organic compounds

1-Methyl-4-[1-(1-phenylethylidene)-hydrazin-2-ylidene]-3,4-dihydro-1H-2λ⁶,1-benzothiazine-2,2-dione

Muhammad Shafiq,[a]* Islam Ullah Khan,[b] Muhammad Zia-ur-Rehman,[c] Tariq Mahmood,[d] Muhammad Ashfaq[e] and Saeed Ahmad[f]

[a]Department of Chemistry, Government College University, Faisalabad 38040, Pakistan, [b]Materials Chemistry Laboratory, Department of Chemistry, GC University, Lahore 54000, Pakistan, [c]Applied Chemistry Research Center, PCSIR Laboratories Complex, Ferozpur Road, Lahore 54600, Pakistan, [d]Department of Chemistry, COMSATS institute of Information Technology, Abbottabad, Pakistan, [e]Department of Chemistry, University of Gujrat, Gujrat 50781, Pakistan, and [f]Department of Chemistry, Gomal University, Dera Ismail Khan, K.P.K, Pakistan

Correspondence e-mail: hafizshafique@hotmail.com

In the title compound, $C_{17}H_{17}N_3O_2S$, the phenyl ring is oriented at dihedral angles of 8.5 (2) and 1.17 (14)°, respectively, to the C=N—N plane and the fused aromatic ring. The thiazine ring adopts an envelope conformation with the S atom at the flap. In the crystal, a weak C—H⋯O interaction connects the molecules, forming a helical chain along the *a* axis.

Related literature

For the synthesis, see: Shafiq *et al.* (2011). For related structures, see: Shafiq *et al.* (2011a,b, 2012).
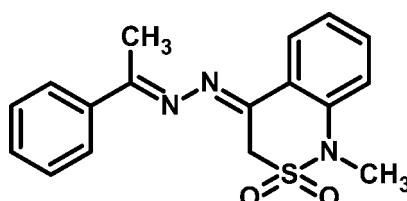
Experimental

Crystal data

C₁₇H₁₇N₃O₂S
M_r = 327.40

Orthorhombic, $P2_12_12_1$
a = 6.6678 (2) Å

b = 12.0783 (6) Å
c = 20.0529 (8) Å
V = 1614.97 (11) Å³
Z = 4

Mo $K\alpha$ radiation
μ = 0.21 mm⁻¹
T = 296 K
0.38 × 0.11 × 0.07 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2007)
T_{min} = 0.923, T_{max} = 0.985

9111 measured reflections
3830 independent reflections
2819 reflections with $I > 2\sigma(I)$
R_{int} = 0.030

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.108
S = 0.97
3828 reflections
210 parameters
H-atom parameters constrained

$\Delta\rho_{max}$ = 0.21 e Å⁻³
$\Delta\rho_{min}$ = −0.27 e Å⁻³
Absolute structure: Flack (1983), 1577 Friedel pairs
Flack parameter: −0.06 (9)

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

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
C8—H8B⋯O1ⁱ	0.97	2.56	3.420 (3)	148

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

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2009); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *PLATON*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IS5153).

References

Bruker (2007). *SADABS*, *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
Shafiq, M., Khan, I. U., Arshad, M. N., Bukhari, I. H. & Ejaz, (2012). *Acta Cryst.* E**68**, o1927.
Shafiq, M., Khan, I. U., Zia-ur-Rehman, M., Arshad, M. N. & Asiri, A. M. (2011a). *Acta Cryst.* E**67**, o2038.
Shafiq, M., Khan, I. U., Zia-ur-Rehman, M., Arshad, M. N. & Asiri, A. M. (2011b). *Acta Cryst.* E**67**, o2092.
Shafiq, M., Zia-ur-Rehman, M., Khan, I. U., Arshad, M. N. & Khan, S. A. (2011). *J. Chil. Chem. Soc.* **56**, 527–531.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.

supplementary materials

1-Methyl-4-[1-(1-phenylethylidene)-hydrazin-2-ylidene]-3,4-dihydro-1*H*-2λ⁶,1-benzothiazine-2,2-dione

