Table 2. *Bond distances* (Å) *and angles* (°) *with e.s.d.'s in parentheses*

Br–C(3)	1·991 (11)	C(6)–C(7)	1·522 (14)
C(1)–C(8)	1·447 (11)	C(7)–C(8)	1·518 (14)
O(2)–C(13)	1·428 (11)	C(8)–C(9)	1·577 (18)
C(1)–C(2)	1·537 (14)	C(8)–C(19)	1·491 (25)
C(1)–C(10)	1·526 (19)	C(9)–C(10)	1·595 (12)
C(2)–C(3)	1·548 (14)	C(9)–C(11)	1·540 (12)
C(3)–C(4)	1·520 (19)	C(10)–C(18)	1·552 (21)
C(4)–C(5)	1·579 (14)	C(11)–C(12)	1·485 (19)
C(4)–C(16)	1·499 (20)	C(12)–C(13)	1·543 (13)
C(4)–C(17)	1·522 (16)	C(13)–C(14)	1·538 (22)
C(5)–C(6)	1·587 (21)	C(13)–C(20)	1·494 (23)
C(5)–C(10)	1·560 (13)	C(14)–C(15)	1·301 (24)

C(2)–C(1)–C(10)	112·8 (8)	C(1)–C(2)–C(3)	108·4 (8)
Br–C(3)–C(2)	107·2 (6)	C(2)–C(3)–C(4)	114·8 (10)
Br–C(3)–C(4)	112·9 (7)	C(3)–C(4)–C(17)	108·9 (12)
C(3)–C(4)–C(16)	112·0 (8)	C(3)–C(4)–C(5)	105·4 (8)
C(16)–C(4)–C(17)	107·1 (9)	C(5)–C(4)–C(17)	108·9 (8)
C(5)–C(4)–C(16)	114·4 (11)	C(4)–C(5)–C(10)	117·4 (7)
C(4)–C(5)–C(6)	113·7 (8)	C(6)–C(5)–C(10)	109·1 (9)
C(5)–C(6)–C(7)	107·7 (10)	C(6)–C(7)–C(8)	111·8 (8)
O(1)–C(8)–C(7)	107·9 (7)	C(7)–C(8)–C(19)	113·5 (10)
C(7)–C(8)–C(19)	113·5 (10)	C(7)–C(8)–C(9)	109·8 (9)
O(1)–C(8)–C(19)	107·3 (9)	O(1)–C(8)–C(9)	101·0 (8)
C(9)–C(8)–C(19)	116·2 (8)	C(8)–C(9)–C(11)	112·6 (9)
C(8)–C(9)–C(10)	112·3 (8)	C(10)–C(9)–C(11)	112·8 (7)
C(5)–C(10)–C(9)	105·4 (7)	C(1)–C(10)–C(9)	106·5 (9)
C(1)–C(10)–C(5)	108·0 (10)	C(9)–C(10)–C(18)	113·2 (9)
C(5)–C(10)–C(18)	114·3 (8)	C(1)–C(10)–C(18)	108·9 (8)
C(9)–C(11)–C(12)	114·7 (9)	C(11)–C(12)–C(13)	117·6 (9)
O(2)–C(13)–C(12)	110·1 (7)	C(12)–C(13)–C(20)	110·4 (9)
C(12)–C(13)–C(14)	108·9 (9)	O(2)–C(13)–C(20)	108·9 (9)
O(2)–C(13)–C(14)	111·8 (8)	C(14)–C(13)–C(20)	110·1 (10)
C(13)–C(14)–C(15)	126·1 (11)		

sample, the structure of isoconcinndiol might differ from (1) in the stereochemistry at C(8) and should be represented by (2) or its C(13) diastereoisomer. The X-ray single-crystal analysis described in this paper confirmed the structure and absolute configuration of (+)-isoconcinndiol as (3*S*,8*R*,13*S*)-labd-14-ene-8,13-diol, depicted in (2).

Fig. 1 is a computer-generated perspective molecular drawing, showing the absolute configuration. Atomic parameters are given in Table 1. Bond distances and angles are listed in Table 2.

The six-membered rings in isoconcinndiol are *trans* fused and are both in a chair conformation. The OH group on C(8) and the side chain on C(9) are equatorial.

The crystal structure is built by hydrogen bonds, comprising an intramolecular O(2)H···O(1), with distance 2·68 (1) Å and angle 165·4 (6)°, and another intermolecular O(1)H···O(2), through symmetry operation $x-\frac{1}{2}, -y+\frac{1}{2}, -z+1$, with distance 2·65 (1) Å and angle 166·9 (6)°.

