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ISSN 2414-3146

# Methyl 2-[(*Z*)-5-methyl-2-oxoindolin-3-ylidene]-hydrazinecarbodithioate

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Received 25 September 2024
Accepted 1 October 2024

Edited by W. T. A. Harrison, University of Aberdeen, United Kingdom

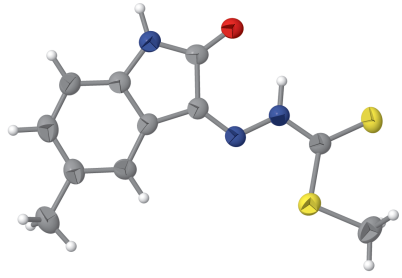
**Keywords:** crystal structure; dithiocarbazate; 5-methylisatin; C═O···C═O interaction.

**CCDC reference:** 2388258

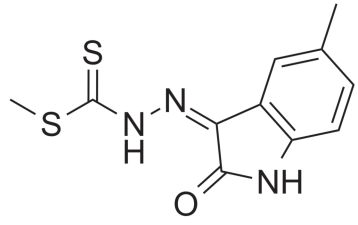
**Structural data:** full structural data are available from iucrdata.iucr.org

The title dithiocarbazate imine, $C_{11}H_{11}N_3OS_2$, was obtained from the condensation reaction of *S*-methyldithiocarbazate (SMDTC) and 5-methylisatin. It shows a *Z* configuration about the imine C═N bond, which is associated with an intramolecular N—H···O hydrogen bond that closes an *S*(6) ring. In the crystal, inversion dimers linked by pairwise N—H···O hydrogen bonds generate $R_2^2(8)$ loops. The extended structure features C—H···S contacts as well as reciprocal carbonyl–carbonyl (C═O···C═O) interactions.

3D view



Chemical scheme




## Structure description

In medicinal chemistry, isatin (1*H*-indole-2,3-dione, $C_8H_5NO_2$) and its derivatives represent an important class of heterocyclic compounds with potential pharmacological properties (Shu *et al.*, 2024). Taking advantage of the versatile reactivity of the isatin nucleus, a huge library of isatin derivatives with various applications is now available. Most of these derivatives have been obtained by utilizing either the high reactivity of its 3-carbonyl group or the nucleophilic nature of its NH group. The NH group can undergo *N*-acylation, *N*-arylation or *N*-alkylation, whereas the C3 carbonyl group can be utilized in the synthesis of hydrazone or imine derivatives as well as oxindoles and spirocyclic compounds (Nath *et al.*, 2020). These derivatives are reported to possess several biological activities and find applications in the field of crystal engineering, supramolecular chemistry and materials science (Mehreen *et al.*, 2022*a*; Ahmed *et al.*, 2019).

Recently, chemists have recognized both one-sided and reciprocal carbonyl–carbonyl interactions as non-covalent interactions of significant interest due to their ability to influence the geometries of small molecules and affect the three dimensional structures of peptides, peptoids, proteins and polyesters (Rahim *et al.*, 2017). Very recently, the use of isatin-derived compounds as potent $\alpha$-glucosidase inhibitors in managing diabetes has been reported, highlighting the role of C═O···C═O interactions in inhibiting

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N4—H4···O2 | 0.98 (2) | 2.01 (6) | 2.754 (6) | 130 (6) |
| N1—H1···O2$^{i}$ | 0.98 (2) | 1.85 (2) | 2.825 (6) | 171 (7) |

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

$\alpha$-glucosidase and controlling postprandial hyperglycemia (Mehreen *et al.*, 2022*b*). As a continuation of our research interests in isatin derivatives, we now report the synthesis and crystal structure of the title compound, $C_{11}H_{11}N_3OS_2$.

The asymmetric unit of the title compound (Fig. 1) comprises one molecule and crystallizes in the monoclinic space group $P2_1/c$. The methyl hydrazinecarbodithioate chain connects to the nine-membered 5-methyisatin ring at C3 and adopts a near planar geometry (r.m.s. deviation from planarity = 0.033 Å). The essentially planar conformation of the molecule is associated with the formation of an intramolecular N4—H4···O2 hydrogen bond (Table 1), which closes an $S(6)$ loop. In the solid state, the compound exists in its thione tautomeric form with the dithiocarbazate fragment adopting a $Z$ conformation about the C=N bond with respect to the 5-methylisatin moiety, while the $S$-methyl group adopts a *syn* conformation relative to the azomethine nitrogen atom. Otherwise, the bond lengths and angles in the title compound may be regarded as normal.

