KOVÀCS, A. L., ANTONINI, E., BRUNORI, M., GIACOMETTI, G. M. & TENTORI, L. (1976). *Colloquium on Myoglobin*, edited by A. G. SCHENECK & C. VANDECASSERIE, pp. 52–74. Bruxelles: Editions de la Facult de Science de l'Université.

MAKINEN, M. W., CHURG, A. K. & GLICK, H. A. (1978). *Proc. Natl Acad. Sci. USA*. In the press.

MATTHEWS, B. W. (1966). *Acta Cryst.* **20**, 230–239.

NORTH, A. C. T., PHILLIPS, D. C. & MATHEWS, F. S. (1968). *Acta Cryst.* A**24**, 351–359.

PADLAN, E. A. & LOVE, W. E. (1968). *Nature (London)*, **220**, 376–378.

PERUTZ, M. F., MUIRHEAD, H., COX, J. M. & GOAMAN, L. C. G. (1968). *Nature (London)*, **219**, 131–139.

ROSSI-FANELLI, A. & ANTONINI, E. (1957). *Biokhimya*, **22**, 335–342.

TENTORI, L., VIVALDI, G., CARTA, S., ANTONINI, E. & BRUNORI, M. (1968). *Nature (London)*, **219**, 487.

VAINSHTEIN, B. K., HARUTYUNYAN, E. H., KURANOVA, I. P., BORISOV, V. V., SOSFENOV, N. I., PAVLOVSKY, A. G., GREBENKO, A. I. & KONAREVA, N. V. (1975). *Nature (London)*, **254**, 163–164.

Acta Cryst. (1978). B**34**, 3662–3666

Nucleic-Acid Constituents.
X.* The Crystal and Molecular Structure of Adenosine-5'-*O*-methylphosphate

BY J. D. HOOGENDORP, G. C. VERSCHOOR AND C. ROMERS

Gorlaeus Laboratoria, X-ray and Electron Diffraction Section, University of Leiden, Leiden, The Netherlands

(*Received* 19 *May* 1978; *accepted* 18 *July* 1978)

Adenosine-5'-*O*-methylphosphate, $C_{11}H_{16}N_5O_7P$, crystallizes in the orthorhombic system with very unusual space group *I*222. The lattice constants at 20°C are $a = 17{\cdot}244$ (8), $b = 13{\cdot}309$ (7) and $c = 15{\cdot}037$ (7) Å. There are eight mononucleotides per unit cell as well as an undefined number of methanol molecules in disordered positions. The space group and structure were determined by Patterson analysis and direct methods. The structure was refined by a least-squares procedure ($R_w = 3{\cdot}8\%$). The adenine moiety has the *anti* configuration ($\chi = 68{\cdot}6°$) with respect to the sugar. The ribose ring has an *S*-conformation [C(2')-*endo*] with pseudorotation angle $P = 171{\cdot}7$ and $\varphi_{\max} = 33{\cdot}9°$. The side-chain orientation is g^+ (*gauche–gauche*) and the backbone is folded. The unusual space group is commented on.

Introduction

This paper is a contribution to a project on synthesis, NMR and ORD studies and X-ray investigations of nucleic-acid constituents. Since the geometry and conformation of the title compound may serve as a reference for the interpretation of NMR measurements of oligonucleotides (Altona and co-workers, unpublished) the crystal structure of adenosine-5'-*O*-methylphosphate (mpA) was decided upon. The chemical synthesis of mpA will be described elsewhere (Oltshoorn, Altona & van Boom, 1979). The chemical formula and the numbering of atoms are indicated in Fig. 1(*a*).

