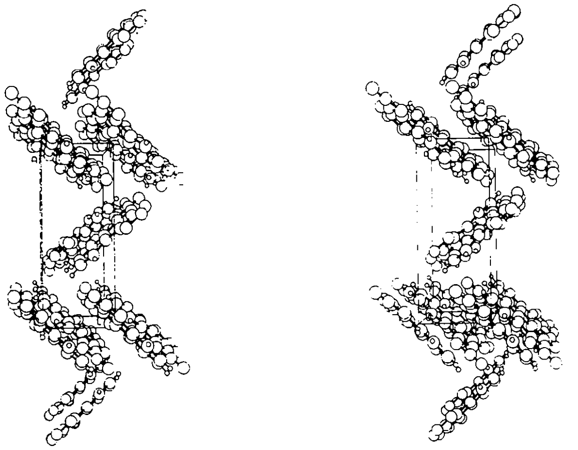

Fig. 2. A stereoview of the packing, viewed down the *b* axis; the long axis is *a*.

A stereoview of the packing of (I) is shown in Fig. 2. Planar molecules are arranged in such a way that they approximately lie on two mutually perpendicular lattice planes forming a see-saw pattern. An examination of intermolecular distances [shortest, N(3)$\cdots$C(8)-($x,y,z+1$) = 3·426 (3) Å] shows that the crystal structure is stabilized by van der Waals interactions only.

This work was supported by a grant (CA 17562) to DvdH from the National Cancer Institute, Department of Health and Human Services, and by grant E-745 to MA from the Robert A. Welch Foundation, Houston, Texas.

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Structure of *N*-Phenylphenothiazine, $C_{18}H_{13}NS$

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(*Received* 20 *November* 1984; *accepted* 12 *April* 1985)

Abstract. $M_r = 275{\cdot}0$, triclinic, $P\bar{1}$, $a = 10{\cdot}369$ (5), $b = 10{\cdot}596$ (6), $c = 15{\cdot}468$ (6) Å, $\alpha = 68{\cdot}26$ (4), $\beta = 65{\cdot}49$ (5), $\gamma = 68{\cdot}04$ (5)°, $V = 1383{\cdot}3$ Å^3, $Z = 4$, $D_x = 1{\cdot}32$ g cm^{-3}, Mo $K\alpha_1$, $\lambda = 0{\cdot}70930$ Å, $\mu = 2{\cdot}1$ cm^{-1}, $F(000) = 576$, $T = 110$ K, final $R = 0{\cdot}055$ for 2921 observed reflections. The title compound is a phenothiazine derivative with two unique molecules in the asymmetric unit. The folding angles between the least-squares planes of the two benzo rings are 162·6 and 150·7°. There are no unusual intramolecular bond lengths or angles.

Introduction. Phenothiazine is the parent molecule of a class of compounds known to possess tranquilizing properties. However, phenothiazine itself and the title compound (I) are not effective drugs. It is well known that an electronegative substituent on the 3-position of the phenothiazine benzo ring and an *N*-substituted propylamine group are necessary for enhanced psychopharmacological activity. There has also been some speculation on the effect of the butterfly folding angle on the tranquilizing activity (Phelps & Cordes, 1974, 1976). The structure determination of *N*-phenylpheno-

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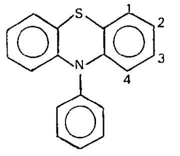
thiazine was undertaken in order to allow comparison with other previously reported substituted phenothiazine structures.



