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# 6-Bromo-1-ethyl-1*H*-2,1-benzothiazin-4(3*H*)-one 2,2-dioxide

**Muhammad Shafiq,[a] M. Nawaz Tahir,[b]* Islam Ullah Khan,[a] Muhammad Nadeem Arshad[a] and Muhammad Safdar[c]**

[a]Government College University, Department of Chemistry, Lahore, Pakistan, [b]University of Sargodha, Department of Physics, Sargodha, Pakistan, and [c]University of Karachi, HEJ research Institute of Chemistry, Karachi, Pakistan
Correspondence e-mail: dmntahir_uos@yahoo.com

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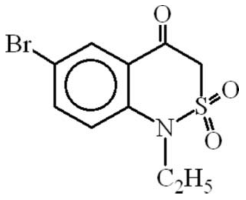
Key indicators: single-crystal X-ray study; $T$ = 296 K; mean $\sigma$(C–C) = 0.004 Å; $R$ factor = 0.038; $wR$ factor = 0.095; data-to-parameter ratio = 18.0.

In the title compound, $C_{10}H_{10}BrNO_3S$, the S atom is four-coordinated in a distorted tetrahedral configuration with nearly equal S=O bond distances; the S—C and S—N bond lengths are 1.755 (3) and 1.649 (3) Å, respectively. The heterocyclic thiazine ring adopts a twist conformation. Adjacent molecules are attached to each other through intermolecular C—H⋯O hydrogen bonds, forming $R_2^2(8)$ and $R_2^2(14)$ ring motifs. The molecules are stabilized by intra- and intermolecular hydrogen bonds, forming a three-dimensional polymeric network.

## Related literature

For previous work on benzothiazines, see: Arshad *et al.* (2008); Shafiq, Khan *et al.* (2008); Shafiq, Tahir *et al.* (2008); Tahir *et al.* (2008). For puckering parameters, see: Cremer & Pople (1975). For graph-set motifs, see: Bernstein *et al.* (1995). For synthesis, see: Lombardino (1972).



## Experimental

*Crystal data*

$C_{10}H_{10}BrNO_3S$
$M_r$ = 304.16
Triclinic, $P\bar{1}$
$a$ = 7.7164 (2) Å
$b$ = 7.9729 (3) Å
$c$ = 10.4579 (3) Å
$\alpha$ = 86.767 (2)°
$\beta$ = 75.773 (1)°
$\gamma$ = 66.912 (2)°
$V$ = 573.13 (3) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 3.76 mm$^{-1}$
$T$ = 296 (2) K
0.28 × 0.16 × 0.12 mm

*Data collection*

Bruker Kappa APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
$T_{min}$ = 0.486, $T_{max}$ = 0.639
12369 measured reflections
2846 independent reflections
1840 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.034

*Refinement*

$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.095
$S$ = 1.02
2846 reflections
158 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.91 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.58 e Å$^{-3}$

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

| $D$—H⋯$A$ | $D$—H | H⋯$A$ | $D$⋯$A$ | $D$—H⋯$A$ |
|---|---|---|---|---|
| C2—H2⋯O1$^{i}$ | 0.9300 | 2.4200 | 3.324 (4) | 165.00 |
| C3—H3⋯O2$^{ii}$ | 0.9300 | 2.5900 | 3.418 (4) | 148.00 |
| C8—H8$A$⋯O3$^{iii}$ | 0.89 (4) | 2.57 (4) | 3.252 (4) | 134 (3) |
| C9—H9$B$⋯O3 | 0.93 (3) | 2.29 (3) | 2.850 (4) | 118 (2) |

Symmetry codes: (i) $x, y+1, z$; (ii) $-x, -y+1, -z$; (iii) $-x, -y, -z+1$.

Data collection: *APEX2* (Bruker, 2007); cell refinement: *APEX2*; 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: *ORTEP-3 for Windows* (Farrugia, 1997) and *PLATON* (Spek, 2003); 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: AT2711).

