

Fig. 2. A view along *a* of the packing of molecules in the unit cell. The H atoms are omitted for clarity.

**Discussion.** The Cu<sup>II</sup> and Pd<sup>II</sup> compounds are isostructural with the corresponding Co<sup>II</sup> (Haider, Hashem, Malik & Hursthouse, 1980) and Ni<sup>II</sup> (Malatesta & Mugnoli, 1981) derivatives. The metal atoms in a square-planar arrangement lie within 0.031 (4) Å (I) and 0.026 (4) Å (II) of the mean plane of the N<sub>2</sub>O<sub>2</sub> atoms. The O/N–M–O/N angles (*cis*) in the square plane are within 5° of the ideal value of 90°. The M–N and M–O bonds are virtually identical in the Co<sup>II</sup> and Ni<sup>II</sup> compounds [Co–O = 1.855 (4), 1.847 (4); Co–N = 1.866 (4), 1.861 (4); Ni–O = 1.851 (4), 1.858 (4); Ni–N = 1.852 (4), 1.859 (4) Å], but longer (by ~0.06 Å) in the Cu<sup>II</sup> and (by ~0.12 Å) in the Pd<sup>II</sup> derivatives, as expected from the relative atomic-radii difference.

As in the case of other tetradentate Schiff-base complexes (Calligaris, Nardin & Randaccio, 1972), the dimensions of the ligand in the present series are independent of the nature of the metal and it shows extensive delocalization. However, compared with the free ligand (Haider, Hashem, Malik & Hursthouse, 1981) the bonds in the chelate rings in all four compounds are systematically modified. The changes in

ligand bonds, effected by metal coordination, although small (<0.06 Å), are real. The N(1)–C(4)–C(5)–N(2) torsion angles are 30.5 (7)° in (I) and 32.6 (7)° in (II). The O(1)–C(1)–C(11)–C(16) and O(2)–C(8)–C(17)–C(22) torsion angles showing the non-planarity of the phenyl rings with the respective chelate rings are 13.6 (7) and –16.1 (7) and 10.9 (7) and –12.2 (7)°, in (I) and (II), respectively. All these values are comparable with those in the Co<sup>II</sup> and Ni<sup>II</sup> compounds.

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## Structure of Trisodium Fructose 1,6-Diphosphate Octahydrate, 3Na<sup>+</sup>·C<sub>6</sub>H<sub>11</sub>O<sub>12</sub>P<sub>2</sub><sup>3-</sup>·8H<sub>2</sub>O

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**Abstract.** *M<sub>r</sub>* = 550.2, monoclinic, *P*2<sub>1</sub>, *a* = 7.085 (1), *b* = 11.645 (3), *c* = 13.290 (3) Å, β = 102.26 (1)°, *U* = 1071.5 Å<sup>3</sup>, *Z* = 2, *D<sub>m</sub>* = 1.708, *D<sub>x</sub>* = 1.704 Mg m<sup>-3</sup>,

Cu *K*α, λ = 1.5418 Å, μ = 3.311 mm<sup>-1</sup>, *F*(000) = 572, *T* = 300 K, final *R* for 2303 unique reflections is 0.055. The phosphate residues at the 1 and 6 positions have

different phosphate ester bond lengths [P(1)—O(1) = 1.591 (3); P(2)—O(6) = 1.622 (3) Å]. The P(2)—O(6) bond length corresponds to a high-energy P~O bond. The conformation about the C(5)—C(6) bond is *gauche-trans* in contrast to *gauche-gauche* about C(1)—C(2). The furanose ring is in the <sup>3</sup>E conformation. The two endocyclic C—O bonds C(2)—O(5) and C(5)—O(5) are nearly equal [1.434 (5); 1.448 (5) Å]. The Na<sup>+</sup> ions bind to the phosphate groups only indirectly through water bridges. The ester oxygen O(1) is also a binding site for a Na<sup>+</sup> cation.

**Introduction.** Fructose 1,6-diphosphate (F1,6-dp) is an intermediate in glycolysis. It is classified as a 'low-energy' phosphate as its free energy of hydrolysis is small,  $-16.7 \text{ kJ mol}^{-1}$ , compared to that of 'high-energy' phosphate such as phosphoenolpyruvate (PEP) ( $-58.5 \text{ kJ mol}^{-1}$ ) (Lehninger, 1973). We report here the structure of Na<sub>3</sub>F1,6-dp. This investigation follows our earlier studies on metal salts of glucose 6-phosphate and glucose 1-phosphate (Katti, Seshadri & Viswamitra, 1982; Narendra, Seshadri & Viswamitra, 1984). This analysis provides the first precise molecular parameters for a fructose attached to a phosphate group.

