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

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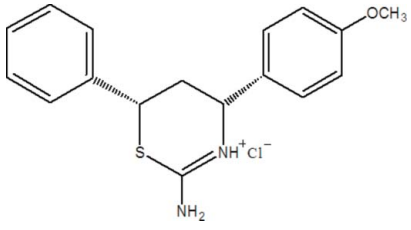
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.004 Å; R factor = 0.056; wR factor = 0.167; data-to-parameter ratio = 17.6.

The title compound, $C_{17}H_{19}N_2OS^+\cdot Cl^-$, was synthesized through a diastereoselective three-component condensation in one pot. The six-membered heterocycle adopts a half-chair conformation which is slightly twisted at 298 K. The cations and the Cl^- anions of the structure are connected through a two-dimensional network of N—H···Cl and C—H···Cl hydrogen bonds. Phenyl rings intercalate between layers, and no $\pi\cdots\pi$ stacking is observed in the structure.

Related literature

For syntheses of related structures, see: Barluenga *et al.* (1991); Sreekumar *et al.* (1997). For pharmacological activities and biological characteristics, see: Bourzat *et al.* (1991); Suárez *et al.* (2006). For related novel compounds and structures, see: Wan *et al.* (2006); Zhu *et al.* (2006).



Experimental

Crystal data

$C_{17}H_{19}N_2OS^+\cdot Cl^-$
M_r = 334.85
Monoclinic, $P2_1/n$
a = 8.4686 (11) Å
b = 18.341 (2) Å
c = 11.1313 (14) Å
β = 102.971 (2)°
V = 1684.8 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.35 mm^{-1}
T = 298 (2) K
0.30 × 0.20 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: none
10217 measured reflections
3673 independent reflections
2879 reflections with $I > 2\sigma(I)$
R_{int} = 0.083

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.056
$wR(F^2)$ = 0.167
S = 1.07
3673 reflections
209 parameters
18 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.56 e Å^{-3}
$\Delta\rho_{min}$ = −0.31 e Å^{-3}

Table 1
Selected torsion angles (°).

S1—C11—N1—C8	2.4 (3)	N1—C11—S1—C10	−8.4 (2)
C9—C8—N1—C11	−25.2 (3)	C9—C10—S1—C11	38.43 (19)

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

D—H···A	D—H	H···A	D···A	D—H···A
C10—H10···Cl1^{i}	0.98	2.80	3.555 (2)	135
N2—H2C···Cl1^{ii}	0.84 (4)	2.38 (4)	3.219 (3)	175 (3)
N1—H1A···Cl1	0.89 (3)	2.38 (3)	3.212 (2)	155 (3)
N2—H2D···Cl1	0.87 (3)	2.50 (3)	3.295 (2)	153 (3)

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

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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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SI2026).

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supplementary materials

Acta Cryst. (2007). E**63**, o3842 [**doi:10.1107/S1600536807033107**]

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

L. Lin, J.-P. Wan and C.-R. Sun

Comment

Sulfur-containing heterocyclic compounds represent a type of valuable structure in the heterocycle family. Thiazine is one of the typical heterocyclic structures of this family with multifunctional characters. Among this class of compounds, 1,3-thiazines are of special importance due to their pharmacological activities (Bourzat *et al.*, 1991) and biological characters (Suárez *et al.*, 2006). Presently, there are sevral methodologies developed for synthesizing certain types of 1,3-thiazine derivatives (Barluenga *et al.*, 1991; Sreekumar *et al.*, 1997). We have recently reported a novel three-component approach of building up the 5,6-dihydro-4*H*-[1,3] thiazine compounds, which starts from aromatic aldehydes, thiourea and styrene with the catalysis of TMSCl (Zhu *et al.*, 2006), as well as a crystal structure of this type (Wan *et al.*, 2006). As a continuous exploration of this novel reaction, we report here the crystal structure of the title compound, a product afforded by the aforementioned diastereoselective three-component condensation (Scheme 1).

