The Crystal and Molecular Structure of Phenothiazine
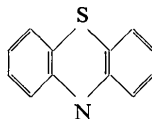
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The structure of phenothiazine,

has been determined from 1046 diffractometer data and refined by least-squares methods to a final residual of 6·1%. The space group is orthorhombic *Pnma* with $a = 7.916 \pm 0.01$, $b = 20.974 \pm 0.01$, $c = 5.894 \pm 0.01$ Å. The four molecules in the unit cell are in special positions with the S and N atoms on mirror planes. The C–S–C angle is $100.9 \pm 0.3°$ and C–S bonds are 1.762 ± 0.006 Å. The molecule has the same folded configuration as chlorpromazine and all other known phenothiazine derivatives, but the dihedral angle between the two planes of the benzene rings has the comparatively high value of 158·5°.

Introduction

Phenothiazine (thiodiphenylamine) is the parent molecule of a very important group of drugs termed the major tranquillizers. As is well known, the introduction into clinical psychiatry by Delay, Deniker & Harl (1952) of chlorpromazine and its analogues has revolutionized the treatment of psychotic conditions and of mental diseases in general.

In 1963 the crystallographic determination of the structures of phenothiazine and certain derivatives was commenced in this laboratory. It was thought that although the phenothiazines have been subjected to extensive clinical tests, comparatively little work had been done on the structural aspects of the drugs; in order to attempt to relate pharmacological properties to molecular structure, accurate molecular models of drugs having different clinical action should be available.

Phenothiazine itself, which lacks both R_1 and R_2 substituents (see Table 5), is not an effective drug. Cell dimensions were reported by Wood, McCale & Williams (1941). Malrieu & Pullman (1964) performed molecular orbital calculations on the modification of the electronic characteristics of the phenothiazine ring as a result of folding, in order to deduce the most probable configuration. Later, short structural analyses of two phenothiazine charge-transfer complexes were reported by Fritchie (1967) and Fritchie & Trus (1968).

A preliminary report was published by Feil, Linck & McDowell (1965) and work on phenothiazine continued in this laboratory; six layer lines had been photographed and intensities had been measured on the Nonius microdensitometer. The project was suspended on the preliminary report of the structure published by Bell, Blount, Briscoe & Freeman (1968). In the course of subsequent correspondence, Briscoe & Freeman (1969) emphasized that as their solved structure was the *monoclinic* form of phenothiazine, it would be of value to continue work on the *orthorhombic* form for comparative purposes, in particular to compare the molecules situated in different environments. During 1974 the solution of orthorhombic phenothiazine was recommenced, more accurate diffractometer data was collected and the results are reported in the present article.

Experimental

The purest phenothiazine powder was obtained from Fluka, Buchs SG, Switzerland. Although crystals were prepared in the first instance by slow evaporation from a solution of carbon tetrachloride, crystals of higher quality were subsequently grown by heating 1 g of the substance dissolved in 50 cm³ methyl alcohol in a reflux condenser for 20 min and allowing to evaporate slowly for a period of three weeks. The pale yellow needle-shaped crystals turned brown slowly on exposure to light, but they proved to be stable over a period of years.

X-ray oscillation and Weissenberg photographs, using Ni-filtered Cu $K\alpha$ radiation, taken about the needle axis showed the unit cell to be orthorhombic with $a = 7.92$, $b = 20.94$, $c = 5.90$ Å, in good agreement with the diffractometer values obtained subsequently; $a = 7.916 \pm 0.01$, $b = 20.974 \pm 0.01$, $c = 5.894 \pm 0.01$ Å. The latter values were used in all calculations.

The conditions for non-extinction were found to be $hk0$, $h = 2n$; $0kl$, $k + l = 2n$; $h00$, $h = 2n$; $0k0$, $k = 2n$; $00l$, $l = 2n$. These lead to either of two possible space

groups, non-centrosymmetric $Pna2_1$ with four equivalent positions, or centrosymmetric $Pnma$ with eight equivalent positions. The $hk0$ intensity data were measured on the microdensitometer and the method of Howells, Phillips & Rogers (1950) was applied. A statistical survey of the intensities of the reflexions gave an $N(z)$ distribution very close indeed to the theoretical curve for a centrosymmetric projection. The measured density was $1·355$ g cm^{-3}; as the calculated value for four molecules per unit cell was $1·352$ g cm^{-3}, the molecules must consequently be in special positions for the centrosymmetric space group.

