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Crystal structure of 6-(*p*-tolyl)benzo[*b*]naphtho-[2,3-*d*]thiophene and of an orthorhombic polymorph of 7-phenylanthra[2,3-*b*]benzo[*d*]thiophene

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CCDC references: 1498519; 1498518

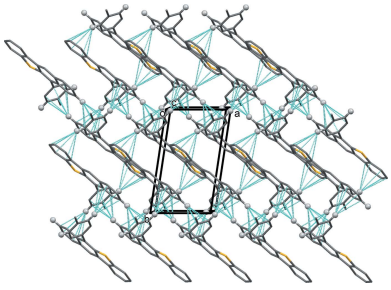
Supporting information: this article has supporting information at journals.iucr.org/e

The title compounds, $C_{23}H_{16}S$, (I), and $C_{26}H_{16}S$, (II), are benzothiophene derivatives in which the benzothiophene moiety is fused with a naphthalene ring system in (I), and with an anthracene ring system in (II). In (I), the mean plane of the benzothiophene ring system makes a dihedral angle of 2.28 (6)° with the naphthalene ring system, and a dihedral angle of 1.28 (6)° with the anthracene ring system in (II), showing that the fused units are essentially planar. In (I), the 4-methylbenzene ring substituent makes a dihedral angle of 71.40 (9)° with the naphthalene ring system, while the phenyl ring substituent in (II) makes a dihedral angle of 67.08 (12)° with the anthracene ring system. In the crystals of both compounds, molecules are linked by C—H···π interactions, leading to the formation of slabs parallel to (001) in (I) and to zigzag chains along [001] in (II). There are also offset π–π interactions present within the slabs in (I). In the crystal of (II), they link the chains, forming sheets parallel to (010). The triclinic polymorph of compound (II) has been reported [Sivasakthikumaran *et al.*, (2012). *J. Org. Chem.* **77**, 9053–9071].

1. Chemical context

The thiophene nucleus has been shown to be an important heterocyclic unit in compounds possessing promising pharmacological characteristics, such as anti-HIV PR inhibitors (Bonini *et al.*, 2005) and anti-breast cancer (Brault *et al.*, 2005) activities. Benzothiophenes are important biologically active molecules. One of the most important drugs based on the benzothiophene system is Raloxifine, used for the prevention and treatment of osteoporosis in postmenopausal women (Jordan, 2003). Benzothiophenes are also present in luminescent components used in organic materials (Russell & Press, 1996).

Naphtho[2,3-*b*]thiophene derivatives have been found to exhibit antiproliferative activity related to the inhibition of tublin polymerization (Zuse *et al.*, 2007, 2006). As a result of their outstanding electronic testability and considerable chemical and environmental stability, thiophene derivatives have been widely used in solar cells (Justin Thomas *et al.*, 2008; Hänsel *et al.*, 2003), organic light-emitting diodes (OLEDs) (Mazzeo *et al.*, 2003), organic field-effect transistors (OFETs) (Zhan *et al.*, 2007) and as NLO devices (Bedworth *et al.*, 1996; Raposo *et al.*, 2011).Against this background, we describe herein the syntheses and crystal structures of the title benzothiophene derivatives.



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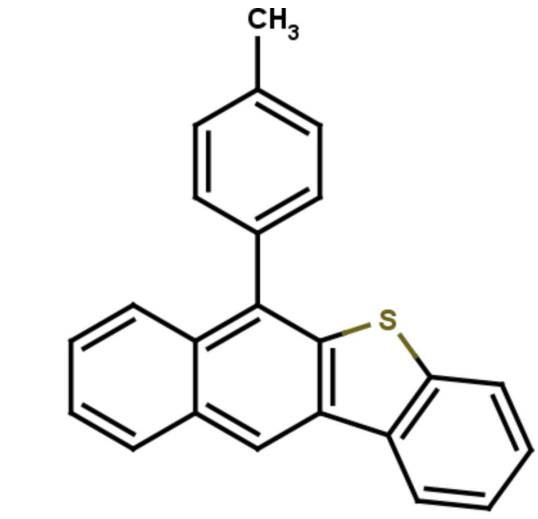
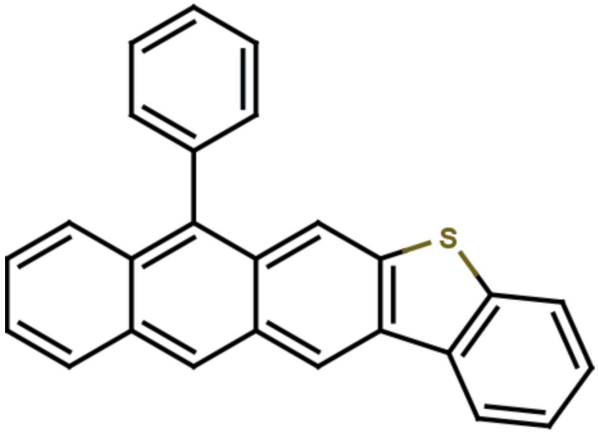


(I)



(II)

2. Structural commentary

The molecular structures of the title compounds, (I) and (II), are illustrated in Figs. 1 and 2, respectively. In both compounds, the benzothiophene ring systems are almost planar with the dihedral angles between the benzene and thiophene rings being 1.85 (11)° in (I) and 0.56 (18)° in (II).

In compound (I), the naphthalene ring system (atoms C1–C3/C10–C16) (r.m.s. deviation = 0.006 Å) makes a a dihedral angle of 2.28 (6)° with the benzothiophene (C3–C10/S1) ring system (r.m.s. deviation = 0.023 Å). The 4-methylbenzene ring substituent (C17–C22) makes a dihedral angle of 71.40 (9)° with the naphthalene ring system

In compound (II), the anthracene ring system (C1–C3/C10–C20) is almost planar (r.m.s. deviation = 0.075 Å) and makes a a dihedral angle of 7.31 (9)° with the benzothiophene (C3–C10/S1) ring system (r.m.s. deviation = 0.012 Å). Here, the phenyl ring substituent (C21–C26) in (II) makes a dihedral angle of 67.08 (12)° with the anthracene ring system, and the anthracene ring is (−)antiperiplanar with respect to the

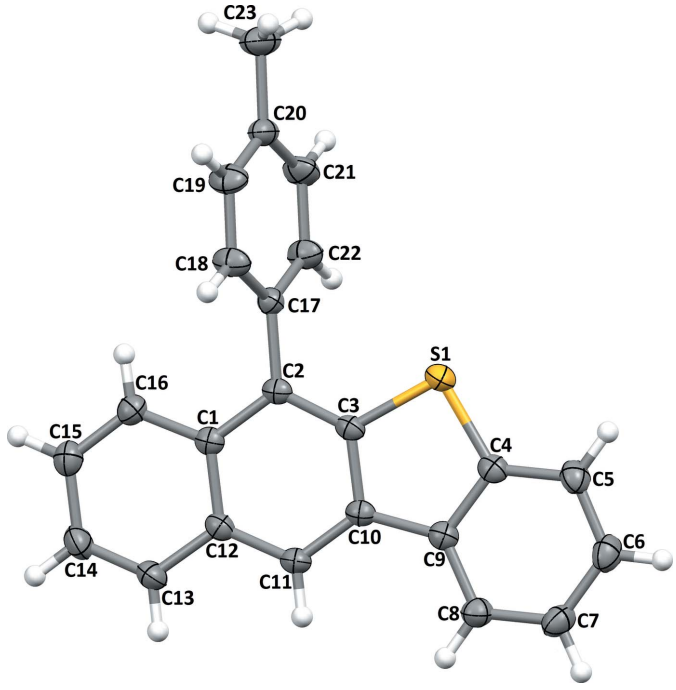


Figure 1
The molecular structure of compound (I), showing the atom labelling. Displacement ellipsoids are drawn at the 30% probability level.

benzothiophene moiety, as indicated by the S1—C3—C10—C11 torsion angle of −176.4 (2)°.

