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Structures of Inorganic Rings as Antitumor Agents. I. Structure of the Two Allotropic Varieties of 1,3,3,5,5-Penta(1-aziridinyl)-$1\lambda^6$,2,4,6,3,5-thiatriazadiphosphorine 1-Oxide, $(NPaz_2)_2(NSOaz)$

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Abstract

The two allotropic varieties of the title compound $N_3P_2SO(NC_2H_4)_5$ have been studied; they are respectively named SOaz(I) and SOaz(II). SOaz(I) crystallizes in the orthorhombic system, space group $P2_12_12_1$, with a = 8·972 (1), b = 23·547 (2), c = 8·028 (1) Å, and Z = 4, V = 1696 Å^3, d_m = 1·40 (5), d_x = 1·419 Mg m^{-3}, μ(Mo $K\alpha$) = 0·39 mm^{-1}, m.p. = 357 K. SOaz(II) is monoclinic, $P2_1/c$, with a = 15·614 (4), b = 14·151 (6), c = 16·310 (6) Å, β = 114·7 (1)°, and Z = 8, V = 3274 Å^3, d_m = 1·45 (5), d_x = 1·471 Mg m^{-3}, μ(Mo $K\alpha$) = 0·41 mm^{-1}, m.p. = 376 K. Both structures have been determined using direct methods and refined to conventional R factors of 0·051 [SOaz(I)] and 0·035 [SOaz(II)] for 1492 and 2242 reflections respectively. SOaz(I) contains one type of $N_3P_2SO(NC_2H_4)_5$ molecule, and SOaz(II) two types, A and B; these three different types of molecule exhibit drastic changes in their conformation. This last fact is explained by the possible rotation around the (P–N) and (S–N) bonds which link the aziridinyl groups to the six-membered ring N_3P_2S.

Introduction

The antitumor activity of some thiatriazadiphosphorines belonging to the $(NPaz_2)_2(NSOX)$ family, namely SOF (X = F), SOPh (X = phenyl) and SOaz (X = az = aziridinyl) against P388 and L1210 leukemias and B16 melanoma has been reported recently (Labarre, Sournies, van de Grampel & van der Huizen, 1979; Sournies, 1980).

Some preliminary studies of the pharmalogical and toxicological behavior of these new antitumor agents have shown that (i) they induce neither mutagenicity (Ames tests) nor teratogenicity (on amphibians) and (ii) that they do not need any peculiar metabolization to be effective *in vivo*. Whereas (i) is of main interest for future clinical trials on humans, (ii) induced us to investigate the possible relationship between the *in vitro* geometric structure and the *in vivo* activity of the drugs.

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The X-ray structures of the SOF and SOPh derivatives have been determined (Cameron, Labarre, van de Grampel & van der Huizen, 1981). This paper deals with the crystal and molecular structures of the third term of the series. *i.e.* SOaz.

Experimental

1. *Synthesis of* SOaz

SOaz was prepared using the procedure which was recently described (van de Grampel, van der Huizen, Jekel, Wiedijk, Labarre & Sournies, 1980). When this preparation was repeated many times we surprisingly obtained two kinds of samples, SOaz(I) and SOaz(II), all the analytical and physico-chemical data of which were identical except for their melting points of 357 and 376 K respectively. We incidentally noticed that we never obtained any sample of SOaz with a melting point different from these two values.

Chemically, SOaz(I) and SOaz(II) are strictly identical and pure, their activity towards animal tumors being identical too. Thus, we could expect that the difference in their melting points would be due to some structural peculiarities, involving either their space groups if the two SOaz are unsolvated in the crystal or an eventual insertion of solvent in the unit cell (clathrate structure): this was indeed observed previously for another anticancer inorganic ring, the hexaaziridinylcyclotri(phosphazene) $N_3P_3az_6$, which may either crystallize unsolvated (Cameron *et al.*, 1981), or give clathrates with carbon tetrachloride ($N_3P_3az_6.3CCl_4$) (Galy, Enjalbert & Labarre, 1980) and with benzene ($2N_3P_3az_6.C_6H_6$) (Cameron, Labarre & Graffeuil, 1982).

2. *Crystal growth*

SOaz(I) and SOaz(II) give spontaneously suitable single crystals at the end of their synthesis (solvent: anhydrous ethyl ether).

