

to incorporate the larger iodide ion. The y coordinates for the C(1), C(2), C(3) side-chain atoms are quite different in the two derivatives. When the cell parameters for both derivatives are compared, it is observed that the iodide substitution causes the molecules to move apart in the a and c directions (along which the hydrogen bonds to the halide are directed) and together in the b direction.

Because of the difference in polarizability between the side chain and glycine-like group, the number of efficient packing arrangements for the leucine molecule in a crystal is limited. The molecules are observed to pack in sheets extending perpendicular to the b axis. The sheets are layered so that the hydrophobic side chains are held together by van der Waals forces and the polar glycine-like groups by hydrogen-bonding forces. The molecular packing arrangement of L-leucine. HI is observed to be similar to that of L-leucine. HBr (Figs. 6 and 7, Subramanian, 1967).

Like the HBr derivative, the charged amino nitrogen atom of L-leucine. HI undergoes what is probably rather weak hydrogen bonding with the two iodide ions, I(II) and I(III), and one oxygen atom O(1) (IV). A third iodide ion, I(IV), directly faces the amino nitrogen atom and does not participate in hydrogen bonding. Hydrogen bonding also occurs between the O(2) oxygen atom and the I(I) iodide ion. Hydrogen-bond

distances for both the HI and HBr derivatives are given in Table 4.

The equation of the mean plane passing through atoms C(5), C(6), O(1) and O(2) is $0.258X + 0.800Y - 0.541Z + 1.37 \text{ \AA} = 0$. The maximum deviation of the above atoms from the calculated mean plane is 0.014 \AA . The amino nitrogen atom, which was not used in the meanplane calculation, deviates by -0.29 \AA .

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The Crystal and Molecular Structure of 2,2',4,4',6,6'-Hexamethyldiphenyl Sulphone (Dimesityl Sulphone)

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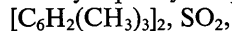
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Crystals of 2,2',4,4',6,6'-hexamethyldiphenyl sulphone are orthorhombic, space group *Pbca*, with eight molecules in a unit cell of dimensions $a = 24.45$, $b = 15.90$, $c = 8.15 \text{ \AA}$. The structure has been determined using photographically recorded X-ray data and refined to an R value of 0.115 for 1349 observed reflexions. Steric interactions between the sulphone and methyl groups lead to abnormal bond lengths, bond angles and non-bonded intramolecular atomic separations.

Introduction

2,2',4,4',6,6'-Hexamethyldiphenyl sulphone,



usually called dimesityl sulphone, is a very unstable compound chemically. The 2,4,6- and 2,4,5-trimethyldiphenyl sulphones convert easily to the 3,4,5 isomer when fused with aluminum chloride (Holt & Pagdin, 1961) but dimesityl sulphone disintegrates totally when

treated with aluminum chloride (Holt, 1970). The instability of dimesityl sulphone is no doubt closely linked with strain in the molecule caused by steric interactions between the sulphone and methyl groups, and the crystal structure has been determined to investigate the nature of these strains.

Experimental

Crystals of dimesityl sulphone were grown from ethyl alcohol as long, orthorhombic needles for which the needle axis has been chosen as the c axis.

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Weissenberg photographs indicate that the space group is $Pbca$ and that the unit-cell dimensions at 20°C , with estimated limits of error, are

$$a = 24.45 \pm 0.06, b = 15.90 \pm 0.05, c = 8.15 \pm 0.04 \text{ \AA}$$

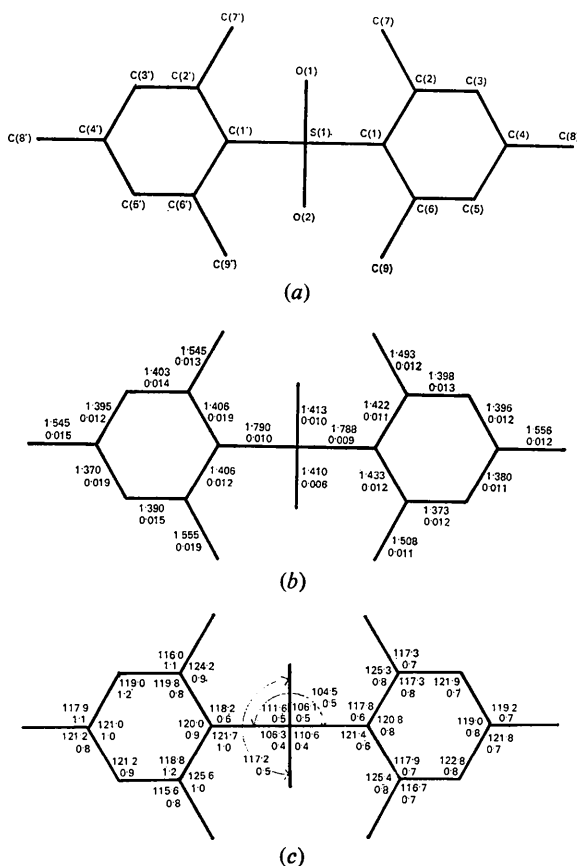


Fig. 1. Dimensions of the molecule. (a) Numbering of the atoms, (b) bond lengths with standard deviations (Å), (c) bond angles with standard deviations (°).

