Table 3. *Comparison of geometries* (Å,°) *of selected phenyltriazenes*

	(I)	(III)	(IV)	(V)	(VI)	(VII)	Average
C1–N1	1·42	1·43	1·43	1·42	1·43	1·42	1·425 (5)
N1–N2	1·27	1·26	1·28	1·26	1·24	1·28	1·27 (1)
N2–N3	1·32	1·35	1·31	1·34	1·38	1·32	1·34 (2)
N3–C7	1·45	—	1·46	1·45	—	—	
N3–C8	1·44	—	1·44	1·45	—	1·45	
C2–C1–N1	116	113	118	115	115	117	116 (2)
C6–C1–N1	125	124	121	125	125	125	124 (2)
C1–N1–N2	112	114	111	112	113	112	112 (1)
N1–N2–N3	115	110	113	114	112	115	113 (2)
N2–N3–C7	116	121	115	112	120	—	
N2–N3–C8	123	—	123	122	119	124	
C7–N3–C8	121	—	120	123	118	—	
C2–C1–N1–N2	−169	−177	−165	−172	−179	−159	
C6–C1–N1–N2	10	1	16	7	1	22	
C1–N1–N2–N3	180	179	179	176	180	180	
N1–N2–N3–C7	−173	−179	−178	−170	173	—	
N1–N2–N3–C8	−4	—	−0	−3	5	−10	

(I) This work; (III) *p*-nitrodiazoaminobenzene (Kondrashev, 1974); (IV) 2-(3,3-dimethyltriazeno)phenyl-1-carboxamide (Edwards *et al.*, 1977); (V) (2,6-*cis*-dimethylpiperidyl)diazobenzene (Lunazzi *et al.*, 1978); (VI) 1,6-bis(*p*-chlorophenyl)-3,4-diacetylhexaaza-1,5-diene (MacKay *et al.*, 1982); (VII) 3-methyl-1-*p*-tolyltriazene (Randall & Schwalbe, 1984).

resonance is strongly correlated with the Hammett constant σ^+, a significant parameter in quantitative structure–activity relationships of triazenes in mutagenesis (Venger *et al.*, 1979) and antitumor activity (Hatheway *et al.*, 1978).

References

BOLHUIS, F. VAN & KIERS, C. TH. (1978). *Acta Cryst.* B**34**, 1015–1016.

COLAPIETRO, M., DOMENICANO, A., MARCIANTE, C. & PORTALONE, G. (1982). *Z. Naturforsch. Teil B*, **37**, 1309–1311.

DENNY, W. A., CAIN, B. F., ATWELL, G. J., HANSCH, C. & LEO, A. (1982). *J. Med. Chem.* **25**, 276–315.

DOMENICANO, A., VACIAGO, A. & COULSON, C. A. (1975). *Acta Cryst.* B**31**, 221–234.

EDWARDS, S. L., CHAPUIS, G., TEMPLETON, D. H. & ZALKIN, A. (1977). *Acta Cryst.* B**33**, 276–278.

FRENZ, B. A. (1978). *The Enraf–Nonius CAD-4 Structure Determination Package – A Real-Time System for Concurrent X-ray Data Collection and Crystal Structure Solution.* In *Computing in Crystallography*, edited by H. SCHENK, R. OLTHOF-HAZEKAMP, H. VAN KONINGSVELD & G. C. BASSI, pp. 64–71. Delft Univ. Press.

HATHEWAY, G. J., HANSCH, C., KIM, K. H., MILSTEIN, S. R., SCHMIDT, C. L., SMITH, R. N. & QUINN, F. R. (1978). *J. Med. Chem.* **21**, 563–574.

HIBERTY, P. C. & OHANESSIAN, G. (1984). *J. Am. Chem. Soc.* **106**, 6963–6968.

International Tables for X-ray Crystallography (1974). Vol. IV. Birmingham: Kynoch Press. (Present distributor Kluwer Academic Publishers, Dordrecht.)

JOHNSON, C. K. (1965). *ORTEP*. Report ORNL-3794. Oak Ridge National Laboratory, Tennessee, USA.

