O(3)—Ba—O(2A)	119.4 (2)	Ba—O(2)—C(3)	113.8 (6)
O(5)—Ba—O(2A)	106.1 (2)	C(3)—O(2)—C(4)	112.9 (7)
O(1A)—Ba—O(2A)	60.2 (2)	Ba—O(3)—C(6)	112.8 (5)
O(4)—Ba—O(3A)	70.8 (2)	Ba—O(4)—C(7)	93.0 (6)
C(7)—Ba—O(3A)	94.2 (2)	C(6)—C(1)—O(1A)	109.1 (10)
O(5)—Ba—O(4A)	134.0 (2)	O(1)—C(2)—C(3)	107.4 (10)
O(5)—Ba—O(5A)	180.0 (1)	O(2)—C(4)—C(5)	108.8 (7)
C(7)—Ba—C(7A)	180.0 (1)	O(3)—C(6)—C(1)	109.6 (10)
Ba—O(1)—C(2)	117.1 (6)	Ba—C(7)—O(5)	64.1 (6)
C(2)—O(1)—C(1A)	111.2 (9)	Ba—C(7)—C(8)	159.5 (7)
Ba—O(2)—C(4)	113.2 (6)	O(5)—C(7)—C(8)	119.3 (9)
Ba—O(3)—C(5)	112.8 (6)	C(7)—C(8)—C(10)	109.4 (10)
C(5)—O(3)—C(6)	113.1 (9)	C(7)—C(8)—C(11)	113.0 (11)
Ba—O(5)—C(7)	93.1 (7)	C(10)—C(8)—C(11)	108.9 (12)
O(1)—Ba—O(3)	119.4 (2)	O(2)—C(3)—C(2)	110.4 (8)
O(1)—Ba—O(4)	101.2 (2)	O(3)—C(5)—C(4)	109.6 (10)
O(3)—Ba—O(4)	109.2 (2)	Ba—C(7)—O(4)	63.1 (5)
O(2)—Ba—O(5)	73.9 (2)	O(4)—C(7)—O(5)	123.8 (9)
O(4)—Ba—O(5)	46.0 (2)	O(4)—C(7)—C(8)	116.9 (7)
O(2)—Ba—C(7)	94.0 (2)	C(7)—C(8)—C(9)	108.7 (9)
O(4)—Ba—C(7)	23.9 (2)	C(9)—C(8)—C(10)	109.8 (14)
O(1)—Ba—O(1A)	180.0 (1)	C(9)—C(8)—C(11)	107.0 (14)
O(3)—Ba—O(1A)	60.6 (2)		

Structure solved by direct methods (*SOLV*) and refined by full-matrix least squares. All non-H atoms anisotropic, all H-atom parameters assumed [*d*(C—H) = 0.960 Å, fixed isotropic U = 0.08 Å^2]. Calculations were performed using *SHELXTL-Plus* (Sheldrick, 1990).

Atomic coordinates and isotropic thermal parameters are given in Table 1, bond lengths and angles in Table 2.

Lists of structure factors, anisotropic thermal parameters and H-atom coordinates have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 55738 (8 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: CR1022]

References

Dyer, R. B., Metcalf, D. H., Ghirardelli, R. G., Palmer, R. A. & Holt, E. M. (1986). *J. Am. Chem. Soc.* **108**, 3621–3627.

Sheldrick, G. M. (1990). *SHELXTL-Plus*, version 4.21/V. Siemens Analytical X-ray Instruments, Inc., Madison, Wisconsin, USA.

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3,4,5-Trihydroxybenzohydroxamic Acid Monohydrate, a Ribonucleotide Reductase Inhibitor

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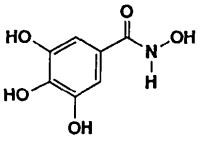
Abstract

The 3,4,5-trihydroxybenzohydroxamic acid molecule consists of two approximately planar parts: the hydroxamic acid moiety and the phenyl ring with the hydroxy substituents. These two planes are twisted relative to each other with a dihedral angle of 34.3 (1)°. The conformation of O=C—N—O is synperiplanar with a torsion angle of −5.4 (4) °. The crystal structure is stabilized by an intensive and complex pattern of hydrogen bonding, in which the water molecule plays a central role.