Muhammad Shafiq, Islam Ullah Khan, Muhammad Zia-ur-Rehman, Tariq Mahmood, Muhammad Ashfaq and Saeed Ahmad

Comment

The present structure is analogue to 1-ethyl-4-[1-(1-phenylethylidene)-hydrazin-2-ylidene]-3,4-dihydro-1*H*- 2λ⁶,1-benzo-thiazine-2,2-dione(II) (Shafiq *et al.*, 2012) and related to 4-hydrazinylidene-1-methyl-3*H*-2λ⁶,1-benzothiazine-2,2-dione (III) (Shafiq, Khan *et al.*, 2011*a*) and 6-bromo-1-methyl-4-[2- (4-methylbenzylidene)hydrazinylidene]-3*H*-2λ⁶, 1-benzo-thiazine-2,2-dione (IV) (Shafiq, Khan *et al.*, 2011*b*). The structure of molecule looks planer as the plane generated from atoms (C1–C7/C9–C15/N1) showes an r.m.s. deviation of 0.0365 Å, while atoms S1 and C16 show maximum deviations of 0.702 (2) and -0.256 (4) Å, respectively. The fused aromatic ring and the mean plane of the thiazine ring are oriented at a dihedral angle of 9.34 (14)° and thiazine ring adopted sofa shape with an r.m.s. deviation of 0.233 (2)°. Comparison of dihedral angles between the phenyl and fused aromatic rings in I and II [*i.e.* 1.17 (14) and 79.33 (2)°, respectively] also explain the planarity of title compound. Similarly dihedral angles between the phenyl and thiazine rings in I and II are 9.34 (2) and 69.74 (6)°, respectively. An intermolecular hydrogen bonding interaction of C—H···O type connects the molecule along the *a* axis and generates a chain structure (Table 1 and Fig. 2). In the group R_2C=N—N=C(CH$_3$)Ar, the configurations around the two double bonds are *Z* and *E*, respectively.

Experimental

In the synthesis of title compound, 4-hydrazinylidene-1- methyl-3*H*-2λ⁶,1-benzothiazine-2,2-dione (Shafiq, Khan *et al.*, 2011*a*) was subjected to react with acetophenone according to literature procedure (Shafiq, Zia-ur-Rehman *et al.*, 2011). The product obtained was then recrystallized in ethylacetate under slow evaporation to obtain single crystals suitable for X-ray diffraction.

Refinement

All H atoms were positioned with idealized geometry with C—H = 0.93 Å for aromatic, 0.96 Å for methyl group and 0.97 Å for methylene and were refined using a riding model, with U_{iso}(H) = 1.2U_{eq}(C) for aromatic and methylene, and U_{iso}(H) = 1.5U_{eq}(C) for methyl carbon atoms. Two reflections (0 1 1) and (0 0 2) were omitted in the final refinement.

Computing details

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT* (Bruker, 2007); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2009); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *PLATON* (Spek, 2009).
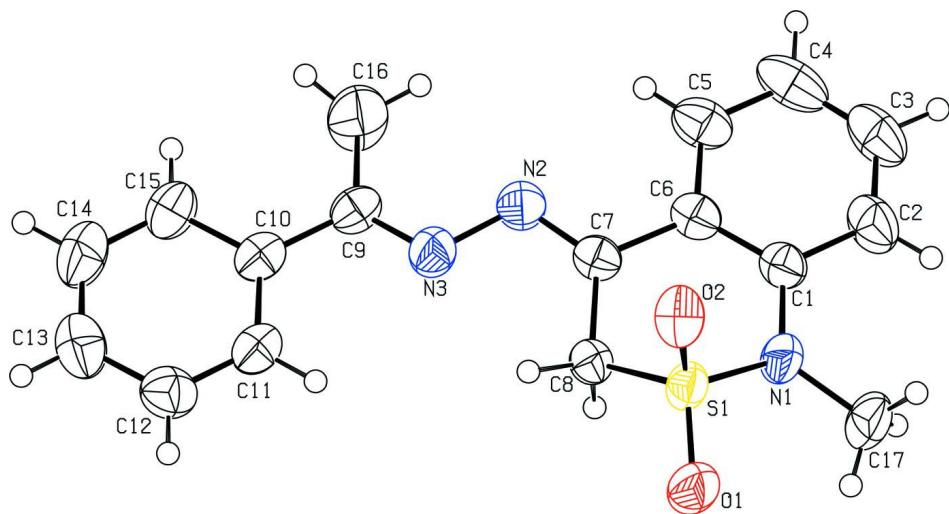
Figure 1

