The novel spiro compound described in this report (V) clearly has structural features which are found in both the oxazolidine and hydantoin drugs. Furthermore, it has been suggested (Camerman & Camerman, 1971) that the spatial properties of the C(5) substituents of compounds such as (II)–(IV) relative to the rest of the molecule may be an important factor in determining the site of action of these drugs. The spatial properties of the oxazolidine residue relative to the hydantoin residue of the spiro compound (V) are very similar to those of the C(5) phenyl substituents of (IV) relative to the hydantoin ring (Camerman & Camerman, 1971). The presence of both oxazolidine and hydantoin ring structures in (V) along with the spatial relationships between these two rings suggests that this spiro compound may have important anticonvulsant and/or antiepileptic properties.

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Structure of 2-Chloro-10-phenylphenothiazine

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Abstract. $C_{18}H_{12}ClNS$, $M_r = 309.82$, monoclinic, $P2_1/c$, $a = 19.689$ (4), $b = 7.240$ (1), $c = 23.582$ (4) Å, $\beta = 116.90$ (1)°, $V = 2997.8$ (9) Å^3, $Z = 8$, $D_x = 1.373$, $D_m = 1.37$ g cm^{-3} (by flotation), $\lambda(Mo\,K\alpha) = 0.7107$ Å, $\mu = 3.78$ cm^{-1}, $F(000) = 1280$, $T = 295$ K. Final $R = 0.036$ for 2929 observed reflections. The central ring of the phenothiazine ring system is in a boat conformation. The folding angle between the least-squares planes of the benzo and the chlorobenzo rings is 153.0 (1) and 153.3 (1)° for the two crystallographically independent molecules in the unit cell. The 10-phenyl substituent is in an equatorial position with respect to the central ring of the phenothiazine ring system.

Introduction. This paper reports the structure of 2-chloro-10-phenylphenothiazine and is a continuation of the structural studies of substituted phenothiazines (Jovanovic, Biehl, de Meester & Chu, 1984). The main objective of these studies is to determine the effect of the substituents on the conformation and configuration of the phenothiazine ring system and to compare the conformation in the solid state with that deduced in solution.

The ^{13}C chemical shifts have been assigned on the basis of model compounds and substituent chemical-shift constants (Jovanovic & Biehl, 1984). The lack of influence of the 2-chloro substituent on the chemical shifts of the C atoms in the unsubstituted benzo ring indicates that the title compound exists in solution in the butterfly conformation.

Experimental. Crystals of the title compound are pale-yellow prisms. Accurate unit-cell parameters by least-squares fit of 15 reflections in range $20 < 2\theta < 30°$, two crystallographically independent molecules in one asymmetric unit of the unit cell, crystal $0.55 \times 0.52 \times 0.15$ mm, automatic Syntex $P2_1$ diffractometer, graphite-monochromatized Mo $K\alpha$ radiation, $\theta/2\theta$ scanning mode, 4185 independent reflections in range $3 < 2\theta < 50°$, hkl range: $h\ -21\rightarrow19$, $k\ 0\rightarrow7$, $l\ 0\rightarrow25$, symmetry-equivalent reflections merged, 2929 observed reflections with $I > 3\sigma(I)$, $\sigma(I)$ from counting statistics; three standard reflections remeasured every 100 reflections showed a random variation of less than 4% in intensity; Lorentz–polarization correction, no absorption or extinction corrections, direct methods (*MULTAN*78, Main, Hull, Lessinger, Germain, Declercq & Woolfson, 1978), refinement by full-matrix least squares using *SHELX*76 (Sheldrick, 1976), anisotropic for non-H, H atoms located in difference Fourier maps, isotropic temperature factors for H, $w = 1/(\sigma^2 F + 0.00036 F^2)$, $\Sigma w(|F_o| - |F_c|)^2$ minimized, $R = 0.036$, $wR = 0.039$ for 2929 observed reflections, $R = 0.056$ using all reflections, $(\Delta/\sigma)_{max} = 0.25$, max. and min. heights in final difference Fourier map 0.17 and -0.20 e Å^{-3}. Atomic scattering factors for C, H, N, S and Cl and effects of anomalous-dispersion correction for S and Cl those stored in *SHELX*76.