The crystal chosen for intensity measurements, of dimensions $0·6 \times 0·7 \times 0·1$ mm, was mounted on a Philips PW 1100 computer-controlled single-crystal diffractometer and exposed to graphite-monochromated Mo $K\alpha$ radiation at a temperature of 20 °C. The counter aperture was set 2° in the detector plane and 1° perpendicular to the plane. The ω-scan mode was used, with scan rate $0·02°$ s^{-1} and scan width $1·2°$, i.e. each integrated intensity was collected over 60 s. Left and right background counts were measured for a period of 30 s each. The θ range set from 3° to 25° resulted in the measured data h,k,l (max) extending to $9,24,7$ respectively. A total number of 1046 reflexions was recorded, including 167 systematically extinct and 259 which were not significantly different from background level and thus rated as less-thans (unobserveds). Three reference reflexions were chosen and recorded at the beginning of the data collection and after every 60 min; the deviation tolerated was less than $1·2\%$ throughout the data collection.

The value of μR for Mo $K\alpha$ radiation was calculated to be $<0·05$; as the corresponding correction factor A^* is $<1·18$ throughout the range of θ, absorption corrections were not applied. The usual corrections were made for Lorentz and polarization factors. Using the sub-program $NORMSF$ (Maslen, 1967) of the X-RAY (1972) program system (updated June 1974 version), preliminary scale and temperature factors $(B=4·15)$ were estimated by Wilson's method. The statistical survey of all intensities gave an $N(z)$ distribution strongly indicative of a centrosymmetric space group.

Solution and refinement of the structure

A three-dimensional Patterson function, sharpened in accordance with the formula

$$|F|^2 = \frac{(\sin^2 \theta/\lambda^2 + 0·16)F_o^2 \exp (B \sin^2 \theta/\lambda^2)}{(\sum f_i)^2}$$

was calculated (McDowell, 1970). The analytical scattering factor values computed from numerical Hartree–Fock wave functions by Cromer & Mann (1968) were used for S, N and C; the values given by Stewart, Davidson & Simpson (1965) were used for H.

The position of the sulphur atom was deduced from the Patterson peaks. Assuming the space group to be $Pnma$, a Fourier synthesis phased on one atom placed

on the mirror plane was computed and the R index was $0·58$, where $R = \sum||F_o|-|F_c||/\sum|F_o|$. All non-hydrogen atoms were located in the second Fourier map and R dropped to $0·32$. Two cycles of full-matrix least-squares refinement of the scale factor, the coordinates and individual isotropic B's of the non-hydrogen atoms, followed by two cycles with individual anisotropic temperature factors brought R down to a value of $0·085$. The sub-program used was $CRYLSQ$ of X-RAY 72 and the function minimized was $R_1 = \sum w(hkl) \{|F_o(hkl) - F_c(hkl)|\}^2$ with equal weights given to all terms in the initial stages.

All hydrogen atoms were clearly identified in a difference Fourier synthesis. Using the sub-programs $WTLSSQ$ and $WTANAL$ of X-RAY 72, a weighting scheme was applied to the reflexions as follows:

$$w(hkl) = \frac{\sin \theta}{A} \cdot \frac{C}{F_o} = X . Y$$

$$X = 1 \text{ for } \sin \theta > A, \ X = \frac{\sin \theta}{A} \text{ for } \sin \theta < A;$$

$$Y = 1 \text{ for } F_o < C, \ Y = \frac{C}{F_o} \text{ for } F_o > C.$$

Table 1. *Observed and calculated structure factors*
Within each group the columns, reading from left to right, contain the values of k, $K|F_o|$, and F_c. An asterisk indicates F_{unobs}.

Values of 0·2 and 20 were chosen for A and C respectively. The hydrogen atoms were assigned isotropic temperature factors derived from the β's of the carbon atoms to which they were bonded. In the last two cycles the coordinates of all atoms and the β's of the non-hydrogen atoms were refined to a final R value of 0·061 for 879 reflexions. In the ultimate cycle, ΔF was less than 2σ for all except 34 reflexions (and $\Delta F < 3\sigma$ for all except five reflexions); the average parameter shifts expressed as fractions of the estimated standard deviations were approximately 0·3. Table 1 lists observed and calculated structure factors; final atomic fractional coordinates and thermal-motion parameters are given in Table 2.