3. *X-ray analysis*

Carefully selected crystals from both experiments, with regular prismatic shapes (all dimensions are within 0·4 to 0·6 mm), were glued on glass fibers and mounted on a Stoe 'reciprocal-lattice explorer' camera. Zr-filtered Mo $K\alpha$ radiation was used.

This photographic study revealed that two allotropic forms of the title compound were obtained: SOaz(I) and SOaz(II). SOaz(I) crystallizes in the orthorhombic system; the space group is $P2_12_12_1$. There is one independent molecule in the cell. SOaz(II) adopts the monoclinic system, systematic reflection absences indicating $P2_1/c$ as the space group. The volume of the cell is twice that of SOaz(I) and two crystallographically independent molecules, SOaz(II*A*) and SOaz(II*B*), exist. Crystallographic data are given in the *Abstract*.

4. *Data collection and computer treatment*

The crystals were transferred to a CAD-4 Enraf–Nonius PDP8/M computer-controlled diffractometer. In each case 25 reflections were used in order to orient the crystals, to check their quality and to refine the cell dimensions.

The conditions for the data collections are summarized in Table 1. The intensities of selected reflections $[I > 2\sigma(I)]$ were corrected for Lorentz and polarization factors but not for absorption.

Atomic scattering factors corrected for anomalous dispersion were obtained from Cromer & Waber (1974) and Cromer & Liberman (1970).

5. *Structure solution and refinement*

Both structures were determined using direct methods included in the *MULTAN* 78 program (Germain, Main & Woolfson, 1971).

The refinement included anisotropic vibration for all the non-H atoms. Difference Fourier syntheses

Table 1. *Conditions for data collection and refinement*

(*a*) Data collection

Temperature: 292 K
Radiation: molybdenum ($\lambda K\bar{\alpha} = 0·71069$ Å)
Monochromatization: highly oriented graphite
Crystal–detector distance: 208 mm
Detector window: height* = 4mm, width* 4 mm

	SOaz(I)	SOaz(II)
Take-off angle	4·0°	4·3°
Scan mode	θ–2θ	θ–2θ
Maximum Bragg angle	28°	21°
Scan angle $\Delta\theta = \Delta\theta_0 + 0·35 \text{ tg } \theta$	$\Delta\theta = 0·65°$	$\Delta\theta = 0·80°$
Values determining the scan speed: $\sigma^*_{\rm pre} = 0·66$, $\sigma^* = 0·018$ $V^*_{\rm pre} = 10°\ {\rm min}^{-1}$	$T_{\rm max} = 40$ s	$T_{\rm max} = 45$ s
Intensity control:		
Reflections	203 $\bar{4}30$ 252	020 200 002
Periodicity: 3600 s		
(*b*) Refinement		
Reflections for cell dimensions	25	25
Recorded reflections	2065	3896
Reflections used	1492	2242
Refined parameters	200	398
Reliability factors		
$R = \sum \lvert kF_o - \lvert F_c\rvert\rvert / \sum kF_o$	0·051	0·035
$R_w = [\sum w(kF_o - \lvert F_c\rvert)^2 / \sum wk^2F_o^2]^{1/2}$	0·063	0·045

* These parameters have been described in Mosset, Bonnet & Galy (1977).

phased by the P, N, S, O and C atoms revealed the H atoms in their expected positions.

In the last refinement cycles the H atoms were positioned geometrically following the indications concerning the bonding of such atoms in aziridinyl groups, *i.e.* (C—H) = 0·97 Å and H—C—H = 116° according to Dermer & Ham (1969), and isotropic thermal parameters were assigned as follows: $B(\mathrm{H}_i) = B_{\mathrm{eq}}(\mathrm{C}_i) + 1$ Å^2.

