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7-(4-Methylphenyl)-5-(methylsulfanyl)-2-phenyl-1,3-benzothiazole-4-carbonitrile

Noor Shahina Begum,[a]* D. E. Vasundhara,[a] V. S. Hegde[b] and I. M. Khazi[b]

[a]Department of Studies in Chemistry, Bangalore University, Bangalore 560 001, India, and [b]Department of Chemistry, Karnatak University, Dharwad 580 003, India
Correspondence e-mail: noorsb@rediffmail.com

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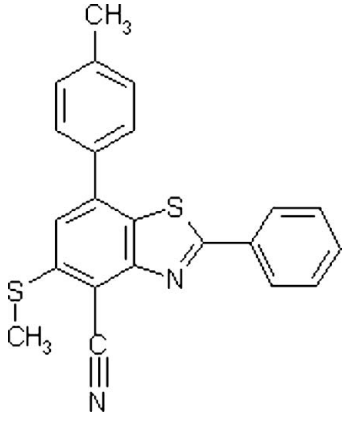
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; R factor = 0.056; wR factor = 0.129; data-to-parameter ratio = 13.8.

In the title compound, $C_{22}H_{16}N_2S_2$, the benzothiazole and tolyl ring systems are inclined at an angle of 31.23 (8)°, and the dihedral angle between the phenyl and benzothiazole rings is 7.567 (2)°. In the crystal structure, intermolecular C—H···N hydrogen bonds link the molecules into a two-dimensional sheet and π–π stacking interactions [perpendicular distance 3.6170 (4) Å] reinforce the crystal cohesion.

Related literature

For related literature, see: Bernstein *et al.* (1995); Bradshaw, Bibby *et al.* (2002); Bradshaw, Chua et al. (2002); Brooker *et al.* (1940); Brownlee *et al.* (1992); Corey & Boger (1978); Hedge *et al.* (2006); Holbová *et al.* (1990); Hutchinson *et al.* (2002); Králová *et al.* (1992); Sidóová & Odlerová (1990).



Experimental

Crystal data

$C_{22}H_{16}N_2S_2$
M_r = 372.49
Monoclinic, $P2_1/c$
a = 11.4142 (11) Å
b = 7.9101 (8) Å
c = 20.553 (2) Å
β = 94.869 (2)°
V = 1849.0 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.30 mm^{-1}
T = 293 (2) K
0.3 × 0.2 × 0.1 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: none
12852 measured reflections
3260 independent reflections
2730 reflections with $I > 2\sigma(I)$
R_{int} = 0.026

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.056
$wR(F^2)$ = 0.129
S = 1.15
3260 reflections
237 parameters
All H-atom parameters refined
$\Delta\rho_{max}$ = 0.26 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C14—H14···N1^{i}	1.045 (5)	2.685 (6)	3.367 (5)	123

Symmetry code: (i) $-x+2, -y+2, -z$.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT-Plus* (Bruker, 1998); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PV2025).

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supplementary materials

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7-(4-Methylphenyl)-5-(methylsulfanyl)-2-phenyl-1,3-benzothiazole-4-carbonitrile

N. S. Begum, D. E. Vasundhara, V. S. Hegde and I. M. Khazi

Comment

Benzothiazoles are bicyclic ring systems with multiple applications. They comprise a novel class of therapeutic compounds shown to exert a wide range of biological activities. Substituted derivatives of benzothiazole demonstrate several interesting pharmacological functions due to their potent capacity to interfere with cellular structures. For instance, the phenyl-substituted benzothiazoles show antitumor activity (Bradshaw, Bibby *et al.*, 2002; Bradshaw, Chua *et al.*, 2002; Hutchinson *et al.*, 2002). They also act as antimicrobial (Holbová *et al.*, 1990; Brownlee *et al.*, 1992) and antimycobacterial (Sidóová & Odlerová, 1990) agents. In adition, they are used in the preparation of dyes (Brooker *et al.*, 1940), organic synthesis of thermostable polymers (Corey & Boger, 1978) and as herbicides which inhibit photosynthesis (Králová *et al.*, 1992). In this paper, we report the structure of the title compound, (I), which has been synthesized in our laboratory.