The crystal structure analysis shows that the product presents a central heterocycle of 5,6-dihydro-4*H*-[1,3]thiazin rather than the isomer tetrahydropyrimidine-2(1*H*)-thione which may give indistinguishable spectral data with the obtained product. From the crystal structure (Figure 1) of the title compound, the core six-member ring 5,6-dihydro-4*H*-[1,3] thiazin adopts a slightly twisted half-chair conformation.

The general identical bond distances of C11—N1 and C11—N2 [1.314 (3)Å and 1.316 (3) Å, respectively] shows that the bond between C11 and N1 is not a normal C═N double bond, instead, the electron cloud symmetrically distributes between N1, C11 and N2. The total value of bond angles N1—C11—S1, N1—C11—N2 and N2—C11—S1 is 359.94°, which implies that N1, C11, N2, S1 locate in the same plane with a normal deviation of 0.06°. From the 2.4 (3)° torsion angles of S1—N1—C11—C8 and −8.4 (2)° of N1—C11—S1—C10, atoms C8 and C10 (Table 1) are found to be placed in the opposite sides of the plane through $N1_{S1}C11$, which also describes the twisted half-chair conformation of this heterocycle. The crystal is mainly stablized by the intermolecular N—H···Cl hydrogen bond, the H atoms at N1 and N2 are involved in the hydrogen bond network and form the crystal packing (Figure 2). Parameters of hydrogen bonds are given in Table 2.

Experimental

4-Methoxylbenzaldehyde (5 mmol), styrene (5 mmol) and thiourea (6 mmol) were located in a flask and 5 mmol TMSCl was added, the mixture was then refluxed and stirred in CH_3CN/DMF (3 mL/1.5 mL) for 10 h. The product deposited directly after completion of the reaction and cooling down to room temperature. The solide was filtered and the analytical pure product was afforded by recystalization of the crude product in ethanol. The proper colorless crystal for the X-ray measurement was obtained through slow evaporation of an ethanol solution.

Refinement

H atoms bonded N atoms were located in difference Fourier maps and their parameters were refined with N—H distances restrained to 0.86 (1) Å. The position of the C-bound H atoms were calculated geometrically and refined using a riding model(C—H=0.93–0.98 Å) with U_{iso}(H) = 1.2U_{eq}(C).

Figures

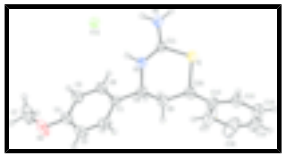

Fig. 1. Molecular structure of the title compound, showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level.

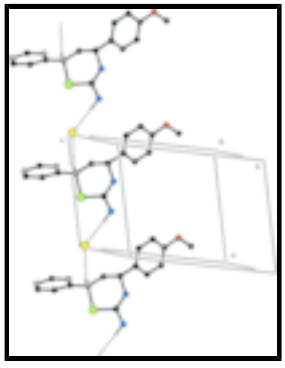

Fig. 2. Selected N—H···Cl and C—H···Cl intermolecular hydrogen bonding interactions along the **a**-axis, indicated as dashed lines.

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

Crystal data

$C_{17}H_{19}N_2OS^+\cdot Cl^-$	F_{000} = 704
M_r = 334.85	D_x = 1.320 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 3831 reflections
a = 8.4686 (11) Å	θ = 2.2–28.0º
b = 18.341 (2) Å	μ = 0.35 mm^{-1}
c = 11.1313 (14) Å	T = 298 (2) K
β = 102.971 (2)º	Block, colourless
V = 1684.8 (4) Å^3	0.30 × 0.20 × 0.20 mm
Z = 4	

Data collection

CCD area-detector diffractometer	2879 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	R_{int} = 0.083
Monochromator: graphite	θ_{max} = 27.0º

T = 298(2) K
phi and ω scans
Absorption correction: none
10217 measured reflections
3673 independent reflections

