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# 2-{(*E*)-[(2*Z*)-(3-Chloro-1-methyl-2,2-dioxo-3,4-dihydro-1*H*-2,1-benzothiazin-4-ylidene)hydrazinylidene]methyl}phenol

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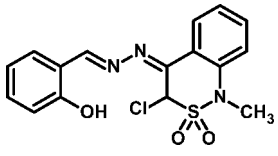
Key indicators: single-crystal X-ray study; $T$ = 296 K; mean $\sigma$(C–C) = 0.006 Å; $R$ factor = 0.073; $wR$ factor = 0.211; data-to-parameter ratio = 18.0.

In the title compound, $C_{16}H_{14}ClN_3O_3S$, the thiazine ring adopts a sofa (half-chair) conformation, with an r.m.s. deviation from the mean plane of 0.23 Å. The S atom and S-bonded C atom exhibit the maximum deviations from the thiazine mean plane [−0.3976 (12) and 0.3179 (14) Å, respectively]. The conformations around the double bonds in the $R_2C{=}N{-}N{=}CHR$ unit are *Z* and *E*. An intramolecular O—H···N hydrogen bond with the hydroxy group as donor generates an *S*(6) ring motif. In the crystal, pairs of weak C—H···O interactions connect the molecules, forming inversion dimers.

## Related literature

For benzothiazine compounds, see: Shafiq, Khan *et al.* (2011); Shafiq, Zia-ur-Rehman *et al.* (2011). For related structures, see: Shafiq *et al.* (2011*a*,*b*). For graph-set notation, see: Bernstein *et al.* (1995).



## Experimental

### Crystal data

$C_{16}H_{14}ClN_3O_3S$
$M_r$ = 363.81
Monoclinic, $P2_1/c$
$a$ = 7.0973 (5) Å
$b$ = 12.0957 (7) Å
$c$ = 18.7396 (13) Å
$\beta$ = 96.058 (4)°
$V$ = 1599.75 (18) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.39 mm$^{-1}$
$T$ = 296 K
0.19 × 0.08 × 0.07 mm

### Data collection

Bruker Kappa APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2007)
$T_{min}$ = 0.930, $T_{max}$ = 0.973
15526 measured reflections
3977 independent reflections
2200 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.061

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.073
$wR(F^2)$ = 0.211
$S$ = 1.03
3977 reflections
221 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 1.13 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.38 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O3—H3*O*···N3 | 0.82 (7) | 1.98 (7) | 2.682 (5) | 143 (7) |
| C9—H9···O1$^{i}$ | 0.95 | 2.55 | 3.394 (5) | 148 |

Symmetry code: (i) $-x, -y+1, -z+1$.

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: *ORTEP-3 for Windows* (Farrugia, 1997) and *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: BH2407).

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# supplementary materials

*Acta Cryst.* (2012). E**68**, o307 [ **doi:10.1107/S1600536811055978** ]

# 2-{(*E*)-[(2*Z*)-(3-Chloro-1-methyl-2,2-dioxo-3,4-dihydro-1*H*-2,1-benzothiazin-4-ylidene)hydrazinylidene]methyl}phenol

**M. Shafiq, I. U. Khan, M. Zia-ur-Rehman, M. N. Arshad and A. M. Asiri**

## Comment

We have recently explored the synthesis of different halogenated benzothiazines (Shafiq, Khan, Arshad *et al.*, 2011), and their Schiff bases (Shafiq, Zia-ur-Rehman *et al.*, 2011). The crystal structure of title compound is being reported in order to study the geometry and different interactions in this class of compounds.

