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4-(4-Methoxyphenyl)naphtho[2,3-*b*]-thiophene

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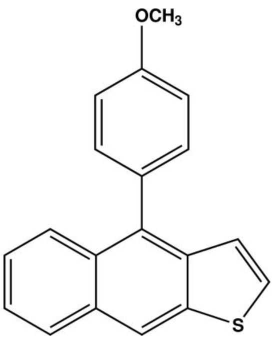
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; disorder in main residue; R factor = 0.054; wR factor = 0.150; data-to-parameter ratio = 13.0.

In the title compound, $C_{19}H_{14}OS$, the naphthothiophene moiety is almost planar except for the S atom of the five-membered ring, which is situated 0.047 (6) Å out of the C_4 plane (with an r.m.s. deviation of fitted atoms = 0.0009 Å). The dihedral angle between the naphthothiophene plane and the attached methoxyphenyl ring is 67.6 (2)°. In the crystal, a C—H$\cdots\pi$ interaction is observed between a methoxyphenyl C—H group and the outer benzene ring of the naphthothiophene moiety. The five-membered ring of the naphthothiophene moiety is disordered, with the S and opposite non-fused C atom approximately exchanging positions, with a site-occupancy factors of 0.808 (3) and 0.187 (3).

Related literature

For related thiophene structures, see: Labat & Halfpenny (2005); Thenmozhi *et al.* (2008). For related heterocyclic compounds, see: Jones *et al.* (1984); Palani *et al.* (2006). For biological activity of naphthothiophenes, see: Zuse *et al.* (2007, 2006); Dallemagne *et al.* (2003); Misra & Amin (1990).



Experimental

Crystal data

$C_{19}H_{14}OS$
M_r = 290.36
Monoclinic, $P2_1/n$
a = 9.2961 (5) Å
b = 15.9931 (7) Å
c = 10.0896 (6) Å
β = 104.580 (3)°
V = 1451.75 (13) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.22 mm^{-1}
T = 293 K
0.30 × 0.20 × 0.20 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
T_{min} = 0.912, T_{max} = 0.961
15008 measured reflections
2553 independent reflections
2223 reflections with $I > 2\sigma(I)$
R_{int} = 0.024

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.054
$wR(F^2)$ = 0.150
S = 1.11
2553 reflections
196 parameters
4 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.33 e Å^{-3}
$\Delta\rho_{min}$ = −0.35 e Å^{-3}

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

Cg is the centroid of the of C5–C10 ring.

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
C17—H17$\cdots Cg^{i}$	0.93	2.82	3.621 (3)	145

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *APEX2* and *SAINT* (Bruker, 2004); data reduction: *SAINT* and *XPREP* (Bruker, 2004); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *Mercury* (Macrae *et al.*, 2008); 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: IM2353).

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supporting information

Acta Cryst. (2012). E**68**, o875–o876 [doi:10.1107/S1600536812005697]

4-(4-Methoxyphenyl)naphtho[2,3-*b*]thiophene

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S1. Comment

Biological evaluation of benzo/naphtho thiophene heterocycles has shown them to act as potential antibiological agents. Naphtho[2,3-*b*]thiophene derivatives were found to exhibit antiproliferative activity related to inhibition of tubulin polymerization (Zuse *et al.* 2007, 2006). Five-membered heterocycles fused to cyclopenta[*c*]thiophene are investigated as new antitumor agents (Dallemagne *et al.* 2003). Benzo[*b*]naphtho[2,1-*d*]thiophene derivatives are found as potentially important metabolites (Misra & Amin, 1990).

