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# Methyl 3-methyl-5-oxo-4-(phenylhydrazono)-4,5-dihydro-1*H*-pyrazole-1-carbodithioate

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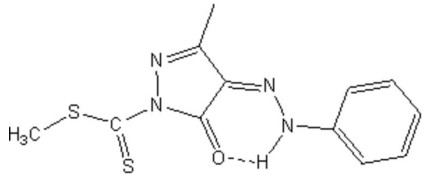
Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(C–C) = 0.002 Å; $R$ factor = 0.031; $wR$ factor = 0.092; data-to-parameter ratio = 13.2.

The title compound, $C_{12}H_{11}N_4OS_2$, has been synthesized by the condensation reaction of 3-oxo-2-(phenylhydrazono)-butanate and *S*-methyldithiocarbazate. The hydrazine unit and the pyrazole ring are coplanar [dihedral angle 3.8 (4)°] due to extensive conjugation and the N—H···O=C intramolecular hydrogen bond. Two adjacent molecules form dimers due to short C—H···O=C [$R_2^2$ (18)] and C—H···S=C [$R_2^2$ (22)] intermolecular interactions. C—H···S—C [$R_2^2$ (14)] interactions link these dimers into ribbons in the [011] direction.

## Related literature

For related literature, see: Bao *et al.* (2006); Bernstein *et al.* (1995); Bose *et al.* (2005); Brassy *et al.* (1974); Liu *et al.* (2007); Shi *et al.* (2005); Yang *et al.* (2003); Zelenak *et al.* (1999).



## Experimental

### Crystal data

$C_{12}H_{12}N_4OS_2$
$M_r$ = 292.40
Triclinic, $P\overline{1}$
$a$ = 5.0915 (8) Å
$b$ = 10.9705 (16) Å
$c$ = 11.9398 (18) Å
$\alpha$ = 93.770 (2)°
$\beta$ = 97.947 (2)°
$\gamma$ = 91.422 (2)°
$V$ = 658.69 (17) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 0.40 mm$^{-1}$
$T$ = 293 (2) K
0.26 × 0.23 × 0.17 mm

### Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2004)
$T_{min}$ = 0.816, $T_{max}$ = 0.874
(expected range = 0.872–0.934)
4799 measured reflections
2304 independent reflections
2035 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.033

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.092
$S$ = 1.02
2304 reflections
174 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.25 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.30 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N1—H1···O1 | 0.86 | 2.06 | 2.751 (2) | 137 |
| C4—H4···O1$^{i}$ | 0.93 | 2.49 | 3.244 (3) | 139 |
| C4—H4···S2$^{i}$ | 0.93 | 2.99 | 3.842 (2) | 152 |

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

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2001).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BV2082).

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# supporting information

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## Methyl 3-methyl-5-oxo-4-(phenylhydrazono)-4,5-dihydro-1*H*-pyrazole-1-carbodithioate

**Xiao-Lan Liu, Yue Zhao, Zhi-Gang Li and Yong-Hong Liu**

### S1. Comment

Pyrazolones compounds are finding increasing numbers of applications as ligands in coordination chemistry (Brassy *et al.*, 1974; Zelenak *et al.*, 1999; Yang *et al.*,2003). For example, they have been applied to the solvent extraction of metal ions (Bose *et al.*, 2005) as ligands in complexes with catalytic activity (Bao *et al.*, 2006) and in the synthesis of rare earth metal complexes with interesting photophysical properties (Shi *et al.* 2005). A related compound, (II), has already been studied (Liu *et al.*, 2007).

Similar to (II), the title compound, (I), has been shown by UV spectroscopy to have extensive conjugation involving four carbon atoms (C2—C5), four nitrogen atoms (N1—N4) and one oxygen (O1). And this has been further confirmed by the determination of its crystal structure (Fig. 1) The bond lengths and angles of the large conjugated system in (I) are similar to the corresponding values in (II). The dihedral angle between the conjugated system and with plane of C1–S1–C2=S2 in (I) is 3.8 (4)° while the value in (II) is 13.1 (3)°. The bond distances of C11—N4 is 1.392 (2) in (I), and the value in (II) is the same with (I), which is shorter than the range of C—N single bonds (1.47–1.40 Å) and might be attributed to a nonclassical $sp^2$-hybrid nitrogen atom and the conjugated system.