θ_{min} = 2.2°
h = −10→10
k = −23→11
l = −14→14

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.056
$wR(F^2)$ = 0.167
S = 1.07
3673 reflections
209 parameters
18 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0886P)^2 + 0.2659P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.56 e Å^{-3}
$\Delta\rho_{min}$ = −0.31 e Å^{-3}
Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit S are based on F^2, conventional *R*-factors *R* are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.1126 (3)	0.15641 (13)	0.6831 (2)	0.0470 (5)
C2	−0.0516 (3)	0.17089 (14)	0.6538 (3)	0.0592 (6)
H2	−0.0986	0.1945	0.7110	0.071*
C3	−0.1468 (3)	0.15095 (16)	0.5416 (3)	0.0699 (8)
H3	−0.2569	0.1616	0.5235	0.084*
C4	−0.0808 (4)	0.11555 (15)	0.4566 (3)	0.0651 (7)
C5	0.0812 (4)	0.09883 (17)	0.4849 (3)	0.0671 (7)
H5	0.1268	0.0736	0.4286	0.081*
C6	0.1766 (3)	0.11966 (16)	0.5978 (2)	0.0616 (7)
H6	0.2865	0.1085	0.6161	0.074*
C7	−0.1175 (6)	0.0664 (2)	0.2539 (3)	0.1092 (15)

H7A	−0.0385	0.0979	0.2312	0.164*
H7B	−0.2027	0.0568	0.1827	0.164*
H7C	−0.0669	0.0213	0.2853	0.164*
C8	0.2155 (3)	0.18024 (13)	0.8061 (2)	0.0474 (5)
H8	0.1594	0.2203	0.8372	0.057*
C9	0.2388 (3)	0.11894 (13)	0.9001 (2)	0.0515 (6)
H9A	0.1337	0.1022	0.9098	0.062*
H9B	0.2926	0.0783	0.8703	0.062*
C10	0.3383 (3)	0.14333 (14)	1.0237 (2)	0.0503 (6)
H10	0.2900	0.1882	1.0472	0.060*
C11	0.5130 (3)	0.20529 (12)	0.86732 (19)	0.0450 (5)
C12	0.3528 (3)	0.08930 (16)	1.1284 (2)	0.0611 (7)
C13	0.4089 (4)	0.1153 (2)	1.2489 (3)	0.0852 (10)
H13	0.4389	0.1640	1.2616	0.102*
C14	0.4202 (5)	0.0698 (3)	1.3481 (3)	0.1091 (15)
H14	0.4570	0.0873	1.4279	0.131*
C15	0.3759 (5)	−0.0027 (3)	1.3278 (4)	0.1068 (14)
H15	0.3872	−0.0342	1.3946	0.128*
C16	0.3156 (7)	−0.0287 (2)	1.2108 (4)	0.1208 (16)
H16	0.2835	−0.0771	1.1985	0.145*
C17	0.3031 (6)	0.01876 (19)	1.1100 (3)	0.1013 (13)
H17	0.2607	0.0020	1.0305	0.122*
Cl1	0.47385 (8)	0.26700 (5)	0.54600 (6)	0.0657 (3)
N1	0.3715 (2)	0.20775 (11)	0.78919 (18)	0.0482 (5)
H1A	0.370 (4)	0.2314 (17)	0.719 (3)	0.072*
N2	0.6421 (3)	0.23294 (14)	0.8372 (2)	0.0578 (6)
H2D	0.630 (4)	0.2502 (17)	0.763 (3)	0.069*
H2C	0.729 (4)	0.2361 (16)	0.892 (3)	0.069*
O1	−0.1827 (3)	0.10034 (15)	0.3452 (2)	0.1001 (9)
S1	0.54606 (8)	0.16402 (4)	1.01166 (5)	0.0545 (2)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0405 (11)	0.0522 (13)	0.0481 (12)	0.0008 (9)	0.0097 (9)	0.0073 (10)
C2	0.0428 (13)	0.0599 (15)	0.0759 (17)	0.0002 (11)	0.0155 (12)	0.0020 (12)
C3	0.0397 (13)	0.0679 (17)	0.094 (2)	−0.0023 (12)	−0.0027 (13)	0.0037 (16)
C4	0.0568 (15)	0.0593 (16)	0.0684 (17)	−0.0120 (12)	−0.0090 (13)	0.0069 (13)
C5	0.0608 (16)	0.0835 (19)	0.0547 (14)	−0.0029 (14)	0.0079 (12)	−0.0102 (14)
C6	0.0426 (13)	0.0855 (19)	0.0540 (14)	0.0044 (12)	0.0050 (10)	−0.0087 (13)
C7	0.144 (4)	0.089 (3)	0.069 (2)	−0.015 (2)	−0.030 (2)	−0.0133 (19)
C8	0.0443 (12)	0.0542 (13)	0.0450 (11)	0.0024 (10)	0.0126 (9)	0.0009 (10)
C9	0.0552 (14)	0.0542 (13)	0.0479 (12)	0.0000 (11)	0.0172 (10)	0.0037 (10)
C10	0.0540 (14)	0.0564 (14)	0.0442 (12)	0.0092 (11)	0.0190 (10)	0.0042 (10)
C11	0.0483 (12)	0.0490 (12)	0.0388 (10)	0.0034 (9)	0.0120 (9)	−0.0026 (9)
C12	0.0631 (16)	0.0752 (18)	0.0516 (13)	0.0158 (13)	0.0264 (12)	0.0149 (13)
C13	0.075 (2)	0.121 (3)	0.0552 (16)	−0.0233 (19)	0.0050 (14)	0.0215 (17)
C14	0.091 (3)	0.165 (4)	0.065 (2)	−0.029 (3)	0.0038 (18)	0.041 (2)