In the triclinic polymorph of compound (II) (Sivasakthikumaran *et al.*, 2012), the major component of the disordered phenyl ring substituent makes a dihedral angle of 79.39 (12)° with the anthracene ring system.

3. Supramolecular features

In the crystals of both compounds, molecules are linked by C—H···π interactions (see Tables 1 and 2), leading to the

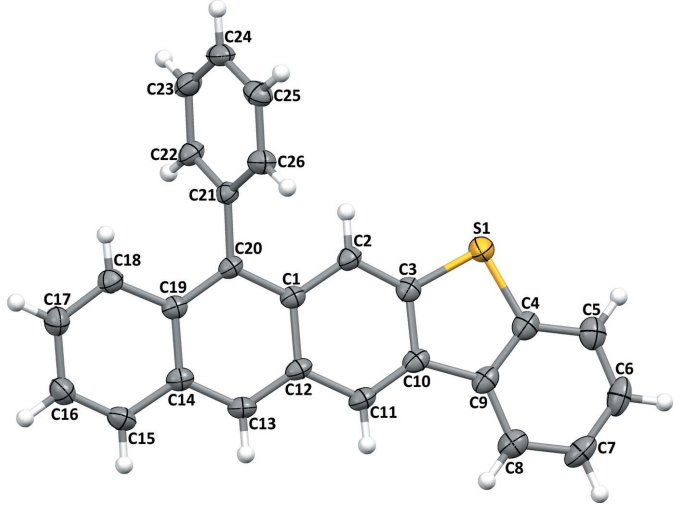


Figure 2
The molecular structure of compound (II), showing the atom labelling. Displacement ellipsoids are drawn at the 30% probability level.

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

*Cg*3, *Cg*4 and *Cg*5 are the centroids of rings (C1/C12–C16), (C4–C6) and (C17–C22), respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C15—H15···*Cg*5^{i}	0.93	2.94	3.763 (3)	148
C19—H19···*Cg*4^{ii}	0.93	2.94	3.753 (3)	147
C21—H21···*Cg*3^{iii}	0.93	2.91	3.721 (3)	146

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

Table 2
Hydrogen-bond geometry (Å, °) for (II).

*Cg*2 and *Cg*3 are the centroids of rings (C1–C3/C10–C12) and (C1/C12–C14/C19/C20), respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C13—H13···*Cg*2^{i}	0.93	2.97	3.885 (4)	168
C15—H15···*Cg*3^{i}	0.93	2.57	3.479 (4)	166

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

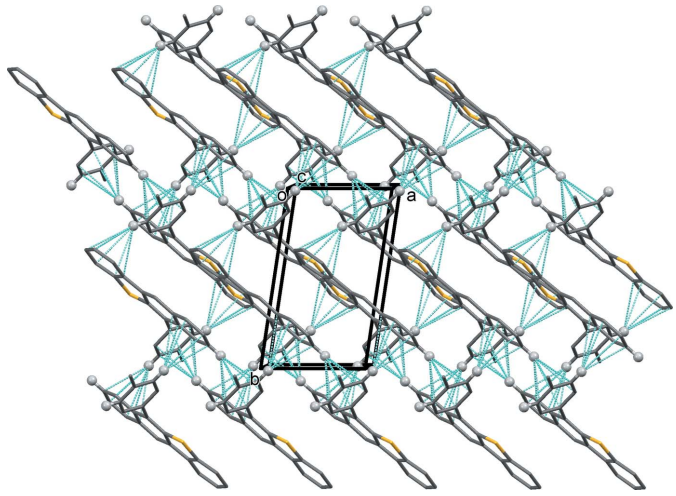


Figure 5
The crystal packing of compound (I), viewed along the *c* axis, showing the C—H···π interactions (represented as turquoise lines) leading to the formation of slabs parallel to (001).

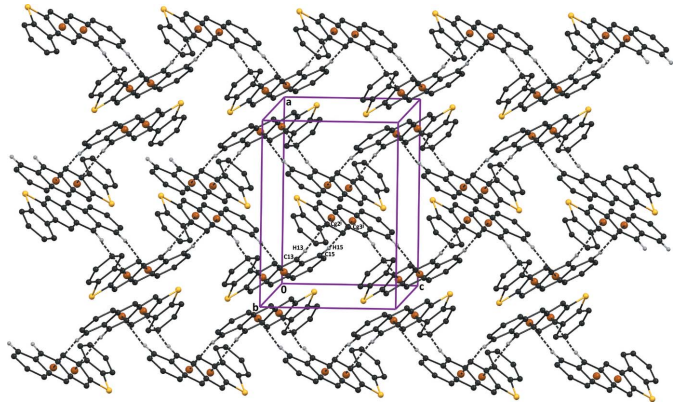


Figure 4
The crystal packing of compound (II), viewed along the *b* axis. The C—H···π interactions are shown as dashed lines (see Table 2 for details) and the centroids as brown balls. H atoms not involved in these interactions have been omitted for clarity.

formation of slabs parallel to (001) in (I), and to zigzag chains along [001] in (II); as illustrated in Figs. 3, 4 and 5. There are also offset π–π interactions present within the slabs in (I) [*Cg*1···*Cg*3^{i} = 3.629 (1) Å, interplanar distance = 3.602 (1) Å, slippage = 0.49 Å; *Cg*2···*Cg*4^{ii} = 3.983 (1), interplanar distance = 3.473 (1), slippage 1.79 Å; *Cg*1, *Cg*2, *Cg*3 and *Cg*4 are the centroids of rings S1/C3/C4/C9/C10, C1–C3/C10–C12, C1/C12–C16 and C4–C9, respectively; symmetry codes: (i) $x+1, y, z$; (ii) $x-1, y, z$]. In the crystal of (II), offset π–π interactions link the chains, forming sheets parallel to (010) [*Cg*2···*Cg*4^{iii} = 3.711 (2) Å, interplanar distance = 3.479 (1) Å, slippage = 1.21 Å; *Cg*3···*Cg*4^{iii} = 3.741 (2) Å, interplanar distance = 3.443 (1) Å, slippage = 1.22 Å; *Cg*2, *Cg*3 and *Cg*4 are the centroids of rings C1–C3/C10–C12, C1/C12–C16 and C4–C9, respectively; symmetry code: (iii) $-x+1, -y+1, -z+1$].

4. Database survey

A search of the Cambridge Structural Database (Version 5.38, update May 2016; Groom *et al.*, 2016) for the naphthobenzothiophene skeleton gave 32 hits. Among these there are five naphthobenzothiophene derivatives that resemble compound

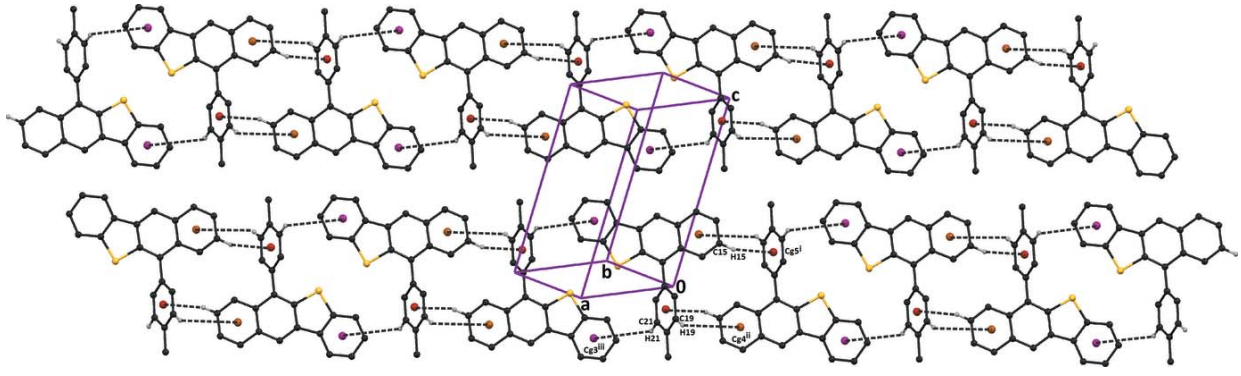


Figure 3
The crystal packing of compound (I). The C—H···π interactions are shown as dashed lines (see Table 1 for details). H atoms not involved in these interactions have been omitted for clarity.