Experimental

mpA was crystallized from a mixture of water, methanol and hydrochloric acid (pH = 3·0). Only one single crystal was found, therefore the density was not determined experimentally. The diffraction symmetry is *mmm* and reflexions *hkl* are absent for $h + k + l$ odd. Since mpA is optically active the space groups to be considered are *I*222 and $I2_12_12_1$. Taking into account the cell dimensions (Table 1) and the lack of symmetry of mpA, it is reasonable to assume that the unit cell contains eight molecules. In a later stage we located an undefined amount of methanol (less than eight

Table 1. *Crystal data at* 20°C

$a = 17{\cdot}244$ (8) Å	*I*222
$b = 13{\cdot}309$ (7)	λ(Mo $K\alpha$) = 0·71069 Å
$c = 15{\cdot}037$ (7)	μ(Mo $K\alpha$) = 2·2 cm^{-1}

$1{\cdot}39 < \text{density} < 1{\cdot}51$ g cm^{-3}

Instrument: three-circle diffractometer, graphite-monochromatized Mo $K\alpha$ radiation, crystal mounted parallel to [010]

Scan method: ω scan between $\theta = 4$ and $\theta = 25{\cdot}5°$

Scanned reflexions	3074
Symmetry-independent	1645
Non-significant ($I < 2\sigma$)	167
Not observed	106
Used in analysis	1372

---

* Part IX: de Graaff, Martens & Romers (1978).

molecules) in disordered positions in the cell. The diffraction data (Mo $K\alpha$ radiation, see Table 1) were reduced to structure factors in the usual way. No absorption correction was applied.

Structure determination and refinement

Attempts to determine the structure with *MULTAN* (Germain, Main & Woolfson, 1971) in terms of $I222$ and $I2_12_12_1$ produced no positive results. Systematic inspection of a sharpened Patterson function indicated the presence of Harker vectors which could be attributed to symmetry-related P atoms in the space group $I222$. A minimum function was calculated shifting over the P–P vectors. The space group was confirmed and a partial solution of the structure obtained. With the exception of one atom the whole structure was, however, found by application of magic integers (Declercq, Germain & Woolfson, 1975).

The least-squares refinement was carried out in the usual way with 9×9 blocks for the heavy atoms. We refer to de Graaff, Admiraal, Koen & Romers (1977) for details concerning scattering, temperature and reliability factors. When the R factor dropped below 10% we discovered six peaks in a Fourier map around the point $\frac{1}{2},0,\frac{1}{2}$. Some of these peaks have mutual distances of ~1·4 Å and none have distances smaller than van der Waals contacts with the nucleotide (see *Packing*). It was impossible to discriminate between O and C for the scattering of these sites and we decided to refine the positional coordinates and the degree of occupancy for each peak, while assigning one isotropic temperature factor to all sites refined. The scattering factor of C was used for these 'atoms'. The high temperature factor ($B = 10\cdot2$ Å^2) and the low degree of occupancy (between 0·17 and 0·96) clearly indicate the disordering of these scatterers.

The H atoms of the nucleotide were partially located in Fourier difference maps and partially introduced at calculated positions. They were refined with isotropic temperature factors.

During the final stages the refinement was hampered by the presence of reflexion 240 in the data set. Its observed intensity was six times the calculated value. Since 200 and 040 are very strong reflexions, it was assumed that 240 suffered from multiple reflexion. Discarding this reflexion resulted in proper convergence with final agreement indices $R = 4\cdot3$ and $R_w = 3\cdot8\%$. The positional parameters of the heavy atoms and their e.s.d.'s are listed in Table 2.*

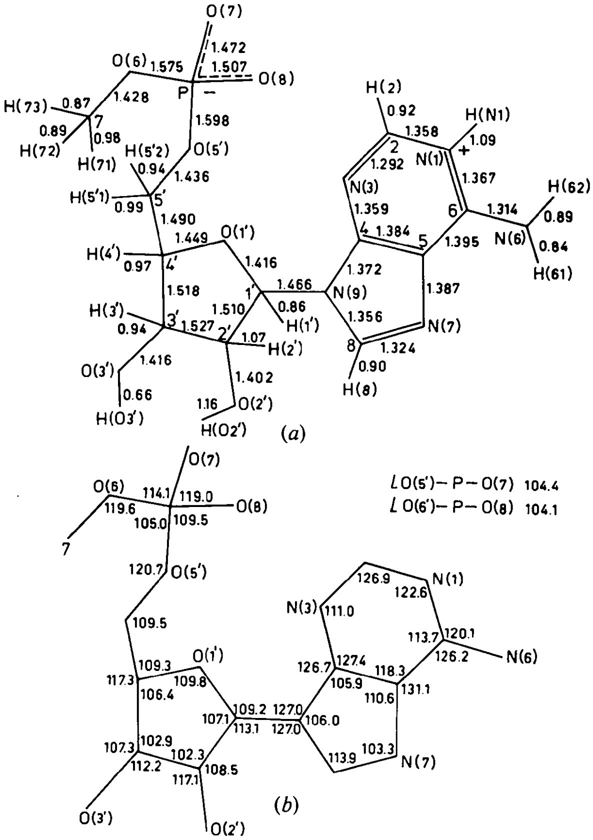


Fig. 1. (*a*) The numbering of atoms of adenosine-5′-*O*-methylphosphate, with bond distances (Å) and (*b*) valence angles (°).