Although there was little doubt that the structure was centrosymmetric, it was thought advisable to check the possibility of the non-centrosymmetric space group as it was considered important to establish with certainty the existence of a mirror plane through the centre of the molecule. The solution and refinement of the structure was therefore repeated entirely
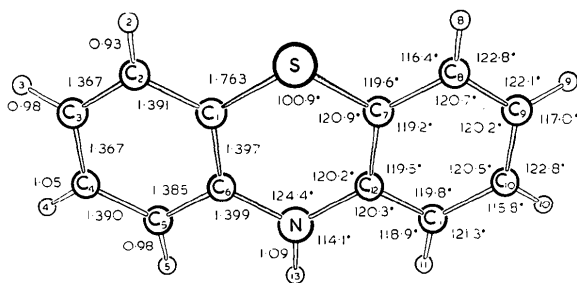
on the assumption that the space group was $Pna2_1$. The lowest R index obtained was 0·078, and there was a tendency to diverge when further cycles were attempted. Bond lengths and angles calculated were unsatisfactory; also it was noted that the majority of the structure factor B values were very small. It can be safely concluded that the molecule lies on a mirror plane in the space group $Pnma$.

Description and discussion of the structure

Bond lengths and angles with associated standard deviations which were calculated from the refined atomic positions of the final cycle are listed in Table 3 and illustrated in Fig. 1. The C–C bonds average $1·383 \pm 0·009$ Å, with maximum deviation 0·011 Å associated with C(3), the atom with highest thermal motion. It was noted that all bond lengths contracted slightly upon inclusion of the H atoms in the refinement. The average value of the C–H bonds is $1·01 \pm 0·06$ Å which is in fair agreement, within the limits of error, with the value of 1·084 Å given by Sutton (1965). The angles within the benzene rings are all very close to 120°; the mean value is $120·0 \pm 0·6°$.

Table 4 gives the equations of the best planes for the aromatic rings, which were calculated by the method of Schomaker, Waser, Marsh & Bergman (1959) using the sub-program $LSQPL$ of X-RAY 72. The maximum displacement of an atom from the plane is 0·01 Å [for C(5)] so that the rings may be regarded as planar, within the limits of precision.

Fig. 2 illustrates the configuration of the molecule which is folded about the S–N axis with a dihedral angle of 158·5°. It does not however 'consist of two

Fig. 1. Bond lengths (Å) and angles.

Table 2. Final atomic fractional coordinates ($\times 10^4$) and thermal parameters ($\times 10^4$) with estimated standard deviations

Anisotropic temperature factor $= \exp\{-(h^2\beta_{11} + k^2\beta_{22} + l^2\beta_{33} + 2hk\beta_{12} + 2hl\beta_{13} + 2kl\beta_{23})\}$ with $\beta_{11} = 2\pi^2 a^{*2} U_{11}$, $\beta_{12} = 2\pi^2 a^* b^* U_{12}$, etc.

	x	y	z	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
S	1346 (2)	2500 (0)	2085 (3)	135 (3)	72 (1)	204 (8)	0 (0)	42 (3)	0 (0)
N	3327 (7)	2500 (0)	−2303 (9)	197 (11)	48 (2)	153 (24)	0 (0)	43 (11)	0 (0)
C(1)	2453 (5)	1852 (3)	893 (7)	107 (6)	56 (2)	220 (21)	−25 (3)	−22 (7)	17 (4)
C(2)	2392 (7)	1259 (4)	1948 (11)	166 (9)	69 (2)	351 (36)	−45 (4)	−14 (12)	54 (6)
C(3)	3083 (9)	734 (4)	934 (14)	246 (12)	51 (2)	621 (53)	−46 (5)	−38 (17)	55 (8)
C(4)	3869 (8)	788 (4)	−1122 (13)	215 (11)	41 (2)	616 (49)	−34 (4)	−35 (15)	−4 (7)
C(5)	3990 (6)	1377 (3)	−2192 (10)	167 (8)	43 (2)	325 (30)	−26 (3)	16 (10)	−18 (5)
C(6)	3267 (5)	1910 (3)	−1200 (7)	117 (6)	44 (2)	206 (21)	−23 (3)	−12 (7)	5 (4)
C(7)	2453 (5)	3148 (3)	893 (7)	107 (6)	56 (2)	220 (21)	25 (3)	−22 (7)	−17 (4)
C(8)	2392 (7)	3741 (4)	1948 (11)	166 (9)	69 (2)	351 (36)	45 (4)	−14 (12)	−54 (6)
C(9)	3083 (9)	4266 (4)	934 (14)	246 (12)	51 (2)	621 (53)	46 (5)	−38 (17)	−55 (8)
C(10)	3869 (8)	4212 (4)	−1122 (13)	215 (11)	41 (2)	616 (49)	34 (4)	−35 (15)	4 (7)
C(11)	3990 (6)	3623 (3)	−2192 (10)	167 (8)	43 (2)	325 (30)	26 (3)	16 (10)	18 (5)
C(12)	3267 (5)	3090 (3)	−1200 (7)	117 (6)	44 (2)	206 (21)	23 (3)	−12 (7)	−5 (4)