Table 3
Experimental details.

	(I)	(II)
Crystal data		
Chemical formula	$C_{23}H_{16}S$	$C_{26}H_{16}S$
M_r	324.42	360.45
Crystal system, space group	Triclinic, $P\overline{1}$	Orthorhombic, *Pccn*
Temperature (K)	296	296
a, b, c (Å)	6.2404 (3), 11.1725 (6), 12.9987 (7)	12.2159 (8), 33.1138 (4), 8.8993 (5)
α, β, γ (°)	109.284 (2), 100.233 (4), 93.925 (2)	90, 90, 90
V (Å^3)	833.90 (8)	3599.9 (3)
Z	2	8
Radiation type	Mo $K\alpha$	Mo $K\alpha$
μ (mm^{-1})	0.19	0.19
Crystal size (mm)	0.30 × 0.25 × 0.20	0.30 × 0.25 × 0.25
Data collection		
Diffractometer	Bruker Kappa APEXII CCD	Bruker Kappa APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2008)	Multi-scan (*SADABS*; Bruker, 2008)
T_{min}, T_{max}	0.944, 0.962	0.946, 0.955
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	15861, 2944, 2407	43542, 3171, 2540
R_{int}	0.024	0.036
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.595	0.595
Refinement		
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.039, 0.113, 1.07	0.059, 0.182, 1.04
No. of reflections	2944	3171
No. of parameters	218	244
H-atom treatment	H-atom parameters constrained	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.21, −0.21	1.06, −0.40

Computer programs: *APEX2* and *SAINT* (Bruker, 2008), *SHELXS97* and *SHELXL97* (Sheldrick, 2008), *ORTEP-3 for Windows* (Farrugia, 2012), *Mercury* (Macrae *et al.*, 2008) and *PLATON* (Spek, 2009).

(I), *viz.* 6-(phenyl)benzo[*b*]naphtho[2,3-*d*]thiophene (NEQMAZ; Silambarasan *et al.*, 2013), 6-(4-methoxyphenyl)benzo[*b*]naphtho[2,3-*d*]thiophene (PECQEV; Silambarasan *et al.*, 2012), 6-(2-thienyl)benzo[*b*]naphtho[2,3-*d*]-thiophene (XIMZUQ; Sivasakthikumaran *et al.*, 2012), 6-(1-benzothiophen-3-yl)benzo[*b*]naphtho[2,3-*d*]thiophene (HIXQUB; Li *et al.*, 2007) and 1,3-dimethylbenzo[*b*]-naphtho[2,3-*d*]thiophene (ROMPUF/ROMPUF01; Umarani *et al.*, 2009/Dhayalan *et al.*, 2009). There are also two anthracene analogues, *viz.* anthra[2,3-*b*]benzo[*d*]thiophene itself (JOHSOP; Du *et al.*, 2008), and 7-(1-benzothiophen-2-yl)anthra[2,3-*b*]benzo[*d*]thiophene (FOLGEU; Rafiq *et al.*, 2014); as well as the triclinic polymorph of compound (II) (XIMZOK; Sivasakthikumaran *et al.*, 2012).

5. Synthesis and crystallization

Compound (I)

The reduction of the diketone (benzothiophen-3-yl)[2-(4-methylbenzoyl)phenyl]methanone (0.85 g, 2.38 mmol) using sodium borohydride (0.49 g, 12.89 mmol) followed by work-up gave the diol. Dipivaloylation of the diol (0.77 g, 2.31 mmol) using pivaloyl chloride (1.39 g, 11.52 mmol) and triethylamine (4.69 g, 45.20 mmol) in the presence of a catalytic amount of DMAP (10 mg) in dry DCM (20 ml) led to the isolation of dipivalate (benzo[*b*]thiophen-3-yl){2-[pivaloyloxy(*p*-tolyl) methyl]phenyl}methyl pivalate as a viscous liquid. Dipivalate (benzo[*b*]thiophen-3-yl){2-[pivaloyloxy(*p*-toyl) methyl]phenyl}methyl pivalate (0.98 g, 1.96 mmol) upon interaction with $ZnBr_2$ (0.02 g, 0.13 mmol) followed by removal of solvent and column chromatographic purification (silica gel; hexane–ethyl acetate, 99:1) gave 6-(*p*-tolyl)benzo[*b*]naphtho[2,3-*d*]thiophene as a pale-green solid (yield 0.53 g, 78%). Single crystals suitable for X-ray diffraction were prepared by slow evaporation of a solution of (I) in ethyl acetate at room temperature (m.p. 391–393 K).

Compound (II)

The reduction of the diketone (2-benzoylphenyl)-(dibenzo[*b*,*d*]thiophen-2-yl)methanone (1.11 g, 2.38 mmol) using sodium borohydride (0.53 g, 13.94 mmol) followed by work-up gave the diol. Dipivaloylation of the diol (1.12 g, 2.82 mmol) using pivaloyl chloride (1.70 g, 14.14 mmol) and triethylamine (5.72 g, 56.56 mmol) in the presence of a catalytic amount of DMAP (10 mg) in dry DCM (20 ml) led to the isolation of dipivalate (dibenzo[*b*,*d*]thiophen-2-yl){2-[phenyl(pivaloyloxy)methyl]phenyl}methyl pivalate as a thick liquid. Dipivalate (dibenzo[*b*,*d*]thiophen-2-yl){2-[phenyl(pivaloyloxy)methyl]phenyl}methyl pivalate (1.28 g, 2.26 mmol) upon interaction with $ZnBr_2$ (0.02 g, 0.13 mmol) followed by removal of solvent and column chromatographic purification (silica gel; hexane–ethyl acetate, 99:1) gave a new orthorhombic polymorph of 7-phenylanthra[2,3-*b*]benzo-[*d*]thiophene (yield 0.83 g, 72%) as a yellow solid. Single crystals suitable for X-ray diffraction were prepared by slow evaporation of a solution of the compound (II) in ethyl acetate at room temperature (m.p. 463–465 K).

6. Refinement

Crystal data, data collection and structure refinement details for compounds (I) and (II) are summarized in Table 3. The C-bound H atoms were included in calculated positions and treated as riding atoms, with C—H = 0.93–0.96 Å and with U_{iso}(H) = 1.5U_{eq}(methyl C) and 1.2U_{eq}(C) for other H atoms.