Measured density = 1.27 g.cm^{-3}

Calculated density = 1.28 g.cm^{-3} with 8 molecules in the unit cell.

Intensity data for the $hk0-hk5$ reflexions were collected by the multiple-film equi-inclination Weissenberg technique using $\text{Cu K}\alpha$ radiation. The intensities of the 1349 observed reflexions were estimated visually by comparison with an intensity wedge. No correction for absorption was applied but it is estimated that errors thereby introduced represent less than 5% in the value of the structure amplitudes.

Determination and refinement of the structure

Wilson (1942) plots were used to estimate an overall temperature factor and thus permit the calculation of suitable sharpening coefficients for Patterson functions. The position of the sulphur atom was deduced from [001] and [010] Patterson projections and then the coordinates of the carbon and oxygen atoms were estimated by trial and error using optical transforms.

Refinement by Fourier series, difference Fourier series and the minimum residual method (Bhuiya & Stanley, 1963) gave values of the residual $R = \sum ||F_o| - |F_c|| / \sum |F_o|$, of 0.12 and 0.16 for the $hk0$ and $h0l$ reflexions respectively. Further refinement, using the full three-dimensional data, was effected entirely by the minimum-residual method. The R value fell from 0.27 to 0.16 in 5 cycles with an isotropic temperature factor. At this stage individual isotropic temperature factors were introduced and refinement continued until the shifts in the positional coordinates were less than one-third of their standard deviation. The final R value was 0.115.

Results and discussion

The final atomic coordinates and temperature factors are given in Table 1 and the observed and calculated

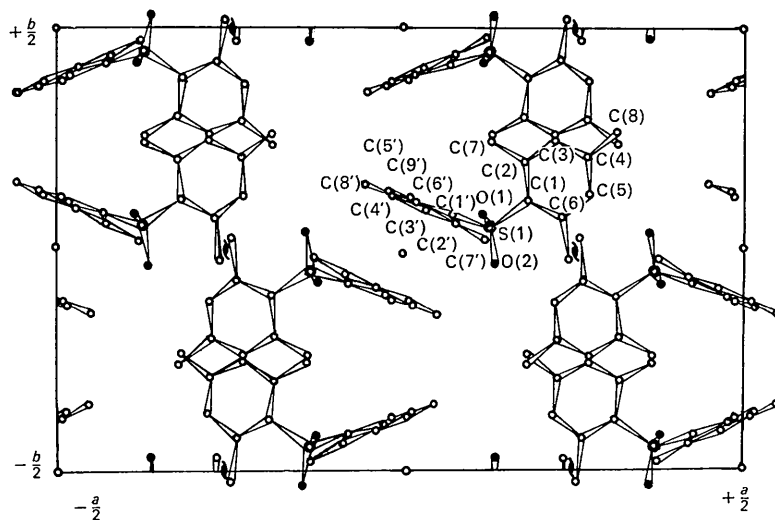


Fig. 2. The arrangement of the molecules viewed along the [001] direction.

Table 1. Final positional coordinates and isotropic temperature factors

	<i>x/a</i>	<i>y/b</i>	<i>z/c</i>	<i>B</i>
C(1)	0.1857	0.1089	0.0699	4.4 Å ²
C(2)	0.1793	0.1977	0.0773	4.7
C(3)	0.2209	0.2438	0.1533	5.3
C(4)	0.2694	0.2060	0.2057	5.3
C(5)	0.2753	0.1201	0.1894	4.9
C(6)	0.2352	0.0696	0.1246	4.5
C(7)	0.1304	0.2453	0.0187	5.6
C(8)	0.3149	0.2616	0.2835	6.4
C(9)	0.2473	-0.0233	0.1165	5.4
C(1)	0.0730	0.0762	0.1165	4.7

Table 1 (cont.)

