C9—C15	1.535 (4)	C26—O7	1.435 (5)
C10—C11	1.529 (5)	C26—C27	1.500 (6)
C12—C13	1.525 (5)	C27—C28	1.497 (6)
C13—C14	1.546 (4)	C28—O8	1.446 (5)
C14—C19	1.543 (4)	C28—C29	1.530 (5)
C14—C15	1.551 (4)	C29—O9	1.418 (4)
C14—C18	1.566 (4)	C29—C30	1.507 (5)
C15—O1	1.454 (3)	C30—O7	1.442 (4)
C15—C16	1.532 (4)	C30—C32	1.511 (6)
C16—C17	1.526 (4)	C31—O8	1.409 (6)
O6—C1—C6	108.6 (3)	C17—C16—C15	106.8 (2)
O6—C1—C2	109.0 (3)	O4—C17—C16	109.4 (2)
C6—C1—C2	110.3 (3)	O4—C17—C18	111.9 (2)
C1—C2—C3	112.5 (3)	C16—C17—C18	108.1 (2)
C2—C3—C11	111.3 (3)	C20—C18—C17	113.8 (2)
C2—C3—C4	113.3 (3)	C20—C18—C14	118.7 (2)
C11—C3—C4	111.0 (3)	C17—C18—C14	103.0 (2)
C7—C4—C3	109.6 (3)	C23—C20—C21	107.1 (3)
C7—C4—C8	110.6 (3)	C23—C20—C18	124.1 (3)
C3—C4—C8	110.0 (2)	C21—C20—C18	128.7 (3)
C7—C4—C5	106.8 (3)	O2—C21—C20	105.1 (3)
C3—C4—C5	107.6 (3)	O3—C22—O2	120.8 (3)
C8—C4—C5	112.2 (3)	O3—C22—C23	130.4 (3)
C6—C5—C4	114.2 (3)	O2—C22—C23	108.8 (3)
C1—C6—C5	112.2 (3)	C20—C23—C22	110.1 (3)
C12—C8—C9	110.0 (3)	O5—C24—O4	121.9 (4)
C12—C8—C4	113.6 (2)	O5—C24—C25	126.5 (4)
C9—C8—C4	111.6 (2)	O4—C24—C25	111.5 (5)
C10—C9—C15	112.0 (2)	O6—C26—O7	110.2 (3)
C10—C9—C8	111.0 (2)	O6—C26—C27	109.6 (3)
C15—C9—C8	113.7 (2)	O7—C26—C27	111.6 (3)
C9—C10—C11	111.6 (3)	C28—C27—C26	115.0 (4)
C10—C11—C3	112.6 (3)	O8—C28—C27	106.3 (3)
C8—C12—C13	112.3 (2)	O8—C28—C29	113.9 (3)
C12—C13—C14	112.9 (3)	C27—C28—C29	110.2 (3)
C19—C14—C13	109.7 (3)	O9—C29—C30	110.7 (3)
C19—C14—C15	115.0 (3)	O9—C29—C28	109.2 (3)
C13—C14—C15	108.1 (2)	C30—C29—C28	109.7 (3)
C19—C14—C18	112.8 (3)	O7—C30—C29	109.9 (3)
C13—C14—C18	107.2 (2)	O7—C30—C32	106.2 (3)
C15—C14—C18	103.7 (2)	C29—C30—C32	115.5 (3)
O1—C15—C16	104.3 (2)	C22—O2—C21	109.0 (2)
O1—C15—C9	108.8 (2)	C24—O4—C17	116.5 (3)
C16—C15—C9	115.0 (2)	C26—O6—C1	114.4 (3)
O1—C15—C14	109.7 (2)	C26—O7—C30	112.4 (3)
C16—C15—C14	103.7 (2)	C31—O8—C28	116.3 (4)
C9—C15—C14	114.7 (2)		
C6—C1—C2—C3	−55.3 (4)	C18—C14—C15—C16	37.9 (3)
C1—C2—C3—C4	55.8 (4)	C13—C14—C15—C9	50.6 (3)
C11—C3—C4—C8	−55.2 (4)	C14—C15—C16—C17	−25.9 (3)
C2—C3—C4—C5	−51.5 (3)	C15—C16—C17—C18	3.8 (3)
C3—C4—C5—C6	51.8 (4)	C16—C17—C18—C14	19.4 (3)
C2—C1—C6—C5	54.9 (4)	C15—C14—C18—C17	−35.1 (3)
C4—C5—C6—C1	−55.4 (5)	C23—C20—C21—O2	0.6 (4)
C3—C4—C8—C9	56.0 (3)	C21—C20—C23—C22	0.4 (4)
C4—C8—C9—C10	−55.7 (3)	O2—C22—C23—C20	−1.3 (4)
C12—C8—C9—C15	49.9 (3)	O6—C26—C27—C28	−74.3 (4)
C8—C9—C10—C11	54.3 (3)	C26—C27—C28—C29	−46.8 (5)
C9—C10—C11—C3	−54.8 (4)	C27—C28—C29—C30	52.0 (4)
C4—C3—C11—C10	55.2 (4)	C28—C29—C30—O7	−60.2 (4)
C9—C8—C12—C13	−54.4 (4)	C23—C22—O2—C21	1.7 (4)
C8—C12—C13—C14	59.4 (4)	C20—C21—O2—C22	−1.4 (4)
C12—C13—C14—C15	−54.9 (3)	C27—C26—O7—C30	−55.5 (4)
C8—C9—C15—C14	−50.2 (3)	C29—C30—O7—C26	62.7 (4)