Acknowledgements

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References

Bedworth, P. V., Cai, Y., Jen, A. & Marder, S. R. (1996). *J. Org. Chem.* **61**, 2242–2246.
Bonini, C., Chiummiento, L., Bonis, M. D., Funicello, M., Lupattelli, P., Suanno, G., Berti, F. & Campaner, P. (2005). *Tetrahedron*, **61**, 6580–6589.
Brault, L., Migianu, E., Néguesque, A., Battaglia, E., Bagrel, D. & Kirsch, G. (2005). *Eur. J. Med. Chem.* **40**, 757–763.
Bruker (2008). *APEX2*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Dhayalan, V., Clement, J. A., Jagan, R. & Mohanakrishnan, A. K. (2009). *Eur. J. Org. Chem.* pp. 531–546.
Du, C., Guo, Y., Liu, Y., Qiu, W., Zhang, H., Gao, X., Liu, Y., Qi, T., Lu, K. & Yu, G. (2008). *Chem. Mater.* **20**, 4188–4190.
Farrugia, L. J. (2012). *J. Appl. Cryst.* **45**, 849–854.
Groom, C. R., Bruno, I. J., Lightfoot, M. P. & Ward, S. C. (2016). *Acta Cryst.* B**72**, 171–179.
Hänsel, H., Zettl, H., Krausch, G., Kisselev, R., Thelakkat, M. & Schmidt, H. W. (2003). *Adv. Mater.* **15**, 2056–2060.
Jordan, V. C. (2003). *J. Med. Chem.* **46**, 1081–1111.
Justin Thomas, K. R., Hsu, Y. C., Lin, J. T., Lee, K. M., Ho, K. C., Lai, C. H., Cheng, Y. M. & Chou, P. T. (2008). *Chem. Mater.* **20**, 1830–1840.
Li, G., Zhou, S., Su, G., Liu, Y. & Wang, P. G. (2007). *J. Org. Chem.* **72**, 9830–9833.
Macrae, C. F., Bruno, I. J., Chisholm, J. A., Edgington, P. R., McCabe, P., Pidcock, E., Rodriguez-Monge, L., Taylor, R., van de Streek, J. & Wood, P. A. (2008). *J. Appl. Cryst.* **41**, 466–470.
Mazzeo, M., Vitale, V., Della Sala, F., Pisignano, D., Anni, M., Barbarella, G., Favaretto, L., Zanelli, A., Cingolani, R. & Gigli, G. (2003). *Adv. Mater.* **15**, 2060–2063.
Rafiq, S. M., Sivasakthikumaran, R. & Mohanakrishnan, A. K. (2014). *Org. Lett.* **16**, 2720–2723.
Raposo, M. M. M., Fonseca, A. M. C., Castro, M. C. R., Belsley, M., Cardoso, M. F. S., Carvalho, L. M. & Coelho, P. J. (2011). *Dyes Pigments*, **91**, 62–73.
Russell, R. K. & Press, J. B. (1996). *Comprehensive Heterocyclic Chemistry II*, Vol. 2, edited by A. R. Katritzky, C. W. Rees & E. F. V. Scriven. pp. 679–729. Oxford: Pergamon Press.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Silambarasan, V., Srinivasan, T., Sivasakthikumaran, R., Mohanakrishnan, A. K. & Velmurugan, D. (2012). *Acta Cryst.* E**68**, o3408–o3409.
Silambarasan, V., Srinivasan, T., Sivasakthikumaran, R., Mohanakrishnan, A. K. & Velmurugan, D. (2013). *Acta Cryst.* E**69**, o36.
Sivasakthikumaran, R., Nandakumar, M. & Mohanakrishnan, A. K. (2012). *J. Org. Chem.* **77**, 9053–9071.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.
Zhan, X., Tan, Z.-A., Domercq, B., An, Z., Zhang, X., Barlow, S., Li, Y.-F., Zhu, D.-B., Kippelen, B. & Marder, S. R. (2007). *J. Am. Chem. Soc.* **129**, 7246–7247.
Zuse, A., Schmidt, P., Baasner, S., Böhm, K. J., Müller, K., Gerlach, M., Günther, E. G., Unger, E. & Prinz, H. (2006). *J. Med. Chem.* **49**, 7816–7825.
Zuse, A., Schmidt, P., Baasner, S., Böhm, K. J., Müller, K., Gerlach, M., Günther, E. G., Unger, E. & Prinz, H. (2007). *J. Med. Chem.* **50**, 6059–6066.

supporting information

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Crystal structure of 6-(*p*-tolyl)benzo[*b*]naphtho[2,3-*d*]thiophene and of an orthorhombic polymorph of 7-phenylanthra[2,3-*b*]benzo[*d*]thiophene

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Computing details

For both compounds, data collection: *APEX2* (Bruker, 2008); cell refinement: *SAINT* (Bruker, 2008); data reduction: *SAINT* (Bruker, 2008); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012) and *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *SHELXL97* (Sheldrick, 2008) and *PLATON* (Spek, 2009).

(I) 6-(*p*-Tolyl)benzo[*b*]naphtho[2,3-*d*]thiophene

Crystal data

$C_{23}H_{16}S$
$M_r = 324.42$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 6.2404$ (3) Å
$b = 11.1725$ (6) Å
$c = 12.9987$ (7) Å
$\alpha = 109.284$ (2)°
$\beta = 100.233$ (4)°
$\gamma = 93.925$ (2)°
$V = 833.90$ (8) Å^3
$Z = 2$
$F(000) = 340$
$D_x = 1.292$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2944 reflections
$\theta = 2.1$–25.0°
$\mu = 0.19$ mm^{-1}
$T = 296$ K
Block, colourless
0.30 × 0.25 × 0.20 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω & φ scans
Absorption correction: multi-scan (SADABS; Bruker, 2008)
$T_{min} = 0.944$, $T_{max} = 0.962$
15861 measured reflections
2944 independent reflections
2407 reflections with $I > 2\sigma(I)$
$R_{int} = 0.024$
$\theta_{max} = 25.0°$, $\theta_{min} = 2.1°$
$h = -7 \rightarrow 7$
$k = -13 \rightarrow 13$
$l = -15 \rightarrow 15$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.039$
$wR(F^2) = 0.113$
$S = 1.07$
2944 reflections
218 parameters
0 restraints
Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map	$w = 1/[\sigma^2(F_o^2) + (0.0484P)^2 + 0.4189P]$ where $P = (F_o^2 + 2F_c^2)/3$
Hydrogen site location: inferred from neighbouring sites	$(\Delta/\sigma)_{max} = 0.002$
H-atom parameters constrained	$\Delta\rho_{max} = 0.21$ e Å^{-3}
	$\Delta\rho_{min} = -0.21$ 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. 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 $F^2 > 2\text{sigma}(F^2)$ 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}
C1	−0.1614 (3)	0.24648 (18)	0.15929 (16)	0.0358 (4)
C2	−0.0247 (3)	0.27515 (17)	0.09112 (15)	0.0344 (4)
C3	0.1606 (3)	0.36306 (18)	0.14305 (15)	0.0355 (4)
C4	0.5130 (3)	0.51269 (19)	0.20179 (16)	0.0401 (5)
C5	0.7116 (3)	0.5852 (2)	0.21532 (19)	0.0504 (5)
H5	0.7718	0.5822	0.1541	0.060*
C6	0.8178 (4)	0.6618 (2)	0.3211 (2)	0.0566 (6)
H6	0.9518	0.7108	0.3316	0.068*
C7	0.7283 (4)	0.6671 (2)	0.4127 (2)	0.0551 (6)
H7	0.8012	0.7209	0.4835	0.066*
C8	0.5328 (4)	0.5937 (2)	0.39951 (18)	0.0474 (5)
H8	0.4743	0.5970	0.4612	0.057*
C9	0.4228 (3)	0.51430 (18)	0.29316 (16)	0.0380 (4)
C10	0.2200 (3)	0.42696 (18)	0.26060 (15)	0.0360 (4)
C11	0.0889 (3)	0.39891 (19)	0.32582 (16)	0.0403 (5)
H11	0.1264	0.4399	0.4028	0.048*
C12	−0.1012 (3)	0.30925 (19)	0.27797 (16)	0.0390 (4)
C13	−0.2388 (4)	0.2784 (2)	0.34417 (18)	0.0485 (5)
H13	−0.2009	0.3178	0.4213	0.058*
C14	−0.4235 (4)	0.1932 (2)	0.2978 (2)	0.0544 (6)
H14	−0.5116	0.1752	0.3430	0.065*
C15	−0.4829 (4)	0.1316 (2)	0.1815 (2)	0.0513 (5)
H15	−0.6102	0.0729	0.1500	0.062*
C16	−0.3550 (3)	0.1575 (2)	0.11515 (18)	0.0437 (5)
H16	−0.3963	0.1154	0.0384	0.052*
C17	−0.0765 (3)	0.21177 (18)	−0.03270 (15)	0.0359 (4)
C18	−0.2468 (4)	0.2399 (2)	−0.10000 (18)	0.0514 (6)
H18	−0.3361	0.2983	−0.0676	0.062*
C19	−0.2881 (4)	0.1835 (2)	−0.21439 (18)	0.0560 (6)
H19	−0.4042	0.2049	−0.2576	0.067*