In the crystal, the molecules of the title compound form inversion dimers through pairwise N1—H1···O2 hydrogen bonds (Table 1) in the common $R_2^2(8)$ motif. There are additional weak, non-classical C7—H7···S11 hydrogen bonds, which link molecules into $C(10)$ chains propagating along [010]. The combination of the chains and inversion dimers forms corrugated sheets lying in the (102) plane (Fig. 2). The aforementioned sheets stack by way of reciprocal carbonyl–carbonyl interactions [C2···O2 = 3.166 (6) Å, C=O···C = 75.1 (3)°, O=C···O = 104.8 (3)°] (Fig. 3). The contact observed differs from the ideal motif-II type interaction (Sahariah & Sarma, 2019) with O2 lying over the adjacent pyrrolone ring (Fig. 4).

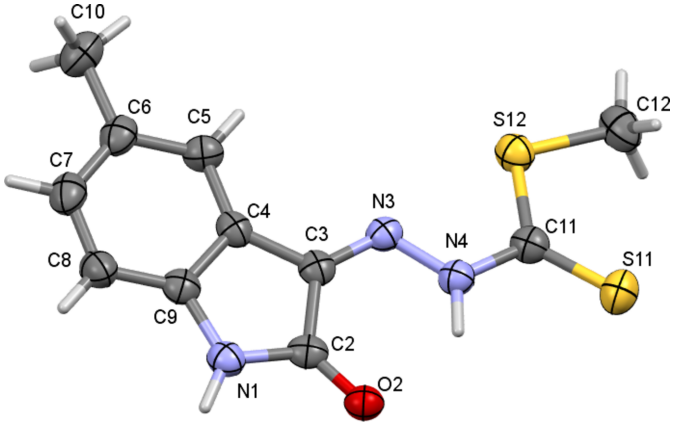



**Figure 1**
The molecular structure of the title compound, showing displacement ellipsoids drawn at the 50% probability level.

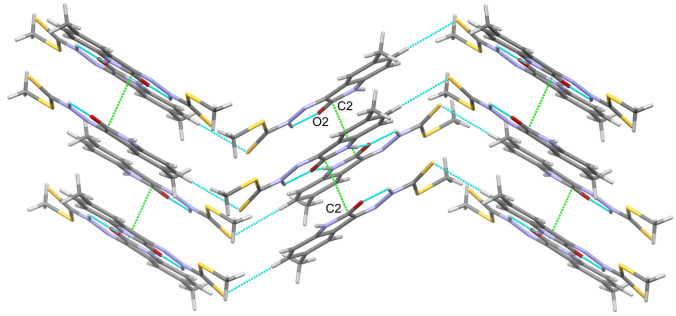



**Figure 3**
View showing the stacking of the corrugated sheets supported by reciprocal carbonyl–carbonyl interactions (green).

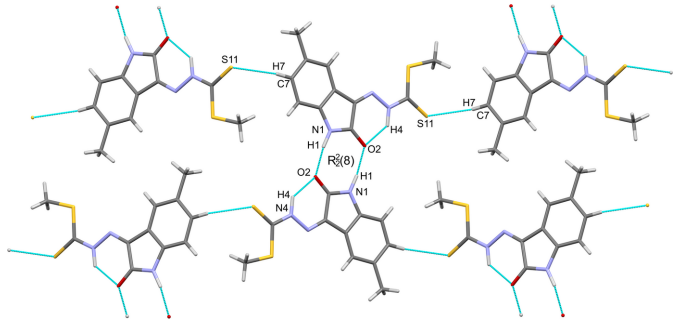



**Figure 2**
View of the N—H···O and C—H···S hydrogen bonds generating $R_2^2(8)$ dimers (centre) and C(10) chains (left to right), which combine to form corrugated (102) sheets.