Comment

The anticancer agent hydroxyurea exerts its ribonucleotide reductase (RNR) inhibitory activity by destroying the tyrosyl free radical in RNR, thereby leaving the enzyme inactive (Atkin, Thelander, Reichard & Lang, 1973; Gräslund, Ehrenberg & Thelander, 1982; Thelander, Gräslund & Thelander, 1985; Howell, Sanders-Loehr, Loehr, Roseman, Mathews & Slabaugh, 1992). In a search for anticancer drugs with the same target of action Elford, Wampler & van't Riet (1979) tested a series of compounds including polyhydroxylated benzohydroxamic acids. 3,4-Dihydroxybenzohydroxamic acid (3,4-OHBHA), 2,3,4-trihydroxybenzohydroxamic acid (2,3,4-OHBHA) and 3,4,5-trihydroxybenzohydroxamic acid (3,4,5-OHBHA) were all found to have strong inhibitory activities on partially purified RNR from Novikoff hepatoma cells. These



3,4,5-OHBHA

compounds were found to have stronger inhibitory effects than hydroxyurea on the mammalian RNR (Elford, van't Riet, Wampler, Lin & Elford, 1981), whereas the *E. coli* RNR and the phage T4 RNR were found to be more sensitive towards hydroxyurea than towards the polyhydroxylated benzohydroxamic acids (Kjøller Larsen, Sjöberg & Thelander, 1982). In an early structure–activity study of hydroxyurea analogues using HeLa cells it was shown that an unsubstituted OH group at the N atom was required for activity (Young, Schochetman, Hodas & Balis, 1967). On the other hand, Elford *et al.* (1979) found that polyhydroxylated benzamides and methyl benzoates were also inhibitors of RNR, indicating that in these compounds the hydroxamic acid moiety is not essential for RNR inhibitory activity. The polyhydroxylated aromatic part of the compounds seems to be the part interfering with the tyrosyl radical of the enzyme.

By testing a series of hydroxyurea analogues (Larsen, 1980; Kjøller Larsen *et al.*, 1982) or polyhydroxybenzene derivatives (Elford *et al.*, 1981) it has been found that the ability of a compound to undergo one-electron oxidation is correlated with its inhibitory activity towards RNR. In addition, the most potent inhibitors were approximately planar molecules. The crystal structure of the small sub-

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unit of *E. coli* RNR, which is the subunit harbouring the tyrosyl free radical, has recently been solved (Nordlund, Sjöberg & Eklund, 1990). No obvious pocket or cleft leading to the tyrosyl radical was found in the protein, and it is not yet known whether the hydroxyurea analogues interact directly with the free radical or by long-range electron transfer. Attempts at crystallization of enzyme–inhibitor complexes are in progress.

The structure of 3,4-OHBHA has been determined previously (Due, Rasmussen & Larsen, 1987) and the compound has been tested in both phase I (Veale *et al.*, 1988) and phase II (Rubens *et al.*, 1991) clinical trials. The structure of 3,4,5-OHBHA was determined in order to compare it with those of salicylohydroxamic acid (2-OHBHA) and 3,4-OHBHA. Crystals of 2,3,4-OHBHA suitable for X-ray work have not yet been obtained.

The bond lengths and angles of 3,4,5-OHBHA (Table 2) are comparable to the values obtained for 3,4-dihydroxybenzohydroxamic acid (Due *et al.*, 1987) and 2-OHBHA (Larsen, 1978). The geometry of the benzene ring is regular. Slight distortions of the valence angles are observed at the hydroxy substituents C3—O3 and C5—O5 (see Table 2). A similar distortion is seen in 3,4-OHBHA where the O4—C4—C5 and C3—C4—O4 angles are 123.51 (9) and 116.14 (8)°, respectively (Due *et al.*, 1987).

The conformation of O=C—N—O is synperiplanar with a torsion angle of −5.4 (4)°. The same conformation is observed in 3,4-OHBHA (Due *et al.*, 1987) and 2-OHBHA (Larsen, 1978) in which the corresponding torsion angles are 10.7 (2) and 6.3 (5)°, respectively, but hydroxamic acids may adopt a synperiplanar as well as an antiperiplanar conformation (Larsen, 1988).