The present structure relates with the already published crystal structures of 4-hydrazinylidene-1-methyl-3*H*-2λ$^6$,1-benzothiazine-2,2-dione (Shafiq, Khan, Zia-ur-Rehman *et al.*, 2011*a*) and 6-bromo-1-methyl-4-[2-(4-methylbenzylidene)hydrazinylidene]-3*H*-2λ$^6$,1-benzothiazine-2,2-dione (Shafiq, Khan, Zia-ur-Rehman *et al.*, 2011*b*). The two fused rings in the title compound (Fig. 1) are oriented at dihedral angle of 7.49 (5)° and the thiazine ring adopts the sofa shape with r.m.s. deviation of about 0.23 Å, and with the maximum deviations arising from S1 [-0.3721 (21) Å] and C8 [0.3118 (26) Å] atoms. The intramolecular hydrogen bonding interaction of O—H···N type generates a six membered ring $S_1^1(6)$ (Bernstein *et al.*, 1995). A weak C—H···O type interaction connects the molecules to form centrosymmetric dimers and generates $R_2^2(16)$ ring motifs (Bernstein *et al.*, 1995; Table 1 and Fig. 2).

The phenol ring is oriented at dihedral angle of 8.17 (4) and 15.58 (5)° with respect to the aromatic ring and thiazine ring, and is twisted by 2.07 (3)° with respect to six membered *S*(6) ring motif generated through the intramolecular O—H···N hydrogen bond.

## Experimental

For the synthesis of title compound, 4-hydrazinylidene-1- methyl-3*H*-2λ$^6$,1-benzothiazine-2,2-dione (Shafiq, Khan, Zia-ur-Rehman *et al.*, 2011*a*) was subjected to react with salicylaldehyde according to literature procedure (Shafiq, Zia-ur-Rehman *et al.*, 2011). The product obtained was then halogenated following another method (Shafiq, Khan, Arshad *et al.*, 2011). Suitable crystals were produced by slow evaporation of a dry ethylacetate solution.

## Refinement

All C-bonded H-atoms were positioned in idealized geometry, with C—H = 0.95 Å for aromatic CH, C—H = 0.98 Å for the methyl group, and C—H = 1 Å for methine C8, and were refined using a riding model with $U_{iso}$(H) = 1.2$U_{eq}$(C) for aromatic groups and C8, and $U_{iso}$(H) = 1.5$U_{eq}$(C16) for the methyl group. Hydroxyl H atom H3O was found in a difference map and refined freely, restraining the O—H bond length to 0.82 (7) Å, with $U_{iso}$(H3O) = 2$U_{eq}$(O3).

## Figures

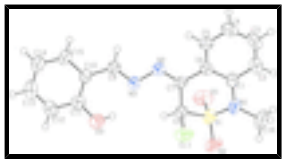

Fig. 1. The molecular structure of the title compound showing 50% displacement ellipsoids.

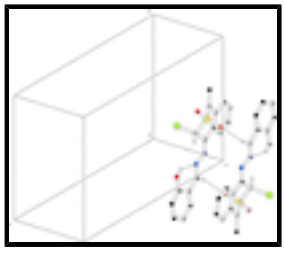

Fig. 2. Perspective view which shows the dimers formed through C—H···O hydrogen bonds (dashed lines).

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*Crystal data*

| | |
|---|---|
| $C_{16}H_{14}ClN_3O_3S$ | $F(000) = 752$ |
| $M_r = 363.81$ | $D_x = 1.511$ Mg m$^{-3}$ |
| Monoclinic, $P2_1/c$ | Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å |
| Hall symbol: -P 2ybc | Cell parameters from 2110 reflections |
| $a = 7.0973$ (5) Å | $\theta = 2.8$–$23.7°$ |
| $b = 12.0957$ (7) Å | $\mu = 0.39$ mm$^{-1}$ |
| $c = 18.7396$ (13) Å | $T = 296$ K |
| $\beta = 96.058$ (4)° | Needle, colourless |
| $V = 1599.75$ (18) Å$^3$ | 0.19 × 0.08 × 0.07 mm |
| $Z = 4$ | |