(I)

Experimental. Yellow, plate-like crystal, approximate dimensions 0·25 × 0·27 × 0·11 mm. Enraf–Nonius CAD-4 diffractometer with graphite-crystal-monochromatized Mo $K\alpha$ radiation. Unit-cell dimensions and successful determination of the structure confirmed with space group as $P\overline{1}$. Lattice constants determined by least-squares fit of 25 reflections with $36 \leq 2\theta \leq 49°$ measured on the diffractometer. Three-dimensional intensity data collected in ω:2θ scan mode; total of 3799 independent reflections, 2921 observed with $I > 3\sigma(I)$; $2 \leq 2\theta \leq 46°$; $-11 \leq h \leq 11$, $-11 \leq k \leq 11$, $0 \leq l \leq 17$. Equivalent reflections were averaged, $R_{\rm int} = 0·014$. Data corrected for Lorentz and polarization effects. Four standard reflections measured every 2 h during data collection (222, 200, 004 and 928) showed no significant change in intensity. ψ absorption correction, 58% min. transmission, 99·5% max. transmission. Structure solved by direct methods using *MULTAN*11/82 (Main, Hull, Lessinger, Germain, Declercq & Woolfson, 1978). Initial E map contained 38 peaks corresponding to all except two non-hydrogen atoms in two unique molecules. The two non-hydrogen atoms and 26 H atoms were located on a difference Fourier map. Subsequent full-matrix least-squares refinement of 465 variables with all coordinates and anisotropic temperature factors for non-hydrogen atoms, coordinates and isotropic thermal parameters for H atoms refined on F led to a final $R = 0·055$, $wR = 0·069$, where $w = 1/\sigma(F)^2$ and $(F)^2 = [(F)^2_{\rm cs} + (0·04)^2(F^2)^2]$, $S = 2·47$. In final least-squares cycle $(\Delta/\sigma)_{\rm max} = 0·00$. Max. and min. peaks in difference Fourier map 0·64 and $-0·70$ e Å^{-3}, respectively. Scattering factors for S and O were corrected for anomalous dispersion and all scattering factors were taken from *International Tables for X-ray Crystallography* (1974). CAD-4 *SDP* (Frenz, 1984) programs used.

Discussion. Final fractional coordinates for the non-hydrogen atoms are given in Table 1.* The numbering system for the molecules is in Fig. 1. Bond lengths and angles are in Table 2.

The compound crystallizes with four molecules in the unit cell. A stereoscopic diagram of the molecular packing in the unit cell is shown in Fig. 2. The shortest intermolecular contact is 2·80 (4) Å. As expected, there are no intermolecular or intramolecular hydrogen bonds. There are no unusual intramolecular bond lengths or angles.

Table 1. *Positional parameters and equivalent isotropic thermal parameters*

$$B_{\rm eq} = \tfrac{4}{3}[a^2B(1,1) + b^2B(2,2) + c^2B(3,3) + ab(\cos\gamma)B(1,2) + ac(\cos\beta)B(1,3) + bc(\cos\alpha)B(2,3)].$$