In (I), the benzothiazole and methylphenyl rings are inclined at an angle of 31.23 (8)° to each other (Fig. 1). The 2-substituted phenyl ring is inclined with respect to benzothiazole ring at an angle of 7.74 (10)°. The methylthio and carbonitrile groups are *cis* to each other. The molecules of (I) are linked by C—H···N hydrogen bonds into two dimensional sheets *via* dimers (Table 1, Fig. 2). Their packing motifs correspond to Etter's descriptors, $R^2_2(14)$ and $R^2_2(22)$ (Bernstein *et al.*, 1995). The molecular packing is further stabilized by π-π stacking interactions between the benzene rings; C13—C13* (* = 2 − *x*,-1/2 + *y*,0.5 − *z*) distance is 3.6170 (4) Å

Experimental

To a suspension of NaH (60%, 0.88 g, 22 mmol) in dry benzene (20 ml) and dry DMF (20 ml) under stirring, a solution of (2-phenyl-1,3-thiazol-4-yl)- acetonitrile (2 g, 10 mmol) in dry benzene (10 ml) was added at 281 K over a period of 15 min and further stirred at 273–361 K for 15 min. Solution of a-oxoketene dithioacetal (10 mmol) in dry DMF (10 ml) was added slowly over 10 min to this mixture with stirring at 273–361 K. The reaction mixture was stirred at room temperature for 4–5 h. The solution was poured into an aqueous ammonium chloride solution (8%, 200 ml), and extracted with benzene (50 ml × 2). The collective extract was washed with water (100 ml × 3), dried over anhydrous sodium sulfate, passed through a silica bed, and concentrated. After standing for 2 h, the crystallized material was separated by filtration and washed with a mixture of benzene and hexane (1:1) to afford a colorless solid, 5-(4-methylphenyl)-3-(methylthio)-5-oxo- 2-(2-phenyl-1,3-thiazol-4-yl)pent-2-enenitrile.

The solution of 5-(4-Methylphenyl)-3-(methylthio)-5-oxo- 2-(2-phenyl-1,3-thiazol-4-yl)pent-2-enenitrile(2.5 mmol) and *p*-toluene sulphonic acid (1 g, 5.3 mmol) in benzene was refluxed for 4–6 h. The reaction mixture (monitored by TLC) was concentrated, dissolved in chloroform, and poured into aqueous sodium bicarbonate solution (6%, 150 ml). The organic layer was separated, washed with water (100 ml × 3), and dried over anhydrous sodium sulfate. The solvent was removed under reduced pressure to yield the greenish yellow oil, which was purified by column chromatography using a benzene-hexane mixture (45:55v/v-80:20v/v) as eluent to furnish a yellow or greenish yellow solid 7-(4-methylphenyl)- 5-(methyl-

thio)-2-phenyl-1,3-benzothiazole-4-carbonitrile (Hedge *et al.*, 2006). Good quality single-crystals of (I) were grown from a chloroform solution by slow evaporation at room temperature.

Refinement

All H atoms were located from Fourier difference maps and refined isotropically.

Figures

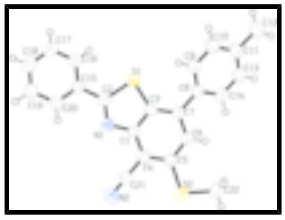

Fig. 1. The molecular structure of (I), showing 50% probability displacement ellipsoids.

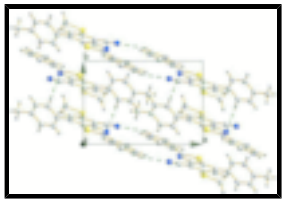

Fig. 2. A view of the unit cell packing of (I).

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Crystal data

$C_{22}H_{16}N_2S_2$	F_{000} = 776
M_r = 372.49	D_x = 1.338 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 500 reflections
a = 11.4142 (11) Å	θ = 1.0–25.0º
b = 7.9101 (8) Å	μ = 0.30 mm^{-1}
c = 20.553 (2) Å	T = 293 (2) K
β = 94.869 (2)º	Rectangular, yellow
V = 1849.0 (3) Å^3	0.3 × 0.2 × 0.1 mm
Z = 4	

Data collection

Bruker SMART CCD area-detector diffractometer	2730 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	R_{int} = 0.026
Monochromator: graphite	θ_{max} = 25.0º
φ and ω scans	θ_{min} = 1.8º
Absorption correction: none	h = −13→13
12852 measured reflections	k = −9→9

3260 independent reflections

$l = -24 \rightarrow 24$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.056$

$wR(F^2) = 0.129$

$S = 1.15$

3260 reflections

237 parameters

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

All H-atom parameters refined

$w = 1/[\sigma^2(F_o^2) + (0.0511P)^2 + 0.8652P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} = 0.001$

