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# 2,9-Dimethylphenanthro[2,1-*b*:6,5-*b*′]dithiophene

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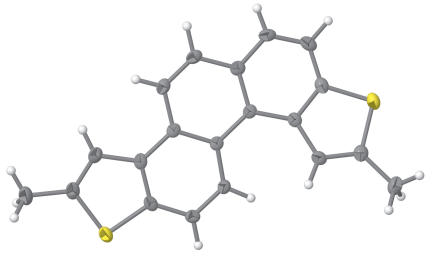
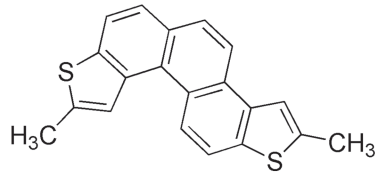
**Structural data:** full structural data are available from iucrdata.iucr.org

The title compound, $C_{20}H_{14}S_2$, was synthesized from a dimethyl-substituted thiophene precursor using an oxidative photocyclization reaction. The molecule has a puckered structure due to steric crowding and the extended structure is consolidated by C—H···$\pi$ interactions between columns of stacked molecules.

3D view



Chemical scheme




## Structure description

Polycyclic aromatic hydrocarbons, or $\pi$-conjugated materials, are an important class of organic compounds that have brought about significant advancements in the field of organic electronics due to their crucial property of conductivity (Wang *et al.*, 2012). Previously, the authors reported on the synthesis of various types of polycyclic aromatic compounds using extended $\pi$-conjugated materials and the evaluation of their organic photoelectronic properties (Moriguchi *et al.*, 2016). More recently, we also reported on the structural properties and crystal structures of heteropolycyclic aromatic compounds for semiconductor materials using X-ray diffraction analysis (Moriguchi *et al.*, 2017*a*; Moriguchi *et al.*, 2017*b*; Moriguchi *et al.*, 2018).

As part of our ongoing studies in this area, this article describes the synthesis and structure determination of the title compound, $C_{20}H_{14}S_2$, (**I**). This compound crystallizes in the non-centrosymmetric space group $P2_12_12_1$, with one molecule in the asymmetric unit (Fig. 1). The shape of the molecule is puckered and the dihedral angle between the terminal thiophene rings (C1–C4/S1 and C16–C19/S2) is 17.26 (9)° (Fig. 3). The dihedral angle between the C4–C9 and C12–C17 aromatic rings is 11.61 (9)°. This molecular distortion may arise due to intramolecular congestion: in particular, the short H3···H14 contact of 1.98 (3) Å, which is relieved by the molecular twisting. In the extended structure, the molecules are linked by C—H···$\pi$ interactions (Table 1), and are not oriented as a $\pi$–$\pi$ stacked structure (Figs. 2 and 3).

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

**Define Cg2/3/5**

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C1—H1B···$Cg3^{i}$ | 1.00 (3) | 2.84 (3) | 3.714 (3) | 147 (2) |
| C7—H7···$Cg2^{ii}$ | 0.91 (2) | 2.962 (19) | 3.767 (2) | 148.3 (15) |
| C10—H10···$Cg5^{ii}$ | 0.99 (2) | 2.960 (19) | 3.427 (2) | 110.1 (13) |

Symmetry codes: (i) $x-1, y, z$; (ii) $-x, y+\frac{1}{2}, -z+\frac{5}{2}$.

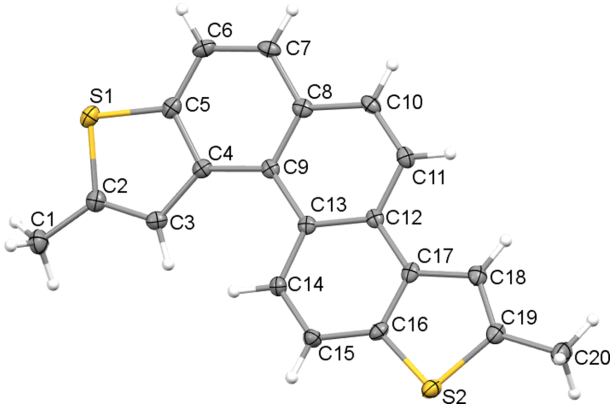



**Figure 1**
The molecular structure of (**I**), with displacement ellipsoids drawn at the 50% probability level.

## Synthesis and crystallization

All reagents and solvents were purchased from commercial sources and were used without further purification. The electron impact (EI) mass spectrum (MS) of the compound was obtained on a Jeol JMS-SX102A spectrometer using dichloromethane (DCM) as the solvent. The instrument was operated in positive ion mode over an $m/z$ range.

