

6-Bromo-1-methyl-4-[2-(4-methylbenzylidene)hydrazinylidene]-3H-2λ⁶,1-benzothiazine-2,2-dione

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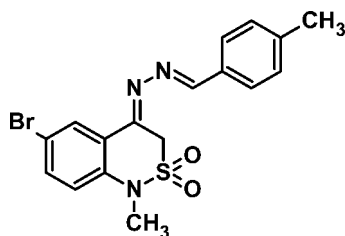
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Key indicators: single-crystal X-ray study; $T = 296$ K; mean $\sigma(\text{C}-\text{C}) = 0.004$ Å; R factor = 0.034; wR factor = 0.078; data-to-parameter ratio = 18.7.

In the title compound, $\text{C}_{17}\text{H}_{16}\text{BrN}_3\text{O}_2\text{S}$, the two fused rings are twisted by a dihedral angle of $6.61(15)^\circ$. The thiazine ring adopts a sofa conformation. The toluene ring is oriented at dihedral angles of $15.5(2)$ and $20.6(2)^\circ$ with respect to the bromobenzene and thiazine rings, respectively. The benzylidene system is approximately planar [r.m.s. deviation = 0.0388 Å]. In the crystal, weak intermolecular $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds connects the molecules into a chain along the b axis.

Related literature

For the synthesis of the title compound, see: Shafiq *et al.* (2011). For related structures, see: Khan *et al.* (2010); Shafiq *et al.* (2009); Arshad *et al.* (2009).



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Experimental

Crystal data

$\text{C}_{17}\text{H}_{16}\text{BrN}_3\text{O}_2\text{S}$
 $M_r = 406.30$
 Monoclinic, $P2_1$
 $a = 9.1077(6)$ Å
 $b = 6.8328(4)$ Å
 $c = 14.1765(9)$ Å
 $\beta = 96.807(3)^\circ$

$V = 876.00(10)$ Å³
 $Z = 2$
 Mo $K\alpha$ radiation
 $\mu = 2.48$ mm⁻¹
 $T = 296$ K
 $0.32 \times 0.12 \times 0.10$ mm

Data collection

Bruker Kappa APEXII CCD diffractometer
 Absorption correction: multi-scan (SADABS; Bruker, 2007)
 $T_{\min} = 0.504$, $T_{\max} = 0.790$

10166 measured reflections
 4119 independent reflections
 2881 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.026$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.034$
 $wR(F^2) = 0.078$
 $S = 0.97$
 4119 reflections
 220 parameters
 1 restraint

H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.29$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.36$ e Å⁻³
 Absolute structure: Flack (1983), 1771 Friedel pairs
 Flack parameter: 0.004 (8)

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{C}17-\text{H}17\text{C}\cdots\text{O}1^i$	0.96	2.64	3.546 (5)	158

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

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.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PV2429).

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supplementary materials

Acta Cryst. (2011). E67, o2092 [doi:10.1107/S1600536811028406]

6-Bromo-1-methyl-4-[2-(4-methylbenzylidene)hydrazinylidene]-3*H*-2λ⁶,1-benzothiazine-2,2-dione

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Comment

In the title molecule (Fig. 1), the thiazine ring adopts a sofa conformation which is similar to the conformation of the corresponding ring in a previously reported compound, 1-propyl-1*H*-2,1-benzothiazin-4(3*H*)-one 2,2-dioxide (Khan *et al.*, 2010). The aromatic ring (C1—C6) in the title compound is twisted at 15.5 (2)° with respect to the toluene ring (C10—C15). The benzylidene moiety (C9—C16/N1/N2) is also very near to planarity as showing the r. m. s. deviation of 0.0388 Å and is oriented at a dihedral angle 15.02 (12)° with respect to the benzene ring (C1—C6). The fused aromatic (C1—C6) and thiazine (C1/C6/C7/C8/N1/S1) rings are twisted at a dihedral angle 6.61 (15)°. The oxygen atom from SO₂ group is involved in weak C—H···O type hydrogen bonding interaction, which connects the molecules in a zig-zag mode along the *b*-axis.

