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

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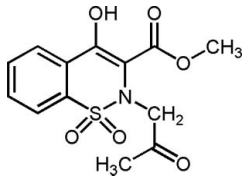
Key indicators: single-crystal X-ray study; T = 120 K; mean σ(C–C) = 0.003 Å; R factor = 0.040; wR factor = 0.101; data-to-parameter ratio = 16.0.

In the molecule of the title compound, $C_{13}H_{13}NO_6S$, the thiazine ring adopts a distorted sofa conformation. The enolic H atom is involved in intramolecular O—H···O hydrogen bonding besides the weaker C—H···O=S and C—H···O=C interactions.

Related literature

For related literature, see: Ahmad *et al.* (2008); Zia-ur-Rehman *et al.* (2005, 2006, 2007); Bihovsky *et al.* (2004); Braun (1923); Fabiola *et al.* (1998); Kojić-Prodić & Ružić-Toroš (1982); Lombardino *et al.* (1971); Turck *et al.* (1996); Weast *et al.* (1984).



Experimental

Crystal data

$C_{13}H_{13}NO_6S$
M_r = 311.30
Orthorhombic, $Pca2_1$
a = 11.7982 (3) Å
b = 8.7206 (2) Å
c = 13.2474 (4) Å
V = 1362.99 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.27 mm^{-1}
T = 120 (2) K
0.50 × 0.30 × 0.15 mm

Data collection

Bruker–Nonius KappaCCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2007)
T_{min} = 0.879, T_{max} = 0.961
12553 measured reflections
3095 independent reflections
2849 reflections with $I > 2\sigma(I)$
R_{int} = 0.041

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.100
S = 1.13
3095 reflections
194 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.57 e Å^{-3}
$\Delta\rho_{min}$ = −0.64 e Å^{-3}
Absolute structure: Flack (1983), 1466 Friedel pairs
Flack parameter: 0.00 (8)

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3···O4	0.84	1.85	2.580 (2)	145
C3—H3A···O1^{i}	0.95	2.37	3.286 (3)	163
C4—H4···O1^{ii}	0.95	2.49	3.267 (3)	139
C11—H11A···O2	0.99	2.46	2.830 (3)	102
C11—H11B···O5	0.99	2.40	2.994 (3)	118

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

Data collection: *COLLECT* (Hooft, 1998); cell refinement: *DENZO* (Otwinowski & Minor, 1997) and *COLLECT*; data reduction: *DENZO* and *COLLECT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *CAMERON* (Watkin *et al.*, 1993); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2729).

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Acta Cryst. (2008). E**64**, o1392 [doi:10.1107/S1600536808019156]

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

Matloob Ahmad, Hamid Latif Siddiqui, Muhammad Zia-ur-Rehman, Graham John Tizzard and Saeed Ahmad

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). Some of the 3,4-dihydro-1,2-benzothiazine-3-carboxylate 1,1-dioxide α-ketomide and P(2)—P(3) peptide mimetic aldehyde compounds act as potent calpain I inhibitors (Bihovsky *et al.*, 2004) while 1,2-benzothiazin-3-yl-quinazolin-4(3*H*)-ones possess antibacterial properties (Zia-ur-Rehman *et al.*, 2006). In continuation of our ongoing work (Zia-ur-Rehman *et al.*, 2007; Ahmad *et al.*, 2008), we herein report the synthesis and crystal structure of the title compound.

In this paper, the structure of the title compound (**I**) is reported (Scheme and figure 1). The thiazine ring, involving two double bonds, exhibits a sofa conformation; with S1/C1/C6/C7 relatively planar and N1 showing significant departure from plane due to its pyramidal geometry. The enolic hydrogen on O3 is involved in intramolecular hydrogen bonding [O3—H3···O4] with the carbonyl oxygen at C4 giving rise to a six-membered hydrogen bond ring (Table 1). The C1—S1 [1.757 (2)Å] bond is shorter than a normal C—S single bond (1.81–2.55Å) (Weast *et al.*, 1984) due to partial double bond character and is in agreement with similar molecules (Kojić-Prodić & Ružić-Toroŝ, 1982; Fabiola *et al.*, 1998]. Each molecule is further linked to neighbouring molecules *via* weaker C—H···O=S and C—H···O=C interactions (Table 1).