**Experimental.** Crystals grown from aqueous solution of compound by diffusion of acetone.  $D_m$  by flotation in acetone/bromoform. Unit-cell dimensions and space group from rotation and Weissenberg photographs; cell parameters from least-squares refinement of 25 high-angle reflections; Enraf-Nonius CAD-4 diffractometer. Max.  $\sin\theta/\lambda = 0.63 \text{ \AA}^{-1}$ , crystal  $0.45 \times 0.62 \times 1.12 \text{ mm}$ ,  $\omega-2\theta$  scan;  $h, k, l$  range  $\pm 8, 0, 14$  and  $0, 16, 2608$  reflections scanned, 2303 unique (including unobserveds) used in analysis;  $R_{\text{int}} = 0.056$ ; two strong reflections (008 and 266) monitored periodically during data collection showed crystal stable to X-rays: max. and min. intensities 40 113 and 38 192; 65 792 and 61 971 respectively. Lorentz and polarization corrections applied. Structure solved by direct methods with *MULTAN* (Main *et al.*, 1980). The two phosphate groups located in *E* map with highest combined figure of merit (2.9411); remaining non-H atoms located from subsequent difference Fourier calculations, full-matrix least-squares refinement (*SHELX76*; Sheldrick, 1976). Further difference Fourier maps revealed all H atoms. Further refinement including H atoms (isotropic) and non-H atoms (anisotropic) converged at  $R = 0.055$ ,  $R_w = 0.061$ ,  $S = 3.18$ ; function minimized  $\sum w(|F_o| - |F_c|)^2$ , where  $w = 1/\sigma^2(F_o)$ . Max. and min. residual electron density in final difference Fourier map 0.66 and  $-0.78 \text{ e \AA}^{-3}$ . Scattering factors for non-H atoms from Cromer & Waber (1965), for H atoms from Stewart, Davidson & Simpson (1965). Max.  $\Delta/\sigma$  for non-H atoms 0.08, for H 3.61.

**Discussion.** Positional parameters for the atoms are given in Table 1.\* Bond lengths and bond angles are listed in Table 2. The molecular structure and the atom numbering scheme are shown in Fig. 1. The hydrogen-bonding environment of the phosphate groups as viewed along *b* is shown in Fig. 2.

*The phosphate group.* As the compound is a trisodium salt, the two phosphate groups are expected to carry three negative charges. The bond lengths P(1)—O(8) and P(1)—O(9) are 1.484 (4) and 1.476 (4) Å, respectively. We may therefore expect a single negative charge to be distributed between these P—O bonds. The three terminal P—O bonds P(2)—O(10), P(2)—O(11) and P(2)—O(12) are nearly equal

\* Lists of structure factors, anisotropic thermal parameters, torsion angles, hydrogen-bond distances and details of least-squares plane calculations have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 39749 (21 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 1. *Fractional coordinates* ( $\times 10^4$ ; for H  $\times 10^3$ ) *with equivalent isotropic temperature factors* ( $\text{\AA}^2 \times 10^2$ )

For H atoms the temperature factors are the refined isotropic values. E.s.d.'s are given in parentheses.

$$U_{\text{eq}} = \frac{1}{3} \sum_i \sum_j U_{ij} \mathbf{a}_i \cdot \mathbf{a}_j$$