	<i>x/a</i>	<i>y/b</i>	<i>z/c</i>	<i>B</i>
C(2')	0.0781	0.0663	0.2872	4.7
C(3')	0.0352	0.0912	0.3907	5.0
C(4')	-0.0125	0.1236	0.3212	5.1
C(5')	-0.0185	0.1287	0.1545	4.7
C(6')	0.0237	0.1059	0.0491	5.3
C(7')	0.1283	0.0267	0.3726	5.1
C(8')	-0.0583	0.1532	0.4383	6.8
C(9')	0.0110	0.1146	-0.1371	6.0
O(1)	0.1227	0.0756	-0.1735	6.1
O(2)	0.1392	-0.0382	0.0153	5.9
S(1)	0.1301	0.0484	-0.0099	4.6

Table 2. Observed and calculated structure factors.

<i>h</i>	<i>k</i>	<i>l</i>	<i> F_o </i>	<i>F_c</i>	<i>h</i>	<i>k</i>	<i>l</i>	<i> F_o </i>	<i>F_c</i>	<i>h</i>	<i>k</i>	<i>l</i>	<i> F_o </i>	<i>F_c</i>	<i>h</i>	<i>k</i>	<i>l</i>	<i> F_o </i>	<i>F_c</i>	<i>h</i>	<i>k</i>	<i>l</i>	<i> F_o </i>	<i>F_c</i>
2	0	0	32.3	-28.0	4	0	0	10.0	20.4	6	0	0	48.9	41.7	8	0	0	213.0	200.2	10	0	0	58.7	-46.2
14	0	0	41.1	38.1	10	0	0	95.0	88.3	18	0	0	48.0	-6.4	20	0	0	95.0	-86.1	22	0	0	33.3	34.0
20	0	0	11.7	-10.7	2	0	0	122.4	-130.0	16	0	0	95.0	72.5	8	1	0	10.3	-13.5	10	1	0	48.0	-27.0
14	1	0	33.3	37.7	16	1	0	11.7	-11.6	18	1	0	11.6	-15.2	20	1	0	11.6	-15.2	22	1	0	35.3	30.3
2	2	0	99.5	85.8	4	2	0	123.3	-141.0	6	2	0	53.8	-49.7	8	2	0	173.3	150.4	10	2	0	79.3	-7.5
4	2	0	29.4	29.3	10	2	0	47.0	45.3	18	2	0	53.8	-49.7	20	2	0	14.7	-14.1	24	2	0	31.5	23.7
14	3	0	16.7	-70.5	6	3	0	44.1	8.1	8	3	0	31.5	-3.5	10	3	0	9.8	-13.1	12	3	0	31.5	-25.0
10	3	0	4.9	-51.8	18	3	0	53.8	-51.7	20	3	0	31.5	-33.7	22	3	0	20.2	-20.2	24	3	0	18.1	25.0
30	3	0	5.0	2.0	0	4	0	32.3	-44.9	2	4	0	218.3	-225.0	4	4	0	187.0	-187.0	6	4	0	55.8	-57.0
10	4	0	58.7	-56.7	12	4	0	42.1	-39.8	14	4	0	11.7	11.4	16	4	0	30.3	28.2	18	4	0	13.7	-13.9
24	4	0	39.5	4.3	2	4	0	175.6	-175.7	4	5	0	39.5	-38.5	6	5	0	39.4	37.7	8	5	0	39.4	37.7
12	5	0	54.8	54.9	14	5	0	30.3	28.3	16	5	0	19.6	-41.6	18	5	0	33.8	-33.6	22	5	0	35.4	-31.4
20	5	0	15.7	-15.1	0	6	0	179.1	-193.2	4	6	0	18.6	14.6	8	6	0	19.6	-21.1	10	6	0	20.6	-20.5
14	6	0	11.7	-10.8	18	6	0	15.7	14.6	20	6	0	37.2	39.0	22	6	0	7.8	-7.9	26	6	0	17.6	-10.4
4	7	0	21.5	42.2	8	7	0	15.7	13.9	8	7	0	15.7	13.9	12	7	0	9.8	-9.8	14	7	0	15.7	13.9
2	7	0	10.8	11.8	24	7	0	10.8	-10.7	0	8	0	9.8	-1.5	2	8	0	23.5	21.4	4	8	0	108.7	114.1
10	8	0	40.1	40.9	12	8	0	13.7	13.8	14	8	0	12.7	-0.0	16	8	0	18.0	-23.0	18	8	0	11.7	12.9
22	8	0	4.8	-5.5	24	8	0	17.0	-11.0	2	9	0	23.5	21.4	4	9	0	23.5	21.4	6	9	0	49.0	51.5
10	9	0	25.5	-27.9	12	9	0	14.7	22.3	14	9	0	20.6	20.7	18	9	0	11.7	11.7	22	9	0	8.8	8.8
26	9	0	5.9	-4.4	0	10	0	41.1	-41.1	2	10	0	7.8	8.8	4	10	0	75.4	81.3	6	10	0	13.7	15.0
10	10	0	23.5	24.1	12	10	0	39.3	39.1	14	10	0	39.2	-40.2	16	10	0	21.5	-25.9	18	10	0	7.8	9.7
22	10	0	10.8	-8.2	24	10	0	9.8	-11.7	26	10	0	8.8	9.4	2	11	0	25.5	26.0	4	11	0	9.8	9.2
12	11	0	42.1	-39.5	10	11	0	38.2	42.8	12	11	0	46.0	-46.5	14	11	0	18.0	19.9	16	11	0	5.9	-4.9
22	11	0	4.9	-4.9	0	12	0	4.9	-4.5	2	12	0	4.5	-4.5	4	12	0	20.0	-23.3	6	12	0	29.4	-34.5