This work was supported by grants from the Spanish CAICYT to JDM and MLR.

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Acta Cryst. (1989). C**45**, 308–311

Structure of Bis(4,4,5,5-tetramethyl-2-thioxo-1,3,2λ^5-dioxaphospholan-2-yl) Disulfide, $[\overline{\mathrm{OC(Me)_2C(Me)_2OP}}(\mathrm{S})\mathrm{S}]_2$

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(*Received* 20 *May* 1988; *accepted* 18 *August* 1988)

Abstract. $C_{12}H_{24}O_4P_2S_4$, $M_r = 422·5$, monoclinic, space group $C2$, $a = 14·913(9)$, $b = 6·847(6)$, $c = 11·427(6)$ Å, $\beta = 120·18(6)°$, $V = 1008·7$ Å^3, $Z = 2$, $D_x = 1·39$ g cm^{-3}, $\lambda(\text{Mo } K\alpha) = 0·71069$ Å, $\mu = 6·195$ cm^{-1}, $T = 295$ K, $F(000) = 444$, $R = 0·0656$ for 957 unique reflections. The molecule has a twofold axis of symmetry and contains a planar zigzag array of S=P–S–S–P=S linkages with two dioxaphospholane

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0108-2701/89/020308-04$03.00

moieties in the *trans* configuration. Important parameters are as follows: S(1)—S(1*) 2·058 (7), P—S(1) 2·082 (6), P—S(2) 1·908 (8), P—O 1·565 (2) Å (average); P—S(1)—S(1*) 108·5 (3), S(1)—P—S(2) 103·3 (4), O(1)—P—O(2) 99·0 (7)°.

Introduction. Structural studies by X-ray diffraction of a large number of main-group as well as transition-metal complexes of *O,O*-dialkyl phosphorodithioate ligands (Wasson, Woltermann & Stoklosa, 1973; Almasi, 1982; Haiduc, 1983; Mehrotra, Srivastava & Chauhan, 1984), carried out during the last two decades, have demonstrated wide variations in the metal–ligand bonding patterns which appear to depend not only on the coordination characteristics of the metal but also on the nature of the alkyl groups in the phosphorodithioate moiety. *O,O*-Alkylene phosphorodithioate ligands (Chauhan, Bhasin, Srivastava & Mehrotra, 1983), which are the cyclic analogues of the above, offer more interesting possibilities due to the variations in the ring size and the shape (Khaskin, 1984).

Although a variety of metal *O,O*-alkylene phosphorodithioates have been isolated in recent years, there is little information on their structural features except for two reports on the crystal structures of $Ph_3SnS(S)\overline{POC(Me)_2C(Me)_2O}$ (Preut, Ngo & Huber, 1987) and $Me_2Sn[S(S)\overline{POC(Me)_2C(Me)_2O}]_2$ (Preut, Ngo & Huber, 1986). These studies indicate that cyclic phosphorodithioates may be equally versatile in their ligating properties. For example, the chelation of the ligand is highly unsymmetrical in the former derivative whereas it is less so in the latter.

A combination of two *O,O*-(tetramethylethylene)-phosphorodithioate moieties yields the title compound (Fig. 1), the structure of which should be unperturbed by the presence of a metal atom and hence be useful as a reference for the corresponding metal complexes.

The only related disulfide for which the crystal structure is known is the open-chain derivative bis(diisopropoxythiophosphoryl) disulfide (Lawton, 1970; Tkachev, Atovmyan & Shchepinov, 1976). The data obtained by the two groups of workers for this compound are almost the same. The backbone of the molecule consists of a zigzag array of S=P—S—S—P=S linkages and tetrahedral arrangement around the P atoms.

Experimental. The title compound was obtained by the interaction of ammonium tetramethylethylenedithiophosphate with iodine in chloroform and crystallized from *n*-hexane (Ahmad, Srivastava & Mehrotra, 1984).

Lattice parameters refined from 20 reflections $9 < \theta < 13°$ collected on an Enraf–Nonius CAD-4 diffractometer, graphite-monochromated Mo $K\alpha$ ($\lambda = 0{\cdot}7107$ Å) radiation, using a yellow crystal *ca* 0·25 × 0·15 × 0·10 mm, sealed in a capillary. Data were collected in the $\omega/2\theta$ mode with $\Delta\theta = (0{\cdot}08 + 0{\cdot}35\tan\theta)°$, two standard reflections (601 and $71\bar{3}$) measured every 1800 s. Of 957 unique reflections, measured for $2 < \theta < 25°$ and $+h(17)$ $+k(8)$ $\pm l(13)$, 487 with $|F^2| > \sigma(F^2)$ were used in the refinement, where $\sigma(F^2) = \{\sigma^2(I) + (0{\cdot}04)^2\}^{1/2}/\mathrm{Lp}$. There was no crystal decay and no absorption correction was made; $[(\sin\theta)/\lambda]_{\max} = 0{\cdot}59$ Å^{-1}.