S2. Experimental

A mixture of mono chloroacetone (1.94 ml; 23.5 mmoles), methyl 4-hydroxy-2*H*-1,2-benzothiazine-3-carboxylate 1,1-dioxide (5.0 g,19.6 mmoles), dimethyl formamide (10.0 ml) and anhydrous sodium carbonate (4.2 g,39.2 mmoles) was stirred under nitrogen atmosphere for 3.0 h at 120 ^{o}C.The contents were then cooled to room temperature and poured over crushed ice.Title compound (I) was precipitated as white precipitates which were washed with excess of water, filtered and dried. Yield: 4.39 g; 72%; *M*.p. 455 K. Crystals were grown by slow evaporation of solution of (**I**) in Chloroform-Methanol (1:1) mixture.

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 (three additional parameters). The following distances were used: Methyl C—H 0.98 Å. ° Methylene C—H 0.99 Å. ° Aromatic C—H 0.95 Å. ° Hydroxyl O—H 0.84 Å. U(H) was set to 1.2U_{eq} of the parent atoms or 1.5U_{eq} for methyl groups.

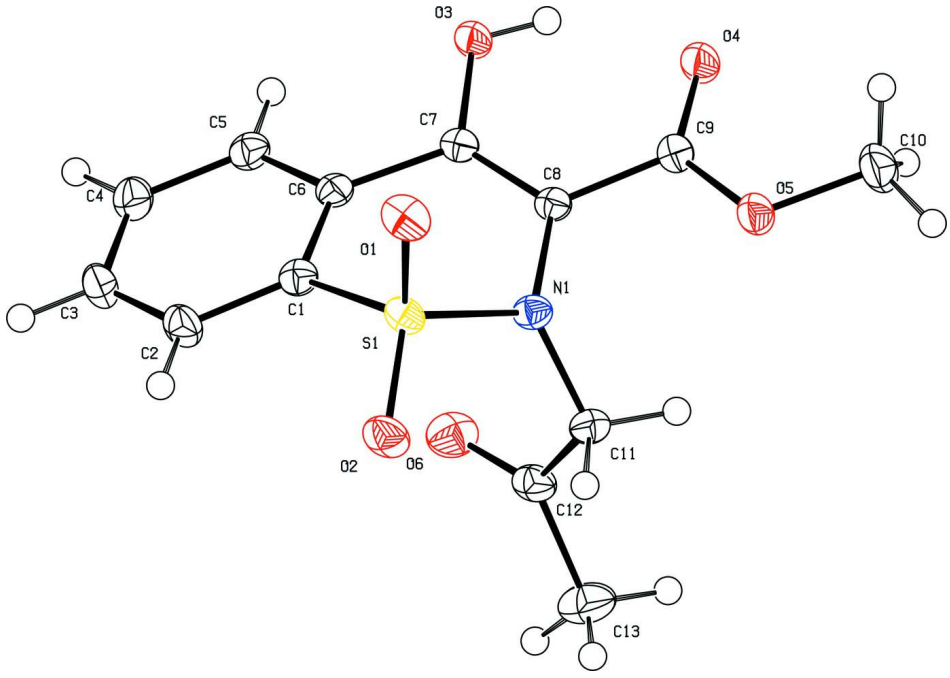

Figure 1

The asymmetric unit of the title compound showing the intramolecular hydrogen bond. Displacement ellipsoids are drawn at the 50% probability level.