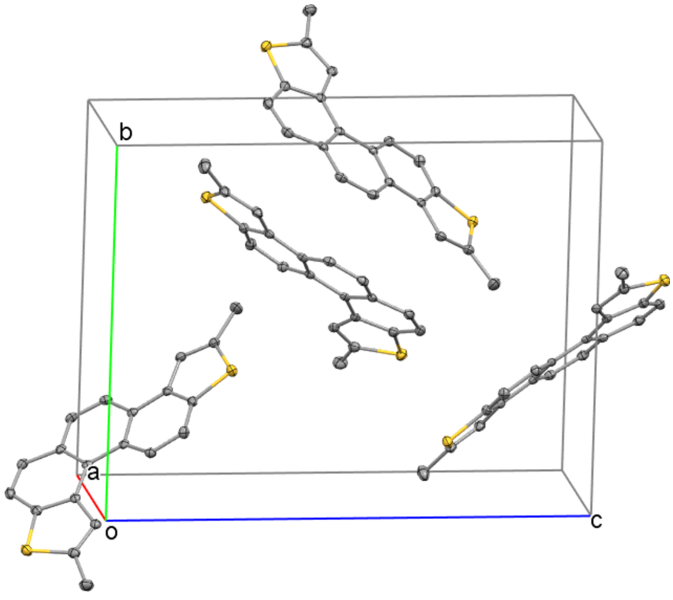



**Figure 2**
Packing diagram of (**I**), with displacement ellipsoids drawn at the 50% probability level. H atoms have been omitted for clarity.

**Table 2**
Experimental details.

| | |
|---|---|
| Crystal data | |
| Chemical formula | $C_{20}H_{14}S_2$ |
| $M_r$ | 318.47 |
| Crystal system, space group | Orthorhombic, $P2_12_12_1$ |
| Temperature (K) | 90 |
| $a, b, c$ (Å) | 6.5043 (17), 13.456 (3), 17.082 (4) |
| $V$ (Å$^3$) | 1495.0 (7) |
| $Z$ | 4 |
| Radiation type | Mo $K\alpha$ |
| $\mu$ (mm$^{-1}$) | 0.35 |
| Crystal size (mm) | 0.45 × 0.10 × 0.10 |
| | |
| Data collection | |
| Diffractometer | Bruker SMART APEX CCD |
| Absorption correction | Multi-scan (*SADABS*; Bruker, 2009) |
| $T_{min}$, $T_{max}$ | 0.611, 0.745 |
| No. of measured, independent and observed [$I \geq 2u(I)$] reflections | 14478, 2666, 2543 |
| $R_{int}$ | 0.037 |
| (sin $\theta/\lambda)_{max}$ (Å$^{-1}$) | 0.598 |
| | |
| Refinement | |
| $R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, $S$ | 0.027, 0.065, 1.08 |
| No. of reflections | 2666 |
| No. of parameters | 255 |
| H-atom treatment | All H-atom parameters refined |
| $\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å$^{-3}$) | 0.20, −0.17 |
| Absolute structure | Hooft *et al.* (2010) |
| Absolute structure parameter | −0.03 (3) |

Computer programs: *APEX2* (Bruker, 2009), *SAINT* (Bruker, 2009), *olex2.solve* (Bourhis *et al.*, 2015), *olex2.refine* (Bourhis *et al.*, 2015) and *OLEX2* (Dolomanov *et al.*, 2009).

