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# 2-[4,5-Bis(butylsulfanyl)-1,3-dithiol-2-ylidene]-5-methyl-5*H*-1,3-dithiolo[4,5-*c*]pyrrole-4-carbaldehyde

**Rui-Bin Hou and Bing-Zhu Yin***

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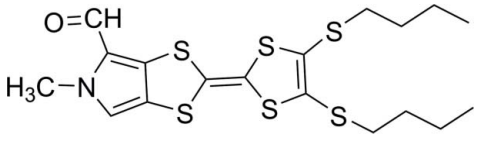
Key indicators: single-crystal X-ray study; $T$ = 291 K; mean $\sigma$(C–C) = 0.006 Å; $R$ factor = 0.051; $wR$ factor = 0.176; data-to-parameter ratio = 20.8.

In the title compound, $C_{18}H_{23}NOS_6$, the dithiolopyrrole ring is almost planar [r.m.s. deviation = 0.044 (3) Å] and makes a dihedral angle of 25.11 (7)° with the dithiole ring. In the crystal, pairs of neighboring molecules are connected by weak intermolecular C—H···O interactions. These dimers are further linked into a chain along [110] by C—H···O interactions.

## Related literature

For background to tetrathiafulvalenes, see: Jeppesen *et al.* (1999); Hansel *et al.* (2004). For the synthesis, see: An *et al.* (2009). For a related structure, see: Leng *et al.* (2009)




## Experimental

### Crystal data

$C_{18}H_{23}NOS_6$
$M_r$ = 461.73
Triclinic, $P\overline{1}$
$a$ = 7.4227 (15) Å
$b$ = 8.8356 (18) Å
$c$ = 17.811 (4) Å
$\alpha$ = 93.44 (3)°
$\beta$ = 99.37 (3)°
$\gamma$ = 105.31 (3)°
$V$ = 1105.1 (4) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 0.63 mm$^{-1}$
$T$ = 291 K
0.12 × 0.11 × 0.10 mm

### Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min}$ = 0.929, $T_{max}$ = 0.940
10707 measured reflections
4956 independent reflections
3298 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.035

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.051
$wR(F^2)$ = 0.176
$S$ = 1.06
4956 reflections
238 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.51 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.44 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C3—H3$B$···O1$^{i}$ | 0.97 | 2.79 | 3.444 (5) | 125 |
| C4—H4$A$···O1$^{i}$ | 0.97 | 2.71 | 3.368 (5) | 126 |
| C18—H18···O1$^{ii}$ | 0.93 | 2.58 | 3.412 (5) | 150 |

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

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NG5074).

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# supporting information

*Acta Cryst.* (2010). E**66**, o3353 [https://doi.org/10.1107/S160053681004910X]

## 2-[4,5-Bis(butylsulfanyl)-1,3-dithiol-2-ylidene]-5-methyl-5*H*-1,3-dithiolo[4,5-*c*]pyrrole-4-carbaldehyde

**Rui-Bin Hou and Bing-Zhu Yin**

### S1. Comment

The tetrathiafulvalenes (TTFs) have become an interesting theme of organic synthesis (Jeppesen *et al.*, 1999). This is due to the high electrical conductivity and super conductor properties of these highly sophisticated compounds. Becher has recently synthesized a series novel donor-$\pi$-acceptor dyads based on the monopyrrolo-TTF (MPTTF), which exhibit good third-order non-linear optical properties (Hansel *et al.* 2004). In this paper, we report the crystal structure of the title compound, which is a key precursor of the dyads.

The title compound, as shown in Fig. 1, all bond lengths and angles are normal and comparable with those reported for the related structure (Leng *et al.*, 2009). In the title compound, the dithiolopyrrole ring and attached C16, C18 and O1 atoms are nearlly coplanar [mean deviation from the mean plane = 0.044 (3) Å. The dihedral angle between the dithiolopyrrole ring and dithiole ring is 25.11 (7) °. In the crystal, weak C—H···O hydrogen bonds (table 1) link the molecules into dimer firstly and the dimers are further linked to form one-dimensional chain along [a+b] direction.

