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4-Benzylidene-2-methyl-11-phenyl-1,2,3,4,11,11a-hexahydropyrido[3,4-*c*]-[1,5]benzothiazepine

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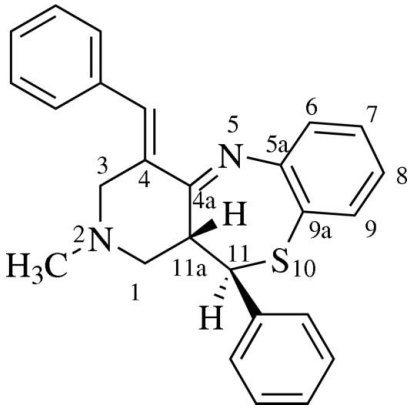
Key indicators: single-crystal X-ray study; T = 273 K; mean σ(C–C) = 0.002 Å; R factor = 0.037; wR factor = 0.100; data-to-parameter ratio = 14.3.

In the title compound, $C_{26}H_{24}N_2S$, the six- and seven-membered heterocyclic rings adopt half-chair and near-boat conformations, respectively. The molecular conformation is influenced by two weak intramolecular C—H···N interactions. The crystal structure is stablized by intermolecular C—H···N and C—H···π interactions.

Related literature

For puckering analysis, see: Cremer & Pople (1975). For background, uses and biological activity of benzothiazepines, see: Jadhav & Ingle (1983); Reddy *et al.* (1993); Satyanarayanan & Rao (1993); DeSarro *et al.* (1995); Chaffman & Brogden (1985); Slade *et al.* (1985); Bock *et al.* (1989); Kantoci *et al.* (1996); Skiles *et al.* (1993). For background, uses and biological activity of piperidines, see: O'Hagan (2000); Kikuchi *et al.* (2005); Kitbunnadaj *et al.* (2005); Christodoulopoulou *et al.* (2005). For reference structural data, see: Allen (2002).



Experimental

Crystal data

$C_{26}H_{24}N_2S$
M_r = 396.53
Monoclinic, $P2_1/c$
a = 11.7545 (6) Å
b = 15.5571 (7) Å
c = 12.1496 (6) Å
β = 106.114 (1)°
V = 2134.46 (18) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.17 mm^{-1}
T = 273 (2) K
0.24 × 0.21 × 0.19 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
20269 measured reflections
3763 independent reflections
3313 reflections with $I > 2\sigma(I)$
R_{int} = 0.023

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.100
S = 1.03
3763 reflections
263 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.15 e Å^{-3}

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

Cg is the centroid of the C20–C25 benzene ring.

D—H···A	D—H	H···A	D···A	D—H···A
C19—H19···N1	0.93	2.40	2.7718 (19)	104
C7—H7···N2	0.98	2.61	3.015 (2)	105
C23—H23···N1^{i}	0.93	2.61	3.389 (2)	142
C3—H3···*Cg*^{ii}	0.93	2.67	3.574 (2)	165
C17—H17···*Cg*^{iii}	0.93	3.03	3.685 (2)	129

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

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL/PC* (Bruker, 2000); program(s) used to refine structure: *SHELXTL/PC*; molecular graphics: *ORTEP-3* (Farrugia, 1997) and *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXTL/PC*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SJ2372).

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supplementary materials

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4-Benzylidene-2-methyl-11-phenyl-1,2,3,4,11,11a-hexahydropyrido[3,4-*c*][1,5]benzothiazepine

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Comment

[1,5]-Benzothiazepines display diverse biological activities such as antibacterial (Jadhav & Ingle, 1983), antifeedant (Reddy *et al.*, 1993), analgesic (Satyanarayanan & Rao, 1993), and anticonvulsant (DeSarro *et al.*, 1995) and hence find a unique place in drug discovery. They also function as calcium antagonists (Chaffman & Brogden, 1985), enzyme inhibitors (Slade *et al.*, 1985), tranquilizers (Bock *et al.*, 1989) and as endogenous natriuretic factors (Kantoci *et al.*, 1996). The [1,5]-benzothiazepine scaffold has been used as a constrained dipeptide mimic in protease inhibitors (Skiles *et al.*, 1993). The piperidine sub-structure is also widely prevalent in many biologically important systems (O'Hagan, 2000; Kikuchi *et al.*, 2005; Kitbunnadaj *et al.*, 2005; Christodoulopoulou *et al.*, 2005). The bio-importance of benzothiazepines and piperidine sub-structures prompted us to report the synthesis and X-ray crystallographic studies of the title compound, (I).