Final hydrogen atomic fractional coordinates ($\times 10^3$) and isotropic temperature factors with estimated standard deviations.

	x	y	z	B		x	y	z	B
H(2)	181 (7)	124 (3)	331 (10)	6·51	H(9)	320 (8)	467 (3)	173 (10)	7·65
H(3)	320 (8)	33 (3)	173 (10)	7·65	H(10)	460 (8)	458 (3)	−182 (10)	7·41
H(4)	460 (8)	42 (3)	−182 (10)	7·41	H(11)	461 (6)	357 (2)	−361 (8)	5·38
H(5)	461 (6)	143 (2)	−361 (8)	5·38	H(13)	408 (9)	250 (0)	−385 (12)	4·93
H(8)	181 (7)	376 (3)	331 (10)	6·51					

Table 3. *Bond lengths and angles with estimated standard deviations*

The e.s.d.'s in the bond lengths $\times 10^3$ and the e.s.d.'s in the bond angles $\times 10$ are given in parentheses.

S——C(1)	1·762 (6) Å	S——C(7)	
N——C(6)	1·399 (6)	N——C(12)	
C(1)–C(2)	1·391 (10)	C(7)—C(8)	
C(2)–C(3)	1·367 (11)	C(8)—C(9)	
C(3)–C(4)	1·367 (11)	C(9)—C(10)	
C(4)–C(5)	1·390 (10)	C(10)–C(11)	
C(5)–C(6)	1·385 (8)	C(11)–C(12)	
C(6)–C(1)	1·397 (6)	C(12)–C(7)	
N——H(13)	1·09 (7)		
C(2)–H(2)	0·93 (6)		
C(3)–H(3)	0·98 (6)	C(8)—H(8)	
C(4)–H(4)	1·05 (6)	C(9)—H(9)	
C(5)–H(5)	0·98 (5)	C(10)–H(10)	
		C(11)–H(11)	

C(1)–S——C(7)	100·9 (3)°		
C(6)–N——C(12)	124·4 (5)		
C(6)–N——H(13)	114·1 (13)		
C(6)–C(1)–S	120·9 (4)	C(12)–N——H(13)	
C(6)–C(1)–C(2)	119·2 (5)	C(12)–C(7)—S	
S——C(1)–C(2)	119·6 (4)	C(12)–C(7)—C(8)	
C(1)–C(2)–C(3)	120·7 (6)	S——C(7)—C(8)	
C(1)–C(2)–H(2)	116·4 (34)	C(7)—C(8)—C(9)	
C(3)–C(2)–H(2)	122·8 (24)	C(7)—C(8)—H(8)	
C(2)–C(3)–C(4)	120·2 (8)	C(9)—C(8)—H(8)	
C(2)–C(3)–H(3)	122·1 (36)	C(8)—C(9)—C(10)	
C(4)–C(3)–H(3)	117·0 (36)	C(8)—C(9)—H(9)	
C(3)–C(4)–C(5)	120·5 (7)	C(10)–C(9)—H(9)	
C(3)–C(4)–H(4)	122·8 (32)	C(9)—C(10)–C(11)	
C(5)–C(4)–H(4)	115·8 (32)	C(9)—C(10)–H(10)	
C(4)–C(5)–C(6)	119·8 (5)	C(11)–C(10)–H(10)	
C(4)–C(5)–H(5)	121·3 (27)	C(10)–C(11)–C(12)	
C(6)–C(5)–H(5)	118·9 (27)	C(10)–C(11)–H(11)	
C(5)–C(6)–C(1)	119·5 (5)	C(12)–C(11)–H(11)	
C(5)–C(6)–N	120·3 (4)	C(11)–C(12)–C(7)	
N——C(6)–C(1)	120·2 (5)	C(11)–C(12)–N	
		N——C(12)–C(7)	

