Table 2. *Bond distances* (Å), *angles* (°), *least-squares planes and dihedral angles* (°)

1	2	3	1–2	1–2–3
O(1)	C(1)	C(4)	1·435 (3)	109·2 (2)
C(21)	C(1)	O(1)	1·521 (3)	111·5 (2)
C(4)	C(1)	C(21)		112·2 (2)
C(2)	O(1)	C(1)	1·370 (3)	117·5 (2)
C(31)	C(3)	C(2)	1·485 (4)	122·6 (2)
C(31)	C(3)	C(41)		119·0 (2)

1	2	3	1–2	1–2–3
C(11)	C(1)	O(1)	1·526 (3)	106·4 (2)
C(4)	C(1)	C(11)	1·525 (5)	105·1 (2)
C(11)	C(1)	C(21)		112·2 (2)
C(3)	C(2)	O(1)	1·328 (4)	121·6 (2)
C(41)	C(3)	C(2)	1·485 (3)	118·4 (2)
O(2)	C(4)	C(1)	1·190 (3)	124·2 (3)

No.	Plane through atoms	Equation of the plane (x along **a**; y in plane ab; z along **c***)	χ^2
1	C(11), C(12), C(13), C(14), C(15), C(16)	$0{\cdot}758x - 0{\cdot}502y - 0{\cdot}417z = -3{\cdot}653$ Å	10
2	C(21), C(22), C(23), C(24), C(25), C(26)	$-0{\cdot}486x + 0{\cdot}139y - 0{\cdot}863z = 6{\cdot}007$ Å	2
3	C(31), C(32), C(33), C(34), C(35), C(36)	$0{\cdot}240x + 0{\cdot}043y - 0{\cdot}970z = 3{\cdot}634$ Å	80
4	C(41), C(42), C(43), C(44), C(45), C(46)	$-0{\cdot}950x - 0{\cdot}306y - 0{\cdot}066z = 10{\cdot}095$ Å	37
5	C(2), C(3), C(31), C(41)	$0{\cdot}891x - 0{\cdot}183y - 0{\cdot}415z = -5{\cdot}517$ Å	1

Dihedral angles: 1,2: 94·5°; 1,3: 55·6°; 1,4: 122·6°; 1,5: 19·9°; 2,3: 43·4°; 2,4: 61·5°; 2,5: 95·8°; 3,4: 100·2°; 3,5: 52·5°; 4,5: 139·7°; ($\sigma \sim 0{\cdot}2°$).

The C–C bond lengths and C–C–C angles in the phenyl groups range from 1·348 (5) to 1·390 (3) Å [mean: 1·374 (4) Å] and from 117·7 (2) to 121·6 (4)° [mean: 120·0 (3)°].

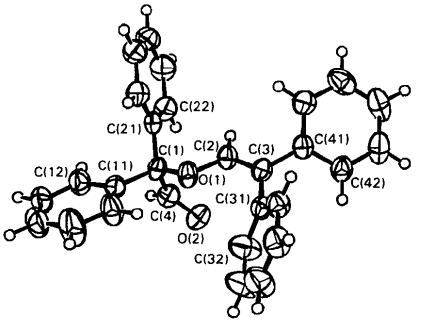

Fig. 1. General view of the molecule.

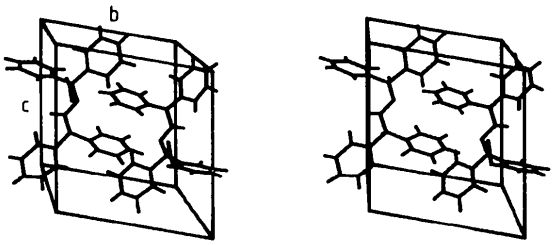

Fig. 2. Stereoscopic view of the unit cell.

atoms;* Table 2 lists bond distances and angles. Fig. 1 shows a general view of the molecule (*ORTEP*II) and Fig. 2 a stereoscopic view of the unit cell (*POP*1).

* Lists of H-atom coordinates, anisotropic thermal parameters, a complete list of bond distances and angles, and structure-factor amplitudes have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 43387 (35 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

References

FRENZ, B. A. (1981). *Enraf–Nonius Structure Determination Package,* 4th ed. Version 18. Enraf–Nonius, Delft, The Netherlands.