## Synthesis and crystallization

The dithiocarbazate precursor (SMDTC) was prepared by the literature method (Das & Livingstone, 1976). The title compound was prepared by adding 5-methylisatin (1.61 g, 10.0 mmol, 1.0 eq) dissolved in hot ethanol (20 ml) to a solution of SMDTC (1.22 g, 10.0 mmol, 1.0 eq) in hot ethanol (35 ml). The mixture was heated (80°C) with continuous stirring for 15 min and later allowed to stand for 20 min at room temperature until a precipitate formed, which was then filtered and dried over silica gel, yielding orange needles of the title compound on recrystallization form ethanol solution (yield: 2.12 g, 80%). m.p. 236–237°C; $^1$H NMR (400 MHz, $d_6$-DMSO) $\delta$: (p.p.m): 2.31 (*s*, 3H), 2.62 (*s*, 3H), 6.84 (*d*, $J$ = 7.96 Hz, 1H), 7.22 (*d*, $J$ = 7.96 Hz, 1H), 7.36 (*s*, 1H), 11.27 (*s*, 1H), 14.00 (*s*, 1H); HRMS *m*/*z* (ESI$^+$), found: $[M+H]^+$ 266.0417, $C_{11}H_{12}N_3OS_2$ requires $[M+H]^+$ 266.0422.

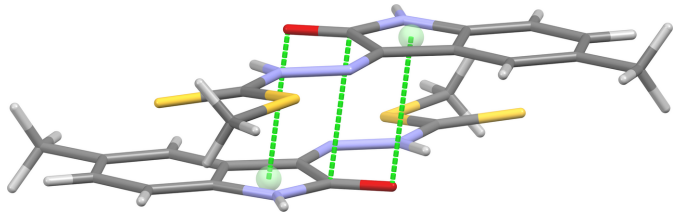


**Figure 4**
Offset geometry of the carbonyl–carbonyl interaction showing how O2 is positioned over the adjacent pyrrolone ring.

## Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The structure was refined as a two-component twin with component 2 rotated by 2.05° around [001] (reciprocal) or [105] (direct), and a refined twin fraction of 0.128 (6).

**Table 2**
Experimental details.

| | |
|---|---|
| Crystal data | |
| Chemical formula | $C_{11}H_{11}N_3OS_2$ |
| $M_r$ | 265.35 |
| Crystal system, space group | Monoclinic, $P2_1/c$ |
| Temperature (K) | 125 |
| $a$, $b$, $c$ (Å) | 4.9897 (4), 21.8014 (19), 11.3394 (9) |
| $\beta$ (°) | 92.995 (8) |
| $V$ (Å$^3$) | 1231.83 (18) |
| $Z$ | 4 |
| Radiation type | Cu $K\alpha$ |
| $\mu$ (mm$^{-1}$) | 3.82 |
| Crystal size (mm) | 0.23 × 0.01 × 0.01 |
| Data collection | |
| Diffractometer | Rigaku XtaLAB P200K |
| Absorption correction | Multi-scan (*CrysAlis PRO*; Rigaku OD, 2023) |
| $T_{min}$, $T_{max}$ | 0.631, 1.000 |
| No. of measured, independent and observed [$I > 2\sigma(I)$] reflections | 23143, 2554, 1548 |
| $R_{int}$ | 0.171 |
| (sin $\theta/\lambda)_{max}$ (Å$^{-1}$) | 0.630 |
| Refinement | |
| $R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, $S$ | 0.079, 0.185, 1.09 |
| No. of reflections | 2554 |
| No. of parameters | 165 |
| No. of restraints | 2 |
| H-atom treatment | H atoms treated by a mixture of independent and constrained refinement |
| $\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å$^{-3}$) | 0.46, −0.63 |

Computer programs: *CrysAlis PRO* (Rigaku OD, 2023), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2019/3* (Sheldrick, 2015*b*), *Mercury* (Macrae *et al.*, 2020), *OLEX2* (Dolomanov *et al.*, 2009) and *publCIF* (Westrip, 2010).

## Funding information

The authors acknowledge Universiti Teknologi MARA for financial support.

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# full crystallographic data

*IUCrData* (2024). **9**, x240967 [https://doi.org/10.1107/S2414314624009672]

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*Crystal data*

$C_{11}H_{11}N_3OS_2$
$M_r = 265.35$
Monoclinic, $P2_1/c$
$a = 4.9897$ (4) Å
$b = 21.8014$ (19) Å
$c = 11.3394$ (9) Å
$\beta = 92.995$ (8)°
$V = 1231.83$ (18) Å$^3$
$Z = 4$
$F(000) = 552$
$D_x = 1.431$ Mg m$^{-3}$
Cu $K\alpha$ radiation, $\lambda = 1.54184$ Å
Cell parameters from 2965 reflections
$\theta = 4.0$–$68.3°$
$\mu = 3.82$ mm$^{-1}$
$T = 125$ K
Needle, orange
0.23 × 0.01 × 0.01 mm