planar halves folded along the N–S axis', as suggested by Fritchie & Trus (1968); both S and N atoms are at significant distances from planes I and II (−0·18 Å for S atom and −0·03 Å for N atom). The hydrogen atom bonded to nitrogen, H(13), is on the opposite side of the planes from S and N, as can be seen from Fig. 2; the sum of the angles about N is 352·6°, thus N forms the apex of a flattened pyramid with C(6), C(12), H(13)

as the base. From molecular orbital calculations, Malrieu & Pullman (1964) deduced that the most probable configuration would be folded with 'H intra', *i.e.* the proton attached to the nitrogen atom would be placed between the two lateral rings. This prediction agrees with the position for H(13) found here.

Table 4. *Mean plane parameters and deviations of atoms from the plane*

Equation of plane I: C(1)–C(6)

$$6·8436x + 3·9102y + 2·7509z = 2·6556$$

Equation of plane II: C(7)–C(12)

$$6·8436x - 3·9102y + 2·7509z = 0·7005$$

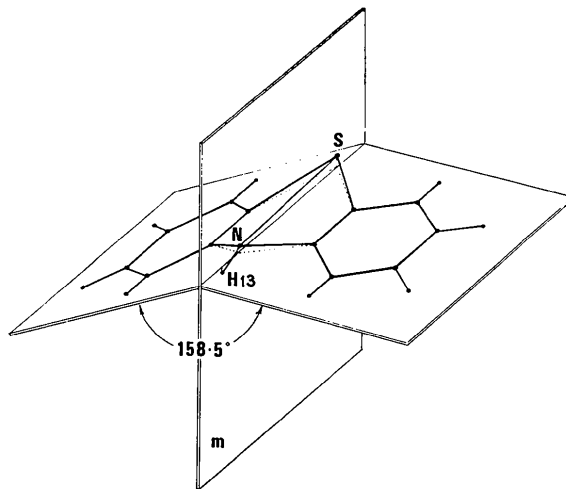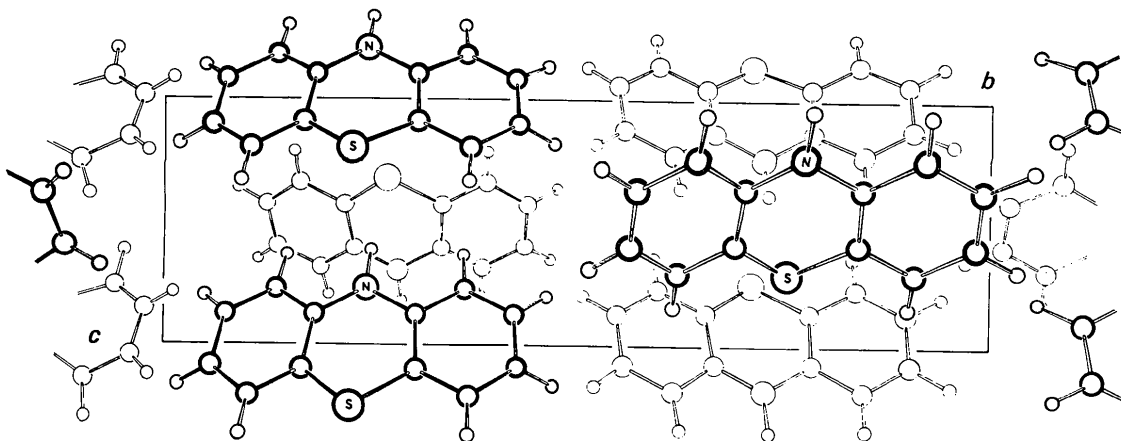|			
C(1)	−0·0071 Å	S	−0·1831 Å
C(2)	0·0095	N	−0·0348
C(3)	−0·0017	H(2)	−0·0244
C(4)	−0·0085	H(3)	0·1333
C(5)	0·0107	H(4)	0·1550
C(6)	−0·0030	H(5)	0·0651
		H(13)	0·0536

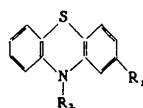Fig. 2. Configuration of phenothiazine molecule.

Fig. 3. The structure viewed down the *a* axis.

