm⁻¹) intensity data. R is 0.068 for 1603 reflections. Of the two endocyclic C—O bonds in the glucose ring, C(5)—O(5) [1.463 (23)] is longer than C(1)—O(5) [1.395 (23) Å]. The pyranose sugar ring takes a ⁴C₁ chair conformation. The Cremer—Pople

puckering parameters are, $\theta = 6.69^\circ$, $Q = 0.619$ Å and $\varphi = 263.7^\circ$. The conformation about the exocyclic C(5)—C(6) bond is *gauche-gauche*, in contrast to *gauche-trans* observed in the structure of glucose 1-phosphate. The phosphate ester bond, P—O(6), is 1.61 (1) Å. It is similar in length to the 'high-energy' P~O bond in phosphoenolpyruvate. The Ba²⁺ ion is surrounded by nine O atoms within a distance of 2.95 Å, of which seven are from water molecules. There is an intramolecular hydrogen bond between the sugar hydroxyl O(4) and phosphate oxygen O(12).

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Introduction

Glucose 6-phosphate (G6P) occupies a central position in the metabolism of carbohydrates in the cell. It is classified as a 'low-energy' phosphate compound as its free energy of hydrolysis is only $-13.8 \text{ kJ mol}^{-1}$, considerably smaller than that of 'high-energy' phosphates such as phosphoenolpyruvate ($-58.5 \text{ kJ mol}^{-1}$) (Lehninger, 1971). We report here the structure of G6P as obtained from X-ray analysis of its monobarium salt. This investigation follows our earlier studies on phosphoenolpyruvate and related phosphates (Katti, Hosur & Viswamitra, 1981; Hosur & Viswamitra, 1981).

Experimental

A crystalline sample of G6P.Ba was obtained from Sigma Chemicals. Unit-cell dimensions and the space group were determined from rotation and Weissenberg photographs. The cell parameters were refined by least squares from 25 high-angle reflections collected on a CAD-4 diffractometer.

The density (2.09 Mg m^{-3}) measured by flotation in acetone and bromoform mixtures was consistent with the presence of seven water molecules and one G6P.Ba in the asymmetric unit. Mo $K\alpha$ intensity data to a 2θ limit of 50° were collected on the diffractometer using a crystal of size $0.05 \times 0.05 \times 0.45 \text{ mm}$, in the ω - 2θ scan mode. Backgrounds for each reflection were measured on each side of the Bragg peak for $\frac{1}{2}$ of the scan angle. Two reflections monitored at regular intervals showed the crystal to be stable to X-rays. The 1603 unique reflections collected in the hkl and $h\bar{k}l$ octants were corrected for Lorentz and polarization effects.

Structure solution and refinement

The structure was solved by Patterson and direct methods with *SHELX 76* (Sheldrick, 1976). The Ba coordinates derived from the Harker section tallied with the strongest peak in the *E* map. The heavy-atom coordinates were used to phase a difference Fourier map. The phosphate group atoms could be clearly identified. The remaining non-H atoms were located from subsequent difference Fourier calculations. *R* for Ba alone was 0.28. Block-diagonal least-squares refinement with anisotropic thermal parameters reduced *R* to 0.071. The peaks in the difference Fourier map computed at this stage were too diffuse to be distinguishable from background and H atoms could not be located unambiguously. They were fixed wherever possible (Table 2) from their expected geometry and were refined with isotropic temperature

Table 1. Fractional coordinates ($\times 10^4$) and equivalent isotropic temperature factors of the non-H atoms

$U_{\text{eq}} = 1/6\pi^2 \sum_i \sum_j \beta_{ij} a_i \cdot a_j$. Average e.s.d. in U_{eq} is 0.008 \AA^2 .