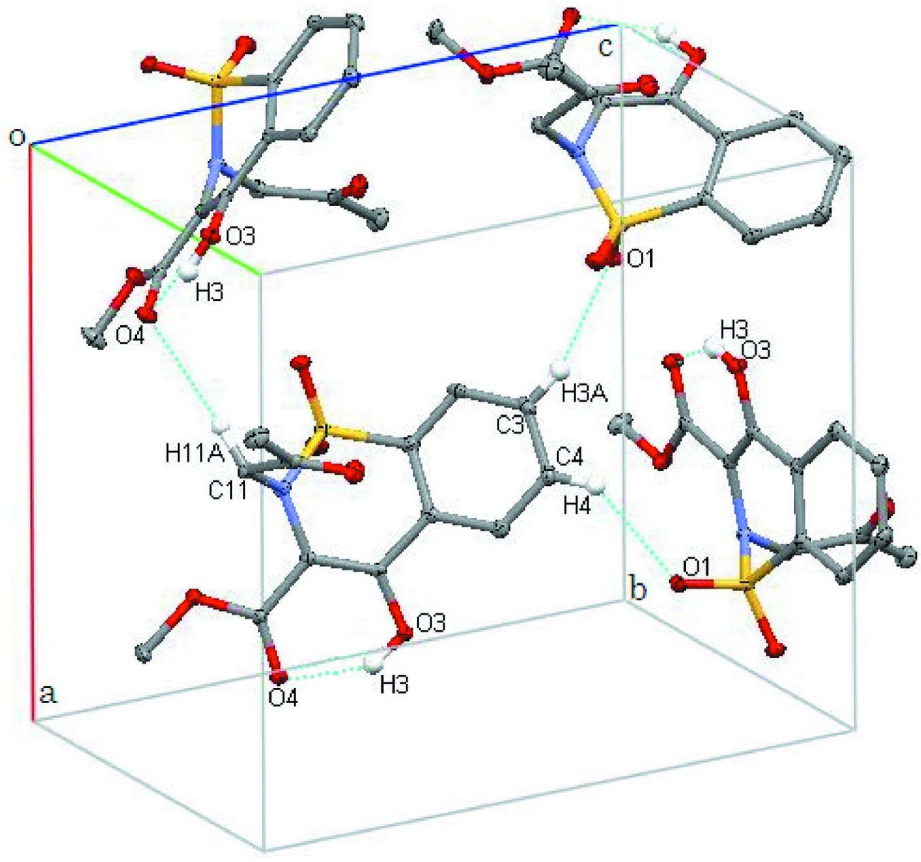

Figure 2

Perspective view of the three-dimensional crystal packing showing hydrogen-bonds and other intermolecular interactions (dashed lines). H atoms not involved in hydrogen bonding have been omitted for clarity.

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

Crystal data

$C_{13}H_{13}NO_6S$
$M_r = 311.30$
Orthorhombic, $Pca2_1$
Hall symbol: P 2c -2ac
$a = 11.7982\ (3)$ Å
$b = 8.7206\ (2)$ Å
$c = 13.2474\ (4)$ Å
$V = 1362.99\ (6)$ Å^3
$Z = 4$
$F(000) = 648$
$D_x = 1.517$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 6916 reflections
$\theta = 2.9–27.5°$
$\mu = 0.27$ mm^{-1}
$T = 120$ K
Block, colourless
0.50 × 0.30 × 0.15 mm

Data collection

Bruker–Nonius KappaCCD diffractometer
Radiation source: Bruker Nonius FR591 Rotating Anode
Graphite monochromator
Detector resolution: 9.091 pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2007)
$T_{min} = 0.879$, $T_{max} = 0.961$
12553 measured reflections
3095 independent reflections
2849 reflections with $I > 2\sigma(I)$
$R_{int} = 0.041$

θ_{max} = 27.5°, θ_{min} = 3.1°
h = −15→15
k = −11→11
l = −17→17

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.100
S = 1.13
3095 reflections
194 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
$w = 1/[\sigma^2(F_o^2) + (0.0621P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.57 e Å^{-3}
$\Delta\rho_{min}$ = −0.64 e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.067 (4)
Absolute structure: Flack (1983), 1466 Friedel pairs
Absolute structure parameter: 0.00 (8)

Special details

Experimental. *SADABS* was used to perform the Absorption correction Estimated minimum and maximum transmission: 0.6723 0.7456 The given Tmin and Tmax were generated using the *SHELX* SIZE command