C20	−0.1618 (4)	0.0964 (2)	−0.26596 (17)	0.0467 (5)
C21	0.0061 (4)	0.0673 (2)	−0.19921 (19)	0.0565 (6)
H21	0.0935	0.0079	−0.2319	0.068*
C22	0.0493 (4)	0.1237 (2)	−0.08442 (18)	0.0514 (6)
H22	0.1652	0.1019	−0.0415	0.062*
C23	−0.2067 (5)	0.0357 (3)	−0.3913 (2)	0.0739 (8)
H23A	−0.0779	0.0023	−0.4136	0.111*
H23B	−0.2443	0.0987	−0.4243	0.111*
H23C	−0.3267	−0.0327	−0.4158	0.111*
S1	0.35084 (8)	0.41019 (5)	0.07515 (4)	0.04430 (18)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0382 (10)	0.0343 (10)	0.0370 (10)	0.0107 (8)	0.0085 (8)	0.0139 (8)
C2	0.0387 (10)	0.0344 (10)	0.0318 (10)	0.0126 (8)	0.0081 (8)	0.0119 (8)
C3	0.0390 (10)	0.0391 (11)	0.0328 (10)	0.0127 (8)	0.0120 (8)	0.0146 (8)
C4	0.0435 (11)	0.0410 (11)	0.0404 (11)	0.0097 (9)	0.0095 (9)	0.0192 (9)
C5	0.0487 (12)	0.0581 (14)	0.0534 (13)	0.0031 (10)	0.0127 (10)	0.0311 (11)
C6	0.0513 (13)	0.0559 (14)	0.0643 (16)	−0.0075 (11)	0.0046 (11)	0.0300 (12)
C7	0.0601 (14)	0.0463 (13)	0.0496 (13)	−0.0078 (11)	−0.0010 (11)	0.0143 (11)
C8	0.0559 (13)	0.0450 (12)	0.0399 (11)	0.0026 (10)	0.0093 (10)	0.0142 (9)
C9	0.0420 (10)	0.0360 (10)	0.0385 (11)	0.0083 (8)	0.0094 (8)	0.0153 (9)
C10	0.0407 (10)	0.0347 (10)	0.0338 (10)	0.0101 (8)	0.0086 (8)	0.0120 (8)
C11	0.0456 (11)	0.0430 (11)	0.0311 (10)	0.0065 (9)	0.0098 (8)	0.0103 (9)
C12	0.0417 (10)	0.0397 (11)	0.0388 (11)	0.0102 (9)	0.0131 (9)	0.0147 (9)
C13	0.0532 (12)	0.0554 (13)	0.0408 (12)	0.0066 (10)	0.0190 (10)	0.0172 (10)
C14	0.0510 (13)	0.0619 (15)	0.0585 (14)	0.0030 (11)	0.0239 (11)	0.0263 (12)
C15	0.0446 (12)	0.0515 (13)	0.0598 (14)	0.0018 (10)	0.0106 (10)	0.0233 (11)
C16	0.0433 (11)	0.0431 (12)	0.0429 (11)	0.0047 (9)	0.0054 (9)	0.0149 (9)
C17	0.0370 (10)	0.0360 (10)	0.0350 (10)	0.0056 (8)	0.0092 (8)	0.0118 (8)
C18	0.0581 (13)	0.0569 (14)	0.0416 (12)	0.0271 (11)	0.0119 (10)	0.0157 (10)
C19	0.0624 (14)	0.0656 (15)	0.0406 (12)	0.0183 (12)	0.0021 (11)	0.0218 (11)
C20	0.0572 (13)	0.0432 (12)	0.0350 (11)	−0.0068 (10)	0.0102 (10)	0.0100 (9)
C21	0.0612 (14)	0.0553 (14)	0.0470 (13)	0.0184 (11)	0.0196 (11)	0.0039 (11)
C22	0.0496 (12)	0.0575 (14)	0.0426 (12)	0.0214 (11)	0.0069 (10)	0.0103 (10)
C23	0.100 (2)	0.0677 (17)	0.0405 (13)	−0.0129 (15)	0.0131 (13)	0.0077 (12)
S1	0.0469 (3)	0.0525 (3)	0.0360 (3)	0.0051 (2)	0.0137 (2)	0.0165 (2)

Geometric parameters (Å, º)

C1—C16	1.411 (3)	C12—C13	1.420 (3)
C1—C2	1.426 (3)	C13—C14	1.349 (3)
C1—C12	1.434 (3)	C13—H13	0.9300
C2—C3	1.373 (3)	C14—C15	1.405 (3)
C2—C17	1.492 (3)	C14—H14	0.9300
C3—C10	1.423 (3)	C15—C16	1.358 (3)
C3—S1	1.7492 (19)	C15—H15	0.9300

C4—C5	1.384 (3)	C16—H16	0.9300
C4—C9	1.397 (3)	C17—C18	1.375 (3)
C4—S1	1.746 (2)	C17—C22	1.376 (3)
C5—C6	1.372 (3)	C18—C19	1.377 (3)
C5—H5	0.9300	C18—H18	0.9300
C6—C7	1.388 (3)	C19—C20	1.370 (3)
C6—H6	0.9300	C19—H19	0.9300
C7—C8	1.373 (3)	C20—C21	1.366 (3)
C7—H7	0.9300	C20—C23	1.508 (3)
C8—C9	1.393 (3)	C21—C22	1.382 (3)
C8—H8	0.9300	C21—H21	0.9300
C9—C10	1.449 (3)	C22—H22	0.9300
C10—C11	1.369 (3)	C23—H23A	0.9600
C11—C12	1.400 (3)	C23—H23B	0.9600
C11—H11	0.9300	C23—H23C	0.9600