*Data collection*

Rigaku XtaLAB P200K diffractometer
Radiation source: Rotating Anode, Rigaku MM-007HF
Rigaku Osmic Confocal Optical System monochromator
Detector resolution: 5.8140 pixels mm$^{-1}$
shutterless scans
Absorption correction: multi-scan (CrysAlisPro; Rigaku OD, 2023)
$T_{min} = 0.631$, $T_{max} = 1.000$
23143 measured reflections
2554 independent reflections
1548 reflections with $I > 2\sigma(I)$
$R_{int} = 0.171$
$\theta_{max} = 76.3°$, $\theta_{min} = 4.1°$
$h = -6 \rightarrow 6$
$k = -27 \rightarrow 27$
$l = 0 \rightarrow 14$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.079$
$wR(F^2) = 0.185$
$S = 1.09$
2554 reflections
165 parameters
2 restraints
Primary atom site location: dual
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + 4.5988P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.46$ e Å$^{-3}$
$\Delta\rho_{min} = -0.63$ e Å$^{-3}$

*Special details*

**Geometry**. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

**Refinement**. Refined as a 2-component twin using an HKLF5 file generated by TWINROTMAT running in PLATON (Spek, 2009), with twin law [-1 0 0 0 -1 0 0.237 0 1]. N—H hydrogen atoms located from $F_{map}$ and refined isotropically with appropriate distance restraints.
The N-bound H atoms were located in a difference map and refined isotropically with a distance restraint. The C-bound H atoms were located geometrically (phenyl C—H =0.95 Å, methyl C—H = 0.98 Å) and refined as riding atoms. The constraint $U_{iso}$(H) = 1.2$U_{eq}$(phenyl C) or 1.5$U_{eq}$(methyl C) was applied in all cases.