The crystal structures of several molecules related to the title compound have been reported (Arshad *et al.*, 2009; Shafiq *et al.*, 2009).

Experimental

The synthesis of the title compound has already been reported (Shafiq *et al.*, 2011). It was recrystallized from a solution in dry ethanol.

Refinement

All H-atoms were positioned at idealized geometry with C_{aromatic}—H = 0.93 Å and C_{methyl}—H = 0.96 Å and were refined using a riding model with $U_{\text{iso}}(\text{H}) = 1.2 U_{\text{eq}}(\text{C})$ for aromatic & $U_{\text{iso}}(\text{H}) = 1.5 U_{\text{eq}}(\text{C})$ for methyl carbon atoms. The reflection 0 0 1 has been omitted in final refinement. An absolute structure was determined (Flack, 1983) using 1771 Friedel pairs.

Figures

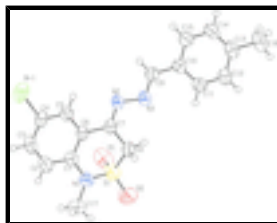


Fig. 1. The *ORTEP* diagram of the title molecule showing the thermal ellipsoids drawn at 50% probability level.

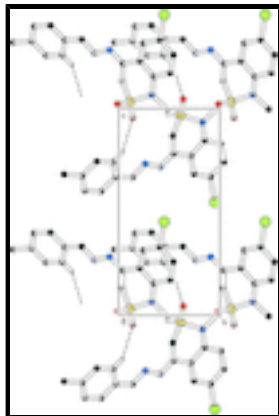


Fig. 2. A unit cell diagram of the title compound showing C—H...O type interactions using dashed lines.

6-Bromo-1-methyl-4-[2-(4-methylbenzylidene)hydrazinylidene]-3H-2λ⁶,1-benzothiazine-2,2-dione

Crystal data

C₁₇H₁₆BrN₃O₂S

M_r = 406.30

Monoclinic, *P*2₁

Hall symbol: P 2yb

a = 9.1077 (6) Å

b = 6.8328 (4) Å

c = 14.1765 (9) Å

β = 96.807 (3)°

V = 876.00 (10) Å³

Z = 2

F(000) = 412

D_x = 1.540 Mg m⁻³

Mo *K*α radiation, λ = 0.71073 Å

Cell parameters from 3801 reflections

θ = 2.3–23.7°

μ = 2.48 mm⁻¹

T = 296 K

Needle, yellow

0.32 × 0.12 × 0.10 mm

Data collection

Bruker Kappa APEXII CCD
diffractometer

Radiation source: fine-focus sealed tube
graphite

φ and ω scans

Absorption correction: multi-scan
(*SADABS*; Bruker, 2007)

T_{min} = 0.504, *T_{max}* = 0.790

10166 measured reflections

4119 independent reflections

2881 reflections with *I* > 2σ(*I*)

R_{int} = 0.026

θ_{max} = 28.3°, θ_{min} = 2.5°

h = -12→12

k = -8→9

l = -18→18

Refinement

Refinement on *F*²

Least-squares matrix: full

R[*F*² > 2σ(*F*²)] = 0.034

wR(*F*²) = 0.078

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

w = 1/[σ²(*F_o*²) + (0.0256*P*)²]