The molecule consists of two approximately planar parts, the phenyl ring including the O-atom substituents and the hydroxamic acid moiety. The maximum deviation from the phenyl ring plane mentioned above is −0.031 (2) Å (the O3 atom). Two of the hydroxy H atoms are situated near to the plane with distances of −0.06 (3) and 0.08 Å for H3 and H4,† respectively, whereas the distance of H5 to the plane is 0.20 (4) Å. The four atoms C1, C7, O7 and N8 of the hydroxamic acid moiety constitute a plane. The distances of O9 and H8 to this plane are 0.116 (2) and 0.21 (4) Å, respectively, and a slight degree of pyramidalization of N8 is observed. The dihedral angle between the plane of the hydroxamic acid moiety and the phenyl ring is 34.3 (1)°. The corresponding angles of 3,4-OHBHA and 2-OHBHA are 11.5 and 3.5°, respectively [calculated from parameters retrieved from the Cambridge Structural Database, January 1992 release (Allen *et al.*, 1979)].

The polyhydroxylated benzohydroxamic acids are much more efficient inhibitors of RNR than are the monohydroxylated derivative 2-OHBHA (Kjøller Larsen *et al.*, 1982; Elford *et al.*, 1981). 2-OHBHA is the most planar of the three componds, but has the lowest ability to undergo one-electron oxidation. The latter property is evidently the most important for effective inhibition of RNR.

The crystal structure is stabilized by a complex three-dimensional pattern of hydrogen bonding in which the water molecule plays a central role (see Fig. 2 and Table 2). The phenyl rings are stacked along the *b* axis. The hydrophilic parts of the 3,4,5-OHBHA molecules are directed towards channels of water molecules forming hydrophilic layers parallel to the (101) crystal planes. The water molecule connects five 3,4,5-OHBHA molecules through hydrogen bonding, being a donor in three and acceptor in two hydrogen bonds. H102† forms a bifurcated hydrogen bond connecting two centrosymmetrically related molecules. Bifurcated hydrogen bonding is also observed for H9 which interacts with O9 as well as O10. Zigzag hydrogen bonding is formed along the *b* axis by H4,†thus connecting two columns of centrosymmetrically related molecules. The hydrogen bonds O3—H3···O7 and N8—H8···O5 further stabilize the structure along the *b* axis. In addition to the complex and intensive intermolecular hydrogen bonding there is intramolecular hydrogen bonding: O4—H4···O3 and O5—H5···O4. Four non-bonded distances in hydrogen-bonding range (< 3.15 Å) are observed between O atoms in the crystal packing (see Table 2).

† See previous footnote.

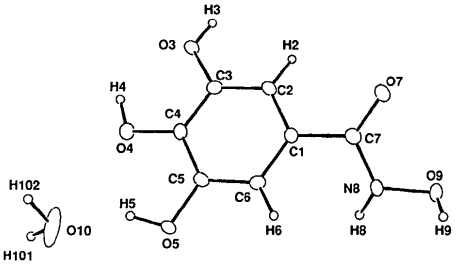

Fig. 1. Molecular structure of 3,4,5-OHBHA (Johnson, 1976) showing the atom labelling. Atomic displacement ellipsoids are drawn at the 50% probability level for non-H atoms.

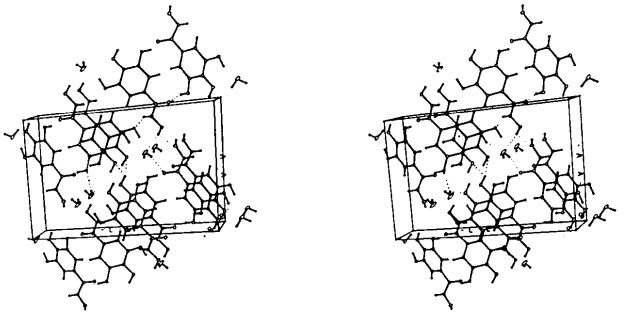

Fig. 2. Crystal packing of 3,4,5-OHBHA with the hydrogen-bonding pattern shown with broken lines.

† The geometry of the hydrogen bonds involving H4 and H102 should be taken with reservation since the positions of these two H atoms were not refined (*cf. Experimental*).