8	12	0	5.9	6.2	14	12	0	9.8	-9.9	10	12	0	9.8	-11.3	20	12	0	6.9	7.5	22	12	0	8.8	-10.1
10	13	0	27.4	-29.0	10	13	0	17.0	-18.8	14	13	0	13.7	-15.5	20	13	0	6.9	-6.9	0	14	0	22.5	-22.4
4	14	0	10.8	-10.8	6	15	0	13.7	-13.6	8	14	0	17.0	-18.5	12	14	0	17.0	-18.5	16	14	0	17.0	-18.5
6	15	0	9.8	-9.2	6	15	0	13.7	-13.6	10	15	0	7.8	9.9	14	15	0	12.7	-12.9	18	15	0	6.9	7.4
8	17	0	6.8	12.9	10	17	0	7.8	12.2	12	17	0	11.7	11.4	1	1	1	150.1	152.1	2	1	1	42.7	-39.6
10	17	0	4.4	-4.4	12	17	0	7.8	12.2	14	17	0	9.3	-18.4	16	17	0	156.6	157.6	18	17	0	17.1	-17.1
19	1	1	58.2	-53.6	20	1	1	30.2	26.8	22	1	1	10.1	9.7	23	1	1	5.8	8.6	24	1	1	14.1	14.7
2	1	1	17.2	-11.4	4	1	1	17.2	-11.4	6	1	1	17.2	-11.4	8	1	1	17.2	-11.4	10	1	1	17.2	-11.4
11	2	1	22.1	-17.8	12	2	1	39.6	-25.4	13	2	1	8.1	9.2	14	2	1	16.5	-11.3	15	2	1	18.6	17.5
11	2	1	37.7	-35.5	18	2	1	44.5	4.7	20	2	1	33.1	-31.4	2	3	1	17.1	16.5	4	3	1	14.3	14.2
12	2	1	13.4	-12.1	24	2	1	12.1	13.8	29	2	1	10.0	1.8	1	3	1	34.8	39.7	2	3	1	43.1	-36.4
4	3	1	40.8	-38.1	5	3	1	20.3	-27.5	6	3	1	31.3	-35.0	7	3	1	6.4	11.1	8	3	1	14.4	14.8
4	3	1	62.4	-57.4	6	3	1	27.4	-32.6	12	3	1	32.3	-35.6	13	3	1	20.7	-23.0	14	3	1	24.7	-28.1
4	3	1	8.8	-10.8	18	3	1	31.3	-35.0	19	3	1	7.1	-7.1	20	3	1	7.1	-7.1	21	3	1	10.1	7.8
23	3	1	5.8	7.9	24	3	1	5.7	-2.4	27	3	1	6.8	-7.7	0	4	1	5.4	-5.4	1	4	1	6.6	-14.5
3	4	1	34.4	-32.9	14	4	1	4.4	-4.6	5	4	1	33.7	-24.0	6	4	1	4.4	-4.6	7	4	1	56.1	-56.5
17	4	1	33.3	-33.3	13	4	1	32.7	-35.3	12	5	1	25.0	-23.5	13	4	1	25.0	-23.5	14	4	1	14.4	-12.0
17	4	1	5.2	-5.7	29	4	1	19.3	10.8	10	4	1	14.4	-14.2	22	4	1	14.4	-14.2	2	5	1	2.5	2.9
6	5	1	13.1	-9.8	6	5	1	10.6	10.4	1	5	1	12.1	-12.1	2	5	1	23.1	-26.0	3	5	1	34.5	-38.4
12	5	1	37.3	-27.6	14	5	1	10.6	10.4	15	5	1	9.3	-8.4	16	5	1	9.3	-8.4	18	5	1	14.4	-13.5
20	5	1	10.6	-17.1	21	5	1	5.9	8.4	23	5	1	12.8	-13.7	24	5	1	14.7	-13.4	0	6	1	35.5	-38.1
4	6	1	12.1	-11.0	4	6	1	12.1	-11.0	8	6	1	33.8	-37.7	7	6	1	10.6	-10.6	10	6	1	27.3	-27.8
10	6	1	13.9	-7.0	11	6	1	17.7	-14.3	12	6	1	10.7	-10.0	13	6	1	24.2	-24.6	14	6	1	5.1	-11.3
17	6	1	6.9	-8.0	19	6	1	10.1	-10.0	21	6	1	12.1	-12.0	24	6	1	12.1	-12.0	2	7	1	7.2	-7.4
8	7	1	26.5	-4.8	7	7	1	10.6	6.3	7	7	1	10.6	6.3	0	7	1	24.8	-25.7	0	7	1	7.8	6.4
3	7	1	4.4	4.8	9	7	1	17.5	-11.2	10	7	1	24.0	-25.5	11	7	1	32.0	-33.1	14	7	1	29.9	29.5
10	7	1	18.6	-11.6	17	7	1	22.2	-22.8	18	7	1	10.1	-10.3	19	7	1	17.6	-17.6	23	7	1	10.3	-10.3
16	8	1	47.8	-47.8	8	8	1	15.8	18.0	7	8	1	20.5	-21.5	4	8	1	40.0	-40.8	4	8	1	15.8	18.0
8	8	1	4.7	-4.8	10	8	1	10.3	-15.4	12	8	1	17.3	14.4	13	8	1	20.3	25.6	14	8	1	5.5	-4.6
16	8	1	18.1	-12.9	17	8	1	10.1	-11.4	1	9	1	13.8	-12.6	2	9	1	4.0	-4.0	3	9	1	48.3	-39.9
11	9	1	44.8	-44.7	9	9	1	15.8	18.0	7	9	1	21.0	-22.1	10	9	1	17.0	-18.1	11	9	1	15.8	18.0
11	9	1	54.5	-51.5	12	9	1	10.3	-14.7	14	9	1	33.5	-33.0	15	9	1	20.8	-20.6	16	9			