The structure was solved by routine direct methods and refined by full-matrix least squares with anisotropic temperature factors. H atoms were located on a difference map and refined with isotropic temperature factors. The weighting scheme was $w = 1/\sigma^2(F)$ and the final residuals were $R = 0{\cdot}0656$, $wR = 0{\cdot}0796$; a final difference map was everywhere $\leq 0{\cdot}5$ e Å^{-3}. 99 parameters were refined for non-hydrogen atoms, $(\Delta/\sigma)_{\max} = 0{\cdot}002$. Programs from the Enraf–Nonius (1979) *Structure Determination Package* were run on a PDP 11/73 computer.

Discussion. The structure of the title compound is shown in Fig. 2 (*PLUTO*; Motherwell & Clegg, 1978). Positional parameters of the non-H atoms and the equivalent values of the anisotropic temperature factors B_{ij} are given in Table 1,† bond lengths and angles in Table 2. The monomeric molecule has a twofold axis of symmetry and exists in the *trans* configuration. It contains a planar zigzag array of linkages with maximum deviations of 0·084 (4) Å from the least-squares plane through the atoms S(1*), S(1), P,S(2),

$$(2)S{=}P{-}S(1){-}S(1^*){-}P{=}S$$

similar to that reported for the open-chain bis(diisopropoxythiophosphoryl) disulfide (Lawton, 1970). The P atom is tetrahedrally coordinated by two O and two S atoms. The dioxaphospholane rings are essentially planar [maximum deviation from the least-squares plane through P, O(1), C(1), C(2), O(2) is 0·19 (2) Å] and the two dioxaphospholane moieties in the molecule are in *trans* configuration. The observed P—S bond lengths, 2·082 (6) and 1·908 (8) Å, correspond to a single and double length respectively. These are of the same order as has been reported for $[(Me_2CHO)_2$-

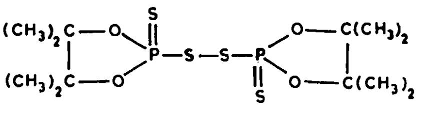

Fig. 1. Structural formula of the title compound.

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† Lists of structure factors, anisotropic thermal parameters, least-squares-planes data and H-atom parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 51353 (11 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

$P(S)S]_2$ [2·072 (2) and 1·908 (3) Å] (Lawton, 1970), $Ph_3SnS(S)\overline{POC(Me)_2C(Me)_2O}$ [2·039 (4) and 1·903 (4) Å] (Preut *et al.*, 1987) and $Me_2Sn[S(S)\overline{POC(Me)_2C(Me)_2O}]_2$ [2·031 (1) and 1·932 (1) Å] (Preut *et al.*, 1986). This indicates that these bonds are not affected by the attachment of Sn to the S atom(s). The S*—S bond length is 2·058 (7) Å and is shorter than the value observed in the case of the corresponding open-chain derivative $[(Me_2CHO)_2P(S)S]_2$ [2·109 (4) Å] (Lawton, 1970). It has been reported that the S—S bond in various sulfur-containing compounds varies in length from 1·89 to 2·58 Å (Abrahams, 1956; Meyer, 1976; Small, Banister & Hauptman, 1981). However, typical S—S bonds between two dicoordinate sulfurs (*e.g.* in *RSSR*, S_8 *etc.*) have lengths in the range of 2·04–2·06 Å (Kice, 1971). Therefore, it appears that in the present compound, the S—S bond is essentially an unperturbed single bond.

The notable deviation in the structure of the title compound from that of the open-chain diisopropyl derivative is the S—S—P angle which is 108·5 (3)° in the former compared with 100·5 (1)° in the latter. However, such variations have been reported earlier in similar systems. For example the S—S—S bond angle in S_8 is 108° whereas the SO_2—S—Ar bond angle in $ArSO_2SAr$ is 100° (Kice, 1971).

Bond lengths and bond angles of the dioxaphospholane rings in the title compound are in the same range as has been found for the corresponding triphenyltin and dimethyltin derivatives (Preut *et al.*, 1986, 1987). Between the molecules in the unit cell, there are no interactions other than van der Waals forces.

