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The Structure of 2-Dimethylamino-6-oxo-4-phenyl-1,3-oxazin-5-carbaldehyde

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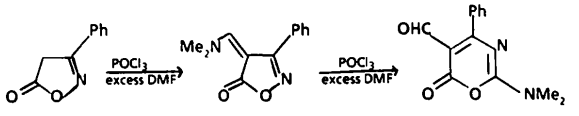
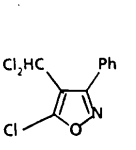
Abstract. $C_{13}H_{12}N_2O_3$, $M_r = 244{\cdot}25$, triclinic, $P\bar{1}$, $a = 8{\cdot}862$ (6), $b = 10{\cdot}041$ (2), $c = 14{\cdot}550$ (1) Å, $\alpha = 97{\cdot}00$ (1), $\beta = 83{\cdot}32$ (2), $\gamma = 116{\cdot}03$ (2)°, $V = 1151{\cdot}8$ (13) Å^3, $Z = 4$, $D_x = 1{\cdot}41$ g cm^{-3}, Cu $K\alpha$, $\lambda = 1{\cdot}5418$ Å, $\mu = 7{\cdot}5$ cm^{-1}, $F(000) = 256$, $T = 123$ K, $R = 0{\cdot}054$ for 3773 unique reflections. The structure has an unusual number of close intermolecular contacts. The dense packing causes significant non-planarity of the oxazine ring in one of the two symmetry-independent molecules, and causes disorder of the aldehyde O and H atoms in the other molecule.

Introduction. Under Vilsmeier conditions, the title compound (3) is formed from 3-phenyl-5(4*H*)-isoxazolone (1) *via* (2) when it is reacted with $POCl_3$–excess *N*,*N*-dimethylformamide (DMF). This

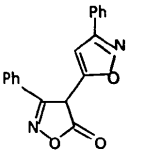


(1) (2) (3)

ring-expanded product was unexpected in the light of a literature report (Kallury & Devi, 1977) that the reaction products are a trichloroisoxazole (4) and a bis-adduct (5). Reactions of (1) with the same and modified conditions were then studied in detail, and mechanisms of the transformations were worked out (Anderson, 1986). In none of the reactions were (4) or (5) ever produced.



(4)



(5)

An X-ray crystallographic study of (3) was performed in order to confirm the structure beyond doubt.

Experimental. Clear chunky prism $0{\cdot}60 \times 0{\cdot}20 \times 0{\cdot}70$ mm; Nicolet $P\bar{1}$ diffractometer controlled by Harris computer; graphite monochromator, Cu $K\alpha$; $2\theta_{max} = 138°$; all 3773 unique reflections measured, 3397 intensities $>2\sigma$; 2° min^{-1} $\theta/2\theta$ step scans, scan widths >3·4°; 10 reflections periodically monitored showed no trend towards deterioration; $\sigma^2(I)$ was approximated by $\sigma^2(I)$ from counting statistics + $(0{\cdot}018I)^2$, where the coefficient of I was calculated from the variations in intensities of the monitored reflections; cell parameters by least-squares fit of Cu $K\alpha_1$ 2θ values [λ(Cu $K\alpha_1$) = 1·5402 Å] for 25 high-2θ reflections (Duchamp, 1977); Lp correction appropriate for a monochromator with 50% perfect character, no absorption correction. The structure was solved by direct methods, using *DIREC* (Duchamp, 1984*a*), H atoms were found in difference maps; except for methyl H atoms, generated positions were used. The aldehyde O and H atoms in the primed molecule are disordered; in a population of molecules, this substituent is rotated