1,3-Bis[2-(2-metylthiophenyl)ethenyl]benzene (1.0 mmol) was dissolved in 200 ml of benzene in a round-bottomed flask at room temperature. To this, iodine (10 mmol) was added, the mixture was stirred and irradiated with UV light using a high-pressure Hg lump for 14 h, quenched with 1.0 mol l$^{-1}$ $Na_2S_2O_3$ solution, allowed to warm to room temperature and extracted twice with AcOEt. The organic layer was washed

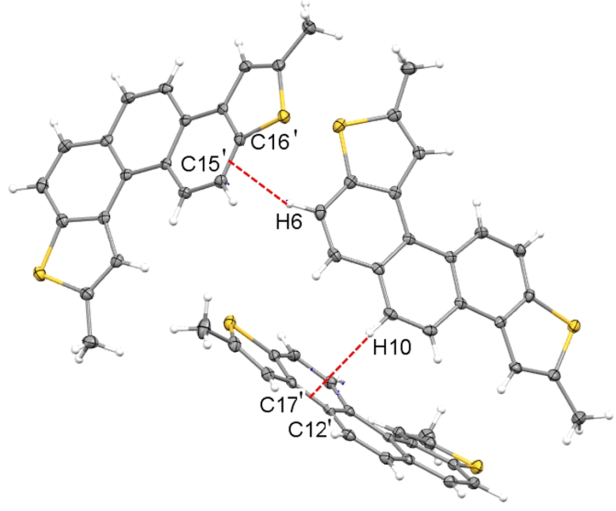



**Figure 3**
View of the packing of (**I**), showing C—H···$\pi$ interactions between adjacent molecules.

once with 50 ml water, twice with 50 ml of brine, dried over $MgSO_4$ and the solvent was removed under reduced pressure. The title compound was obtained using silica gel (Wako gel C-300) column chromatography (200 mg, 63% yield) with $CH_2Cl_2$ as an eluent. Suitable single crystals of (**I**) in the form of yellow prisms were obtained at room temperature from a solution of dichloromethane–*n*-hexane (1/1 *v*/*v*). MS(EI): $M^+$ 318.

## Refinement

Key crystallographic data are listed in Table 2. The H atoms were located in difference maps and their positions were freely refined.

## Acknowledgements

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# full crystallographic data

*IUCrData* (2026). **11**, x260700 [https://doi.org/10.1107/S2414314626007005]

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### 2,9-Dimethylphenanthro[2,1-*b*:6,5-*b′*]dithiophene

*Crystal data*

$C_{20}H_{14}S_2$
$M_r$ = 318.47
Orthorhombic, $P2_12_12_1$
$a$ = 6.5043 (17) Å
$b$ = 13.456 (3) Å
$c$ = 17.082 (4) Å
$V$ = 1495.0 (7) Å$^3$
$Z$ = 4
$F$(000) = 665.274
$D_x$ = 1.415 Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å
Cell parameters from 6305 reflections
$\theta$ = 2.4–25.1°
$\mu$ = 0.35 mm$^{-1}$
$T$ = 90 K
Prism, clear light yellow
0.45 × 0.10 × 0.10 mm

*Data collection*

Bruker SMART APEX CCD diffractometer
Radiation source: sealed tube
Graphite monochromator
Detector resolution: 8 pixels mm$^{-1}$
$\omega$ scans
Absorption correction: multi-scan SADABS (Bruker, 2009)
$T_{min}$ = 0.611, $T_{max}$ = 0.745
14478 measured reflections
2666 independent reflections
2543 reflections with $I \geq 2u(I)$
$R_{int}$ = 0.037
$\theta_{max}$ = 25.1°, $\theta_{min}$ = 2.4°
$h$ = −7→7
$k$ = −16→16
$l$ = −20→20

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.027
$wR(F^2)$ = 0.065
$S$ = 1.08
2666 reflections
255 parameters
0 restraints
0 constraints
Primary atom site location: iterative
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0346P)^2 + 0.2686P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.20 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.17 e Å$^{-3}$
Absolute structure: Hooft *et al.* (2010)
Absolute structure parameter: −0.03 (3)