Discussion. The final atomic parameters are given in Table 1.* The identification of the atoms and the conformation of the molecule are shown in the *ORTEP* (Johnson, 1965) drawing of Fig. 1. The bond lengths and bond angles are presented in Table 2. They are similar to those reported for other N(10)-substituted 2-chlorophenothiazines, such as chlorpromazine (McDowell, 1969) and chlorpromazine sulfoxide (Hough, Hjorth & Dahl, 1985). There are no significant differences in bond lengths and bond angles between the two crystallographically independent molecules in the title compound, except, for no apparent reason, the bond length of C(8)–C(9) is larger [1.402 (4) Å] in molecule (1) than in molecule (2) [1.373 (5) Å].

The central phenothiazine ring is in the boat conformation as shown by the torsion angles in Fig. 1 and the puckering parameters (Cremer & Pople, 1975). For molecule (1), these parameters are $q_2 = 0.448$ (2), $q_3 = -0.081$ (2), $Q = 0.456$ (2) Å, $\varphi_2 = 125.7$ (3) and $\theta = 100.3$ (3)°, while for molecule (2), these parameters take the values 0.461 (2), -0.075 (2), 0.467 (2) Å, 121.5 (3) and 99.3 (3)°, respectively. For

ideal boat conformation, the puckering parameters are $q_2 = Q$, $q_3 = 0$ Å, $\varphi_2 = 120$ and $\theta = 90°$. The 10-phenyl substituent is in an equatorial position relative to the central ring. The deviations of the atoms from the least-squares planes calculated for the benzo and phenyl

Table 1. *Fractional atomic coordinates with equivalent isotropic thermal parameters for the non-*H *and isotropic for the* H *atoms (e.s.d.'s in parentheses)*