Two adjacent molecules form dimers due to short C—H···O=C [$R^2_2$ (18)] and C—H···S=C [$R^2_2$ (22)] (Bernstein *et al.*, 1995) intermolecular interactions. C—H···S—C [$R^2_2$ (14)] interactions link these dimers into ribbons in the (011) direction (Table 1).

### S2. Experimental

The title compound was synthesized by refluxing an ethanol solution of ethyl 3-oxo-2-(phenylhydrazono)butanate and *S*-methyldithiocarbazate (1:1) for 24 h. After 12 h at room temperature, the precipitate was collected by filtration and recrystallized from ethanol (yield 86.7%).The yellow crystals suitable for X-ray analysis were obtained by slow evaporation of a dichloromethane solution at 293 K (m.p. 396.2–397.7 K). Analysis calculated for $C_{12}H_{11}N_4OS_2$: C49.47, H 3.81, N 19.23%; found: C 49.63, H 3.56, N 19.14%. IR (KBr,$cm^{-1}$): 3250(w, NH), 1630 (*vs*, O?C), 1520 (s, N?C), 1275(S?C). UV ($\lambda_{max}$, in $CHCl_3$, nm): 396 (K-band, $1.87\times 10^4$). $^1$H NMR (600 MHz, $CDCl_3$, $\delta$, p.p.m.): 9.64 (m, 5H, ArH), 6.91 (s, H, NH), 3.96 (s, 3H, $SCH_3$), 1.13 (s, 3H, $CH_3$).

### S3. Refinement

The H atoms were placed in calculated positions and refined as riding, with C—H=0.93–0.97 Å and N—H=0.91 Å, and refined using a riding model, with $U_{iso}$(H) =1.2$U_{eq}$(C, N) and 1.5$U_{eq}$(methyl C).

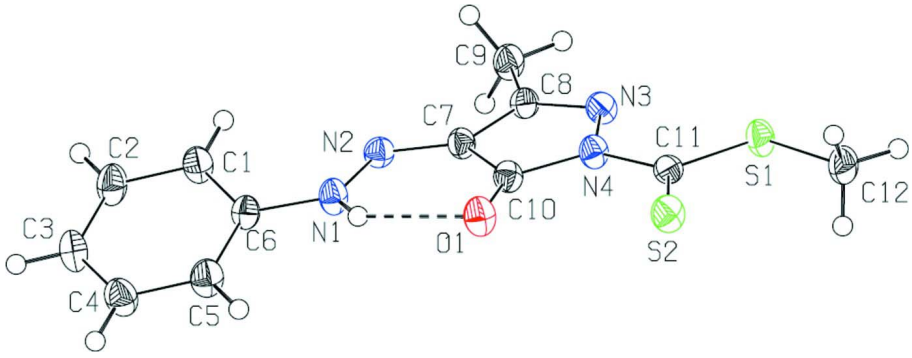



**Figure 1**

The molecular of (I) structure of the title compound, showing 50% probability ellipsoids. The C — H ··· N intramolecular hydrogen bond is shown dashed.