$S = 0.97$	where $P = (F_o^2 + 2F_c^2)/3$
4119 reflections	$(\Delta/\sigma)_{\max} = 0.018$
220 parameters	$\Delta\rho_{\max} = 0.29 \text{ e } \text{\AA}^{-3}$
1 restraint	$\Delta\rho_{\min} = -0.36 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods	Absolute structure: Flack (1983), 1771 Friedel pairs Flack parameter: 0.004 (8)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Br1	1.13358 (4)	1.44957 (7)	0.45270 (2)	0.08174 (14)
S1	0.72100 (10)	1.11072 (10)	0.03233 (5)	0.0611 (2)
O1	0.8404 (3)	0.9855 (3)	0.02125 (18)	0.0855 (8)
O2	0.6089 (3)	1.1379 (5)	-0.04538 (16)	0.0999 (9)
N1	0.7821 (3)	1.3277 (3)	0.06656 (16)	0.0589 (6)
N2	0.7702 (3)	0.9100 (3)	0.28328 (17)	0.0519 (6)
N3	0.6650 (3)	0.7615 (3)	0.26789 (18)	0.0556 (6)
C1	0.8667 (3)	1.3470 (4)	0.1553 (2)	0.0464 (6)
C2	0.9579 (4)	1.5101 (4)	0.1724 (2)	0.0590 (8)
H2	0.9654	1.5998	0.1238	0.071*
C3	1.0369 (4)	1.5402 (4)	0.2599 (2)	0.0625 (8)
H3	1.0959	1.6509	0.2707	0.075*
C4	1.0285 (3)	1.4062 (4)	0.3312 (2)	0.0539 (7)
C5	0.9427 (3)	1.2426 (4)	0.31626 (19)	0.0472 (7)
H5	0.9405	1.1516	0.3648	0.057*
C6	0.8585 (3)	1.2109 (4)	0.22905 (18)	0.0422 (6)
C7	0.7585 (3)	1.0412 (4)	0.21833 (19)	0.0430 (6)
C8	0.6452 (3)	1.0352 (4)	0.13283 (19)	0.0529 (7)
H8A	0.5630	1.1198	0.1430	0.063*
H8B	0.6077	0.9029	0.1235	0.063*
C9	0.6761 (3)	0.6340 (4)	0.3337 (2)	0.0497 (7)
H9	0.7494	0.6483	0.3847	0.060*
C10	0.5776 (3)	0.4669 (4)	0.33129 (17)	0.0448 (6)
C11	0.4620 (3)	0.4417 (5)	0.25878 (18)	0.0513 (6)
H11	0.4457	0.5356	0.2112	0.062*