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å$^2$)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| S1 | −0.04847 (9) | 0.63225 (4) | 1.13345 (3) | 0.02673 (13) |
| S2 | 0.15028 (9) | 0.18292 (4) | 0.70895 (3) | 0.02671 (13) |
| C1 | −0.3530 (4) | 0.68925 (17) | 1.02692 (15) | 0.0332 (5) |
| H1a | −0.377 (4) | 0.701 (2) | 0.9739 (18) | 0.062 (9)* |
| H1b | −0.484 (5) | 0.660 (2) | 1.0463 (16) | 0.067 (9)* |

| | | | | |
|---|---|---|---|---|
| H1c | −0.336 (5) | 0.751 (2) | 1.0483 (16) | 0.068 (9)* |
| C20 | 0.4911 (4) | 0.05841 (19) | 0.68237 (14) | 0.0383 (6) |
| H20a | 0.628 (5) | 0.047 (2) | 0.6963 (16) | 0.055 (8)* |
| H20b | 0.424 (5) | −0.007 (2) | 0.6861 (16) | 0.066 (9)* |
| H20c | 0.484 (4) | 0.0714 (19) | 0.6294 (16) | 0.055 (8)* |
| C2 | −0.1704 (3) | 0.62557 (14) | 1.04301 (11) | 0.0245 (4) |
| C3 | −0.0746 (3) | 0.56109 (13) | 0.99428 (11) | 0.0214 (4) |
| H3 | −0.121 (3) | 0.5547 (14) | 0.9429 (11) | 0.018 (5)* |
| C4 | 0.1031 (3) | 0.51287 (13) | 1.02696 (10) | 0.0193 (4) |
| C5 | 0.1397 (3) | 0.54895 (13) | 1.10359 (11) | 0.0224 (4) |
| C19 | 0.3958 (3) | 0.13846 (14) | 0.73123 (11) | 0.0264 (5) |
| C18 | 0.4745 (3) | 0.18496 (14) | 0.79448 (11) | 0.0240 (4) |
| H18 | 0.598 (3) | 0.1690 (15) | 0.8135 (11) | 0.020 (5)* |
| C17 | 0.3420 (3) | 0.25900 (13) | 0.82838 (10) | 0.0201 (4) |
| C16 | 0.1569 (3) | 0.26534 (13) | 0.78785 (10) | 0.0215 (4) |
| C6 | 0.3123 (3) | 0.52437 (14) | 1.14820 (11) | 0.0252 (4) |
| H6 | 0.332 (3) | 0.5511 (15) | 1.2015 (13) | 0.030 (6)* |
| C7 | 0.4554 (4) | 0.46387 (14) | 1.11539 (11) | 0.0237 (4) |
| H7 | 0.572 (3) | 0.4467 (14) | 1.1416 (11) | 0.015 (5)* |
| C15 | −0.0010 (3) | 0.32809 (14) | 0.81307 (11) | 0.0225 (4) |
| H15 | −0.128 (4) | 0.3298 (15) | 0.7842 (12) | 0.031 (6)* |
| C14 | 0.0304 (3) | 0.38536 (13) | 0.87894 (11) | 0.0208 (4) |
| H14 | −0.086 (3) | 0.4230 (13) | 0.8932 (10) | 0.013 (5)* |
| C10 | 0.5811 (3) | 0.35708 (14) | 1.00967 (11) | 0.0227 (4) |
| H10 | 0.710 (3) | 0.3506 (14) | 1.0398 (11) | 0.025 (6)* |
| C11 | 0.5574 (3) | 0.30801 (14) | 0.94137 (11) | 0.0222 (4) |