Fig. 1 shows the *ORTEP* representation of the molecular structure of the title compound with atoms at the 40% probability level. The five membered ring of the naphtho-thiophene moiety is disordered with sulfur (S1) and carbon (C2) approximately exchanging positions. The two portions of the moiety were assigned variable occupancy factors during refinement with sum of their occupancies restrained as 1 resulting in a refined s.o.f. ratio of 81% and 19%. In the naphtho thiophene moiety, S1 of the five membered ring in the major component is observed 0.047 (6) Å out of the (C1–C4) plane (0.058 (7) Å for the minor component). The latter atoms show a r.m.s. deviation of 0.0009 Å or 0.009 Å for the major and minor component, respectively. The dihedral angle between the mean plane of the naphtho-thiophene moiety and the methoxy-phenyl ring is 67.6 (2)°. Fig. 2 shows the packing of molecules in the unit cell. There is a C—H···π interaction between H17 (symmcode: 1.5 - *x*, -0.5 + *y*, 1.5 - *z*) and the phenyl ring (C5–C10). The distance between the H atom and centroid of the phenyl ring is 2.822 Å. Except for this C—H···π interaction, the packing is featureless.

S2. Experimental

To a solution of (2-(acetoxy(4-methoxyphenyl)methyl)phenyl) (thiophen-2-yl)methylacetate (0.5 g, 1.12 mmol) in anhydrous dichloromethane (20 ml), $BF_3 \times Et_2O$ (40 mg) was added. The reaction mixture was then stirred at room temperature for 4 h under N_2 atmosphere. Removal of the solvent followed by column chromatography (n-hexane/ethyl-acetate 98:2) led to the isolation of the product 4-(4-methoxyphenyl)naphtho[2,3-*b*]thiophene (yield: 56%). The product was recrystallized from chloroform and was obtained as a colourless crystals.

S3. Refinement

As S1 and C2 are disordered, refinement is carried out with a second component for the thiophene ring with atoms C2′, C1′, S1′ located near S1, C1 and C2, respectively. Disordered pairs of the same sites were restrained to have same thermal parameter. The distance C3—S1′ was restrained to be 1.70 Å. Similarily, distances C1—C2′ and C2′—C12 were restrained to be around 1.4 Å and 1.52 Å during the refinement. The two components were assigned variable occupancy factors during refinement with the sum of their occupancies restrained as 1 resulting in a refined s.o.f. ratio of 81% and 19%. H atoms were constrained as riding atoms with d(C—H) = 0.93 Å and $U_{iso}(H) = 1.2U_{eq}(C)$ for aromatic CH groups and 0.96 Å and $U_{iso}(H) = 1.5U_{eq}(C)$ for the methyl group.