In the crystal structure, the average C—N, C—S and C—C bond distances in the piperidine and the seven membered rings, are in good agreement with the literature values (Allen, 2002). The half-chair conformation of the piperidine ring is confirmed by the puckering analysis [q_2 = 0.2830 (16) Å, φ_2 = 330.1 (3)°, q3 = 0.4437 (16) Å; Cremer & Pople, 1975]. Further, the seven membered heterocyclic ring is in a near-boat conformation [q_2 = 1.1402 (13) Å, φ_2 = 190.00 (8)°, q_3 = 0.2060 (15) Å, φ_3 = 231.2 (4)°; Cremer & Pople, 1975] (Fig. 1). The phenyl rings C13/C18 and C20/C25 are oriented with a dihedral angle of 71.07 (5)° to each other. The molecular conformation is further stabilized by two intramolecular C—H···N interactions (Table 2). The crystal packing is stablized by intermolecular C—H···N and two C—H···π interactions, with no evidence of significant π···π stacking interactions (Fig. 2).

Experimental

A mixture of *o*-aminothiophenol (1 mmol), (*E*)-1-methyl-3,5-bis-(phenylmethylidene)-4-piperidone (1 mmol) and a catalytic amount of acetic acid (30 mol %) was thoroughly mixed in an open glass tube. The tube containing the mixture was placed over a silica bath in a microwave oven irradiated for 6 min at 600 W. The progress of the reaction was monitored after every minute of irradiation by TLC with petroleum ether:ethyl acetate (4:1 *v*/*v* mixture) as eluent. After each irradiation, the reaction mixture was cooled to room temperature and mixed well. After completion of the reaction (TLC), the yellow solid was recrystallized from ethanol to obtain pure 2-methyl-11-phenyl-4-(phenylmethylidene)-1,2,3,4,11,11*a*-hexahydropyrido [3,4-*c*][1,5]benzothiazepine.

Refinement

All the H atoms were positioned geometrically and refined using a riding model, with C—H = 0.93–0.98 Å and U_{iso}(H) = 1.2–1.5 U_{eq} (parent atom).

Figures

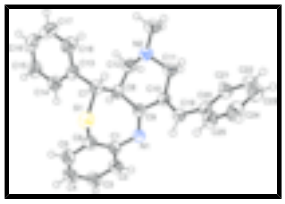

Fig. 1. The molecular structure of the title compound (I) with the numbering scheme for the atoms and 50% probability displacement ellipsoids.

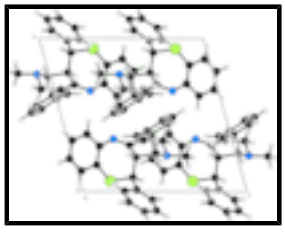

Fig. 2. Packing diagram of the molecules viewed down the *b*-axis.

4-Benzylidene-2-methyl-11-phenyl-1,2,3,4,11,11*a*- hexahydropyrido[3,4-*c*][1,5]benzothiazepine

Crystal data

$C_{26}H_{24}N_2S$	F_{000} = 840
M_r = 396.53	D_x = 1.234 Mg m^{-3}
Monoclinic, $P2_1/c$	Melting point: 200 K
Hall symbol: -P 2ybc	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 11.7545 (6) Å	Cell parameters from 3953 reflections
b = 15.5571 (7) Å	θ = 2.4–24.7º
c = 12.1496 (6) Å	μ = 0.17 mm^{-1}
β = 106.114 (1)º	*T* = 273 (2) K
V = 2134.46 (18) Å^3	Block, colourless
Z = 4	0.24 × 0.21 × 0.19 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer	3313 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	R_{int} = 0.023
Monochromator: graphite	θ_{max} = 25.0º
T = 273(2) K	θ_{min} = 1.8º
ω scans	*h* = −13→13
Absorption correction: none	*k* = −18→18
20269 measured reflections	*l* = −14→14
3763 independent reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map

Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.037$	H-atom parameters constrained
$wR(F^2) = 0.100$	$w = 1/[\sigma^2(F_o^2) + (0.0483P)^2 + 0.5835P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.03$	$(\Delta/\sigma)_{max} < 0.001$
3763 reflections	$\Delta\rho_{max} = 0.20$ e Å^{-3}
263 parameters	$\Delta\rho_{min} = -0.15$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	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 $F^2 > 2$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	0.29637 (14)	0.06177 (9)	0.18099 (12)	0.0432 (3)
C2	0.37430 (16)	0.09676 (11)	0.12553 (13)	0.0527 (4)
H2	0.4553	0.0889	0.1565	0.063*
C3	0.33360 (19)	0.14289 (12)	0.02532 (15)	0.0635 (5)
H3	0.3871	0.1676	−0.0091	0.076*
C4	0.2142 (2)	0.15224 (12)	−0.02348 (15)	0.0667 (5)
H4	0.1867	0.1821	−0.0921	0.080*
C5	0.13503 (17)	0.11747 (11)	0.02894 (14)	0.0589 (5)
H5	0.0542	0.1242	−0.0047	0.071*
C6	0.17397 (14)	0.07245 (9)	0.13153 (13)	0.0466 (4)
C7	0.09214 (13)	0.06832 (9)	0.32994 (13)	0.0437 (3)
H7	0.0717	0.0239	0.3784	0.052*
C8	0.22410 (12)	0.08956 (9)	0.38307 (12)	0.0398 (3)
H8	0.2432	0.1404	0.3441	0.048*
C9	0.30253 (12)	0.01647 (9)	0.36584 (12)	0.0391 (3)
C10	0.33643 (12)	−0.05010 (9)	0.45629 (12)	0.0405 (3)
C11	0.33162 (14)	−0.02641 (10)	0.57538 (13)	0.0467 (4)
H11A	0.3207	−0.0781	0.6159	0.056*
H11B	0.4063	−0.0006	0.6169	0.056*
C12	0.24955 (14)	0.11058 (10)	0.51039 (13)	0.0463 (4)
H12A	0.3297	0.1322	0.5392	0.056*
H12B	0.1955	0.1548	0.5212	0.056*