The molecular structure of the title compound, with 50% displacement ellipsoids for non-H atoms.
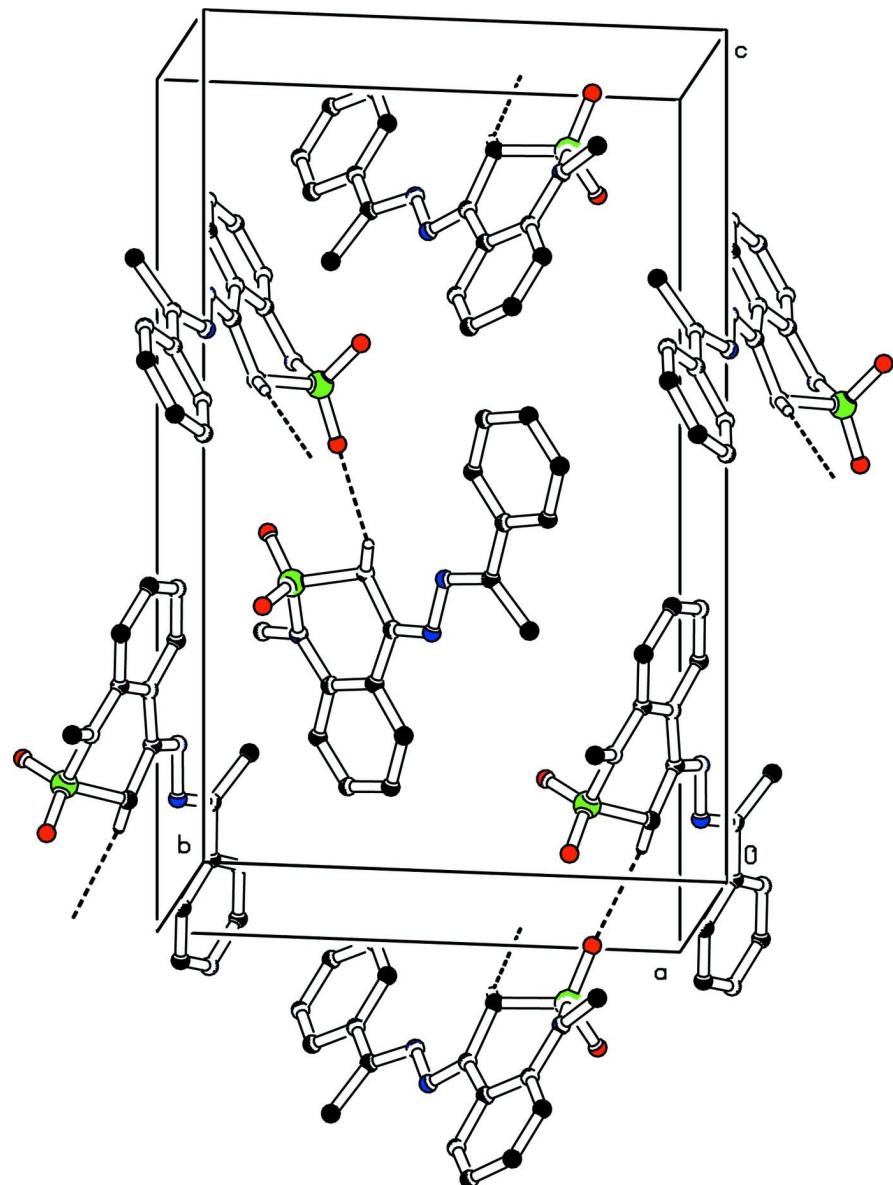
Figure 2

A packing diagram, showing C—H···O hydrogen bonds (dashed lines).