Experimental

Crystal data

$C_7H_7NO_5.H_2O$
M_r = 203.15
Monoclinic
$P2_1/n$
a = 11.5961 (8) Å
b = 3.6323 (4) Å
c = 18.531 (1) Å
β = 94.020 (6)°
V = 778.6 (2) Å^3
Z = 4
D_x = 1.733 Mg m^{-3}
Cu $K\alpha$ radiation
λ = 1.5418 Å

Cell parameters from 22 reflections
θ = 39.91–46.17°
μ = 1.2944 mm^{-1}
T = 110 K
Rectangular thin plates
0.40 × 0.10 × 0.04 mm
Colourless
Crystal source: synthesized as described by van't Riet *et al.* (1979); single crystals obtained by slow cooling of a hot aqueous solution

Data collection

Enraf–Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
4298 measured reflections
1609 independent reflections
1231 observed reflections [$>5\sigma$]
R_{int} = 0.022
θ_{max} = 75.00°

$h = -14 \rightarrow 14$
$k = -4 \rightarrow 4$
$l = -23 \rightarrow 23$
3 standard reflections monitored every 300 reflections
frequency: 166 min
intensity variation: −4.0%

Refinement

Refinement on F
Final R = 0.045
wR = 0.064
S = 2.091
1231 reflections
155 parameters
All H-atom parameters refined except H102 and H4 for which both positional and displacement parameters were fixed

$w = 1/[\sigma^2(F)+(0.02F)^2+2.00]$
$(\Delta/\sigma)_{max}$ = 0.00
$\Delta\rho_{max}$ = 0.798 e Å^{-3}
$\Delta\rho_{min}$ = −0.819 e Å^{-3}
Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV, Table 2.3.1)

All H atoms were found in a difference Fourier map after refinement of positional and anisotropic displacement parameters for the non-H atoms. It was not possible to refine the positions of H4 and H102. Refinement of the occupancy for H102 was tried but was not successful. H102 and H4 were then fixed at the positions found in a difference Fourier map, calculated after refinement of all other parameters. Data reduction: *BEGIN*, *SDP* (B. A. Frenz & Associates, Inc., 1982). Program(s) used to solve structure: *SHELXS86* (Sheldrick, 1990). Program(s) used to refine structure: *LSFM*, *SDP* (B. A. Frenz & Associates, Inc., 1982). Molecular graphics: *ORTEP*II (Johnson, 1976).

Table 1. *Fractional atomic coordinates and equivalent isotropic thermal parameters* (Å^2)

$B_{eq} = 4/3\Sigma_i\Sigma_j\beta_{ij}\mathbf{a}_i.\mathbf{a}_j.$

	x	y	z	B_{eq}
O3	0.4263 (1)	0.5576 (6)	0.37376 (8)	1.36 (3)
O4	0.3993 (1)	0.2770 (6)	0.50631 (9)	1.43 (3)
O5	0.1797 (1)	0.0761 (5)	0.54529 (8)	1.02 (3)
O7	0.0154 (1)	0.4181 (5)	0.24199 (8)	1.36 (3)
O9	−0.1831 (1)	0.6263 (6)	0.29423 (9)	1.57 (3)
O10	0.3516 (2)	−0.2028 (7)	0.6358 (1)	3.58 (4)
N8	−0.0858 (2)	0.5377 (6)	0.3390 (1)	1.17 (3)
C1	0.1130 (2)	0.3939 (6)	0.3609 (1)	0.81 (3)
C2	0.2219 (2)	0.4892 (7)	0.3395 (1)	0.92 (4)
C3	0.3175 (2)	0.4545 (7)	0.3882 (1)	0.95 (4)
C4	0.3057 (2)	0.3120 (6)	0.4573 (1)	0.90 (4)
C5	0.1964 (2)	0.2138 (6)	0.4780 (1)	0.86 (4)
C6	0.0999 (2)	0.2586 (6)	0.4302 (1)	0.92 (4)
C7	0.0114 (2)	0.4496 (6)	0.3084 (1)	0.96 (4)

Table 2. *Selected bond lengths* (Å), *bond angles* (°), *torsion angles* (°), *contact distances* (Å) *and hydrogen-bond geometry* (Å, °)