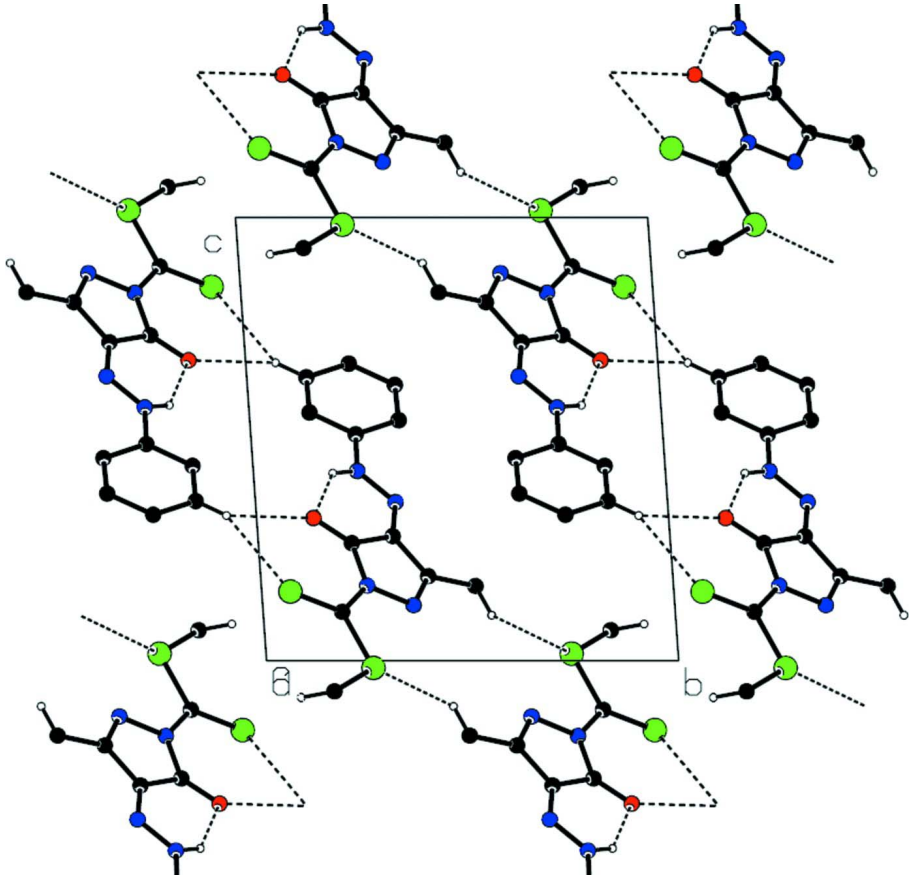
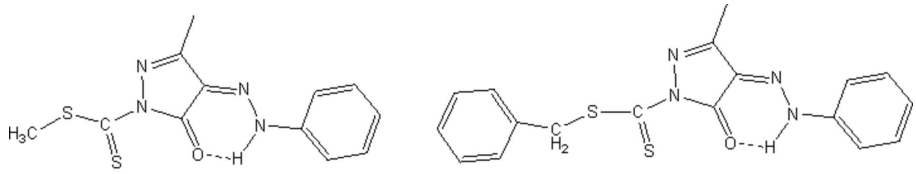



**Figure 2**

Packing diagram of (I), showing the formation of $R^2_2$ (18), and $R^2_2$ (22) and $R^2_2$ (14) ring *via* the short intermolecular interaction of C—H···O=C and C—H···S=C, and C—H···S—C, respectively, viewed along *a* axis. H atoms not involved in hydrogen bonding have been omitted.



(I) (II)

**Figure 3**

The structures of (I) and (II).

## Methyl 3-methyl-5-oxo-4-(phenylhydrazono)-4,5-dihydro-1*H*-pyrazole-1-carbodithioate

*Crystal data*

$C_{12}H_{12}N_4OS_2$
$M_r = 292.40$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 5.0915\ (8)$ Å
$b = 10.9705\ (16)$ Å
$c = 11.9398\ (18)$ Å
$\alpha = 93.770\ (2)°$
$\beta = 97.947\ (2)°$
$\gamma = 91.422\ (2)°$
$V = 658.69\ (17)$ Å$^3$
$Z = 2$
$F(000) = 304.0$
$D_x = 1.474$ Mg m$^{-3}$
Melting point: 397 K
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3332 reflections
$\theta = 2.4–28.2°$
$\mu = 0.40$ mm$^{-1}$
$T = 293$ K
Block, yellow
0.26 × 0.23 × 0.17 mm

*Data collection*

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
phi and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2004)
$T_{min} = 0.816$, $T_{max} = 0.874$
4799 measured reflections
2304 independent reflections
2035 reflections with $I > 2\sigma(I)$
$R_{int} = 0.033$
$\theta_{max} = 25.0°$, $\theta_{min} = 1.9°$
$h = -5\rightarrow6$
$k = -12\rightarrow13$
$l = -13\rightarrow14$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.031$
$wR(F^2) = 0.092$
$S = 1.02$
2304 reflections
174 parameters
0 restraints
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
$w = 1/[\sigma^2(F_o^2) + (0.0578P)^2 + 0.115P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.25$ e Å$^{-3}$
$\Delta\rho_{min} = -0.30$ e Å$^{-3}$