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 (Å²)

	x	y	z	U_{iso}*/U_{eq}
S1	0.12520 (4)	0.72682 (5)	0.71113 (5)	0.01779 (15)
O1	0.14000 (12)	0.85887 (19)	0.64793 (13)	0.0249 (4)
O2	0.21431 (12)	0.61542 (17)	0.71678 (14)	0.0255 (4)
O3	−0.19773 (12)	0.91805 (17)	0.77253 (12)	0.0204 (3)
H3	−0.2440	0.8985	0.7261	0.031*
O4	−0.27020 (12)	0.78295 (17)	0.61171 (13)	0.0229 (4)
O5	−0.15104 (13)	0.62248 (18)	0.53092 (12)	0.0234 (4)
O6	−0.03227 (14)	0.48788 (19)	0.85565 (13)	0.0287 (4)
N1	0.00988 (15)	0.63873 (19)	0.67500 (15)	0.0172 (4)
C1	0.08889 (18)	0.7943 (2)	0.83187 (17)	0.0173 (4)
C2	0.16859 (19)	0.8042 (3)	0.90839 (18)	0.0231 (5)
H2	0.2436	0.7675	0.8984	0.028*
C3	0.1371 (2)	0.8685 (3)	0.9994 (2)	0.0258 (5)
H3A	0.1909	0.8765	1.0525	0.031*
C4	0.0269 (2)	0.9218 (3)	1.01423 (18)	0.0244 (5)
H4	0.0061	0.9659	1.0771	0.029*
C5	−0.05253 (19)	0.9105 (2)	0.93717 (17)	0.0195 (4)
H5	−0.1274	0.9473	0.9476	0.023*

C6	−0.02314 (17)	0.8457 (2)	0.84476 (17)	0.0169 (4)
C7	−0.10643 (17)	0.8267 (2)	0.76334 (17)	0.0156 (4)
C8	−0.09225 (18)	0.7266 (2)	0.68505 (15)	0.0155 (4)
C9	−0.17931 (18)	0.7142 (2)	0.60656 (16)	0.0172 (4)
C10	−0.2356 (2)	0.6047 (3)	0.4522 (2)	0.0327 (6)
H10A	−0.3074	0.5716	0.4822	0.049*
H10B	−0.2098	0.5275	0.4035	0.049*
H10C	−0.2465	0.7029	0.4176	0.049*
C11	0.00404 (19)	0.4701 (2)	0.67907 (18)	0.0202 (4)
H11A	0.0763	0.4277	0.6532	0.024*
H11B	−0.0572	0.4350	0.6335	0.024*
C12	−0.01724 (18)	0.4058 (2)	0.78301 (19)	0.0216 (5)
C13	−0.0175 (2)	0.2338 (3)	0.7899 (2)	0.0329 (6)
H13A	−0.0154	0.2028	0.8609	0.049*
H13B	0.0492	0.1928	0.7549	0.049*
H13C	−0.0864	0.1935	0.7582	0.049*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0125 (2)	0.0212 (2)	0.0196 (2)	0.00081 (16)	0.0010 (2)	0.0031 (3)
O1	0.0198 (8)	0.0285 (8)	0.0263 (10)	−0.0038 (6)	0.0031 (6)	0.0092 (7)
O2	0.0170 (7)	0.0302 (8)	0.0293 (9)	0.0066 (5)	−0.0005 (7)	−0.0005 (8)
O3	0.0159 (7)	0.0222 (7)	0.0232 (8)	0.0050 (5)	−0.0035 (6)	−0.0042 (7)
O4	0.0176 (8)	0.0256 (7)	0.0256 (8)	0.0052 (6)	−0.0034 (6)	−0.0057 (7)
O5	0.0237 (9)	0.0267 (9)	0.0198 (8)	0.0058 (6)	−0.0048 (6)	−0.0056 (7)
O6	0.0361 (10)	0.0257 (8)	0.0243 (9)	0.0012 (7)	0.0043 (7)	0.0048 (7)
N1	0.0148 (9)	0.0162 (7)	0.0205 (9)	0.0014 (6)	0.0018 (7)	0.0003 (7)
C1	0.0173 (10)	0.0157 (8)	0.0190 (10)	−0.0019 (7)	0.0016 (9)	0.0019 (9)
C2	0.0164 (11)	0.0253 (10)	0.0276 (12)	−0.0014 (8)	−0.0053 (9)	0.0016 (10)
C3	0.0267 (13)	0.0267 (12)	0.0241 (12)	−0.0015 (9)	−0.0110 (9)	0.0007 (10)
C4	0.0310 (13)	0.0232 (10)	0.0191 (11)	0.0003 (9)	−0.0031 (9)	−0.0014 (9)
C5	0.0205 (11)	0.0158 (9)	0.0222 (10)	−0.0019 (7)	0.0009 (9)	0.0011 (9)
C6	0.0181 (11)	0.0119 (8)	0.0208 (11)	−0.0029 (7)	−0.0013 (8)	0.0036 (8)
C7	0.0129 (9)	0.0150 (9)	0.0188 (10)	−0.0008 (7)	0.0016 (8)	0.0030 (8)
C8	0.0137 (9)	0.0141 (9)	0.0188 (11)	−0.0009 (7)	0.0004 (8)	0.0021 (8)
C9	0.0161 (10)	0.0187 (9)	0.0168 (10)	−0.0009 (8)	0.0005 (8)	0.0004 (8)
C10	0.0323 (14)	0.0408 (12)	0.0250 (12)	0.0121 (11)	−0.0117 (10)	−0.0120 (12)
C11	0.0205 (10)	0.0168 (9)	0.0234 (11)	0.0035 (8)	−0.0005 (8)	−0.0019 (9)
C12	0.0144 (11)	0.0200 (10)	0.0303 (13)	0.0005 (7)	−0.0008 (9)	0.0035 (10)
C13	0.0332 (15)	0.0194 (11)	0.0460 (17)	0.0012 (9)	0.0037 (12)	0.0042 (11)