$\Delta\rho_{max} = 0.26$ e Å^{-3}

$\Delta\rho_{min} = -0.19$ 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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.9027 (2)	0.7127 (4)	−0.02928 (14)	0.0446 (7)
C2	0.8276 (3)	0.6166 (4)	0.05881 (15)	0.0467 (7)
C3	1.0029 (3)	0.7342 (4)	0.01428 (14)	0.0452 (7)
C4	0.9041 (3)	0.7583 (4)	−0.09522 (15)	0.0483 (7)
C5	1.0078 (3)	0.8232 (4)	−0.11692 (15)	0.0531 (8)
C6	1.1065 (3)	0.8403 (4)	−0.07267 (16)	0.0520 (8)
H6	1.175 (3)	0.877 (4)	−0.0863 (17)	0.058 (10)*
C7	1.1080 (3)	0.8004 (4)	−0.00666 (15)	0.0455 (7)
C8	1.2178 (3)	0.8258 (4)	0.03667 (15)	0.0466 (7)
C9	1.2497 (3)	0.7210 (5)	0.08930 (17)	0.0526 (8)
H9	1.205 (3)	0.630 (4)	0.0988 (15)	0.055 (9)*
C10	1.3538 (3)	0.7431 (5)	0.12779 (19)	0.0594 (9)
H10	1.374 (4)	0.662 (5)	0.165 (2)	0.082 (12)*
C11	1.4303 (3)	0.8725 (5)	0.11495 (17)	0.0589 (9)
C12	1.5458 (4)	0.8981 (9)	0.1561 (3)	0.0849 (14)
H12A	1.535 (4)	0.999 (7)	0.185 (3)	0.117 (17)*
H12B	1.598 (5)	0.901 (8)	0.131 (3)	0.13 (2)*
H12C	1.561 (5)	0.810 (7)	0.191 (3)	0.13 (2)*
C13	1.3986 (3)	0.9782 (5)	0.06248 (19)	0.0616 (10)
H13	1.445 (3)	1.068 (5)	0.0526 (17)	0.055 (9)*
C14	1.2947 (3)	0.9560 (4)	0.02381 (18)	0.0547 (8)
H14	1.276 (3)	1.041 (5)	−0.0146 (16)	0.045 (9)*