### S2. Experimental

The title compound was prepared according to literature (An *et al.*, 2009). Crystals suitable for single-crystal X-ray diffraction were grown by recrystallization from mixture of dichloromethane and petroleum (60–90 °C).

### S3. Refinement

Carbon-bound H-atoms were placed in calculated positions with C—H = 0.93–0.97 A and were included in the refinement in the riding model with $U_{iso}$(H) = 1.2 or 1.5 $U_{eq}$(C).

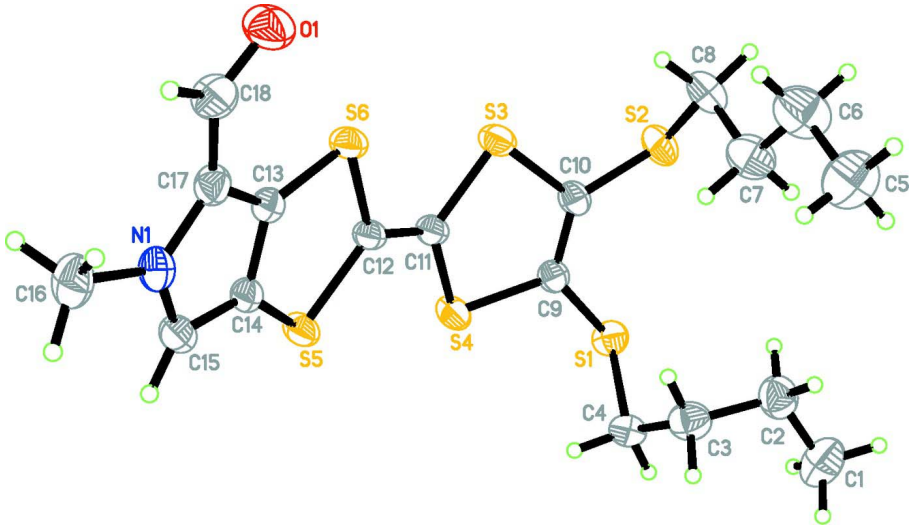


**Figure 1**

The asymmetric of title compound, with the atom numbering. Displacement ellipsoids of non-H atoms are drawn at the 30% probalility level.

**2-[4,5-Bis(butylsulfanyl)-1,3-dithiol-2-ylidene]-5-methyl-5*H*- 1,3-dithiolo[4,5-*c*]pyrrole-4-carbaldehyde**

*Crystal data*

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$\gamma = 105.31\ (3)°$
$V = 1105.1\ (4)$ Å$^3$
$Z = 2$
$F(000) = 484$
$D_x = 1.388$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 7048 reflections
$\theta = 3.2–27.4°$
$\mu = 0.63$ mm$^{-1}$
$T = 291$ K
Block, yellow
0.12 × 0.11 × 0.10 mm