Geometric parameters (Å, º)

S1—O2	1.4335 (14)	C4—C5	1.389 (3)
S1—O1	1.4345 (17)	C4—H4	0.9500
S1—N1	1.6341 (19)	C5—C6	1.392 (3)
S1—C1	1.757 (2)	C5—H5	0.9500

O3—C7	1.345 (2)	C6—C7	1.469 (3)
O3—H3	0.8400	C7—C8	1.366 (3)
O4—C9	1.231 (3)	C8—C9	1.465 (3)
O5—C9	1.325 (3)	C10—H10A	0.9800
O5—C10	1.452 (3)	C10—H10B	0.9800
O6—C12	1.212 (3)	C10—H10C	0.9800
N1—C8	1.434 (3)	C11—C12	1.508 (3)
N1—C11	1.473 (3)	C11—H11A	0.9900
C1—C2	1.385 (3)	C11—H11B	0.9900
C1—C6	1.406 (3)	C12—C13	1.503 (3)
C2—C3	1.381 (4)	C13—H13A	0.9800
C2—H2	0.9500	C13—H13B	0.9800
C3—C4	1.394 (4)	C13—H13C	0.9800
C3—H3A	0.9500		

O2—S1—O1	119.03 (10)	O3—C7—C6	113.72 (18)
O2—S1—N1	107.90 (9)	C8—C7—C6	123.24 (18)
O1—S1—N1	107.93 (10)	C7—C8—N1	120.98 (18)
O2—S1—C1	110.99 (11)	C7—C8—C9	119.99 (18)
O1—S1—C1	106.99 (10)	N1—C8—C9	118.93 (18)
N1—S1—C1	102.77 (10)	O4—C9—O5	123.7 (2)
C7—O3—H3	109.5	O4—C9—C8	122.39 (19)
C9—O5—C10	115.80 (17)	O5—C9—C8	113.86 (18)
C8—N1—C11	119.38 (17)	O5—C10—H10A	109.5
C8—N1—S1	114.92 (13)	O5—C10—H10B	109.5
C11—N1—S1	119.83 (15)	H10A—C10—H10B	109.5
C2—C1—C6	121.9 (2)	O5—C10—H10C	109.5
C2—C1—S1	121.44 (17)	H10A—C10—H10C	109.5
C6—C1—S1	116.52 (16)	H10B—C10—H10C	109.5
C3—C2—C1	118.8 (2)	N1—C11—C12	114.36 (18)
C3—C2—H2	120.6	N1—C11—H11A	108.7
C1—C2—H2	120.6	C12—C11—H11A	108.7
C2—C3—C4	120.6 (2)	N1—C11—H11B	108.7
C2—C3—H3A	119.7	C12—C11—H11B	108.7
C4—C3—H3A	119.7	H11A—C11—H11B	107.6
C5—C4—C3	120.1 (2)	O6—C12—C13	122.8 (2)
C5—C4—H4	119.9	O6—C12—C11	121.97 (18)
C3—C4—H4	119.9	C13—C12—C11	115.3 (2)
C6—C5—C4	120.4 (2)	C12—C13—H13A	109.5