C15	0.7422 (3)	0.5403 (4)	0.09969 (15)	0.0481 (7)
C16	0.7639 (3)	0.5262 (5)	0.16663 (18)	0.0615 (9)
H16	0.832 (3)	0.560 (4)	0.1869 (17)	0.064 (11)*
C17	0.6819 (4)	0.4536 (6)	0.2037 (2)	0.0732 (12)
H17	0.699 (3)	0.449 (5)	0.248 (2)	0.075 (13)*
C18	0.5773 (4)	0.3960 (6)	0.1740 (2)	0.0717 (11)
H18	0.522 (3)	0.346 (4)	0.1975 (16)	0.065 (10)*
C19	0.5544 (3)	0.4091 (5)	0.1075 (2)	0.0662 (10)
H19	0.479 (3)	0.366 (5)	0.0883 (19)	0.082 (12)*
C20	0.6359 (3)	0.4809 (5)	0.07039 (19)	0.0587 (9)
H20	0.621 (3)	0.491 (4)	0.0263 (18)	0.059 (10)*
C21	0.8001 (3)	0.7345 (5)	−0.13869 (16)	0.0536 (8)
C22	1.1479 (5)	0.9563 (8)	−0.2095 (3)	0.0882 (15)
H22A	1.171 (5)	1.083 (8)	−0.183 (3)	0.15 (2)*
H22B	1.145 (3)	0.976 (5)	−0.249 (2)	0.077 (13)*
H22C	1.204 (5)	0.870 (7)	−0.201 (3)	0.13 (2)*
N1	0.8054 (2)	0.6455 (4)	−0.00331 (13)	0.0476 (6)
N2	0.7190 (3)	0.7147 (5)	−0.17417 (16)	0.0748 (10)
S1	0.96953 (7)	0.67111 (11)	0.09166 (4)	0.0508 (3)
S2	1.00579 (9)	0.87246 (18)	−0.20032 (5)	0.0879 (4)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0435 (16)	0.0431 (17)	0.0476 (18)	0.0030 (13)	0.0067 (14)	0.0010 (13)
C2	0.0461 (17)	0.0455 (18)	0.0485 (18)	0.0039 (14)	0.0035 (14)	−0.0013 (14)
C3	0.0469 (16)	0.0458 (18)	0.0431 (17)	0.0071 (13)	0.0044 (14)	0.0016 (13)
C4	0.0467 (18)	0.0505 (19)	0.0475 (17)	0.0046 (14)	0.0033 (14)	0.0045 (15)
C5	0.0530 (19)	0.059 (2)	0.0469 (18)	0.0035 (15)	0.0044 (15)	0.0078 (15)
C6	0.0445 (18)	0.057 (2)	0.054 (2)	−0.0019 (15)	0.0057 (15)	0.0068 (16)
C7	0.0450 (16)	0.0420 (17)	0.0497 (18)	0.0039 (13)	0.0049 (14)	0.0010 (14)
C8	0.0453 (16)	0.0473 (18)	0.0476 (18)	0.0040 (14)	0.0071 (14)	−0.0036 (14)
C9	0.0471 (18)	0.054 (2)	0.057 (2)	−0.0050 (16)	0.0040 (16)	0.0005 (16)
C10	0.054 (2)	0.067 (2)	0.056 (2)	0.0049 (18)	0.0008 (17)	−0.002 (2)
C11	0.0469 (18)	0.073 (2)	0.057 (2)	0.0010 (17)	0.0042 (16)	−0.0173 (18)
C12	0.057 (3)	0.114 (4)	0.082 (3)	−0.009 (3)	−0.006 (2)	−0.018 (3)
C13	0.054 (2)	0.063 (2)	0.069 (2)	−0.0132 (18)	0.0139 (19)	−0.0110 (19)
C14	0.053 (2)	0.051 (2)	0.061 (2)	0.0006 (16)	0.0084 (16)	−0.0004 (17)
C15	0.0475 (17)	0.0498 (18)	0.0475 (18)	0.0017 (14)	0.0071 (14)	−0.0012 (14)
C16	0.055 (2)	0.077 (3)	0.052 (2)	−0.0065 (19)	0.0001 (17)	0.0034 (18)
C17	0.078 (3)	0.091 (3)	0.053 (2)	−0.008 (2)	0.015 (2)	0.012 (2)
C18	0.066 (2)	0.080 (3)	0.072 (3)	−0.009 (2)	0.024 (2)	0.008 (2)
C19	0.056 (2)	0.074 (3)	0.070 (3)	−0.0126 (19)	0.0108 (19)	−0.004 (2)
C20	0.056 (2)	0.069 (2)	0.051 (2)	−0.0031 (17)	0.0042 (17)	−0.0007 (18)
C21	0.0526 (19)	0.064 (2)	0.0448 (19)	0.0011 (16)	0.0080 (16)	0.0060 (16)
C22	0.077 (3)	0.116 (5)	0.074 (3)	−0.010 (3)	0.022 (3)	0.033 (3)
N1	0.0458 (14)	0.0511 (17)	0.0459 (16)	0.0019 (12)	0.0037 (12)	0.0006 (13)
N2	0.0580 (19)	0.106 (3)	0.058 (2)	−0.0108 (18)	−0.0041 (16)	0.0010 (18)

S1	0.0471 (5)	0.0616 (5)	0.0436 (5)	−0.0010 (4)	0.0030 (3)	0.0013 (4)
S2	0.0671 (6)	0.1441 (12)	0.0514 (6)	−0.0234 (6)	−0.0009 (5)	0.0296 (6)

Geometric parameters (Å, °)