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# supplementary materials

*Acta Cryst.* (2009). E**65**, o393 [ **doi:10.1107/S1600536809002621** ]

# 6-Bromo-1-ethyl-1*H*-2,1-benzothiazin-4(3*H*)-one 2,2-dioxide

**M. Shafiq, M. N. Tahir, I. U. Khan, M. N. Arshad** and **M. Safdar**

## Comment

Our group is involved in synthesizing various derivatives of benzothiazine molecule (Shafiq, Khan *et al.*, 2008; Shafiq, Tahir *et al.*, 2008; Tahir *et al.*, 2008; Arshad *et al.*, 2008) and their characterization by X-ray studies. We, here, report the title compound (I), (Fig 1), in this context.

In the title compound, the bromo-substituated benzene ring A (C1–C6), is almost planar with alternate distortions at individual C atoms. The Br atom is at a distance of 0.073 (4) Å from the r.m.s. plane of ring A. The thiazine ring B (S1/N1/C1/C6–C8) is in the twisted form. The maximum puckering (Cremer & Pople, 1975) amplitude, $Q_T$, of ring A and ring B is 0.674 (2) Å. There exist an intramolecular H-bond of C—H···O type between the methylene group and the $SO_2$ moiety. The intermolecular H-bonds [C8—H8A···.O3] and [C3—H3···.O2] (Table 1), joint the adjacent molecules forming ring motifs, (Bernstein *et al.*, 1995), $R_2^2(8)$ and $R_2^2(14)$, respectively. The three asymmetric units joint in this way, are further linked through [C2—H2···O1] H-bonds with carbonyl moiety (Fig 2).

## Experimental

The title compound was prepared in a three step scheme following the reported procedure (Lombardino, 1972). Starting material used was methyl-2-amino-5-bromo benzoate. It was reacted with methane sulfonyl chloride taking equimolar quantities, in dichloromethane. The pH was kept alkaline with triethylamine. The product of this step was then *N*-ethylated (ethyl iodide) and cyclized as reported in the above mentioned reference, to get the title compound which was recrystallized in ethanol for X-ray diffraction studies.

## Refinement

The H atoms of methylene group were located from a difference Fourier map and refined freely. H atoms were positioned geometrically, with C—H = 0.93 and 0.96 Å for aromatic and methyl H, and constrained to ride on their parent atoms, with $U_{iso}(H) = xU_{eq}(C)$, where x = 1.5 for methyl H, and x = 1.2 for all other H atoms.

## Figures

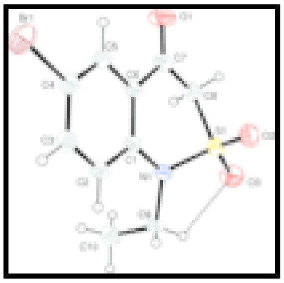

Fig. 1. *ORTEP* drawing of the title compound, with the atom numbering scheme. The thermal ellipsoids are drawn at the 50% probability level. H atoms are shown by small circles of arbitrary radii. The dotted line shows the intramolecular H-bond.

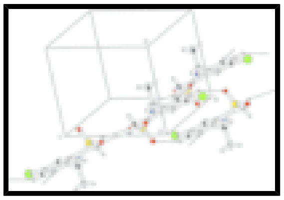

Fig. 2. The partial packing figure (*PLATON*: Spek, 2003) which shows that intermolecular H-bonds form the ring motifs.