*Data collection*

Rigaku R-AXIS RAPID diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega$ scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min} = 0.929$, $T_{max} = 0.940$
10707 measured reflections
4956 independent reflections
3298 reflections with $I > 2\sigma(I)$
$R_{int} = 0.035$
$\theta_{max} = 27.5°$, $\theta_{min} = 3.2°$
$h = -9\rightarrow9$
$k = -11\rightarrow11$
$l = -23\rightarrow23$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.051$
$wR(F^2) = 0.176$
$S = 1.06$
4956 reflections
238 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
$w = 1/[\sigma^2(F_o^2) + (0.103P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.51$ e Å$^{-3}$
$\Delta\rho_{min} = -0.44$ 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 (Å$^2$)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| C1 | 1.3588 (7) | 0.8577 (6) | 0.3605 (3) | 0.0992 (16) |
| H1A | 1.4403 | 0.8569 | 0.3239 | 0.149* |
| H1B | 1.4309 | 0.8665 | 0.4113 | 0.149* |
| H1C | 1.3067 | 0.9459 | 0.3554 | 0.149* |
| C2 | 1.2000 (6) | 0.7069 (5) | 0.3463 (2) | 0.0746 (11) |
| H2A | 1.2529 | 0.6206 | 0.3598 | 0.090* |
| H2B | 1.1120 | 0.7139 | 0.3802 | 0.090* |
| C3 | 1.0910 (6) | 0.6676 (5) | 0.2657 (2) | 0.0685 (10) |
| H3A | 1.0039 | 0.5628 | 0.2612 | 0.082* |
| H3B | 1.1798 | 0.6642 | 0.2317 | 0.082* |
| C4 | 0.9789 (5) | 0.7804 (5) | 0.2387 (2) | 0.0612 (9) |
| H4A | 0.9227 | 0.7494 | 0.1851 | 0.073* |
| H4B | 1.0656 | 0.8853 | 0.2429 | 0.073* |
| C5 | 1.0794 (8) | 0.1668 (7) | 0.4134 (3) | 0.1074 (17) |
| H5A | 1.0622 | 0.1460 | 0.3588 | 0.161* |
| H5B | 1.1150 | 0.0815 | 0.4370 | 0.161* |
| H5C | 1.1778 | 0.2634 | 0.4305 | 0.161* |
| C6 | 0.8994 (9) | 0.1813 (7) | 0.4347 (3) | 0.1053 (17) |
| H6A | 0.7974 | 0.0886 | 0.4120 | 0.126* |
| H6B | 0.9111 | 0.1849 | 0.4899 | 0.126* |
| C7 | 0.8498 (7) | 0.3235 (6) | 0.4094 (3) | 0.0837 (13) |
| H7A | 0.8372 | 0.3194 | 0.3542 | 0.100* |
| H7B | 0.9524 | 0.4161 | 0.4317 | 0.100* |
| C8 | 0.6652 (7) | 0.3397 (5) | 0.4319 (2) | 0.0735 (11) |
| H8A | 0.6734 | 0.3350 | 0.4866 | 0.088* |
| H8B | 0.5604 | 0.2521 | 0.4059 | 0.088* |
| C9 | 0.6295 (5) | 0.6022 (4) | 0.26157 (16) | 0.0458 (7) |
| C10 | 0.5642 (5) | 0.4948 (4) | 0.30804 (17) | 0.0483 (7) |
| C11 | 0.4100 (4) | 0.3654 (3) | 0.17027 (16) | 0.0445 (7) |
| C12 | 0.3512 (4) | 0.2543 (3) | 0.10934 (16) | 0.0438 (7) |
| C13 | 0.2413 (4) | −0.0068 (3) | 0.02430 (17) | 0.0440 (7) |
| C14 | 0.3053 (4) | 0.1071 (3) | −0.02319 (16) | 0.0439 (7) |

