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(4*RS*,6*SR*)-2-Amino-6-phenyl-4-*p*-tolyl-5,6-dihydro-4*H*-1,3-thiazin-3-ium chloride

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Key indicators

Single-crystal X-ray study
T = 173 K
Mean σ(C–C) = 0.004 Å
R factor = 0.044
wR factor = 0.119
Data-to-parameter ratio = 18.3

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

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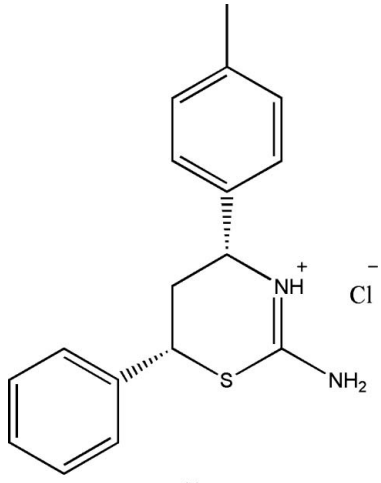
The title compound, $C_{17}H_{19}N_2S^+\cdot Cl^-$, is a 5,6-dihydro-4*H*-1,3-thiazine derivative in which two benzene rings replace H atoms at positions 4 and 6 of the central ring, which adopts a slightly twisted half-chair conformation at 173 K. The crystal structure is stabilized by weak intermolecular N—H···Cl hydrogen bonds.

Comment

Multicomponent reactions (MCRs) are now playing an increasingly important role in research in both organic and medicinal fields (Kappe, 2000). As one of the products obtained from the three-component reactions we are studying (Zhu *et al.*, 2006), thiazine derivatives also attract great interest of chemists for their biological activities (Kieć-Kononowicz *et al.*, 2001; Bózsing *et al.*, 1996). In addition, in terms of organic syntheis, thiazine and its derivatives are important intermediates for the synthesis of more functionalized compounds.



(I)

Fig. 1 shows the asymmetric unit of the title compound, (I). At the centre of the cation, the thiazine ring adopts a slightly twisted half-chair conformation. Identical C4—N1 and C4—N2 bond distances (Table 1) imply that the electron distribution between N1/C4/N2 is symmetrical. The torsion angles listed in Table 1 place C1 and C2 on opposite sides of the mean plane through S1/C4/N1/C3, with C2 slightly further from this plane than C1. Two chiral centers are found in the cation (C3 and C1); the relative configurations are 4*R* at C3 and 6*S* at C1, according to the crystal structure.

The H atoms at both N1 and N2 take part in intermolecular hydrogen bonds (Table 2). The crystal packing illustrates that the crystal structure is stabilized mainly by a network of intermolecular N—H···Cl hydrogen bonds.

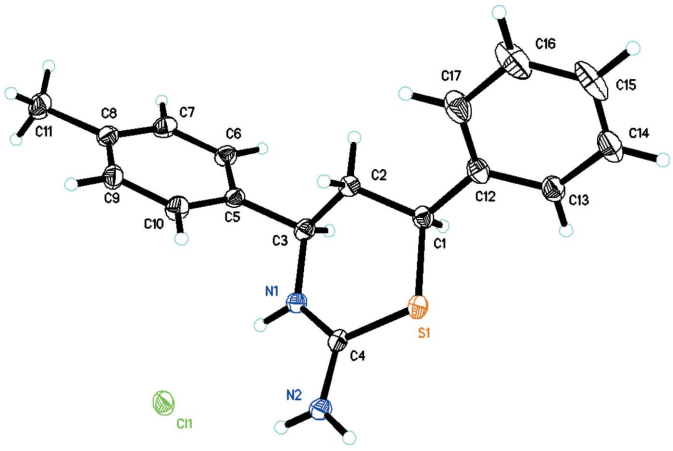


Figure 1
The asymmetric unit of the title compound, showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level.