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approximately 180°. Least-squares refinement included: coordinates and anisotropic thermal parameters for non-H atoms, except for disordered atoms O(5′) and O(5″), which were kept isotropic. Occupancy factors were fixed and repeatedly adjusted until temperature factors would refine to approximately equal values. H-atom parameters were included in the calculations but were not refined. The function minimized in the refinement was $\sum w(F_o^2 - F_c^2)^2$, where weights w were $1/\sigma^2(F_o^2)$. Atomic form factors were from Doyle & Turner (1968), and, for H, from Stewart, Davidson & Simpson (1965). In the final refinement cycle, all shifts were $<0{\cdot}30\sigma$. Occupancies were 72% for O(5′) and H(*H5′*), and 28% for O(5″) and H(*H5″*). $wR = 0{\cdot}116$, $R = 0{\cdot}054$, $S = 3{\cdot}30$; final difference Fourier map peaks were $<0{\cdot}3$ e Å^{-3}. The *CRYM* system of computer programs was used (Duchamp, 1984*b*).

Discussion. Final atomic parameters are listed in Table 1.* Fig. 1 shows conformation and numbering for one of the two symmetry-independent molecules. Bond distances and angles and selected torsion angles are given in Table 2. The other molecule (primed numbers) has similar conformation with respect to the orientation of the phenyl group. The aldehyde O and H atoms in this molecule are disordered; in the major species (72% occupancy), the C(5′)–C(*H5′*) bond is rotated approximately 180° from the conformation in Fig. 1. Table 2 lists close intermolecular contacts. Both O(5′) and O(5″) have several short intermolecular contacts, in fact they are the shortest distances in the table, which probably is related to the disorder observed.

Although many of the close contacts are similar for the two molecules, and although both phenyl groups have very similar orientations, the molecules are not related by crystallographic symmetry. The packing drawing, Fig. 2, shows that each pair of molecules is related by an approximate twofold-axis-plus-translation, but this is not crystallographic symmetry.

The oxazine ring is significantly non-planar, especially in the unprimed molecule, as torsion angles show. In the primed (disordered) molecule, the deviations from the best plane for ring atoms range from −0·034 to 0·037 Å; in the unprimed molecule the range is −0·038 to 0·081 Å. Substituents O(6), N(2) and C(*H5*) deviate from the best planes by −0·032, 0·080, and 0·252 Å in the primed molecule, and by −0·168, 0·284, and 0·443 Å, respectively, in the unprimed molecule. The ring in the unprimed molecule (no disorder) is folded along a line between C(2) and C(5); atoms C(2), O(1), C(6), O(6) and C(5) are coplanar, and atoms C(2), N(3), C(4), C(1*P*) and C(5) are coplanar; the angle between these planes is about 14°. The *N*-dimethyl substituent and the aldehyde substituent are bent away from the ring in the opposite direction from the phenyl and carbonyl, so that the

Table 1. *Fractional coordinates* (×10⁴) *and* B_{eq} [*B for* O(5′) *and* O(5″)]; *e.s.d.'s are in parentheses*