| H11 | 0.655 (3) | 0.2674 (15) | 0.9225 (11) | 0.023 (5)* |
| C9 | 0.2457 (3) | 0.44063 (12) | 0.99489 (11) | 0.0176 (4) |
| C13 | 0.2158 (3) | 0.38424 (13) | 0.92283 (10) | 0.0176 (4) |
| C8 | 0.4253 (3) | 0.42170 (13) | 1.03969 (10) | 0.0205 (4) |
| C12 | 0.3746 (3) | 0.31869 (13) | 0.89681 (10) | 0.0184 (4) |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| S1 | 0.0315 (3) | 0.0248 (2) | 0.0239 (2) | 0.0001 (2) | 0.0038 (2) | −0.0052 (2) |
| S2 | 0.0352 (3) | 0.0251 (2) | 0.0199 (2) | 0.0027 (2) | −0.0002 (2) | −0.0034 (2) |
| C1 | 0.0330 (13) | 0.0281 (11) | 0.0384 (13) | 0.0082 (11) | 0.0022 (11) | −0.0012 (10) |
| C20 | 0.0516 (18) | 0.0365 (13) | 0.0269 (12) | 0.0172 (12) | −0.0013 (11) | −0.0066 (10) |
| C2 | 0.0261 (10) | 0.0200 (9) | 0.0275 (10) | −0.0017 (9) | 0.0033 (9) | 0.0010 (8) |
| C3 | 0.0258 (11) | 0.0176 (9) | 0.0207 (10) | −0.0041 (8) | −0.0023 (9) | 0.0013 (8) |
| C4 | 0.0228 (11) | 0.0155 (9) | 0.0197 (9) | −0.0051 (7) | 0.0022 (7) | 0.0025 (7) |
| C5 | 0.0262 (11) | 0.0187 (9) | 0.0223 (9) | −0.0043 (8) | 0.0045 (9) | −0.0002 (7) |
| C19 | 0.0369 (13) | 0.0197 (9) | 0.0226 (9) | 0.0063 (9) | 0.0025 (9) | 0.0033 (8) |
| C18 | 0.0275 (11) | 0.0198 (9) | 0.0248 (9) | 0.0054 (9) | 0.0011 (9) | 0.0054 (9) |
| C17 | 0.0263 (10) | 0.0153 (8) | 0.0187 (8) | −0.0001 (8) | 0.0063 (9) | 0.0047 (7) |
| C16 | 0.0290 (10) | 0.0186 (9) | 0.0169 (8) | −0.0026 (8) | 0.0018 (9) | 0.0003 (7) |
| C6 | 0.0322 (12) | 0.0233 (9) | 0.0202 (10) | −0.0066 (9) | −0.0022 (9) | −0.0002 (8) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C7 | 0.0239 (10) | 0.0220 (10) | 0.0251 (10) | −0.0033 (9) | −0.0076 (9) | 0.0060 (8) |
| C15 | 0.0191 (11) | 0.0265 (10) | 0.0218 (9) | −0.0018 (8) | −0.0012 (8) | −0.0004 (8) |
| C14 | 0.0195 (9) | 0.0200 (9) | 0.0229 (9) | 0.0014 (8) | 0.0013 (8) | −0.0007 (8) |
| C10 | 0.0210 (11) | 0.0200 (9) | 0.0271 (10) | 0.0006 (8) | −0.0028 (9) | 0.0068 (8) |
| C11 | 0.0219 (10) | 0.0161 (9) | 0.0286 (10) | 0.0012 (9) | 0.0026 (9) | 0.0038 (8) |