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*Crystal data*

$C_{10}H_{10}BrNO_3S$

$M_r = 304.16$

Triclinic, $P\bar{1}$

Hall symbol: -P 1

$a = 7.7164$ (2) Å

$b = 7.9729$ (3) Å

$c = 10.4579$ (3) Å

$\alpha = 86.767$ (2)°

$\beta = 75.773$ (1)°

$\gamma = 66.912$ (2)°

$V = 573.13$ (3) Å$^3$

$Z = 2$

$F_{000} = 304$

$D_x = 1.762$ Mg m$^{-3}$

Mo *K*α radiation
$\lambda = 0.71073$ Å

Cell parameters from 2847 reflections

$\theta = 2.0–28.3$°

$\mu = 3.76$ mm$^{-1}$

$T = 296$ (2) K

Needle, colourless

0.28 × 0.16 × 0.12 mm

*Data collection*

Bruker Kappa APEXII CCD diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

Detector resolution: 7.40 pixels mm$^{-1}$

$T = 296(2)$ K

ω scans

Absorption correction: multi-scan (SADABS; Bruker, 2005)

$T_{min} = 0.486$, $T_{max} = 0.639$

12369 measured reflections

2846 independent reflections

1840 reflections with $I > 2\sigma(I)$

$R_{int} = 0.034$

$\theta_{max} = 28.3$°

$\theta_{min} = 2.0$°

$h = -10 \rightarrow 9$

$k = -10 \rightarrow 10$

$l = -13 \rightarrow 13$

*Refinement*

Refinement on $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.038$

$wR(F^2) = 0.095$

$S = 1.02$

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0388P)^2 + 0.3304P]$
where $P = (F_o^2 + 2F_c^2)/3$

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

| | |
|---|---|
| 2846 reflections | $\Delta\rho_{max}$ = 0.91 e Å$^{-3}$ |
| 158 parameters | $\Delta\rho_{min}$ = −0.57 e Å$^{-3}$ |
| Primary atom site location: structure-invariant direct methods | Extinction correction: none |

### *Special details*

**Geometry**. Bond distances, angles *etc*. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

**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* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Br1 | 0.36240 (6) | 0.15247 (6) | −0.35948 (3) | 0.0686 (2) |
| S1 | −0.00069 (12) | 0.19519 (10) | 0.32296 (7) | 0.0435 (3) |
| O1 | 0.2170 (4) | −0.2056 (3) | 0.0770 (3) | 0.0705 (10) |
| O2 | −0.1737 (3) | 0.2464 (3) | 0.2787 (2) | 0.0578 (8) |
| O3 | −0.0156 (4) | 0.2267 (3) | 0.4583 (2) | 0.0668 (10) |
| N1 | 0.1437 (4) | 0.2891 (3) | 0.2351 (2) | 0.0450 (9) |
| C1 | 0.1999 (4) | 0.2535 (4) | 0.0977 (3) | 0.0358 (9) |
| C2 | 0.2376 (5) | 0.3826 (4) | 0.0126 (3) | 0.0444 (10) |
| C3 | 0.2876 (5) | 0.3511 (4) | −0.1214 (3) | 0.0471 (11) |
| C4 | 0.3017 (4) | 0.1895 (4) | −0.1739 (3) | 0.0423 (10) |
| C5 | 0.2710 (4) | 0.0580 (4) | −0.0934 (3) | 0.0416 (10) |
| C6 | 0.2210 (4) | 0.0869 (4) | 0.0432 (3) | 0.0361 (9) |
| C7 | 0.1935 (4) | −0.0623 (4) | 0.1248 (3) | 0.0427 (10) |
| C8 | 0.1398 (6) | −0.0343 (4) | 0.2718 (3) | 0.0493 (11) |
| C9 | 0.1564 (5) | 0.4465 (4) | 0.2950 (3) | 0.0465 (11) |
| C10 | 0.3622 (5) | 0.4137 (5) | 0.2925 (4) | 0.0635 (14) |
| H2 | 0.22872 | 0.49140 | 0.04727 | 0.0533* |
| H3 | 0.31214 | 0.43846 | −0.17724 | 0.0564* |
| H5 | 0.28342 | −0.05116 | −0.12983 | 0.0499* |
| H8A | 0.065 (5) | −0.092 (5) | 0.313 (4) | 0.0591* |
| H8B | 0.247 (5) | −0.063 (5) | 0.306 (3) | 0.0591* |
| H9A | 0.092 (5) | 0.550 (5) | 0.245 (3) | 0.0558* |
| H9B | 0.085 (5) | 0.457 (4) | 0.382 (3) | 0.0558* |
| H10A | 0.43344 | 0.41151 | 0.20285 | 0.0948* |
| H10B | 0.36403 | 0.50981 | 0.34278 | 0.0948* |
| H10C | 0.42109 | 0.29879 | 0.33010 | 0.0948* |