The structure shown in Fig. 2 closely resembles that of the phenothiazine nucleus as found in chlorpromazine, thiethylperazine and thioridazine, except that the dihedral angle in phenothiazine is greater, as can be seen from Table 5, which lists for comparative purposes important parameters of phenothiazine and eight derivatives of known structure. Seven of the derivatives have dihedral angles between 135° and 145° with a mean value of 138·9°. It is surprising to find that methoxypromazine, with properties very similar to chlorpromazine, has a configuration much closer to that of phenothiazine.

Characteristic of this type of compound are the contracted C–S bond lengths and the C–S–C angles in which there is a remarkable uniformity (Table 5). All bonds have values between 1·75 and 1·78 Å with average 1·767 Å; all angles lie between 97·3 and 100·9° with mean value 98·7°. Orthorhombic phenothiazine, although close to monoclinic phenothiazine and methoxypromazine, has the highest value of 100·9°. In every case the S atom is displaced from the planes of the aromatic rings, symmetrically in both phenothiazines, asymmetrically in most of the other compounds with a tendency toward greater displacement

Table 5. *Comparison of bond lengths and angles in phenothiazine and certain derivatives*

Compound	Drug action	R₁	R₂	Space group	C-S-C (degrees)	C-S (Å)	Distance of S from planes (Å)	C-N (Å)	Mean C-C in benzene rings (Å)	Dihedral angle (degrees)	Reference
Phenothiazine (monoclinic)		-H	-H	$P2_1$	99.6±0.4	1.770±0.005	0.18, 0.17	1.404±0.007	1.387	153.3	(a)
Phenothiazine (orthorhombic)		-H	-H	$Pnma$	100.9±0.3	1.762·0.006	0.18, 0.18	1.399·0.006	1.383	158.5	(b)
Diethazine	Antiparkinsonian	-H	-CH₂-CH₂-N(CH₂-CH₃)₂	$P2_1/c$	97.5	1.766	0.09, 0.06	1.415	1.397	138.0	(c)
Isothazine	Antiparkinsonian	-H	-CH₂-CH₂-N(CH₂-CH₃)₂	$P2_1/c$	98.1·0.2	1.766±0.004		1.420·0.004	1.389	138.5	(d)
Thiazinamium	Antihistamine, anticholinergic	-H	-CH₂-CH-N(CH₃)...	$P2_1/c$	98.0	1.772·0.006	0.06, 0.14	1.411·0.007	1.386	135.6	(e)
Promethazine	Antihistamine	-H	-CH₂-CH-N(CH₃)₂	$I\bar4$	98.8	1.766·0.005	0.03, 0.02	1.414·0.006	1.384	140.6	(f)
Methoxypromazine	Neuroleptic	-O-CH₃	-CH₂-CH₂-CH₂-N(CH₃)₂	Pca	99.8·0.3	1.758·0.007	0.28, 0.19	1.413±0.007	1.383	157.7	(g)
Chlorpromazine	Neuroleptic	-Cl	-CH₂-CH₂-CH₂-N(CH₃)₂	Pca	97.3·0.3	1.75±0.01	0.14, 0.02	1.405·0.010	1.400	139.4	(h)
Thiethylperazine	Anti-emetic	-S-CH₂-CH₃	-CH₂-CH₂-CH₂-N(N-CH₃)	$P2_12_12_1$	99.0±0.7	1.78·0.015	0.14, 0.0	1.425±0.015	1.395	139.0	(i)
Thioridazine	Neuroleptic	-S-CH₃	-CH₂-CH₂C...	$Pna2_1$	99.0±0.4 / 97.8±0.4	1.774±0.008 / 1.769·0.008	0.08, 0.14 / 0.10, 0.01	1.411±0.009 / 1.407±0.009	1.386 / 1.389	145.8 / 134.4	(j)*
					98.7	1.767		1.411	1.389		

(a) Bell, Blount, Briscoe & Freeman (1968)
(b) Present work
(c) Marsau (1971)
(d) Marsau & Calas (1971)
(e) Marsau & Cam (1973)
(f) Marsau & Busetta (1973)
(g) Marsau & Gauthier (1973)
(h) McDowell (1969)
(i) McDowell (1970)
(j) McDowell (1975). *The first and second rows are values for molecules I and II respectively.
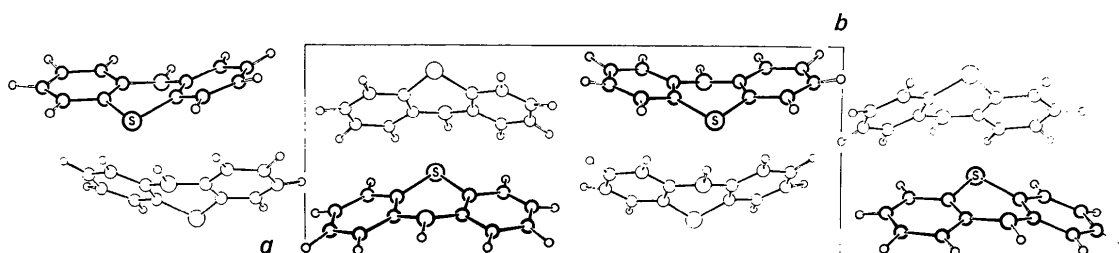