Table 2 (cont.)

h	k	l	F _{hkl}	F _c	h	k	l	F _{hkl}	F _c	h	k	l	F _{hkl}	F _c	h	k	l	F _{hkl}	F _c	h	k	l	F _{hkl}	F _c				
13 12 2	15.3	12.2	22	22	13 12 2	15.3	12.2	22	22	2 13 2	8.0	0.4	4 13 2	8.0	4 13 2	8.0	4 13 2	8.0	4 13 2	8.0	4 13 2	8.0	4 13 2	8.0				
13 12 2	15.3	12.2	22	22	13 12 2	15.3	12.2	22	22	0 14 2	20.0	-30.0	4 14 2	21.3	4 14 2	21.3	4 14 2	21.3	4 14 2	21.3	4 14 2	21.3	4 14 2	21.3				
13 14 2	11.1	8.5	10	10	13 14 2	11.1	8.5	10	10	18 14 2	11.1	10.4	6 15 2	22.7	6 15 2	22.7	6 15 2	22.7	6 15 2	22.7	6 15 2	22.7	6 15 2	22.7				
8 15 2	9.0	6.5	10	10	13 15 2	8.0	10.7	13	13	14 15 2	10.9	-13.0	18 15 2	11.1	12.1	4 10 2	6.2	4 10 2	6.2	4 10 2	6.2	4 10 2	6.2	4 10 2	6.2			
2 17 1	1.3	10.0	1	1	2 13 1	11.9	-47.7	2	2	4 1 3	30.2	31.7	4 1 3	30.2	31.7	5 1 3	28.7	5 1 3	28.7	5 1 3	28.7	5 1 3	28.7	5 1 3	28.7			
7 1 3	37.7	-31.5	7	7	7 1 3	37.7	-31.5	7	7	0 1 3	15.7	-13.8	10 1 3	20.0	-22.0	11 1 3	54.9	-57.7	11 1 3	54.9	-57.7	11 1 3	54.9	-57.7	11 1 3	54.9		
12 1 3	0.1	-4.1	14	14	15 1 3	8.8	-8.3	15	15	13 3 0	1.1	39.4	10 1 3	12.1	12.2	17 1 3	16.2	-12.0	18 1 3	10.2	-12.1	18 1 3	10.2	-12.1	18 1 3	10.2		
19 1 3	30.8	-30.7	24	24	23 1 3	13.3	13.1	23	23	27 1 3	5.2	-5.5	27 1 3	5.2	-5.5	2 2 3	74.2	-77.5	1 2 3	26.7	28.8	1 2 3	26.7	28.8	1 2 3	26.7		
2 2 3	21.6	-23.1	3	3	2 3 3	49.1	-53.0	4	4	5 2 3	18.8	14.1	6 2 3	16.9	-22.0	7 2 3	38.8	-39.4	7 2 3	38.8	-39.4	7 2 3	38.8	-39.4	7 2 3	38.8		
8 2 3	50.4	53.4	9	9	9 2 3	9.1	-6.0	10	10	11 2 3	4.8	7.7	12 2 3	6.2	10.0	14 2 3	29.7	30.2	14 2 3	29.7	30.2	14 2 3	29.7	30.2	14 2 3	29.7		
15 2 3	14.7	13.0	16	16	2 3 3	8.6	-8.8	17	17	13 2 3	13.3	-17.1	18 2 3	5.0	7.0	10 2 3	14.7	14.7	20 2 3	6.7	8.6	20 2 3	6.7	8.6	20 2 3	6.7		
21 2 3	11.9	9.7	23	23	3 3 3	8.0	10.5	24	24	4 3 3	16.2	8.2	25 2 3	5.9	-7.0	27 2 3	8.8	7.9	1 3 3	57.4	59.8	1 3 3	57.4	59.8	1 3 3	57.4		
3 3 3	32.0	-30.9	4	4	4 3 3	37.5	-37.0	5	5	5 3 3	45.4	-52.8	6 3 3	21.3	20.1	7 3 3	65.4	67.7	0 3 3	1.3	-0.1	0 3 3	1.3	-0.1	0 3 3	1.3		
10 3 3	4.7	-7.2	11	11	11 3 3	32.0	-24.0	12	12	13 3 3	21.5	18.4	13 3 3	19.4	-13.0	14 3 3	10.7	10.0	15 3 3	37.1	42.5	15 3 3	37.1	42.5	15 3 3	37.1		