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

	x	*y*	*z*	B_{eq}(Å²)
O(1)	2295 (2)	4599 (1)	98 (1)	1·74 (4)
C(2)	1412 (2)	5104 (2)	745 (1)	1·59 (6)
N(2)	1904 (2)	6555 (2)	789 (1)	1·76 (6)
C(*M1*)	1091 (3)	7244 (2)	1499 (1)	2·23 (7)
C(*M2*)	3318 (2)	7502 (2)	177 (1)	2·10 (7)
N(3)	126 (2)	4252 (2)	1287 (1)	1·63 (5)
C(4)	−121 (2)	2827 (2)	1293 (1)	1·51 (6)
C(5)	904 (2)	2238 (2)	775 (1)	1·57 (6)
C(*H5*)	926 (2)	860 (2)	973 (1)	1·78 (6)
O(5)	1784 (2)	291 (2)	545 (1)	2·21 (5)
C(6)	2090 (2)	3103 (2)	68 (1)	1·71 (6)
O(6)	2921 (2)	2777 (2)	−545 (1)	2·34 (5)
C(1*P*)	−1591 (2)	1935 (2)	1915 (1)	1·61 (6)
C(2*P*)	−1920 (2)	2633 (2)	2754 (1)	1·85 (7)
C(3*P*)	−3277 (2)	1850 (2)	3356 (1)	2·28 (7)
C(4*P*)	−4340 (2)	377 (2)	3116 (1)	2·46 (7)
C(5*P*)	−4049 (2)	−303 (2)	2270 (2)	2·36 (7)
C(6*P*)	−2671 (2)	465 (2)	1666 (1)	1·97 (7)
O(1′)	−2152 (2)	421 (1)	4948 (1)	1·88 (5)
C(2′)	−1523 (2)	−130 (2)	4182 (1)	1·66 (6)
N(2′)	−2417 (2)	−1550 (2)	3959 (1)	1·78 (5)
C(*M1′*)	−1914 (3)	−2264 (2)	3117 (1)	2·25 (7)
C(*M2′*)	−4023 (2)	−2429 (2)	4470 (1)	2·29 (7)
N(3′)	−131 (2)	667 (2)	3681 (1)	1·69 (5)
C(4′)	726 (2)	2113 (2)	3966 (1)	1·74 (6)
C(5′)	282 (2)	2773 (2)	4789 (1)	1·82 (6)
C(*H5′*)	1300 (3)	4222 (3)	5225 (2)	2·84 (8)
O(5′)	2724 (3)	5051 (2)	5100 (2)	3·00 (4)*
O(5″)	1154 (7)	4905 (7)	5775 (4)	3·17 (10)*
C(6′)	−1276 (2)	1919 (2)	5300 (1)	2·01 (7)
O(6′)	−1942 (2)	2280 (2)	5990 (1)	2·84 (6)
C(1*P′*)	2159 (2)	2931 (2)	3304 (1)	1·79 (6)
C(2*P′*)	3099 (2)	2211 (2)	2842 (1)	2·04 (7)
C(3*P′*)	4373 (2)	2904 (3)	2174 (1)	2·45 (7)
C(4*P′*)	4697 (2)	4306 (3)	1945 (1)	2·69 (8)
C(5*P′*)	3758 (3)	5027 (2)	2394 (1)	2·54 (8)
C(6*P′*)	2501 (2)	4354 (2)	3080 (1)	2·13 (7)

* O(5′) and O(5″) were kept isotropic; values are *B*, not B_{eq}.

* Lists of structure factors, anisotropic thermal parameters, H-atom coordinates, torsion angles, close intermolecular contacts, and deviations from best planes have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 44335 (23 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

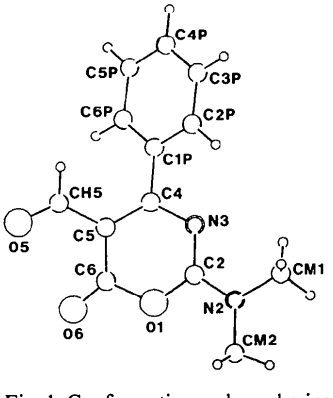

Fig. 1. Conformation and numbering.

Table 2. *Bond lengths* (Å) *and angles* (°), *selected torsion angles* (°) *and intermolecular contacts* <3·3 Å *between non-*H *atoms*