C15	0.111 (3)	0.131 (3)	0.082 (2)	0.024 (3)	0.030 (2)	0.056 (2)
C16	0.193 (5)	0.077 (2)	0.114 (3)	0.029 (3)	0.081 (3)	0.028 (2)
C17	0.183 (4)	0.068 (2)	0.0658 (18)	0.017 (2)	0.055 (2)	0.0091 (16)
Cl1	0.0469 (4)	0.1019 (6)	0.0482 (4)	−0.0092 (3)	0.0106 (3)	0.0103 (3)
N1	0.0471 (11)	0.0553 (11)	0.0413 (10)	−0.0030 (8)	0.0080 (8)	0.0062 (8)
N2	0.0464 (12)	0.0820 (16)	0.0438 (11)	−0.0053 (11)	0.0078 (9)	0.0043 (11)
O1	0.0846 (17)	0.1022 (18)	0.0880 (16)	−0.0109 (13)	−0.0347 (13)	−0.0072 (14)
S1	0.0502 (4)	0.0734 (5)	0.0401 (3)	0.0089 (3)	0.0106 (3)	0.0058 (3)

Geometric parameters (Å, °)

C1—C6	1.372 (4)	C9—H9B	0.97
C1—C2	1.380 (3)	C10—C12	1.514 (3)
C1—C8	1.513 (3)	C10—S1	1.834 (3)
C2—C3	1.375 (4)	C10—H10	0.98
C2—H2	0.93	C11—N1	1.314 (3)
C3—C4	1.366 (5)	C11—N2	1.316 (3)
C3—H3	0.93	C11—S1	1.741 (2)
C4—O1	1.371 (3)	C12—C17	1.362 (5)
C4—C5	1.372 (4)	C12—C13	1.402 (4)
C5—C6	1.386 (4)	C13—C14	1.370 (5)
C5—H5	0.93	C13—H13	0.93
C6—H6	0.93	C14—C15	1.386 (7)
C7—O1	1.407 (5)	C14—H14	0.93
C7—H7A	0.96	C15—C16	1.373 (6)
C7—H7B	0.96	C15—H15	0.93
C7—H7C	0.96	C16—C17	1.405 (5)
C8—N1	1.465 (3)	C16—H16	0.93
C8—C9	1.519 (3)	C17—H17	0.93
C8—H8	0.98	N1—H1A	0.89 (3)
C9—C10	1.510 (3)	N2—H2D	0.86 (3)
C9—H9A	0.97	N2—H2C	0.84 (4)
C6—C1—C2	117.7 (2)	C9—C10—C12	116.1 (2)
C6—C1—C8	122.1 (2)	C9—C10—S1	110.06 (15)
C2—C1—C8	120.2 (2)	C12—C10—S1	106.17 (17)
C3—C2—C1	121.2 (3)	C9—C10—H10	108.1
C3—C2—H2	119.4	C12—C10—H10	108.1
C1—C2—H2	119.4	S1—C10—H10	108.1
C4—C3—C2	120.5 (3)	N1—C11—N2	120.3 (2)
C4—C3—H3	119.7	N1—C11—S1	124.04 (18)
C2—C3—H3	119.7	N2—C11—S1	115.60 (18)
C3—C4—O1	116.8 (3)	C17—C12—C13	119.6 (3)
C3—C4—C5	119.4 (3)	C17—C12—C10	122.5 (3)
O1—C4—C5	123.8 (3)	C13—C12—C10	117.7 (3)
C4—C5—C6	119.7 (3)	C14—C13—C12	120.7 (4)
C4—C5—H5	120.1	C14—C13—H13	119.6
C6—C5—H5	120.1	C12—C13—H13	119.6
C1—C6—C5	121.5 (2)	C13—C14—C15	119.0 (4)
C1—C6—H6	119.2	C13—C14—H14	120.5