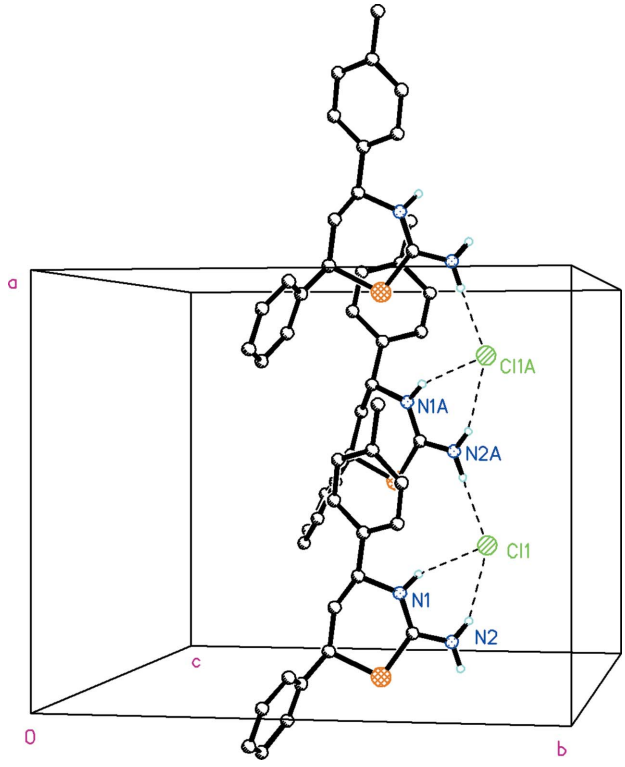


Figure 2
The packing diagram, with intermolecular N—H···Cl hydrogen-bond interactions indicated by dashed lines. For clarity, H atoms bonded to C atoms have been omitted.

Experimental

The title compound was synthesized from a three-component one-pot reaction involving benzaldehyde, styrene and thiourea. Details of the synthesis and purification of the compound are described elsewhere (Zhu *et al.* 2006). Suitable crystals were obtained by slow evaporation of an ethanol solution at room temperature over a period of a week.

Crystal data

$C_{17}H_{19}N_2S^+\cdot Cl^-$
M_r = 318.85
Orthorhombic, *Pbca*
a = 12.0026 (15) Å
b = 14.5838 (17) Å
c = 18.364 (2) Å
V = 3214.4 (7) Å^3
Z = 8
D_x = 1.318 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.36 mm^{-1}
T = 173 (2) K
Block, colorless
0.48 × 0.43 × 0.37 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.845, T_{max} = 0.878
16907 measured reflections
3502 independent reflections
2344 reflections with $I > 2\sigma(I)$
R_{int} = 0.053
θ_{max} = 27.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.120
S = 1.04
3502 reflections
191 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0529P)^2 + 1.9742P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.46 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

C1—C2	1.507 (3)	C4—N2	1.315 (3)
C1—S1	1.831 (2)	C4—N1	1.316 (3)
C2—C3	1.518 (3)	C4—S1	1.737 (2)
C3—N1	1.471 (3)		
C2—C1—S1	109.74 (17)	C5—C3—C2	111.09 (19)
C1—C2—C3	112.9 (2)	N1—C4—S1	124.41 (18)
N1—C3—C5	109.49 (19)	C4—N1—C3	128.0 (2)
N1—C3—C2	110.73 (19)	C4—S1—C1	101.76 (11)
S1—C4—N1—C3	0.4 (3)	N1—C4—S1—C1	−7.2 (2)
C2—C3—N1—C4	−23.1 (3)	C2—C1—S1—C4	37.38 (19)

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1*A*···Cl1	0.88	2.36	3.169 (2)	154
N2—H2*C*···Cl1	0.88	2.47	3.241 (2)	147
N2—H2*D*···Cl1^{i}	0.88	2.29	3.164 (2)	176

Symmetry code: (i) $x+\frac{1}{2}, y, -z+\frac{3}{2}$.

H atoms bonded to N atoms were located in difference Fourier maps, and then idealized and refined as riding, with N—H = 0.88 Å. The positions of the C-bound H atoms were calculated geometrically and refined using a riding model (C—H = 0.93–0.98 Å). U_{iso}(H) = 1.5U_{eq}(C) for methyl atoms and U_{iso}(H) = 1.2U_{eq}(C,N) for all other H atoms.

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2002); software used to prepare material for publication: *SHELXTL*.

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