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C12	0.3723 (4)	0.2815 (4)	0.2565 (2)	0.0572 (8)
H12	0.2944	0.2689	0.2082	0.069*
C13	0.3960 (4)	0.1366 (4)	0.3257 (2)	0.0607 (8)
C14	0.5088 (4)	0.1620 (4)	0.3977 (2)	0.0614 (8)
H14	0.5244	0.0681	0.4454	0.074*
C15	0.5999 (3)	0.3245 (4)	0.4010 (2)	0.0562 (7)
H15	0.6763	0.3382	0.4503	0.067*
C16	0.2981 (4)	-0.0437 (6)	0.3201 (3)	0.0892 (11)
H16A	0.3586	-0.1589	0.3278	0.134*
H16B	0.2389	-0.0476	0.2594	0.134*
H16C	0.2347	-0.0387	0.3695	0.134*
C17	0.7742 (4)	1.4824 (6)	-0.0046 (3)	0.0913 (12)
H17A	0.7455	1.6028	0.0230	0.137*
H17B	0.7025	1.4480	-0.0572	0.137*
H17C	0.8693	1.4984	-0.0264	0.137*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0823 (2)	0.0930 (2)	0.0655 (2)	-0.0207 (2)	-0.00971 (15)	-0.02718 (19)
S1	0.0823 (6)	0.0609 (4)	0.0395 (4)	-0.0132 (4)	0.0050 (4)	-0.0079 (3)
O1	0.1165 (19)	0.0679 (16)	0.0801 (16)	-0.0059 (15)	0.0453 (14)	-0.0163 (13)
O2	0.135 (2)	0.106 (2)	0.0500 (14)	-0.0347 (17)	-0.0242 (15)	0.0036 (13)
N1	0.0768 (18)	0.0526 (13)	0.0453 (13)	-0.0107 (13)	-0.0011 (12)	0.0057 (11)
N2	0.0566 (14)	0.0422 (13)	0.0553 (14)	-0.0149 (11)	-0.0005 (11)	0.0018 (11)
N3	0.0606 (16)	0.0462 (13)	0.0585 (15)	-0.0122 (11)	0.0003 (12)	0.0013 (11)
C1	0.0480 (17)	0.0447 (14)	0.0479 (16)	-0.0029 (12)	0.0112 (13)	-0.0047 (12)
C2	0.069 (2)	0.0496 (17)	0.0604 (19)	-0.0148 (15)	0.0168 (16)	0.0001 (13)
C3	0.063 (2)	0.0513 (16)	0.074 (2)	-0.0220 (14)	0.0096 (17)	-0.0113 (16)
C4	0.0504 (16)	0.0603 (19)	0.0498 (16)	-0.0115 (14)	0.0015 (12)	-0.0193 (14)
C5	0.0506 (17)	0.0493 (15)	0.0419 (15)	-0.0055 (12)	0.0064 (13)	-0.0036 (12)
C6	0.0419 (16)	0.0429 (13)	0.0422 (14)	-0.0058 (12)	0.0077 (12)	-0.0066 (11)
C7	0.0435 (16)	0.0438 (13)	0.0420 (14)	-0.0043 (12)	0.0063 (12)	-0.0083 (12)
C8	0.0521 (18)	0.0549 (15)	0.0515 (17)	-0.0131 (13)	0.0055 (14)	-0.0046 (13)
C9	0.0485 (16)	0.0483 (15)	0.0516 (16)	-0.0026 (13)	0.0036 (13)	-0.0007 (13)
C10	0.0486 (15)	0.0410 (13)	0.0463 (14)	0.0012 (14)	0.0120 (11)	0.0020 (13)
C11	0.0622 (17)	0.0427 (13)	0.0493 (14)	-0.0018 (17)	0.0083 (13)	0.0008 (15)
C12	0.060 (2)	0.0536 (16)	0.0583 (17)	-0.0074 (15)	0.0075 (15)	-0.0110 (15)
C13	0.064 (2)	0.0451 (15)	0.076 (2)	-0.0061 (15)	0.0235 (18)	-0.0048 (15)
C14	0.067 (2)	0.0470 (16)	0.073 (2)	-0.0025 (15)	0.0199 (18)	0.0145 (15)
C15	0.0551 (19)	0.0550 (16)	0.0592 (18)	0.0025 (15)	0.0101 (14)	0.0057 (15)
C16	0.088 (2)	0.0594 (18)	0.123 (3)	-0.027 (2)	0.025 (2)	-0.007 (3)
C17	0.094 (3)	0.085 (3)	0.089 (3)	-0.005 (2)	-0.015 (2)	0.034 (2)

Geometric parameters (\AA , $^\circ$)

Br1—C4	1.892 (3)	C8—H8A	0.9700
S1—O1	1.407 (3)	C8—H8B	0.9700
S1—O2	1.423 (3)	C9—C10	1.450 (4)