Fig. 4. The structure viewed down the *c* axis.

from the ring containing a substituent R_1, or from the ring towards which the 'tail' or R_2 substituent is oriented. It is also of interest to compare the averaged C–C lengths in the benzene rings, as it can be noted that the majority are shorter than the value of 1·394 Å reported for benzene (Sutton, 1965).

Some intramolecular non-bonded distances and intermolecular contacts less than 4 Å are listed in Table 6, from which it can be seen that there are no abnormally short contacts. In Figs. 3 and 4 the molecular packing in the unit cell is viewed along the a and c axes respectively. The molecules are arranged in sheets perpendicular to the a axis.

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Table 6. *Intramolecular and intermolecular distances*

The superscripts denote the equivalent positions at (i) $x, y, z - 1$, (ii) $x, y, z + 1$, (iii) $\frac{1}{2} + x, y, \frac{1}{2} - z$, (iv) $-\frac{1}{2} + x, y, -\frac{1}{2} - z$, (v) $-\frac{1}{2} + x, y, \frac{1}{2} - z$, (vi) $\frac{1}{2} + x, y, -\frac{1}{2} - z$, (vii) $\bar{x}, \bar{y} - 1, \bar{z}$, (viii) $\frac{1}{2} - x, -1 - y, \frac{1}{2} + z$, (ix) $\frac{1}{2} - x, -1 - y, -\frac{1}{2} + z$.

H(2)–H(3)	2·399 Å	H(4)–H(5)	2·356 Å
H(3)–H(4)	2·379	H(5)–H(13)	2·294
S——H(13^{iv})	2·619	C(3)–H(4^{vii})	3·086
S——C(1^v)	3·573	C(3)–H(2^{iii})	3·163
S——C(6^v)	3·654	C(3)–H(5^{iv})	3·398
S——N^{ii}	3·661	C(3)–H(3^{ix})	3·479
S——N^{iv}	3·695	C(3)–H(4^{viii})	3·483
S——N^v	3·895	C(3)–H(4^{iv})	3·729
S——S^{iii}	3·988	C(3)–H(5^{ii})	3·731
		C(3)–C(4^{viii})	3·948
N——H(13^{iv})	3·432		
N——H(5^{iv})	3·743	C(4)–H(2^{iii})	3·008
N——N^{vi}	3·965	C(4)–H(3^{ix})	3·118
		C(4)–H(4^{vii})	3·306
C(1)–H(5^{iv})	2·769	C(4)–H(3^{vii})	3·313
C(1)–H(13^{iv})	3·230	C(4)–H(5^{iv})	3·631
C(1)–H(13^{ii})	3·619	C(4)–H(4^{iv})	3·672
C(1)–C(5^{iv})	3·642	C(4)–H(2^i)	3·785
C(1)–H(2^{iii})	3·708	C(4)–C(4^{vii})	3·985
C(1)–H(5^{ii})	3·770		
		C(5)–H(2^i)	3·178
C(2)–H(5^{iv})	2·974	C(5)–H(2^{iii})	3·207
C(2)–H(5^{ii})	3·173	C(5)–H(5^v)	3·500
C(2)–H(2^{iii})	3·498	C(5)–C(6^{vi})	3·689
C(2)–C(5^{ii})	3·687	C(5)–C(5^{vi})	3·975
C(2)–C(3^v)	3·796	C(5)–C(5^{iv})	3·975
C(2)–H(13^{ii})	3·832		
C(2)–C(4^v)	3·848	C(6)–H(5^{iv})	3·068
C(2)–C(5^{iv})	3·895	C(6)–H(13^{iv})	3·540
C(2)–H(4^{viii})	3·929	C(6)–H(2^{iii})	3·568
C(2)–H(3^v)	3·985	C(6)–H(2^i)	3·713

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