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{eq}}/U_{\text{iso}}$
P(1)	3494 (1)	3629	2480 (1)	1.80 (10)
O(7)	2855 (6)	4849 (4)	2030 (3)	3.55 (12)
O(8)	4983 (5)	3160 (4)	1958 (2)	2.79 (10)
O(9)	1712 (5)	2961 (5)	2449 (3)	3.68 (13)
P(2)	12441 (1)	3826 (1)	7494 (1)	1.07 (10)
O(10)	13903 (4)	4148 (3)	6866 (2)	2.01 (10)
O(11)	12281 (5)	2530 (3)	7593 (2)	1.78 (10)
O(12)	12736 (5)	4469 (3)	8512 (2)	2.13 (10)
O(1)	4598 (4)	3863 (3)	3635 (2)	1.88 (10)
C(1)	3743 (5)	4565 (4)	4310 (3)	1.33 (10)
C(2)	5307 (6)	5341 (4)	4926 (3)	1.28 (11)
C(3)	6127 (6)	6233 (4)	4279 (3)	1.28 (10)
C(4)	8161 (6)	6452 (4)	4937 (3)	1.57 (11)
O(5)	6945 (4)	4645 (3)	5366 (2)	1.64 (10)
C(5)	8734 (6)	5257 (4)	5394 (3)	1.30 (10)
C(6)	9899 (7)	5317 (4)	6477 (3)	1.88 (12)
O(6)	10310 (4)	4153 (3)	6834 (2)	1.71 (10)
O(2)	4588 (5)	5910 (3)	5691 (2)	1.81 (10)
O(3)	4902 (4)	7204 (3)	4106 (3)	1.87 (10)
O(4)	9562 (5)	6874 (4)	4398 (3)	2.84 (11)
Na(1)	8212 (3)	2492 (2)	-529 (2)	2.67 (10)
Na(2)	8319 (3)	5261 (2)	-331 (2)	2.81 (10)
Na(3)	2708 (3)	7658 (2)	5177 (2)	2.56 (10)
O <sup>W</sup> (1)	5272 (5)	1375 (4)	8812 (3)	2.63 (10)
O <sup>W</sup> (2)	4642 (6)	1185 (3)	823 (3)	2.68 (10)
O <sup>W</sup> (3)	8584 (6)	3128 (6)	3410 (3)	4.62 (15)
O <sup>W</sup> (4)	9255 (5)	8812 (4)	37 (2)	2.79 (10)
O <sup>W</sup> (5)	9548 (5)	1480 (4)	1031 (3)	2.80 (10)
O <sup>W</sup> (6)	9685 (5)	6254 (4)	1260 (3)	2.82 (10)
O <sup>W</sup> (7)	7554 (5)	3933 (4)	8133 (3)	2.72 (10)
O <sup>W</sup> (8)	6148 (5)	3818 (4)	137 (3)	3.11 (11)
H(1)	329 (9)	403 (7)	478 (5)	0.75 (48)
H'(1)	274 (11)	500 (8)	399 (6)	3.43 (70)
H(3)	638 (6)	592 (4)	347 (3)	0.99 (30)
H(4)	804 (8)	702 (6)	550 (4)	0.47 (44)
H(5)	962 (7)	484 (5)	491 (5)	0.07 (7)
H(6)	1102 (10)	578 (9)	666 (5)	2.56 (65)
H'(6)	897 (9)	549 (7)	693 (5)	0.10 (60)
H <sup>W</sup> (8)	585 (11)	1383 (10)	1077 (6)	1.84 (73)
H' <sup>W</sup> (8)	502 (13)	396 (12)	935 (7)	2.16 (107)
O(7)H	378 (11)	535 (8)	187 (6)	3.52 (74)
O(2)H	442 (11)	586 (9)	643 (6)	3.75 (73)
O(3)H	546 (11)	777 (9)	367 (6)	2.59 (74)
O(4)H	930 (11)	695 (9)	366 (6)	2.75 (72)