Table 2. SOaz(I): *fractional atomic coordinates and equivalent isotropic thermal parameters for the non*-H *atoms, with e.s.d.'s in parentheses*

$$B_{\mathrm{eq}} = \tfrac{4}{3}\textstyle\sum_i \sum_j \beta_{ij}\,\mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	B_{eq} (Å^2)
S	0·5251 (2)	0·9427 (1)	0·1454 (3)	2·93 (6)
P(1)	0·5818 (3)	0·8275 (1)	0·1962 (3)	3·13 (7)
P(2)	0·3276 (2)	0·8767 (1)	0·3322 (3)	3·09 (7)
O	0·5041 (7)	0·9750 (2)	−0·0057 (8)	4·2 (2)
N(1)	0·6183 (8)	0·8879 (3)	0·1150 (10)	3·7 (3)
N(2)	0·4312 (8)	0·8241 (3)	0·2974 (10)	3·5 (2)
N(3)	0·3776 (8)	0·9349 (3)	0·2397 (9)	3·5 (3)
N(4)	0·6305 (8)	0·9800 (3)	0·2766 (10)	3·6 (3)
N(5)	0·7302 (9)	0·8083 (3)	0·3031 (10)	4·2 (3)
N(6)	0·5813 (10)	0·7773 (3)	0·0542 (11)	4·6 (3)
N(7)	0·3139 (10)	0·8853 (3)	0·5383 (11)	4·4 (3)
N(8)	0·1532 (8)	0·8605 (3)	0·2813 (12)	4·5 (3)
C(1)	0·7476 (12)	1·0150 (4)	0·2008 (14)	5·0 (4)
C(2)	0·6148 (13)	1·0423 (4)	0·2695 (16)	5·9 (4)
C(3)	0·7513 (16)	0·8279 (6)	0·4746 (16)	7·4 (6)
C(4)	0·7149 (15)	0·7689 (6)	0·4412 (17)	6·9 (6)
C(5)	0·6657 (18)	0·7859 (5)	−0·1053 (15)	6·3 (5)
C(6)	0·5038 (16)	0·7879 (5)	−0·1074 (15)	6·4 (5)
C(7)	0·2778 (14)	0·9420 (5)	0·6060 (14)	6·1 (5)
C(8)	0·4269 (14)	0·9203 (5)	0·6159 (14)	5·6 (5)
C(9)	0·1063 (14)	0·8703 (6)	0·1103 (17)	6·6 (5)
C(10)	0·0512 (12)	0·9067 (5)	0·2391 (20)	7·0 (5)

In the final stages of refinement, an overall extinction parameter was calculated: 0·257 × 10^{-7} for SOaz(I) and 0·129 × 10^{-7} for SOaz(II).

The final R values are indicated in Table 1, corresponding in both cases to final difference maps exhibiting peaks lower than 0·4 e Å^{-3}.

Final positional parameters are collected in Table 2 for SOaz(I) and Table 3 for SOaz(II).*

Important bond lengths and bond angles of the molecule in its different conformations, *i.e.* SOaz(I), SOaz(II*A*) and SOaz(II*B*), are given in Table 4.

Description of the structures and discussion

A perspective view of the SOaz(I) molecule is shown in Fig. 1. The figure, obtained using the program *ORTEP* (Johnson, 1965), shows the numbering of the atoms, which is identical for both structures SOaz(I) and SOaz(II) (molecules *A* and *B*).

These three molecules, with quasi-planar six-membered rings (Table 5), do not possess any symmetry. Table 4 gives a comparison of the details of these molecules, the main differences being at the

Table 3. SOaz(II): *fractional atomic coordinates and equivalent isotropic thermal parameters for the non*-H *atoms, with e.s.d.'s in parentheses*