Table 3. *Hydrogen-bonding geometry* (Å, °)

D—H···*A*	H···*A*	*D*···*A*	*D*—H···*A*
O1—HO1···O*W*2^{i}	2.05 (3)	2.821 (5)	149 (3)
O9—HO9···O*W*1	1.95 (3)	2.741 (5)	174 (3)
O*W*1—H1*W*1···O3^{ii}	2.06 (3)	2.847 (5)	166 (3)
O*W*1—H2*W*1···O1^{iii}	1.80 (3)	2.825 (5)	162 (3)
O*W*2—H1*W*2···O9	1.83 (3)	2.793 (5)	168 (3)
O*W*2—H2*W*2···O5^{ii}	1.82 (3)	2.837 (5)	163 (3)

Symmetry codes: (i) $x - \frac{1}{2}, \frac{3}{2} - y, 2 - z$; (ii) $\frac{1}{2} - x, 2 - y, \frac{1}{2} + z$; (iii) $\frac{3}{2} - x, 2 - y, \frac{1}{2} + z$.

Data collection: *P*4 diffractometer software. Cell refinement: *XSCANS* (Siemens, 1991). Data reduction: *XSCANS*. Program(s) used to solve structure: *SHELXS*86 (Sheldrick, 1985). Program(s) used to refine structure: *SHELXL*93 (Sheldrick, 1993). Molecular graphics: *SHELXTL-Plus* (Sheldrick, 1990). Software used to prepare material for publication: *SHELXL*93.

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Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: HR1054). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Bis(phenylsulfonyl)methane, $(PhSO_2)_2CH_2$, and Dibromobis(phenylsulfonyl)methane, $(PhSO_2)_2CBr_2$

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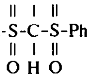
Abstract

In bis(phenylsulfonyl)methane, $C_{13}H_{12}O_4S_2$, the central C—S bond lengths are 1.786 (2) and 1.786 (3) Å, while

in dibromobis(phenylsulfonyl)methane, $C_{13}H_{10}Br_2O_4S_2$, the central C—S bond lengths are 1.872 (5) and 1.854 (5) Å. The unusual structural features reported for $(PhSO_2)_2CI_2$ [Stergioudis, Bozopoulos, Kavounis & Rentzeperis (1989). *Z. Kristallogr.* **189**, 57–63] are not reproduced in either of the title compounds.