1-Methyl-4-[1-(1-phenylethylidene)-hydrazin-2-ylidene]-3,4-dihydro-1H- 2λ⁶,1-benzothiazine-2,2-dione

Crystal data

$C_{17}H_{17}N_3O_2S$	$F(000) = 688$
$M_r = 327.40$	$D_x = 1.347$ Mg m^{-3}
Orthorhombic, $P2_12_12_1$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: P 2ac 2ab	Cell parameters from 2415 reflections
$a = 6.6678$ (2) Å	$\theta = 2.6$–21.1°
$b = 12.0783$ (6) Å	$\mu = 0.21$ mm^{-1}
$c = 20.0529$ (8) Å	$T = 296$ K
$V = 1614.97$ (11) Å^3	Needle, colorless
$Z = 4$	$0.38 \times 0.11 \times 0.07$ mm

Data collection

Bruker Kappa APEXII CCD diffractometer	9111 measured reflections
Radiation source: fine-focus sealed tube	3830 independent reflections
Graphite monochromator	2819 reflections with $I > 2\sigma(I)$
φ and ω scans	$R_{\text{int}} = 0.030$
Absorption correction: multi-scan (*SADABS*; Bruker, 2007)	$\theta_{\text{max}} = 28.3°$, $\theta_{\text{min}} = 2.0°$
	$h = -8 \rightarrow 6$
	$k = -16 \rightarrow 13$
$T_{\text{min}} = 0.923$, $T_{\text{max}} = 0.985$	$l = -26 \rightarrow 18$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	
$R[F^2 > 2\sigma(F^2)] = 0.045$	H-atom parameters constrained
$wR(F^2) = 0.108$	$w = 1/[\sigma^2(F_o^2) + (0.0554P)^2 + 0.0282P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.97$	
3828 reflections	$(\Delta/\sigma)_{\text{max}} = 0.007$
210 parameters	$\Delta\rho_{\text{max}} = 0.21$ e Å^{-3}
0 restraints	$\Delta\rho_{\text{min}} = -0.27$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Absolute structure: Flack (1983), 1577 Friedel pairs
Secondary atom site location: difference Fourier map	Flack parameter: −0.06 (9)

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 $F^2 > \sigma(F^2)$ 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	−0.0436 (3)	0.1646 (2)	0.19872 (12)	0.0434 (6)
C2	−0.1882 (4)	0.1755 (3)	0.24813 (14)	0.0607 (8)
H2	−0.2979	0.2216	0.2412	0.073*
C3	−0.1708 (5)	0.1190 (3)	0.30686 (14)	0.0689 (9)
H3	−0.2704	0.1259	0.3390	0.083*
C4	−0.0087 (5)	0.0522 (3)	0.31910 (14)	0.0703 (9)
H4	0.0036	0.0154	0.3596	0.084*
C5	0.1365 (5)	0.0404 (2)	0.27030 (12)	0.0592 (7)
H5	0.2473	−0.0044	0.2785	0.071*
C6	0.1196 (4)	0.09462 (19)	0.20875 (11)	0.0425 (5)
C7	0.2735 (3)	0.07398 (19)	0.15723 (11)	0.0401 (5)
C8	0.2426 (3)	0.12341 (18)	0.08901 (11)	0.0394 (5)
H8A	0.1559	0.0756	0.0629	0.047*
H8B	0.3705	0.1291	0.0662	0.047*
C9	0.6894 (3)	−0.07684 (19)	0.12801 (12)	0.0448 (6)

