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Methyl 4-hydroxy-2-propyl-2H-1,2-benzothiazine-3-carboxylate 1,1-dioxide

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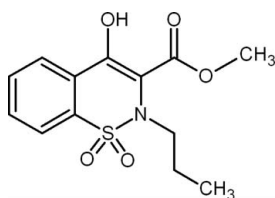
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 Key indicators: single-crystal X-ray study; $T = 296$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.036; wR factor = 0.094; data-to-parameter ratio = 17.7.

In the title compound, $\text{C}_{13}\text{H}_{15}\text{NO}_5\text{S}$, the thiazine ring adopts a distorted half-chair conformation. The enolic H atom is involved in an intramolecular $\text{O}-\text{H}\cdots\text{O}$ hydrogen bond, forming a six-membered ring. In the crystal, molecules are linked through weak intermolecular $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds, resulting in zigzag chains lying along the c axis.

Related literature

For the syntheses of related compounds, see: Bihovsky *et al.* (2004); Braun (1923); Lombardino *et al.* (1971); Zia-ur-Rehman *et al.* (2005, 2009). For the biological activity of benzothiazines, see: Turck *et al.* (1996); Zia-ur-Rehman *et al.* (2006). For related structures, see: Fabiola *et al.* (1998); Zia-ur-Rehman *et al.* (2007).



Experimental

Crystal data

 $\text{C}_{13}\text{H}_{15}\text{NO}_5\text{S}$
 $M_r = 297.32$

 Orthorhombic, $Pca2_1$
 $a = 12.4398$ (6) Å

 $b = 8.7538$ (5) Å

 $c = 12.7288$ (7) Å

 $V = 1386.11$ (13) Å³
 $Z = 4$

 Mo $K\alpha$ radiation

 $\mu = 0.25$ mm⁻¹
 $T = 296$ K

 $0.39 \times 0.36 \times 0.11$ mm

Data collection

Bruker APEXII CCD area-detector diffractometer

Absorption correction: multi-scan (SADABS; Sheldrick, 1996)

 $T_{\min} = 0.908$, $T_{\max} = 0.973$

 8843 measured reflections
 3252 independent reflections

 2540 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.028$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.036$
 $wR(F^2) = 0.094$
 $S = 1.03$

3252 reflections

184 parameters

1 restraint

H-atom parameters constrained

 $\Delta\rho_{\text{max}} = 0.16$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.22$ e Å⁻³

Absolute structure: Flack (1983),

1451 Friedel pairs

 Flack parameter: -0.08 (8)

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{O3}-\text{H3A}\cdots\text{O4}$	0.82	1.84	2.558 (2)	145
$\text{C3}-\text{H3}\cdots\text{O2}^i$	0.93	2.48	3.358 (3)	158

 Symmetry code: (i) $-x + \frac{3}{2}, y, z - \frac{1}{2}$

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) and Mercury (Macrae *et al.*, 2006); 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: IS2482).

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supporting information

Acta Cryst. (2009). E65, o3025 [doi:10.1107/S1600536809046236]

Methyl 4-hydroxy-2-propyl-2*H*-1,2-benzothiazine-3-carboxylate 1,1-dioxide**Muhammad Nadeem Arshad, Muhammad Zia-ur-Rehman and Islam Ullah Khan****S1. Comment**

Benzothiazine 1,1-dioxides are known to possess a versatile range of biological activities and have been synthesized continuously since the very first synthesis in 1923 (Braun, 1923). Among these, Piroxicam (Lombardino *et al.*, 1971; Zia-ur-Rehman *et al.*, 2005), and Meloxicam (Turck *et al.*, 1996) are familiar for their analgesic and anti-inflammatory activities and are being used world wide as non-steroidal anti-inflammatory drugs (NSAIDs). Few of its derivatives are also known as potent calpain I inhibitors (Bihovsky *et al.*, 2004), while benzothiazine-3-yl-quinazolin-4-ones showed marked activity against *Bacillus subtilis* (Zia-ur-Rehman *et al.*, 2006). As part of a research program synthesizing various bioactive benzothiazines (Zia-ur-Rehman *et al.*, 2005, 2006, 2009), we herein report the crystal structure of the title compound, (**I**).