*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 (Å²)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| S1 | 1.11220 (9) | 0.25831 (4) | −0.01602 (4) | 0.02887 (16) |
| S2 | 1.21824 (9) | 0.06971 (4) | 0.15622 (4) | 0.03043 (16) |
| O1 | 0.8212 (2) | 0.13832 (11) | 0.32205 (10) | 0.0297 (3) |
| N2 | 0.4418 (3) | 0.33971 (12) | 0.35801 (12) | 0.0232 (3) |
| N1 | 0.4384 (3) | 0.25235 (13) | 0.42827 (12) | 0.0257 (3) |
| H1 | 0.5430 | 0.1925 | 0.4233 | 0.031* |
| N3 | 0.7936 (3) | 0.36637 (13) | 0.12557 (13) | 0.0248 (3) |
| N4 | 0.8960 (3) | 0.25697 (13) | 0.16941 (12) | 0.0237 (3) |
| C8 | 0.6255 (3) | 0.40665 (15) | 0.19108 (14) | 0.0230 (4) |
| C6 | 0.2679 (3) | 0.25469 (15) | 0.51098 (14) | 0.0235 (4) |
| C10 | 0.7816 (3) | 0.22690 (15) | 0.26553 (14) | 0.0229 (4) |
| C11 | 1.0712 (3) | 0.19198 (15) | 0.11056 (14) | 0.0232 (4) |
| C5 | 0.2180 (4) | 0.14648 (16) | 0.56018 (16) | 0.0310 (4) |
| H5 | 0.3012 | 0.0755 | 0.5397 | 0.037* |
| C7 | 0.6034 (3) | 0.32719 (15) | 0.28113 (14) | 0.0225 (4) |
| C9 | 0.4760 (4) | 0.51969 (16) | 0.16867 (16) | 0.0289 (4) |
| H9A | 0.5274 | 0.5542 | 0.1028 | 0.043* |
| H9B | 0.5153 | 0.5779 | 0.2328 | 0.043* |
| H9C | 0.2891 | 0.4998 | 0.1560 | 0.043* |
| C1 | 0.1473 (4) | 0.36136 (16) | 0.54284 (15) | 0.0283 (4) |
| H1A | 0.1827 | 0.4341 | 0.5110 | 0.034* |
| C2 | −0.0262 (4) | 0.35827 (17) | 0.62250 (16) | 0.0325 (4) |
| H2 | −0.1079 | 0.4293 | 0.6440 | 0.039* |
| C3 | −0.0791 (4) | 0.25008 (17) | 0.67044 (15) | 0.0315 (4) |
| H3 | −0.1974 | 0.2485 | 0.7232 | 0.038* |
| C12 | 1.3501 (4) | 0.15958 (18) | −0.06889 (16) | 0.0328 (4) |
| H12A | 1.5066 | 0.1599 | −0.0139 | 0.049* |
| H12B | 1.3958 | 0.1882 | −0.1382 | 0.049* |
| H12C | 1.2751 | 0.0779 | −0.0829 | 0.049* |
| C4 | 0.0444 (4) | 0.14470 (17) | 0.63963 (16) | 0.0326 (4) |
| H4 | 0.0107 | 0.0724 | 0.6724 | 0.039* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| S1 | 0.0259 (3) | 0.0330 (3) | 0.0306 (3) | 0.00503 (19) | 0.01298 (19) | 0.00305 (19) |
| S2 | 0.0270 (3) | 0.0285 (3) | 0.0381 (3) | 0.00935 (19) | 0.0109 (2) | 0.0028 (2) |
| O1 | 0.0298 (7) | 0.0309 (7) | 0.0310 (7) | 0.0109 (5) | 0.0090 (5) | 0.0079 (6) |
| N2 | 0.0242 (8) | 0.0215 (7) | 0.0241 (8) | 0.0028 (6) | 0.0040 (6) | 0.0016 (6) |
| N1 | 0.0289 (8) | 0.0239 (8) | 0.0274 (8) | 0.0102 (6) | 0.0110 (6) | 0.0060 (6) |