	Molecule *A*				Molecule *B*			
	x	y	z	B_{eq} (Å^2)	x	y	z	B_{eq} (Å^2)
S	0·9109 (1)	0·7149 (1)	0·6892 (1)	2·80 (6)	0·6150 (1)	0·2965 (1)	0·1985 (1)	2·66 (6)
P(1)	0·8514 (1)	0·7980 (1)	0·8123 (1)	3·01 (6)	0·6618 (1)	0·1798 (1)	0·0830 (1)	2·70 (6)
P(2)	0·7980 (1)	0·8773 (1)	0·6430 (1)	2·97 (6)	0·6760 (1)	0·1110 (1)	0·2477 (1)	2·51 (6)
O	1·0028 (2)	0·7000 (3)	0·6919 (2)	3·9 (2)	0·5240 (2)	0·3284 (3)	0·1877 (2)	4·0 (2)
N(1)	0·9133 (3)	0·7248 (3)	0·7845 (3)	3·1 (2)	0·6193 (3)	0·2749 (3)	0·1070 (3)	3·0 (2)
N(2)	0·7969 (3)	0·8749 (3)	0·7388 (3)	3·4 (2)	0·6896 (3)	0·0997 (3)	0·1575 (3)	2·9 (2)
N(3)	0·8563 (3)	0·7942 (3)	0·6223 (3)	3·0 (2)	0·6530 (3)	0·2168 (3)	0·2699 (3)	2·6 (2)
N(4)	0·8553 (3)	0·6117 (3)	0·6518 (3)	3·3 (2)	0·6834 (3)	0·3906 (3)	0·2307 (3)	3·5 (2)
N(5)	0·7827 (3)	0·7340 (3)	0·8464 (3)	3·5 (2)	0·7530 (3)	0·2021 (3)	0·0596 (3)	3·2 (2)
N(6)	0·9161 (3)	0·8534 (4)	0·9075 (3)	4·4 (2)	0·5870 (3)	0·1357 (3)	−0·0147 (3)	3·2 (2)
N(7)	0·8382 (3)	0·9814 (3)	0·6288 (3)	3·3 (2)	0·7680 (3)	0·0769 (3)	0·3384 (3)	2·8 (2)
N(8)	0·6884 (3)	0·8690 (3)	0·5663 (4)	4·9 (2)	0·5952 (3)	0·0329 (3)	0·2449 (3)	3·5 (2)
C(1)	0·8184 (4)	0·5946 (5)	0·5539 (4)	4·6 (3)	0·7173 (4)	0·4137 (4)	0·3321 (4)	4·1 (3)
C(2)	0·7539 (4)	0·6137 (4)	0·5967 (4)	4·3 (3)	0·7826 (4)	0·3788 (4)	0·2966 (4)	4·1 (3)
C(3)	0·6968 (5)	0·7770 (5)	0·8459 (5)	5·1 (3)	0·8162 (4)	0·2807 (4)	0·1052 (4)	4·3 (3)
C(4)	0·6899 (4)	0·7060 (5)	0·7785 (5)	4·9 (3)	0·7545 (4)	0·2886 (5)	0·0096 (4)	4·9 (3)
C(5)	1·0112 (5)	0·8867 (6)	0·9240 (6)	7·0 (4)	0·5222 (4)	0·1979 (5)	−0·0859 (4)	4·6 (3)
C(6)	1·0006 (5)	0·8075 (7)	0·9765 (5)	6·7 (4)	0·4863 (4)	0·1343 (5)	−0·0373 (4)	4·7 (3)
C(7)	0·8915 (5)	0·9884 (5)	0·5733 (5)	5·0 (4)	0·8339 (4)	0·0052 (4)	0·3296 (4)	4·1 (3)
C(8)	0·9421 (5)	0·9947 (5)	0·6726 (5)	5·2 (4)	0·8624 (4)	0·1053 (5)	0·3469 (4)	4·2 (3)
C(9)	0·6210 (5)	0·9470 (5)	0·5517 (5)	5·8 (4)	0·5327 (5)	0·0536 (4)	0·2895 (5)	4·8 (3)
C(10)	0·6538 (5)	0·9222 (5)	0·4812 (5)	6·7 (4)	0·4957 (4)	0·0588 (5)	0·1908 (5)	4·5 (3)

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* Lists of structure factors, anisotropic thermal parameters and H-atom coordinates have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 36095 (28 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 4. *Comparison of molecular parameters with e.s.d.'s in parentheses, for* $N_3P_2SOaz_5$ *of* SOaz(I), $N_3P_2SOaz_5$ *forms A and B of* SOaz(II) *and* $N_3P_3az_6$ *of the complex* $N_3P_3az_6.3CCl_4$ (*Galy et al.*, 1980)