C13	0.01197 (13)	0.14416 (10)	0.33121 (13)	0.0447 (4)
C14	0.00314 (15)	0.21251 (10)	0.25636 (15)	0.0532 (4)
H14	0.0450	0.2113	0.2017	0.064*
C15	−0.06740 (17)	0.28267 (11)	0.26193 (17)	0.0641 (5)
H15	−0.0722	0.3282	0.2113	0.077*
C16	−0.13015 (16)	0.28550 (13)	0.34154 (19)	0.0675 (5)
H16	−0.1770	0.3329	0.3455	0.081*
C17	−0.12324 (16)	0.21824 (14)	0.4148 (2)	0.0727 (6)
H17	−0.1662	0.2197	0.4686	0.087*
C18	−0.05269 (15)	0.14734 (12)	0.41019 (17)	0.0617 (5)
H18	−0.0490	0.1018	0.4606	0.074*
C19	0.36293 (13)	−0.12880 (9)	0.42549 (13)	0.0427 (3)
H19	0.3607	−0.1351	0.3488	0.051*
C20	0.39499 (13)	−0.20618 (9)	0.49633 (13)	0.0431 (3)
C21	0.46410 (14)	−0.20436 (10)	0.60939 (14)	0.0488 (4)
H21	0.4967	−0.1526	0.6417	0.059*
C22	0.48494 (17)	−0.27838 (12)	0.67437 (15)	0.0598 (5)
H22	0.5311	−0.2760	0.7501	0.072*
C23	0.43823 (18)	−0.35534 (12)	0.62834 (17)	0.0644 (5)
H23	0.4508	−0.4048	0.6731	0.077*
C24	0.37244 (17)	−0.35901 (11)	0.51521 (18)	0.0650 (5)
H24	0.3414	−0.4112	0.4833	0.078*
C25	0.35245 (15)	−0.28542 (10)	0.44919 (15)	0.0537 (4)
H25	0.3101	−0.2888	0.3723	0.064*
C26	0.23128 (18)	0.05341 (13)	0.68957 (15)	0.0645 (5)
H26A	0.3036	0.0812	0.7305	0.097*
H26B	0.2220	0.0011	0.7281	0.097*
H26C	0.1656	0.0909	0.6866	0.097*
N1	0.34257 (11)	0.00985 (8)	0.27801 (10)	0.0434 (3)
N2	0.23539 (11)	0.03366 (8)	0.57301 (11)	0.0460 (3)
S1	0.06776 (4)	0.02108 (3)	0.18734 (4)	0.05483 (15)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0541 (9)	0.0349 (7)	0.0391 (8)	0.0064 (6)	0.0107 (7)	−0.0005 (6)
C2	0.0592 (10)	0.0541 (10)	0.0462 (9)	0.0038 (8)	0.0169 (8)	0.0035 (7)
C3	0.0853 (14)	0.0591 (11)	0.0500 (10)	0.0038 (10)	0.0253 (9)	0.0089 (8)
C4	0.0968 (15)	0.0574 (11)	0.0424 (9)	0.0151 (10)	0.0133 (10)	0.0093 (8)
C5	0.0670 (11)	0.0531 (10)	0.0460 (9)	0.0134 (9)	−0.0020 (8)	−0.0053 (8)
C6	0.0558 (9)	0.0369 (8)	0.0428 (8)	0.0051 (7)	0.0065 (7)	−0.0071 (6)
C7	0.0422 (8)	0.0352 (8)	0.0535 (9)	−0.0026 (6)	0.0128 (7)	0.0018 (6)
C8	0.0414 (8)	0.0315 (7)	0.0460 (8)	0.0002 (6)	0.0113 (6)	0.0005 (6)
C9	0.0378 (7)	0.0357 (7)	0.0421 (8)	−0.0002 (6)	0.0083 (6)	0.0002 (6)
C10	0.0394 (8)	0.0407 (8)	0.0413 (8)	0.0026 (6)	0.0110 (6)	0.0022 (6)
C11	0.0515 (9)	0.0442 (8)	0.0439 (8)	0.0041 (7)	0.0124 (7)	0.0022 (7)
C12	0.0477 (9)	0.0391 (8)	0.0518 (9)	0.0004 (7)	0.0133 (7)	−0.0070 (7)
C13	0.0346 (7)	0.0426 (8)	0.0550 (9)	−0.0025 (6)	0.0091 (7)	−0.0035 (7)

C14	0.0541 (9)	0.0494 (9)	0.0548 (9)	0.0074 (7)	0.0129 (8)	0.0009 (7)
C15	0.0654 (11)	0.0494 (10)	0.0674 (11)	0.0139 (8)	0.0018 (9)	−0.0020 (9)
C16	0.0439 (10)	0.0619 (12)	0.0889 (14)	0.0109 (8)	0.0055 (9)	−0.0193 (11)
C17	0.0495 (10)	0.0807 (14)	0.0966 (15)	−0.0021 (10)	0.0346 (10)	−0.0204 (12)
C18	0.0512 (10)	0.0609 (11)	0.0793 (12)	−0.0030 (8)	0.0283 (9)	0.0022 (9)
C19	0.0456 (8)	0.0427 (8)	0.0406 (8)	0.0045 (6)	0.0131 (6)	0.0030 (6)
C20	0.0431 (8)	0.0410 (8)	0.0488 (8)	0.0060 (6)	0.0186 (7)	0.0035 (7)
C21	0.0533 (9)	0.0441 (9)	0.0499 (9)	0.0065 (7)	0.0157 (7)	0.0040 (7)
C22	0.0705 (12)	0.0605 (11)	0.0513 (10)	0.0143 (9)	0.0218 (8)	0.0140 (8)
C23	0.0758 (12)	0.0501 (10)	0.0765 (13)	0.0116 (9)	0.0366 (10)	0.0235 (9)
C24	0.0674 (12)	0.0410 (9)	0.0892 (14)	−0.0002 (8)	0.0262 (10)	0.0033 (9)
C25	0.0536 (10)	0.0454 (9)	0.0605 (10)	0.0060 (7)	0.0134 (8)	−0.0008 (8)
C26	0.0765 (12)	0.0706 (12)	0.0510 (10)	0.0053 (10)	0.0254 (9)	−0.0085 (9)
N1	0.0465 (7)	0.0415 (7)	0.0422 (7)	0.0067 (5)	0.0122 (6)	0.0047 (5)
N2	0.0510 (7)	0.0451 (7)	0.0439 (7)	0.0029 (6)	0.0166 (6)	−0.0030 (6)
S1	0.0492 (3)	0.0455 (2)	0.0643 (3)	−0.00796 (17)	0.0067 (2)	−0.01459 (19)