KAZITSYNA, L. A., USTYNYUK, YU. K., GURMAN, V. S., PERGUSHOV, V. I. & GRUZDNEVA, V. N. (1977). *Dokl. Acad. Nauk SSSR*, **233**, 213–219.

KONDRASHEV, YU. D. (1974). *Zh. Strukt. Khim.* **15**, 441–446.

LUNAZZI, L., CERIONI, G., FORESTI, E. & MACCIANTELLI, D. (1978). *J. Chem. Soc. Perkin Trans.* 2, pp. 686–691.

MACKAY, D., MCINTYRE, D. D. & TAYLOR, N. J. (1982). *J. Org. Chem.* **47**, 532–535.

MAIN, P., FISKE, S. J., HULL, S. E., LESSINGER, L., GERMAIN, G., DECLERCQ, J.-P. & WOOLFSON, M. M. (1982). *MULTAN82. A System of Computer Programs for the Automatic Solution of Crystal Structures from X-ray Diffraction Data.* Univs. of York, England, and Louvain, Belgium.

MERLINO, S. & SARTORI, F. (1982). *Acta Cryst.* B**38**, 1476–1480.

MOTHERWELL, W. D. S. & CLEGG, W. (1978). *PLUTO78*. Program for plotting molecular and crystal structures. Univ. of Cambridge, England.

RANDALL, A. J. & SCHWALBE, C. H. (1984). *J. Chem. Soc. Perkin Trans.* 2, pp. 251–253.

SHELDRICK, G. (1976). *SHELX76*. Program for crystal structure determination. Univ. of Cambridge, England.

VENGER, B. H., HANSCH, C., HATHEWAY, G. J. & AMREIN, Y. U. (1979). *J. Med. Chem.* **22**, 473–476.

Acta Cryst. (1988). C**44**, 1653–1656

Structure of 2-Bromo-4-(2-chlorophenyl)-6*H*-thieno[3,2-*f*][1,2,4]triazolo-[4,3-*a*][1,4]diazepine (I) and of its 9-Cyclohexyl Derivative (II)*

BY HELEN J. KEMMISH AND THOMAS A. HAMOR

Department of Chemistry, University of Birmingham, Birmingham B15 2TT, England

(*Received* 25 *March* 1988; *accepted* 11 *May* 1988)

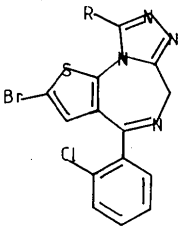
Abstract. (I) $C_{14}H_8BrClN_4S$, $M_r = 379{\cdot}7$, monoclinic, $P2_1/c$, $a = 12{\cdot}385\ (2)$, $b = 8{\cdot}674\ (1)$, $c = 14{\cdot}335\ (2)$ Å, $\beta = 104{\cdot}91\ (1)°$, $V = 1488{\cdot}1$ Å^3, $Z = 4$, $D_x = 1{\cdot}695$ g cm^{-3}, λ(Mo $K\alpha$) = 0·71069 Å, $\mu = 29{\cdot}8$ cm^{-1}, $F(000) = 752$, $T = 293$ K, $R = 0{\cdot}045$ for 2110 reflections [$I > 2{\cdot}5\sigma(I)$]. (II) $C_{20}H_{18}BrClN_4S$, $M_r = 461{\cdot}8$, monoclinic, $P2_1/c$, $a = 8{\cdot}140\ (1)$, $b = 14{\cdot}982\ (7)$, $c = 16{\cdot}095\ (9)$ Å, $\beta = 99{\cdot}09\ (3)°$, $V = 1938{\cdot}2$ Å^3, $Z = 4$, $D_x = 1{\cdot}583$ g cm^{-3}, λ(Mo $K\alpha$) = 0·71069 Å, $\mu = 23{\cdot}0$ cm^{-1}, $F(000) = 936$, $T = 293$ K, $R = 0{\cdot}028$ for 2544 reflections [$I > 2{\cdot}5\sigma(I)$]. The angle between the

* Contribution from the Crystallography Unit, Universities of Aston and Birmingham.