O(1)–C(2)	1·348 (2)	O(1′)–C(2′)	1·354 (2)
O(1)–C(6)	1·427 (1)	O(1′)–C(6′)	1·417 (2)
C(2)–N(2)	1·321 (1)	C(2′)–N(2′)	1·313 (2)
C(2)–N(3)	1·324 (2)	C(2′)–N(3′)	1·327 (2)
N(2)–C(*M*1)	1·467 (2)	N(2′)–C(*M*1)	1·467 (2)
N(2)–C(*M*2)	1·472 (2)	N(2′)–C(*M*2′)	1·473 (3)
N(3)–C(4)	1·350 (1)	N(3′)–C(4′)	1·347 (2)
C(4)–C(5)	1·396 (2)	C(4′)–C(5′)	1·397 (2)
C(4)–C(1*P*)	1·489 (3)	C(4′)–C(1*P*′)	1·486 (3)
C(5)–C(*H*5)	1·456 (1)	C(5′)–C(*H*5′)	1·445 (3)
C(5)–C(6)	1·444 (2)	C(5′)–C(6′)	1·439 (3)
C(*H*5)–O(5)	1·216 (2)	C(*H*5′)–O(5′)	1·175 (3)
C(6)–O(6)	1·196 (2)	C(6′)–O(6′)	1·204 (2)
C(1*P*)–C(2*P*)	1·398 (2)	C(1*P*′)–C(2*P*′)	1·395 (2)
C(1*P*)–C(6*P*)	1·392 (2)	C(1*P*′)–C(6*P*′)	1·397 (2)
C(2*P*)–C(3*P*)	1·387 (3)	C(2*P*′)–C(3*P*′)	1·387 (3)
C(3*P*)–C(4*P*)	1·387 (2)	C(3*P*′)–C(4*P*′)	1·384 (2)
C(4*P*)–C(5*P*)	1·387 (3)	C(4*P*′)–C(5*P*′)	1·390 (2)
C(5*P*)–C(6*P*)	1·395 (3)	C(5*P*′)–C(6*P*′)	1·392 (3)
		C(*H*5′)–O(5″)	1·023 (6)

C(2)–O(1)–C(6)	120·5 (1)	C(2′)–O(1′)–C(6′)	120·6 (1)
O(1)–C(2)–N(2)	114·3 (1)	O(1′)–C(2′)–N(2′)	114·3 (2)
O(1)–C(2)–N(3)	124·6 (1)	O(1′)–C(2′)–N(3′)	124·4 (1)
N(2)–C(2)–N(3)	121·1 (1)	N(2′)–C(2′)–N(3′)	121·3 (1)
C(2)–N(2)–C(*M*1)	119·2 (1)	C(2′)–N(2′)–C(*M*1′)	119·6 (2)
C(2)–N(2)–C(*M*2)	121·2 (1)	C(2′)–N(2′)–C(*M*2′)	122·1 (1)
C(*M*1)–N(2)–C(*M*2)	119·5 (1)	C(*M*1′)–N(2′)–C(*M*2′)	118·0 (1)
C(2)–N(3)–C(4)	116·6 (1)	C(2′)–N(3′)–C(4′)	117·5 (1)
N(3)–C(4)–C(5)	123·6 (2)	N(3′)–C(4′)–C(5′)	123·2 (2)
N(3)–C(4)–C(1*P*)	113·6 (1)	N(3′)–C(4′)–C(1*P*′)	112·9 (1)
C(5)–C(4)–C(1*P*)	122·8 (1)	C(5′)–C(4′)–C(1*P*′)	123·9 (1)
C(4)–C(5)–C(*H*5)	122·7 (2)	C(4′)–C(5′)–C(*H*5′)	126·1 (2)
C(4)–C(5)–C(6)	118·0 (1)	C(4′)–C(5′)–C(6′)	118·4 (1)
C(*H*5)–C(5)–C(6)	119·0 (1)	C(*H*5′)–C(5′)–C(6′)	115·3 (2)
C(5)–C(*H*5)–O(5)	125·7 (2)	C(5′)–C(*H*5′)–O(5′)	132·2 (2)
O(1)–C(6)–C(5)	114·6 (1)	O(1′)–C(6′)–C(5′)	115·4 (1)
O(1)–C(6)–O(6)	114·4 (1)	O(1′)–C(6′)–O(6′)	114·8 (2)
C(5)–C(6)–O(6)	131·0 (1)	C(5′)–C(6′)–O(6′)	129·7 (2)
C(4)–C(1*P*)–C(2*P*)	118·2 (1)	C(4′)–C(1*P*′)–C(2*P*′)	118·9 (1)
C(4)–C(1*P*)–C(6*P*)	122·0 (2)	C(4′)–C(1*P*′)–C(6*P*′)	121·5 (1)
C(2*P*)–C(1*P*)–C(6*P*)	119·7 (2)	C(2*P*′)–C(1*P*′)–C(6*P*′)	119·4 (2)
C(1*P*)–C(2*P*)–C(3*P*)	120·3 (1)	C(1*P*′)–C(2*P*′)–C(3*P*′)	120·5 (1)
C(2*P*)–C(3*P*)–C(4*P*)	120·0 (2)	C(2*P*′)–C(3*P*′)–C(4*P*′)	120·1 (2)
C(3*P*)–C(4*P*)–C(5*P*)	119·7 (2)	C(3*P*′)–C(4*P*′)–C(5*P*′)	119·8 (2)
C(4*P*)–C(5*P*)–C(6*P*)	120·8 (2)	C(4*P*′)–C(5*P*′)–C(6*P*′)	120·5 (1)
C(1*P*)–C(6*P*)–C(5*P*)	119·3 (2)	C(1*P*′)–C(6*P*′)–C(5*P*′)	119·6 (1)
		C(5′)–C(*H*5′)–O(5″)	136·9 (4)

