Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2-Amino-5-(4-methoxybenzyl)-4-methyl-1,3-thiazolium chloride

Daniel E. Lynch[a]* and Ian McClenaghan[b]†

[a]School of Natural and Environmental Sciences, Coventry University, Coventry CV1 5FB, England, and [b]Spa Contract Synthesis, School of Natural and Environmental Sciences, Coventry University, Coventry CV1 5FB, England

† E-mail: 106355.1670@CompuServe.com.

Correspondence e-mail: apx106@coventry.ac.uk

Received 31 October 2000
Accepted 14 November 2000
Online 1 December 2000

The structure of the title compound, $C_{12}H_{15}ClN_2OS$, (I), comprises a twisted thiazolium base that associates to a free Cl ion *via* N—H···Cl hydrogen-bonding interactions. The dihedral angle between the two ring systems is 79.65 (7)°.

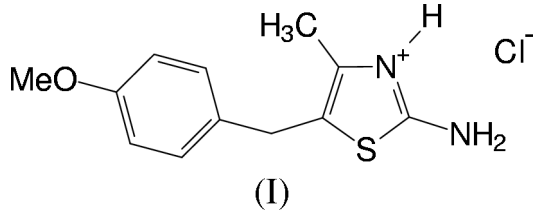
Key indicators

Single-crystal X-ray study
T = 151 K
Mean σ(C–C) = 0.003 Å
R factor = 0.050
wR factor = 0.136
Data-to-parameter ratio = 16.6

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Experimental

The title compound, (I), was prepared by Spa Contract Synthesis. Crystals of (I) were grown from a dimethylformamide solution.



(I)

Crystal data

$C_{12}H_{15}ClN_2OS$
M_r = 270.77
Monoclinic, $P2_1/n$
a = 7.5746 (15) Å
b = 11.878 (2) Å
c = 14.519 (3) Å
β = 100.47 (3)°
V = 1284.6 (4) Å^3
Z = 4
D_x = 1.400 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 10172 reflections
θ = 1.0–27.5°
μ = 0.45 mm^{-1}
T = 150 (2) K
Needle, colourless
0.20 × 0.08 × 0.06 mm

Data collection

Enraf–Nonius KappaCCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SORTAV*; Blessing, 1995)
T_{min} = 0.916, T_{max} = 0.974
6971 measured reflections
2796 independent reflections
2125 reflections with $I > 2\sigma(I)$
R_{int} = 0.073
θ_{max} = 27.5°
$h = -9 \rightarrow 9$
$k = -14 \rightarrow 15$
$l = -18 \rightarrow 18$
Intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.136
S = 1.01
2796 reflections
168 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0691P)^2 + 0.1620P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.40 e Å^{-3}
$\Delta\rho_{min}$ = −0.55 e Å^{-3}

Table 1
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3···Cl1^{i}	0.84 (3)	2.33 (3)	3.155 (2)	167 (3)
N21—H21···Cl1^{ii}	0.85 (3)	2.40 (3)	3.162 (2)	150 (2)
N21—H22···Cl1^{iii}	0.91 (3)	2.30 (3)	3.193 (2)	168 (3)

Symmetry codes: (i) $-\frac{1}{2}-x, y-\frac{1}{2}, \frac{3}{2}-z$; (ii) $x-\frac{1}{2}, \frac{1}{2}-y, z-\frac{1}{2}$; (iii) $\frac{1}{2}-x, y-\frac{1}{2}, \frac{3}{2}-z$.

All H atoms were included in the refinement, at calculated positions, as riding models with C—H set to 0.95 (Ar–H), 0.98 (CH_3) and 0.99 Å (CH_2), except for the H atoms involved in the hydrogen-bonding interactions which were located on difference syntheses and both positional and displacement parameters refined.

Data collection: *DENZO* (Otwinowski & Minor, 1997) and *COLLECT* (Hooft, 1998); cell refinement: *DENZO* and *COLLECT*; data reduction: *DENZO*and *COLLECT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); software used to prepare material for publication: *SHELXL*97.

The authors thank the EPSRC National Crystallography Service (Southampton).

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