Geometric parameters (Å, °)

C1—C2	1.390 (2)	C13—C18	1.381 (2)
C1—C6	1.407 (2)	C13—C14	1.384 (2)
C1—N1	1.4076 (19)	C14—C15	1.384 (2)
C2—C3	1.379 (2)	C14—H14	0.9300
C2—H2	0.9300	C15—C16	1.370 (3)
C3—C4	1.371 (3)	C15—H15	0.9300
C3—H3	0.9300	C16—C17	1.362 (3)
C4—C5	1.376 (3)	C16—H16	0.9300
C4—H4	0.9300	C17—C18	1.390 (3)
C5—C6	1.392 (2)	C17—H17	0.9300
C5—H5	0.9300	C18—H18	0.9300
C6—S1	1.7684 (17)	C19—C20	1.467 (2)
C7—C13	1.513 (2)	C19—H19	0.9300
C7—C8	1.541 (2)	C20—C21	1.388 (2)
C7—S1	1.8298 (16)	C20—C25	1.392 (2)
C7—H7	0.9800	C21—C22	1.379 (2)
C8—C9	1.5145 (19)	C21—H21	0.9300
C8—C12	1.527 (2)	C22—C23	1.370 (3)
C8—H8	0.9800	C22—H22	0.9300
C9—N1	1.2844 (18)	C23—C24	1.378 (3)
C9—C10	1.482 (2)	C23—H23	0.9300
C10—C19	1.342 (2)	C24—C25	1.380 (2)
C10—C11	1.509 (2)	C24—H24	0.9300
C11—N2	1.461 (2)	C25—H25	0.9300
C11—H11A	0.9700	C26—N2	1.463 (2)
C11—H11B	0.9700	C26—H26A	0.9600
C12—N2	1.452 (2)	C26—H26B	0.9600
C12—H12A	0.9700	C26—H26C	0.9600
C12—H12B	0.9700		
C2—C1—C6	118.69 (14)	C18—C13—C7	119.99 (15)