Table 2. *Fractional coordinates* (×10^4) *of the heavy atoms, with e.s.d.'s in digits of the last decimal given in parentheses*

	x	*y*	*z*
C(1′)	3728 (2)	−3760 (3)	1532 (3)
C(2′)	3216 (2)	−3647 (3)	2341 (3)
C(3′)	2525 (3)	−4314 (3)	2109 (3)
C(4′)	2566 (2)	−4204 (3)	1106 (3)
C(5′)	1887 (3)	−3473 (4)	757 (3)
C(2)	6190 (3)	−3372 (4)	1083 (3)
C(4)	4997 (2)	−2850 (3)	1239 (3)
C(5)	5189 (2)	−1848 (3)	1129 (3)
C(6)	5967 (2)	−1601 (3)	1000 (3)
C(7)	609 (4)	−1159 (6)	1191 (6)
C(8)	3967 (3)	−1904 (3)	1311 (3)
N(1)	6448 (2)	−2416 (3)	967 (3)
N(3)	5483 (2)	−3653 (3)	1219 (2)
N(6)	6251 (2)	−691 (3)	906 (3)
N(7)	4533 (2)	−1248 (2)	1179 (2)
N(9)	4208 (2)	−2873 (2)	1359 (2)
O(1′)	3233 (2)	−3928 (2)	796 (2)
O(2′)	3649 (2)	−3909 (2)	3095 (2)
O(3′)	2672 (2)	−5341 (3)	2291 (3)
O(5′)	2070 (2)	−2483 (2)	1076 (2)
O(6)	1037 (1)	−1384 (2)	403 (2)
O(7)	2346 (2)	−703 (2)	928 (2)
O(8)	2178 (2)	−1769 (2)	−477 (2)
P	1943 (1)	−1521 (1)	458 (1)

---

* Lists of structure factors, anisotropic thermal parameters for the heavy atoms, positional and isotropic thermal parameters for hydrogen and 'methanol' atoms have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 33829 (7 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Discussion of the structure

Taking into account a 40% underestimation due to the block-diagonal refinement the e.s.d.'s of P—O, C—O, C—N, C—C and C(7)—O(6) distances are 0·003, 0·008, 0·008, 0·009 and 0·013 Å, respectively. The e.s.d.'s of valence and torsion angles are about 0·5 and 0·6°.

The bond distances and valence angles are indicated in Fig. 1(*a*) and (*b*). As usual the ribose ring C—C distances are rather small. The average value [1·518(5) Å] does not deviate significantly from that [1·523(4) Å] observed by Sundaralingam (1965) in his survey on nucleosides. He also commented on the length of C(4')—C(5') and found that its mean value (1·516 Å) differs significantly from the commonly observed single-bond C—C value of 1·533 Å (*Tables of Interatomic Distances and Configuration in Molecules and Ions*, 1965). In our case this bond is exceptionally short (1·490 Å). The differences in lengths between the bonds P—O(5') and P—O(6) [0·023(4) Å] and between P—O(7) and P—O(8) [0·029(4) Å] are highly significant. The former difference is frequently observed in phosphodiesters, the latter is probably a consequence of the very strong N(1)—H···O(8) hydrogen bond of length 2·626 Å.

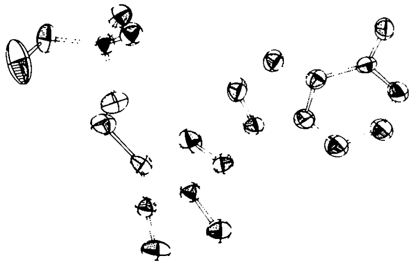


Fig. 2. *ORTEP* projection of the molecule mpA.

