Related literature. This structure determination was undertaken to establish the course of a reaction, which may also be used to prepare a series of analogous compounds (DuBoisson, 1986).

The authors thank the SERC for financial support with equipment.

References

BROWN, J. N. & TREFONAS, L. M. (1973). *Acta Cryst.* B29, 237–241.

CSSR (1984). *Crystal Structure Search and Retrieval Instruction Manual.* SERC Daresbury Laboratory, Warrington, England.

DUBOISSON, R. A. (1986). PhD Thesis, Univ., of Manchester, England.

FALSHAW, C. P., HASHI, N. A. & TAYLOR, G. A. (1985). *J. Chem. Soc. Perkin Trans.* 1, pp. 1837–1843.

MAIN, P., FISKE, S. J., HULL, S. E., LESSINGER, L., GERMAIN, G., DECLERCQ, J.-P. & WOOLFSON, M. M. (1980). *MULTAN*80. *A System of Computer Programs for the Automatic Solution of Crystal Structures from X-ray Difraction Data.* Univs. of York, England, and Louvain, Belgium.

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

SHELDRICK, G. M. (1976). *SHELX*76. Program for crystal structure determination. Univ. of Cambridge, England.

Acta Cryst. (1991). C47, 232–233

Structure of *N*-Methyl-2-(4-methoxyphenylthio)benzylammonium Chloride

BY BOHDAN SCHNEIDER

Pharmaceutical and Biochemical Research Institute, Kouřimská 17, 13060 *Praha* 3, *Czechoslovakia*

AND JINDŘICH HAŠEK AND JIŘÍ JEČNÝ

Institute of Macromolecular Chemistry, Czechoslovak Academy of Sciences, Heyrovského nám 2, 16206 *Praha* 6, *Czechoslovakia*

(*Received* 8 *March* 1990; *accepted* 27 *June* 1990)

Abstract. $C_{15}H_{18}NOS^+.Cl^-$, $M_r = 295{\cdot}8$, orthorhombic, $P2_12_12_1$, $a = 5{\cdot}167$ (1), $b = 10{\cdot}748$ (4), $c = 27{\cdot}278$ (8) Å, $V = 1515{\cdot}0$ (9) Å^3, $Z = 4$, $D_x = 1{\cdot}297$ Mg m^{-3}, Cu $K\alpha$ radiation ($\lambda = 1{\cdot}5418$ Å), $\mu = 3{\cdot}456$ mm^{-1}, $F(000) = 624$, $T = 295$ K, $R = 0{\cdot}065$, $wR = 0{\cdot}085$ for 1440 observed reflections. The dihedral angle between the phenyl rings is 100·9 (2)°. Strong intermolecular contacts N9—H92···Cl [N9···Cl 3·141 (5) Å, N9—H92···Cl 147 (6)°] and N9—H91···Cl^i [N9···Cl^i 3·079 (5) Å, N9—H91···Cl^i 154 (6)° where i is the equivalent position $x - 1$, y, z] join ammonium cations and chloride anions into chains parallel to the a axis. The methyl group attached to N9 is not in the generally preferred *anti* conformation but is approximately *gauche* [C7—C8—N9—C10 −82·4 (6)°]. The C8 atom lies in the mean plane of the first phenyl ring [deviation 0·004 (5) Å] and the atoms O15, C16 lie near the mean plane of the second phenyl ring [deviations: 0·046 (5) and 0·019 (7) Å]. The atom S1 deviates by −0·106 (2) Å from the first and by 0·172 (2) Å from the second plane.

Experimental. Colorless, needle-shaped and extremely fragile crystals were grown from an ethanol–heptane solution (9:1) by slow evaporation at room temperature. Crystal dimensions 0·40 × 0·17 × 0·14 mm, Syntex $P2_1$ diffractometer, graphite-monochromated Cu $K\alpha$ radiation. Cell constants by least squares using 21 reflections with $9 \le 2\theta \le 26°$. Cell dimensions and space group $P2_12_12_1$ independently determined also by Weissenberg and oscillation techniques. Only 1546 unique reflections collected using $\theta/2\theta$ scans, 1440 with $F \ge 3{\cdot}92\sigma(F)$, $0 \le 2\theta \le 132°$, $0 \le h \le 6$; $0 \le k \le 12$; $0 \le l \le 32$. No absorption corrections applied ($\mu r = 0{\cdot}82$). No significant variation in three standard reflections (200, 016, 008 measured after every 40 reflections) were observed.