*Data collection*

| | |
|---|---|
| Bruker Kappa APEXII CCD diffractometer | 3977 independent reflections |
| Radiation source: fine-focus sealed tube | 2200 reflections with $I > 2\sigma(I)$ |
| graphite | $R_{int} = 0.061$ |
| φ and ω scans | $\theta_{max} = 28.3°$, $\theta_{min} = 2.9°$ |
| Absorption correction: multi-scan (*SADABS*; Bruker, 2007) | $h = -8 \rightarrow 9$ |
| $T_{min} = 0.930$, $T_{max} = 0.973$ | $k = -16 \rightarrow 16$ |
| 15526 measured reflections | $l = -24 \rightarrow 25$ |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Primary atom site location: structure-invariant direct methods |
| Least-squares matrix: full | Secondary atom site location: difference Fourier map |

| | |
|---|---|
| $R[F^2 > 2\sigma(F^2)] = 0.073$ | Hydrogen site location: inferred from neighbouring sites |
| $wR(F^2) = 0.211$ | H atoms treated by a mixture of independent and constrained refinement |
| $S = 1.03$ | $w = 1/[\sigma^2(F_o^2) + (0.0873P)^2 + 1.6824P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| 3977 reflections | $(\Delta/\sigma)_{max} < 0.001$ |
| 221 parameters | $\Delta\rho_{max} = 1.13$ e Å$^{-3}$ |
| 0 restraints | $\Delta\rho_{min} = -0.38$ e Å$^{-3}$ |
| 0 constraints | |

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

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Cl1 | 0.51356 (17) | 0.73641 (10) | 0.42510 (7) | 0.0613 (4) |
| S1 | 0.16021 (16) | 0.83188 (8) | 0.46237 (6) | 0.0466 (3) |
| O1 | −0.0316 (4) | 0.7950 (3) | 0.46762 (18) | 0.0589 (9) |
| O2 | 0.1931 (5) | 0.9186 (2) | 0.41328 (19) | 0.0646 (10) |
| O3 | 0.2121 (6) | 0.4788 (3) | 0.27384 (18) | 0.0632 (10) |
| N1 | 0.2779 (5) | 0.8598 (3) | 0.5392 (2) | 0.0486 (9) |
| N2 | 0.2405 (5) | 0.5211 (3) | 0.48831 (18) | 0.0410 (8) |
| N3 | 0.2244 (5) | 0.4863 (2) | 0.41731 (18) | 0.0409 (8) |
| C1 | 0.2935 (6) | 0.7761 (3) | 0.5927 (2) | 0.0393 (9) |
| C2 | 0.3168 (7) | 0.8064 (4) | 0.6654 (2) | 0.0546 (12) |
| H2 | 0.3185 | 0.8823 | 0.6784 | 0.066* |
| C3 | 0.3368 (7) | 0.7278 (5) | 0.7172 (3) | 0.0625 (14) |
| H3 | 0.3541 | 0.7496 | 0.7662 | 0.075* |
| C4 | 0.3327 (7) | 0.6172 (4) | 0.7003 (2) | 0.0576 (12) |
| H4 | 0.3462 | 0.5629 | 0.7371 | 0.069* |
| C5 | 0.3090 (6) | 0.5861 (4) | 0.6295 (2) | 0.0466 (10) |
| H5 | 0.3059 | 0.5097 | 0.6178 | 0.056* |
| C6 | 0.2894 (5) | 0.6638 (3) | 0.5745 (2) | 0.0349 (8) |
| C7 | 0.2647 (5) | 0.6248 (3) | 0.4995 (2) | 0.0340 (8) |
| C8 | 0.2740 (6) | 0.7083 (3) | 0.4402 (2) | 0.0402 (9) |
| H8 | 0.2059 | 0.6776 | 0.3950 | 0.048* |
| C9 | 0.2063 (6) | 0.3806 (3) | 0.4143 (2) | 0.0399 (9) |
| H9 | 0.2041 | 0.3408 | 0.4579 | 0.048* |
| C10 | 0.1889 (5) | 0.3193 (3) | 0.3476 (2) | 0.0383 (9) |
| C11 | 0.1917 (6) | 0.3688 (3) | 0.2807 (2) | 0.0448 (10) |
| C12 | 0.1740 (7) | 0.3036 (4) | 0.2194 (3) | 0.0570 (12) |
| H12 | 0.1764 | 0.3368 | 0.1736 | 0.068* |
| C13 | 0.1532 (7) | 0.1921 (4) | 0.2249 (3) | 0.0628 (14) |
| H13 | 0.1388 | 0.1487 | 0.1824 | 0.075* |
| C14 | 0.1526 (7) | 0.1407 (4) | 0.2903 (3) | 0.0568 (12) |
| H14 | 0.1393 | 0.0628 | 0.2932 | 0.068* |
| C15 | 0.1715 (6) | 0.2043 (3) | 0.3513 (3) | 0.0464 (10) |
| H15 | 0.1728 | 0.1695 | 0.3968 | 0.056* |
| C16 | 0.3125 (10) | 0.9768 (4) | 0.5597 (3) | 0.0839 (18) |