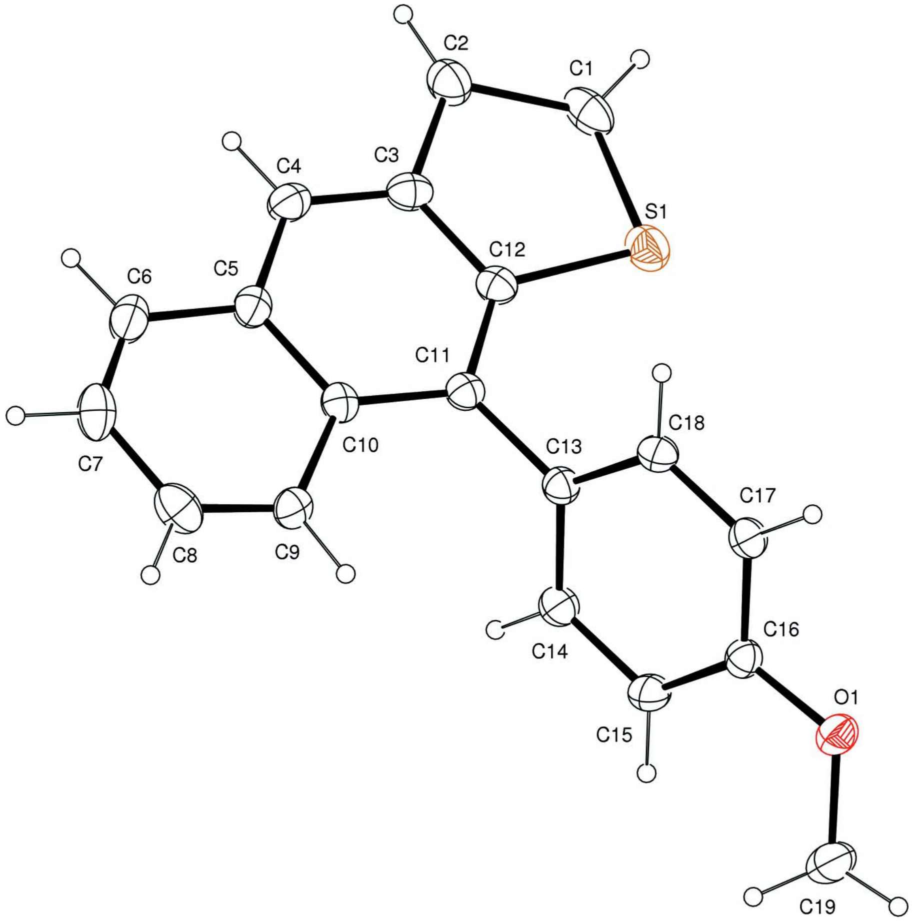

Figure 1

ORTEP plot of the title compound with thermal ellipsoids drawn at the 40% probability level.

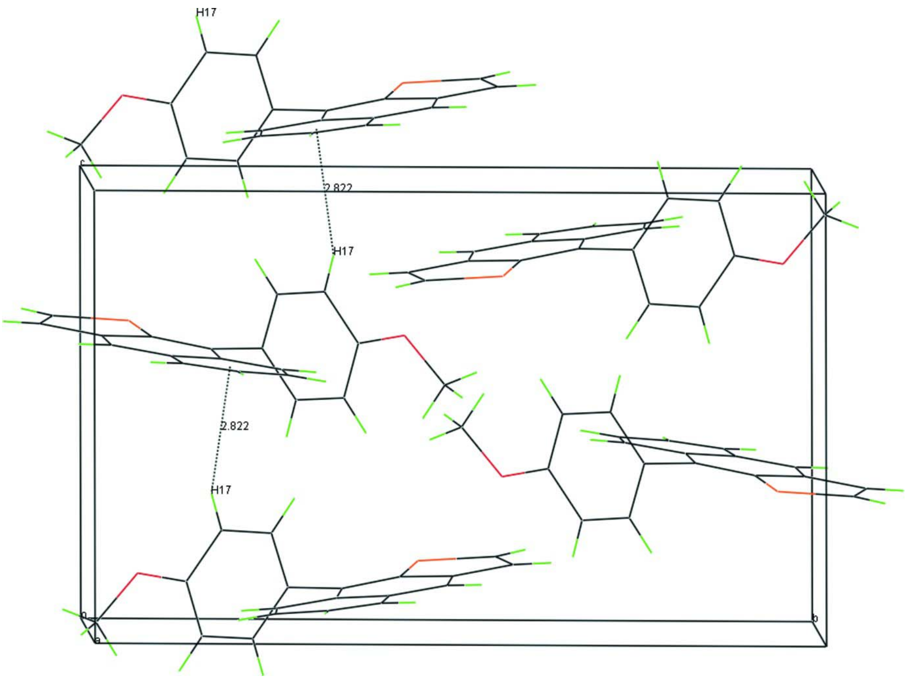

Figure 2

Molecular packing diagram. C—H···π interactions are shown as dotted lines.