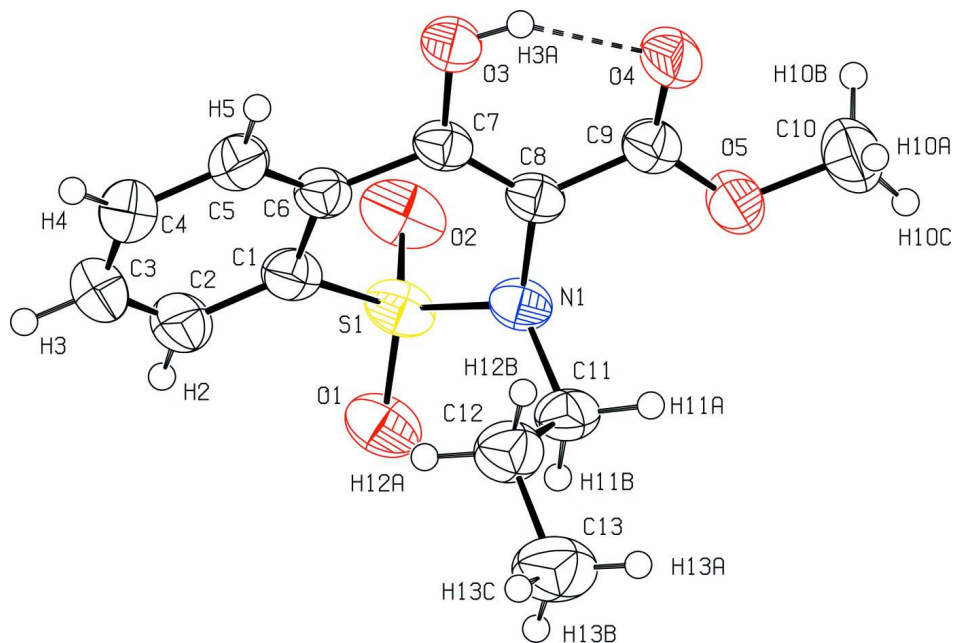
In the molecule of the title compound (Fig. 1), the thiazine ring exhibits a distorted half-chair conformation with S1/C1/C6/C7 atoms lying in a plane and N1 showing significant departure from the plane due to its pyramidal geometry projecting the propyl group approximately perpendicular to the ring. Like other 1,2-benzothiazine 1,1-dioxide derivatives (Fabiola *et al.*, 1998; Zia-ur-Rehman *et al.*, 2007), the enolic hydrogen on O3 is involved in intramolecular hydrogen bonding (Table 1). Also, C7—C8 bond length [1.346 (3) Å] (very close to normal C—C bond 1.36 Å) indicates a partial double-bond character indicating the dominance of enolic form in the molecule. The C1—S1 bond distance [1.759 (3) Å] is as expected for typical C(*sp*²)—S bond (1.751 Å). Each molecule is linked to neighbouring molecules *via* weaker C—H···O=S interactions giving rise to zigzag chains along the *c* axis (Fig. 2).