| | | | | |
|---|---|---|---|---|
| H16A | 0.2108 | 1.0030 | 0.5869 | 0.126* |
| H16B | 0.3153 | 1.0217 | 0.5163 | 0.126* |
| H16C | 0.4343 | 0.9831 | 0.5893 | 0.126* |
| H3O | 0.235 (11) | 0.509 (6) | 0.313 (4) | 0.126* |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Cl1 | 0.0542 (7) | 0.0619 (7) | 0.0709 (9) | 0.0012 (6) | 0.0213 (6) | 0.0147 (6) |
| S1 | 0.0503 (7) | 0.0366 (5) | 0.0514 (7) | 0.0043 (5) | −0.0005 (5) | 0.0050 (5) |
| O1 | 0.0359 (17) | 0.073 (2) | 0.066 (2) | 0.0084 (15) | −0.0010 (14) | 0.0259 (17) |
| O2 | 0.086 (3) | 0.0398 (17) | 0.066 (2) | −0.0017 (16) | −0.0010 (18) | 0.0182 (15) |
| O3 | 0.094 (3) | 0.0417 (18) | 0.054 (2) | 0.0080 (17) | 0.0063 (19) | 0.0097 (15) |
| N1 | 0.060 (2) | 0.0312 (17) | 0.052 (2) | 0.0033 (16) | −0.0057 (17) | −0.0064 (15) |
| N2 | 0.049 (2) | 0.0353 (17) | 0.038 (2) | −0.0009 (15) | 0.0044 (15) | −0.0005 (14) |
| N3 | 0.052 (2) | 0.0315 (16) | 0.040 (2) | −0.0002 (14) | 0.0060 (15) | −0.0033 (14) |
| C1 | 0.035 (2) | 0.041 (2) | 0.041 (2) | 0.0017 (17) | −0.0009 (17) | −0.0064 (18) |
| C2 | 0.055 (3) | 0.062 (3) | 0.045 (3) | 0.001 (2) | 0.001 (2) | −0.016 (2) |
| C3 | 0.058 (3) | 0.095 (4) | 0.034 (3) | −0.005 (3) | 0.004 (2) | −0.015 (3) |
| C4 | 0.061 (3) | 0.075 (3) | 0.037 (3) | −0.004 (2) | 0.004 (2) | 0.011 (2) |
| C5 | 0.051 (3) | 0.046 (2) | 0.042 (3) | −0.0043 (19) | 0.0007 (19) | 0.0059 (19) |
| C6 | 0.032 (2) | 0.040 (2) | 0.033 (2) | −0.0003 (16) | 0.0024 (15) | 0.0014 (17) |
| C7 | 0.036 (2) | 0.0306 (18) | 0.035 (2) | 0.0025 (15) | 0.0018 (16) | 0.0031 (16) |
| C8 | 0.051 (2) | 0.0322 (19) | 0.037 (2) | 0.0031 (17) | 0.0035 (18) | 0.0001 (17) |
| C9 | 0.042 (2) | 0.035 (2) | 0.043 (2) | 0.0007 (17) | 0.0047 (18) | 0.0022 (17) |
| C10 | 0.037 (2) | 0.0342 (19) | 0.043 (2) | 0.0021 (16) | 0.0013 (17) | −0.0020 (17) |
| C11 | 0.042 (2) | 0.042 (2) | 0.050 (3) | 0.0069 (18) | −0.0001 (19) | 0.0010 (19) |
| C12 | 0.061 (3) | 0.069 (3) | 0.040 (3) | 0.007 (2) | 0.000 (2) | −0.006 (2) |
| C13 | 0.059 (3) | 0.063 (3) | 0.066 (3) | 0.003 (2) | 0.004 (2) | −0.026 (3) |
| C14 | 0.056 (3) | 0.043 (2) | 0.072 (3) | −0.005 (2) | 0.011 (2) | −0.015 (2) |
| C15 | 0.046 (3) | 0.035 (2) | 0.059 (3) | −0.0032 (18) | 0.007 (2) | −0.007 (2) |
| C16 | 0.123 (5) | 0.040 (3) | 0.086 (4) | −0.004 (3) | −0.005 (4) | −0.016 (3) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| Cl1—C8 | 1.786 (4) | C5—C6 | 1.391 (5) |
| S1—O2 | 1.430 (3) | C5—H5 | 0.9500 |
| S1—O1 | 1.445 (3) | C6—C7 | 1.475 (5) |
| S1—N1 | 1.623 (4) | C7—C8 | 1.509 (5) |
| S1—C8 | 1.770 (4) | C8—H8 | 1.0000 |
| O3—C11 | 1.346 (5) | C9—C10 | 1.447 (5) |
| O3—H3O | 0.82 (7) | C9—H9 | 0.9500 |
| N1—C1 | 1.420 (5) | C10—C11 | 1.391 (6) |
| N1—C16 | 1.479 (6) | C10—C15 | 1.399 (5) |
| N2—C7 | 1.280 (5) | C11—C12 | 1.388 (6) |
| N2—N3 | 1.389 (5) | C12—C13 | 1.362 (7) |
| N3—C9 | 1.286 (5) | C12—H12 | 0.9500 |
| C1—C6 | 1.399 (5) | C13—C14 | 1.374 (7) |
| C1—C2 | 1.405 (6) | C13—H13 | 0.9500 |