C10	0.8400 (3)	−0.08935 (19)	0.07412 (12)	0.0446 (6)
C11	0.8205 (4)	−0.0311 (2)	0.01409 (12)	0.0485 (6)
H11	0.7109	0.0153	0.0078	0.058*
C12	0.9605 (4)	−0.0414 (2)	−0.03551 (13)	0.0573 (7)
H12	0.9457	−0.0014	−0.0748	0.069*
C13	1.1223 (4)	−0.1103 (3)	−0.02763 (15)	0.0666 (8)
H13	1.2158	−0.1178	−0.0617	0.080*
C14	1.1456 (4)	−0.1680 (3)	0.03080 (16)	0.0723 (8)
H14	1.2560	−0.2141	0.0365	0.087*
C15	1.0061 (4)	−0.1578 (2)	0.08111 (15)	0.0571 (7)
H15	1.0234	−0.1975	0.1204	0.068*
C16	0.6984 (5)	−0.1505 (3)	0.18763 (15)	0.0859 (11)
H16A	0.6132	−0.1214	0.2220	0.129*
H16B	0.8339	−0.1541	0.2037	0.129*
H16C	0.6538	−0.2234	0.1756	0.129*
C17	−0.2573 (3)	0.2746 (2)	0.12031 (13)	0.0601 (8)
H17A	−0.3647	0.2230	0.1275	0.090*
H17B	−0.2542	0.2957	0.0742	0.090*
H17C	−0.2782	0.3391	0.1474	0.090*
N1	−0.0679 (3)	0.22309 (19)	0.13822 (10)	0.0543 (6)
N2	0.4234 (3)	0.01227 (18)	0.17172 (10)	0.0500 (5)
N3	0.5596 (3)	−0.00040 (18)	0.11964 (10)	0.0508 (5)
O1	0.0707 (2)	0.29407 (17)	0.03230 (9)	0.0663 (6)
O2	0.2661 (2)	0.32168 (14)	0.13476 (9)	0.0559 (5)
S1	0.13459 (7)	0.25435 (5)	0.09576 (3)	0.04299 (16)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0355 (12)	0.0530 (15)	0.0417 (13)	−0.0110 (11)	0.0034 (10)	−0.0029 (11)
C2	0.0496 (15)	0.073 (2)	0.0592 (17)	−0.0102 (14)	0.0168 (12)	−0.0038 (15)
C3	0.072 (2)	0.080 (2)	0.0548 (18)	−0.0237 (17)	0.0264 (15)	−0.0051 (16)
C4	0.103 (2)	0.063 (2)	0.0452 (16)	−0.0274 (18)	0.0170 (17)	0.0015 (14)
C5	0.0776 (17)	0.0510 (16)	0.0489 (16)	−0.0075 (15)	0.0031 (15)	0.0062 (12)
C6	0.0466 (13)	0.0416 (13)	0.0392 (12)	−0.0097 (11)	0.0021 (11)	−0.0003 (10)
C7	0.0427 (12)	0.0382 (12)	0.0395 (13)	−0.0067 (10)	0.0019 (10)	0.0023 (10)
C8	0.0385 (12)	0.0417 (12)	0.0380 (12)	−0.0005 (9)	0.0027 (10)	0.0002 (11)
C9	0.0459 (13)	0.0354 (13)	0.0531 (14)	−0.0007 (10)	−0.0081 (11)	0.0037 (11)
C10	0.0443 (13)	0.0360 (12)	0.0536 (14)	−0.0027 (10)	−0.0086 (11)	−0.0010 (10)
C11	0.0454 (13)	0.0447 (15)	0.0555 (16)	0.0030 (11)	−0.0077 (11)	0.0006 (12)
C12	0.0661 (17)	0.0553 (17)	0.0506 (16)	−0.0018 (14)	−0.0047 (14)	−0.0050 (13)
C13	0.0637 (17)	0.067 (2)	0.0694 (19)	0.0017 (16)	0.0120 (16)	−0.0144 (17)
C14	0.0625 (17)	0.064 (2)	0.090 (2)	0.0226 (16)	0.0003 (18)	−0.0040 (17)
C15	0.0568 (15)	0.0448 (15)	0.0695 (18)	0.0119 (12)	−0.0036 (14)	0.0044 (13)
C16	0.096 (2)	0.080 (2)	0.081 (2)	0.0307 (19)	0.0198 (18)	0.0376 (19)
C17	0.0329 (12)	0.075 (2)	0.0724 (18)	0.0058 (12)	−0.0040 (11)	−0.0046 (15)
N1	0.0322 (9)	0.0787 (17)	0.0521 (12)	0.0092 (10)	0.0048 (8)	0.0099 (12)
N2	0.0512 (12)	0.0504 (13)	0.0486 (12)	0.0059 (10)	0.0022 (9)	0.0078 (10)
N3	0.0485 (11)	0.0534 (13)	0.0506 (13)	0.0095 (10)	0.0044 (9)	0.0074 (10)
O1	0.0577 (10)	0.0845 (15)	0.0567 (11)	0.0191 (10)	0.0038 (9)	0.0243 (10)