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

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Br1 | 0.0779 (3) | 0.0861 (3) | 0.0329 (2) | −0.0249 (2) | −0.0092 (2) | 0.0002 (2) |
| S1 | 0.0540 (5) | 0.0443 (4) | 0.0344 (4) | −0.0260 (4) | −0.0036 (3) | 0.0030 (3) |
| O1 | 0.113 (2) | 0.0401 (13) | 0.0672 (17) | −0.0416 (15) | −0.0168 (15) | −0.0010 (12) |
| O2 | 0.0464 (14) | 0.0583 (14) | 0.0673 (16) | −0.0232 (12) | −0.0074 (12) | 0.0063 (12) |
| O3 | 0.098 (2) | 0.0734 (16) | 0.0341 (13) | −0.0463 (15) | −0.0033 (12) | 0.0009 (11) |
| N1 | 0.0626 (17) | 0.0467 (14) | 0.0332 (14) | −0.0347 (14) | −0.0012 (12) | −0.0045 (11) |
| C1 | 0.0391 (16) | 0.0356 (15) | 0.0340 (16) | −0.0178 (13) | −0.0056 (12) | −0.0001 (12) |
| C2 | 0.0552 (19) | 0.0351 (15) | 0.0453 (19) | −0.0238 (15) | −0.0057 (15) | 0.0010 (13) |
| C3 | 0.051 (2) | 0.0462 (18) | 0.0429 (19) | −0.0212 (16) | −0.0075 (15) | 0.0110 (15) |
| C4 | 0.0425 (18) | 0.0510 (18) | 0.0307 (16) | −0.0164 (15) | −0.0074 (13) | 0.0015 (14) |
| C5 | 0.0439 (18) | 0.0377 (16) | 0.0418 (18) | −0.0139 (14) | −0.0098 (14) | −0.0056 (14) |
| C6 | 0.0419 (17) | 0.0324 (15) | 0.0369 (16) | −0.0182 (13) | −0.0082 (13) | 0.0005 (12) |
| C7 | 0.0487 (19) | 0.0354 (16) | 0.0491 (19) | −0.0198 (14) | −0.0158 (15) | 0.0050 (14) |
| C8 | 0.061 (2) | 0.0436 (18) | 0.047 (2) | −0.0254 (18) | −0.0137 (17) | 0.0121 (15) |
| C9 | 0.056 (2) | 0.0423 (17) | 0.0440 (19) | −0.0255 (17) | −0.0033 (16) | −0.0115 (15) |
| C10 | 0.065 (2) | 0.066 (2) | 0.071 (3) | −0.033 (2) | −0.023 (2) | −0.004 (2) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| Br1—C4 | 1.893 (3) | C6—C7 | 1.477 (4) |
| S1—O2 | 1.421 (3) | C7—C8 | 1.496 (4) |
| S1—O3 | 1.420 (2) | C9—C10 | 1.499 (6) |
| S1—N1 | 1.649 (3) | C2—H2 | 0.9300 |
| S1—C8 | 1.755 (3) | C3—H3 | 0.9300 |
| O1—C7 | 1.202 (4) | C5—H5 | 0.9300 |
| N1—C1 | 1.406 (4) | C8—H8A | 0.89 (4) |
| N1—C9 | 1.481 (4) | C8—H8B | 0.92 (4) |
| C1—C2 | 1.393 (4) | C9—H9A | 0.98 (4) |
| C1—C6 | 1.409 (4) | C9—H9B | 0.93 (3) |
| C2—C3 | 1.369 (4) | C10—H10A | 0.9600 |
| C3—C4 | 1.383 (4) | C10—H10B | 0.9600 |
| C4—C5 | 1.364 (4) | C10—H10C | 0.9600 |
| C5—C6 | 1.393 (4) | | |
| Br1···Br1$^{i}$ | 3.5704 (5) | C2···H9A | 2.61 (3) |
| Br1···H8B$^{ii}$ | 3.00 (4) | C2···H10A | 2.8500 |
| O1···C2$^{iii}$ | 3.324 (4) | C9···H2 | 2.5500 |
| O2···C6 | 3.254 (4) | C10···H2 | 2.9400 |
| O2···C10$^{iv}$ | 3.263 (5) | H2···O1$^{ix}$ | 2.4200 |
| O2···C3$^{v}$ | 3.418 (4) | H2···C9 | 2.5500 |
| O3···C8$^{vi}$ | 3.252 (4) | H2···C10 | 2.9400 |
| O1···H9A$^{iii}$ | 2.84 (4) | H2···H9A | 2.0600 |
| O1···H2$^{iii}$ | 2.4200 | H2···H10A | 2.4300 |
| O1···H5 | 2.4700 | H3···O2$^{v}$ | 2.5900 |