| | | | |
|---|---|---|---|
| C2—C3 | 1.355 (7) | C14—C15 | 1.372 (6) |
| C2—H2 | 0.9500 | C14—H14 | 0.9500 |
| C3—C4 | 1.375 (7) | C15—H15 | 0.9500 |
| C3—H3 | 0.9500 | C16—H16A | 0.9800 |
| C4—C5 | 1.371 (6) | C16—H16B | 0.9800 |
| C4—H4 | 0.9500 | C16—H16C | 0.9800 |
| O2—S1—O1 | 119.2 (2) | C7—C8—S1 | 109.6 (3) |
| O2—S1—N1 | 108.3 (2) | C7—C8—Cl1 | 111.1 (3) |
| O1—S1—N1 | 113.8 (2) | S1—C8—Cl1 | 110.0 (2) |
| O2—S1—C8 | 111.0 (2) | C7—C8—H8 | 108.7 |
| O1—S1—C8 | 102.2 (2) | S1—C8—H8 | 108.7 |
| N1—S1—C8 | 100.35 (19) | Cl1—C8—H8 | 108.7 |
| C11—O3—H3O | 111 (5) | N3—C9—C10 | 123.1 (4) |
| C1—N1—C16 | 120.1 (4) | N3—C9—H9 | 118.4 |
| C1—N1—S1 | 118.1 (3) | C10—C9—H9 | 118.4 |
| C16—N1—S1 | 119.0 (3) | C11—C10—C15 | 118.8 (4) |
| C7—N2—N3 | 116.8 (3) | C11—C10—C9 | 123.3 (4) |
| C9—N3—N2 | 110.0 (3) | C15—C10—C9 | 117.9 (4) |
| C6—C1—C2 | 119.1 (4) | O3—C11—C12 | 118.9 (4) |
| C6—C1—N1 | 121.5 (3) | O3—C11—C10 | 121.6 (4) |
| C2—C1—N1 | 119.4 (4) | C12—C11—C10 | 119.5 (4) |
| C3—C2—C1 | 120.3 (4) | C13—C12—C11 | 120.1 (5) |
| C3—C2—H2 | 119.8 | C13—C12—H12 | 119.9 |
| C1—C2—H2 | 119.8 | C11—C12—H12 | 119.9 |
| C2—C3—C4 | 121.3 (4) | C12—C13—C14 | 121.7 (5) |
| C2—C3—H3 | 119.4 | C12—C13—H13 | 119.2 |
| C4—C3—H3 | 119.4 | C14—C13—H13 | 119.2 |
| C5—C4—C3 | 119.1 (4) | C15—C14—C13 | 118.7 (4) |
| C5—C4—H4 | 120.4 | C15—C14—H14 | 120.6 |
| C3—C4—H4 | 120.4 | C13—C14—H14 | 120.6 |
| C4—C5—C6 | 121.6 (4) | C14—C15—C10 | 121.2 (4) |
| C4—C5—H5 | 119.2 | C14—C15—H15 | 119.4 |
| C6—C5—H5 | 119.2 | C10—C15—H15 | 119.4 |
| C5—C6—C1 | 118.5 (4) | N1—C16—H16A | 109.5 |
| C5—C6—C7 | 118.8 (3) | N1—C16—H16B | 109.5 |
| C1—C6—C7 | 122.7 (3) | H16A—C16—H16B | 109.5 |
| N2—C7—C6 | 118.1 (3) | N1—C16—H16C | 109.5 |
| N2—C7—C8 | 123.4 (3) | H16A—C16—H16C | 109.5 |
| C6—C7—C8 | 118.5 (3) | H16B—C16—H16C | 109.5 |
| O2—S1—N1—C1 | −169.2 (3) | C5—C6—C7—C8 | −170.6 (4) |
| O1—S1—N1—C1 | 55.7 (4) | C1—C6—C7—C8 | 9.6 (6) |
| C8—S1—N1—C1 | −52.7 (3) | N2—C7—C8—S1 | 142.6 (3) |
| O2—S1—N1—C16 | 29.7 (5) | C6—C7—C8—S1 | −39.0 (4) |
| O1—S1—N1—C16 | −105.4 (4) | N2—C7—C8—Cl1 | −95.6 (4) |
| C8—S1—N1—C16 | 146.1 (4) | C6—C7—C8—Cl1 | 82.8 (4) |
| C7—N2—N3—C9 | 178.1 (4) | O2—S1—C8—C7 | 170.5 (3) |
| C16—N1—C1—C6 | −170.4 (4) | O1—S1—C8—C7 | −61.3 (3) |
| S1—N1—C1—C6 | 28.6 (5) | N1—S1—C8—C7 | 56.1 (3) |

