Acta Crystallographica Section E
**Structure Reports Online**
ISSN 1600-5368

# Methyl 4-acetoxy-2-methyl-2*H*-1,2-benzothiazine-3-carboxylate 1,1-dioxide

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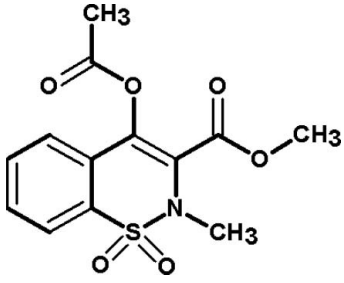
Received 12 December 2007; accepted 7 February 2008

Key indicators: single-crystal X-ray study; $T$ = 120 K; mean $\sigma$(C–C) = 0.004 Å; $R$ factor = 0.051; $wR$ factor = 0.146; data-to-parameter ratio = 15.7.

In the title compound, $C_{13}H_{13}NO_6S$, the thiazine ring adopts a distorted half-chair conformation. Each molecule is linked to its neighbour through intermolecular C—H···O hydrogen bonds.

## Related literature

For related literature, see: Fabiola *et al.* (1998); Golič & Leban (1987); Kojić-Prodić & Ružić-Toroš (1982); Rajagopal & Seshadri (1990); Reck *et al.* (1988); Rehman *et al.* (2005, 2006); Turck *et al.* (1996).



## Experimental

### Crystal data

$C_{13}H_{13}NO_6S$
$M_r$ = 311.30
Monoclinic, $P2_1/c$
$a$ = 6.8917 (5) Å
$b$ = 24.1814 (17) Å
$c$ = 8.2861 (5) Å
$\beta$ = 97.876 (4)°
$V$ = 1367.86 (16) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.26 mm$^{-1}$
$T$ = 120 (2) K
0.40 × 0.20 × 0.20 mm

### Data collection

Bruker Nonius KappaCCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2007)
$T_{min}$ = 0.902, $T_{max}$ = 0.949
12265 measured reflections
3032 independent reflections
2183 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.057

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.145
$S$ = 1.03
3032 reflections
193 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.36 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.55 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C13—H13$A$···O4$^{i}$ | 0.98 | 2.48 | 3.387 (3) | 153 |
| C5—H5···O1$^{i}$ | 0.95 | 2.48 | 3.349 (3) | 151 |

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

Data collection: *COLLECT* (Nonius, 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* (Pearce & Watkin, 1993); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

The authors acknowledge financial support from the Higher Education Commission of Pakistan and the University of the Punjab, Lahore.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: KP2156).

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# supplementary materials

*Acta Cryst.* (2008). E**64**, o594 [ **doi:10.1107/S1600536808004029** ]

# Methyl 4-acetoxy-2-methyl-2*H*-1,2-benzothiazine-3-carboxylate 1,1-dioxide

**M. Ahmad, H. L. Siddiqui, S. Ahmad, M. Irfan Ashiq and G. J. Tizzard**

## Comment

Among the vast class of benzothiazines, 1,2-benzothiazine1,1-dioxides are the most versatile compounds due to their applications in various fields such as pharmaceuticals (Turck *et al.*, 1996), dyes (Rajagopal & Seshadri, 1990) and fungicides. In continuation of our investigation of the chemistry of 1,2-benzothiazine 1,1-dioxide derivatives (Rehman *et al.*, 2005; Rehman *et al.*, 2006) we have synthesized the title compound (**I**) and its crystal structure is reported here.

In (**I**) (Fig. 1), the benzene ring of the benzothiazine nucleus is planar (the maximum least square deviation from the plane of the atoms involved is 0.01 Å) while the thiazine ring adopts a distorted half chair conformation. N1 has a pyramidal geometry projecting the methyl group approximately perpendicular to the thiazine ring. Atoms O1, O3 and O5 lie approximately in the plane of the ring while O2 lies almost perpendicular to it.

The C7—O3 bond length in (I) is longer [1.389 (3)] than in the related molecules having no substitution at O3 [1.352 (9) Å; Golič & Leban, 1987; 1.350 (9) Å; Reck *et al.*, 1988].

C9—O4 bond length [1.201 (13) Å] is observed to be shorter than in its previously reported non acylated analogue [1.262 (10) Å; Golič & Leban, 1987] due to no involvement of O4 electrons in the hydrogen bonding. O4 lies almost perpendicular to the thiazine ring and the bond angle C7—C8—C9 [127.3 (2) Å] is greater than observed in the related hydrogen bonded oxicams [121.0 (3) Å; Kojić-Prodić & Ružić-Toroš, 1982; 120.9 (2) Å, Fabiola *et al.*, 1998]. Molecules are linked by C—H···O hydrogen bonds (Table1) forming a chain along *a* axis.