17 3 3	6.3	-7.4	19	19	19 3 3	14.0	-14.1	20	20	20 3 3	16.7	-7.5	23 3 3	12.0	11.9	27 3 3	9.9	-9.5	1 4 3	19.4	-18.1	1 4 3	19.4	-18.1	1 4 3	19.4		
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19 4 3	14.7	14.8	21	21	21 4 3	20.0	20.0	24 4 3	9.1	4.6	25 4 3	7.0	-10.0	25 4 3	7.0	-10.0	1 5 3	10.0	24.1	2 5 3	13.1	6.4	2 5 3	13.1	6.4	2 5 3	13.1	
3 5 3	29.9	-25.3	4	4	4 5 3	15.8	19.4	5 5 3	20.2	-27.2	6 5 3	25.3	33.0	7 5 3	18.8	28.8	7 5 3	18.8	28.8	8 5 3	11.1	11.2	8 5 3	11.1	11.2	8 5 3	11.1	
9 5 3	20.7	17.7	10	10	10 5 3	5.2	4.9	11 5 3	14.7	-13.6	12 5 3	9.7	11.7	15 5 3	15.8	15.7	17 5 3	15.8	15.7	17 5 3	15.8	15.7	17 5 3	15.8	15.7	17 5 3	15.8	
25 5 3	8.8	2.3	26	26	26 5 3	9.6	-5.1	0 6 3	20.3	22.4	1 6 3	21.2	-18.3	2 6 3	7.4	7.3	3 6 3	29.0	-22.3	3 6 3	29.0	-22.3	3 6 3	29.0	-22.3	3 6 3	29.0	
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1 6 3	16.7	-19.0	12	12	12 6 3	12.6	-14.5	13 6 3	24.7	23.5	17 6 3	14.0	-13.8	18 6 3	12.5	-14.3	19 6 3	11.5	-11.6	19 6 3	11.5	-11.6	19 6 3	11.5	-11.6	19 6 3	11.5	
21 6 3	13.0	12.0	25	25	25 6 3	18.4	-18.1	2 7 3	18.6	-18.4	2 7 3	18.6	-18.4	4 7 3	3.8	8.0	6 7 3	28.7	29.1	6 7 3	28.7	29.1	6 7 3	28.7	29.1	6 7 3	28.7	
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15 8 3	17.4	-17.5	17	17	17 8 3	14.9	-14.1	18 8 3	10.7	-6.4	19 8 3	22.7	-21.0	0 9 3	16.2	8.1	2 9 3	16.2	8.1	2 9 3	16.2	8.1	2 9 3	16.2	8.1	2 9 3	16.2	
9 9 3	17.1	-17.5	2	2	2 9 3	19.5	-21.8	3 9 3	23.0	19.5	5 9 3	39.1	30.8	6 9 3	13.6	-13.8	7 9 3	34.9	-38.4	7 9 3	34.9	-38.4	7 9 3	34.9	-38.4	7 9 3	34.9	
11 9 3	13.5	13.8	12	12	12 9 3	6.5	-2.7	13 9 3	9.3	9.6	4 9 3	6.6	4.6	15 9 3	27.5	-28.4	19 9 3	9.1	8.0	23 9 3	9.1	8.0	23 9 3	9.1	8.0	23 9 3	9.1	
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9 10 3	11.2	-13.0	10	10	10 10 3	12.2	-14.1	11 10 3	6.2	-2.9	12 10 3	5.2	1.2	14 10 3	5.2	1.2	15 10 3	11.2	-11.4	15 10 3	11.2	-11.4	15 10 3	11.2	-11.4	15 10 3	11.2	
17 10 3	9.2	-11.3	18	18	18 10 3	6.3	3.5	20 10 3	7.0	7.9	1 11 3	22.4	-26.1	2 11 3	12.5	-16.5	3 11 3	12.5	-16.5	3 11 3	12.5	-16.5	3 11 3	12.5	-16.5	3 11 3	12.5	