| C9 | 0.0183 (9) | 0.0133 (8) | 0.0212 (9) | −0.0028 (7) | 0.0020 (8) | 0.0049 (7) |
| C13 | 0.0198 (10) | 0.0147 (9) | 0.0184 (9) | −0.0024 (7) | 0.0027 (7) | 0.0049 (7) |
| C8 | 0.0241 (11) | 0.0146 (9) | 0.0227 (9) | −0.0025 (8) | −0.0001 (8) | 0.0060 (7) |
| C12 | 0.0192 (9) | 0.0156 (8) | 0.0205 (8) | −0.0015 (8) | 0.0030 (8) | 0.0061 (8) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| S1—C2 | 1.739 (2) | C18—C17 | 1.439 (3) |
| S1—C5 | 1.736 (2) | C17—C16 | 1.392 (3) |
| S2—C19 | 1.747 (2) | C17—C12 | 1.434 (2) |
| S2—C16 | 1.7459 (18) | C16—C15 | 1.397 (3) |
| C1—H1a | 0.93 (3) | C6—H6 | 0.99 (2) |
| C1—H1b | 1.00 (3) | C6—C7 | 1.358 (3) |
| C1—H1c | 0.92 (3) | C7—H7 | 0.91 (2) |
| C1—C2 | 1.490 (3) | C7—C8 | 1.426 (3) |
| C20—H20a | 0.94 (3) | C15—H15 | 0.96 (2) |
| C20—H20b | 0.99 (3) | C15—C14 | 1.379 (3) |
| C20—H20c | 0.92 (3) | C14—H14 | 0.941 (19) |
| C20—C19 | 1.497 (3) | C14—C13 | 1.420 (3) |
| C2—C3 | 1.354 (3) | C10—H10 | 0.99 (2) |
| C3—H3 | 0.931 (19) | C10—C11 | 1.349 (3) |
| C3—C4 | 1.438 (3) | C10—C8 | 1.431 (3) |
| C4—C5 | 1.416 (3) | C11—H11 | 0.90 (2) |
| C4—C9 | 1.451 (3) | C11—C12 | 1.419 (3) |
| C5—C6 | 1.396 (3) | C9—C13 | 1.459 (3) |
| C19—C18 | 1.349 (3) | C9—C8 | 1.419 (3) |
| C18—H18 | 0.89 (2) | C13—C12 | 1.429 (2) |
| | | | |
| C5—S1—C2 | 91.55 (10) | C12—C17—C16 | 119.94 (17) |
| C16—S2—C19 | 91.54 (9) | C17—C16—S2 | 111.49 (14) |
| H1b—C1—H1a | 105 (2) | C15—C16—S2 | 127.14 (16) |
| H1c—C1—H1a | 104 (2) | C15—C16—C17 | 121.29 (17) |
| H1c—C1—H1b | 109 (2) | H6—C6—C5 | 121.4 (13) |
| C2—C1—H1a | 114.3 (17) | C7—C6—C5 | 117.89 (18) |
| C2—C1—H1b | 112.8 (16) | C7—C6—H6 | 120.7 (13) |
| C2—C1—H1c | 111 (2) | H7—C7—C6 | 121.3 (12) |
| H20b—C20—H20a | 105 (2) | C8—C7—C6 | 121.2 (2) |
| H20c—C20—H20a | 109 (2) | C8—C7—H7 | 117.4 (12) |
| H20c—C20—H20b | 102 (2) | H15—C15—C16 | 119.1 (12) |
| C19—C20—H20a | 111.5 (17) | C14—C15—C16 | 118.73 (18) |
| C19—C20—H20b | 115.3 (17) | C14—C15—H15 | 122.1 (12) |
| C19—C20—H20c | 113.0 (16) | H14—C14—C15 | 113.2 (11) |
| C1—C2—S1 | 119.84 (15) | C13—C14—C15 | 123.40 (18) |