	x	y	z	$B_{\rm eq}$(Å^2)
S(1)	0·33201 (9)	0·11943 (8)	0·53766 (6)	2·25 (2)
S(1′)	−0·85560 (8)	0·37062 (8)	0·95159 (6)	2·24 (2)
N(1)	0·2574 (3)	0·4375 (2)	0·5103 (2)	1·70 (6)
N(1′)	−0·5661 (2)	0·2600 (3)	0·9919 (2)	1·67 (6)
C(1)	0·3807 (3)	0·2474 (3)	0·4268 (2)	1·81 (8)
C(1′)	−0·6887 (3)	0·2765 (3)	0·8810 (2)	1·79 (8)
C(2′)	−0·6843 (3)	0·2551 (3)	0·7978 (2)	2·27 (8)
C(2)	0·4677 (3)	0·2016 (3)	0·3430 (2)	1·98 (8)
C(3′)	−0·5533 (4)	0·1920 (3)	0·7359 (2)	2·47 (9)
C(3)	0·5331 (3)	0·2910 (3)	0·2575 (2)	2·14 (8)
C(4)	0·5013 (3)	0·4301 (3)	0·2560 (2)	2·22 (9)
C(4′)	−0·4272 (3)	0·1487 (3)	0·7617 (2)	2·32 (9)
C(5)	0·4077 (3)	0·4799 (3)	0·3374 (2)	1·91 (8)
C(5′)	−0·4315 (3)	0·1677 (3)	0·8454 (2)	1·96 (8)
C(6′)	−0·5605 (3)	0·2334 (3)	0·9076 (2)	1·69 (8)
C(6)	0·3442 (3)	0·3897 (3)	0·4261 (2)	1·58 (7)
C(7′)	−0·8321 (3)	0·2950 (3)	1·0675 (2)	1·90 (8)
C(7)	0·1795 (3)	0·2221 (3)	0·6101 (2)	2·04 (8)
C(8)	0·0829 (3)	0·1522 (3)	0·6928 (2)	2·44 (9)
C(8′)	−0·9553 (3)	0·2862 (3)	1·1516 (3)	2·27 (9)
C(9′)	−0·9448 (4)	0·2474 (4)	1·2431 (3)	2·61 (9)
C(9)	−0·0333 (4)	0·2260 (4)	0·7556 (3)	2·8 (1)
C(10′)	−0·8081 (4)	0·2147 (4)	1·2533 (3)	2·8 (1)
C(10)	−0·0587 (4)	0·3694 (4)	0·7356 (3)	2·69 (9)
C(11′)	−0·6836 (3)	0·2176 (3)	1·1708 (2)	2·23 (9)
C(11)	0·0361 (3)	0·4395 (3)	0·6534 (2)	2·19 (8)
C(12′)	−0·6924 (3)	0·2554 (3)	1·0773 (2)	1·77 (8)
C(12)	0·1568 (3)	0·3668 (3)	0·5907 (2)	1·86 (8)
C(13)	0·2373 (3)	0·5827 (3)	0·5056 (2)	1·71 (8)
C(13′)	−0·4261 (3)	0·2338 (3)	1·0051 (2)	1·64 (8)
C(14′)	−0·3638 (3)	0·3443 (3)	0·9733 (2)	1·77 (8)
C(14)	0·3158 (3)	0·6107 (3)	0·5464 (2)	1·95 (8)
C(15′)	−0·2319 (3)	0·3230 (3)	0·9854 (2)	2·04 (8)
C(15)	0·2989 (3)	0·7499 (3)	0·5410 (2)	2·12 (8)
C(16′)	−0·1599 (3)	0·1885 (3)	1·0282 (2)	2·12 (8)
C(16)	0·2036 (3)	0·8577 (3)	0·4968 (2)	2·25 (8)
C(17)	0·1233 (3)	0·8285 (3)	0·4574 (2)	2·19 (9)
C(17′)	−0·2213 (3)	0·0774 (3)	1·0586 (2)	2·15 (8)
C(18′)	−0·3545 (3)	0·0990 (3)	1·0474 (2)	1·98 (8)
C(18)	0·1407 (3)	0·6901 (3)	0·4616 (2)	1·95 (8)

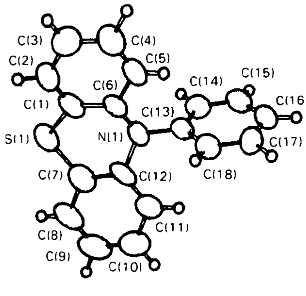


Fig. 1. Atomic labeling scheme in one molecular unit of the title compound. The thermal ellipsoids are drawn at the 90% probability level and the H atoms have been plotted with arbitrary radii.

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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 42184 (43 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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