| | | | |
|---|---|---|---|
| C16—N1—C1—C2 | 8.4 (6) | O2—S1—C8—Cl1 | 48.0 (3) |
| S1—N1—C1—C2 | −152.5 (3) | O1—S1—C8—Cl1 | 176.2 (2) |
| C6—C1—C2—C3 | 0.6 (7) | N1—S1—C8—Cl1 | −66.4 (2) |
| N1—C1—C2—C3 | −178.3 (4) | N2—N3—C9—C10 | −179.2 (3) |
| C1—C2—C3—C4 | −0.8 (8) | N3—C9—C10—C11 | 0.5 (6) |
| C2—C3—C4—C5 | 0.4 (8) | N3—C9—C10—C15 | 179.5 (4) |
| C3—C4—C5—C6 | 0.1 (7) | C15—C10—C11—O3 | −178.6 (4) |
| C4—C5—C6—C1 | −0.3 (6) | C9—C10—C11—O3 | 0.4 (6) |
| C4—C5—C6—C7 | 179.9 (4) | C15—C10—C11—C12 | 1.0 (6) |
| C2—C1—C6—C5 | −0.1 (6) | C9—C10—C11—C12 | −180.0 (4) |
| N1—C1—C6—C5 | 178.8 (4) | O3—C11—C12—C13 | 180.0 (4) |
| C2—C1—C6—C7 | 179.7 (4) | C10—C11—C12—C13 | 0.3 (7) |
| N1—C1—C6—C7 | −1.4 (6) | C11—C12—C13—C14 | −1.2 (8) |
| N3—N2—C7—C6 | −177.7 (3) | C12—C13—C14—C15 | 0.7 (8) |
| N3—N2—C7—C8 | 0.7 (6) | C13—C14—C15—C10 | 0.8 (7) |
| C5—C6—C7—N2 | 7.9 (5) | C11—C10—C15—C14 | −1.6 (6) |
| C1—C6—C7—N2 | −171.9 (4) | C9—C10—C15—C14 | 179.3 (4) |