C1—N1	1.379 (4)	C12—H12A	1.01 (6)
C1—C3	1.402 (4)	C12—H12B	0.82 (6)
C1—C4	1.404 (4)	C12—H12C	1.01 (6)
C2—N1	1.301 (4)	C13—C14	1.381 (5)
C2—C15	1.470 (4)	C13—H13	0.92 (4)
C2—S1	1.755 (3)	C14—H14	1.05 (3)
C3—C7	1.409 (4)	C15—C16	1.382 (5)
C3—S1	1.740 (3)	C15—C20	1.389 (5)
C4—C5	1.397 (4)	C16—C17	1.380 (5)
C4—C21	1.436 (5)	C16—H16	0.89 (4)
C5—C6	1.394 (4)	C17—C18	1.372 (6)
C5—S2	1.756 (3)	C17—H17	0.91 (4)
C6—C7	1.392 (4)	C18—C19	1.373 (5)
C6—H6	0.90 (4)	C18—H18	0.92 (4)
C7—C8	1.487 (4)	C19—C20	1.374 (5)
C8—C9	1.387 (4)	C19—H19	0.98 (4)
C8—C14	1.393 (4)	C20—H20	0.91 (3)
C9—C10	1.382 (5)	C21—N2	1.140 (4)
C9—H9	0.91 (3)	C22—S2	1.778 (5)
C10—C11	1.385 (5)	C22—H22A	1.16 (7)
C10—H10	1.01 (4)	C22—H22B	0.83 (4)
C11—C13	1.388 (5)	C22—H22C	0.94 (6)
C11—C12	1.518 (5)		
N1—C1—C3	116.1 (3)	H12A—C12—H12C	98 (4)
N1—C1—C4	123.2 (3)	H12B—C12—H12C	112 (5)
C3—C1—C4	120.7 (3)	C14—C13—C11	121.7 (3)
N1—C2—C15	123.3 (3)	C14—C13—H13	117 (2)
N1—C2—S1	115.6 (2)	C11—C13—H13	121 (2)
C15—C2—S1	121.1 (2)	C13—C14—C8	120.6 (4)
C1—C3—C7	121.3 (3)	C13—C14—H14	117.5 (19)
C1—C3—S1	108.6 (2)	C8—C14—H14	121.9 (19)
C7—C3—S1	130.1 (2)	C16—C15—C20	118.7 (3)
C5—C4—C1	118.8 (3)	C16—C15—C2	122.0 (3)
C5—C4—C21	121.8 (3)	C20—C15—C2	119.2 (3)
C1—C4—C21	119.4 (3)	C17—C16—C15	120.7 (4)
C6—C5—C4	119.2 (3)	C17—C16—H16	118 (2)
C6—C5—S2	123.9 (2)	C15—C16—H16	121 (2)
C4—C5—S2	116.9 (2)	C18—C17—C16	119.8 (4)
C7—C6—C5	123.8 (3)	C18—C17—H17	122 (2)
C7—C6—H6	116 (2)	C16—C17—H17	118 (2)
C5—C6—H6	120 (2)	C17—C18—C19	120.2 (4)
C6—C7—C3	116.2 (3)	C17—C18—H18	121 (2)
C6—C7—C8	119.5 (3)	C19—C18—H18	118 (2)
C3—C7—C8	124.2 (3)	C18—C19—C20	120.2 (4)

C9—C8—C14	117.5 (3)	C18—C19—H19	117 (2)
C9—C8—C7	122.6 (3)	C20—C19—H19	122 (2)
C14—C8—C7	119.9 (3)	C19—C20—C15	120.4 (3)
C10—C9—C8	121.8 (3)	C19—C20—H20	121 (2)
C10—C9—H9	116 (2)	C15—C20—H20	119 (2)
C8—C9—H9	122 (2)	N2—C21—C4	178.6 (3)
C9—C10—C11	120.7 (4)	S2—C22—H22A	116 (3)
C9—C10—H10	119 (2)	S2—C22—H22B	102 (3)
C11—C10—H10	120 (2)	H22A—C22—H22B	107 (4)
C10—C11—C13	117.8 (3)	S2—C22—H22C	109 (4)
C10—C11—C12	121.6 (4)	H22A—C22—H22C	114 (5)
C13—C11—C12	120.6 (4)	H22B—C22—H22C	107 (4)
C11—C12—H12A	107 (3)	C2—N1—C1	110.5 (3)
C11—C12—H12B	108 (4)	C3—S1—C2	89.17 (15)
H12A—C12—H12B	118 (5)	C5—S2—C22	104.5 (2)
C11—C12—H12C	113 (3)		
N1—C1—C3—C7	179.5 (3)	C6—C7—C8—C14	31.5 (4)
C4—C1—C3—C7	−0.6 (5)	C3—C7—C8—C14	−149.7 (3)
N1—C1—C3—S1	−1.6 (3)	C14—C8—C9—C10	−0.2 (5)
C4—C1—C3—S1	178.3 (2)	C7—C8—C9—C10	177.9 (3)
N1—C1—C4—C5	−179.1 (3)	C7—C8—C14—C13	−178.1 (3)
C3—C1—C4—C5	1.0 (5)	N1—C2—C15—C16	−173.5 (3)
N1—C1—C4—C21	−0.2 (5)	S1—C2—C15—C16	7.7 (4)
C3—C1—C4—C21	179.9 (3)	N1—C2—C15—C20	6.3 (5)
C1—C4—C5—C6	0.2 (5)	S1—C2—C15—C20	−172.5 (3)
C21—C4—C5—C6	−178.7 (3)	C20—C15—C16—C17	0.4 (6)
C1—C4—C5—S2	178.2 (2)	C2—C15—C16—C17	−179.8 (4)
C21—C4—C5—S2	−0.7 (4)	C2—C15—C20—C19	−180.0 (3)
C4—C5—C6—C7	−1.8 (5)	C15—C2—N1—C1	−178.1 (3)
S2—C5—C6—C7	−179.7 (3)	S1—C2—N1—C1	0.7 (4)
C5—C6—C7—C3	2.1 (5)	C3—C1—N1—C2	0.6 (4)
C5—C6—C7—C8	−179.1 (3)	C4—C1—N1—C2	−179.3 (3)
C1—C3—C7—C6	−0.8 (4)	C1—C3—S1—C2	1.6 (2)
S1—C3—C7—C6	−179.5 (2)	C7—C3—S1—C2	−179.6 (3)
C1—C3—C7—C8	−179.6 (3)	N1—C2—S1—C3	−1.4 (3)
S1—C3—C7—C8	1.6 (5)	C15—C2—S1—C3	177.5 (3)
C6—C7—C8—C9	−146.5 (3)	C6—C5—S2—C22	−3.8 (4)
C3—C7—C8—C9	32.3 (5)	C4—C5—S2—C22	178.2 (3)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C14—H14···N1^{i}	1.045 (5)	2.685 (6)	3.367 (5)	123