| O2 | 0.0494 (9) | 0.0457 (10) | 0.0726 (12) | −0.0038 (8) | 0.0088 (9) | −0.0036 (9) |
| S1 | 0.0344 (3) | 0.0471 (3) | 0.0475 (3) | 0.0042 (3) | 0.0046 (2) | 0.0087 (3) |

Geometric parameters (Å, º)

C1—C2	1.389 (3)	C10—C11	1.400 (3)
C1—C6	1.392 (3)	C11—C12	1.369 (3)
C1—N1	1.413 (3)	C11—H11	0.9300
C2—C3	1.366 (4)	C12—C13	1.371 (4)
C2—H2	0.9300	C12—H12	0.9300
C3—C4	1.371 (4)	C13—C14	1.372 (4)
C3—H3	0.9300	C13—H13	0.9300
C4—C5	1.384 (4)	C14—C15	1.378 (4)
C4—H4	0.9300	C14—H14	0.9300
C5—C6	1.402 (3)	C15—H15	0.9300
C5—H5	0.9300	C16—H16A	0.9600
C6—C7	1.477 (3)	C16—H16B	0.9600
C7—N2	1.280 (3)	C16—H16C	0.9600
C7—C8	1.507 (3)	C17—N1	1.453 (3)
C8—S1	1.743 (2)	C17—H17A	0.9600
C8—H8A	0.9700	C17—H17B	0.9600
C8—H8B	0.9700	C17—H17C	0.9600
C9—N3	1.277 (3)	N1—S1	1.6402 (19)
C9—C10	1.483 (3)	N2—N3	1.392 (3)
C9—C16	1.491 (3)	O1—S1	1.4251 (18)
C10—C15	1.389 (3)	O2—S1	1.4288 (18)
C2—C1—C6	119.8 (2)	C11—C12—C13	120.5 (3)
C2—C1—N1	119.0 (2)	C11—C12—H12	119.8
C6—C1—N1	121.14 (19)	C13—C12—H12	119.8
C3—C2—C1	120.6 (3)	C14—C13—C12	119.7 (3)
C3—C2—H2	119.7	C14—C13—H13	120.1
C1—C2—H2	119.7	C12—C13—H13	120.1
C2—C3—C4	121.0 (3)	C13—C14—C15	120.2 (3)
C2—C3—H3	119.5	C13—C14—H14	119.9
C4—C3—H3	119.5	C15—C14—H14	119.9
C3—C4—C5	119.1 (3)	C14—C15—C10	121.1 (3)
C3—C4—H4	120.5	C14—C15—H15	119.4
C5—C4—H4	120.5	C10—C15—H15	119.4
C4—C5—C6	121.2 (3)	C9—C16—H16A	109.5
C4—C5—H5	119.4	C9—C16—H16B	109.5
C6—C5—H5	119.4	H16A—C16—H16B	109.5
C1—C6—C5	118.3 (2)	C9—C16—H16C	109.5
C1—C6—C7	123.0 (2)	H16A—C16—H16C	109.5
C5—C6—C7	118.8 (2)	H16B—C16—H16C	109.5
N2—C7—C6	118.8 (2)	N1—C17—H17A	109.5
N2—C7—C8	122.9 (2)	N1—C17—H17B	109.5
C6—C7—C8	118.23 (19)	H17A—C17—H17B	109.5
C7—C8—S1	110.21 (16)	N1—C17—H17C	109.5
C7—C8—H8A	109.6	H17A—C17—H17C	109.5