$$U_{eq} = (U_{11} + U_{22} + U_{33})/3.$$

	x	y	z	$U_{eq}/U(Å^2)$
C(1)1	0.8101 (2)	0.3605 (4)	0.1455 (1)	0.0496 (7)*
C(2)1	0.7436 (2)	0.3379 (4)	0.1511 (1)	0.0587 (7)
Cl(2)1	0.72419 (5)	0.1273 (1)	0.17555 (4)	0.0831 (2)
C(3)1	0.6911 (2)	0.4782 (5)	0.1361 (1)	0.0651 (8)
C(4)1	0.7055 (2)	0.6397 (5)	0.1130 (1)	0.0649 (9)
C(4a)1	0.7707 (1)	0.6671 (4)	0.1061 (1)	0.0505 (6)
S(5)1	0.78627 (4)	0.8812 (1)	0.07995 (4)	0.0679 (2)
C(5a)1	0.8452 (1)	0.8140 (4)	0.0457 (1)	0.0476 (6)
C(6)1	0.8459 (2)	0.9204 (4)	-0.0023 (1)	0.0537 (7)
C(7)1	0.9002 (2)	0.8938 (4)	-0.0237 (1)	0.0639 (8)
C(8)1	0.9530 (2)	0.7580 (4)	0.0027 (1)	0.0621 (8)
C(9)1	0.9501 (2)	0.6418 (4)	0.0491 (1)	0.0530 (7)
C(9a)1	0.8963 (1)	0.6672 (3)	0.0712 (1)	0.0419 (6)
N(10)1	0.8935 (1)	0.5522 (3)	0.1185 (1)	0.0471 (5)
C(10a)1	0.8255 (1)	0.5244 (4)	0.1236 (1)	0.0446 (6)
C(1')1	0.9549 (1)	0.4198 (4)	0.1489 (1)	0.0443 (6)
C(2')1	1.0162 (2)	0.4666 (5)	0.2047 (1)	0.0548 (7)
C(3')1	1.0768 (2)	0.3466 (6)	0.2319 (2)	0.0655 (10)
C(4')1	1.0763 (2)	0.1815 (5)	0.2042 (2)	0.0759 (10)
C(5')1	1.0148 (2)	0.1333 (4)	0.1482 (2)	0.0697 (9)
C(6')1	0.9539 (2)	0.2533 (4)	0.1207 (1)	0.0574 (7)
C(1)2	0.5962 (1)	0.6081 (4)	0.4020 (1)	0.0479 (6)
C(2)2	0.5734 (1)	0.6252 (4)	0.4494 (1)	0.0526 (7)
Cl(2)2	0.52854 (5)	0.8272 (1)	0.45406 (4)	0.0822 (2)
C(3)2	0.5861 (2)	0.4851 (5)	0.4929 (1)	0.0584 (8)
C(4)2	0.6213 (2)	0.3264 (4)	0.4882 (1)	0.0534 (7)
C(4a)2	0.6439 (1)	0.3047 (4)	0.4411 (1)	0.0464 (6)
S(5)2	0.68083 (5)	0.0909 (1)	0.43427 (4)	0.0684 (2)
C(5a)2	0.7378 (1)	0.1629 (4)	0.3987 (1)	0.0468 (6)
C(6)2	0.8001 (2)	0.0566 (5)	0.4077 (2)	0.0571 (8)
C(7)2	0.8410 (2)	0.0919 (5)	0.3747 (2)	0.0684 (9)
C(8)2	0.8208 (2)	0.2383 (5)	0.3335 (2)	0.0695 (9)
C(9)2	0.7605 (2)	0.3489 (4)	0.3256 (1)	0.0575 (8)
C(9a)2	0.7173 (1)	0.3143 (4)	0.3573 (1)	0.0445 (6)
N(10)2	0.6537 (1)	0.4240 (3)	0.3480 (1)	0.0482 (5)
C(10a)2	0.6317 (1)	0.4472 (3)	0.3970 (1)	0.0430 (6)
C(1')2	0.6279 (1)	0.5598 (4)	0.2981 (1)	0.0480 (6)
C(2')2	0.5652 (2)	0.5218 (5)	0.2416 (1)	0.0552 (8)
C(3')2	0.5407 (2)	0.6511 (6)	0.1933 (2)	0.0719 (11)
C(4')2	0.5781 (2)	0.8163 (6)	0.2016 (2)	0.0842 (11)
C(5')2	0.6406 (2)	0.8546 (5)	0.2580 (2)	0.0789 (11)
C(6')2	0.6649 (2)	0.7260 (4)	0.3057 (2)	0.0631 (8)
H(1)1	0.841 (1)	0.259 (3)	0.158 (1)	0.051 (8)
H(3)1	0.648 (2)	0.454 (4)	0.142 (1)	0.061 (9)
H(4)1	0.677 (2)	0.746 (4)	0.106 (1)	0.081 (10)
H(6)1	0.811 (1)	1.021 (4)	-0.019 (1)	0.063 (8)
H(7)1	0.902 (2)	0.977 (4)	-0.056 (1)	0.077 (10)
H(8)1	0.990 (1)	0.744 (3)	-0.010 (1)	0.036 (7)
H(9)1	0.987 (1)	0.549 (4)	0.067 (1)	0.060 (8)
H(2')1	1.018 (1)	0.588 (4)	0.224 (1)	0.059 (8)
H(3')1	1.116 (2)	0.378 (4)	0.267 (1)	0.078 (11)
H(4')1	1.118 (2)	0.100 (4)	0.223 (1)	0.080 (10)
H(5')1	1.010 (2)	0.006 (5)	0.127 (1)	0.095 (11)
H(6')1	0.913 (1)	0.226 (3)	0.079 (1)	0.055 (8)
H(1)2	0.587 (1)	0.709 (4)	0.372 (1)	0.056 (8)
H(3)2	0.571 (1)	0.505 (3)	0.523 (1)	0.047 (8)
H(4)2	0.631 (1)	0.220 (3)	0.516 (1)	0.054 (8)
H(6)2	0.812 (2)	-0.042 (4)	0.436 (1)	0.072 (10)
H(7)2	0.878 (2)	0.010 (4)	0.376 (1)	0.072 (10)
H(8)2	0.849 (1)	0.269 (4)	0.312 (1)	0.058 (8)
H(9)2	0.749 (1)	0.447 (3)	0.302 (1)	0.047 (8)
H(2')2	0.541 (1)	0.408 (3)	0.235 (1)	0.037 (7)
H(3')2	0.500 (2)	0.620 (5)	0.158 (2)	0.102 (13)
H(4')2	0.564 (2)	0.899 (4)	0.171 (1)	0.079 (11)
H(5')2	0.666 (2)	0.968 (4)	0.263 (1)	0.079 (10)
H(6')2	0.710 (2)	0.748 (4)	0.346 (1)	0.080 (10)