S1—N1	1.637 (3)	C9—H9	0.9300
S1—C8	1.734 (3)	C10—C15	1.384 (4)
N1—C1	1.402 (4)	C10—C11	1.392 (4)
N1—C17	1.457 (4)	C11—C12	1.364 (4)
N2—C7	1.281 (3)	C11—H11	0.9300
N2—N3	1.394 (3)	C12—C13	1.392 (4)
N3—C9	1.271 (3)	C12—H12	0.9300
C1—C2	1.394 (4)	C13—C14	1.371 (5)
C1—C6	1.408 (4)	C13—C16	1.518 (5)
C2—C3	1.374 (4)	C14—C15	1.384 (4)
C2—H2	0.9300	C14—H14	0.9300
C3—C4	1.373 (4)	C15—H15	0.9300
C3—H3	0.9300	C16—H16A	0.9600
C4—C5	1.366 (4)	C16—H16B	0.9600
C5—C6	1.392 (4)	C16—H16C	0.9600
C5—H5	0.9300	C17—H17A	0.9600
C6—C7	1.471 (4)	C17—H17B	0.9600
C7—C8	1.496 (4)	C17—H17C	0.9600
O1—S1—O2	119.10 (17)	S1—C8—H8B	109.5
O1—S1—N1	110.09 (15)	H8A—C8—H8B	108.1
O2—S1—N1	107.38 (15)	N3—C9—C10	121.9 (3)
O1—S1—C8	107.40 (14)	N3—C9—H9	119.1
O2—S1—C8	110.87 (15)	C10—C9—H9	119.1
N1—S1—C8	100.39 (13)	C15—C10—C11	118.3 (3)
C1—N1—C17	122.0 (3)	C15—C10—C9	119.9 (3)
C1—N1—S1	118.89 (18)	C11—C10—C9	121.7 (3)
C17—N1—S1	117.7 (2)	C12—C11—C10	121.0 (3)
C7—N2—N3	113.6 (2)	C12—C11—H11	119.5
C9—N3—N2	113.0 (2)	C10—C11—H11	119.5
C2—C1—N1	118.9 (3)	C11—C12—C13	120.7 (3)
C2—C1—C6	118.8 (3)	C11—C12—H12	119.6
N1—C1—C6	122.2 (2)	C13—C12—H12	119.6
C3—C2—C1	120.9 (3)	C14—C13—C12	118.4 (3)
C3—C2—H2	119.5	C14—C13—C16	121.7 (3)
C1—C2—H2	119.5	C12—C13—C16	119.9 (3)
C2—C3—C4	119.7 (3)	C13—C14—C15	121.3 (3)
C2—C3—H3	120.1	C13—C14—H14	119.3
C4—C3—H3	120.1	C15—C14—H14	119.3
C5—C4—C3	120.8 (3)	C14—C15—C10	120.2 (3)
C5—C4—Br1	119.2 (2)	C14—C15—H15	119.9
C3—C4—Br1	120.0 (2)	C10—C15—H15	119.9
C4—C5—C6	120.7 (3)	C13—C16—H16A	109.5
C4—C5—H5	119.7	C13—C16—H16B	109.5
C6—C5—H5	119.7	H16A—C16—H16B	109.5
C5—C6—C1	119.0 (2)	C13—C16—H16C	109.5
C5—C6—C7	118.9 (2)	H16A—C16—H16C	109.5
C1—C6—C7	122.0 (2)	H16B—C16—H16C	109.5
N2—C7—C6	118.7 (2)	N1—C17—H17A	109.5
N2—C7—C8	123.6 (2)	N1—C17—H17B	109.5

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C6—C7—C8	117.7 (2)	H17A—C17—H17B	109.5
C7—C8—S1	110.75 (19)	N1—C17—H17C	109.5
C7—C8—H8A	109.5	H17A—C17—H17C	109.5
S1—C8—H8A	109.5	H17B—C17—H17C	109.5
C7—C8—H8B	109.5		
O1—S1—N1—C1	-64.2 (3)	N3—N2—C7—C6	177.0 (2)
O2—S1—N1—C1	164.7 (2)	N3—N2—C7—C8	-1.1 (4)
C8—S1—N1—C1	48.8 (2)	C5—C6—C7—N2	-11.9 (4)
O1—S1—N1—C17	102.5 (3)	C1—C6—C7—N2	171.1 (3)
O2—S1—N1—C17	-28.6 (3)	C5—C6—C7—C8	166.3 (2)
C8—S1—N1—C17	-144.5 (3)	C1—C6—C7—C8	-10.6 (4)
C7—N2—N3—C9	-178.8 (2)	N2—C7—C8—S1	-139.9 (2)
C17—N1—C1—C2	-6.8 (4)	C6—C7—C8—S1	41.9 (3)
S1—N1—C1—C2	159.2 (2)	O1—S1—C8—C7	58.5 (2)
C17—N1—C1—C6	170.8 (3)	O2—S1—C8—C7	-169.9 (2)
S1—N1—C1—C6	-23.1 (4)	N1—S1—C8—C7	-56.6 (2)
N1—C1—C2—C3	176.7 (3)	N2—N3—C9—C10	-179.8 (2)
C6—C1—C2—C3	-1.1 (4)	N3—C9—C10—C15	175.6 (3)
C1—C2—C3—C4	1.3 (5)	N3—C9—C10—C11	-2.7 (4)
C2—C3—C4—C5	0.2 (5)	C15—C10—C11—C12	0.3 (4)
C2—C3—C4—Br1	-178.6 (2)	C9—C10—C11—C12	178.6 (3)
C3—C4—C5—C6	-1.8 (4)	C10—C11—C12—C13	-1.4 (4)
Br1—C4—C5—C6	177.0 (2)	C11—C12—C13—C14	2.1 (4)
C4—C5—C6—C1	2.0 (4)	C11—C12—C13—C16	-178.0 (3)
C4—C5—C6—C7	-175.1 (2)	C12—C13—C14—C15	-1.7 (4)
C2—C1—C6—C5	-0.5 (4)	C16—C13—C14—C15	178.4 (3)
N1—C1—C6—C5	-178.2 (2)	C13—C14—C15—C10	0.6 (4)
C2—C1—C6—C7	176.5 (2)	C11—C10—C15—C14	0.1 (4)
N1—C1—C6—C7	-1.2 (4)	C9—C10—C15—C14	-178.2 (2)