4 11 3	6.3	-5.1	5	5	5 11 3	20.2	28.7	6 11 3	9.1	-12.5	7 11 3	26.7	-20.3	9 11 3	14.7	-16.1	11 11 3	24.5	-25.8	11 11 3	24.5	-25.8	11 11 3	24.5	-25.8	11 11 3	24.5	
11 11 3	26.5	-29.7	19	19	19 11 3	13.0	15.0	20 11 3	9.1	-5.2	3 12 3	10.0	15.1	4 12 3	13.3	13.5	5 12 3	16.1	-16.0	5 12 3	16.1	-16.0	5 12 3	16.1	-16.0	5 12 3	16.1	
0 12 3	19.2	-19.0	13	13	13 12 3	12.2	-15.0	17 12 3	8.0	4.0	18 12 3	7.1	7.1	19 12 3	13.8	-22.3	2 13 3	8.2	9.9	8 13 3	8.2	9.9	8 13 3	8.2	9.9	8 13 3	8.2	
3 13 3	26.7	20.3	4	4	4 13 3	9.4	-12.0	5 13 3	13.0	9.0	6 13 3	10.0	8.0	7 13 3	9.4	-9.8	8 13 3	9.4	-9.8	8 13 3	9.4	-9.8	8 13 3	9.4	-9.8	8 13 3	9.4	
9 13 3	13.3	-16.7	11	11	11 13 3	27.6	20.0	12 13 3	19.4	7.6	15 13 3	8.5	-9.3	19 13 3	8.4	10.7	2 14 3	14.9	-15.9	2 14 3	14.9	-15.9	2 14 3	14.9	-15.9	2 14 3	14.9	
1 14 3	4.5	6.4	6	6	6 14 3	9.2	-9.2	7 14 3	14.8	-15.8	7 14 3	14.8	-15.8	8 14 3	10.5	-11.8	9 14 3	10.5	-11.8	9 14 3	10.5	-11.8	9 14 3	10.5	-11.8	9 14 3	10.5	
13 14 3	8.4	-9.5	14	14	14 14 3	4.2	-7.4	17 14 3	11.2	9.1	1 15 3	12.7	-11.1	3 15 3	6.5	6.0	4 15 3	6.4	7.6	4 15 3	6.4	7.6	4 15 3	6.4	7.6	4 15 3	6.4	
7 15 3	13.8	-13.1	15	15	15 15 3	4.5	-3.8	0 16 3	4.5	-2.5	2 16 3	8.7	-4.6	4 16 3	8.5	5.0	8 16 3	8.0	2.7	8 16 3	8.0	2.7	8 16 3	8.0	2.7	8 16 3	8.0	
12 16 3	8.6	1.4	2	2	2 16 3	19.9	-16.9	3 16 3	41.0	-79.0	4 16 3	127.7	-129.6	5 16 3	39.0	35.0	6 16 3	33.4	29.3	6 16 3	33.4	29.3	6 16 3	33.4	29.3	6 16 3	33.4	
7 17 3	0.4	-47.1	8	8	8 17 3	19.8	19.8	9 17 3	22.0	21.9	10 17 3	49.8	-49.3	13 17 3	0.4	-0.4	13 17 3	0.4	-0.4	13 17 3	0.4	-0.4	13 17 3	0.4	-0.4	13 17 3	0.4	
14 17 3	23.0	29.3	15	15	15 17 3	25.0	27.7	16 17 3	13.5	17.7	17 17 3	0.4	35.8	-35.8	18 17 3	19.6	-17.0	22 17 3	0.4	17.5	22 17 3	0.4	17.5	22 17 3	0.4	17.5	22 17 3	0.4
2 18 3	9.0	-8.8	27	27	27 18 3	4.0	4.9	1 19 3	25.1	-25.0	2 19 3	8.1	8.1	3 19 3	19.9	19.7	4 19 3	39.7	-43.4	4 19 3	39.7	-43.4	4 19 3	39.7	-43.4	4 19 3	39.7	
5 19 3	23.2	-21.0	6	6	6 19 3	49.0	-47.6	7 19 3	8.5	-8.4	8 19 3	21.1	-18.4	9 19 3	22.5	-22.6	10 19 3	17.1										