0108-2701/88/091653-04$03.00

mean planes of the phenyl and thieno rings is 88·8 (8)° in (I) and 88·3 (5)° in (II). The triazolo ring is planar to within ±0·002 Å in both compounds; the seven-membered ring adopts a cycloheptatriene-like boat conformation with bow and stern angles of 55·4 (8) and 29·2 (8)° in (I), and 55·3 (5) and 32·9 (5)° in (II). Bond lengths and angles are normal.

Introduction. The title compounds (Weber, Bauer, Langbein & Daniel, 1978) are related to the psychotropic 5-phenyl-1,4-benzodiazepin-2-one and triazolobenzodiazepine drugs, but differ from these in containing a thiene ring instead of the normal benzene ring fused to the seven-membered heterocyclic system. Compounds (I) and (II) have a high affinity for the benzodiazepine receptor (Squires & Braestrup, 1977), binding more strongly than the triazolobenzodiazepines alprazolam (Hester, Duchamp & Chidester, 1971) by factors of *ca* 5 and 2 respectively, and estazolam (Meguro & Kuwada, 1970) by factors of *ca* 25 and 10 respectively. The title compounds also bind more strongly than diazepam by factors of approximately 15 and 16 respectively. The crystal structure of the 9-methyl analogue, brotizolam, which has found use as a hypnotic, has been determined previously (Butcher & Hamor, 1985).



(I) R = H
(II) R = cyclohexyl

Experimental. Compound (I): crystals from ethanol, Enraf–Nonius CAD-4 diffractometer, crystal size 0·15 × 0·25 × 0·5 mm, cell dimensions from setting angles of 24 reflections ($14 \le \theta \le 22°$), graphite-monochromated Mo $K\alpha$ radiation, no absorption correction, 3412 unique reflections scanned by ω–2θ scans up to $\theta = 27·5°$, 2110 considered observed [$I > 2·5\sigma(I)$], index range h −16 to 15, k 0 to 11, l 0 to 18. Two standard reflections, measured every 2 h, showed no significant change in intensity. Structure solved by direct methods; H atoms located from difference Fourier maps; refinement by least squares on F values, H atoms isotropically, other species with anisotropic vibration parameters; final calculated shifts all $< 0·3\sigma$, $R = 0·045$, $wR = 0·056$ for the 2110 observed reflections; weighting scheme $w = 1/[\sigma^2(F) + 0·001F^2]$; residual electron density in final difference map ±0·7 e Å^{-3}, no correction for secondary extinction.

Compound (II): crystals from ethanol; diffractometer measurements and structure solution and refinement details as for compound (I) except: crystal size 0·4 × 0·5 × 0·6 mm, θ for cell refinement 11–14°, 3036 unique reflections scanned, 2544 considered observed, $\theta_{max} = 24°$, index range h ±9, k 0 to 17, l 0 to 18. No crystal deterioration. Final $R = 0·028$, $wR = 0·040$ for the 2544 observed reflections, $\Delta/\sigma < 0·3$, residual electron density ±0·5 e Å^{-3}.

Table 1. *Fractional atomic coordinates* (Br × 10^5, *others* × 10^4) *with e.s.d.'s in parentheses and equivalent isotropic temperature factors* (Å^2 × 10^3)

$U_{eq} = \frac{1}{3}(U_{11} + U_{22} + U_{33} + 2U_{13}\cos\beta)$.