	<i>x</i>	<i>y</i>	<i>z</i>	U_{eq} (\AA^2)
Ba	664 (1)	2723 (1)	4314 (1)	0.017
P	2332 (4)	5015 (6)	1357 (5)	0.017
O(11)	1861 (10)	4837 (16)	2906 (13)	0.024
O(12)	3489 (12)	4260 (17)	1402 (18)	0.036
O(13)	1439 (11)	4593 (18)	-167 (16)	0.034
O(6)	2527 (11)	6861 (14)	1346 (16)	0.024
C(6)	3118 (12)	7575 (24)	159 (18)	0.018
O(5)	3875 (10)	9751 (15)	1866 (15)	0.023
C(1)	4814 (16)	10706 (24)	2518 (23)	0.026
O(1)	4386 (12)	11984 (16)	3274 (16)	0.031
C(2)	5716 (13)	9861 (20)	3827 (20)	0.015
O(2)	6656 (10)	10844 (14)	4353 (14)	0.018
C(3)	6099 (16)	8344 (21)	3101 (22)	0.022
O(3)	6888 (8)	7537 (17)	4316 (13)	0.023
C(4)	5001 (14)	7401 (18)	2403 (19)	0.019
O(4)	5329 (12)	6006 (15)	1697 (17)	0.030
C(5)	4211 (17)	8379 (22)	1053 (21)	0.026
W(1)	8882 (11)	4964 (16)	3627 (15)	0.026
W(2)	9413 (11)	2597 (30)	6747 (16)	0.049
W(3)	9770 (10)	2854 (29)	951 (15)	0.043
W(4)	1974 (14)	1418 (18)	9339 (19)	0.043
W(5)	1670 (15)	408 (21)	2643 (21)	0.054
W(6)	6826 (12)	4099 (17)	4223 (20)	0.038
W(7)	8834 (12)	373 (17)	3400 (17)	0.036

Table 2. Fractional coordinates ($\times 10^3$) and isotropic temperature factors of the H atoms

Average e.s.d. in *U* is 0.040 \AA^2 .

	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> (\AA^2)
H(1)	531 (13)	1100 (19)	173 (18)	0.006
H(2)	532 (20)	974 (31)	453 (30)	0.056
H(3)	634 (21)	876 (33)	251 (29)	0.058
H(4)	459 (12)	716 (18)	339 (18)	0.007
H(5)	473 (13)	860 (19)	32 (18)	0.007
H(6)	324 (17)	695 (25)	-47 (24)	0.034
H'(6)	248 (13)	823 (19)	-29 (19)	0.006

Table 3. Bond lengths (\AA)

C(1)-C(2)	1.532 (25)	C(5)-O(5)	1.463 (23)
C(1)-O(1)	1.419 (24)	O(5)-C(1)	1.395 (23)
C(2)-C(3)	1.551 (25)	C(5)-C(6)	1.513 (26)
C(2)-O(2)	1.392 (21)	C(6)-O(6)	1.472 (20)
C(3)-C(4)	1.537 (25)	O(6)-P	1.608 (14)
C(3)-O(3)	1.402 (22)	P-O(11)	1.527 (12)
C(4)-C(5)	1.546 (24)	P-O(12)	1.514 (16)
C(4)-O(4)	1.430 (21)	P-O(13)	1.508 (14)

Table 4. Bond angles (°)

O(5)—C(1)—O(1)	107.3 (15)	C(4)—C(5)—O(5)	106.7 (14)
O(5)—C(1)—C(2)	111.6 (15)	C(5)—O(5)—C(1)	112.4 (14)
O(1)—C(1)—C(2)	108.3 (15)	C(4)—C(5)—C(6)	115.1 (15)
C(1)—C(2)—C(3)	110.0 (14)	O(5)—C(5)—C(6)	107.8 (14)
C(1)—C(2)—O(2)	108.6 (14)	C(5)—C(6)—O(6)	110.2 (14)
O(2)—C(2)—C(3)	110.5 (14)	C(6)—O(6)—P	120.6 (11)
C(2)—C(3)—O(3)	110.1 (14)	O(6)—P—O(11)	100.7 (7)
O(3)—C(3)—C(4)	112.6 (14)	O(6)—P—O(12)	107.1 (8)
C(2)—C(3)—C(4)	107.2 (14)	O(6)—P—O(13)	108.0 (8)
C(3)—C(4)—C(5)	108.3 (14)	O(11)—P—O(12)	116.0 (8)
C(3)—C(4)—O(4)	108.3 (13)	O(11)—P—O(13)	111.6 (8)
O(4)—C(4)—C(5)	109.5 (13)	O(12)—P—O(13)	112.4 (8)

Table 5. Torsion angles (°)

Average e.s.d. is 1.4°.