Table 2. Distances and angles

Bond lengths (Å)			
P(1)—O(7)	1.570 (5)	C(2)—O(2)	1.397 (5)
P(1)—O(8)	1.484 (4)	C(2)—C(3)	1.539 (6)
P(1)—O(9)	1.476 (4)	C(2)—O(5)	1.434 (5)
P(1)—O(1)	1.591 (3)	C(3)—C(4)	1.540 (6)
P(2)—O(10)	1.509 (3)	C(3)—O(3)	1.414 (6)
P(2)—O(11)	1.521 (4)	C(4)—C(5)	1.538 (6)
P(2)—O(12)	1.521 (3)	C(4)—O(4)	1.429 (6)
P(2)—O(6)	1.622 (3)	C(5)—O(5)	1.448 (5)
C(1)—O(1)	1.439 (5)	C(5)—C(6)	1.501 (6)
C(1)—C(2)	1.526 (6)	C(6)—O(6)	1.445 (6)
Bond angles (°)			
O(7)—P(1)—O(8)	109.3 (2)	C(1)—C(2)—O(2)	109.6 (3)
O(7)—P(1)—O(9)	106.9 (2)	C(3)—C(2)—O(5)	103.9 (3)
O(7)—P(1)—O(1)	104.8 (2)	C(3)—C(2)—O(2)	109.0 (3)
O(8)—P(1)—O(9)	118.8 (2)	O(5)—C(2)—O(2)	111.1 (3)
O(8)—P(1)—O(1)	105.1 (2)	C(2)—C(3)—C(4)	102.3 (3)
O(9)—P(1)—O(1)	111.1 (2)	C(2)—C(3)—O(3)	109.8 (3)
O(10)—P(2)—O(11)	111.5 (2)	C(4)—C(3)—O(3)	115.3 (3)
O(10)—P(2)—O(12)	112.9 (2)	C(3)—C(4)—C(5)	102.2 (3)
O(10)—P(2)—O(6)	108.2 (2)	C(3)—C(4)—O(4)	116.0 (4)
O(11)—P(2)—O(12)	114.2 (2)	C(5)—C(4)—O(4)	110.8 (4)
O(11)—P(2)—O(6)	101.6 (2)	C(2)—O(5)—C(5)	111.1 (3)
O(12)—P(2)—O(6)	107.5 (2)	C(4)—C(5)—O(5)	106.2 (3)
P(1)—O(1)—C(1)	120.8 (3)	C(4)—C(5)—C(6)	112.4 (4)
O(1)—C(1)—C(2)	108.5 (3)	O(5)—C(5)—C(6)	110.3 (3)
C(1)—C(2)—C(3)	114.7 (3)	C(5)—C(6)—O(6)	107.6 (3)
C(1)—C(2)—O(5)	108.4 (3)	P(2)—O(6)—C(6)	119.8 (3)

Sodium coordination distances (Å): average e.s.d. = 0.005 Å

Na(1)—OW(1 <sup>h</sup> )	2.454	Na(2)—OW(2 <sup>h</sup> )	2.325
—OW(4 <sup>h</sup> )	2.348	—OW(4 <sup>h</sup> )	2.381
—OW(5 <sup>h</sup> )	2.398	—OW(5 <sup>h</sup> )	2.400
—OW(6 <sup>h</sup> )	2.420	—OW(6 <sup>h</sup> )	2.424
—OW(7 <sup>h</sup> )	2.417	—OW(7 <sup>h</sup> )	2.526
—OW(8 <sup>h</sup> )	2.420	—OW(8 <sup>h</sup> )	2.446

Na(3)—O(1 <sup>h</sup> )	2.612
—O(2 <sup>h</sup> )	2.449
—O(3 <sup>h</sup> )	2.379
—O(4 <sup>h</sup> )	2.428
—O(5 <sup>h</sup> )	2.452
—OW(3 <sup>h</sup> )	2.322

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

[1.509 (3), 1.521 (4), 1.521 (3) Å], as found in Na<sub>2</sub> glucose 1-phosphate (Narendra *et al.*, 1984). Presumably the two negative charges are distributed between O(10), O(11) and O(12). The longest of the terminal P—O bonds, P(1)—O(7) = 1.570 (5) Å, is close to the P—O(H) distance of 1.564 Å found in Na phosphoenolpyruvate (Katti, Hosur & Viswamitra, 1981). The phosphates at the 1 and 6 positions have different phosphate ester bond lengths [P(1)—O(1) = 1.591 (3); P(2)—O(6) = 1.622 (3) Å]. The P(2)—O(6) bond length corresponds to a high-energy P~O bond (Katti *et al.*, 1981). The average O—P—O angle is 109.5°, range 101.6–118.8°.

*The furanose ring.* The furanose ring is in the <sup>3</sup>E conformation (Stoddart, 1971) as found in the fructofuranosyl moiety of sucrose (Brown & Levy, 1973), with C(3) displaced from the O(5)—C(2)—C(4)—C(5) plane by 0.580 (4) Å on the opposite side (*exo*) of C(6) and O(2) as in sucrose. The two endocyclic C—O bonds C(2)—O(5) and C(5)—O(5) are nearly equal. The internal C(2)—O(5)—C(5) angle [111.1 (3)°] is the only internal angle in the furanose ring to be close to the

tetrahedral bond angle (Sundaralingam, 1965). The Cremer—Pople (1975) puckering parameters are  $Q_2 = 0.372 (1) \text{ \AA}$  and  $\phi_2 = 254.17 (16)^\circ$ .

The torsion angles O(1)—C(1)—C(2)—O(5) and O(1)—C(1)—C(2)—C(3) are  $-50.0 (4)$  and  $65.6 (4)^\circ$  respectively. The conformation about the C(1)—C(2) bond is therefore *gauche-gauche* (*gg*). The torsion angles O(6)—C(6)—C(5)—O(5) and O(6)—C(6)—C(5)—C(4) are  $60.2 (4)$  and  $178.6 (3)^\circ$  and the conformation about the C(5)—C(6) bond is therefore *gauche-trans* (*gt*).