S(1)–C(1)	1·763 (2)	C(7′)–C(12′)	1·407 (3)
S(1)–C(7)	1·757 (2)	C(7)–C(8)	1·407 (3)
S(1′)–C(1′)	1·769 (2)	C(7)–C(12)	1·394 (3)
S(1′)–C(7′)	1·751 (2)	C(8)–C(9)	1·376 (4)
N(1)–C(6)	1·393 (3)	C(8′)–C(9′)	1·358 (4)
N(1)–C(12)	1·419 (3)	C(9′)–C(10′)	1·390 (4)
N(1)–C(13)	1·452 (3)	C(9)–C(10)	1·376 (4)
N(1′)–C(6′)	1·408 (3)	C(10′)–C(11′)	1·388 (3)
N(1′)–C(12′)	1·423 (3)	C(10)–C(11)	1·394 (3)
N(1′)–C(13′)	1·458 (3)	C(11′)–C(12′)	1·383 (3)
C(1)–C(2)	1·378 (3)	C(11)–C(12)	1·388 (3)
C(1)–C(6)	1·407 (3)	C(13)–C(14)	1·375 (3)
C(1′)–C(2′)	1·367 (4)	C(13)–C(18)	1·379 (3)
C(1′)–C(6′)	1·416 (3)	C(13′)–C(14′)	1·381 (3)
C(2′)–C(3′)	1·387 (4)	C(13′)–C(18′)	1·392 (3)
C(2)–C(3)	1·384 (3)	C(14′)–C(15′)	1·381 (3)
C(3′)–C(4′)	1·388 (4)	C(14)–C(15)	1·393 (3)
C(3)–C(4)	1·379 (3)	C(15′)–C(16′)	1·394 (3)
C(4)–C(5)	1·378 (3)	C(15)–C(16)	1·374 (4)
C(4′)–C(5′)	1·363 (4)	C(16′)–C(17′)	1·383 (3)
C(5)–C(6)	1·406 (3)	C(16)–C(17)	1·384 (3)
C(5′)–C(6′)	1·390 (3)	C(17)–C(18)	1·389 (3)
C(7′)–C(8′)	1·399 (3)	C(17′)–C(18′)	1·386 (3)
C(1)–S(1)–C(7)	101·3 (1)	S(1)–C(7)–C(12)	122·2 (2)
C(1′)–S(1′)–C(7′)	99·4 (1)	C(8)–C(7)–C(12)	120·1 (2)
C(6)–N(1)–C(12)	123·0 (2)	C(7)–C(8)–C(9)	120·2 (2)
C(6)–N(1)–C(13)	118·3 (2)	C(7′)–C(8′)–C(9′)	121·6 (2)
C(12)–N(1)–C(13)	116·4 (2)	C(8′)–C(9′)–C(10′)	119·2 (2)
C(6′)–N(1′)–C(12′)	120·7 (2)	C(8)–C(9)–C(10)	120·0 (2)
C(6′)–N(1′)–C(13′)	116·9 (2)	C(9′)–C(10′)–C(11′)	120·1 (3)
C(12′)–N(1′)–C(13′)	117·6 (2)	C(9)–C(10)–C(11)	120·1 (3)
S(1)–C(1)–C(2)	117·7 (2)	C(10′)–C(11′)–C(12′)	121·4 (2)
S(1)–C(1)–C(6)	120·8 (2)	C(10)–C(11)–C(12)	120·9 (2)
C(2)–C(1)–C(6)	121·2 (2)	N(1′)–C(12′)–C(7′)	119·7 (2)
S(1′)–C(1′)–C(2′)	118·9 (2)	N(1′)–C(12′)–C(11′)	122·2 (2)
S(1′)–C(1′)–C(6′)	119·7 (2)	C(7′)–C(12′)–C(11′)	118·1 (2)
C(2′)–C(1′)–C(6′)	121·2 (2)	N(1)–C(12)–C(7)	120·7 (2)
C(1′)–C(2′)–C(3′)	120·9 (2)	N(1)–C(12)–C(11)	120·6 (2)
C(1)–C(2)–C(3)	121·2 (2)	C(7)–C(12)–C(11)	118·6 (2)
C(2′)–C(3′)–C(4′)	118·2 (3)	N(1)–C(13)–C(14)	118·7 (2)
C(2)–C(3)–C(4)	118·2 (2)	N(1)–C(13)–C(18)	120·4 (2)
C(3)–C(4)–C(5)	121·4 (2)	C(14)–C(13)–C(18)	120·9 (2)
C(3′)–C(4′)–C(5′)	121·1 (3)	N(1′)–C(13′)–C(14′)	119·1 (2)
C(4)–C(5)–C(6)	121·2 (2)	N(1′)–C(13′)–C(18′)	120·8 (2)
C(4′)–C(5′)–C(6′)	121·9 (2)	C(14′)–C(13′)–C(18′)	120·1 (2)
N(1′)–C(6′)–C(1′)	120·5 (2)	C(13′)–C(14′)–C(15′)	120·4 (2)
N(1′)–C(6′)–C(5′)	122·9 (2)	C(13)–C(14)–C(15)	119·2 (2)
C(1′)–C(6′)–C(5′)	116·6 (2)	C(14′)–C(15′)–C(16′)	119·7 (2)
N(1)–C(6)–C(1)	121·9 (2)	C(14)–C(15)–C(16)	120·4 (2)
N(1)–C(6)–C(5)	121·4 (2)	C(15′)–C(16′)–C(17′)	119·8 (2)
C(1)–C(6)–C(5)	116·6 (2)	C(15)–C(16)–C(17)	120·0 (2)
S(1′)–C(7′)–C(8′)	119·4 (2)	C(16)–C(17)–C(18)	119·9 (2)
S(1′)–C(7′)–C(12′)	120·8 (2)	C(16′)–C(17′)–C(18′)	120·5 (2)
C(8′)–C(7′)–C(12′)	119·5 (2)	C(13′)–C(18′)–C(17′)	119·4 (2)
S(1)–C(7)–C(8)	117·6 (2)	C(13)–C(18)–C(17)	119·6 (2)