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| S11 | 0.1241 (3) | 0.27752 (7) | −0.01332 (14) | 0.0469 (4) |
| S12 | −0.0419 (3) | 0.32382 (7) | 0.22526 (13) | 0.0413 (4) |
| O2 | 0.7445 (7) | 0.43673 (16) | 0.0099 (3) | 0.0370 (9) |
| N1 | 0.8229 (9) | 0.5243 (2) | 0.1228 (4) | 0.0368 (11) |
| H1 | 0.962 (11) | 0.542 (3) | 0.075 (6) | 0.09 (3)* |
| N3 | 0.3151 (9) | 0.4171 (2) | 0.1850 (4) | 0.0333 (10) |
| N4 | 0.3199 (9) | 0.3741 (2) | 0.0983 (4) | 0.0348 (10) |
| H4 | 0.440 (12) | 0.378 (3) | 0.033 (5) | 0.09 (3)* |
| C2 | 0.6980 (10) | 0.4710 (2) | 0.0933 (5) | 0.0332 (12) |
| C3 | 0.4865 (10) | 0.4614 (2) | 0.1812 (5) | 0.0325 (12) |
| C4 | 0.5034 (10) | 0.5136 (2) | 0.2617 (5) | 0.0330 (12) |
| C5 | 0.3648 (11) | 0.5306 (2) | 0.3595 (5) | 0.0364 (12) |
| H5 | 0.227148 | 0.505107 | 0.387426 | 0.044* |
| C6 | 0.4315 (12) | 0.5858 (3) | 0.4162 (5) | 0.0410 (14) |
| C7 | 0.6350 (12) | 0.6224 (3) | 0.3727 (6) | 0.0460 (15) |
| H7 | 0.678915 | 0.659976 | 0.411573 | 0.055* |
| C8 | 0.7741 (12) | 0.6058 (3) | 0.2752 (5) | 0.0430 (14) |
| H8 | 0.909675 | 0.631488 | 0.246180 | 0.052* |
| C9 | 0.7089 (11) | 0.5509 (2) | 0.2222 (5) | 0.0354 (12) |
| C10 | 0.2876 (13) | 0.6062 (3) | 0.5235 (5) | 0.0503 (16) |
| H10A | 0.195041 | 0.645094 | 0.506230 | 0.075* |
| H10B | 0.418146 | 0.611821 | 0.590187 | 0.075* |
| H10C | 0.156207 | 0.574984 | 0.543505 | 0.075* |
| C11 | 0.1427 (11) | 0.3261 (3) | 0.0983 (5) | 0.0363 (12) |
| C12 | −0.2434 (12) | 0.2564 (3) | 0.1973 (6) | 0.0517 (16) |
| H12A | −0.344567 | 0.260750 | 0.121366 | 0.078* |
| H12B | −0.368701 | 0.251475 | 0.260409 | 0.078* |
| H12C | −0.126802 | 0.220314 | 0.195053 | 0.078* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| S11 | 0.0550 (9) | 0.0417 (8) | 0.0435 (8) | 0.0003 (7) | −0.0028 (7) | −0.0055 (7) |
| S12 | 0.0400 (8) | 0.0386 (8) | 0.0453 (8) | −0.0014 (6) | 0.0031 (6) | 0.0030 (7) |
| O2 | 0.035 (2) | 0.038 (2) | 0.037 (2) | 0.0033 (17) | 0.0029 (17) | 0.0032 (17) |
| N1 | 0.033 (2) | 0.035 (2) | 0.043 (3) | 0.002 (2) | 0.002 (2) | 0.003 (2) |
| N3 | 0.034 (2) | 0.033 (2) | 0.033 (2) | 0.004 (2) | 0.0005 (19) | 0.0010 (19) |
| N4 | 0.035 (2) | 0.034 (2) | 0.036 (3) | 0.001 (2) | 0.002 (2) | 0.001 (2) |
| C2 | 0.031 (3) | 0.035 (3) | 0.034 (3) | 0.008 (2) | 0.000 (2) | 0.009 (2) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C3 | 0.031 (3) | 0.031 (3) | 0.035 (3) | 0.005 (2) | −0.004 (2) | 0.005 (2) |
| C4 | 0.030 (3) | 0.031 (3) | 0.037 (3) | 0.001 (2) | −0.004 (2) | 0.006 (2) |
| C5 | 0.039 (3) | 0.038 (3) | 0.033 (3) | 0.003 (2) | 0.004 (2) | 0.006 (2) |
| C6 | 0.044 (3) | 0.034 (3) | 0.045 (3) | 0.009 (3) | −0.004 (3) | −0.003 (3) |
| C7 | 0.044 (3) | 0.039 (3) | 0.055 (4) | 0.008 (3) | −0.009 (3) | −0.008 (3) |
| C8 | 0.037 (3) | 0.037 (3) | 0.055 (4) | −0.001 (3) | 0.004 (3) | −0.002 (3) |
| C9 | 0.032 (3) | 0.037 (3) | 0.036 (3) | 0.005 (2) | −0.003 (2) | 0.004 (2) |
| C10 | 0.063 (4) | 0.045 (3) | 0.043 (3) | 0.010 (3) | 0.001 (3) | −0.005 (3) |
| C11 | 0.037 (3) | 0.034 (3) | 0.038 (3) | 0.003 (2) | 0.001 (2) | 0.006 (2) |
| C12 | 0.045 (4) | 0.036 (3) | 0.074 (5) | −0.002 (3) | −0.001 (3) | 0.010 (3) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| S11—C11 | 1.649 (6) | C5—H5 | 0.9500 |
| S12—C11 | 1.750 (6) | C5—C6 | 1.396 (8) |
| S12—C12 | 1.799 (6) | C6—C7 | 1.402 (8) |
| O2—C2 | 1.237 (6) | C6—C10 | 1.511 (8) |
| N1—H1 | 0.98 (2) | C7—H7 | 0.9500 |
| N1—C2 | 1.354 (7) | C7—C8 | 1.384 (8) |
| N1—C9 | 1.412 (7) | C8—H8 | 0.9500 |
| N3—N4 | 1.360 (6) | C8—C9 | 1.372 (8) |
| N3—C3 | 1.292 (7) | C10—H10A | 0.9800 |
| N4—H4 | 0.98 (2) | C10—H10B | 0.9800 |
| N4—C11 | 1.370 (7) | C10—H10C | 0.9800 |
| C2—C3 | 1.503 (7) | C12—H12A | 0.9800 |
| C3—C4 | 1.460 (7) | C12—H12B | 0.9800 |
| C4—C5 | 1.387 (7) | C12—H12C | 0.9800 |
| C4—C9 | 1.400 (7) | | |
| | | | |
| C11—S12—C12 | 101.1 (3) | C8—C7—C6 | 122.3 (6) |
| C2—N1—H1 | 122 (5) | C8—C7—H7 | 118.8 |
| C2—N1—C9 | 110.5 (4) | C7—C8—H8 | 121.3 |
| C9—N1—H1 | 128 (5) | C9—C8—C7 | 117.4 (5) |
| C3—N3—N4 | 117.0 (4) | C9—C8—H8 | 121.3 |
| N3—N4—H4 | 121 (4) | C4—C9—N1 | 110.5 (5) |
| N3—N4—C11 | 119.3 (4) | C8—C9—N1 | 127.7 (5) |
| C11—N4—H4 | 119 (4) | C8—C9—C4 | 121.8 (5) |
| O2—C2—N1 | 127.3 (5) | C6—C10—H10A | 109.5 |
| O2—C2—C3 | 126.1 (5) | C6—C10—H10B | 109.5 |
| N1—C2—C3 | 106.6 (5) | C6—C10—H10C | 109.5 |
| N3—C3—C2 | 128.0 (5) | H10A—C10—H10B | 109.5 |
| N3—C3—C4 | 125.4 (5) | H10A—C10—H10C | 109.5 |
| C4—C3—C2 | 106.6 (4) | H10B—C10—H10C | 109.5 |
| C5—C4—C3 | 133.9 (5) | S11—C11—S12 | 127.0 (3) |
| C5—C4—C9 | 120.4 (5) | N4—C11—S11 | 120.0 (4) |
| C9—C4—C3 | 105.8 (5) | N4—C11—S12 | 112.9 (4) |
| C4—C5—H5 | 120.6 | S12—C12—H12A | 109.5 |
| C4—C5—C6 | 118.7 (5) | S12—C12—H12B | 109.5 |