C(6)–O(1)–C(2)–N(3)	−11·6 (3)	C(6′)–O(1′)–C(2′)–N(3′)	−3·7 (2)
O(1)–C(2)–N(3)–C(4)	11·5 (3)	O(1′)–C(2′)–N(3′)–C(4′)	1·4 (2)
C(2)–N(3)–C(4)–C(5)	0·8 (3)	C(2′)–N(3′)–C(4′)–C(5′)	4·4 (2)
N(3)–C(4)–C(5)–C(6)	−12·1 (3)	N(3′)–C(4′)–C(5′)–C(6′)	−7·6 (2)
C(4)–C(5)–C(6)–O(1)	11·3 (2)	C(4′)–C(5′)–C(6′)–O(1′)	5·0 (2)
C(2)–O(1)–C(6)–C(5)	−0·5 (2)	C(2′)–O(1′)–C(6′)–C(5′)	0·3 (2)
C(6)–O(1)–C(2)–N(2)	170·1 (2)	C(6′)–O(1′)–C(2′)–N(2′)	176·7 (1)
N(2)–C(2)–N(3)–C(4)	−170·3 (2)	N(2′)–C(2′)–N(3′)–C(4′)	−179·0 (1)
C(2)–N(3)–C(4)–C(1*P*)	−179·8 (2)	C(2′)–N(3′)–C(4′)–C(1*P*′)	−174·1 (1)
C(1*P*)–C(4)–C(5)–C(6)	168·5 (2)	C(1*P*′)–C(4′)–C(5′)–C(6′)	170·7 (2)
N(3)–C(4)–C(5)–C(*H*5)	162·5 (2)	N(3′)–C(4′)–C(5′)–C(*H*5′)	167·7 (2)
C(1*P*)–C(4)–C(5)–C(*H*5)	−16·9 (3)	C(1*P*′)–C(4′)–C(5′)–C(*H*5′)	−14·0 (3)
C(4)–C(5)–C(6)–O(6)	−168·0 (2)	C(4′)–C(5′)–C(6′)–O(6′)	−175·9 (2)
C(2)–O(1)–C(6)–O(6)	178·9 (2)	C(2′)–O(1′)–C(6′)–O(6′)	−179·0 (1)
N(3)–C(4)–C(1*P*)–C(2*P*)	−36·8 (2)	N(3′)–C(4′)–C(1*P*′)–C(2*P*′)	−37·5 (2)
N(3)–C(4)–C(1*P*)–C(6*P*)	140·4 (2)	N(3′)–C(4′)–C(1*P*′)–C(6*P*′)	137·4 (2)
C(5)–C(4)–C(1*P*)–C(2*P*)	142·6 (2)	C(5′)–C(4′)–C(1*P*′)–C(2*P*′)	144·0 (2)
C(5)–C(4)–C(1*P*)–C(6*P*)	−40·2 (3)	C(5′)–C(4′)–C(1*P*′)–C(6*P*′)	−41·1 (3)
C(*H*5)–C(5)–C(6)–O(1)	−163·5 (2)	C(*H*5′)–C(5′)–C(6′)–O(1′)	−170·8 (1)
C(*H*5)–C(5)–C(6)–O(6)	17·2 (3)	C(*H*5′)–C(5′)–C(6′)–O(6′)	8·3 (3)
C(4)–C(5)–C(*H*5)–O(5)	179·6 (2)	C(4′)–C(5′)–C(*H*5′)–O(5′)	−12·5 (3)
C(6)–C(5)–C(*H*5)–O(5)	−5·9 (3)	C(6′)–C(5′)–C(*H*5′)–O(5′)	162·9 (2)
C(4′)–C(5′)–C(*H*5′)–O(5″)	173·4 (4)	C(6′)–C(5′)–C(*H*5′)–O(5″)	−11·2 (5)