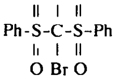
Comment

In compounds of the type $X(MR_3)_2$, the geometry of the central M—X—M fragment depends, for given M, very markedly upon the nature of X. Thus for MR_3 = $SiPh_3$, the M—X—M angle varies from 180° (imposed by a centre of inversion) for X = O (Glidewell & Liles, 1978), through 138.1 (4)° for X = NH (Glidewell & Holden, 1981) to 128.8 (7)° for X = CH_2 (Glidewell & Liles, 1982). Similarly, for MR_3 = SO_2Ar, the M—X—M angle is 127.7 (3)° for X = NH and Ar = Ph (Cotton & Stokeley, 1970), 111.5 (7)° for X = CH_2 and Ar = 4-BrC_6H_4 (Berthou, Jéminet & Laurent, 1972) and 120.7 (3)° for X = $C{=}CH_2$ and Ar = Ph (De Lucchi, Pasquato, Modena & Valle, 1985). An interesting member of this latter series has X = CI_2, but the reported structure for $(PhSO_2)_2CI_2$ shows a number of highly unusual features (Stergioudis, Bozopoulos, Kavounis & Rentzeperis, 1989). Firstly, the two central S—C bonds are very different in length [1.72 (2) and 1.83 (2) Å], whereas in each of $(PhSO_2)_2NH$ (Cotton & Stokeley, 1970) and $(PhSO_2)_2C{=}CH_2$ (De Lucchi, Pasquato, Modena & Valle, 1985), the two independent values are identical within experimental uncertainty, and in $(4\text{-}BrC_6H_4SO_2)_2CH_2$ (Berthou, Jéminet & Laurent, 1972) the molecule lies on a crystallographic twofold axis. Second, the O—S—O angles in $(PhSO_2)_2CI_2$ are reported as 110.0 (8) and 112.4 (7)°, whereas in all other neutral disulfones (Cotton & Stokeley, 1970; Berthou, Jéminet & Laurent, 1972; De Lucchi, Pasquato, Modena & Valle, 1985; Foss, Kvammen & Marøy, 1985), the O—S—O angles lie in the range 118.5 (3)–121.0 (3)°. Third, the non-bonding I···S distances span a wide range from 3.09 (2) to 3.42 (2) Å. In view of these unusual results, we have now determined the structure of the parent compound of this series, bis(phenylsulfonyl)methane, $(PhSO_2)_2CH_2$, (I), and that of dibromobis(phenylsulfonyl)methane, $(PhSO_2)_2CBr_2$, (II), which is very closely related to $(PhSO_2)_2CI_2$.



$$\mathrm{Ph{-}\overset{\overset{O}{\|}}{\underset{\underset{O}{\|}}{S}}{-}\overset{\overset{H}{|}}{\underset{\underset{H}{|}}{C}}{-}\overset{\overset{O}{\|}}{\underset{\underset{O}{\|}}{S}}{-}Ph}$$

(I)



$$\mathrm{Ph{-}\overset{\overset{O}{\|}}{\underset{\underset{O}{\|}}{S}}{-}\overset{\overset{Br}{|}}{\underset{\underset{Br}{|}}{C}}{-}\overset{\overset{O}{\|}}{\underset{\underset{O}{\|}}{S}}{-}Ph}$$

(II)

Compounds (I) and (II) both crystallize in the monoclinic space group $P2_1/n$ with four isolated molecules in the unit cell and molecular volumes of 345 (1) and 389.9 (3) $Å^3$, respectively. Although the compounds are similar in constitution, their unit cells are entirely different. In compound (I), the central bond lengths C(1)—S(1) and C(1)—S(2), although independent, have the same values [1.786 (2) and 1.786 (3) Å], identical to the mean value reported for such C—S bonds by Allen *et al.* (1987). The S(1)—C(11) and S(2)—C(21) distances are 1.759 (3) and 1.759 (2) Å, respectively, again virtually identical to the mean value (1.763 Å) reported for C(aryl)—SO_2—C bonds. The S—C—S angle is 115.5 (1)°, with a non-bonding S···S distance of 3.021 (3) Å; the two O—S—O angles are 119.3 (1)° at S(1) and 119.0 (1)° at S(2), entirely consistent with all those reported previously (Cotton & Stokeley, 1970; Berthou, Jéminet & Laurent, 1972; De Lucchi, Pasquato, Modena & Valle, 1985; Foss, Kvammen & Marøy, 1985) with the exception of those in $(PhSO_2)_2CI_2$ (Stergioudis, Bozopoulos, Kavounis & Rentzeperis, 1989).