	x	y	z	U_{eq}
Compound (I)				
Br	38717 (5)	−20115 (7)	55552 (4)	74
Cl	3047 (1)	4405 (2)	3562 (1)	82
S	1797 (1)	102 (1)	5261 (1)	43
N(1)	340 (2)	2050 (3)	4069 (2)	33
N(2)	−946 (3)	3632 (4)	4276 (2)	49
N(3)	−1207 (3)	3202 (4)	3305 (2)	43
N(5)	710 (3)	2017 (4)	2054 (2)	40
C(1)	−29 (3)	2942 (4)	4708 (3)	42
C(3)	−432 (3)	2260 (4)	3203 (3)	35
C(4)	−298 (3)	1464 (5)	2322 (3)	43
C(6)	1658 (3)	1657 (4)	2600 (3)	37
C(7)	2776 (3)	−169 (5)	3895 (3)	47
C(8)	2831 (3)	−671 (5)	4796 (3)	47
C(10)	1284 (3)	1099 (4)	4200 (2)	33
C(11)	1878 (3)	862 (4)	3541 (3)	38
C(1′)	2669 (3)	2087 (5)	2260 (3)	41
C(2′)	3351 (4)	3306 (5)	2652 (3)	52
C(3′)	4276 (4)	3677 (6)	2318 (4)	64
C(4′)	4495 (4)	2845 (7)	1591 (4)	67
C(5′)	3833 (4)	1645 (6)	1183 (4)	59
C(6′)	2913 (4)	1254 (5)	1505 (3)	47
Compound (II)				
Br	−23603 (3)	3615 (2)	−51258 (2)	46
Cl	3730 (1)	638 (1)	−6691 (1)	48
S	−202 (1)	1998 (1)	−5383 (1)	34
N(1)	1599 (2)	2907 (1)	−6428 (1)	29
N(2)	3391 (3)	4006 (1)	−6306 (1)	42
N(3)	2561 (3)	3991 (1)	−7134 (1)	41
N(5)	803 (2)	2148 (1)	−8207 (1)	35
C(1)	2808 (3)	3363 (2)	−5894 (1)	32
C(3)	1505 (3)	3335 (1)	−7186 (1)	33
C(4)	328 (3)	3033 (2)	−7932 (2)	37
C(6)	670 (3)	1493 (2)	−7715 (1)	31
C(7)	−947 (3)	878 (2)	−6593 (2)	33
C(8)	−1191 (3)	1049 (2)	−5810 (1)	32
C(10)	578 (3)	2174 (1)	−6304 (1)	29
C(11)	86 (3)	1535 (2)	−6896 (1)	29
C(1′)	1190 (3)	600 (2)	−7996 (1)	32
C(2′)	2575 (3)	157 (2)	−7581 (2)	35
C(3′)	3166 (4)	−619 (2)	−7881 (2)	42
C(4′)	2316 (4)	−983 (2)	−8603 (2)	46
C(5′)	897 (4)	−580 (2)	−9023 (2)	44
C(6′)	330 (3)	210 (2)	−8728 (2)	41
C(1C)	3428 (3)	3128 (2)	−5000 (1)	31
C(2C)	4340 (4)	2232 (2)	−4927 (2)	41
C(3C)	4966 (4)	2004 (2)	−4014 (2)	51
C(4C)	6085 (4)	2736 (2)	−3590 (2)	54
C(5C)	5191 (4)	3620 (2)	−3658 (2)	49
C(6C)	4529 (4)	3860 (2)	−4562 (2)	42

Atomic scattering factors were taken from *International Tables for X-ray Crystallography* (1974). Computations were carried out with *SHELX*78 (Sheldrick, 1978) and *PLUTO*78 (Motherwell & Clegg, 1978) on the Birmingham University Honeywell DPS 8/70 computer and on the CDC7600 at the University of Manchester Regional Computer Centre.

Discussion. Atomic parameters for molecules (I) and (II) are listed in Table 1, and bond lengths and selected

Table 2. *Bond lengths* (Å) *and selected bond angles* (°) *with e.s.d.'s in parentheses and selected torsion angles* (°) *for compounds* (I) *and* (II)

For torsion angles, e.s.d.'s are *ca* 0·7° in (I) and 0·5° in (II).