| | | | |
|---|---|---|---|
| C6—C5—H5 | 120.6 | S12—C12—H12C | 109.5 |
| C5—C6—C7 | 119.3 (5) | H12A—C12—H12B | 109.5 |
| C5—C6—C10 | 120.8 (5) | H12A—C12—H12C | 109.5 |
| C7—C6—C10 | 119.9 (5) | H12B—C12—H12C | 109.5 |
| C6—C7—H7 | 118.8 | | |

| | | | |
|---|---|---|---|
| O2—C2—C3—N3 | −1.0 (8) | C3—C4—C9—N1 | −0.8 (6) |
| O2—C2—C3—C4 | −179.2 (5) | C3—C4—C9—C8 | 177.6 (5) |
| N1—C2—C3—N3 | 178.2 (5) | C4—C5—C6—C7 | 0.2 (8) |
| N1—C2—C3—C4 | 0.1 (5) | C4—C5—C6—C10 | −179.7 (5) |
| N3—N4—C11—S11 | 173.7 (4) | C5—C4—C9—N1 | 179.3 (5) |
| N3—N4—C11—S12 | −7.1 (6) | C5—C4—C9—C8 | −2.3 (8) |
| N3—C3—C4—C5 | 2.1 (9) | C5—C6—C7—C8 | −0.2 (9) |
| N3—C3—C4—C9 | −177.7 (5) | C6—C7—C8—C9 | −1.0 (9) |
| N4—N3—C3—C2 | −1.5 (7) | C7—C8—C9—N1 | −179.7 (5) |
| N4—N3—C3—C4 | 176.3 (5) | C7—C8—C9—C4 | 2.2 (8) |
| C2—N1—C9—C4 | 0.9 (6) | C9—N1—C2—O2 | 178.6 (5) |
| C2—N1—C9—C8 | −177.3 (5) | C9—N1—C2—C3 | −0.6 (5) |
| C2—C3—C4—C5 | −179.7 (5) | C9—C4—C5—C6 | 1.0 (8) |
| C2—C3—C4—C9 | 0.5 (5) | C10—C6—C7—C8 | 179.7 (5) |
| C3—N3—N4—C11 | 179.9 (5) | C12—S12—C11—S11 | 0.1 (5) |
| C3—C4—C5—C6 | −178.8 (5) | C12—S12—C11—N4 | −179.0 (4) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N4—H4···O2 | 0.98 (2) | 2.01 (6) | 2.754 (6) | 130 (6) |
| N1—H1···O2$^{i}$ | 0.98 (2) | 1.85 (2) | 2.825 (6) | 171 (7) |

Symmetry code: (i) −*x*+2, −*y*+1, −*z*.