In contrast, in compound (II), the central bond lengths C(1)—S(1) and C(1)—S(2) are 1.872 (5) and 1.854 (5) Å, respectively, far higher than the upper quartile value for bonds of this type (1.797 Å) but not significantly different from each other, unlike those reported for $(PhSO_2)_2CI_2$. However, the bond distances from sulfur to the aryl rings, S(1)—C(11) and S(2)—C(21), are 1.762 (5) and 1.763 (5) Å, respectively, not significantly different from those in (I) and entirely typical. Similarly, the S—O bond lengths in both (I) [1.429–1.434, mean 1.432 (2) Å] and (II) [1.414–1.433, mean 1.423 (8) Å] differ little, either from each other or from the mean value for previously reported examples (1.436 Å); the O—S—O angles in (II) are 120.1 (2)° at S(1) and 120.1 (3)° at S(2), again typical of the majority of previously reported examples. The second unusual feature in (II), in addition to the very long central C—S bonds, is the shortness of the C—Br bonds: 1.905 (5) and 1.916 (4) Å. These values are both well below the mean [1.966 (2) Å] and lower quartile [1.951 (2) Å] values for C—Br bonds of all types, and are similar only to those for bonds involving Br and a C atom in a cyclopropane ring, for which the upper and lower quartile values are 1.914 (2) and 1.900 (2) Å, respectively.

The shortness of the C—Br bonds, although not immediately explicable in simple terms, may be related to the long central C—S bonds. If the C—S bonds are stretched as a result of limiting non-bonding contacts with the Br atoms, the non-bonding S···Br distances would be expected to be very similar. This is indeed found, with all four distances in the range 3.009 (5)–3.086 (5) Å, with the mean, 3.060 (2) Å, very close to the sum of the limiting one-angle radii for S and Br [3.04 (2) Å] (Glidewell, 1979). In $(PhSO_2)_2CI_2$, the mean value of the non-bonding S···I distances is 3.19 (2) Å, close to the sum of the one-angle radii for I and S (3.20 Å).

The conformations of both (I) and (II) are such that C(2) is *trans* to S(1), with torsion angles C(21)—S(2)—C(1)—S(1) of −177.5 (1)° in (I) and 177.5 (3)° in (II) for the asymmetric units defined in Tables 1 and 2, while one of the sulfonyl O atoms bonded to S(1) is *trans* to S(2), with O—S—C—S torsion angles of 176.1 (1) and 179.0 (2)° in (I) and (II), respectively. Thus, neither (I) nor (II) exhibits any molecular symmetry in the crystal. In this respect, these compounds differ from $(BrC_6H_4SO_2)_2CH_2$ (Berthou, Jéminet & Laurent, 1972) and $(PhSO_2)_2S$ (Foss, Kvammen & Marøy, 1985) where the molecules lie on twofold axes, and also from $(PhSO_2)_2NH$ (Cotton & Stokeley, 1970) where the molecules exhibit approximate, although not crystallographic, twofold symmetry.

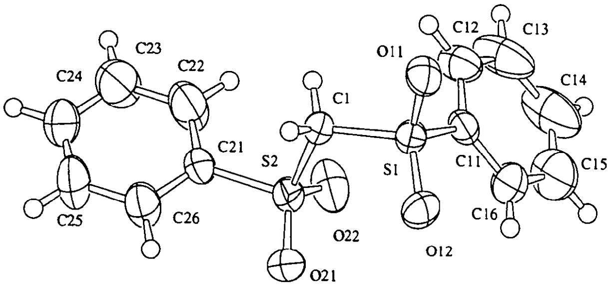


Fig. 1. Perspective view of the molecule of bis(phenylsulfonyl)-methane, showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% level for non-H atoms; H atoms are shown as small spheres of arbitrary size.