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O3—H3O···N3 | 0.82 (7) | 1.98 (7) | 2.682 (5) | 143 (7) |
| C9—H9···O1$^{i}$ | 0.95 | 2.55 | 3.394 (5) | 148. |

Symmetry codes: (i) −*x*, −*y*+1, −*z*+1.

**Fig. 1**

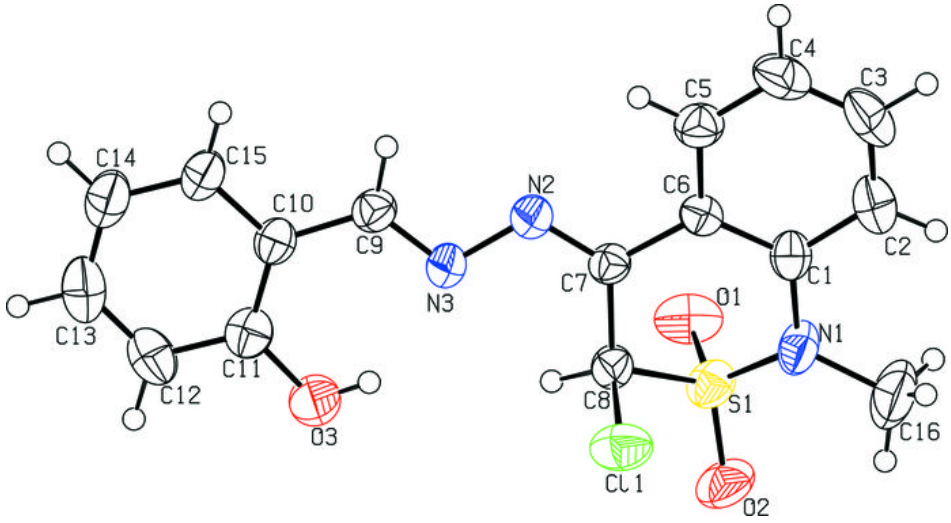
C4
C5
C3
C14
C15
C10
C9
N2
C6
C2
C1
C7
O1
N3
C13
C11
N1
C12
C8
S1
C16
O3
Cl1
O2

**Fig. 2**