* The standard deviations of U_{eq}'s were calculated according to Schomaker & Marsh (1983).

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* Lists of structure factors, anisotropic thermal parameters and least-squares planes have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 42766 (26 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

rings are given in Table 3 (deposited). The tricyclic phenothiazine ring is folded along the S(5)···N(10) line. The angle between the two benzo rings is virtually identical in the two crystallographically independent molecules: 153·0 (1) and 153·3 (1)°, and has a similar magnitude to those in other 10-phenyl substituted phenothiazines (Chu, Yang & van der Helm, 1976; Jovanovic, Biehl, de Meester & Chu, 1984). The phenyl ring is nearly parallel to the plane bisecting the tricyclic ring. In molecule (1), the phenyl ring makes an angle of −72·8 (1)° with the chlorobenzo group and of 80·6 (1)° with the benzo group. The corresponding values in molecule (2) are 77·9 (1) and 75·4 (1)°.

The packing of the molecules in the unit cell is shown in the stereoscopic drawing of Fig. 2. There are no intermolecular distances less than the van der Waals distances.

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

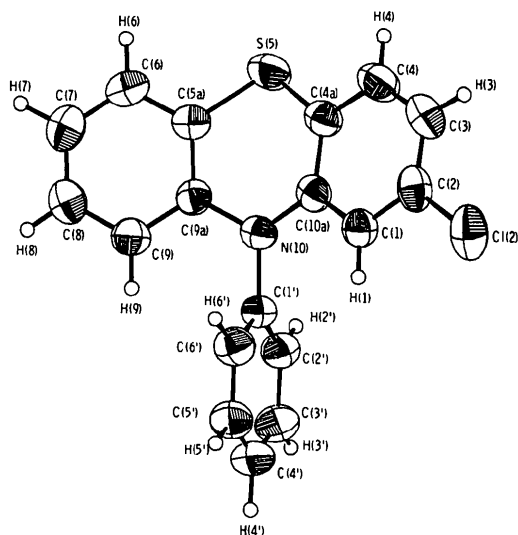|			
C(1)1–C(2)1	1·384 (4)	C(1)2–C(2)2	1·386 (3)
C(1)1–C(10a)1	1·381 (4)	C(1)2–C(10a)2	1·391 (4)
C(2)1–Cl(2)1	1·732 (3)	C(2)2–Cl(2)2	1·738 (3)
C(2)1–C(3)1	1·376 (5)	C(2)2–C(3)2	1·383 (4)
C(3)1–C(4)1	1·373 (5)	C(3)2–C(4)2	1·372 (5)
C(4)1–C(4a)1	1·379 (4)	C(4)2–C(4a)2	1·380 (4)
C(4a)1–S(5)1	1·747 (3)	C(4a)2–S(5)2	1·748 (3)
C(4a)1–C(10a)1	1·414 (3)	C(4a)2–C(10a)2	1·406 (3)
S(5)1–C(5a)1	1·755 (3)	S(5)2–C(5a)2	1·757 (3)
C(5a)1–C(6)1	1·374 (4)	C(5a)2–C(6)2	1·381 (5)
C(5a)1–C(9a)1	1·399 (3)	C(5a)2–C(9a)2	1·400 (3)
C(6)1–C(7)1	1·387 (4)	C(6)2–C(7)2	1·373 (6)
C(7)1–C(8)1	1·360 (4)	C(7)2–C(8)2	1·370 (6)
C(8)1–C(9)1	1·402 (4)	C(8)2–C(9)2	1·373 (5)
C(9)1–C(9a)1	1·388 (4)	C(9)2–C(9a)2	1·386 (4)
C(9a)1–N(10)1	1·413 (3)	C(9a)2–N(10)2	1·414 (3)
N(10)1–C(10a)1	1·412 (3)	N(10)2–C(10a)2	1·416 (3)
N(10)1–C(1')1	1·453 (3)	N(10)2–C(1')2	1·438 (3)
C(1')1–C(2')1	1·366 (4)	C(1')2–C(2')2	1·374 (4)
C(1')1–C(6')1	1·373 (4)	C(1')2–C(6')2	1·376 (5)