Symmetry operations listed are performed on the first atom; distances are in Å.

O(5′)···C(*M*2′)	$x-1, y-1, z$	3·017 (3)
C(*M*1)···O(5)	$x, y-1, z$	3·294 (2)
C(5)···O(5)	$-x, -y, -z$	3·222 (2)
C(*H*5)···O(5)	$-x, -y, -z$	3·188 (2)
O(5)···C(6*P*)	$-x, -y, -z$	3·299 (2)
C(2*P*)···O(5″)	$-x, 1-y, 1-z$	2·955 (5)
C(3*P*)···O(5″)	$-x, 1-y, 1-z$	3·151 (5)
O(5″)···O(5″)	$-x, 1-y, 1-z$	3·289 (8)
C(*H*5′)···O(5″)	$-x, 1-y, 1-z$	3·214 (5)

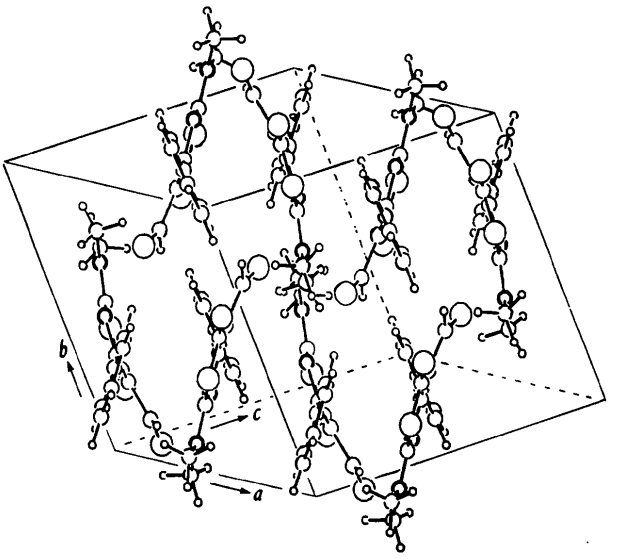

Fig. 2. Packing.

molecule has a slight saddle shape. The crystal structure of an oxazine ring with carbonyl, NH_2, $S-CH_3$, and cyano substituents was reported recently (Kristinsson, Winkler, Rihs & Fritz, 1985), and two symmetry-independent molecules in this structure were planar to within experimental error. An oxadiazine ring with three *N*-dimethyl substituents (Rushton, Schwalbe & Stevens, 1983) is planar. The observed C–O distances, 1·366 (6) and 1·386 (5) Å, and the mean C–N distance, 1·32 Å, are similar to the C–O and C–N distances in the analogous part of the structure reported here. The intramolecular distance between O(5) and O(6) is 2·855 (2) Å; if they were in the same plane this distance would be 2·76 Å. It is doubtful that repulsion between the carbonyl O atoms could be responsible for the ring distortion, however. Sasvári & Simon (1973) reported a carbonyl O···carbonyl O intramolecular distance of 2·81 Å for carbonyl and $COOC_2H_3$ substituents of a pyrimidine ring and the system was quite planar. Bravic & Bideau (1978) found a carbonyl···carbonyl distance of 2·79 Å with substituents of a flat pyran ring (in this case the $COOCH_2CH_3$ substituent was rotated about 14°). The molecules in the structure reported here are densely packed, as can be seen from the short intermolecular contacts listed in Table 2; packing forces, especially the aldehyde–aldehyde contacts between molecules related by the center of symmetry at the origin, are the probable cause for the observed ring distortion.