4-(4-Methoxyphenyl)naphtho[2,3-*b*]thiophene

Crystal data

$C_{19}H_{14}OS$
$M_r = 290.36$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 9.2961\ (5)$ Å
$b = 15.9931\ (7)$ Å
$c = 10.0896\ (6)$ Å
$\beta = 104.580\ (3)°$
$V = 1451.75\ (13)$ Å^3
$Z = 4$
$F(000) = 608$
$D_x = 1.328$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4322 reflections
$\theta = 2.7–24.5°$
$\mu = 0.22$ mm^{-1}
$T = 293$ K
Block, pale yellow
0.30 × 0.20 × 0.20 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω and φ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
$T_{\min} = 0.912$, $T_{\max} = 0.961$
15008 measured reflections
2553 independent reflections
2223 reflections with $I > 2\sigma(I)$
$R_{\text{int}} = 0.024$
$\theta_{\max} = 25.0°$, $\theta_{\min} = 2.4°$
$h = -11 \rightarrow 11$
$k = -19 \rightarrow 19$
$l = -11 \rightarrow 11$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.054$
$wR(F^2) = 0.150$
$S = 1.11$
2553 reflections
196 parameters
4 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
$w = 1/[\sigma^2(F_o^2) + (0.0618P)^2 + 1.0365P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.33$ e Å^{-3}
$\Delta\rho_{\min} = -0.35$ 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*	$U_{\rm iso}$*/$U_{\rm eq}$	Occ. (<1)
C1	0.5082 (5)	−0.0475 (3)	0.6960 (6)	0.0644 (14)	0.808 (3)
H1	0.4432	−0.0894	0.7079	0.077*	0.808 (3)
C2	0.6679 (6)	−0.0682 (3)	0.6871 (5)	0.0614 (3)	0.808 (3)
H2	0.7162	−0.1196	0.6943	0.074*	0.808 (3)
S1	0.45408 (12)	0.05754 (8)	0.68296 (10)	0.0614 (3)	0.808 (3)
C1′	0.461 (3)	−0.0280 (15)	0.677 (3)	0.0644 (14)	0.187 (3)
H1′	0.3766	−0.0550	0.6898	0.077*	0.187 (3)
C2′	0.4755 (15)	0.0563 (14)	0.646 (3)	0.0614 (3)	0.187 (3)
H2′	0.3939	0.0917	0.6199	0.074*	0.187 (3)
S1′	0.6213 (5)	−0.0676 (3)	0.6865 (5)	0.0614 (3)	0.187 (3)
C3	0.7222 (3)	0.01533 (15)	0.6642 (3)	0.0490 (6)	
C4	0.8635 (3)	0.02564 (16)	0.6515 (3)	0.0515 (6)	
H4	0.9258	−0.0204	0.6564	0.062*	
C5	0.9148 (3)	0.10577 (17)	0.6308 (2)	0.0461 (6)	
C6	1.0633 (3)	0.1195 (2)	0.6226 (3)	0.0605 (8)	
H6	1.1268	0.0741	0.6279	0.073*	
C7	1.1118 (3)	0.1930 (2)	0.6081 (3)	0.0631 (8)	
H7	1.2106	0.1997	0.6059	0.076*	
C8	1.0209 (3)	0.2633 (2)	0.5954 (3)	0.0630 (8)	
H8	1.0603	0.3153	0.5833	0.076*	
C9	0.8833 (3)	0.25843 (16)	0.6001 (2)	0.0452 (6)	
H9	0.8252	0.3064	0.5910	0.054*	
C10	0.8187 (3)	0.17623 (15)	0.6198 (2)	0.0407 (5)	
C11	0.6717 (3)	0.16559 (15)	0.6331 (2)	0.0409 (5)	
C12	0.6285 (3)	0.08554 (15)	0.6572 (2)	0.0437 (6)	