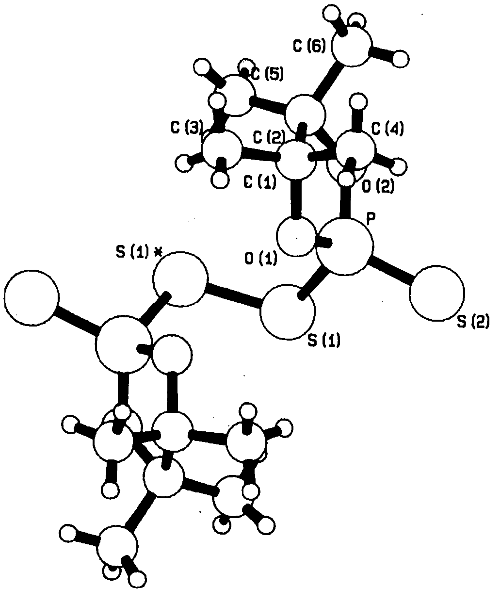

Fig. 2. Molecular structure (*PLUTO*; Motherwell & Clegg, 1978) of the title compound.

Table 1. *Positional parameters and their e.s.d.'s*

	x	*y*	*z*	B_{eq}(Å^2)
S(1)	−0·0219 (4)	0·1761	0·0723 (5)	5·2 (1)
S(2)	0·0073 (3)	0·3905 (14)	0·3313 (5)	6·7 (2)
P	0·0719 (3)	0·3743 (10)	0·2237 (4)	3·5 (1)
O(1)	0·0851 (7)	0·5554 (20)	0·1551 (10)	3·5 (3)
O(2)	0·1892 (7)	0·3025 (19)	0·3025 (10)	3·9 (3)
C(1)	0·1935 (12)	0·6294 (29)	0·2233 (15)	3·5 (5)
C(2)	0·2582 (9)	0·4348 (27)	0·2792 (14)	3·0 (4)
C(3)	0·2068 (12)	0·7269 (37)	0·1128 (19)	5·3 (6)
C(4)	0·2091 (14)	0·7686 (39)	0·3284 (21)	6·3 (7)
C(5)	0·2844 (11)	0·3253 (45)	0·1832 (16)	6·8 (7)
C(6)	0·3569 (14)	0·4614 (36)	0·4179 (18)	5·4 (6)

Anisotropically refined atoms are given in the form of the equivalent isotropic equivalent displacement parameter defined as (4/3) × $[a^{2*}B(1,1) + b^{2*}B(2,2) + c^{2*}B(3,3) + ab(\cos\gamma)B(1,2) + ac(\cos\beta)B(1,3) + bc(\cos\alpha)B(2,3)]$.

Table 2. *Intramolecular distances* (Å) *and angles* (°)

S(1)—S(1*)	2·058 (7)	O(2)—C(2)	1·49 (2)
S(1)—P	2·082 (6)	C(1)—C(2)	1·58 (2)
S(2)—P	1·908 (8)	C(1)—C(3)	1·53 (3)
P—O(1)	1·54 (2)	C(1)—C(4)	1·46 (3)
P—O(2)	1·59 (2)	C(2)—C(5)	1·53 (4)
O(1)—C(1)	1·48 (2)	C(2)—C(6)	1·54 (2)
S(1*)—S(1)—P	108·5 (3)	O(1)—C(1)—C(4)	109 (2)
S(1)—P—S(2)	103·3 (4)	C(2)—C(1)—C(3)	113 (2)
S(1)—P—O(1)	107·7 (5)	C(2)—C(1)—C(4)	114 (1)
S(1)—P—O(2)	110·7 (6)	C(3)—C(1)—C(4)	111 (2)
S(2)—P—O(1)	121·2 (8)	O(2)—C(2)—C(1)	104 (1)
S(2)—P—O(2)	114·9 (6)	O(2)—C(2)—C(5)	106 (2)
O(1)—P—O(2)	99·0 (7)	O(2)—C(2)—C(6)	106 (1)
P—O(1)—C(1)	113·0 (9)	C(1)—C(2)—C(5)	117 (2)
P—O(2)—C(2)	112 (1)	C(1)—C(2)—C(6)	113 (2)
O(1)—C(1)—C(2)	102 (1)	C(5)—C(2)—C(6)	110 (1)
O(1)—C(1)—C(3)	106 (2)		

Numbers in parentheses are estimated standard deviations in the least significant digits.

* Symmetry element is −*x*, *y*, −*z*.