S2. Experimental

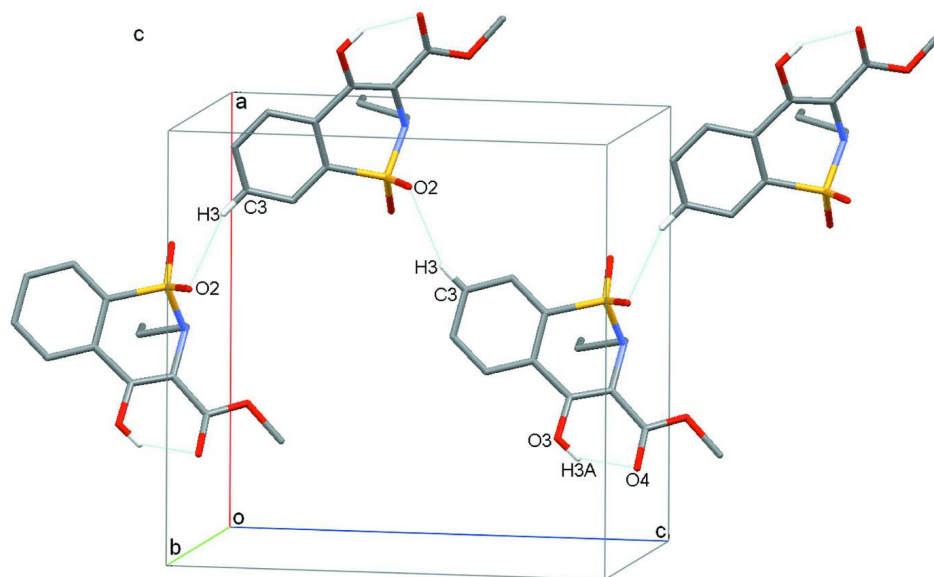
Propyl iodide (5.10 g, 30.0 mmol) was added drop wise to the mixture of methyl 4-hydroxy-2*H*-1,2-benzothiazine-3-carboxylate-1,1-dioxide (3.83 g, 15.0 mmol), anhydrous potassium carbonate (1.68 g, 30.0 mmol) and dimethylformamide (20.0 ml) in a round bottom flask. Contents were stirred at room temperature for 7 h under nitrogen atmosphere and poured over ice cooled water (300 ml) resulting in an immediate formation of a white solid, which was filtered and washed with cold water. Crystallization from methanol yielded pure compound.

S3. Refinement

All hydrogen atoms were identified in the difference map and subsequently fixed in ideal positions and treated as riding on their parent atoms. In the case of the methyl and hydroxyl H atoms the torsion angles were freely refined. The following distances were used: C—H = 0.98 Å for methyl, C—H = 0.95 Å for aromatic and O—H = 0.84 Å for hydroxyl. $U_{\text{iso}}(\text{H})$ was set to $1.2U_{\text{eq}}$ of the parent atoms or $1.5U_{\text{eq}}$ for methyl groups.


Figure 1

The molecular structure of (I), with displacement ellipsoids at the 50% probability level.


Figure 2

Perspective view of the crystal packing showing C—H...O hydrogen-bonded interactions (dashed lines). H atoms not involved in hydrogen bonding have been omitted for clarity.

Methyl 4-hydroxy-2-propyl-2*H*-1,2-benzothiazine-3-carboxylate 1,1-dioxide

Crystal data

$C_{13}H_{15}NO_5S$

$M_r = 297.32$

Orthorhombic, $Pca2_1$

Hall symbol: $P\ 2c\ -2ac$

$a = 12.4398\ (6)\ \text{\AA}$

$b = 8.7538\ (5)\ \text{\AA}$

$c = 12.7288 (7) \text{ \AA}$
 $V = 1386.11 (13) \text{ \AA}^3$
 $Z = 4$
 $F(000) = 624$
 $D_x = 1.425 \text{ Mg m}^{-3}$
 Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$

Cell parameters from 2980 reflections

$\theta = 2.3\text{--}25.3^\circ$
 $\mu = 0.25 \text{ mm}^{-1}$
 $T = 296 \text{ K}$
 Rods, yellow
 $0.39 \times 0.36 \times 0.11 \text{ mm}$

Data collection

Bruker APEXII CCD area-detector
 diffractometer
 Radiation source: fine-focus sealed tube
 Graphite monochromator
 φ and ω scans
 Absorption correction: multi-scan
 (SADABS; Sheldrick, 1996)
 $T_{\min} = 0.908$, $T_{\max} = 0.973$

8843 measured reflections
 3252 independent reflections
 2540 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.028$
 $\theta_{\max} = 28.3^\circ$, $\theta_{\min} = 2.9^\circ$
 $h = -16 \rightarrow 10$
 $k = -11 \rightarrow 11$
 $l = -16 \rightarrow 15$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.036$
 $wR(F^2) = 0.094$
 $S = 1.03$
 3252 reflections
 184 parameters
 1 restraint
 Primary atom site location: structure-invariant
 direct methods
 Secondary atom site location: difference Fourier
 map