C1—C2	1.394 (3)	O3—C3	1.361 (3)
C1—C6	1.394 (3)	O4—C4	1.371 (3)
C1—C7	1.489 (3)	O5—C5	1.371 (3)
C2—C3	1.386 (3)	O7—C7	1.240 (3)
C3—C4	1.398 (3)	N8—C7	1.336 (3)
C4—C5	1.396 (3)	O9—N8	1.390 (2)
C5—C6	1.386 (3)		
C1—C2—C3	119.5 (2)	O3—C3—C4	115.8 (2)
C1—C6—C5	119.6 (2)	O4—C4—C3	121.1 (2)
C2—C1—C6	120.6 (2)	O4—C4—C5	119.2 (2)
C2—C1—C7	118.1 (2)	O5—C5—C6	117.8 (2)
C2—C3—C4	120.3 (2)	O5—C5—C4	122.1 (2)
C3—C4—C5	119.7 (2)	O7—C7—C1	123.6 (2)
C4—C5—C6	120.2 (2)	O7—C7—N8	122.4 (2)
C6—C1—C7	121.3 (2)	N8—C7—C1	114.1 (2)
O3—C3—C2	124.0 (2)	O9—N8—C7	118.4 (2)
C2—C1—C7—N8	−147.3 (2)	H9—O9—N8—C7	123 (3)
O9—N8—C7—O7	−5.4 (4)		
O9···O9^{i}	2.835 (3)	O4···O10	3.047 (3)
O3···O4^{ii}	2.959 (2)	O9···O10^{iii}	3.005 (3)

D	H	A	$D\cdots A$	H···A	D—H···A
O3	H3	O7^{i}	2.641 (2)	1.83 (3)	162 (3)
O4	H4	O3	2.698 (2)	2.22	115
O4	H4	O4^{iv}	3.104 (3)	2.74	107
O4	H4	O4^{ii}	2.865 (3)	2.15	139
O5	H5	O4	2.792 (2)	2.30 (3)	112 (3)
O5	H5	O10	2.710 (3)	1.82 (3)	154 (3)
N8	H8	O5^{v}	2.842 (3)	2.07 (3)	146 (3)
O9	H9	O9^{vi}	2.835 (3)	2.42 (4)	112 (3)
O9	H9	O10^{vii}	2.867 (3)	2.07 (4)	163 (3)
O10	H101	O7^{viii}	2.834 (3)	2.03 (4)	163 (4)
O10	H102	O3^{iv}	2.896 (3)	2.07	135
O10	H102	O4^{ix}	3.134 (3)	2.34	133

Symmetry code: (i) $-x+0.5, y+0.5, -z+0.5$; (ii) $-x+1, -y+1, -z+1$; (iii) $x-0.5, -y+0.5, z-0.5$; (iv) $-x+1, -y, -z+1$; (v) $-x, -y+1, -z+1$ (vi) $-x-0.5, y-0.5, -z+0.5$ (vii) $-x, -y, -z+1$; (viii) $x+0.5, -y+0.5, z+0.5$; (ix) $x, y-1, z$.

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Lists of structure factors, anisotropic thermal parameters, H-atom coordinates, complete geometry and least-squares-planes data have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 55790 (12 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: AB1042]

References

Allen, F. H., Bellard, S., Brice, M. D., Cartwright, B. A., Doubleday, A., Higgs, H., Hummelink, T., Hummelink-Peters, B. G., Kennard, O., Motherwell, W. D. S., Rodgers, J. R. & Watson, D. G. (1979). *Acta Cryst.* B**35**, 2331-2339.

Atkin, C. L., Thelander, L., Reichard, P. & Lang, G. (1973). *J. Biol. Chem.* **248**, 7464-7472.

B. A. Frenz & Associates, Inc. (1982). *SDP Structure Determination Package*. College Station, Texas, USA, and Enraf-Nonius, Delft, The Netherlands.

Due, L., Rasmussen, H. & Larsen, I. K. (1987). *Acta Cryst.* C**43**, 582-585.

Elford, H. L., van't Riet, B., Wampler, G. L., Lin, A. L. & Elford, R. M. (1981). *Adv. Enzyme Regul.* **19**, 151-168.

Elford, H. L., Wampler, G. L. & van't Riet, B. (1979). *Cancer Res.* **39**, 844-851.

Gräslund, A., Ehrenberg, A. & Thelander, L. (1982). *J. Biol. Chem.* **257**, 5711-5715.

Howell, M. L., Sanders-Loehr, J., Loehr, T. M., Roseman, N. A., Mathews, M. K. & Slabaugh, M. B. (1992). *J. Biol. Chem.* **267**, 1705-1711.

Johnson, C. K. (1976). *ORTEP*II. Report ORNL-5138. Oak Ridge National Laboratory, Tennessee, USA.

Kjøller Larsen, I., Sjöberg, B.-M. & Thelander, L. (1982). *Eur. J. Biochem.* **125**, 75-81.

Larsen, I. K. (1978). *Acta Cryst.* B**34**, 962-964.