| | | | | | | |
|---|---|---|---|---|---|---|
| N3 | 0.0239 (8) | 0.0216 (7) | 0.0305 (8) | 0.0047 (6) | 0.0081 (6) | 0.0032 (6) |
| N4 | 0.0205 (8) | 0.0248 (8) | 0.0274 (8) | 0.0068 (6) | 0.0076 (6) | 0.0028 (6) |
| C8 | 0.0211 (9) | 0.0240 (9) | 0.0245 (9) | 0.0017 (7) | 0.0058 (7) | 0.0000 (7) |
| C6 | 0.0240 (9) | 0.0262 (9) | 0.0213 (8) | 0.0053 (7) | 0.0049 (7) | 0.0029 (7) |
| C10 | 0.0186 (9) | 0.0273 (9) | 0.0230 (9) | 0.0022 (7) | 0.0033 (7) | 0.0013 (7) |
| C11 | 0.0168 (9) | 0.0251 (9) | 0.0278 (9) | −0.0009 (7) | 0.0058 (7) | −0.0034 (7) |
| C5 | 0.0372 (11) | 0.0253 (9) | 0.0334 (10) | 0.0102 (8) | 0.0113 (8) | 0.0058 (8) |
| C7 | 0.0214 (9) | 0.0238 (9) | 0.0234 (9) | 0.0022 (7) | 0.0068 (7) | 0.0013 (7) |
| C9 | 0.0334 (10) | 0.0244 (9) | 0.0316 (10) | 0.0074 (8) | 0.0124 (8) | 0.0037 (7) |
| C1 | 0.0320 (10) | 0.0273 (9) | 0.0281 (9) | 0.0062 (8) | 0.0103 (8) | 0.0060 (7) |
| C2 | 0.0358 (11) | 0.0339 (10) | 0.0310 (10) | 0.0125 (8) | 0.0134 (8) | 0.0042 (8) |
| C3 | 0.0301 (10) | 0.0410 (11) | 0.0265 (10) | 0.0069 (8) | 0.0116 (8) | 0.0077 (8) |
| C12 | 0.0268 (10) | 0.0398 (11) | 0.0339 (10) | 0.0033 (8) | 0.0136 (8) | −0.0034 (8) |
| C4 | 0.0370 (11) | 0.0304 (10) | 0.0333 (10) | 0.0041 (8) | 0.0113 (8) | 0.0096 (8) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| S1—C11 | 1.7555 (18) | C10—C7 | 1.462 (2) |
| S1—C12 | 1.7960 (18) | C5—C4 | 1.384 (3) |
| S2—C11 | 1.6403 (17) | C5—H5 | 0.9300 |
| O1—C10 | 1.224 (2) | C9—H9A | 0.9600 |
| N2—N1 | 1.3159 (19) | C9—H9B | 0.9600 |
| N2—C7 | 1.318 (2) | C9—H9C | 0.9600 |
| N1—C6 | 1.401 (2) | C1—C2 | 1.386 (3) |
| N1—H1 | 0.8600 | C1—H1A | 0.9300 |
| N3—C8 | 1.303 (2) | C2—C3 | 1.387 (3) |
| N3—N4 | 1.4227 (19) | C2—H2 | 0.9300 |
| N4—C11 | 1.392 (2) | C3—C4 | 1.383 (3) |
| N4—C10 | 1.411 (2) | C3—H3 | 0.9300 |
| C8—C7 | 1.442 (2) | C12—H12A | 0.9600 |
| C8—C9 | 1.491 (2) | C12—H12B | 0.9600 |
| C6—C1 | 1.390 (2) | C12—H12C | 0.9600 |
| C6—C5 | 1.392 (2) | C4—H4 | 0.9300 |
| | | | |
| C11—S1—C12 | 100.91 (8) | C8—C7—C10 | 106.59 (15) |
| N1—N2—C7 | 116.78 (14) | C8—C9—H9A | 109.5 |
| N2—N1—C6 | 121.45 (14) | C8—C9—H9B | 109.5 |
| N2—N1—H1 | 119.3 | H9A—C9—H9B | 109.5 |
| C6—N1—H1 | 119.3 | C8—C9—H9C | 109.5 |
| C8—N3—N4 | 107.13 (14) | H9A—C9—H9C | 109.5 |
| C11—N4—C10 | 129.66 (14) | H9B—C9—H9C | 109.5 |
| C11—N4—N3 | 118.47 (14) | C2—C1—C6 | 119.35 (17) |
| C10—N4—N3 | 111.69 (13) | C2—C1—H1A | 120.3 |
| N3—C8—C7 | 111.47 (15) | C6—C1—H1A | 120.3 |
| N3—C8—C9 | 121.65 (16) | C1—C2—C3 | 120.54 (17) |
| C7—C8—C9 | 126.86 (15) | C1—C2—H2 | 119.7 |
| C1—C6—C5 | 120.19 (17) | C3—C2—H2 | 119.7 |
| C1—C6—N1 | 121.47 (16) | C4—C3—C2 | 119.84 (18) |