O(11)—P—O(6)—C(6)	172.4	O(1)—C(1)—C(2)—C(3)	173.3
O(12)—P—O(6)—C(6)	50.7	C(1)—C(2)—C(3)—O(3)	-177.5
O(13)—P—O(6)—C(6)	-70.6	O(2)—C(2)—C(3)—O(3)	62.5
P—O(6)—C(6)—C(5)	-118.3	C(1)—C(2)—C(3)—C(4)	-54.7
O(6)—C(6)—C(5)—O(5)	-70.3	O(2)—C(2)—C(3)—C(4)	-174.7
O(6)—C(6)—C(5)—C(4)	48.6	C(2)—C(3)—C(4)—O(4)	178.9
C(5)—O(5)—C(1)—O(1)	-179.8	O(3)—C(3)—C(4)—O(4)	-59.9
C(5)—O(5)—C(1)—C(2)	-61.2	C(2)—C(3)—C(4)—C(5)	60.2
C(1)—O(5)—C(5)—C(6)	-170.9	O(3)—C(3)—C(4)—C(5)	-178.6
C(1)—O(5)—C(5)—C(4)	65.0	C(3)—C(4)—C(5)—C(6)	176.3
O(5)—C(1)—C(2)—O(2)	176.5	O(4)—C(4)—C(5)—C(6)	58.4
O(1)—C(1)—C(2)—O(2)	-65.6	C(3)—C(4)—C(5)—O(5)	-64.1
O(5)—C(1)—C(2)—C(3)	55.4	O(4)—C(4)—C(5)—O(5)	177.9

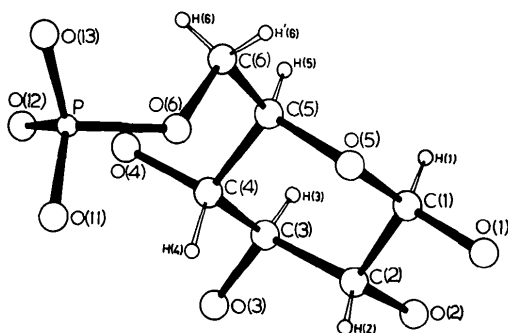


Fig. 1. The structure of the G6P dianion, showing the numbering of the atoms.

factors. Final cycles of refinement with a Cruickshank (1961) weighting scheme converged at $R = 0.068$. The function minimized was $\sum w(|F_o| - k|F_c|)^2$, where $w = 1/(a + b|F_o| + c|F_c|^2)$ with $a = 4.402$, $b = -0.131$, $c = 0.001$. Scattering factors for non-H atoms were computed using Cromer & Waber (1965) constants and those for H were taken from Stewart, Davidson & Simpson (1965). For Ba anomalous-dispersion corrections $f' = -0.613$, $f'' = 2.282$ (Cromer & Liberman, 1970) were also included.

Positional parameters for the heavier atoms are given in Table 1, and those for H in Table 2.* Bond lengths and angles are listed in Tables 3 and 4, and torsion angles in Table 5. The chemical structure and the numbering scheme are shown in Fig. 1.

Molecular geometry

The glucose ring

Of the two endocyclic C—O bonds, C(5)—O(5) [1.463 (23)] is longer than C(1)—O(5) [1.395 (23) Å]. The difference in the bond lengths in the present structure is somewhat greater than that in other glucose structures (0.004–0.031 Å). In the structures of β -D-glucose (Chu & Jeffrey, 1968), methyl tetraacetyl- β -D-glucoside (Zugenmaier & Rappenecker, 1978) and α -D-glucose (Brown & Levy, 1979) the bonds are nearly equal.

The C(1)—O(1) distance (Table 3) does not follow the usual trend of being shorter than the other exocyclic C—O(H) distances. A correlation between C(1)—O(1) bond shortening and the difference in the ring C—O bonds, C(5)—O(5) and C(1)—O(5), has been drawn by Berman, Chu & Jeffrey (1967). They observe that a 'normal' C(1)—O(1) bond is accompanied by a pronounced difference in the ring C—O bonds. The C—O distances in the present structure are in line with this observation.