Larsen, I. K. (1980). *Acta Chem. Scand. Ser. B*, **34**, 209-212.

Larsen, I. K. (1988). *Acta Cryst.* B**44**, 527-533.

Nordlund, P., Sjöberg, B.-M. & Eklund, H. (1990). *Nature (London)*, **345**, 593-598.

Riet, B. van't, Wampler, G. L. & Elford, H. L. (1979). *J. Med. Chem.* **22**, 589-592.

Rubens, R. D., Kaye, S. B., Soukop, M., Williams, C. J., Brampton, M. H. & Harris, A. L. (1991). *Br. J. Cancer*, **64**, 1187-1188.

Sheldrick, G. M. (1990). *Acta Cryst.* A**46**, 467-473.

Thelander, M., Gräslund, A. & Thelander, L. (1985). *J. Biol. Chem.* **260**, 2737-2741.

Veale, D., Carmichael, J., Cantwell, B. M. J, Elford, H. L., Blackie, R., Kerr, D. J., Kaye, S. B. & Harris, A. L. (1988). *Br. J. Cancer*, **58**, 70-72.

Young, C. W., Schochetman, G., Hodas, S. & Balis, E. M. (1967). *Cancer Res.* **27**, 535-540.

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Isopropylammonium Dihydrogenmonophosphate and Isopropylammonium Monohydrogenphosphite

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Abstract

The atomic arrangements in isopropylammonium dihydrogenmonophosphate and isopropylammonium monohydrogenphosphite are described. In the phosphate, the distances between the H_2PO_4 groups are rather short (P—P = 4.238 and 4.218 Å) so that these entities form (through strong hydrogen bonds) infinite $(H_2PO_4)_n$ chains parallel to the **a** direction. In spite of the significantly longer (4.769 Å) P—P distance, the $(HPO_3H)_n$ groups in the phosphite compound also form infinite chains running parallel to the **a** direction. In the phosphate derivative, linear arrays of the isopropylammonium groups spread parallel to the **c** direction, *i.e.* perpendicular to the phosphoric chain, while in the phosphite compound the arrays of the organic component and the phosphoric chains are parallel.

Comment

Both arrangements are characterized principally by the existence of infinite phosphoric chains, $(H_2PO_4)_n$ for the phosphate and $(HPO_3H)_n$ in the case of the phosphite. In both structures, isopropylammonium groups are arranged in linear arrays, but the organization of these arrays relative to the phosphoric chains is fundamentally different in the two derivatives. In the phosphate, the phosphoric chains spread along the **a** direction, while the organic component arrays are parallel to the **c** direction. Fig. 1 shows the general organization of this arrangement projected along **c**. In contrast, both the $(HPO_3H)_n$ chains and the arrays of isopropylammonium groups in the phosphite compound are parallel to the **a** direction. In the phosphate, each H_2PO_4 group is connected to its two adjacent neighbours by relatively strong hydrogen bonds (2.567 and 2.631 Å) corresponding to O—O distances slightly longer than those observed inside the PO_4 tetrahedron. The short P—P distances observed in the chain (4.238 and 4.218 Å) are easily explained by the geometry of these hydrogen bonds. In the phosphite, the P—P distance is significantly longer (4.769 Å) because the infinite $(HPO_3H)_n$ chain is more stretched, each PO_3H tetrahedron being bonded to its two neighbours by only one hydrogen bond. Fig. 2 depicts the general organization of the phosphite derivative. Tables 2 and 4 give the main interatomic distances and bond angles in these two arrangements, includ-

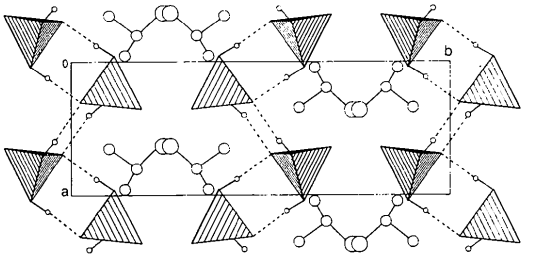

Fig. 1. Projection along the **c** direction of the atomic arrangement of the phosphate compound. The hatched tetrahedra denote the PO_4 groups. The open circles represent, in decreasing order of size, N, C and H atoms. Inside the phosphoric chain, hydrogen bonds are represented by solid and dashed lines. The H atoms of the organic components have been omitted.

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