C16—C1—C2	122.80 (18)	C14—C13—H13	119.2
C16—C1—C12	117.81 (17)	C12—C13—H13	119.2
C2—C1—C12	119.39 (17)	C13—C14—C15	120.2 (2)
C3—C2—C1	117.87 (17)	C13—C14—H14	119.9
C3—C2—C17	120.13 (17)	C15—C14—H14	119.9
C1—C2—C17	121.99 (17)	C16—C15—C14	120.2 (2)
C2—C3—C10	123.09 (17)	C16—C15—H15	119.9
C2—C3—S1	125.07 (15)	C14—C15—H15	119.9
C10—C3—S1	111.84 (14)	C15—C16—C1	121.9 (2)
C5—C4—C9	121.40 (19)	C15—C16—H16	119.1
C5—C4—S1	125.91 (16)	C1—C16—H16	119.1
C9—C4—S1	112.68 (15)	C18—C17—C22	117.15 (19)
C6—C5—C4	118.5 (2)	C18—C17—C2	122.18 (17)
C6—C5—H5	120.8	C22—C17—C2	120.65 (17)
C4—C5—H5	120.8	C17—C18—C19	121.4 (2)
C5—C6—C7	121.0 (2)	C17—C18—H18	119.3
C5—C6—H6	119.5	C19—C18—H18	119.3
C7—C6—H6	119.5	C20—C19—C18	121.4 (2)
C8—C7—C6	120.6 (2)	C20—C19—H19	119.3
C8—C7—H7	119.7	C18—C19—H19	119.3
C6—C7—H7	119.7	C21—C20—C19	117.3 (2)
C7—C8—C9	119.6 (2)	C21—C20—C23	121.5 (2)
C7—C8—H8	120.2	C19—C20—C23	121.2 (2)
C9—C8—H8	120.2	C20—C21—C22	121.7 (2)
C8—C9—C4	118.95 (19)	C20—C21—H21	119.1
C8—C9—C10	128.82 (18)	C22—C21—H21	119.1
C4—C9—C10	112.23 (17)	C17—C22—C21	121.0 (2)
C11—C10—C3	118.90 (18)	C17—C22—H22	119.5
C11—C10—C9	129.40 (18)	C21—C22—H22	119.5
C3—C10—C9	111.69 (17)	C20—C23—H23A	109.5
C10—C11—C12	120.75 (18)	C20—C23—H23B	109.5
C10—C11—H11	119.6	H23A—C23—H23B	109.5

C12—C11—H11	119.6	C20—C23—H23C	109.5
C11—C12—C13	121.63 (19)	H23A—C23—H23C	109.5
C11—C12—C1	120.00 (17)	H23B—C23—H23C	109.5
C13—C12—C1	118.37 (18)	C4—S1—C3	91.52 (9)
C14—C13—C12	121.6 (2)		

C16—C1—C2—C3	−179.76 (17)	C10—C11—C12—C1	−0.5 (3)
C12—C1—C2—C3	−0.2 (3)	C16—C1—C12—C11	−179.63 (17)
C16—C1—C2—C17	−0.5 (3)	C2—C1—C12—C11	0.8 (3)
C12—C1—C2—C17	179.12 (16)	C16—C1—C12—C13	0.1 (3)
C1—C2—C3—C10	−0.6 (3)	C2—C1—C12—C13	−179.48 (18)
C17—C2—C3—C10	−179.96 (16)	C11—C12—C13—C14	179.1 (2)
C1—C2—C3—S1	179.27 (13)	C1—C12—C13—C14	−0.6 (3)
C17—C2—C3—S1	−0.1 (3)	C12—C13—C14—C15	0.6 (4)
C9—C4—C5—C6	−1.3 (3)	C13—C14—C15—C16	−0.1 (3)
S1—C4—C5—C6	179.61 (17)	C14—C15—C16—C1	−0.4 (3)
C4—C5—C6—C7	−0.3 (3)	C2—C1—C16—C15	179.98 (18)
C5—C6—C7—C8	1.3 (4)	C12—C1—C16—C15	0.4 (3)
C6—C7—C8—C9	−0.7 (3)	C3—C2—C17—C18	−108.5 (2)
C7—C8—C9—C4	−0.9 (3)	C1—C2—C17—C18	72.2 (3)
C7—C8—C9—C10	178.1 (2)	C3—C2—C17—C22	70.1 (3)
C5—C4—C9—C8	1.9 (3)	C1—C2—C17—C22	−109.1 (2)
S1—C4—C9—C8	−178.87 (15)	C22—C17—C18—C19	−0.7 (3)
C5—C4—C9—C10	−177.24 (18)	C2—C17—C18—C19	177.9 (2)
S1—C4—C9—C10	2.0 (2)	C17—C18—C19—C20	0.3 (4)
C2—C3—C10—C11	0.9 (3)	C18—C19—C20—C21	0.4 (4)
S1—C3—C10—C11	−179.04 (15)	C18—C19—C20—C23	−179.5 (2)
C2—C3—C10—C9	179.87 (17)	C19—C20—C21—C22	−0.6 (4)
S1—C3—C10—C9	0.0 (2)	C23—C20—C21—C22	179.3 (2)
C8—C9—C10—C11	−1.4 (3)	C18—C17—C22—C21	0.5 (3)
C4—C9—C10—C11	177.64 (19)	C2—C17—C22—C21	−178.2 (2)
C8—C9—C10—C3	179.71 (19)	C20—C21—C22—C17	0.2 (4)
C4—C9—C10—C3	−1.2 (2)	C5—C4—S1—C3	177.47 (19)
C3—C10—C11—C12	−0.3 (3)	C9—C4—S1—C3	−1.69 (15)
C9—C10—C11—C12	−179.05 (18)	C2—C3—S1—C4	−178.95 (17)
C10—C11—C12—C13	179.71 (18)	C10—C3—S1—C4	0.96 (14)

Hydrogen-bond geometry (Å, º)

Cg3, Cg4 and Cg5 are the centroids of rings (C1/C12–C16), (C4–C6) and (C17–C22), respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C15—H15···*Cg*5^{i}	0.93	2.94	3.763 (3)	148
C19—H19···*Cg*4^{ii}	0.93	2.94	3.753 (3)	147
C21—H21···*Cg*3^{iii}	0.93	2.91	3.721 (3)	146

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

(II) 7-Phenylanthra[2,3-*b*]benzo[*d*]thiophene

Crystal data

$C_{26}H_{16}S$
$M_r = 360.45$
Orthorhombic, *Pccn*
Hall symbol: -P 2ab 2ac
$a = 12.2159$ (8) Å
$b = 33.1138$ (4) Å
$c = 8.8993$ (5) Å
$V = 3599.9$ (3) Å^3
$Z = 8$
$F(000) = 1504$
$D_x = 1.330$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3171 reflections
$\theta = 2.5$–$25.0°$
$\mu = 0.19$ mm^{-1}
$T = 296$ K
Block, colourless
0.30 × 0.25 × 0.25 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω & φ scans
Absorption correction: multi-scan (SADABS; Bruker, 2008)
$T_{min} = 0.946$, $T_{max} = 0.955$
43542 measured reflections
3171 independent reflections
2540 reflections with $I > 2\sigma(I)$
$R_{int} = 0.036$
$\theta_{max} = 25.0°$, $\theta_{min} = 2.5°$
$h = -14 \rightarrow 14$
$k = -39 \rightarrow 39$
$l = -10 \rightarrow 9$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.059$
$wR(F^2) = 0.182$
$S = 1.04$
3171 reflections
244 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
$w = 1/[\sigma^2(F_o^2) + (0.0831P)^2 + 5.3659P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 1.06$ e Å^{-3}
$\Delta\rho_{min} = -0.40$ 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. 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 $F^2 > 2$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	0.4387 (2)	0.40078 (9)	0.4515 (3)	0.0366 (7)
C2	0.4905 (3)	0.42302 (9)	0.3361 (3)	0.0412 (7)
H2	0.5423	0.4107	0.2749	0.049*
C3	0.4643 (3)	0.46257 (9)	0.3144 (3)	0.0422 (7)
C4	0.4365 (3)	0.53427 (10)	0.2336 (4)	0.0494 (8)