C(2')1–C(3')1	1·377 (6)	C(2')2–C(3')2	1·382 (6)
C(3')1–C(4')1	1·360 (6)	C(3')2–C(4')2	1·371 (6)
C(4')1–C(5')1	1·373 (6)	C(4')2–C(5')2	1·371 (6)
C(5')1–C(6')1	1·382 (5)	C(5')2–C(6')2	1·369 (6)
C(2)1–C(1)1–C(10a)1	121·0 (3)	C(2)2–C(1)2–C(10a)2	120·1 (2)
C(1)1–C(2)1–Cl(2)1	119·7 (2)	C(1)2–C(2)2–Cl(2)2	119·1 (2)
C(1)1–C(2)1–C(3)1	121·4 (3)	C(1)2–C(2)2–C(3)2	121·1 (2)
Cl(2)1–C(2)1–C(3)1	118·8 (2)	Cl(2)2–C(2)2–C(3)2	119·8 (2)
C(2)1–C(3)1–C(4)1	117·7 (3)	C(2)2–C(3)2–C(4)2	118·9 (3)
C(3)1–C(4)1–C(4a)1	122·7 (3)	C(3)2–C(4)2–C(4a)2	121·3 (3)
C(41)–C(4a)1–S(5)1	119·4 (2)	C(4)2–C(4a)2–S(5)2	118·3 (2)
C(4)1–C(4a)1–C(10a)1	119·2 (2)	C(4)2–C(4a)2–C(10a)2	120·2 (2)
S(5)1–C(4a)1–C(10a)1	121·2 (2)	S(5)2–C(4a)2–C(10a)2	121·4 (2)
C(4a)1–S(5)1–C(5a)1	100·1 (1)	C(4a)2–S(5)2–C(5a)2	99·4 (1)
S(5)1–C(5a)1–C(6)1	118·6 (2)	S(5)2–C(5a)2–C(6)2	118·4 (2)
S(5)1–C(5a)1–C(9a)1	120·6 (2)	S(5)2–C(5a)2–C(9a)2	121·4 (2)
C(6)1–C(5a)1–C(9a)1	120·4 (2)	C(6)2–C(5a)2–C(9a)2	120·0 (3)
C(5a)1–C(6)1–C(7)1	121·2 (3)	C(5a)2–C(6)2–C(7)2	121·1 (4)
C(6)1–C(7)1–C(8)1	119·3 (3)	C(6)2–C(7)2–C(8)2	119·3 (4)
C(7)1–C(8)1–C(9)1	119·9 (3)	C(7)2–C(8)2–C(9)2	120·2 (4)
C(8)1–C(9)1–C(9a)1	121·4 (3)	C(8)2–C(9)2–C(9a)2	121·7 (3)
C(5a)1–C(9a)1–C(9)1	117·5 (2)	C(5a)2–C(9a)2–C(9)2	117·6 (2)
C(5a)1–C(9a)1–N(10)1	120·7 (2)	C(5a)2–C(9a)2–N(10)2	120·2 (2)
C(9)1–C(9a)1–N(10)1	121·8 (2)	C(9)2–C(9a)2–N(10)2	122·1 (2)
C(9a)1–N(10)1–C(10a)1	121·9 (2)	C(9a)2–N(10)2–C(10a)2	121·1 (2)
C(9a)1–N(10)1–C(1')1	117·2 (2)	C(9a)2–N(10)2–C(1')2	118·1 (2)
C(10a)–N(10)1–C(1')1	118·3 (2)	C(10a)–N(10)2–C(1')2	117·5 (2)
C(1)1–C(10a)1–C(4a)1	118·0 (2)	C(1)2–C(10a)2–C(4a)2	118·4 (2)
C(1)1–C(10a)1–N(10)1	122·1 (2)	C(1)2–C(10a)2–N(10)2	121·3 (2)
C(4a)1–C(10a)1–N(10)1	119·9 (2)	C(4a)2–C(10a)2–N(10)2	120·2 (2)
N(10)1–C(1')1–C(2')1	119·1 (2)	N(10)2–C(1')2–C(2')2	119·1 (2)
N(10)1–C(1')1–C(6')1	120·9 (2)	N(10)2–C(1')2–C(6')2	121·4 (3)
C(2')1–C(1')1–C(6')1	119·8 (3)	C(2')2–C(1')2–C(6')2	119·5 (3)
C(1')1–C(2')1–C(3')1	119·6 (3)	C(1')2–C(2')2–C(3')2	119·3 (3)
C(2')1–C(3')1–C(4')1	120·9 (4)	C(2')2–C(3')2–C(4')2	120·6 (4)
C(3')1–C(4')1–C(5')1	119·8 (4)	C(3')2–C(4')2–C(5')2	120·2 (4)
C(4')1 C(5')1 C(6')1	119·5 (4)	C(4')2–C(5')2–C(6')2	119·1 (4)
C(1')1–C(6')1–C(5')1	120·4 (3)	C(1')2–C(6')2–C(5')2	121·3 (3)