## Experimental

Acetyl chloride (1.57 g; 10 mmol) was slowly added to a mixture of methyl 4-hydroxy-2-methyl-2*H*-1,2-benzothiazine-3-carboxylate1,1-dioxide (1.345 g; 5 mmol), triethylamine (0.71 g; 7 mmol) and carbon tetrachloride (25 ml) under nitrogen atmosphere at 273 K. The mixture was stirred for a period of three hours at room temperature and the solvent was evaporated under vacuum. A residue was poured over ice-water mixture to get the white coloured product which was washed with cold water and recrystallized from chloroform-methanol mixture (1:1). Yield 1.31 g; 84°; m.p. 422 K.

## Figures

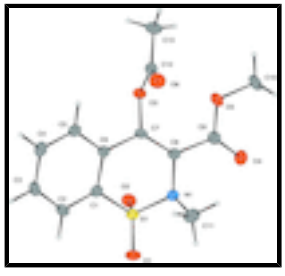

Fig. 1. The molecular structure of (I), showing displacement ellipsoids at the 50% probability level for non-H atoms. Dashed lines denote hydrogen bonds.

## Methyl 4-acetoxy-2-methyl-2*H*-1,2-benzothiazine-3-carboxylate 1,1-dioxide

*Crystal data*

| | |
|---|---|
| $C_{13}H_{13}NO_6S$ | $F(000) = 648$ |
| $M_r = 311.30$ | $D_x = 1.512$ Mg m$^{-3}$ |
| Monoclinic, $P2_1/c$ | Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å |
| Hall symbol: -P 2ybc | Cell parameters from 15145 reflections |
| $a = 6.8917$ (5) Å | $\theta = 2.9$–$27.5°$ |
| $b = 24.1814$ (17) Å | $\mu = 0.26$ mm$^{-1}$ |
| $c = 8.2861$ (5) Å | $T = 120$ K |
| $\beta = 97.876$ (4)° | Block, colourless |
| $V = 1367.86$ (16) Å$^3$ | 0.40 × 0.20 × 0.20 mm |
| $Z = 4$ | |

*Data collection*

| | |
|---|---|
| Bruker Nonius CCD camera on κ-goniostat diffractometer | 3032 independent reflections |
| Radiation source: Bruker Nonius FR591 Rotating Anode | 2183 reflections with $I > 2\sigma(I)$ |
| graphite | $R_{int} = 0.057$ |
| Detector resolution: 9.091 pixels mm$^{-1}$ | $\theta_{max} = 27.5°$, $\theta_{min} = 3.0°$ |
| φ and ω scans to fill the asymmetric unit | $h = -8 \rightarrow 8$ |
| Absorption correction: multi-scan (*SADABS*; Sheldrick, 2007) | $k = -31 \rightarrow 30$ |
| $T_{min} = 0.902$, $T_{max} = 0.949$ | $l = -10 \rightarrow 9$ |
| 12265 measured reflections | |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Primary atom site location: structure-invariant direct methods |
| Least-squares matrix: full | Secondary atom site location: difference Fourier map |
| $R[F^2 > 2\sigma(F^2)] = 0.050$ | Hydrogen site location: inferred from neighbouring sites |
| $wR(F^2) = 0.145$ | H-atom parameters constrained |
| $S = 1.03$ | $w = 1/[\sigma^2(F_o^2) + (0.0764P)^2 + 0.6225P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| 3032 reflections | $(\Delta/\sigma)_{max} = 0.001$ |
| 193 parameters | $\Delta\rho_{max} = 0.36$ e Å$^{-3}$ |
| 0 restraints | $\Delta\rho_{min} = -0.55$ e Å$^{-3}$ |