C5	0.4359 (3)	0.57228 (11)	0.1701 (4)	0.0581 (9)
H5	0.4836	0.5788	0.0923	0.070*
C6	0.3634 (4)	0.60010 (11)	0.2244 (5)	0.0667 (11)
H6	0.3614	0.6257	0.1819	0.080*
C7	0.2930 (3)	0.59091 (11)	0.3413 (5)	0.0626 (11)
H7	0.2442	0.6103	0.3762	0.075*
C8	0.2948 (3)	0.55284 (10)	0.4065 (4)	0.0532 (9)
H8	0.2479	0.5466	0.4855	0.064*
C9	0.3679 (3)	0.52414 (9)	0.3515 (4)	0.0454 (8)
C10	0.3829 (3)	0.48249 (9)	0.4034 (4)	0.0416 (7)
C11	0.3348 (3)	0.46241 (9)	0.5176 (4)	0.0442 (8)
H11	0.2827	0.4754	0.5764	0.053*
C12	0.3627 (2)	0.42151 (9)	0.5490 (4)	0.0400 (7)
C13	0.3191 (3)	0.40108 (10)	0.6711 (4)	0.0432 (7)
H13	0.2707	0.4145	0.7344	0.052*
C14	0.3452 (2)	0.36119 (9)	0.7016 (3)	0.0402 (7)
C15	0.3034 (3)	0.34053 (11)	0.8295 (4)	0.0492 (8)
H15	0.2612	0.3547	0.8986	0.059*
C16	0.3231 (3)	0.30128 (11)	0.8533 (4)	0.0548 (9)
H16	0.2945	0.2886	0.9379	0.066*
C17	0.3869 (3)	0.27908 (11)	0.7506 (4)	0.0557 (9)
H17	0.3987	0.2517	0.7666	0.067*
C18	0.4313 (3)	0.29732 (10)	0.6286 (4)	0.0464 (8)
H18	0.4737	0.2822	0.5626	0.056*
C19	0.4146 (2)	0.33940 (9)	0.5989 (3)	0.0379 (7)
C20	0.4605 (2)	0.35934 (9)	0.4753 (3)	0.0359 (7)
C21	0.5279 (2)	0.33716 (8)	0.3628 (3)	0.0362 (7)
C22	0.6302 (3)	0.32209 (9)	0.3981 (4)	0.0466 (8)
H22	0.6588	0.3261	0.4938	0.056*
C23	0.6905 (3)	0.30109 (10)	0.2926 (4)	0.0538 (9)
H23	0.7593	0.2912	0.3180	0.065*
C24	0.6502 (3)	0.29467 (10)	0.1514 (4)	0.0530 (9)
H24	0.6904	0.2799	0.0817	0.064*
C25	0.5496 (3)	0.31020 (11)	0.1135 (4)	0.0534 (9)
H25	0.5224	0.3064	0.0169	0.064*
C26	0.4887 (3)	0.33134 (10)	0.2176 (4)	0.0478 (8)
H26	0.4208	0.3418	0.1905	0.057*
S1	0.52265 (8)	0.49395 (3)	0.18065 (10)	0.0547 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0346 (15)	0.0381 (15)	0.0371 (15)	0.0019 (12)	−0.0045 (13)	−0.0064 (13)
C2	0.0445 (17)	0.0402 (16)	0.0391 (17)	0.0081 (13)	−0.0050 (14)	−0.0058 (13)
C3	0.0466 (18)	0.0413 (17)	0.0388 (17)	0.0005 (14)	−0.0070 (14)	−0.0041 (13)
C4	0.0527 (19)	0.0462 (18)	0.0492 (19)	0.0015 (15)	−0.0137 (17)	−0.0067 (15)
C5	0.063 (2)	0.055 (2)	0.056 (2)	−0.0056 (18)	−0.0142 (18)	0.0020 (17)
C6	0.079 (3)	0.0383 (19)	0.083 (3)	−0.0056 (18)	−0.031 (2)	0.0072 (19)

C7	0.057 (2)	0.0421 (19)	0.089 (3)	0.0117 (16)	−0.016 (2)	−0.0154 (19)
C8	0.0470 (19)	0.0497 (19)	0.063 (2)	−0.0002 (15)	−0.0075 (16)	−0.0095 (17)
C9	0.0474 (18)	0.0382 (16)	0.0506 (19)	0.0015 (14)	−0.0136 (15)	−0.0088 (14)
C10	0.0424 (16)	0.0400 (16)	0.0425 (17)	0.0043 (13)	−0.0097 (14)	−0.0108 (14)
C11	0.0428 (17)	0.0422 (16)	0.0477 (19)	0.0079 (14)	−0.0018 (15)	−0.0117 (14)
C12	0.0371 (15)	0.0397 (16)	0.0431 (17)	0.0068 (12)	−0.0045 (13)	−0.0131 (13)
C13	0.0381 (16)	0.0488 (18)	0.0429 (17)	0.0036 (13)	0.0049 (14)	−0.0106 (14)
C14	0.0320 (15)	0.0461 (17)	0.0424 (17)	0.0001 (13)	−0.0032 (13)	−0.0085 (14)
C15	0.0404 (17)	0.064 (2)	0.0436 (18)	−0.0002 (15)	0.0069 (15)	−0.0034 (16)
C16	0.056 (2)	0.060 (2)	0.048 (2)	−0.0037 (17)	0.0068 (17)	0.0067 (17)
C17	0.063 (2)	0.0480 (19)	0.056 (2)	−0.0015 (16)	0.0022 (18)	0.0074 (17)
C18	0.0499 (19)	0.0428 (17)	0.0463 (18)	0.0039 (14)	0.0009 (15)	−0.0041 (14)
C19	0.0346 (15)	0.0414 (16)	0.0378 (16)	0.0013 (12)	−0.0052 (13)	−0.0063 (13)
C20	0.0337 (14)	0.0350 (14)	0.0390 (16)	0.0047 (12)	−0.0053 (12)	−0.0070 (12)
C21	0.0395 (16)	0.0313 (14)	0.0378 (16)	0.0015 (12)	−0.0001 (13)	−0.0026 (12)
C22	0.0503 (19)	0.0420 (17)	0.0473 (19)	0.0103 (14)	−0.0043 (15)	−0.0079 (14)
C23	0.0486 (19)	0.0469 (18)	0.066 (2)	0.0118 (15)	0.0052 (17)	−0.0024 (17)
C24	0.058 (2)	0.0461 (18)	0.055 (2)	0.0043 (16)	0.0195 (18)	−0.0078 (16)
C25	0.062 (2)	0.058 (2)	0.0407 (18)	−0.0048 (17)	0.0045 (16)	−0.0088 (16)
C26	0.0431 (17)	0.055 (2)	0.0450 (18)	0.0027 (15)	0.0013 (15)	−0.0070 (15)
S1	0.0709 (6)	0.0480 (5)	0.0453 (5)	0.0081 (4)	0.0074 (4)	0.0035 (4)

Geometric parameters (Å, º)

C1—C20	1.414 (4)	C13—H13	0.9300
C1—C2	1.414 (4)	C14—C15	1.423 (5)
C1—C12	1.444 (4)	C14—C19	1.440 (4)
C2—C3	1.362 (4)	C15—C16	1.338 (5)
C2—H2	0.9300	C15—H15	0.9300
C3—C10	1.431 (4)	C16—C17	1.408 (5)
C3—S1	1.734 (3)	C16—H16	0.9300
C4—C5	1.380 (5)	C17—C18	1.356 (5)
C4—C9	1.385 (5)	C17—H17	0.9300
C4—S1	1.764 (4)	C18—C19	1.433 (4)
C5—C6	1.366 (6)	C18—H18	0.9300
C5—H5	0.9300	C19—C20	1.400 (4)
C6—C7	1.384 (6)	C20—C21	1.489 (4)
C6—H6	0.9300	C21—C22	1.382 (4)
C7—C8	1.388 (5)	C21—C26	1.392 (4)
C7—H7	0.9300	C22—C23	1.381 (5)
C8—C9	1.393 (5)	C22—H22	0.9300
C8—H8	0.9300	C23—C24	1.366 (5)
C9—C10	1.466 (4)	C23—H23	0.9300
C10—C11	1.350 (5)	C24—C25	1.374 (5)
C11—C12	1.424 (4)	C24—H24	0.9300
C11—H11	0.9300	C25—C26	1.380 (5)
C12—C13	1.386 (5)	C25—H25	0.9300
C13—C14	1.386 (4)	C26—H26	0.9300