C2—C1—N1	118.53 (14)	C14—C13—C7	121.72 (14)
C6—C1—N1	122.46 (14)	C15—C14—C13	120.71 (17)
C3—C2—C1	121.18 (17)	C15—C14—H14	119.6
C3—C2—H2	119.4	C13—C14—H14	119.6
C1—C2—H2	119.4	C16—C15—C14	120.48 (18)
C4—C3—C2	119.96 (18)	C16—C15—H15	119.8
C4—C3—H3	120.0	C14—C15—H15	119.8
C2—C3—H3	120.0	C17—C16—C15	119.39 (17)
C3—C4—C5	120.05 (16)	C17—C16—H16	120.3
C3—C4—H4	120.0	C15—C16—H16	120.3
C5—C4—H4	120.0	C16—C17—C18	120.72 (18)
C4—C5—C6	121.04 (17)	C16—C17—H17	119.6
C4—C5—H5	119.5	C18—C17—H17	119.6
C6—C5—H5	119.5	C13—C18—C17	120.43 (18)
C5—C6—C1	119.03 (16)	C13—C18—H18	119.8
C5—C6—S1	118.63 (13)	C17—C18—H18	119.8
C1—C6—S1	122.01 (12)	C10—C19—C20	128.81 (14)
C13—C7—C8	112.69 (12)	C10—C19—H19	115.6
C13—C7—S1	112.87 (11)	C20—C19—H19	115.6
C8—C7—S1	110.95 (10)	C21—C20—C25	118.01 (14)
C13—C7—H7	106.6	C21—C20—C19	123.24 (14)
C8—C7—H7	106.6	C25—C20—C19	118.73 (14)
S1—C7—H7	106.6	C22—C21—C20	120.76 (16)
C9—C8—C12	110.19 (12)	C22—C21—H21	119.6
C9—C8—C7	111.20 (11)	C20—C21—H21	119.6
C12—C8—C7	111.20 (12)	C23—C22—C21	120.57 (17)
C9—C8—H8	108.0	C23—C22—H22	119.7
C12—C8—H8	108.0	C21—C22—H22	119.7
C7—C8—H8	108.0	C22—C23—C24	119.57 (16)
N1—C9—C10	118.36 (13)	C22—C23—H23	120.2
N1—C9—C8	123.54 (13)	C24—C23—H23	120.2
C10—C9—C8	118.10 (12)	C23—C24—C25	120.20 (17)
C19—C10—C9	117.79 (13)	C23—C24—H24	119.9
C19—C10—C11	124.30 (13)	C25—C24—H24	119.9
C9—C10—C11	117.80 (12)	C24—C25—C20	120.77 (17)
N2—C11—C10	111.84 (12)	C24—C25—H25	119.6
N2—C11—H11A	109.2	C20—C25—H25	119.6
C10—C11—H11A	109.2	N2—C26—H26A	109.5
N2—C11—H11B	109.2	N2—C26—H26B	109.5
C10—C11—H11B	109.2	H26A—C26—H26B	109.5
H11A—C11—H11B	107.9	N2—C26—H26C	109.5
N2—C12—C8	109.61 (12)	H26A—C26—H26C	109.5
N2—C12—H12A	109.7	H26B—C26—H26C	109.5
C8—C12—H12A	109.7	C9—N1—C1	120.30 (13)
N2—C12—H12B	109.7	C12—N2—C11	109.67 (12)
C8—C12—H12B	109.7	C12—N2—C26	111.93 (13)
H12A—C12—H12B	108.2	C11—N2—C26	110.40 (13)
C18—C13—C14	118.27 (15)	C6—S1—C7	103.88 (7)
C6—C1—C2—C3	1.5 (2)	C7—C13—C14—C15	−177.57 (15)