The structure was solved by direct methods using *SHELXS*86 (Sheldrick, 1986) and refined with *SHELX*76 (Sheldrick, 1976). An isotropic refinement based on $|F|$ with all non-H atoms gave $R = 0{\cdot}15$. H atoms were refined to reasonable positions without any constraints ($R = 0{\cdot}135$). However, H91 and H92 required fixed temperature factors $U = 0{\cdot}1$ Å^2 (Table 1). Anisotropic refinement of non-H atoms and isotropic refinement of H atoms (243 variables) converged at $R = 0{\cdot}065$, $wR = 0{\cdot}064$ and $S = 2{\cdot}4$ using 1440 F's with $F \ge 3{\cdot}92\sigma(F)$ (and at $R = 0{\cdot}069$, $wR = 0{\cdot}064$ for all unique reflections), $w^{-1} = \sigma^2(F) + 0{\cdot}0009F^2$, $(\Delta/\sigma)_{max} = 0{\cdot}18$. The maximum and minimum peaks in the final difference map were 0·35, −0·85 e Å^{-3}. Atomic scattering factors were taken

0108-2701/91/010232-02$03.00

Table 1. *Fractional atomic coordinates* ($\times 10^4$) *and equivalent isotropic temperature factors for non-*H *atoms* ($Å^2 \times 10^3$) *with e.s.d.'s in parentheses*

$U_{eq} = (1/3)\sum_i \sum_j U_{ij} a_i^* a_j^* \mathbf{a}_i.\mathbf{a}_j.$

	x	y	z	U_{eq}
S1	182 (3)	7544 (1)	8827 (1)	67 (1)
Cl	4386 (3)	7426 (1)	7493 (1)	71 (1)
C2	1641 (11)	9045 (4)	8805 (2)	49 (1)
C3	3674 (13)	9386 (5)	9110 (2)	56 (2)
C4	4651 (13)	10588 (5)	9098 (2)	59 (2)
C5	3578 (15)	11461 (5)	8782 (3)	65 (2)
C6	1542 (13)	11111 (5)	8477 (2)	56 (2)
C7	566 (10)	9909 (4)	8481 (2)	46 (1)
C8	−1645 (11)	9564 (5)	8145 (2)	50 (1)
N9	−687 (9)	8963 (4)	7682 (1)	50 (1)
C10	184 (18)	9856 (6)	7299 (2)	74 (2)
C11	2582 (11)	6569 (5)	9093 (2)	55 (1)
C12	2638 (13)	6381 (5)	9607 (2)	59 (2)
C13	4330 (14)	5546 (5)	9803 (2)	60 (2)
C14	6020 (12)	4859 (4)	9506 (2)	54 (2)
O15	7559 (10)	4021 (4)	9738 (1)	72 (1)
C16	9357 (16)	3324 (6)	9460 (3)	77 (2)
C17	5979 (13)	5045 (5)	9001 (2)	57 (2)
C18	4283 (13)	5905 (5)	8806 (2)	57 (2)

Table 2. *Selected bond lengths* (Å), *bond angles and torsion angles* (°) *of N-methyl-2-(4-methoxyphenylthio)benzylammonium chloride*

S1—C2	1·782 (5)	N9—H91	1·08 (8)
S1—C11	1·778 (6)	N9—H92	0·93 (9)
C7—C8	1·511 (7)	C14—O15	1·358 (7)
C8—N9	1·502 (6)	O15—C16	1·414 (9)
N9—C10	1·488 (8)		

C2—S1—C11	104·6 (3)	C2—C7—C8	121·4 (4)
S1—C2—C3	122·6 (4)	C7—C8—N9	111·5 (4)
S1—C2—C7	117·1 (4)	C8—N9—C10	114·3 (4)
S1—C11—C12	120·1 (4)	C8—N9—H91	111 (5)
S1—C11—C18	121·1 (4)	C8—N9—H92	112 (4)
C3—C2—C7	120·3 (5)	C13—C14—C17	119·1 (5)
C12—C11—C18	118·5 (5)	C13—C14—O15	116·4 (4)
C2—C7—C6	118·6 (5)	C14—O15—C16	119·1 (5)