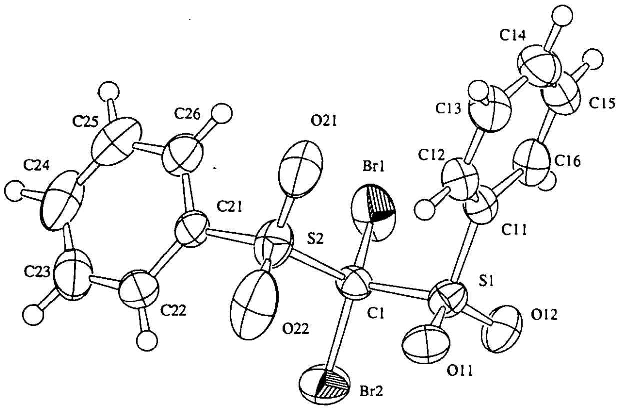


Fig. 2. Perspective view of the molecule of dibromobis(phenylsulfonyl)methane, showing the atom-labelling scheme. Atoms are depicted as in Fig. 1.

Experimental

Compound (I) was prepared by hydrogen peroxide oxidation (Kohler & Tishler, 1935) of bis(phenylthio)methane (Shriner, Struck & Jorison, 1930). Compound (II) was prepared by bromination of (I) (Kohler & Tishler, 1935). Crystals of (I) and (II) suitable for X-ray diffraction were grown by slow evaporation of solutions in dry ethanol.

Compound (I)

Crystal data

$C_{13}H_{12}O_4S_2$
$M_r = 296.36$
Monoclinic
$P2_1/n$
$a = 5.824 (6)$ Å
$b = 23.038 (3)$ Å
$c = 10.589 (5)$ Å
$\beta = 103.59 (5)°$
$V = 1381 (1)$ Å^3
$Z = 4$
$D_x = 1.425$ Mg m^{-3}

Mo $K\alpha$ radiation
$\lambda = 0.7107$ Å
Cell parameters from 19 reflections
$\theta = 13.9–19.1°$
$\mu = 0.391$ mm^{-1}
$T = 293.2$ K
Needle
0.70 × 0.15 × 0.10 mm
Colourless

Data collection

AFC-7*S* diffractometer
$\omega/2\theta$ scans
Absorption correction: ψ scan (North, Phillips & Mathews, 1968)
$T_{\min} = 0.928$, $T_{\max} = 1.000$
2557 measured reflections
2302 independent reflections
1782 observed reflections [$I \geq 3\sigma(I)$]

$R_{\rm int} = 0.0112$
$\theta_{\max} = 25.0°$
$h = 0 \rightarrow 6$
$k = 0 \rightarrow 27$
$l = -12 \rightarrow 12$
3 standard reflections monitored every 150 reflections intensity decay: 1.05%

Refinement

Refinement on *F*
$R = 0.033$
$wR = 0.045$
$S = 1.95$
1782 reflections
173 parameters
H-atom parameters not refined
Weighting scheme based on measured e.s.d.'s
$(\Delta/\sigma)_{\max} = 0.001$

$\Delta\rho_{\max} = 0.25$ e Å^{-3}
$\Delta\rho_{\min} = -0.25$ e Å^{-3}
Extinction correction: type II, Gaussian, isotropic (Zachariasen, 1967)
Extinction coefficient: 18.2
Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV)

Compound (II)

Crystal data

$C_{13}H_{10}Br_2O_4S_2$
$M_r = 454.15$
Monoclinic
$P2_1/n$
$a = 8.215 (1)$ Å
$b = 10.234 (1)$ Å
$c = 18.589 (1)$ Å
$\beta = 93.72 (1)°$
$V = 1559.6 (3)$ Å^3
$Z = 4$
$D_x = 1.934$ Mg m^{-3}

Mo $K\alpha$ radiation
$\lambda = 0.7107$ Å
Cell parameters from 20 reflections
$\theta = 23.5–26.4°$
$\mu = 5.491$ mm^{-1}
$T = 293.2$ K
Block
0.60 × 0.20 × 0.20 mm
Colourless