Symmetry codes: (i) −*x*+2, −*y*+2, −*z*.

Fig. 1

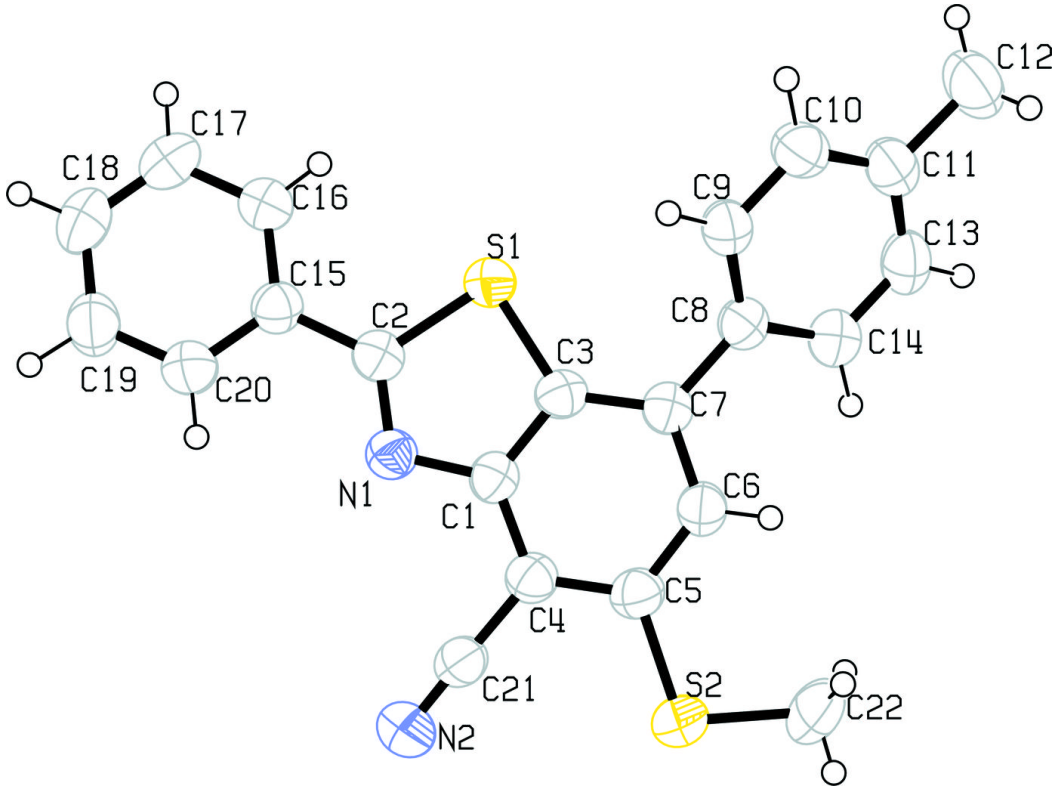
C12
C10
C11
C17
C18
C16
C9
C13
S1
C15
C2
C8
C3
C14
C19
C20
C7
N1
C6
C1
C5
C4
C21
S2
C22
N2

Fig. 2