C13	0.5697 (2)	0.23754 (15)	0.6292 (2)	0.0409 (5)
C14	0.5147 (3)	0.28478 (16)	0.5126 (3)	0.0484 (6)
H14	0.5416	0.2712	0.4325	0.058*
C15	0.4202 (3)	0.35206 (17)	0.5124 (3)	0.0490 (6)
H15	0.3842	0.3830	0.4328	0.059*
C16	0.3800 (3)	0.37276 (15)	0.6307 (2)	0.0426 (6)
C17	0.4321 (3)	0.32557 (16)	0.7474 (3)	0.0461 (6)
H17	0.4038	0.3387	0.8269	0.055*
C18	0.5258 (3)	0.25921 (16)	0.7463 (2)	0.0457 (6)
H18	0.5606	0.2281	0.8259	0.055*
C19	0.2441 (4)	0.4937 (2)	0.5322 (3)	0.0717 (9)
H19A	0.3303	0.5160	0.5086	0.107*
H19B	0.1878	0.5385	0.5576	0.107*
H19C	0.1838	0.4645	0.4548	0.107*
O1	0.2893 (2)	0.43755 (11)	0.64381 (19)	0.0548 (5)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.057 (4)	0.077 (3)	0.056 (3)	−0.031 (2)	0.010 (3)	0.005 (2)
C2	0.0525 (6)	0.0696 (6)	0.0625 (7)	−0.0089 (4)	0.0150 (4)	0.0068 (5)
S1	0.0525 (6)	0.0696 (6)	0.0625 (7)	−0.0089 (4)	0.0150 (4)	0.0068 (5)
C1′	0.057 (4)	0.077 (3)	0.056 (3)	−0.031 (2)	0.010 (3)	0.005 (2)
C2′	0.0525 (6)	0.0696 (6)	0.0625 (7)	−0.0089 (4)	0.0150 (4)	0.0068 (5)
S1′	0.0525 (6)	0.0696 (6)	0.0625 (7)	−0.0089 (4)	0.0150 (4)	0.0068 (5)
C3	0.0631 (16)	0.0428 (14)	0.0391 (13)	0.0014 (12)	0.0091 (11)	0.0000 (10)
C4	0.0606 (16)	0.0466 (14)	0.0472 (14)	0.0126 (12)	0.0137 (12)	0.0023 (12)
C5	0.0438 (13)	0.0570 (15)	0.0371 (13)	0.0057 (11)	0.0094 (10)	−0.0017 (11)
C6	0.0478 (15)	0.080 (2)	0.0544 (17)	0.0155 (15)	0.0140 (12)	0.0006 (15)
C7	0.0409 (14)	0.084 (2)	0.0650 (18)	−0.0075 (14)	0.0153 (13)	−0.0171 (16)
C8	0.074 (2)	0.0624 (18)	0.0568 (17)	−0.0210 (15)	0.0235 (15)	−0.0096 (14)
C9	0.0533 (15)	0.0466 (14)	0.0373 (12)	0.0071 (11)	0.0145 (11)	−0.0074 (10)
C10	0.0422 (12)	0.0470 (13)	0.0331 (11)	−0.0018 (10)	0.0096 (9)	−0.0044 (10)
C11	0.0443 (13)	0.0436 (13)	0.0341 (12)	0.0007 (10)	0.0085 (10)	−0.0003 (10)
C12	0.0447 (13)	0.0463 (14)	0.0378 (12)	−0.0039 (11)	0.0062 (10)	0.0018 (10)
C13	0.0390 (12)	0.0432 (13)	0.0406 (13)	−0.0014 (10)	0.0101 (10)	0.0012 (10)
C14	0.0562 (15)	0.0538 (15)	0.0377 (13)	0.0060 (12)	0.0165 (11)	0.0018 (11)
C15	0.0533 (14)	0.0518 (15)	0.0405 (13)	0.0071 (12)	0.0091 (11)	0.0084 (11)
C16	0.0380 (12)	0.0423 (13)	0.0470 (14)	−0.0008 (10)	0.0100 (10)	−0.0010 (11)
C17	0.0497 (14)	0.0503 (14)	0.0408 (13)	0.0018 (11)	0.0162 (11)	−0.0008 (11)
C18	0.0496 (14)	0.0489 (14)	0.0383 (13)	0.0030 (11)	0.0105 (11)	0.0062 (11)
C19	0.081 (2)	0.0627 (19)	0.073 (2)	0.0271 (16)	0.0225 (17)	0.0152 (16)
O1	0.0584 (11)	0.0520 (11)	0.0562 (11)	0.0144 (9)	0.0185 (9)	0.0041 (9)

Geometric parameters (Å, º)