| | | | |
|---|---|---|---|
| C5—C6—N1 | 118.34 (15) | C4—C3—H3 | 120.1 |
| O1—C10—N4 | 128.54 (16) | C2—C3—H3 | 120.1 |
| O1—C10—C7 | 128.36 (16) | S1—C12—H12A | 109.5 |
| N4—C10—C7 | 103.10 (14) | S1—C12—H12B | 109.5 |
| N4—C11—S2 | 123.30 (13) | H12A—C12—H12B | 109.5 |
| N4—C11—S1 | 111.28 (12) | S1—C12—H12C | 109.5 |
| S2—C11—S1 | 125.42 (10) | H12A—C12—H12C | 109.5 |
| C4—C5—C6 | 119.86 (17) | H12B—C12—H12C | 109.5 |
| C4—C5—H5 | 120.1 | C3—C4—C5 | 120.22 (17) |
| C6—C5—H5 | 120.1 | C3—C4—H4 | 119.9 |
| N2—C7—C8 | 126.19 (15) | C5—C4—H4 | 119.9 |
| N2—C7—C10 | 127.11 (15) | | |

| | | | |
|---|---|---|---|
| C7—N2—N1—C6 | −178.00 (16) | N1—C6—C5—C4 | −178.05 (17) |
| C8—N3—N4—C11 | 176.70 (14) | N1—N2—C7—C8 | 175.26 (16) |
| C8—N3—N4—C10 | 1.18 (19) | N1—N2—C7—C10 | −0.4 (3) |
| N4—N3—C8—C7 | −0.49 (19) | N3—C8—C7—N2 | −176.75 (16) |
| N4—N3—C8—C9 | −178.93 (15) | C9—C8—C7—N2 | 1.6 (3) |
| N2—N1—C6—C1 | −17.1 (3) | N3—C8—C7—C10 | −0.3 (2) |
| N2—N1—C6—C5 | 162.07 (16) | C9—C8—C7—C10 | 178.02 (17) |
| C11—N4—C10—O1 | 3.6 (3) | O1—C10—C7—N2 | −2.5 (3) |
| N3—N4—C10—O1 | 178.51 (16) | N4—C10—C7—N2 | 177.36 (16) |
| C11—N4—C10—C7 | −176.20 (16) | O1—C10—C7—C8 | −178.85 (17) |
| N3—N4—C10—C7 | −1.32 (18) | N4—C10—C7—C8 | 0.97 (18) |
| C10—N4—C11—S2 | −9.6 (3) | C5—C6—C1—C2 | −1.1 (3) |
| N3—N4—C11—S2 | 175.85 (12) | N1—C6—C1—C2 | 178.01 (17) |
| C10—N4—C11—S1 | 170.68 (14) | C6—C1—C2—C3 | 0.2 (3) |
| N3—N4—C11—S1 | −3.90 (19) | C1—C2—C3—C4 | 0.8 (3) |
| C12—S1—C11—N4 | 178.32 (12) | C2—C3—C4—C5 | −0.8 (3) |
| C12—S1—C11—S2 | −1.43 (14) | C6—C5—C4—C3 | −0.1 (3) |
| C1—C6—C5—C4 | 1.1 (3) | | |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N1—H1···O1 | 0.86 | 2.06 | 2.751 (2) | 137 |
| C4—H4···O1$^{i}$ | 0.93 | 2.49 | 3.244 (3) | 139 |
| C4—H4···S2$^{i}$ | 0.93 | 2.99 | 3.842 (2) | 152 |

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