Hydrogen site location: inferred from
 neighbouring sites
 H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.0496P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.16 \text{ e \AA}^{-3}$
 $\Delta\rho_{\min} = -0.22 \text{ e \AA}^{-3}$
 Absolute structure: Flack (1983), 1451 Friedel
 pairs
 Absolute structure parameter: $-0.08 (8)$

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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.58950 (17)	0.7963 (3)	0.8319 (2)	0.0442 (5)
C2	0.66903 (18)	0.8114 (3)	0.7577 (2)	0.0565 (6)
H2	0.7391	0.7816	0.7726	0.068*
C3	0.6434 (2)	0.8714 (3)	0.6609 (3)	0.0703 (8)
H3	0.6967	0.8829	0.6103	0.084*
C4	0.5396 (2)	0.9145 (3)	0.6385 (2)	0.0622 (7)
H4	0.5230	0.9536	0.5725	0.075*
C5	0.45981 (19)	0.9001 (3)	0.71319 (19)	0.0509 (6)
H5	0.3900	0.9308	0.6976	0.061*

C6	0.48305 (15)	0.8403 (3)	0.81103 (17)	0.0407 (5)
C7	0.39979 (15)	0.8187 (3)	0.89165 (18)	0.0398 (5)
C8	0.40966 (15)	0.7206 (2)	0.97246 (19)	0.0389 (5)
C9	0.32273 (17)	0.7043 (3)	1.04807 (18)	0.0443 (5)
C10	0.2568 (3)	0.5866 (3)	1.2006 (3)	0.0755 (8)
H10A	0.1955	0.5455	1.1645	0.113*
H10B	0.2378	0.6825	1.2322	0.113*
H10C	0.2794	0.5165	1.2542	0.113*
C11	0.50112 (17)	0.4660 (3)	0.9658 (2)	0.0493 (5)
H11A	0.4465	0.4214	1.0107	0.059*
H11B	0.5695	0.4204	0.9848	0.059*
C12	0.4761 (2)	0.4257 (3)	0.8530 (2)	0.0589 (7)
H12A	0.5279	0.4748	0.8072	0.071*
H12B	0.4052	0.4639	0.8350	0.071*
C13	0.4794 (3)	0.2548 (3)	0.8355 (3)	0.0812 (10)
H13A	0.4297	0.2057	0.8823	0.122*
H13B	0.5507	0.2178	0.8490	0.122*
H13C	0.4600	0.2325	0.7641	0.122*
N1	0.50637 (13)	0.6325 (2)	0.98684 (13)	0.0423 (5)
O1	0.70303 (11)	0.6188 (2)	0.95391 (16)	0.0633 (5)
O2	0.62415 (13)	0.8534 (2)	1.02728 (17)	0.0676 (6)
O3	0.31275 (12)	0.90699 (18)	0.87688 (13)	0.0532 (4)
H3A	0.2671	0.8861	0.9211	0.080*
O4	0.23788 (13)	0.7728 (2)	1.03972 (15)	0.0586 (5)
O5	0.34308 (13)	0.60963 (19)	1.12699 (13)	0.0547 (4)
S1	0.61649 (4)	0.72551 (7)	0.95848 (6)	0.04848 (16)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0361 (10)	0.0384 (12)	0.0580 (13)	-0.0019 (9)	0.0015 (10)	-0.0081 (10)
C2	0.0407 (13)	0.0523 (15)	0.0765 (17)	-0.0002 (11)	0.0107 (12)	-0.0006 (13)
C3	0.0666 (18)	0.0632 (18)	0.081 (2)	0.0040 (15)	0.0342 (15)	0.0044 (15)
C4	0.0709 (17)	0.0561 (17)	0.0595 (16)	0.0069 (13)	0.0155 (14)	0.0104 (13)
C5	0.0502 (13)	0.0437 (14)	0.0587 (15)	0.0032 (10)	0.0017 (11)	0.0047 (11)
C6	0.0369 (10)	0.0354 (12)	0.0499 (13)	-0.0005 (9)	0.0016 (9)	-0.0056 (10)
C7	0.0322 (10)	0.0402 (12)	0.0471 (12)	0.0021 (8)	-0.0027 (9)	-0.0072 (9)
C8	0.0315 (8)	0.0412 (11)	0.0439 (14)	0.0042 (8)	-0.0029 (9)	-0.0057 (10)
C9	0.0403 (12)	0.0447 (12)	0.0480 (12)	0.0016 (10)	0.0004 (10)	-0.0040 (11)
C10	0.0678 (16)	0.095 (2)	0.0642 (17)	0.0176 (16)	0.0203 (13)	0.0219 (18)
C11	0.0443 (10)	0.0444 (12)	0.0592 (13)	0.0112 (9)	-0.0031 (11)	0.0016 (13)
C12	0.0590 (14)	0.0499 (16)	0.0677 (17)	-0.0024 (11)	-0.0011 (13)	-0.0091 (12)
C13	0.077 (2)	0.059 (2)	0.107 (3)	-0.0003 (14)	0.0020 (18)	-0.0210 (19)
N1	0.0350 (9)	0.0465 (11)	0.0455 (12)	0.0077 (7)	-0.0061 (7)	-0.0044 (8)
O1	0.0354 (7)	0.0806 (12)	0.0740 (11)	0.0161 (7)	-0.0059 (9)	-0.0045 (11)
O2	0.0468 (10)	0.0802 (14)	0.0760 (12)	-0.0004 (8)	-0.0149 (8)	-0.0329 (11)
O3	0.0378 (8)	0.0548 (10)	0.0669 (11)	0.0137 (7)	0.0065 (7)	0.0114 (8)
O4	0.0413 (9)	0.0678 (11)	0.0669 (11)	0.0144 (8)	0.0100 (8)	0.0109 (9)