*Special details*

**Experimental**. *SADABS* was used to perform the Absorption correction Estimated minimum and maximum transmission: 0.6195 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 (Å$^2$)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| C1 | 0.5172 (4) | 0.43090 (10) | 0.7387 (3) | 0.0183 (5) |
| C2 | 0.7043 (4) | 0.45347 (10) | 0.7686 (3) | 0.0213 (6) |
| H2 | 0.7629 | 0.4616 | 0.8766 | 0.026* |
| C3 | 0.8032 (4) | 0.46376 (10) | 0.6369 (3) | 0.0213 (5) |
| H3 | 0.9315 | 0.4790 | 0.6544 | 0.026* |
| C4 | 0.7153 (4) | 0.45192 (10) | 0.4788 (3) | 0.0219 (6) |
| H4 | 0.7836 | 0.4597 | 0.3893 | 0.026* |
| C5 | 0.5299 (4) | 0.42895 (9) | 0.4508 (3) | 0.0183 (5) |
| H5 | 0.4719 | 0.4211 | 0.3425 | 0.022* |
| C6 | 0.4276 (4) | 0.41729 (9) | 0.5809 (3) | 0.0167 (5) |
| C7 | 0.2364 (3) | 0.39001 (9) | 0.5570 (3) | 0.0162 (5) |
| C8 | 0.1613 (4) | 0.36162 (10) | 0.6749 (3) | 0.0181 (5) |
| C9 | −0.0253 (4) | 0.32911 (10) | 0.6577 (3) | 0.0202 (6) |
| C10 | −0.2808 (4) | 0.28845 (11) | 0.4788 (3) | 0.0301 (6) |
| H10A | −0.2544 | 0.2510 | 0.5215 | 0.045* |
| H10B | −0.3298 | 0.2865 | 0.3622 | 0.045* |
| H10C | −0.3793 | 0.3061 | 0.5364 | 0.045* |
| C11 | 0.3594 (4) | 0.30948 (11) | 0.8954 (3) | 0.0294 (7) |
| H11A | 0.2711 | 0.2784 | 0.8643 | 0.044* |
| H11B | 0.3914 | 0.3107 | 1.0143 | 0.044* |
| H11C | 0.4800 | 0.3048 | 0.8464 | 0.044* |
| C12 | 0.1291 (4) | 0.35858 (10) | 0.2862 (3) | 0.0207 (6) |
| C13 | −0.0222 (4) | 0.37189 (12) | 0.1456 (3) | 0.0307 (7) |
| H13A | −0.0128 | 0.3455 | 0.0572 | 0.046* |
| H13B | −0.0008 | 0.4094 | 0.1073 | 0.046* |
| H13C | −0.1526 | 0.3695 | 0.1796 | 0.046* |
| N1 | 0.2622 (3) | 0.36187 (8) | 0.8366 (2) | 0.0185 (5) |
| O1 | 0.4912 (3) | 0.41115 (8) | 1.04687 (19) | 0.0263 (4) |
| O2 | 0.2249 (3) | 0.46261 (7) | 0.8823 (2) | 0.0234 (4) |
| O3 | 0.1272 (2) | 0.39845 (6) | 0.40526 (18) | 0.0184 (4) |

| | | | | |
|---|---|---|---|---|
| O4 | −0.0967 (3) | 0.31203 (8) | 0.7727 (2) | 0.0353 (5) |
| O5 | −0.1014 (3) | 0.32064 (7) | 0.5028 (2) | 0.0266 (4) |
| O6 | 0.2420 (3) | 0.32061 (7) | 0.3014 (2) | 0.0282 (5) |
| S1 | 0.37225 (9) | 0.42031 (2) | 0.89441 (7) | 0.0197 (2) |