| | | | |
|---|---|---|---|
| C3—C2—S1 | 111.69 (15) | C13—C14—H14 | 123.3 (11) |
| C3—C2—C1 | 128.44 (19) | C11—C10—H10 | 120.3 (11) |
| H3—C3—C2 | 119.4 (12) | C8—C10—H10 | 117.9 (11) |
| C4—C3—C2 | 114.84 (17) | C8—C10—C11 | 121.75 (19) |
| C4—C3—H3 | 125.6 (12) | H11—C11—C10 | 121.9 (13) |
| C5—C4—C3 | 109.83 (17) | C12—C11—C10 | 120.67 (19) |
| C9—C4—C3 | 132.02 (16) | C12—C11—H11 | 117.5 (13) |
| C9—C4—C5 | 118.10 (17) | C13—C9—C4 | 125.57 (17) |
| C4—C5—S1 | 111.97 (15) | C8—C9—C4 | 116.27 (16) |
| C6—C5—S1 | 124.00 (14) | C8—C9—C13 | 118.12 (16) |
| C6—C5—C4 | 123.95 (18) | C9—C13—C14 | 123.58 (17) |
| C20—C19—S2 | 120.21 (17) | C12—C13—C14 | 117.14 (16) |
| C18—C19—S2 | 111.24 (15) | C12—C13—C9 | 119.14 (16) |
| C18—C19—C20 | 128.6 (2) | C10—C8—C7 | 118.00 (18) |
| H18—C18—C19 | 121.4 (13) | C9—C8—C7 | 122.06 (18) |
| C17—C18—C19 | 114.60 (19) | C9—C8—C10 | 119.93 (17) |
| C17—C18—H18 | 124.0 (13) | C11—C12—C17 | 120.30 (17) |
| C16—C17—C18 | 111.12 (17) | C13—C12—C17 | 119.49 (17) |
| C12—C17—C18 | 128.86 (19) | C13—C12—C11 | 120.08 (16) |
| | | | |
| S1—C2—C3—C4 | 0.09 (16) | C19—C18—C17—C16 | 0.72 (19) |
| S1—C5—C4—C3 | 3.52 (15) | C19—C18—C17—C12 | 177.42 (15) |
| S1—C5—C4—C9 | −178.57 (12) | C18—C17—C16—C15 | 176.11 (15) |
| S1—C5—C6—C7 | −175.12 (16) | C18—C17—C12—C11 | −0.5 (2) |
| S2—C19—C18—C17 | −0.14 (16) | C18—C17—C12—C13 | −176.35 (18) |
| S2—C16—C17—C18 | −0.96 (15) | C17—C16—C15—C14 | 0.8 (2) |
| S2—C16—C17—C12 | −177.99 (11) | C17—C12—C11—C10 | −173.85 (17) |
| S2—C16—C15—C14 | 177.40 (16) | C17—C12—C13—C14 | 0.78 (18) |
| C1—C2—C3—C4 | 178.1 (2) | C17—C12—C13—C9 | 176.65 (15) |
| C20—C19—C18—C17 | −179.9 (2) | C16—C15—C14—C13 | 0.1 (2) |
| C2—C3—C4—C5 | −2.33 (19) | C6—C7—C8—C10 | −178.76 (18) |
| C2—C3—C4—C9 | −179.85 (15) | C6—C7—C8—C9 | 0.1 (2) |
| C3—C4—C5—C6 | −173.39 (14) | C7—C8—C10—C11 | 174.71 (17) |
| C3—C4—C9—C13 | −12.7 (2) | C7—C8—C9—C13 | −172.10 (16) |
| C3—C4—C9—C8 | 169.6 (2) | C15—C14—C13—C9 | −176.58 (17) |
| C4—C5—C6—C7 | 1.4 (2) | C15—C14—C13—C12 | −0.9 (2) |
| C4—C9—C13—C14 | −7.2 (2) | C14—C13—C9—C8 | 170.49 (17) |
| C4—C9—C13—C12 | 177.26 (17) | C14—C13—C12—C11 | −175.03 (16) |
| C4—C9—C8—C7 | 5.76 (19) | C10—C11—C12—C13 | 1.9 (2) |
| C4—C9—C8—C10 | −175.41 (15) | C10—C8—C9—C13 | 6.72 (19) |
| C5—C6—C7—C8 | −3.8 (2) | C11—C12—C13—C9 | 0.84 (19) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C1—H1B···*Cg*3$^{i}$ | 1.00 (3) | 2.84 (3) | 3.714 (3) | 147 (2) |

| | | | | |
|---|---|---|---|---|
| C7—H7···*Cg*2$^{ii}$ | 0.91 (2) | 2.962 (19) | 3.767 (2) | 148.3 (15) |
| C10—H10···*Cg*5$^{ii}$ | 0.99 (2) | 2.960 (19) | 3.427 (2) | 110.1 (13) |

Symmetry codes: (i) $x-1, y, z$; (ii) $-x, y+1/2, -z+5/2$.