International Tables for X-ray Crystallography (1974). Vol. IV, Tables 2.2B and 2.3.1. Birmingham: Kynoch Press. (Present distributor D. Reidel, Dordrecht.)

JOHNSON, C. K. (1976). *ORTEP*II. Report ORNL-5138. Oak Ridge National Laboratory, Tennessee.

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 Diffraction Data.* Univs. of York, England, and Louvain, Belgium.

NEUMANN, W. P. & STAPEL, R. (1986). *Chem. Ber.* **119**, 3422–3431.

WAAL, B. W. VAN DE (1976). *POP*1. *Plot of Packing Program.* Twente Univ. of Technology, The Netherlands.

Acta Cryst. (1987). C**43**, 375–376

Structure of *S*-Benzyl-L-cysteine Methyl Ester Hydrochloride

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Abstract. $C_{11}H_{16}NO_2S^+.Cl^-$, $M_r = 261{\cdot}7$, monoclinic, $P2_1$, $a = 15{\cdot}327$ (11), $b = 8{\cdot}741$ (3), $c = 5{\cdot}211$ (2) Å, $\beta = 100{\cdot}01$ (5)°, $V = 687{\cdot}5$ (6) Å^3, $Z = 2$, $D_x = 1{\cdot}26$ g cm^{-3}, $F(000) = 276$, λ(Mo $K\alpha$) = 0·7107 Å, $\mu = 4{\cdot}12$ cm^{-1}, room temperature, $R = 0{\cdot}0374$ for 977 unique reflections. Cl^- ions link the organic cations

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Table 1. *Atomic positional* ($\times 10^4$) *and equivalent isotropic thermal parameters* (Å^2)

$B_{eq} = \frac{4}{3}\sum_i\sum_j \beta_{ij}\mathbf{a}_i.\mathbf{a}_j$.

	x	y	z	B_{eq}
Cl(1)	540 (1)	0	11493 (2)	4·39
N(2)	126 (3)	6614 (6)	3739 (8)	3·60
S(3)	2610 (1)	7427 (2)	7794 (3)	5·76
O(4)	1977 (2)	4812 (5)	2391 (7)	5·42
O(5)	1141 (3)	3872 (4)	5073 (9)	6·02
C(6)	2310 (5)	3283 (8)	2006 (17)	7·89
C(7)	1404 (3)	4929 (6)	3966 (8)	3·86
C(8)	1112 (3)	6567 (5)	4230 (9)	3·48
C(9)	1425 (3)	7175 (6)	6994 (8)	4·31
C(10)	2731 (4)	9187 (11)	6029 (18)	9·51
C(11)	3660 (4)	9719 (7)	6644 (11)	5·61
C(12)	3989 (6)	10672 (11)	8706 (17)	9·36
C(13)	4930 (7)	11128 (11)	9123 (18)	9·68
C(14)	5415 (6)	10495 (10)	7587 (21)	9·24
C(15)	5131 (7)	9596 (17)	5690 (21)	11·67
C(16)	4253 (6)	9202 (12)	5219 (16)	8·72

Table 2. *Selected bond distances* (Å) *and bond angles* (°)

N(2)–H(2*A*)	0·921 (5)	H(2*B*)–N(2)–H(2*A*)	102·8 (41)
N(2)–H(2*B*)	0·917 (62)	H(2*C*)–N(2)–H(2*A*)	103·4 (41)
N(2)–H(2*C*)	0·904 (69)	H(2*C*)–N(2)–H(2*B*)	117·6 (45)
N(2)–C(8)	1·489 (6)	C(8)–N(2)–H(2*A*)	113·3 (24)
O(4)–C(6)	1·457 (8)	C(8)–N(2)–H(2*B*)	111·2 (31)
O(4)–C(7)	1·306 (5)	C(8)–N(2)–H(2*C*)	108·4 (31)
O(5)–C(7)	1·196 (6)	C(9)–S(3)–C(10)	100·0 (3)
S(3)–C(9)	1·805 (4)		
S(3)–C(10)	1·818 (7)		