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

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C1 | 0.0191 (13) | 0.0190 (12) | 0.0169 (12) | 0.0010 (10) | 0.0030 (10) | 0.0017 (9) |
| C2 | 0.0201 (14) | 0.0197 (12) | 0.0222 (13) | −0.0006 (10) | −0.0035 (10) | −0.0003 (10) |
| C3 | 0.0138 (13) | 0.0196 (12) | 0.0302 (14) | −0.0010 (10) | 0.0021 (10) | 0.0026 (11) |
| C4 | 0.0205 (14) | 0.0207 (12) | 0.0260 (13) | 0.0023 (10) | 0.0082 (10) | 0.0032 (10) |
| C5 | 0.0193 (14) | 0.0183 (12) | 0.0175 (12) | 0.0029 (10) | 0.0034 (10) | 0.0009 (9) |
| C6 | 0.0162 (13) | 0.0149 (11) | 0.0182 (12) | 0.0021 (9) | −0.0003 (10) | 0.0017 (9) |
| C7 | 0.0146 (12) | 0.0198 (12) | 0.0135 (11) | 0.0019 (10) | −0.0006 (9) | −0.0019 (9) |
| C8 | 0.0204 (14) | 0.0183 (12) | 0.0151 (11) | 0.0004 (10) | 0.0009 (9) | −0.0017 (9) |
| C9 | 0.0214 (14) | 0.0197 (12) | 0.0201 (13) | 0.0000 (10) | 0.0047 (10) | −0.0040 (10) |
| C10 | 0.0250 (16) | 0.0325 (15) | 0.0320 (15) | −0.0132 (12) | 0.0013 (12) | −0.0068 (12) |
| C11 | 0.0372 (17) | 0.0243 (14) | 0.0257 (14) | 0.0046 (12) | 0.0006 (12) | 0.0038 (11) |
| C12 | 0.0186 (14) | 0.0267 (13) | 0.0175 (12) | −0.0040 (11) | 0.0046 (10) | −0.0015 (10) |
| C13 | 0.0280 (16) | 0.0437 (17) | 0.0190 (13) | −0.0027 (13) | −0.0015 (11) | −0.0039 (12) |
| N1 | 0.0192 (12) | 0.0202 (10) | 0.0157 (10) | −0.0012 (8) | 0.0013 (8) | 0.0007 (8) |
| O1 | 0.0243 (11) | 0.0390 (11) | 0.0141 (9) | −0.0034 (8) | −0.0023 (7) | 0.0010 (8) |
| O2 | 0.0248 (10) | 0.0230 (9) | 0.0223 (9) | 0.0011 (7) | 0.0031 (7) | −0.0041 (7) |
| O3 | 0.0176 (9) | 0.0218 (9) | 0.0152 (8) | 0.0003 (7) | −0.0003 (7) | −0.0008 (7) |
| O4 | 0.0386 (13) | 0.0458 (12) | 0.0225 (10) | −0.0196 (10) | 0.0080 (9) | 0.0008 (9) |
| O5 | 0.0222 (10) | 0.0351 (10) | 0.0223 (9) | −0.0119 (8) | 0.0020 (7) | −0.0044 (8) |
| O6 | 0.0308 (11) | 0.0284 (10) | 0.0259 (10) | 0.0028 (8) | 0.0054 (8) | −0.0049 (8) |
| S1 | 0.0207 (4) | 0.0234 (3) | 0.0147 (3) | −0.0017 (2) | 0.0014 (2) | −0.0012 (2) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| C1—C2 | 1.391 (3) | C10—O5 | 1.451 (3) |
| C1—C6 | 1.407 (3) | C10—H10A | 0.9800 |
| C1—S1 | 1.755 (3) | C10—H10B | 0.9800 |
| C2—C3 | 1.386 (4) | C10—H10C | 0.9800 |
| C2—H2 | 0.9500 | C11—N1 | 1.484 (3) |
| C3—C4 | 1.396 (3) | C11—H11A | 0.9800 |
| C3—H3 | 0.9500 | C11—H11B | 0.9800 |
| C4—C5 | 1.384 (3) | C11—H11C | 0.9800 |
| C4—H4 | 0.9500 | C12—O6 | 1.199 (3) |
| C5—C6 | 1.396 (3) | C12—O3 | 1.380 (3) |
| C5—H5 | 0.9500 | C12—C13 | 1.488 (3) |
| C6—C7 | 1.463 (3) | C13—H13A | 0.9800 |
| C7—C8 | 1.353 (3) | C13—H13B | 0.9800 |
| C7—O3 | 1.389 (3) | C13—H13C | 0.9800 |
| C8—N1 | 1.422 (3) | N1—S1 | 1.644 (2) |
| C8—C9 | 1.498 (3) | O1—S1 | 1.4258 (17) |
| C9—O4 | 1.203 (3) | O2—S1 | 1.4354 (18) |