*Sodium coordination.* There are three crystallographically independent sodium ions in the structure. The Na<sup>+</sup> ions do not interact directly with the phosphate O atoms. Na(1) and Na(2) are completely surrounded by water molecules and interact with phosphate O atoms through water bridges as found in Na<sub>2</sub> deoxycytidine 5'-phosphate 7H<sub>2</sub>O (Pandit, Seshadri & Viswamitra, 1983). Na(3) interacts through OW(3), the exocyclic hydroxyl oxygen atoms, phosphate ester oxygen O(1) and ring oxygen O(5).

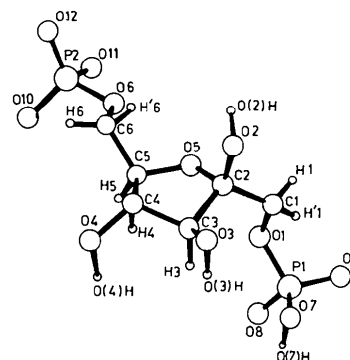


Fig. 1. Molecular structure and atomic numbering.

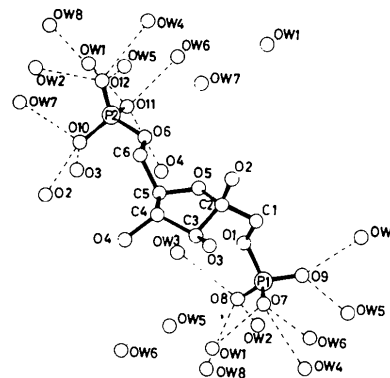


Fig. 2. The environment of the two phosphate groups. Dotted lines indicate hydrogen bonds.

*Hydrogen bonding.*\* There is no intramolecular hydrogen bonding. The phosphate groups are involved in extensive hydrogen bonding with water molecules and exocyclic hydroxyls as shown in Fig. 2. The ring oxygen O(5) and phosphate ester oxygen O(1) are not involved in hydrogen bonding. The phosphate ester oxygen O(6) accepts a hydrogen bond from water molecule OW(7). Each of the three furanose hydroxyl groups has two close contacts – to a Na<sup>+</sup> ion and a phosphate oxygen. The symmetry-related molecules are linked by O(3)···O(10) and O(4)···O(11) hydrogen bonds.

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\* See deposition footnote.

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### Structure of the Hydrated Complex between Lanthanum Chloride and 1,5,12,16,23,26,29,32-Octaoxa[10<sup>3,14</sup>][5.5]orthocyclophane, C<sub>24</sub>H<sub>30</sub>O<sub>8</sub>·LaCl<sub>x</sub>(OH)<sub>3-x</sub>·yH<sub>2</sub>O

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**Abstract.**  $M_r = 763.6$  for  $x = 2.5$  (1),  $y = 4.5$  (2), triclinic,  $P\bar{1}$ ,  $a = 11.325$  (2),  $b = 12.934$  (3),  $c = 11.551$  (4) Å,  $\alpha = 104.80$  (2),  $\beta = 100.62$  (2),  $\gamma = 101.15$  (2)°,  $U = 1555$  Å<sup>3</sup>,  $Z = 2$ ,  $D_m = 1.637$ ,  $D_x = 1.631$  g cm<sup>-3</sup>,  $\lambda(\text{Mo } K\alpha) = 0.71069$  Å,  $\mu(\text{Mo } K\alpha) = 16.5$  cm<sup>-1</sup>,  $F(000) = 744$ ,  $T = 295$  K,  $R = 0.032$  for

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4038 observations (all data with  $3^\circ < \theta \leq 22.5^\circ$ ). Each unit cell contains a pseudocentrosymmetric 'dimer'  $[\text{Cl}(\text{C}_{24}\text{H}_{30}\text{O}_8)\text{LaX}]_2$  where X is the site occupied by Cl<sup>-</sup> in one half and OH<sup>-</sup> in the other half, with an O—H···Cl hydrogen bond across the centre of symmetry. The La atom is ten-coordinated by the eight O atoms of the ligand in an end-capped trigonal prism with Cl and X on two faces. Another Cl<sup>-</sup> anion and water molecules occupy disordered sites in channels through the crystal.

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