C11—S1—C2—C3	−22·7 (5)	C2—C7—C8—N9	−84·5 (6)
C11—S1—C2—C7	160·5 (4)	C7—C8—N9—C10	−82·4 (6)
C2—S1—C11—C12	91·9 (5)	C7—C8—N9—H91	160 (5)
C2—S1—C11—C18	−93·4 (5)	C7—C8—N9—H92	56 (6)
S1—C2—C3—C4	−176·4 (4)	C12—C13—C14—O15	−177·7 (5)
S1—C2—C7—C6	175·8 (4)	C13—C14—O15—C16	−178·3 (6)
S1—C2—C7—C8	−3·2 (6)	C14—O15—C16—H161	−165 (4)
S1—C11—C12—C13	174·0 (5)	S1—C11—C18—C17	−173·1 (5)

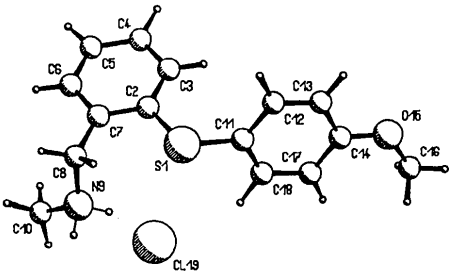

Fig. 1. Perspective view of a single molecule of *N*-methyl-2-(4-methoxyphenylthio)benzylammonium chloride with the labelling scheme.

from *International Tables for X-ray Crystallography* (1974, Vol. IV).

The final fractional coordinates and equivalent isotropic temperature factors are listed in Table 1.* The *PLUTO* (Motherwell, 1978) drawing of a single molecule of the title compound is depicted in Fig. 1. Intra- and intermolecular geometrical parameters were computed by the program *PARST* (Nardelli, 1983). Selected bond lengths, angles and torsion angles are listed in Table 2.

Related literature. The title compound is a selective inhibitor of the serotonine re-uptake in comparison with the noradrenaline re-uptake. It belongs to the 'second generation antidepressants' (Enna & Eison, 1987) which have a more specific mechanism of action and less side effects compared with the older tricyclic antidepressants. Most second generation antidepressants influence serotonergic nerve functions whereas noradrenaline functions are not affected.

Potentially antidepressive properties were recently found in a group of aminoalkyldiphenyl sulfides (Jílek *et al.*, 1989). They show a high affinity to both imipramine and desipramine binding sites in the rat brain and inhibit the re-uptake of 5-hydroxytryptamine as well as of noradrenaline in the rat brain structures. A few, however, are specific for the uptake inhibition of a single amine only. A discussion of the structural behaviour of aminoalkyldiphenyl sulfides found in the Cambridge Structural Database (Allen *et al.*, 1979) can be found in Schneider, Rejholec & Kuchař (1990).

* Lists of structure factors, anisotropic thermal parameters, a stereo packing diagram and H-atom parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 53339 (12 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

References

ALLEN, F. H., BELLARD, S., BRICE, M. D., CARTWRIGHT, B. A., DOUBLEDAY, A., HIGGS, H., HUMMELINK, T., HUMMELILNK-PETERS, B. G., KENNARD, O., MOTHERWELL, W. D. S., RODGERS, J. R. & WATSON, D. G. (1979). *Acta Cryst.* B**35**, 2331–2339.

ENNA, S. J. & EISON, M. S. (1987). *Handb. Psychopharmacol.* **19**, 609–631.

JÍLEK, J., ŠINDELÁŘ, K., POMYKÁČEK, J., KMONÍČEK, V., ŠEDIVÝ, Z., HRUBANTOVÁ, M., HOLUBEK, J., SVÁTEK, E., RYSKA, M., KORUNA, I., VALCHÁŘ, M., DLABAČ, A., METYŠOVÁ, J., DLOHOŽKOVÁ. N. & PROTIVA, M. (1989). *Collect. Czech. Chem. Commun.* **54**, 3294–3338.

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

NARDELLI, M. (1983). *Comput. Chem.* **7**, 95–98.

SCHNEIDER, B., REJHOLEC, V. & KUCHAŘ, M. (1990). *Collect. Czech. Chem. Commun.* Submitted.

SHELDRICK, G. M. (1976). *SHELX*76. Program for crystal structure determination. Univ. of Cambridge, England.

SHELDRICK, G. M. (1986). *SHELXS*86. Program for the solution of crystal structures. Univ. of Cambridge, England.