| | | | | |
|---|---|---|---|---|
| C15 | 0.2900 (5) | 0.0300 (4) | −0.09493 (18) | 0.0525 (8) |
| H15 | 0.3207 | 0.0776 | −0.1381 | 0.063* |
| C16 | 0.1719 (6) | −0.2460 (5) | −0.1579 (2) | 0.0688 (10) |
| H16A | 0.0363 | −0.2788 | −0.1743 | 0.103* |
| H16B | 0.2154 | −0.3354 | −0.1440 | 0.103* |
| H16C | 0.2307 | −0.2022 | −0.1989 | 0.103* |
| C17 | 0.1886 (5) | −0.1548 (4) | −0.01838 (19) | 0.0510 (7) |
| C18 | 0.1247 (6) | −0.3038 (4) | 0.0080 (2) | 0.0639 (9) |
| H18 | 0.0960 | −0.3934 | −0.0267 | 0.077* |
| N1 | 0.2228 (4) | −0.1257 (3) | −0.09119 (15) | 0.0526 (7) |
| O1 | 0.1051 (5) | −0.3211 (3) | 0.07376 (16) | 0.0820 (9) |
| S1 | 0.79120 (13) | 0.78869 (10) | 0.29159 (5) | 0.0561 (3) |
| S2 | 0.61844 (16) | 0.52311 (12) | 0.40750 (5) | 0.0659 (3) |
| S3 | 0.38334 (14) | 0.32527 (10) | 0.26366 (5) | 0.0567 (3) |
| S4 | 0.52382 (14) | 0.56342 (9) | 0.16415 (4) | 0.0536 (2) |
| S5 | 0.37538 (13) | 0.30352 (9) | 0.01664 (4) | 0.0524 (2) |
| S6 | 0.24240 (13) | 0.05437 (9) | 0.11878 (4) | 0.0516 (2) |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C1 | 0.068 (3) | 0.109 (4) | 0.115 (4) | 0.023 (3) | 0.011 (3) | −0.006 (3) |
| C2 | 0.074 (3) | 0.087 (3) | 0.069 (3) | 0.035 (2) | 0.011 (2) | 0.010 (2) |
| C3 | 0.073 (3) | 0.068 (2) | 0.066 (2) | 0.018 (2) | 0.023 (2) | −0.0010 (19) |
| C4 | 0.061 (2) | 0.070 (2) | 0.0535 (19) | 0.0135 (18) | 0.0181 (17) | 0.0137 (17) |
| C5 | 0.099 (4) | 0.107 (4) | 0.122 (5) | 0.039 (3) | 0.027 (3) | −0.005 (3) |
| C6 | 0.125 (5) | 0.117 (4) | 0.099 (4) | 0.061 (4) | 0.046 (3) | 0.022 (3) |
| C7 | 0.103 (4) | 0.083 (3) | 0.072 (3) | 0.031 (3) | 0.027 (3) | 0.009 (2) |
| C8 | 0.094 (3) | 0.082 (3) | 0.050 (2) | 0.032 (2) | 0.012 (2) | 0.0188 (19) |
| C9 | 0.0491 (17) | 0.0483 (16) | 0.0380 (15) | 0.0111 (14) | 0.0081 (13) | −0.0007 (12) |
| C10 | 0.0561 (19) | 0.0532 (17) | 0.0366 (15) | 0.0176 (15) | 0.0089 (14) | 0.0004 (13) |
| C11 | 0.0497 (18) | 0.0417 (15) | 0.0383 (15) | 0.0053 (13) | 0.0094 (13) | 0.0053 (12) |
| C12 | 0.0484 (17) | 0.0414 (14) | 0.0378 (14) | 0.0038 (13) | 0.0107 (13) | 0.0066 (12) |
| C13 | 0.0437 (16) | 0.0421 (15) | 0.0410 (15) | 0.0058 (13) | 0.0039 (13) | 0.0028 (12) |
| C14 | 0.0460 (17) | 0.0414 (15) | 0.0388 (15) | 0.0052 (13) | 0.0042 (13) | 0.0038 (12) |
| C15 | 0.060 (2) | 0.0524 (18) | 0.0425 (16) | 0.0105 (16) | 0.0079 (15) | 0.0079 (14) |
| C16 | 0.072 (3) | 0.064 (2) | 0.061 (2) | 0.0154 (19) | 0.0018 (19) | −0.0205 (18) |
| C17 | 0.0520 (19) | 0.0439 (16) | 0.0504 (18) | 0.0074 (14) | 0.0010 (14) | 0.0021 (13) |
| C18 | 0.072 (2) | 0.0439 (17) | 0.069 (2) | 0.0075 (17) | 0.0110 (19) | 0.0014 (16) |
| N1 | 0.0560 (17) | 0.0517 (15) | 0.0452 (14) | 0.0140 (13) | 0.0012 (12) | −0.0056 (12) |
| O1 | 0.109 (2) | 0.0570 (15) | 0.0691 (18) | 0.0038 (15) | 0.0158 (17) | 0.0148 (13) |
| S1 | 0.0593 (5) | 0.0486 (4) | 0.0552 (5) | 0.0078 (4) | 0.0121 (4) | −0.0066 (4) |
| S2 | 0.0881 (7) | 0.0735 (6) | 0.0349 (4) | 0.0241 (5) | 0.0069 (4) | 0.0004 (4) |
| S3 | 0.0694 (6) | 0.0540 (5) | 0.0389 (4) | 0.0006 (4) | 0.0148 (4) | 0.0056 (3) |
| S4 | 0.0736 (6) | 0.0425 (4) | 0.0383 (4) | 0.0066 (4) | 0.0071 (4) | 0.0051 (3) |
| S5 | 0.0704 (6) | 0.0412 (4) | 0.0381 (4) | 0.0023 (4) | 0.0097 (4) | 0.0066 (3) |
| S6 | 0.0623 (5) | 0.0431 (4) | 0.0422 (4) | −0.0001 (4) | 0.0128 (4) | 0.0074 (3) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| C1—C2 | 1.504 (6) | C9—C10 | 1.342 (5) |
| C1—H1A | 0.9600 | C9—S1 | 1.756 (3) |
| C1—H1B | 0.9600 | C9—S4 | 1.757 (3) |
| C1—H1C | 0.9600 | C10—S2 | 1.739 (3) |
| C2—C3 | 1.500 (5) | C10—S3 | 1.767 (3) |
| C2—H2A | 0.9700 | C11—C12 | 1.350 (4) |
| C2—H2B | 0.9700 | C11—S4 | 1.749 (3) |
| C3—C4 | 1.510 (5) | C11—S3 | 1.753 (3) |
| C3—H3A | 0.9700 | C12—S5 | 1.757 (3) |
| C3—H3B | 0.9700 | C12—S6 | 1.769 (3) |
| C4—S1 | 1.818 (3) | C13—C14 | 1.391 (4) |
| C4—H4A | 0.9700 | C13—C17 | 1.399 (4) |
| C4—H4B | 0.9700 | C13—S6 | 1.734 (3) |
| C5—C6 | 1.482 (7) | C14—C15 | 1.385 (4) |
| C5—H5A | 0.9600 | C14—S5 | 1.744 (3) |
| C5—H5B | 0.9600 | C15—N1 | 1.344 (4) |
| C5—H5C | 0.9600 | C15—H15 | 0.9300 |
| C6—C7 | 1.475 (7) | C16—N1 | 1.475 (4) |
| C6—H6A | 0.9700 | C16—H16A | 0.9600 |
| C6—H6B | 0.9700 | C16—H16B | 0.9600 |
| C7—C8 | 1.528 (6) | C16—H16C | 0.9600 |
| C7—H7A | 0.9700 | C17—N1 | 1.387 (4) |
| C7—H7B | 0.9700 | C17—C18 | 1.413 (5) |
| C8—S2 | 1.807 (4) | C18—O1 | 1.217 (5) |
| C8—H8A | 0.9700 | C18—H18 | 0.9300 |
| C8—H8B | 0.9700 | | |