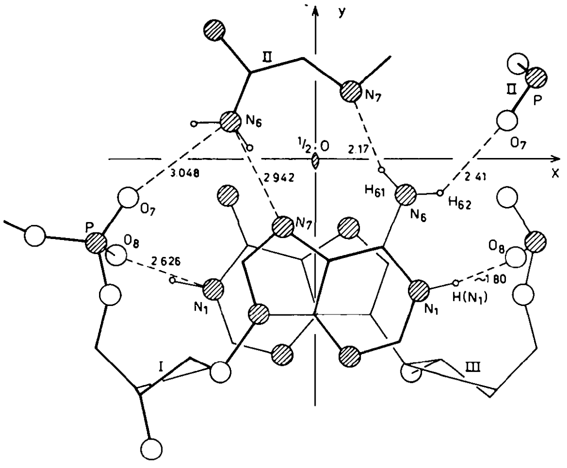


Fig. 3. A part of the crystal structure viewed in a projection along [001]. Shown are the molecules (I) at *x,y,z*; (II) at 1 − *x*, −*y*, *z* and (III) at 1 − *x*, *y*, −*z*.

An *ORTEP* (Johnson, 1965) projection of the molecule is presented in Fig. 2. Evidently the backbone is folded, while the adenine base is oriented *anti* (χ = 68·6°) with respect to the furanoside ring. A number of torsion angles are listed in Table 3. It follows that the ribose ring has an *S* conformation [C(2')-*endo*] with the phase angle of pseudorotation (Altona & Sundaralingam, 1972) P = 171·7° and $\varphi_{\max}$ = 33·7°. The side-chain moiety —O(5')—C(5')H_2— has a *gauche–gauche* (g^+) orientation with respect to O(1') and C(3'). The same conformational features were observed in sodium uridine-5'-*O*-methylphosphate (mpU; Hoogendorp & Romers, 1978). However, in contrast to mpU, the backbone of which assumes the right-handed arrangement of *B*-DNA, the backbone of mpA is left handed. A second important difference is the base–base stacking (see next section) which is absent in mpU.

Packing

We have refrained from depicting the complicated three-dimensional structure, preferring to show the most relevant part (Fig. 3) in projection along [001]. Three molecules (I), (II) and (III) are shown in part in positions *x,y,z*; 1 − *x*, −*y*, *z* and 1 − *x*, *y*, −*z*. The amino group [H(61)—N(6)—H(62)] plays a dominant role in the linkage of molecules by means of hydrogen bridges. Both H(61) and H(62) are involved. The former is donated to N(7), the latter to O(7). The hydrogen bond N(6)—H(61)···N(7), of length 2·942 Å, is comparable to N—H···N bridges found in xanthane hydride (2·98 Å, Stanford, 1963), 9-ethylguanine–1-methylcytosine (2·91 Å; O'Brien, 1963), 9-methyladenine–1-methylthymine (2·924 Å; Hoogsteen, 1963), adenosine–5-bromouridine (2·80 Å; Haschemeyer & Sobell, 1965) and hydrazinium chloride (2·95 Å; Sakurai & Tomiie, 1952). Although the N(6)—H(62)···O(7) bond, of length 3·048 Å, is rather weak, its existence is essential to explain the observed bending of the backbone. A

Table 3. *Selected torsion angles* (°) *of mpA*

Notation	Designation	Angle	Conformation
τ_0	C(4')—O(1')—C(1')—C(2')	−15·8	*S*-type
τ_1	O(1')—C(1')—C(2')—C(3')	30·3	C(2')-*endo*
τ_2	C(1')—C(2')—C(3')—C(4')	−32·6	P = 171·0
τ_3	C(2')—C(3')—C(4')—O(1')	24·2	$\varphi_{\max}$ = 33·7
τ_4	C(3')—C(4')—O(1')—C(1')	−5·6	
ψ'	O(3')—C(3')—C(4')—C(5')	143·5	
ψ	C(3')—C(4')—C(5')—O(5')	60·6	g^+(*gauche–gauche*)
φ	C(4')—C(5')—O(5')—P	143·3	
ω	C(5')—O(5')—P—O(6)	71·6	
ω'	O(5')—P—O(6)—C(7)	63·5	
	O(1')—C(4')—C(5')—O(5')	299·4	
χ	O(1')—C(1')—N(9)—C(8)	68·6	*anti*
	O(2')—C(2')—C(3')—O(3')	−36·4	
	O(2')—C(2')—C(3')—C(4')	151·3	
	O(2')—C(2')—C(1')—O(1')	154·9	