The pyranose ring has the 4C_1 chair conformation (Figs. 1 and 2) with C(4) and C(1) displaced from the C(2)—C(3)—C(5)—O(5) plane by -0.76 and 0.65 Å (Table 6). The Cremer & Pople (1975) puckering parameters are $Q = 0.619$ Å, $\theta = 6.69^\circ$ and $\varphi = 263.7^\circ$. The distortion from perfect chair form is towards the 1S_3 skew geometry. Crystal-structure studies have shown a wide range of values for φ , within

* Lists of structure factors, anisotropic thermal parameters and bond lengths and angles involving H atoms have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 36467 (14 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 6. Least-squares plane and deviations of atoms (Å)

Average e.s.d. in atom deviation is 0.019 Å.

Equation of plane: $0.5391X + 0.5638Y - 0.6257Z = 6.0948$

C(1)	0.654	C(4)	-0.762
C(2)	0.023*	C(5)	0.031*
C(3)	-0.026*	O(5)	-0.013*

* Atoms included in least-squares plane.

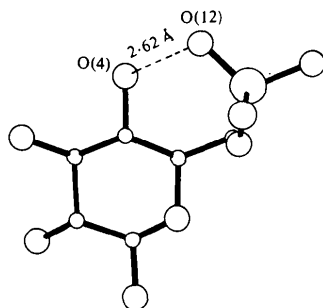


Fig. 2. Perspective view showing the intramolecular hydrogen bond between phosphate oxygen and sugar hydroxyl oxygen.

the constraint of the 4C_1 chair conformation. Recent theoretical work by Kildeby, Melberg & Rasmussen (1977) also show that the 4C_1 chair form is the minimum-energy conformer for D-sugars.

Conformation about the exocyclic C(5)–C(6) bond

The torsion angles O(6)–C(6)–C(5)–O(5) and O(6)–C(6)–C(5)–C(4) are -70.3 and 48.6° respectively. The conformation about the C(5)–C(6) bond is therefore *gauche-gauche*. It is significantly different from the *gauche-trans* geometry (52.0 , 174.7°) in glucose 1-phosphate (Beever & Maconochie, 1965).

Phosphate group

The phosphate group exists as a dianion as the compound is a Ba^{2+} salt. The three terminal P–O bonds are nearly equal (Table 3) and the negative charges are, therefore, likely to be distributed between O(11), O(12) and O(13).

The phosphate ester bond P–O(6) is 1.608 (14) Å which is comparable to the high-energy P~O bonds in the crystal structure of monosodium phosphoenolpyruvate [1.595 (5), 1.610 (6) Å] (Katti *et al.*, 1981). The phosphate group takes a staggered conformation about this bond.

Conformation about the C(6)–O(6) bond

The torsion angle C(5)–C(6)–O(6)–P is -118.3° , so that the conformation about C(6)–O(6) departs considerably from an ideal *trans* (180°) geometry, commonly observed in furanose nucleotide structures (Sundaralingam, 1969). The smaller angle is probably a consequence of the intramolecular hydrogen bond which occurs between the phosphate O(12) and the sugar O(4).

Ba^{2+} coordination

The Ba^{2+} ion is surrounded by nine ligands within a distance of 2.95 Å (Table 7). Of these seven are water

Table 7. Barium coordination distances (Å)

Average e.s.d. is 0.015 Å.

	Distance (Å)	Symmetry	Translation		
			a	b	c
Ba...W(1)	2.827	1	-1	0	0
Ba...W(1)	2.912	2	1	-1	0
Ba...W(2)	2.775	1	-1	0	0
Ba...W(3)	2.773	1	-1	0	0
Ba...W(7)	2.943	1	-1	0	0
Ba...W(7)	2.950	2	1	0	1
Ba...O(11)	2.734	1	0	0	0
Ba...W(5)	2.846	1	0	0	0
Ba...O(3)	2.881	2	1	-1	1

Symmetry code: (1) x, y, z ; (2) $\bar{x}, \frac{1}{2} + y, \bar{z}$.

molecules. The other two are the phosphate O(11) and the sugar O(3). Ninefold coordination for Ba^{2+} has also been reported in the structures of hydrated barium cytidine 5'-phosphate [$Ba(5'-CMP)$] (Hogle, Sundaralingam & Lin, 1980), barium tetrathionate dihydrate (Foss, Furberg & Zachariassen, 1954) and $Ba(H_2PO_4)_2$ (Durif & Guitel, 1978). In the $Ba(5'-CMP)$ structure, the cation in the general position coordinates preferentially to water molecules.