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Structure of the Radiation Protection Agent *S*-2-(3-Aminopropylamino)ethylphosphorothioic Acid (WR 2721)

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Abstract. $C_5H_{15}N_2O_3PS.3H_2O$, $M_r = 268{\cdot}3$, orthorhombic, $P2_12_12_1$, $a = 6{\cdot}762$ (1), $b = 8{\cdot}458$ (1), $c = 21{\cdot}564$ (3) Å, $V = 1233{\cdot}3$ Å^3, $Z = 4$, $D_x = 1{\cdot}445$ g cm^{-3}, Cu $K\alpha$, $\lambda = 1{\cdot}54178$ Å, $\mu = 36{\cdot}1$ cm^{-1}, $F(000) = 576$, room temperature, final $R = 3{\cdot}55\%$ for 1075 reflections with $|F_o| > 3\sigma$. The overall conformation of the molecule is folded with an intramolecular hydrogen bond between N(3) and O(1) of the SPO_3 group. The folded conformation of the molecule has a chiral twist. The molecule is a double zwitterion with the two phosphate hydrogens moved to the two nitrogen atoms, and the three P–O bonds are of equal length at 1·52 Å. The S–P bond is unusually long at 2·12 Å. Each H atom on each N atom and in each water molecule participates in hydrogen bonding. One of the N(7) hydrogen atoms forms a bifurcated intermolecular hydrogen bond to two of the phosphate O atoms.

Introduction. The title compound (WR 2721) was developed by the Walter Reed Army Institute of Research and the National Cancer Institute as a protective agent against the damaging and/or lethal effects of ionizing radiation (Sweeney, 1979). WR 2721 increases the radiation resistance of normal tissues to X- or γ-radiation by a factor of 1·2 to 3·4 (Yuhas, Spellman & Culo, 1980). Yuhas (1970) has demonstrated a dose reduction factor of 2·7 by WR 2721 against 30-day mortality in C57B1/6J mice. WR 2721 has been studied in clinical trials as a radioprotector of normal tissues in oncology radiation therapy (Constine, Zagars, Rubin & Kligerman, 1986) and has also been studied as an adjunctive therapy for alkylating agents in oncology patients (Glick, Glover, Weiler, Norfleet, Yuhas & Kligerman, 1984; Glover, Glick, Weiler, Fox, Turrisi & Kligerman, 1986) and for patients with cystic fibrosis (Tabachink, Peterson & Cerami, 1980). Through a route that bypasses the blood brain barrier, WR 2721 is being studied for its potential to provide radioprotection to healthy central nervous system tissues (Spence, Krohn, Edmondson, Steele & Rasey, 1986).

Although WR 2721 is the best known radioprotective agent, it has limitations for its proposed use as a radioprotectant for military personnel. Clinical trials of oncology patients show that most patients experience nausea and a small percentage (5%) experience significant hypotension (Kligerman *et al.*, 1984). The radioprotection of an oral dose, the desired route of administration for the military, of WR 2721 in large species such as the monkey is poor (Davidson, Grenan & Sweeney, 1980). In addition, the duration of radioprotection of WR 2721 in animal studies is relatively short, the best protection in the mouse occurring within 15 to 180 min post i.p. dosing with protection rapidly diminishing past 180 min (Davidson, Grenan & Sweeney, 1980). The three-dimensional structure of WR 2721 was established to provide information with respect to overall conformation and to the interatomic distance between potentially pharmacologically active N and S atoms, information which may lead to improved radioprotectants.

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