		SOaz(II)		
	SOaz(I)	*A*	*B*	$N_3P_3az_6$
P(1)–N(1)	1·598 (7) Å	1·607 (4) Å	1·620 (4) Å	1·592 (3) Å
P(1)–N(2)	1·578 (7)	1·580 (4)	1·583 (4)	1·588 (2)
P(2)–N(2)	1·574 (7)	1·569 (4)	1·580 (4)	1·588 (2)
P(2)–N(3)	1·623 (7)	1·601 (4)	1·616 (4)	1·592 (3)
S–N(1)	1·557 (7)	1·544 (4)	1·553 (4)	1·587 (3)
S–N(3)	1·535 (7)	1·548 (4)	1·550 (4)	1·587 (3)
P(1)–N(5)	1·648 (8)	1·666 (5)	1·651 (4)	1·676 (4)
N(5) C(3)	1·464 (13)	1·470 (7)	1·467 (7)	1·468 (6)
N(5)–C(4)	1·452 (15)	1·463 (7)	1·476 (7)	1·467 (6)
C(3) C(4)	1·452 (18)	1·460 (9)	1·455 (8)	1·465 (7)
P(1)–N(6)	1·642 (8)	1·654 (5)	1·655 (4)	1·677 (3)
N(6)–C(5)	1·501 (15)	1·471 (8)	1·471 (7)	1·469 (5)
N(6)–C(6)	1·491 (14)	1·479 (9)	1·456 (7)	1·461 (6)
C(5)–C(6)	1·453 (18)	1·460 (11)	1·458 (8)	1·466 (7)
P(2)–N(7)	1·672 (9)	1·656 (4)	1·645 (4)	1·677 (3)
N(7)–C(7)	1·478 (13)	1·468 (7)	1·493 (7)	1·469 (5)
N(7)–C(8)	1·448 (13)	1·486 (7)	1·477 (7)	1·461 (6)
C(7)–C(8)	1·435 (16)	1·479 (9)	1·476 (9)	1·466 (7)
P(2)–N(8)	1·662 (7)	1·648 (5)	1·663 (5)	1·676 (4)
N(8)–C(9)	1·455 (15)	1·474 (8)	1·471 (7)	1·468 (6)
N(8)–C(10)	1·463 (12)	1·469 (8)	1·476 (7)	1·467 (6)
C(9)–C(10)	1·432 (18)	1·481 (10)	1·467 (9)	1·465 (7)
S–O	1·444 (6)	1·433 (3)	1·430 (4)	
S–N(4)	1·666 (7)	1·677 (5)	1·657 (5)	1·675 (4)
N(4)–C(1)	1·468 (12)	1·474 (7)	1·456 (7)	1·468 (6)
N(4)–C(2)	1·473 (11)	1·459 (7)	1·455 (7)	1·468 (6)
C(1)–C(2)	1·461 (15)	1·470 (8)	1·454 (8)	1·464 (8)
N(1)–P(1)–N(2)	115·5 (4)°	115·2 (2)°	114·7 (2)°	116·6 (2)°
P(1)–N(2)–P(2)	123·8 (6)	122·9 (3)	122·8 (3)	123·4 (2)
N(2)–P(2)–N(3)	114·9 (4)	115·9 (2)	115·5 (2)	116·6 (2)
P(2)–N(3)–S	124·4 (4)	125·1 (3)	123·9 (3)	123·2 (2)
N(3)–S–N(1)	116·2 (4)	114·7 (2)	115·0 (2)	116·8 (2)
S–N(1)–P(1)	124·3 (5)	125·3 (3)	125·6 (3)	123·2 (2)
N(5)–P(1)–N(6)	99·6 (4)	99·8 (2)	100·3 (2)	99·0 (2)
P(1)–N(5)–C(3)	120·5 (8)	119·1 (4)	119·3 (4)	117·7 (3)
P(1)–N(5)–C(4)	119·8 (8)	117·8 (4)	120·0 (4)	118·1 (3)
C(3)–N(5)–C(4)	59·7 (8)	59·7 (4)	59·3 (4)	59·9 (3)
P(1)–N(6)–C(5)	119·6 (7)	119·9 (4)	120·6 (4)	118·4 (3)
P(1)–N(6)–C(6)	119·0 (7)	120·4 (5)	120·1 (4)	118·0 (3)
C(5)–N(6)–C(6)	58·1 (7)	59·3 (5)	59·8 (4)	60·1 (3)
N(7)–P(2)–N(8)	101·7 (5)	106·9 (3)	101·4 (2)	99·0 (2)
P(2)–N(7)–C(7)	119·4 (7)	119·5 (4)	119·4 (4)	118·4 (3)
P(2)–N(7)–C(8)	116·4 (7)	116·5 (4)	117·8 (4)	118·0 (3)
C(7)–N(7)–C(8)	58·7 (7)	60·1 (4)	59·6 (4)	60·1 (3)
P(2)–N(8)–C(9)	118·0 (8)	120·9 (4)	120·5 (4)	117·7 (3)
P(2)–N(8)–C(10)	118·3 (6)	122·4 (5)	116·7 (4)	118·1 (3)
C(9)–N(8)–C(10)	58·8 (8)	60·4 (4)	59·7 (4)	59·9 (3)
O–S–N(4)	109·1 (4)	104·0 (2)	104·1 (2)	98·9 (3)
S–N(4)–C(1)	116·2 (6)	116·5 (4)	118·1 (4)	117·8 (3)
S–N(4)–C(2)	116·5 (7)	118·1 (4)	119·8 (4)	118·2 (3)
C(1)–N(4)–C(2)	59·6 (6)	60·2 (4)	59·9 (4)	59·8 (3)