| | | | |
|---|---|---|---|
| C9—O5 | 1.334 (3) | | |
| C2—C1—C6 | 122.4 (2) | O5—C10—H10C | 109.5 |
| C2—C1—S1 | 122.25 (18) | H10A—C10—H10C | 109.5 |
| C6—C1—S1 | 115.33 (18) | H10B—C10—H10C | 109.5 |
| C3—C2—C1 | 118.3 (2) | N1—C11—H11A | 109.5 |
| C3—C2—H2 | 120.8 | N1—C11—H11B | 109.5 |
| C1—C2—H2 | 120.8 | H11A—C11—H11B | 109.5 |
| C2—C3—C4 | 120.4 (2) | N1—C11—H11C | 109.5 |
| C2—C3—H3 | 119.8 | H11A—C11—H11C | 109.5 |
| C4—C3—H3 | 119.8 | H11B—C11—H11C | 109.5 |
| C5—C4—C3 | 120.8 (2) | O6—C12—O3 | 121.9 (2) |
| C5—C4—H4 | 119.6 | O6—C12—C13 | 128.5 (2) |
| C3—C4—H4 | 119.6 | O3—C12—C13 | 109.5 (2) |
| C4—C5—C6 | 120.3 (2) | C12—C13—H13A | 109.5 |
| C4—C5—H5 | 119.9 | C12—C13—H13B | 109.5 |
| C6—C5—H5 | 119.9 | H13A—C13—H13B | 109.5 |
| C5—C6—C1 | 117.9 (2) | C12—C13—H13C | 109.5 |
| C5—C6—C7 | 121.9 (2) | H13A—C13—H13C | 109.5 |
| C1—C6—C7 | 120.2 (2) | H13B—C13—H13C | 109.5 |
| C8—C7—O3 | 121.0 (2) | C8—N1—C11 | 116.50 (18) |
| C8—C7—C6 | 123.9 (2) | C8—N1—S1 | 115.14 (15) |
| O3—C7—C6 | 114.97 (19) | C11—N1—S1 | 117.95 (17) |
| C7—C8—N1 | 119.5 (2) | C12—O3—C7 | 119.17 (18) |
| C7—C8—C9 | 127.3 (2) | C9—O5—C10 | 115.4 (2) |
| N1—C8—C9 | 113.2 (2) | O1—S1—O2 | 119.20 (10) |
| O4—C9—O5 | 124.0 (2) | O1—S1—N1 | 108.13 (11) |
| O4—C9—C8 | 123.0 (2) | O2—S1—N1 | 107.37 (10) |
| O5—C9—C8 | 113.0 (2) | O1—S1—C1 | 110.97 (12) |
| O5—C10—H10A | 109.5 | O2—S1—C1 | 108.25 (11) |
| O5—C10—H10B | 109.5 | N1—S1—C1 | 101.39 (11) |
| H10A—C10—H10B | 109.5 | | |
| C6—C1—C2—C3 | 1.3 (4) | C7—C8—N1—C11 | −108.8 (3) |
| S1—C1—C2—C3 | −175.79 (18) | C9—C8—N1—C11 | 72.3 (3) |
| C1—C2—C3—C4 | 0.4 (4) | C7—C8—N1—S1 | 35.6 (3) |
| C2—C3—C4—C5 | −1.1 (4) | C9—C8—N1—S1 | −143.34 (17) |
| C3—C4—C5—C6 | 0.1 (4) | O6—C12—O3—C7 | −10.5 (3) |
| C4—C5—C6—C1 | 1.6 (3) | C13—C12—O3—C7 | 170.6 (2) |
| C4—C5—C6—C7 | −176.3 (2) | C8—C7—O3—C12 | −86.4 (3) |
| C2—C1—C6—C5 | −2.3 (3) | C6—C7—O3—C12 | 98.0 (2) |
| S1—C1—C6—C5 | 175.01 (17) | O4—C9—O5—C10 | −0.2 (4) |
| C2—C1—C6—C7 | 175.6 (2) | C8—C9—O5—C10 | 178.9 (2) |
| S1—C1—C6—C7 | −7.1 (3) | C8—N1—S1—O1 | −170.76 (17) |
| C5—C6—C7—C8 | 157.1 (2) | C11—N1—S1—O1 | −27.0 (2) |
| C1—C6—C7—C8 | −20.7 (4) | C8—N1—S1—O2 | 59.42 (19) |
| C5—C6—C7—O3 | −27.4 (3) | C11—N1—S1—O2 | −156.78 (18) |
| C1—C6—C7—O3 | 154.8 (2) | C8—N1—S1—C1 | −54.01 (19) |
| O3—C7—C8—N1 | −169.13 (19) | C11—N1—S1—C1 | 89.79 (19) |
| C6—C7—C8—N1 | 6.2 (4) | C2—C1—S1—O1 | −28.5 (2) |

| | | | |
|---|---|---|---|
| O3—C7—C8—C9 | 9.6 (4) | C6—C1—S1—O1 | 154.23 (17) |
| C6—C7—C8—C9 | −175.1 (2) | C2—C1—S1—O2 | 104.1 (2) |
| C7—C8—C9—O4 | −168.4 (3) | C6—C1—S1—O2 | −73.2 (2) |
| N1—C8—C9—O4 | 10.4 (3) | C2—C1—S1—N1 | −143.1 (2) |
| C7—C8—C9—O5 | 12.4 (4) | C6—C1—S1—N1 | 39.6 (2) |
| N1—C8—C9—O5 | −168.8 (2) | | |

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C13—H13A···O4$^{i}$ | 0.98 | 2.49 | 3.387 (3) | 153 |
| C5—H5···O1$^{i}$ | 0.95 | 2.48 | 3.349 (3) | 151 |

Symmetry codes: (i) *x*, *y*, *z*−1.

**Fig. 1**