second factor contributing to this folding is the exceptionally short hydrogen bond N(1)—H(N1)$\cdots$O(8), of length 2·626 Å. Similar, short N—H$\cdots$O bonds are, however, observed in adenine hydrochloride (2·62 Å; Broomhead, 1951), glycl-L-tryptophan (2·68 Å; Pasternak, 1956), hydroxy-L-proline (2·69 Å; Donohue & Trueblood, 1952) and 6-amido-3-pyridazone (2·64 Å, Cucka & Small, 1954).

Table 4 contains a survey of all intermolecular contacts, *e.g.* hydrogen bonds (with molecules II–VII), base–base stacking (III), methanol contacts (VIII–XI) and hydrophobic contacts (XII–XV). In his survey of solid-state stacking of purine bases Bugg (1972) distinguishes two stacking patterns in which the imidazole rings point either in parallel or in opposite directions. The stacking in mpA is of the latter type. In comparison with the shown examples in Bugg's review the stacking of adenine in mpA is nearly perfect. The mutual distance of the bases is ~3·50 Å. Superficial inspection of Table 4 suggests a close packing with 14 neighbouring molecules. However, the relatively few H$\cdots$H contacts (~2·6 Å) are very weak. If we ignore these hydrophobic interactions the coordination is reduced to ten. This results in an unstable structure in terms of Kitaigorodsky's (1961) theory of close packing. The methanol molecules serve as inclusion compounds in clathrates: without these molecules the structure would contain big holes with a radius of ~5 Å in positions $\frac{1}{2},0,\frac{1}{2}$ and $0,\frac{1}{2},0$.

Table 4. *Intermolecular distances* (Å)

Bond	Operation	Distance	Molecule
Hydrogen bonds			
N(6)$\cdots$O(7)	$1-x,\ -y,\ z$	3·048	II
N(6)$\cdots$N(7)	$1-x,\ -y,\ z$	2·942	II
N(1)$\cdots$O(8)	$1-x,\ y,\ -z$	2·626	III
O(2')$\cdots$O(8)	$\frac{1}{2}-x,\ -\frac{1}{2}-y,\ \frac{1}{2}+z$	2·730	IV
O(8)$\cdots$O(2')	$\frac{1}{2}-x,\ -\frac{1}{2}-y,\ -\frac{1}{2}+z$	2·730	V
O(3')$\cdots$O(7)	$\frac{1}{2}-x,\ -\frac{1}{2}+y,\ \frac{1}{2}-z$	2·722	VI
O(7)$\cdots$O(3')	$\frac{1}{2}-x,\ \frac{1}{2}+y,\ \frac{1}{2}-z$	2·722	VII
Base–base stacking, several interactions			
	$1-x,\ y,\ -z$	~3·50	III
O(1')$\cdots$C(2)	$1-x,\ y,\ -z$	3·085	III
C(6')$\cdots$O(8)	$1-x,\ y,\ -z$	3·305	III
Methanol contacts			
	$-\frac{1}{2}+x,\ -\frac{1}{2}-y,\ \frac{1}{2}-z$		VIII
	$\frac{1}{2}+x,\ -\frac{1}{2}-y,\ \frac{1}{2}-z$		IX
	$x,\ -y,\ 1-z$		X
	$1-x,\ y,\ 1-z$		XI
Hydrophobic contacts			
H(4')$\cdots$H(4')	$x,\ -1-y,\ -z$	2·61	XII
H(4')$\cdots$H(5'1)	$x,\ -1-y,\ -z$	2·76	XII
H(71)$\cdots$H(73)	$-x,\ -y,\ z$	2·51	XIII
H(71)$\cdots$H(71)	$-x,\ -y,\ z$	2·77	XIII
H(73)$\cdots$H(73)	$-x,\ -y,\ z$	2·92	XIII
H(61)$\cdots$H(61)	$x,\ -y,\ -z$	2·72	XIV
H(62)$\cdots$H(62)	$x,\ -y,\ -z$	2·89	XIV
H(4')$\cdots$H(2)	$1-x,\ -1-y,\ z$	2·56	XV
H(1')$\cdots$H(2)	$1-x,\ -1-y,\ z$	2·86	XV
H(2)$\cdots$O(3')	$1-x,\ -1-y,\ z$	2·58	XV