We are grateful to Dr P. B. Hitchcock (Visiting Scientist under ALIS Program between Universities of Rajasthan and Sussex) for his valuable guidance in solving the above structure, to UGC, New Delhi, for providing X-ray facilities under the COSIST programme and to CSIR, New Delhi, for the award of an SRF to one of the authors (JSY).

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Acta Cryst. (1989). C**45**, 311–314

Structures of Three DNA Cross-Linking Agents, Ethane-1,2-di(methylsulfonate), Propane-1,3-di(methylsulfonate) and *n*-Butane-1,4-di(methylsulfonate)

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(*Received* 4 *July* 1988; *accepted* 21 *September* 1988)

Abstract. (I): $C_4H_{10}O_6S_2$, $M_r = 218{\cdot}25$, $P2_1/c$, $a = 7{\cdot}2611\ (9)$, $b = 5{\cdot}8726\ (4)$, $c = 10{\cdot}6628\ (19)$ Å, $\beta = 103{\cdot}95\ (1)^\circ$, $V = 441{\cdot}3\ (2)$ Å^3, $Z = 2$, $D_m = 1{\cdot}65$, $D_x = 1{\cdot}642$ Mg m^{-3}, λ(Cu $K\alpha$) = 1·54184 Å, $\mu = 5{\cdot}43$ mm^{-1}, $F(000) = 228$, $R = 0{\cdot}0336$ and $wR = 0{\cdot}0346$ for 745 unique reflections with $F \geq 3\sigma(F)$, $T = 298$ K. (II): $C_5H_{12}O_6S_2$, $M_r = 232{\cdot}28$, $P2_1/c$, $a = 11{\cdot}030\ (1)$, $b = 8{\cdot}452\ (1)$, $c = 11{\cdot}162\ (1)$ Å, $\beta = 104{\cdot}65\ (1)^\circ$, $V = 1006{\cdot}8\ (3)$ Å^3, $Z = 4$, $D_m = 1{\cdot}54$, $D_x = 1{\cdot}532$ Mg m^{-3}, λ(Cu $K\alpha$) = 1·54184 Å, $\mu = 4{\cdot}79$ mm^{-1}, $F(000) = 488$, $R = 0{\cdot}0418$ and $wR = 0{\cdot}0430$ for 1666 unique reflections with $F \geq 3\sigma(F)$, $T = 298$ K. (III): $C_6H_{14}O_6S_2$, $M_r = 246{\cdot}30$, $P\bar{1}$, $a = 5{\cdot}6147\ (9)$, $b = 6{\cdot}8343\ (6)$, $c = 7{\cdot}5434\ (6)$ Å, $\alpha = 110{\cdot}61\ (1)$, $\beta = 92{\cdot}08\ (1)$, $\gamma = 76{\cdot}15\ (1)^\circ$, $V = 262{\cdot}7\ (3)$ Å^3, $Z = 1$, $D_m = 1{\cdot}56$, $D_x = 1{\cdot}557$ Mg m^{-3}, λ(Cu $K\alpha$) = 1·54184 Å, $\mu = 4{\cdot}79$ mm^{-1}, $F(000) = 130$, $R = 0{\cdot}0397$ and $wR = 0{\cdot}0425$ for 907 unique reflections with $F \geq 3\sigma(F)$, $T = 298$ K. All three compounds have a common conformation in the $C.O.SO_2.CH_3$ part of the molecules due to weak O···H interactions. Compounds (I) and (III) have a *trans* conformation about the central C—C bond, whereas (II) is *cis*.

Introduction. Several members of the series of dimethanesulfonic acid esters of general formula $CH_3.SO_2.O.(CH_2)_n.O.SO_2.CH_3$ ($n = 1$–10) have long been known to be active against a number of proliferating cell systems in experimental animals (Fox, 1975). Their antitumour and immunosuppressive activities vary greatly with the length of the central methylene chain. Antitumour activity was observed in the case of the four-carbon chain member, BDMS ($n = 4$), against the Walker 256 rodent carcinoma (Haddow & Timmis, 1951). More recent work has shown that maximum *in vitro* cytotoxicity against Yoshida lymphosarcoma cells occurs with hexanedimethanesulfonate ($n = 6$), and the highest *in vivo* antitumour therapeutic index is for octanedimethanesulfonate ($n = 8$) (Bedford & Fox, 1983). With the exception of EDMS ($n = 2$), DNA cross-linking has been observed with all the other members of this series (Bedford & Fox, 1983; Hartley & Fox, 1986). The relationship between this cross-linking and the antitumour and cytotoxic properties of

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