	(I)	(II)
Br–C(8)	1·864 (4)	1·873 (2)
Cl–C(2′)	1·734 (5)	1·741 (2)
S–C(8)	1·724 (4)	1·722 (2)
S–C(10)	1·722 (3)	1·723 (2)
N(1)–C(1)	1·365 (5)	1·381 (3)
N(1)–C(3)	1·369 (5)	1·370 (3)
N(1)–C(10)	1·404 (4)	1·410 (3)
N(2)–N(3)	1·395 (5)	1·395 (3)
N(2)–C(1)	1·292 (5)	1·301 (3)
N(3)–C(3)	1·298 (5)	1·300 (3)
N(5)–C(4)	1·477 (5)	1·469 (3)
N(5)–C(6)	1·271 (5)	1·276 (3)
C(3)–C(4)	1·486 (5)	1·483 (3)
C(6)–C(11)	1·477 (5)	1·472 (3)
C(6)–C(1′)	1·502 (5)	1·494 (3)
C(7)–C(8)	1·349 (6)	1·332 (3)
C(7)–C(11)	1·415 (5)	1·428 (3)
C(10)–C(11)	1·355 (5)	1·365 (3)
C(1′)–C(2′)	1·379 (6)	1·383 (3)
C(1′)–C(6′)	1·398 (6)	1·400 (3)
C(2′)–C(3′)	1·388 (7)	1·376 (4)
C(3′)–C(4′)	1·352 (8)	1·368 (4)
C(4′)–C(5′)	1·361 (7)	1·382 (4)
C(5′)–C(6′)	1·377 (6)	1·380 (4)
C(1)–C(1*C*)		1·490 (3)
C(1*C*)–C(2*C*)		1·530 (4)
C(1*C*)–C(6*C*)		1·517 (3)
C(2*C*)–C(3*C*)		1·517 (4)
C(3*C*)–C(4*C*)		1·517 (4)
C(4*C*)–C(5*C*)		1·507 (5)
C(5*C*)–C(6*C*)		1·513 (4)
C(10)–N(1)–C(3)	124·2 (3)	122·6 (2)
N(1)–C(3)–C(4)	120·3 (3)	121·1 (2)
C(3)–C(4)–N(5)	110·9 (3)	110·6 (2)
C(4)–N(5)–C(6)	118·0 (3)	117·1 (2)
N(5)–C(6)–C(11)	126·9 (3)	126·4 (2)
C(6)–C(11)–C(10)	124·1 (3)	123·6 (2)
C(11)–C(10)–N(1)	125·3 (3)	124·2 (2)
C(11)–C(10)–S	113·4 (3)	112·6 (2)
C(10)–S–C(8)	89·8 (2)	89·8 (1)
S–C(8)–C(7)	112·7 (3)	113·9 (2)
C(8)–C(7)–C(11)	112·9 (4)	111·9 (2)
C(7)–C(11)–C(10)	111·3 (3)	111·7 (2)
C(3)–N(1)–C(1)	104·9 (3)	104·9 (2)
N(1)–C(1)–N(2)	110·1 (4)	109·3 (2)
C(1)–N(2)–N(3)	107·7 (3)	108·3 (2)
N(2)–N(3)–C(3)	107·0 (3)	106·9 (2)
N(3)–C(3)–N(1)	110·2 (3)	110·6 (2)
C(10)–N(1)–C(3)–C(4)	−0·4	−1·2
N(1)–C(3)–C(4)–N(5)	−65·1	−66·8
C(3)–C(4)–N(5)–C(6)	69·6	67·4
C(4)–N(5)–C(6)–C(11)	−6·6	0·0
N(5)–C(6)–C(11)–C(10)	−37·3	−44·3
C(6)–C(11)–C(10)–N(1)	4·2	5·1
C(11)–C(10)–N(1)–C(3)	33·8	35·8
C(11)–C(6)–C(1′)–C(2′)	−75·0	−66·6
N(5)–C(6)–C(1′)–C(2′)	104·8	112·4

bond and torsion angles are in Table 2.* The atomic numbering scheme used in this paper is illustrated in Fig. 1.

Bond lengths and angles generally agree well with those found in brotizolam (Butcher & Hamor, 1985). The N(1)–C(3) bond is shortened from the normal single-bond value of *ca* 1·47 Å to 1·37 Å and there is a planar disposition of bonds about N(1) and C(3); thus the geometry of this bond resembles a double bond, as for benzodiazepin-2-ones (Hamor & Martin, 1983). The angle C(10)–N(1)–C(3) [124·2 (3) in (I), 122·6 (2)° in (II)] is similar to that found in N(1)–Me substituted benzodiazepines but some 3–5° smaller than the corresponding angle in N(1)–H substituted compounds (Chananont, Hamor & Martin, 1981).