C1—C2	1.545 (6)	C8—C9	1.294 (4)
C1—S1	1.749 (5)	C8—H8	0.9300

C1—H1	0.9300	C9—C10	1.479 (3)
C2—C3	1.468 (5)	C9—H9	0.9300
C2—H2	0.9300	C10—C11	1.417 (3)
S1—C12	1.764 (3)	C11—C12	1.381 (3)
C1′—C2′	1.399 (10)	C11—C13	1.486 (3)
C1′—S1′	1.60 (3)	C13—C14	1.384 (3)
C1′—H1′	0.9300	C13—C18	1.387 (3)
C2′—C12	1.474 (10)	C14—C15	1.389 (4)
C2′—H2′	0.9300	C14—H14	0.9300
S1′—C3	1.673 (5)	C15—C16	1.378 (4)
C3—C4	1.362 (4)	C15—H15	0.9300
C3—C12	1.412 (4)	C16—O1	1.363 (3)
C4—C5	1.401 (4)	C16—C17	1.379 (3)
C4—H4	0.9300	C17—C18	1.375 (3)
C5—C6	1.420 (4)	C17—H17	0.9300
C5—C10	1.425 (3)	C18—H18	0.9300
C6—C7	1.281 (4)	C19—O1	1.419 (3)
C6—H6	0.9300	C19—H19A	0.9600
C7—C8	1.392 (4)	C19—H19B	0.9600
C7—H7	0.9300	C19—H19C	0.9600

C2—C1—S1	117.7 (4)	C11—C10—C5	119.9 (2)
C2—C1—H1	121.2	C11—C10—C9	123.6 (2)
S1—C1—H1	121.2	C5—C10—C9	116.4 (2)
C3—C2—C1	100.8 (4)	C12—C11—C10	117.3 (2)
C3—C2—H2	129.6	C12—C11—C13	120.7 (2)
C1—C2—H2	129.6	C10—C11—C13	122.0 (2)
C1—S1—C12	89.8 (2)	C11—C12—C3	122.9 (2)
C2′—C1′—S1′	105 (2)	C11—C12—C2′	126.8 (10)
C2′—C1′—H1′	127.7	C3—C12—C2′	108.8 (10)
S1′—C1′—H1′	127.7	C11—C12—S1	125.5 (2)
C1′—C2′—C12	115.9 (19)	C3—C12—S1	111.67 (19)
C1′—C2′—H2′	122.1	C2′—C12—S1	13.0 (10)
C12—C2′—H2′	122.1	C14—C13—C18	117.6 (2)
C1′—S1′—C3	103.0 (9)	C14—C13—C11	122.8 (2)
C4—C3—C12	119.8 (2)	C18—C13—C11	119.6 (2)
C4—C3—C2	120.3 (3)	C13—C14—C15	121.5 (2)
C12—C3—C2	120.0 (3)	C13—C14—H14	119.2
C4—C3—S1′	134.1 (3)	C15—C14—H14	119.2
C12—C3—S1′	106.1 (3)	C16—C15—C14	119.6 (2)
C2—C3—S1′	13.9 (3)	C16—C15—H15	120.2
C3—C4—C5	119.8 (2)	C14—C15—H15	120.2
C3—C4—H4	120.1	O1—C16—C15	125.2 (2)
C5—C4—H4	120.1	O1—C16—C17	115.2 (2)
C4—C5—C6	121.5 (3)	C15—C16—C17	119.6 (2)
C4—C5—C10	120.3 (2)	C18—C17—C16	120.2 (2)
C6—C5—C10	118.2 (3)	C18—C17—H17	119.9
C7—C6—C5	121.6 (3)	C16—C17—H17	119.9