C5—C6—H6	119.2	C15—C14—H14	120.5
O1—C7—H7A	109.5	C16—C15—C14	121.2 (3)
O1—C7—H7B	109.5	C16—C15—H15	119.4
H7A—C7—H7B	109.5	C14—C15—H15	119.4
O1—C7—H7C	109.5	C15—C16—C17	119.1 (4)
H7A—C7—H7C	109.5	C15—C16—H16	120.4
H7B—C7—H7C	109.5	C17—C16—H16	120.4
N1—C8—C1	109.66 (18)	C12—C17—C16	120.2 (4)
N1—C8—C9	111.24 (19)	C12—C17—H17	119.9
C1—C8—C9	111.7 (2)	C16—C17—H17	119.9
N1—C8—H8	108.1	C11—N1—C8	128.1 (2)
C1—C8—H8	108.1	C11—N1—H1A	115 (2)
C9—C8—H8	108.1	C8—N1—H1A	117 (2)
C10—C9—C8	111.6 (2)	C11—N2—H2D	117 (2)
C10—C9—H9A	109.3	C11—N2—H2C	119 (2)
C8—C9—H9A	109.3	H2D—N2—H2C	124 (3)
C10—C9—H9B	109.3	C4—O1—C7	118.3 (3)
C8—C9—H9B	109.3	C11—S1—C10	101.48 (11)
H9A—C9—H9B	108.0		
C6—C1—C2—C3	−1.8 (4)	C9—C10—C12—C13	−164.8 (3)
C8—C1—C2—C3	178.7 (2)	S1—C10—C12—C13	72.5 (3)
C1—C2—C3—C4	0.6 (4)	C17—C12—C13—C14	2.5 (5)
C2—C3—C4—O1	−177.4 (3)	C10—C12—C13—C14	178.0 (3)
C2—C3—C4—C5	1.1 (4)	C12—C13—C14—C15	0.3 (6)
C3—C4—C5—C6	−1.7 (4)	C13—C14—C15—C16	−2.5 (7)
O1—C4—C5—C6	176.7 (3)	C14—C15—C16—C17	1.8 (7)
C2—C1—C6—C5	1.2 (4)	C13—C12—C17—C16	−3.2 (6)
C8—C1—C6—C5	−179.3 (2)	C10—C12—C17—C16	−178.5 (3)
C4—C5—C6—C1	0.5 (5)	C15—C16—C17—C12	1.1 (7)
C6—C1—C8—N1	40.5 (3)	N2—C11—N1—C8	−179.9 (2)
C2—C1—C8—N1	−140.0 (2)	S1—C11—N1—C8	2.4 (3)
C6—C1—C8—C9	−83.2 (3)	C1—C8—N1—C11	−149.2 (2)
C2—C1—C8—C9	96.3 (3)	C9—C8—N1—C11	−25.2 (3)
N1—C8—C9—C10	58.5 (3)	C3—C4—O1—C7	177.6 (3)
C1—C8—C9—C10	−178.66 (19)	C5—C4—O1—C7	−0.8 (5)
C8—C9—C10—C12	173.1 (2)	N1—C11—S1—C10	−8.4 (2)
C8—C9—C10—S1	−66.3 (2)	N2—C11—S1—C10	173.75 (19)
C9—C10—C12—C17	10.5 (4)	C9—C10—S1—C11	38.43 (19)
S1—C10—C12—C17	−112.1 (3)	C12—C10—S1—C11	164.80 (17)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C10—H10···Cl1^{i}	0.98	2.80	3.555 (2)	135
N2—H2C···Cl1^{ii}	0.84 (4)	2.38 (4)	3.219 (3)	175 (3)
N1—H1A···Cl1	0.89 (3)	2.38 (3)	3.212 (2)	155 (3)
N2—H2D···Cl1	0.87 (3)	2.50 (3)	3.295 (2)	153 (3)