Hydrogen bonding and molecular packing

The hydrogen-bonding interactions are summarized in Table 8. The hydroxyl groups take part in hydrogen bonds both as acceptors and as donors. The hydroxyl

Table 8. Hydrogen-bond distances (Å)

Average e.s.d. is 0.02 Å.

	Distance (Å)	Symmetry	Translation		
			a	b	c
O(1)...O(12)	2.58	1	0	1	0
O(4)...O(12)	2.62	1	0	0	0
O(2)...O(11)	2.70	2	1	0	1
O(3)...O(1)	2.82	2	1	-1	1
W(1)...W(4)	2.76	2	1	0	1
W(1)...W(6)	2.70	1	0	0	0
W(2)...O(11)	2.87	2	1	-1	1
W(2)...W(5)	2.84	2	1	0	1
W(3)...O(13)	2.81	1	1	0	0
W(3)...O(6)	3.03	2	1	-1	0
W(4)...O(13)	2.86	1	0	0	1
W(4)...W(5)	2.99	1	0	0	1
W(5)...O(5)	2.89	1	0	-1	0
W(5)...W(6)	3.04	2	1	-1	1
W(6)...O(2)	2.81	1	0	-1	0
W(6)...O(4)	2.94	1	0	0	0
W(6)...O(3)	2.96	1	0	0	0
W(7)...O(2)	2.90	1	0	-1	0
W(7)...O(13)	2.73	2	1	-1	0

Symmetry code: (1) x, y, z ; (2) $\bar{x}, \frac{1}{2} + y, \bar{z}$.

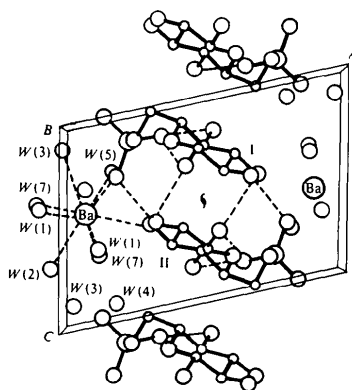


Fig. 3. The packing arrangement in the unit cell viewed along *b*.

O(4) forms an intramolecular hydrogen bond with phosphate O(12) (2.62 Å). No such intramolecular interaction is observed in the structure of glucose 1-phosphate (Beever & Maconochie, 1965). The ring oxygen O(5) accepts a hydrogen bond from the water molecule *W*(5). The distance between the ester oxygen O(6) and the water molecule *W*(3) is 3.03 Å. Since the H atoms of *W*(3) have not been located, it is uncertain whether hydrogen bonding is involved.

The packing arrangement as viewed along *b* is shown in Fig. 3. The molecules (I) and (II), related by the twofold screw axis, are linked to each other through O(1)···O(3) and O(2)···O(11) hydrogen bonds. The O(1)···O(12) interaction connects the molecules along *b*. These three hydrogen bonds arrange the molecules in a spiral fashion around the screw axis. Ba²⁺ ions and water molecules link adjacent columns of G6P molecules.

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Structure of Tricarbonyl(dimethyl 4-methyl-1-oxo-1,3-pentadiene-2,3-dicarboxylate)iron

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Abstract

C₁₃H₁₂FeO₈, *M_r* = 352.08, monoclinic, *P*2₁/*c*, *a* = 7.191 (3), *b* = 21.346 (7), *c* = 10.361 (4) Å, β = 0567-7408/82/041140-05\$01.00

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109.18 (2)°, *V* = 1502 Å³, *Z* = 4, *D_c* = 1.557 g cm⁻³, μ(Mo *K*α) = 10.703 cm⁻¹, *F*(000) = 720. The crystal structure has been determined and refined from 1496 diffractometer data to an *R* value of 0.048. The crystal © 1982 International Union of Crystallography