conformational level, the aziridinyl groups 'rotating' around the P–N and S–N directions.

A joint view of the projections on the planes through the rings of these three SOaz molecules and of $N_3P_3az_6$ as determined from the $N_3P_3az_6.3CCl_4$ clathrate (Galy *et al.*, 1980) is given in Fig. 2; it readily illustrates the different conformations adopted in each case by the aziridinyl groups.

The packing of the molecules (without H atoms) in both allotropic forms SOaz(I) and (II) is visualized from the projections onto the planes (001) and (010) (Figs. 3 and 4); for SOaz(II) half of the cell content was drawn for the sake of clarity (the helicoidal twofold axes have not been used).

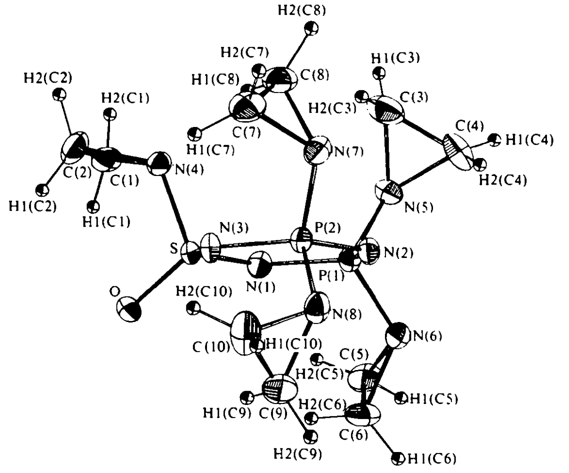

Fig. 1. A perspective view of the molecule SOaz(I).

Table 5. *Equations of the best plane for the rings* N_3P_2S *and distances of atoms* (Å) *to the best plane*

Atoms defining the plane: SN(1)P(1)N(2)P(2)N(3)

SOaz(I): $-0{\cdot}5089x - 0{\cdot}2321y - 0{\cdot}8290z + 8{\cdot}4656 = 0$
SOaz(II*A*): $-0{\cdot}7332x - 0{\cdot}5924y - 0{\cdot}3339z + 16{\cdot}4599 = 0$
SOaz(II*B*): $-0{\cdot}8555x - 0{\cdot}3413y - 0{\cdot}3894z + 9{\cdot}6538 = 0$

		SOaz(II)	
	SOaz(I)	*A*	*B*
S	−0·046 (3)	−0·043 (3)	0·019 (2)
N(1)	0·030 (3)	0·039 (3)	0·060 (5)
P(1)	−0·014 (2)	−0·064 (4)	−0·050 (5)
N(2)	0·019 (5)	0·029 (5)	−0·029 (3)
P(2)	−0·027 (3)	0·002 (2)	0·102 (5)
N(3)	0·041 (4)	−0·033 (5)	−0·100 (5)
O	0·880 (6)	−0·855 (4)	1·080 (3)
N(4)	−1·604 (8)	1·572 (5)	−1·347 (5)
N(5)	−1·297 (8)	1·388 (5)	1·377 (5)
N(6)	1·208 (9)	−1·137 (5)	1·157 (3)
N(7)	−1·384 (9)	1·322 (5)	−0·956 (5)
N(8)	1·196 (9)	−1·332 (5)	1·559 (5)