C6—C5—H5	119.8	C12—C13—H13B	109.5
C4—C5—H5	119.8	H13A—C13—H13B	109.5
C5—C6—C1	118.06 (19)	C12—C13—H13C	109.5
C5—C6—C7	121.68 (19)	H13A—C13—H13C	109.5
C1—C6—C7	120.2 (2)	H13B—C13—H13C	109.5
O3—C7—C8	123.04 (19)		

O2—S1—N1—C8	167.94 (15)	C5—C6—C7—O3	20.3 (3)
O1—S1—N1—C8	−62.23 (17)	C1—C6—C7—O3	−161.46 (18)

C1—S1—N1—C8	50.61 (17)	C5—C6—C7—C8	−160.21 (19)
O2—S1—N1—C11	15.1 (2)	C1—C6—C7—C8	18.0 (3)
O1—S1—N1—C11	144.91 (16)	O3—C7—C8—N1	175.91 (18)
C1—S1—N1—C11	−102.25 (17)	C6—C7—C8—N1	−3.5 (3)
O2—S1—C1—C2	31.3 (2)	O3—C7—C8—C9	−0.6 (3)
O1—S1—C1—C2	−100.01 (18)	C6—C7—C8—C9	−179.97 (18)
N1—S1—C1—C2	146.46 (18)	C11—N1—C8—C7	118.1 (2)
O2—S1—C1—C6	−152.25 (15)	S1—N1—C8—C7	−34.9 (2)
O1—S1—C1—C6	76.41 (16)	C11—N1—C8—C9	−65.4 (3)
N1—S1—C1—C6	−37.13 (17)	S1—N1—C8—C9	141.61 (16)
C6—C1—C2—C3	−0.9 (3)	C10—O5—C9—O4	−0.7 (3)
S1—C1—C2—C3	175.34 (17)	C10—O5—C9—C8	179.00 (18)
C1—C2—C3—C4	0.3 (3)	C7—C8—C9—O4	−5.5 (3)
C2—C3—C4—C5	0.1 (3)	N1—C8—C9—O4	177.96 (18)
C3—C4—C5—C6	0.2 (3)	C7—C8—C9—O5	174.79 (18)
C4—C5—C6—C1	−0.7 (3)	N1—C8—C9—O5	−1.8 (3)
C4—C5—C6—C7	177.53 (19)	C8—N1—C11—C12	−73.3 (3)
C2—C1—C6—C5	1.1 (3)	S1—N1—C11—C12	78.4 (2)
S1—C1—C6—C5	−175.30 (15)	N1—C11—C12—O6	2.6 (3)
C2—C1—C6—C7	−177.19 (19)	N1—C11—C12—C13	−176.96 (19)
S1—C1—C6—C7	6.4 (2)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3···O4	0.84	1.85	2.580 (2)	145
C3—H3*A*···O1^{i}	0.95	2.37	3.286 (3)	163
C4—H4···O1^{ii}	0.95	2.49	3.267 (3)	139
C11—H11*A*···O2	0.99	2.46	2.830 (3)	102
C11—H11*B*···O5	0.99	2.40	2.994 (3)	118

Symmetry codes: (i) *x*+1/2, −*y*, *z*; (ii) −*x*, −*y*+2, *z*+1/2.