Symmetry codes: (i) *x*−1/2, −*y*+1/2, *z*+1/2; (ii) *x*+1/2, −*y*+1/2, *z*+1/2.

Fig. 1

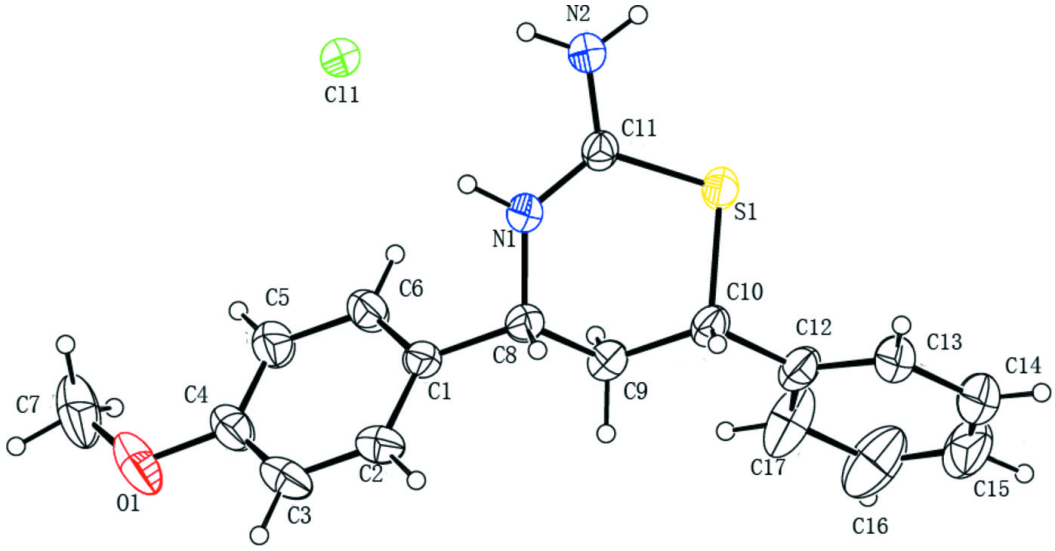
N2
Cl1
C11
S1
N1
C10
C5
C6
C12
C13
C14
C8
C1
C9
C7
C4
C2
C17
C15
O1
C3
C16

Fig. 2