| | | | |
|---|---|---|---|
| C2—C1—H1A | 109.5 | C7—C8—H8B | 109.3 |
| C2—C1—H1B | 109.5 | S2—C8—H8B | 109.3 |
| H1A—C1—H1B | 109.5 | H8A—C8—H8B | 107.9 |
| C2—C1—H1C | 109.5 | C10—C9—S1 | 125.3 (2) |
| H1A—C1—H1C | 109.5 | C10—C9—S4 | 117.4 (2) |
| H1B—C1—H1C | 109.5 | S1—C9—S4 | 116.88 (18) |
| C3—C2—C1 | 115.1 (4) | C9—C10—S2 | 125.1 (3) |
| C3—C2—H2A | 108.5 | C9—C10—S3 | 116.0 (2) |
| C1—C2—H2A | 108.5 | S2—C10—S3 | 118.30 (19) |
| C3—C2—H2B | 108.5 | C12—C11—S4 | 123.3 (2) |
| C1—C2—H2B | 108.5 | C12—C11—S3 | 123.5 (2) |
| H2A—C2—H2B | 107.5 | S4—C11—S3 | 113.19 (16) |
| C2—C3—C4 | 115.4 (3) | C11—C12—S5 | 121.2 (2) |
| C2—C3—H3A | 108.4 | C11—C12—S6 | 121.7 (2) |
| C4—C3—H3A | 108.4 | S5—C12—S6 | 117.09 (16) |
| C2—C3—H3B | 108.4 | C14—C13—C17 | 108.2 (3) |
| C4—C3—H3B | 108.4 | C14—C13—S6 | 118.5 (2) |
| H3A—C3—H3B | 107.5 | C17—C13—S6 | 133.4 (3) |
| C3—C4—S1 | 114.2 (3) | C15—C14—C13 | 107.6 (3) |