O5	0.0484 (9)	0.0677 (11)	0.0480 (9)	0.0105 (8)	0.0071 (7)	0.0092 (8)
S1	0.0309 (2)	0.0583 (3)	0.0562 (3)	0.0046 (2)	-0.0086 (3)	-0.0146 (3)

Geometric parameters (Å, °)

C1—C2	1.374 (3)	C10—O5	1.439 (3)
C1—C6	1.404 (3)	C10—H10A	0.9600
C1—S1	1.759 (3)	C10—H10B	0.9600
C2—C3	1.376 (4)	C10—H10C	0.9600
C2—H2	0.9300	C11—N1	1.483 (3)
C3—C4	1.375 (4)	C11—C12	1.511 (4)
C3—H3	0.9300	C11—H11A	0.9700
C4—C5	1.380 (3)	C11—H11B	0.9700
C4—H4	0.9300	C12—C13	1.513 (4)
C5—C6	1.382 (3)	C12—H12A	0.9700
C5—H5	0.9300	C12—H12B	0.9700
C6—C7	1.470 (3)	C13—H13A	0.9600
C7—O3	1.344 (2)	C13—H13B	0.9600
C7—C8	1.346 (3)	C13—H13C	0.9600
C8—N1	1.441 (3)	N1—S1	1.6339 (19)
C8—C9	1.455 (3)	O1—S1	1.4268 (15)
C9—O4	1.219 (3)	O2—S1	1.425 (2)
C9—O5	1.327 (3)	O3—H3A	0.8200
C2—C1—C6	121.5 (2)	H10A—C10—H10C	109.5
C2—C1—S1	121.76 (19)	H10B—C10—H10C	109.5
C6—C1—S1	116.72 (17)	N1—C11—C12	114.2 (2)
C1—C2—C3	119.0 (2)	N1—C11—H11A	108.7
C1—C2—H2	120.5	C12—C11—H11A	108.7
C3—C2—H2	120.5	N1—C11—H11B	108.7
C4—C3—C2	120.5 (2)	C12—C11—H11B	108.7
C4—C3—H3	119.7	H11A—C11—H11B	107.6
C2—C3—H3	119.7	C11—C12—C13	111.4 (2)
C3—C4—C5	120.5 (3)	C11—C12—H12A	109.3
C3—C4—H4	119.8	C13—C12—H12A	109.3
C5—C4—H4	119.8	C11—C12—H12B	109.3
C4—C5—C6	120.4 (2)	C13—C12—H12B	109.3
C4—C5—H5	119.8	H12A—C12—H12B	108.0
C6—C5—H5	119.8	C12—C13—H13A	109.5
C5—C6—C1	118.1 (2)	C12—C13—H13B	109.5
C5—C6—C7	122.04 (19)	H13A—C13—H13B	109.5
C1—C6—C7	119.8 (2)	C12—C13—H13C	109.5
O3—C7—C8	123.2 (2)	H13A—C13—H13C	109.5
O3—C7—C6	113.3 (2)	H13B—C13—H13C	109.5
C8—C7—C6	123.46 (18)	C8—N1—C11	117.79 (16)
C7—C8—N1	120.99 (19)	C8—N1—S1	113.92 (15)
C7—C8—C9	120.03 (18)	C11—N1—S1	119.13 (14)
N1—C8—C9	118.98 (19)	C7—O3—H3A	109.5