C20—C1—C2	122.0 (3)	C13—C14—C19	119.2 (3)
C20—C1—C12	119.5 (3)	C15—C14—C19	118.6 (3)
C2—C1—C12	118.5 (3)	C16—C15—C14	121.9 (3)
C3—C2—C1	119.9 (3)	C16—C15—H15	119.0
C3—C2—H2	120.1	C14—C15—H15	119.0
C1—C2—H2	120.1	C15—C16—C17	120.2 (3)
C2—C3—C10	121.9 (3)	C15—C16—H16	119.9
C2—C3—S1	125.2 (3)	C17—C16—H16	119.9
C10—C3—S1	112.9 (2)	C18—C17—C16	120.6 (3)
C5—C4—C9	121.9 (3)	C18—C17—H17	119.7
C5—C4—S1	125.7 (3)	C16—C17—H17	119.7
C9—C4—S1	112.3 (3)	C17—C18—C19	121.6 (3)
C6—C5—C4	118.3 (4)	C17—C18—H18	119.2
C6—C5—H5	120.9	C19—C18—H18	119.2
C4—C5—H5	120.9	C20—C19—C18	123.1 (3)
C5—C6—C7	121.4 (3)	C20—C19—C14	119.9 (3)
C5—C6—H6	119.3	C18—C19—C14	117.0 (3)
C7—C6—H6	119.3	C19—C20—C1	120.0 (3)
C6—C7—C8	120.3 (3)	C19—C20—C21	121.1 (3)
C6—C7—H7	119.9	C1—C20—C21	118.8 (3)
C8—C7—H7	119.9	C22—C21—C26	118.2 (3)
C7—C8—C9	118.9 (4)	C22—C21—C20	121.7 (3)
C7—C8—H8	120.6	C26—C21—C20	120.1 (3)
C9—C8—H8	120.6	C23—C22—C21	120.6 (3)
C8—C9—C4	119.3 (3)	C23—C22—H22	119.7
C8—C9—C10	127.7 (3)	C21—C22—H22	119.7
C4—C9—C10	113.0 (3)	C22—C23—C24	120.8 (3)
C11—C10—C3	119.5 (3)	C22—C23—H23	119.6
C11—C10—C9	130.2 (3)	C24—C23—H23	119.6
C3—C10—C9	110.3 (3)	C25—C24—C23	119.3 (3)
C10—C11—C12	120.8 (3)	C25—C24—H24	120.3
C10—C11—H11	119.6	C23—C24—H24	120.3
C12—C11—H11	119.6	C24—C25—C26	120.5 (3)
C13—C12—C11	121.7 (3)	C24—C25—H25	119.8
C13—C12—C1	119.1 (3)	C26—C25—H25	119.8
C11—C12—C1	119.2 (3)	C25—C26—C21	120.5 (3)
C12—C13—C14	122.0 (3)	C25—C26—H26	119.7
C12—C13—H13	119.0	C21—C26—H26	119.7
C14—C13—H13	119.0	C3—S1—C4	91.43 (16)
C13—C14—C15	122.2 (3)		

C20—C1—C2—C3	177.9 (3)	C13—C14—C15—C16	175.5 (3)
C12—C1—C2—C3	−3.1 (4)	C19—C14—C15—C16	−2.7 (5)
C1—C2—C3—C10	−1.6 (5)	C14—C15—C16—C17	0.1 (5)
C1—C2—C3—S1	178.5 (2)	C15—C16—C17—C18	1.6 (6)
C9—C4—C5—C6	−1.4 (5)	C16—C17—C18—C19	−0.5 (5)
S1—C4—C5—C6	179.9 (3)	C17—C18—C19—C20	179.0 (3)

C4—C5—C6—C7	0.8 (6)	C17—C18—C19—C14	−2.1 (5)
C5—C6—C7—C8	0.1 (6)	C13—C14—C19—C20	4.3 (4)
C6—C7—C8—C9	−0.5 (5)	C15—C14—C19—C20	−177.5 (3)
C7—C8—C9—C4	−0.1 (5)	C13—C14—C19—C18	−174.7 (3)
C7—C8—C9—C10	−179.9 (3)	C15—C14—C19—C18	3.6 (4)
C5—C4—C9—C8	1.1 (5)	C18—C19—C20—C1	178.8 (3)
S1—C4—C9—C8	180.0 (2)	C14—C19—C20—C1	−0.1 (4)
C5—C4—C9—C10	−179.2 (3)	C18—C19—C20—C21	2.0 (4)
S1—C4—C9—C10	−0.2 (3)	C14—C19—C20—C21	−176.9 (3)
C2—C3—C10—C11	3.8 (5)	C2—C1—C20—C19	174.5 (3)
S1—C3—C10—C11	−176.4 (2)	C12—C1—C20—C19	−4.5 (4)
C2—C3—C10—C9	−177.4 (3)	C2—C1—C20—C21	−8.6 (4)
S1—C3—C10—C9	2.5 (3)	C12—C1—C20—C21	172.4 (3)
C8—C9—C10—C11	−3.0 (6)	C19—C20—C21—C22	−69.3 (4)
C4—C9—C10—C11	177.3 (3)	C1—C20—C21—C22	113.8 (3)
C8—C9—C10—C3	178.4 (3)	C19—C20—C21—C26	111.1 (3)
C4—C9—C10—C3	−1.4 (4)	C1—C20—C21—C26	−65.7 (4)
C3—C10—C11—C12	−1.0 (5)	C26—C21—C22—C23	−1.4 (5)
C9—C10—C11—C12	−179.6 (3)	C20—C21—C22—C23	179.0 (3)
C10—C11—C12—C13	176.1 (3)	C21—C22—C23—C24	−0.2 (5)
C10—C11—C12—C1	−3.7 (4)	C22—C23—C24—C25	1.6 (5)
C20—C1—C12—C13	4.9 (4)	C23—C24—C25—C26	−1.4 (5)
C2—C1—C12—C13	−174.1 (3)	C24—C25—C26—C21	−0.2 (5)
C20—C1—C12—C11	−175.3 (3)	C22—C21—C26—C25	1.6 (5)
C2—C1—C12—C11	5.7 (4)	C20—C21—C26—C25	−178.8 (3)
C11—C12—C13—C14	179.5 (3)	C2—C3—S1—C4	177.6 (3)
C1—C12—C13—C14	−0.7 (5)	C10—C3—S1—C4	−2.2 (2)
C12—C13—C14—C15	177.9 (3)	C5—C4—S1—C3	−179.7 (3)
C12—C13—C14—C19	−3.9 (5)	C9—C4—S1—C3	1.4 (3)

Hydrogen-bond geometry (Å, º)

Cg2 and Cg3 are the centroids of rings (C1–C3/C10–C12) and (C1/C12–C14/C19/C20), respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C13—H13···*Cg*2^{i}	0.93	2.97	3.885 (4)	168
C15—H15···*Cg*3^{i}	0.93	2.57	3.479 (4)	166

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