Disregarding the compound dimethyltin dichloride (DMTC; Graybeal & Berta, 1969) the space groups $I222$ and $I2_12_12_1$ are absent among more than 10 000 known inorganic structures. The presented structure of DMTC with space group $I2_12_12_1$ is doubtful (R factor >0·27) and Davies, Milledge, Puxley & Smith (1970) propose a different structure with space group *Imma*. A search of 16 198 organic structures in the Cambridge Crystallographic Data File produced one structure, 1-cyanoacenaphthylene photodimer (DYAN; Courseille, Busetta, Hospital & Castellan, 1972) with space group $I222$. Recently two more structures with space group $I222$ were published: 5-[*N*-(L-leucyl)amino]uridine (LEUC; Narayanan & Berman, 1977) and a mixed-valence platinum–chloro complex with cyclohexanediamine as ligands (PLAT; Larsen & Toftlund, 1977).

Interestingly Kitaigorodsky (1961) excludes $I2_12_12_1$ as a possible space group for close packing, but accepts $I222$ for 'limitingly close packing' of molecules with symmetry 222. The latter condition is fulfilled in the complex PLAT containing tetragonal ligands about the Pt atom at the special position 0,0,0, but only partially in the photodimer CYAN with molecular symmetry 2. However, CYAN can also be considered as a disordered tetramer of symmetry 222. The third example, LEUC, does not conform to Kitaigorodsky's rule. Its structure consists of infinite double layers of molecules perpendicular to [010]. By means of lattice translations and the dyad parallel to [010] each LEUC molecule is hydrogen bonded with six neighbouring molecules. The double layers are formed under the operation of the two other dyads parallel to [100] and [001]. The double layers are kept together by interactions with water molecules (hydrophilic region) and the leucyl moieties (hydrophobic region). Interactions between different double layers complete the coordination of LEUC molecules to twelvefold.

Inspection of Fig. 3 reveals the following features in mpA: (i) the base–base stacked pair (I) and (III) can be considered as a dimer of symmetry 2; (ii) by means of hydrogen bridges this pair is connected to molecules (II) and (XIV) (not shown in Fig. 3); (iii) this tightly connected tetramer has symmetry 222 and is a candidate for close packing in the space group $I222$. In view of the weak H$\cdots$H interactions between the different tetramers the observed structure can hardly be considered as a stable one.

The first author acknowledges financial support from the Organization of Pure Scientific Research in the Netherlands (ZWO). We thank Dr Olga Kennard for information given by the Cambridge Crystallographic Data File and Dr R. A. G. de Graaff for assistance with 'magic integer' calculations and Mrs Marja Visser for assistance during the first stage of the investigation.

References

Altona, C. & Sundaralingam, M. (1972). *J. Am. Chem. Soc.* **94**, 8205–8212.

Broomhead, J. M. (1951). *Acta Cryst.* **4**, 92–100.

Bugg, C. E. (1972). *The Purines–Theory and Experiment*, edited by E. D. Bergmann & B. Pulmann. *Jerusalem Symp. Quantum Chem. Biochem.* **4**.

Courseille, C., Busetta, B., Hospital, M. & Castellan, A. (1972). *Cryst. Struct. Commun.* **1**, 337–340.

Cucka, P. & Small, R. W. H. (1954). *Acta Cryst.* **7**, 199–203.

Davies, A. G., Milledge, H. J., Puxley, D. C. & Smith, P. J. (1970). *J. Chem. Soc. A*, pp. 2862–2866.

Declercq, J. P., Germain, G. & Woolfson, M. M. (1975). *Acta Cryst.* A**31**, 367–372.

Donohue, J. & Trueblood, K. N. (1952). *Acta Cryst.* **5**, 419–431.