The seven-membered ring is in a cycloheptatriene-like boat conformation, the other two double bonds being N(5)–C(6), 1·271 (5) Å in (I) and 1·276 (3) Å in (II) and C(10)–C(11), 1·355 (5) Å in (I) and 1·365 (3) Å in (II). The 'boat' may be described in terms of the angles between the central plane, consisting of atoms N(1), C(3), N(5), C(6) and the 'bow' and 'stern' planes, atoms C(3), C(4), N(5) and C(6), C(11), C(10), N(1), respectively. The bow and stern angles of 55·4 (8) and 29·2 (8)°, respectively in (I), and 55·3 (5) and 32·9 (5)° in (II), compare with values of 56·8 and 29·2° in brotizolam and 54 and 31° in estazolam (Kamiya, Wada & Nishikawa, 1973). The ring in these compounds is thus slightly flatter than is generally found in 1,4-benzodiazepin-2-ones, which do not have an extra ring fused across the N(1)–C(2) bond [N(1)–C(3) in the present numbering scheme], where the bow and stern angles of the seven-membered ring are in the ranges 58–64 and 32–40°, respectively (Hamor & Martin, 1983). The deviation parameter, Δ, defined in Hamor & Martin (1983), which gives a

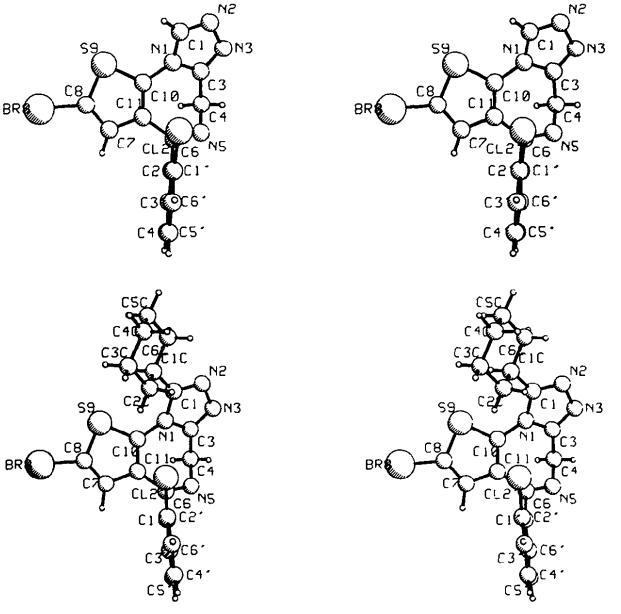


Fig. 1. Stereoscopic view of molecule (I) (upper diagram) and (II) (lower diagram) in a direction perpendicular to the mean plane of the thieno ring.

*Lists of structure factors, anisotropic thermal parameters, H-atom parameters and bond angles have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 51023 (34 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

measure of the deviation of the ring from an ideal cycloheptatriene boat with mirror symmetry, in terms of the endocyclic torsion angles, is 4·3° for (I) and 4·5° for (II). These values are typical of those found in 1,4-benzodiazepin-2-ones (Hamor & Martin, 1983) and also similar to that in brotizolam (3·0°).

The triazolo, phenyl and thieno rings are all planar to within ±0·015 Å. The phenyl ring is steeply inclined to the thieno plane, interplanar angle 88·8 (8)° in (I) and 88·3 (5)° in (II). These angles compare with values of 73–86° in 2′-chloro-substituted 1,4-benzodiazepines and 71·7° in brotizolam. Unlike the situation in the crystal structure of brotizolam, the Cl atom lies on the opposite side of the thieno plane from the bow atom, C(4) [compare Fig. 1 with Fig. 1 in Butcher & Hamor (1985)]. The orientations of the phenyl rings in compounds (I) and (II) thus correspond to that normally found in the crystal structures of 5-phenyl-1,4-benzodiazepines and triazolobenzodiazepines (Hamor & Martin, 1983). The 1-cyclohexyl substituent of compound (II) adopts a normal chair conformational, torsion angles in the range ±54·2 to ±56·8°.

We thank Dr K. H. Weber, Boehringer-Ingelheim KG, for materials, Dr I. L. Martin, Medical Research Council Centre, Cambridge, for affinity measurements and the SERC for financial support to HJK.