| | | | |
|---|---|---|---|
| O2···H10C$^{iv}$ | 2.9000 | H5···O1 | 2.4700 |
| O2···H5$^{vii}$ | 2.7400 | H5···O2$^{vii}$ | 2.7400 |
| O2···H3$^{v}$ | 2.5900 | H8A···O3$^{vi}$ | 2.57 (4) |
| O3···H9B | 2.29 (3) | H8B···Br1$^{ii}$ | 3.00 (4) |
| O3···H8A$^{vi}$ | 2.57 (4) | H9A···O1$^{ix}$ | 2.84 (4) |
| O3···H9B$^{viii}$ | 2.90 (3) | H9A···C2 | 2.61 (3) |
| C2···O1$^{ix}$ | 3.324 (4) | H9A···H2 | 2.0600 |
| C2···C10 | 3.348 (5) | H9B···O3 | 2.29 (3) |
| C2···C2$^{v}$ | 3.472 (5) | H9B···O3$^{viii}$ | 2.90 (3) |
| C3···O2$^{v}$ | 3.418 (4) | H9B···H9B$^{viii}$ | 2.49 (4) |
| C6···O2 | 3.254 (4) | H10A···C1 | 2.9900 |
| C8···O3$^{vi}$ | 3.252 (4) | H10A···C2 | 2.8500 |
| C10···C2 | 3.348 (5) | H10A···H2 | 2.4300 |
| C10···O2$^{x}$ | 3.263 (5) | H10C···O2$^{x}$ | 2.9000 |
| C1···H10A | 2.9900 | | |