N1—C1—C2—C3	175.19 (15)	C13—C14—C15—C16	−0.3 (3)
C1—C2—C3—C4	−2.4 (3)	C14—C15—C16—C17	−0.5 (3)
C2—C3—C4—C5	1.6 (3)	C15—C16—C17—C18	0.5 (3)
C3—C4—C5—C6	−0.1 (3)	C14—C13—C18—C17	−0.9 (3)
C4—C5—C6—C1	−0.8 (2)	C7—C13—C18—C17	177.61 (16)
C4—C5—C6—S1	−174.25 (13)	C16—C17—C18—C13	0.2 (3)
C2—C1—C6—C5	0.1 (2)	C9—C10—C19—C20	−177.79 (14)
N1—C1—C6—C5	−173.37 (14)	C11—C10—C19—C20	−1.7 (3)
C2—C1—C6—S1	173.30 (12)	C10—C19—C20—C21	−37.0 (2)
N1—C1—C6—S1	−0.1 (2)	C10—C19—C20—C25	141.75 (17)
C13—C7—C8—C9	−172.25 (12)	C25—C20—C21—C22	−3.1 (2)
S1—C7—C8—C9	−44.57 (14)	C19—C20—C21—C22	175.63 (15)
C13—C7—C8—C12	64.57 (16)	C20—C21—C22—C23	0.3 (3)
S1—C7—C8—C12	−167.75 (10)	C21—C22—C23—C24	1.7 (3)
C12—C8—C9—N1	−146.74 (14)	C22—C23—C24—C25	−0.9 (3)
C7—C8—C9—N1	89.50 (17)	C23—C24—C25—C20	−2.0 (3)
C12—C8—C9—C10	32.18 (17)	C21—C20—C25—C24	3.9 (2)
C7—C8—C9—C10	−91.58 (15)	C19—C20—C25—C24	−174.85 (15)
N1—C9—C10—C19	−27.1 (2)	C10—C9—N1—C1	168.39 (13)
C8—C9—C10—C19	153.97 (13)	C8—C9—N1—C1	−12.7 (2)
N1—C9—C10—C11	156.60 (14)	C2—C1—N1—C9	139.08 (15)
C8—C9—C10—C11	−22.37 (19)	C6—C1—N1—C9	−47.5 (2)
C19—C10—C11—N2	−142.28 (15)	C8—C12—N2—C11	70.45 (15)
C9—C10—C11—N2	33.80 (19)	C8—C12—N2—C26	−166.67 (13)
C9—C8—C12—N2	−55.62 (16)	C10—C11—N2—C12	−57.75 (16)
C7—C8—C12—N2	68.15 (15)	C10—C11—N2—C26	178.47 (14)
C8—C7—C13—C18	−103.94 (17)	C5—C6—S1—C7	−122.43 (13)
S1—C7—C13—C18	129.40 (14)	C1—C6—S1—C7	64.30 (13)
C8—C7—C13—C14	74.55 (19)	C13—C7—S1—C6	94.25 (11)
S1—C7—C13—C14	−52.11 (17)	C8—C7—S1—C6	−33.33 (12)
C18—C13—C14—C15	0.9 (2)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C19—H19···N1	0.93	2.40	2.7718 (19)	104
C7—H7···N2	0.98	2.61	3.015 (2)	105
C23—H23···N1^{i}	0.93	2.61	3.389 (2)	142
C3—H3···Cg^{ii}	0.93	2.67	3.574 (2)	165
C17—H17···Cg^{iii}	0.93	3.03	3.685 (2)	129

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

Fig. 1

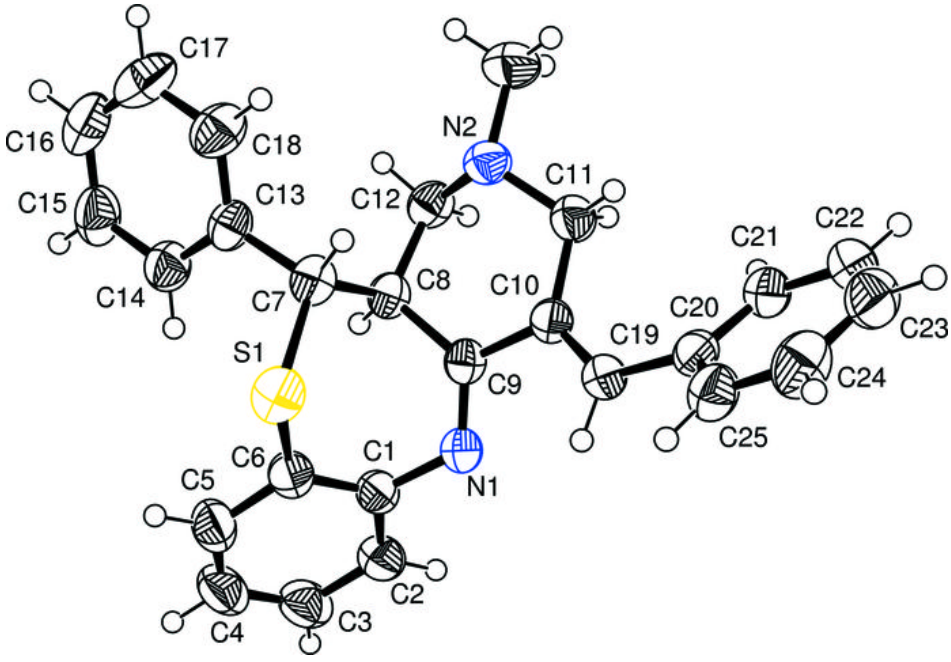
C17
C16
C18
C15
C13
C14
C7
S1
C6
C5
C4
C3
C2
C1
N1
C12
N2
C11
C8
C10
C9
C19
C20
C21
C22
C23
C24
C25

Fig. 2