Fig. 1. *ORTEP* drawing of molecule (1), one of the two crystallographically independent molecules. Thermal ellipsoids are scaled at the 50% probability level. H atoms are represented as circles of arbitrary radius. The torsion angles are:

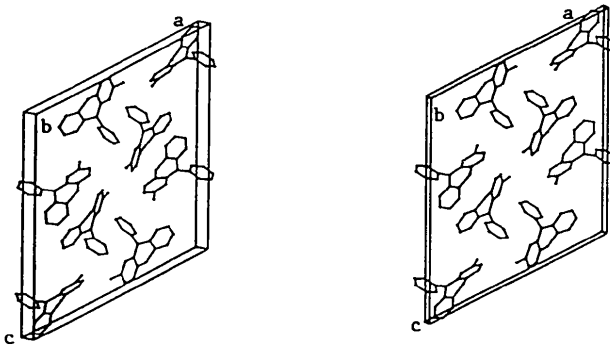|	Molecule (1)	Molecule (2)
N(10)–C(10)–C(4a)–S(5)	−1·6 (4)°	−4·0 (4)°
C(10a)–C(4a)–S(5)–C(5a)	29·2 (3)	30·8 (3)
C(4a)–S(5)–C(5a)–C(9a)	−33·3 (3)	−32·0 (3)
S(5)–C(5a)–C(9a)–N(10)	9·8 (4)	6·1 (4)
C(5a)–C(9a)–N(10)–C(10a)	27·1 (4)	30·4 (4)
C(9a)–N(10)–C(10a)–C(4a)	−31·5 (4)	−31·6 (4)
C(9a)–N(10)–C(1')–C(2')	94·3 (4)	101·5 (4)
C(9a)–N(10)–C(1')–C(6')	−82·2 (4)	−78·2 (5)
C(10a)–N(10)–C(1')–C(2')	−103·7 (4)	−98·8 (4)
C(10a)–N(10)–C(1')–C(6')	79·8 (4)	81·6 (5)

Fig. 2. Stereoscopic drawing of the molecular packing in the cell. The H atoms are omitted for clarity.