| | | | |
|---|---|---|---|
| O2—S1—O3 | 118.87 (16) | S1—C8—C7 | 112.1 (2) |
| O2—S1—N1 | 110.91 (14) | N1—C9—C10 | 111.6 (3) |
| O2—S1—C8 | 106.97 (18) | C1—C2—H2 | 120.00 |
| O3—S1—N1 | 107.50 (16) | C3—C2—H2 | 120.00 |
| O3—S1—C8 | 111.51 (15) | C2—C3—H3 | 120.00 |
| N1—S1—C8 | 99.36 (16) | C4—C3—H3 | 120.00 |
| S1—N1—C1 | 117.1 (2) | C4—C5—H5 | 120.00 |
| S1—N1—C9 | 118.39 (19) | C6—C5—H5 | 120.00 |
| C1—N1—C9 | 121.6 (2) | S1—C8—H8A | 104 (2) |
| N1—C1—C2 | 120.3 (3) | S1—C8—H8B | 104 (2) |
| N1—C1—C6 | 121.0 (3) | C7—C8—H8A | 113 (3) |
| C2—C1—C6 | 118.7 (3) | C7—C8—H8B | 112 (2) |
| C1—C2—C3 | 120.7 (3) | H8A—C8—H8B | 111 (3) |
| C2—C3—C4 | 120.1 (3) | N1—C9—H9A | 104 (2) |
| Br1—C4—C3 | 119.3 (2) | N1—C9—H9B | 105 (2) |
| Br1—C4—C5 | 120.0 (2) | C10—C9—H9A | 115 (2) |
| C3—C4—C5 | 120.7 (3) | C10—C9—H9B | 110 (3) |
| C4—C5—C6 | 120.1 (3) | H9A—C9—H9B | 111 (3) |
| C1—C6—C5 | 119.6 (3) | C9—C10—H10A | 109.00 |
| C1—C6—C7 | 122.9 (3) | C9—C10—H10B | 110.00 |
| C5—C6—C7 | 117.4 (3) | C9—C10—H10C | 109.00 |
| O1—C7—C6 | 122.2 (3) | H10A—C10—H10B | 109.00 |
| O1—C7—C8 | 119.4 (3) | H10A—C10—H10C | 109.00 |
| C6—C7—C8 | 118.4 (3) | H10B—C10—H10C | 109.00 |

| | | | |
|---|---|---|---|
| O2—S1—N1—C1 | −56.8 (3) | N1—C1—C6—C5 | 178.0 (3) |
| O2—S1—N1—C9 | 104.3 (2) | N1—C1—C6—C7 | −2.4 (5) |
| O3—S1—N1—C1 | 171.7 (2) | C2—C1—C6—C5 | −2.6 (5) |
| O3—S1—N1—C9 | −27.2 (3) | C2—C1—C6—C7 | 177.1 (3) |
| C8—S1—N1—C1 | 55.5 (3) | C1—C2—C3—C4 | −0.2 (6) |
| C8—S1—N1—C9 | −143.4 (3) | C2—C3—C4—Br1 | 177.9 (3) |
| O2—S1—C8—C7 | 61.0 (3) | C2—C3—C4—C5 | −1.7 (6) |

| | | | |
|---|---|---|---|
| O3—S1—C8—C7 | −167.5 (3) | Br1—C4—C5—C6 | −178.2 (3) |
| N1—S1—C8—C7 | −54.3 (3) | C3—C4—C5—C6 | 1.3 (5) |
| S1—N1—C1—C2 | 149.4 (3) | C4—C5—C6—C1 | 0.8 (5) |
| S1—N1—C1—C6 | −31.2 (4) | C4—C5—C6—C7 | −178.8 (3) |
| C9—N1—C1—C2 | −11.1 (5) | C1—C6—C7—O1 | −178.0 (3) |
| C9—N1—C1—C6 | 168.3 (3) | C1—C6—C7—C8 | 0.4 (5) |
| S1—N1—C9—C10 | 125.2 (3) | C5—C6—C7—O1 | 1.7 (5) |
| C1—N1—C9—C10 | −74.6 (4) | C5—C6—C7—C8 | 180.0 (3) |
| N1—C1—C2—C3 | −178.3 (3) | O1—C7—C8—S1 | −150.2 (3) |
| C6—C1—C2—C3 | 2.2 (5) | C6—C7—C8—S1 | 31.4 (5) |

Symmetry codes: (i) −*x*+1, −*y*, −*z*−1; (ii) −*x*+1, −*y*, −*z*; (iii) *x*, *y*−1, *z*; (iv) *x*−1, *y*, *z*; (v) −*x*, −*y*+1, −*z*; (vi) −*x*, −*y*, −*z*+1; (vii) −*x*, −*y*, −*z*; (viii) −*x*, −*y*+1, −*z*+1; (ix) *x*, *y*+1, *z*; (x) *x*+1, *y*, *z*.