Data collection

AFC-7*S* diffractometer
$\omega/2\theta$ scans
Absorption correction: ψ scan (North, Phillips & Mathews, 1968)
$T_{\min} = 0.925$, $T_{\max} = 0.999$
3718 measured reflections
1749 independent reflections
1370 observed reflections [$I \geq 3\sigma(I)$]

$R_{\rm int} = 0.045$
$\theta_{\max} = 22.7°$
$h = -7 \rightarrow 7$
$k = -11 \rightarrow 11$
$l = -19 \rightarrow 19$
3 standard reflections monitored every 150 reflections intensity decay: 10.2%

Refinement

Refinement on F
$R = 0.029$
$wR = 0.030$
$S = 2.86$
1370 reflections
191 parameters
H-atom parameters not refined
Weighting scheme based on measured e.s.d.'s
$(\Delta/\sigma)_{\text{max}} = 0.001$
$\Delta\rho_{\text{max}} = 0.81$ e Å^{-3}
$\Delta\rho_{\text{min}} = -0.60$ e Å^{-3}
Extinction correction: type II, Gaussian, isotropic (Zachariasen, 1967)
Extinction coefficient: 1.34
Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV)

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

$$U_{\text{eq}} = (1/3)\Sigma_i\Sigma_j U_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	U_{eq}
S(1)	0.3077 (1)	0.06592 (3)	0.63616 (6)	0.0391 (3)
S(2)	0.3806 (1)	0.11093 (3)	0.38052 (6)	0.0458 (3)
O(11)	0.1473 (3)	0.02780 (8)	0.6793 (2)	0.0526 (9)
O(12)	0.5565 (3)	0.05471 (8)	0.6749 (2)	0.0532 (9)
O(21)	0.6205 (3)	0.0917 (1)	0.4028 (2)	0.066 (1)
O(22)	0.3341 (4)	0.16910 (8)	0.4142 (2)	0.070 (1)
C(1)	0.2222 (4)	0.0634 (1)	0.4628 (2)	0.040 (1)
C(11)	0.2545 (5)	0.1372 (1)	0.6812 (2)	0.043 (1)
C(12)	0.0286 (5)	0.1596 (1)	0.6476 (3)	0.063 (1)
C(13)	−0.0081 (7)	0.2151 (2)	0.6892 (5)	0.097 (2)
C(14)	0.1781 (9)	0.2455 (2)	0.7657 (5)	0.111 (3)
C(15)	0.4003 (8)	0.2223 (2)	0.7985 (4)	0.098 (2)
C(16)	0.4414 (5)	0.1679 (1)	0.7552 (3)	0.063 (1)
C(21)	0.2414 (5)	0.0988 (1)	0.2164 (2)	0.047 (1)
C(22)	0.0223 (7)	0.1211 (2)	0.1685 (3)	0.099 (2)
C(23)	−0.0885 (7)	0.1116 (2)	0.0389 (4)	0.118 (3)
C(24)	0.0252 (7)	0.0820 (2)	−0.0394 (3)	0.082 (2)
C(25)	0.2432 (7)	0.0597 (1)	0.0102 (3)	0.074 (2)
C(26)	0.3539 (6)	0.0673 (1)	0.1398 (3)	0.061 (2)

Table 2. *Fractional atomic coordinates and equivalent isotropic displacement parameters* (Å^2) *for* (II)