Hydrogen-bond geometry (\AA , $^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C17—H17C \cdots O1 ⁱ	0.96	2.64	3.546 (5)	158.

Symmetry codes: (i) $-x+2, y+1/2, -z$.

Fig. 1

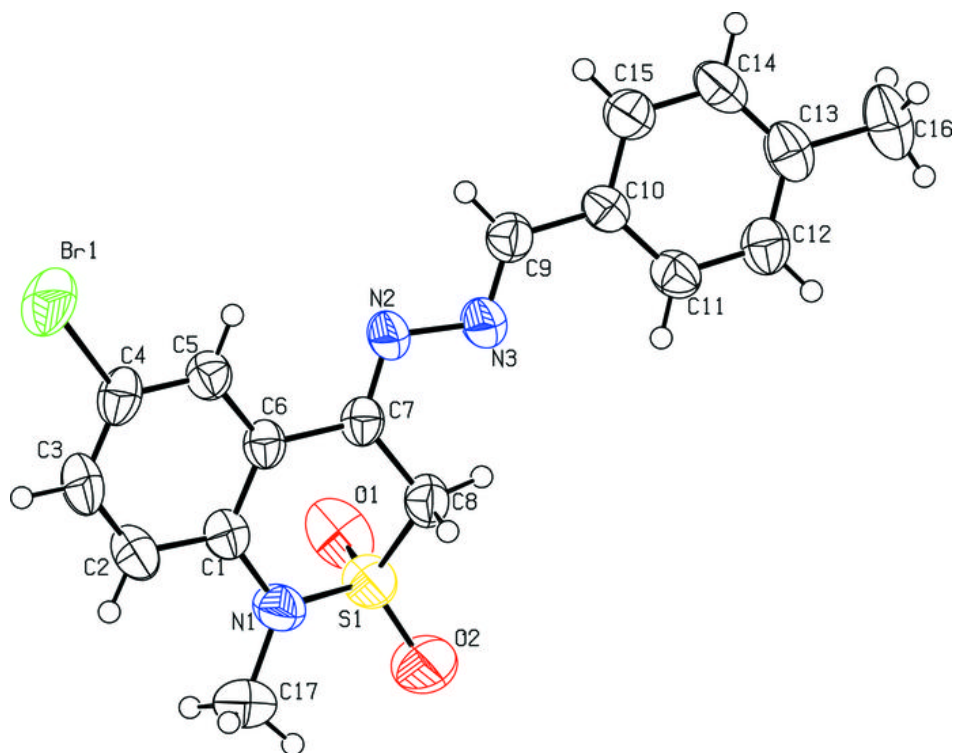


Fig. 2