S1—C8—H8A	109.6	H17B—C17—H17C	109.5
C7—C8—H8B	109.6	C1—N1—C17	121.73 (19)
S1—C8—H8B	109.6	C1—N1—S1	117.79 (15)
H8A—C8—H8B	108.1	C17—N1—S1	119.25 (17)
N3—C9—C10	115.9 (2)	C7—N2—N3	113.76 (19)
N3—C9—C16	124.3 (2)	C9—N3—N2	115.0 (2)
C10—C9—C16	119.7 (2)	O1—S1—O2	118.72 (12)
C15—C10—C11	117.4 (2)	O1—S1—N1	107.15 (10)
C15—C10—C9	121.8 (2)	O2—S1—N1	110.61 (11)
C11—C10—C9	120.8 (2)	O1—S1—C8	111.07 (12)
C12—C11—C10	121.0 (2)	O2—S1—C8	107.78 (10)
C12—C11—H11	119.5	N1—S1—C8	99.87 (11)
C10—C11—H11	119.5		
C6—C1—C2—C3	0.7 (4)	C11—C12—C13—C14	−1.0 (4)
N1—C1—C2—C3	179.1 (2)	C12—C13—C14—C15	0.7 (5)
C1—C2—C3—C4	1.4 (5)	C13—C14—C15—C10	−0.2 (5)
C2—C3—C4—C5	−1.5 (5)	C11—C10—C15—C14	−0.1 (4)
C3—C4—C5—C6	−0.5 (4)	C9—C10—C15—C14	−179.5 (2)
C2—C1—C6—C5	−2.6 (3)	C2—C1—N1—C17	−13.5 (4)
N1—C1—C6—C5	179.0 (2)	C6—C1—N1—C17	164.9 (2)
C2—C1—C6—C7	176.5 (2)	C2—C1—N1—S1	153.8 (2)
N1—C1—C6—C7	−1.8 (3)	C6—C1—N1—S1	−27.8 (3)
C4—C5—C6—C1	2.5 (4)	C6—C7—N2—N3	−179.38 (19)
C4—C5—C6—C7	−176.7 (2)	C8—C7—N2—N3	2.9 (3)
C1—C6—C7—N2	176.9 (2)	C10—C9—N3—N2	−178.1 (2)
C5—C6—C7—N2	−3.9 (3)	C16—C9—N3—N2	1.0 (4)
C1—C6—C7—C8	−5.3 (3)	C7—N2—N3—C9	−167.5 (2)
C5—C6—C7—C8	173.8 (2)	C1—N1—S1—O1	169.67 (19)
N2—C7—C8—S1	−145.02 (19)	C17—N1—S1—O1	−22.8 (2)
C6—C7—C8—S1	37.3 (2)	C1—N1—S1—O2	−59.5 (2)
N3—C9—C10—C15	170.5 (2)	C17—N1—S1—O2	108.0 (2)
C16—C9—C10—C15	−8.7 (4)	C1—N1—S1—C8	53.8 (2)
N3—C9—C10—C11	−8.9 (3)	C17—N1—S1—C8	−138.6 (2)
C16—C9—C10—C11	172.0 (3)	C7—C8—S1—O1	−169.41 (15)
C15—C10—C11—C12	−0.2 (4)	C7—C8—S1—O2	58.95 (17)
C9—C10—C11—C12	179.2 (2)	C7—C8—S1—N1	−56.59 (17)
C10—C11—C12—C13	0.7 (4)		

Hydrogen-bond geometry (Å, º)

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
C8—H8B⋯O1[i]	0.97	2.56	3.420 (3)	148

Symmetry code: (i) x+1/2, −y+1/2, −z.