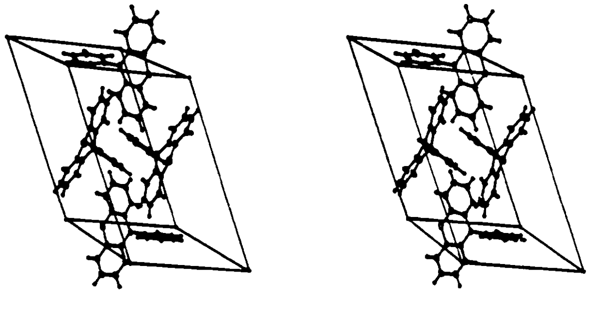

Fig. 2. Stereoview of the molecular packing of the contents of the unit cell.

The phenyl ring is bonded equatorially to the phenothiazine skeleton at the N. The phenyl-ring plane nearly bisects the benzo planes in each of the two molecules [78·6 (4) and 84·6 (4)° in the unprimed molecule and 81·7 (4) and 79·3 (4)° in the primed molecule]. The folding angles between the two least-squares planes of the two benzo rings are 162·6 (5) and 150·7 (5)°. These fold angles are significantly larger than comparable angles in similar compounds which show some tranquilizing activity [*i.e.* chlorpromazine free base, 134·2° (McDowell, 1969); promethazine HBr, 140·4° (Marsau & Busetta, 1973); perphenazine, 140·7° (McDowell, 1978); phenothiazine-10-propionic acid, 138·0° (Malmstrom & Cordes, 1972); *etc.*]. However, they are not inconsistent with some substituted phenothiazines that show considerably flattened skeletons [*i.e.* methoxypromazine, 157·7° (Marsau & Gauthier, 1973); 1-ethylphenothiazine, 154·8° (Chu, Napoleone, Ternay & Chang, 1982); *N*-methylphenothiazine, 165·4° (Chu & van der Helm, 1974); *etc.*]. Of these, methoxypromazine is the only one that shows any tranquilizing activity. The crystal packing is without significant intermolecular contacts that would contribute to the flattening of the molecules and the folding angle between the benzo rings does not appear to correlate with tranquilizing activity.

This research was partially supported by the National Institutes of Health, MBRS program (RR08008) and by the donors of the Petroleum Research Fund administered by the American Chemical Society. We wish to thank Dr E. D. Stevens and the University of New Orleans for allowing us to collect data on their instrument.

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