Hydrogen-bonding distances (Å)		Symmetry codes
Cl(1^{i})···H(2*A*)	2·166 (48)	(i) $-x, \frac{1}{2}+y, 1-z$
Cl(1^{ii})···H(2*B*)	2·271 (65)	(ii) $-x, \frac{1}{2}+y, 2-z$
O(5^{iii})···H(2*C*)	2·239 (71)	(iii) $-x, \frac{1}{2}+y, 1-z$

along **c** by means of two $Cl^-\cdots H{-}N^+$ hydrogen bonds [Cl···H 2·17 (5) and 2·27 (7) Å]. The third H atom linked to N participates in a hydrogen bond with the carbonyl O atom of a neighbouring cation [NH···O 2·24 (7) Å]. Bond lengths in the phenyl ring range from 1·279 (14) to 1·475 (13) Å, associated with high [maximum $U_{ii} = 0{\cdot}184$ (13) Å^2] atomic thermal parameters. Other bond lengths and bond angles are normal.

Experimental. Colourless elongated plate, 0·08 × 0·25 × 0·40 mm, Syntex $P2_1$ diffractometer, graphite-monochromated Mo $K\alpha$ radiation, lattice parameters from least-squares refinement of 25 reflections with $2\theta < 30°$, data collected to $2\theta = 47°$ with $\omega/2\theta$ scans, one standard reflection measured every 50 without significant deviation from its mean intensity, index range $-17 \le h \le 16$, $0 \le k \le 9$, $0 \le l \le 5$. 1093 unique reflections measured of which 977 with $I > 2{\cdot}5\sigma(I)$ used in refinement. No absorption correction applied.

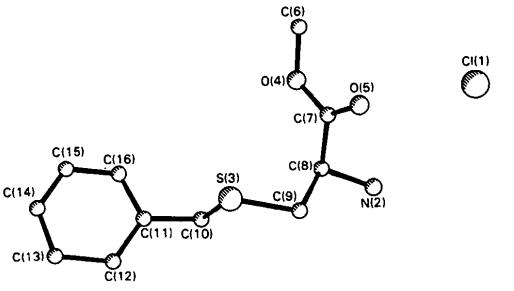

Fig. 1. View of the molecule showing the atom numbering.

Final $R = 0{\cdot}0374$, $wR = 0{\cdot}0394$, $\sum w(\Delta F)^2$ minimized, $w = 2{\cdot}3249/[\sigma^2(F) + 0{\cdot}000407F^2]$, max. $\Delta/\sigma < 0{\cdot}02$, max. and min. electron densities in final difference map 0·18, −0·12 e Å^{-3}. Structure solved by direct methods and refined by full-matrix least-squares techniques. All non-H atoms refined with anisotropic thermal parameters. H atoms constrained to idealized positions except those linked to N, which was located on difference map and refined isotropically. Computer programs used: *MULTAN*11/84 (Main, Germain & Woolfson, 1984), *SHELX* (Sheldrick, 1976), and *PLUTO* (Motherwell & Clegg, 1978), atomic scattering factors from *SHELX*. Atomic coordinates and equivalent isotropic temperature factors are given in Table 1.* Selected bond distances and bond angles are in Table 2. A view of the molecule is given in Fig. 1.

Related literature. For the preparation, properties and uses of the title compound see Maclaren, Savige & Swan (1958) and Boissonnas, Guttmann, Jaquenoud & Waller (1955). The title compound is an intermediate in the synthesis of oxytocin and somatostatin analogues.

*Lists of structure factors, anisotropic thermal parameters, H-atom parameters and complete bond length and angle data have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 43380 (7 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

References

BOISSONNAS, R. A., GUTTMANN, S., JAQUENOUD, P. A. & WALLER, J. P. (1955). *Helv. Chim. Acta*, **38**, 1491–1501.

MACLAREN, J. A., SAVIGE, W. E. & SWAN, J. M. (1958). *Aust. J. Chem.* **11**, 345–359.

MAIN, P., GERMAIN, G. & WOOLFSON, M. M. (1984). *MULTAN*11/84. *A System of Computer Programs for the Automatic Solution of Crystal Structures from X-ray Diffraction 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.