References

BUTCHER, H. J. & HAMOR, T. A. (1985). *Acta Cryst.* C**41**, 265–266.

CHANANONT, P., HAMOR, T. A. & MARTIN, I. L. (1981). *Acta Cryst.* B**37**, 1371–1375.

HAMOR, T. A. & MARTIN, I. L. (1983). *Progress in Medicinal Chemistry*, Vol. 20, edited by G. P. ELLIS & G. B. WEST, pp. 157–223. Amsterdam: Elsevier.

HESTER, J. B. JR, DUCHAMP, D. J. & CHIDESTER, C. G. (1971). *Tetrahedron Lett.* pp. 1609–1612.

International Tables for X-ray Crystallography (1974). Vol. IV. Birmingham: Kynoch Press. (Present distributor Kluwer Academic Publishers, Dordrecht.)

KAMIYA, K., WADA, Y. & NISHIKAWA, M. (1973). *Chem. Pharm. Bull.* **21**, 1520–1529.

MEGURO, K. & KUWADA, Y. (1970). *Tetrahedron Lett.* pp. 4039–4042.

MOTHERWELL, W. D. S. & CLEGG, W. (1978). *PLUTO*78. Program for plotting molecular and crystal structures. Univ. of Cambridge, England.

SHELDRICK, G. M. (1978). *SHELX*78. Program for crystal structure determination. Univ. of Cambridge, England.

SQUIRES, R. F. & BRAESTRUP, C. (1977). *Nature (London)*, **266**, 732–734.

WEBER, K. H., BAUER, A., LANGBEIN, A. & DANIEL, H. (1978). *Justus Liebigs Ann. Chem.* pp. 1257–1265.

Acta Cryst. (1988). C**44**, 1656–1658

9-Amino-1,2,3,4-tetrahydroacridine Hydrochloride Monohydrate (THA.HCl)

BY DAVID E. ZACHARIAS AND JENNY P. GLUSKER

The Institute for Cancer Research, The Fox Chase Cancer Center, Philadelphia, PA 19111, *USA*

(*Received* 9 *February* 1988; *accepted* 3 *May* 1988)

Abstract. $C_{13}H_{15}N_2^+.Cl^-.H_2O$, $M_r = 252{\cdot}74$, monoclinic, $P2_1/c$, $a = 8{\cdot}776$ (2), $b = 8{\cdot}514$ (1), $c = 18{\cdot}046$ (4) Å, $\beta = 107{\cdot}09$ (2)°, $V = 1288{\cdot}8$ (5) Å^3, $Z = 4$, $D_x = 1{\cdot}302$ Mg m^{-3}, λ(Cu $K\alpha$) = 1·5418 Å, $\mu = 0{\cdot}238$ mm^{-1}, $F(000) = 536$, $T = 293$ K, final $R = 0{\cdot}042$ for 2080 observed data. Atoms C2 and C3 of the reduced ring are disordered. The crystal structure has an extensive network of hydrogen bonds in which the water molecule donates its H atoms to two Cl ions and accepts the H atom from the protonated ring N atom. The amino group also donates its H atoms in hydrogen bonding to two Cl ions.

Introduction. The compound 9-amino-1,2,3,4-tetrahydroacridine hydrochloride, THA.HCl (tacrine hydrochloride), a cholinesterase inhibitor, has been of recent interest as a drug for the treatment of Alzheimer's disease, an affliction that causes a progressively increasing loss of memory and intellectual function (Coyle, Price & DeLong, 1983; Summers, Majovski, Marsh, Tachiki & Kling, 1986). Unfortunately, it causes an elevation in the amount of the enzyme transaminase in the liver, and for the present its use has been discontinued.

We report here the crystal structure of this compound and compare it to the crystal structure of the less-saturated analog 9-aminoacridine hydrochloride (9AA.HCl) (Talacki, Carrell & Glusker, 1974) which is a known mutagen.

Experimental. The compound, THA.HCl, was purchased from Aldrich Chemical Company and used directly. A crystal of dimensions 0·30 × 0·30 × 0·35 mm was used for data collection with a Syntex $P\bar{1}$

0108-2701/88/091656-03$03.00