Germain, G., Main, P. & Woolfson, M. M. (1971). *Acta Cryst.* A**27**, 368–376.

Graaff, R. A. G. de, Admiraal, G., Koen, E. H. & Romers, C. (1977), *Acta Cryst.* B**33**, 2459–2464.

Graaff, R. A. G. de, Martens, F. B. & Romers, C. (1978). *Acta Cryst.* B**34**, 3012–3015.

Graybeal, J. D. & Berta, D. A. (1969). *Natl Bur. Stand. US Spec. Publ.* **301**, 393.

Haschemeyer, A. E. V. & Sobell, H. M. (1965). *Acta Cryst.* **18**, 525–532.

Hoogendorp, J. D. & Romers, C. (1978). *Acta Cryst.* B**34**, 2724–2728.

Hoogsteen, K. (1963). *Acta Cryst.* **16**, 907–916.

Johnson, C. K. (1965). *ORTEP*. Report ORNL-3794. Oak Ridge National Laboratory, Tennessee.

Kitaigorodsky, A. I. (1961). *Organic Chemical Crystallography*, p. 99. New York: Consultants Bureau.

Larsen, K. P. & Toftlund, H. (1977). *Acta Chem. Scand. Ser. A*, **31**, 182–186.

Narayanan, P. & Berman, H. M. (1977). *Acta Cryst.* B**33**, 2047–2051.

O'Brien, E. J. (1963). *J. Mol. Biol.* **7**, 107–110.

Oltshoorn, C. S. M., Altona, C. & van Boom, J. H. (1979). To be published.

Pasternak, R. A. (1956). *Acta Cryst.* **9**, 341–349.

Sakurai, K. & Tomiie, Y. (1952). *Acta Cryst.* **16**, 1157–1162.

Stanford, D. H. Jr (1963). *Acta Cryst.* **16**, 1157–1162.

Sundaralingam, M. (1965). *J. Am. Chem. Soc.* **87**, 599–606.

Tables of Interatomic Distances and Configuration in Molecules and Ions (1965). Spec. Publ. No. 18. London: The Chemical Society.

Acta Cryst. (1978). B**34**, 3666–3671

Structure Cristalline du Sophorose [*O*-*β*-D-Glucosyl-(1 → 2)-*α*-D-glucose]

Par Jacqueline Ohanessian, François Longchambon et Florence Arene

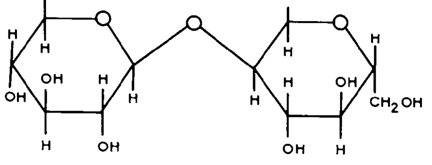
UER Expérimentale Santé, Médecine et Biologie Humaine, Université Paris XIII, 74 *rue Marcel Cachin*, 93000 *Bobigny, France*

(*Reçu le* 31 *mars* 1978, *accepté le* 21 *juillet* 1978)

Sophorose crystallizes in the orthorhombic space group $P2_12_12_1$ with a = 22·046 (4), b = 14·436 (2), c = 4·8657 (4) Å. The three-dimensional crystal structure obtained by direct methods was refined by least-squares calculations to a weighted R value of 0·045. The glucosyl units are in the $^4C_1$ chair conformation. Observed bond distances, bond angles and hydrogen bonds are consistent with those from other recent structure determinations of pyranose sugars. There is no intramolecular hydrogen bond.

Introduction

Nous avons entrepris l'étude d'un disaccharide de synthèse, le sophorose [*O*-*β*-D-glucosyl-(1→2)-α-D-glucose].



La particularité de ce composé relève de la présence de la liaison osidique *β*(1→2) car, à l'heure actuelle, aucun exemple de détermination structurale par diffraction des rayons X n'est connu. Une telle étude prolonge celles poursuivies au laboratoire sur le mélibiose (Neuman & Gillier-Pandraud, 1976; Kanters, Roelofsen, Doesburg & Koops, 1976), le turanose (Neuman, Avenel & Gillier-Pandraud, 1978) et le mélézitose (Avenel, Neuman & Gillier-Pandraud, 1976).

Partie expérimentale

De longues aiguilles de sophorose se sont développées rapidement dans une solution d'un produit commercial