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Structure of 10-(*m*-Tolyl)-5,10-dihydrophenarsazine

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Abstract. $C_{19}H_{16}AsN$, $M_r = 333 \cdot 27$, monoclinic, $P2_1/c$, $a = 17 \cdot 309$ (3), $b = 5 \cdot 974$ (1), $c = 16 \cdot 546$ (2) Å, $\beta = 115 \cdot 65$ (1)°, $V = 1542 \cdot 3$ (4) Å^3, $Z = 4$, $D_x = 1 \cdot 435$ g cm^{-3}, $\lambda(\text{Mo } K\alpha) = 0 \cdot 7107$ Å, $\mu = 21 \cdot 6$ cm^{-1}, $F(000) = 680$, $T = 295$ K. Final $R = 0 \cdot 031$ for 1935 observed reflections. The central phenarsazine ring is in a flattened boat conformation. The dihedral angle between the two benzo planes is 160·6 (2)°. The *m*-tolyl substituent is in an axial position relative to the central ring. The bond lengths and angles are in good agreement with those found in 10-(3-methoxyphenyl)-5,10-dihydrophenarsazine.

Introduction. As part of our continuing structural studies of substituted phenarsazines and phenothiazines, we have recently determined the structure of 10-(3-methoxyphenyl)-5,10-dihydrophenarsazine (de Meester, Chu, Jovanovic & Biehl, 1985). We report here the structure of 10-(*m*-tolyl)-5,10-dihydrophenarsazine.

Experimental. Crystals of the title compound are colorless rectangular plates elongated in the [010] direction. Lattice parameters from least-squares refinement of 15 reflections in range $15 < 2\theta < 20°$, crystal faces 100, $\bar{1}00$, 010, $0\bar{1}0$, 001 and $00\bar{1}$, crystal dimensions $0 \cdot 55 \times 0 \cdot 20 \times 0 \cdot 11$ mm, automatic Syntex $P2_1$ diffractometer, graphite-monochromatized Mo $K\alpha$ radiation, $\theta/2\theta$ scanning mode, 2714 independent reflections in range $3 < 2\theta < 50°$, *hkl* range:

$-20 \le h \le 18$, $0 \le k \le 7$, $0 \le l \le 19$, 1937 observed reflections with $I > 3\sigma(I)$, $\sigma(I)$ from counting statistics; three standard reflections ($12\bar{3}$, 106 and $40\bar{8}$) remeasured every 100 reflections showed no change in intensity greater than $2\sigma(I)$; Lorentz–polarization correction, absorption correction (transmission-factor range 0·583 to 0·783), no extinction correction; Structure solved by standard Patterson and difference Fourier methods; refinement by full-matrix least squares using *SHELX*76 (Sheldrick, 1976), anisotropic for non-H, isotropic for H atoms, $w = 1/[\sigma^2(F) + 0 \cdot 00146F^2]$, $\sum w(|F_o| - |F_c|)^2$ minimized; during final refinement, two strong reflections (200 and 310) discarded due to measurement errors; $R = 0 \cdot 031$, $wR = 0 \cdot 033$ for 1935 observed reflections, $(\Delta/\sigma)_{max} = 0 \cdot 25$, $\Delta\rho_{max} = 0 \cdot 28$ e Å^{-3}. Atomic scattering factors for C, H and N those stored in *SHELX*76, for As *International Tables for X-ray Crystallography* (1974); effects of anomalous-dispersion correction for As (from same source) included in calculation of F_c.

Discussion. The final atomic parameters are given in Table 1.† The identification of the atoms and the configuration of the molecule are shown in the *ORTEP* (Johnson, 1965) drawing of Fig. 1. The bond lengths and bond angles are listed in Table 2. They are in good

† Lists of structure factors, anisotropic thermal parameters and least-squares planes have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 42767 (16 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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