| | | | |
|---|---|---|---|
| C3—C4—H4A | 108.7 | C15—C14—S5 | 135.4 (2) |
| S1—C4—H4A | 108.7 | C13—C14—S5 | 117.0 (2) |
| C3—C4—H4B | 108.7 | N1—C15—C14 | 107.9 (3) |
| S1—C4—H4B | 108.7 | N1—C15—H15 | 126.0 |
| H4A—C4—H4B | 107.6 | C14—C15—H15 | 126.0 |
| C6—C5—H5A | 109.5 | N1—C16—H16A | 109.5 |
| C6—C5—H5B | 109.5 | N1—C16—H16B | 109.5 |
| H5A—C5—H5B | 109.5 | H16A—C16—H16B | 109.5 |
| C6—C5—H5C | 109.5 | N1—C16—H16C | 109.5 |
| H5A—C5—H5C | 109.5 | H16A—C16—H16C | 109.5 |
| H5B—C5—H5C | 109.5 | H16B—C16—H16C | 109.5 |
| C7—C6—C5 | 112.5 (5) | N1—C17—C13 | 105.7 (3) |
| C7—C6—H6A | 109.1 | N1—C17—C18 | 126.9 (3) |
| C5—C6—H6A | 109.1 | C13—C17—C18 | 127.3 (3) |
| C7—C6—H6B | 109.1 | O1—C18—C17 | 123.6 (3) |
| C5—C6—H6B | 109.1 | O1—C18—H18 | 118.2 |
| H6A—C6—H6B | 107.8 | C17—C18—H18 | 118.2 |
| C6—C7—C8 | 112.7 (4) | C15—N1—C17 | 110.6 (3) |
| C6—C7—H7A | 109.0 | C15—N1—C16 | 124.0 (3) |
| C8—C7—H7A | 109.0 | C17—N1—C16 | 125.0 (3) |
| C6—C7—H7B | 109.0 | C9—S1—C4 | 101.26 (16) |
| C8—C7—H7B | 109.0 | C10—S2—C8 | 102.69 (17) |
| H7A—C7—H7B | 107.8 | C11—S3—C10 | 94.65 (15) |
| C7—C8—S2 | 111.8 (3) | C11—S4—C9 | 94.30 (15) |
| C7—C8—H8A | 109.3 | C14—S5—C12 | 93.61 (14) |
| S2—C8—H8A | 109.3 | C13—S6—C12 | 93.09 (14) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C3—H3*B*···O1$^{i}$ | 0.97 | 2.79 | 3.444 (5) | 125 |
| C4—H4*A*···O1$^{i}$ | 0.97 | 2.71 | 3.368 (5) | 126 |
| C18—H18···O1$^{ii}$ | 0.93 | 2.58 | 3.412 (5) | 150 |

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