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C2—H2···O1$^{ix}$ | 0.9300 | 2.4200 | 3.324 (4) | 165.00 |
| C3—H3···O2$^{v}$ | 0.9300 | 2.5900 | 3.418 (4) | 148.00 |
| C8—H8A···O3$^{vi}$ | 0.89 (4) | 2.57 (4) | 3.252 (4) | 134 (3) |
| C9—H9B···O3 | 0.93 (3) | 2.29 (3) | 2.850 (4) | 118 (2) |

Symmetry codes: (ix) *x*, *y*+1, *z*; (v) −*x*, −*y*+1, −*z*; (vi) −*x*, −*y*, −*z*+1.

**Fig. 1**

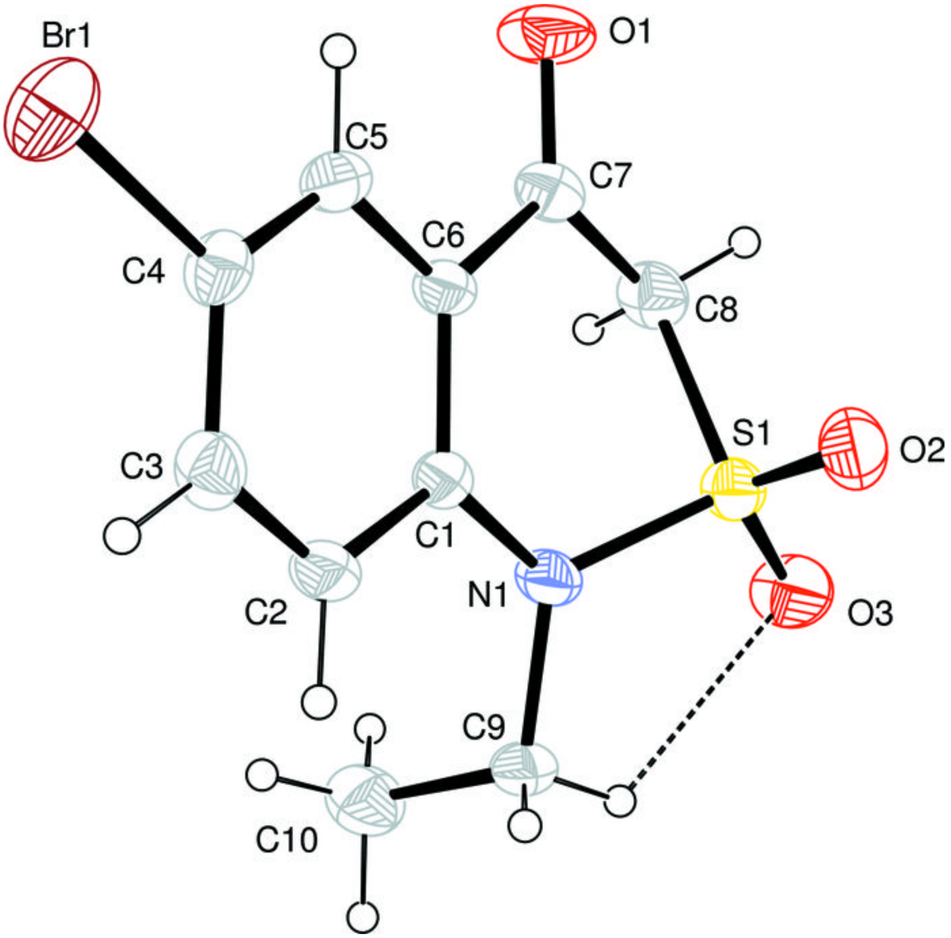

**Fig. 2**