C7—C6—H6	119.2
C5—C6—H6	119.2
C6—C7—C8	121.9 (3)
C6—C7—H7	119.1
C8—C7—H7	119.1
C9—C8—C7	122.1 (3)
C9—C8—H8	119.0
C7—C8—H8	119.0
C8—C9—C10	119.8 (2)
C8—C9—H9	120.1
C10—C9—H9	120.1
C17—C18—C13	121.5 (2)
C17—C18—H18	119.3
C13—C18—H18	119.3
O1—C19—H19A	109.5
O1—C19—H19B	109.5
H19A—C19—H19B	109.5
O1—C19—H19C	109.5
H19A—C19—H19C	109.5
H19B—C19—H19C	109.5
C16—O1—C19	118.1 (2)

S1—C1—C2—C3	−1.9 (5)
C2—C1—S1—C12	2.4 (4)
S1′—C1′—C2′—C12	−11 (3)
C2′—C1′—S1′—C3	4 (2)
C1—C2—C3—C4	179.4 (3)
C1—C2—C3—C12	0.2 (4)
C1—C2—C3—S1′	−5.9 (12)
C1′—S1′—C3—C4	−174.8 (13)
C1′—S1′—C3—C12	4.3 (13)
C1′—S1′—C3—C2	179 (2)
C12—C3—C4—C5	−0.3 (4)
C2—C3—C4—C5	−179.4 (3)
S1′—C3—C4—C5	178.8 (3)
C3—C4—C5—C6	177.4 (2)
C3—C4—C5—C10	−1.5 (4)
C4—C5—C6—C7	−177.8 (3)
C10—C5—C6—C7	1.2 (4)
C5—C6—C7—C8	−1.9 (5)
C6—C7—C8—C9	1.2 (5)
C7—C8—C9—C10	0.2 (4)
C4—C5—C10—C11	1.5 (3)
C6—C5—C10—C11	−177.4 (2)
C4—C5—C10—C9	179.2 (2)
C6—C5—C10—C9	0.2 (3)
C8—C9—C10—C11	176.7 (2)
C8—C9—C10—C5	−0.9 (3)
C5—C10—C11—C12	0.3 (3)
C9—C10—C11—C12	−177.2 (2)
C5—C10—C11—C13	177.0 (2)
C9—C10—C11—C13	−0.5 (3)
C10—C11—C12—C3	−2.1 (3)
C13—C11—C12—C3	−178.9 (2)
C10—C11—C12—C2′	−166.3 (12)
C13—C11—C12—C2′	17.0 (13)
C10—C11—C12—S1	177.76 (18)
C13—C11—C12—S1	1.0 (3)
C4—C3—C12—C11	2.2 (4)
C2—C3—C12—C11	−178.7 (3)
S1′—C3—C12—C11	−177.1 (3)
C4—C3—C12—C2′	168.8 (11)
C2—C3—C12—C2′	−12.0 (11)
S1′—C3—C12—C2′	−10.5 (11)
C4—C3—C12—S1	−177.7 (2)
C2—C3—C12—S1	1.4 (3)
S1′—C3—C12—S1	3.0 (3)
C1′—C2′—C12—C11	−179.4 (19)
C1′—C2′—C12—C3	15 (3)
C1′—C2′—C12—S1	−90 (5)
C1—S1—C12—C11	178.0 (3)
C1—S1—C12—C3	−2.1 (3)
C1—S1—C12—C2′	78 (4)
C12—C11—C13—C14	−116.0 (3)
C10—C11—C13—C14	67.3 (3)
C12—C11—C13—C18	63.7 (3)
C10—C11—C13—C18	−112.9 (3)
C18—C13—C14—C15	0.7 (4)
C11—C13—C14—C15	−179.6 (2)
C13—C14—C15—C16	0.1 (4)
C14—C15—C16—O1	179.5 (2)
C14—C15—C16—C17	−1.1 (4)
O1—C16—C17—C18	−179.3 (2)
C15—C16—C17—C18	1.2 (4)
C16—C17—C18—C13	−0.4 (4)
C14—C13—C18—C17	−0.5 (4)
C11—C13—C18—C17	179.7 (2)
C15—C16—O1—C19	−6.8 (4)
C17—C16—O1—C19	173.7 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C17—H17···*Cg*^{i}	0.93	2.82	3.621 (3)	145

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