$$U_{\text{eq}} = (1/3)\Sigma_i\Sigma_j U_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	U_{eq}
Br(1)	0.75772 (7)	0.34804 (7)	0.26208 (3)	0.0706 (5)
Br(2)	1.00733 (8)	0.14360 (6)	0.20734 (4)	0.0730 (5)
S(1)	0.8121 (2)	0.3119 (1)	0.10071 (7)	0.0444 (9)
S(2)	1.0824 (2)	0.4359 (2)	0.20297 (8)	0.0537 (9)
O(11)	0.9405 (4)	0.2990 (3)	0.0531 (2)	0.054 (2)
O(12)	0.6903 (4)	0.2122 (3)	0.1034 (2)	0.060 (2)
O(21)	1.0079 (5)	0.5589 (4)	0.1896 (2)	0.090 (2)
O(22)	1.2060 (5)	0.3915 (5)	0.1590 (2)	0.092 (2)
C(1)	0.9151 (5)	0.3144 (4)	0.1935 (3)	0.038 (3)
C(11)	0.7159 (6)	0.4644 (5)	0.0865 (2)	0.039 (3)
C(12)	0.7994 (6)	0.5618 (5)	0.0525 (3)	0.045 (3)
C(13)	0.7194 (7)	0.6774 (6)	0.0372 (3)	0.057 (3)
C(14)	0.5604 (8)	0.6935 (6)	0.0555 (3)	0.060 (4)
C(15)	0.4793 (7)	0.5962 (7)	0.0881 (3)	0.057 (3)
C(16)	0.5557 (6)	0.4788 (6)	0.1040 (3)	0.049 (3)
C(21)	1.1581 (6)	0.4293 (5)	0.2938 (3)	0.041 (3)
C(22)	1.2849 (7)	0.3458 (5)	0.3133 (3)	0.055 (3)
C(23)	1.3496 (8)	0.3491 (6)	0.3835 (4)	0.075 (4)
C(24)	1.2886 (9)	0.4343 (7)	0.4322 (3)	0.078 (4)
C(25)	1.1619 (8)	0.5163 (7)	0.4115 (4)	0.076 (4)
C(26)	1.0948 (7)	0.5148 (6)	0.3416 (3)	0.058 (3)

Table 3. *Selected geometric parameters* (Å, °)

	(I)	(II)
S(1)—O(11)	1.433 (2)	1.426 (3)
S(1)—O(12)	1.434 (2)	1.433 (4)
S(2)—O(21)	1.431 (2)	1.414 (4)
S(2)—O(22)	1.429 (2)	1.419 (4)
S(1)—C(1)	1.786 (2)	1.872 (5)
S(2)—C(1)	1.786 (3)	1.854 (5)
S(1)—C(11)	1.759 (3)	1.762 (5)
S(2)—C(21)	1.759 (2)	1.763 (5)
C(1)—Br(1)		1.905 (5)
C(1)—Br(2)		1.916 (4)
O(11)—S(1)—O(12)	119.3 (1)	120.1 (2)
O(11)—S(1)—C(1)	105.2 (1)	105.4 (2)
O(11)—S(1)—C(11)	108.5 (1)	109.4 (2)
O(12)—S(1)—C(1)	107.9 (1)	104.6 (2)
O(12)—S(1)—C(11)	108.7 (1)	109.2 (2)
C(1)—S(1)—C(11)	106.6 (1)	107.3 (2)
O(21)—S(2)—O(22)	119.0 (1)	120.1 (3)
O(21)—S(2)—C(1)	109.0 (1)	105.7 (2)
O(21)—S(2)—C(21)	108.6 (1)	108.9 (3)
O(22)—S(2)—C(1)	107.7 (1)	106.5 (2)
O(22)—S(2)—C(21)	109.0 (1)	108.5 (3)
C(1)—S(2)—C(21)	102.3 (1)	106.2 (2)
S(1)—C(1)—S(2)	115.5 (1)	112.6 (2)
Br(1)—C(1)—Br(2)		110.8 (2)
Br(1)—C(1)—S(1)		109.5 (2)
Br(1)—C(1)—S(2)		110.3 (2)
Br(2)—C(1)—S(1)		105.2 (2)
Br(2)—C(1)—S(2)		108.4 (2)

Data reduction, structure solution and refinement, and preparation of material for publication: *TEXSAN* (Molecular Structure Corporation, 1985, 1992). Data for (II) were corrected for decay. Molecular graphics: *ORTEP*II (Johnson, 1976).

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates, complete geometry for (I) and bond distances and angles involving non-H atoms for (II) have been deposited with the IUCr (Reference: AB1250). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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