O4—C9—O5	122.6 (2)	C9—O5—C10	115.99 (19)
O4—C9—C8	122.6 (2)	O2—S1—O1	119.30 (11)
O5—C9—C8	114.85 (18)	O2—S1—N1	108.17 (11)
O5—C10—H10A	109.5	O1—S1—N1	108.37 (10)
O5—C10—H10B	109.5	O2—S1—C1	107.40 (13)
H10A—C10—H10B	109.5	O1—S1—C1	109.72 (11)
O5—C10—H10C	109.5	N1—S1—C1	102.59 (9)
C6—C1—C2—C3	0.1 (4)	N1—C8—C9—O5	1.8 (3)
S1—C1—C2—C3	-178.3 (2)	N1—C11—C12—C13	176.1 (2)
C1—C2—C3—C4	-0.5 (4)	C7—C8—N1—C11	-108.9 (2)
C2—C3—C4—C5	0.9 (4)	C9—C8—N1—C11	72.3 (3)
C3—C4—C5—C6	-0.9 (4)	C7—C8—N1—S1	37.8 (3)
C4—C5—C6—C1	0.5 (3)	C9—C8—N1—S1	-141.04 (17)
C4—C5—C6—C7	-178.1 (2)	C12—C11—N1—C8	63.6 (3)
C2—C1—C6—C5	-0.1 (3)	C12—C11—N1—S1	-81.3 (2)
S1—C1—C6—C5	178.34 (18)	O4—C9—O5—C10	2.7 (3)
C2—C1—C6—C7	178.5 (2)	C8—C9—O5—C10	-177.5 (2)
S1—C1—C6—C7	-3.0 (3)	C8—N1—S1—O2	61.60 (18)
C5—C6—C7—O3	-21.8 (3)	C11—N1—S1—O2	-152.19 (18)
C1—C6—C7—O3	159.7 (2)	C8—N1—S1—O1	-167.73 (15)
C5—C6—C7—C8	158.4 (2)	C11—N1—S1—O1	-21.5 (2)
C1—C6—C7—C8	-20.2 (3)	C8—N1—S1—C1	-51.72 (16)
O3—C7—C8—N1	-177.71 (19)	C11—N1—S1—C1	94.49 (18)
C6—C7—C8—N1	2.1 (3)	C2—C1—S1—O2	100.0 (2)
O3—C7—C8—C9	1.1 (3)	C6—C1—S1—O2	-78.46 (19)
C6—C7—C8—C9	-179.1 (2)	C2—C1—S1—O1	-31.1 (2)
C7—C8—C9—O4	2.6 (3)	C6—C1—S1—O1	150.46 (17)
N1—C8—C9—O4	-178.5 (2)	C2—C1—S1—N1	-146.1 (2)
C7—C8—C9—O5	-177.1 (2)	C6—C1—S1—N1	35.43 (19)

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O3—H3A \cdots O4	0.82	1.84	2.558 (2)	145
C3—H3 \cdots O2 ⁱ	0.93	2.48	3.358 (3)	158

Symmetry code: (i) $-x+3/2, y, z-1/2$.