It is noticeable, as regards the molecular structures of SOaz(I), SOaz(II*A*) and SOaz(II*B*), that the conformations of their aziridinyl ligands differ drastically from one allotropic form to the other and, moreover, differ also from those which were observed in SOF and SOPh (Cameron *et al.*, 1981), when the aziridinyl pairs on P are considered. In other words, the molecule of SOaz appears to be versatile as regards its aziridinyl groups. There is, at the moment, no ready explanation for the adoption of either the one or the other conformation when the synthesis is repeated using exactly the same experimental conditions. However, the SOaz molecule seems to be extremely flexible in terms of the orientation of its 'wings', more so than the $N_3P_3az_6$ molecule (*cf.* Galy *et al.*, 1980; Cameron *et al.*, 1981, 1982).

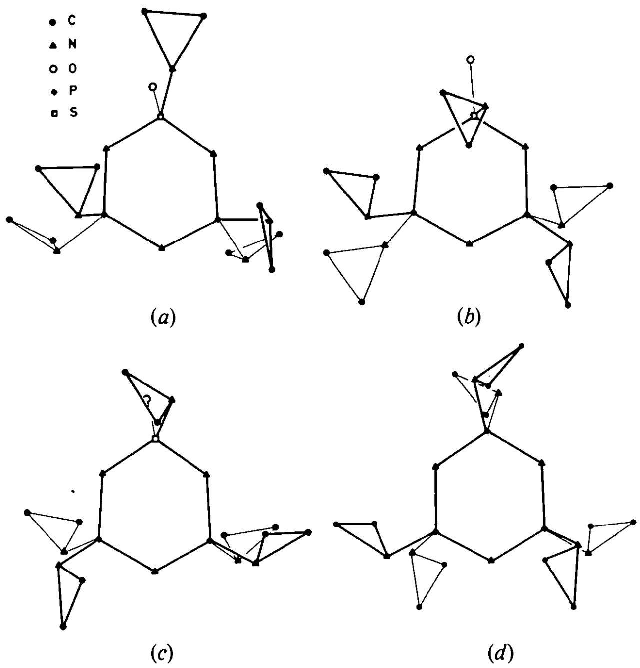

Fig. 2. Projection on the ring plane of the three SOaz molecule types and $N_3P_3az_6$ (from the anticlathrate $N_3P_3az_6.3CCl_4$). (*a*) SOaz(I). (*b*) SOaz(II*A*). (*c*) SOaz(II*B*). (*d*) $N_3P_3az_6$.

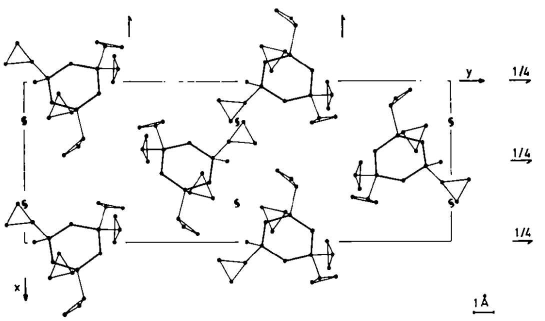

Fig. 3. Projection onto the (001) plane of the SOaz(I) structure.

Such flexibilities, as demonstrated by X-ray structures, perhaps allow SOaz and $N_3P_3az_6$ to adapt themselves to many dialkylating sites of DNA (assumed to be the target) and this would possibly explain the wide spectrum of activity of these two drugs on the various kinds of animal tumors.

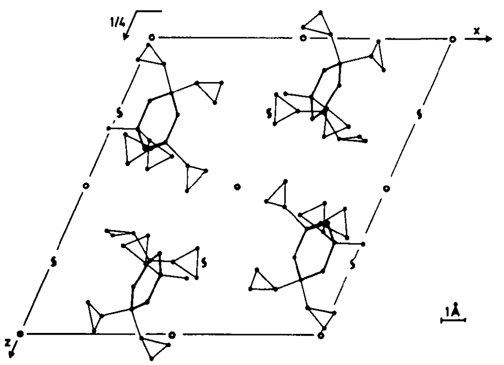

Fig. 4. Projection onto the (010) plane of the SOaz(II) structure.

A detailed discussion about molecular conformation–antitumor activity relationships will follow these systematic investigations and preliminary papers devoted to these inorganic ring systems.

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