shank (1953) and of Darlow (1960). Two carbon-carbon distances in one of the aromatic rings are rather larger than would be expected and this suggests that the standard deviations may be slightly underestimated. No corrections were made for libration effects.

Non-bonded intramolecular distances in the crowded region around the sulphone group are shown in Table 3 and it is clear that the sulphone group is involved in serious steric interactions with the methyl groups attached to C(2), C(2'), C(6) and C(6'). The four sulphur-methyl carbon distances, two of the oxygen-methyl carbon distances and two of the methyl carbon-aromatic carbon distances are 0.3 to 0.5 Å shorter than those found in normal van der Waals contacts. Further strains are indicated in Fig. 1(c) where the bond-angles C(1)-C(2)-C(7), C(1')-C(2')-C(7'), C(1)-C(6)-C(9) and C(1')-C(6')-C(9') are all about 5° greater than the normal 120°; at each angle the methyl group has been forced away from the sulphone group.

Table 3. *Non-bonded intramolecular distances in the region of the sulphone group.*

Distance		Distance	
C(7)-O(1)	3.13 Å	C(7')-O(1)	4.52 Å
C(7)-O(2)	4.51	C(7')-O(2)	3.10
C(7)-S(1)	3.14	C(7')-S(1)	3.14
C(7)-C(1')	3.13	C(7')-C(1)	3.14
C(7)-C(2')	3.84	C(7')-C(2')	3.81
C(7)-C(6')	3.37	C(7')-C(6')	3.43
C(7)-C(9')	3.80	C(7')-C(9')	3.67
C(9)-O(1)	4.16	C(9')-O(1)	2.82
C(9)-O(2)	2.78	C(9')-O(2)	4.15
C(9)-S(1)	3.25	C(9')-S(1)	3.27

The angular dispositions of C(1), C(1'), O(1) and O(2) about S(1) depart significantly from a regular tetrahedral arrangement with the usual large O(1)-S(1)-O(2) bond angle found in sulphone groups (117.2°) and a small C(1)-S(1)-C(1') bond angle (104.5°). The sulphur-carbon distances are about 0.025 Å longer than values found in sulphones and it seems probable that this is further evidence of strain in the molecule.

The least-squares best planes passing through the six carbon atoms of each aromatic ring, with deviations of atoms from these planes, are given in Table 4. Despite the steric strain within the molecule the individual aromatic

rings are approximately planar, but the sulphur and some of the methyl carbon atoms are displaced considerable distances from the best planes. The two aromatic rings are mutually inclined at an angle of 77°.

Table 4. *Least-squares best planes through atoms in aromatic ring I [C(1), C(2), . . . C(6)] and aromatic ring II [C(1'), C(2'), . . . C(6')]*

$$\begin{aligned} \text{I} & 0.4091X + 0.1213Y - 0.9044Z = 1.573 \text{ \AA} \\ \text{II} & 0.3695X + 0.9283Y - 0.0421Z = 1.801 \end{aligned}$$

Displacements of atoms from best planes

Displacement from I		Displacement from II	
C(1)	-0.021 Å	C(1')	0.023 Å
C(2)	0.031	C(2')	-0.007
C(3)	-0.024	C(3')	-0.016
C(4)	0.002	C(4')	0.020
C(5)	0.016	C(5')	-0.003
C(6)	-0.005	C(6')	-0.018
C(7)	0.066	C(7')	0.055
C(8)	-0.009	C(8')	0.084
C(9)	-0.004	C(9')	0.120
S(1)	-0.106	S(1)	0.085

In view of the foregoing evidence of extensive strain it is hardly surprising that the molecule is unstable.

The structure of the molecule, with its environment when viewed along [001], is shown in Fig. 2.

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