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1,2-Bis(2-methyl-5-phenyl-3-thienyl)-benzene

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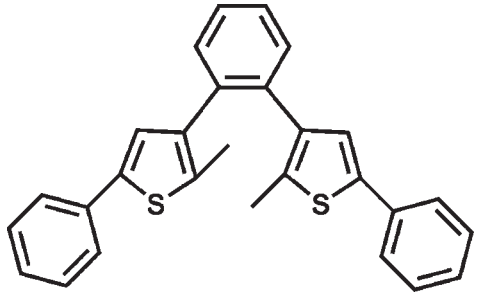
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.004 Å; R factor = 0.041; wR factor = 0.108; data-to-parameter ratio = 15.2.

In the molecule of the title compound, $C_{28}H_{22}S_2$, the two thiophene rings are twisted with respect to the central benzene ring, making dihedral angles of 71.59 (12) and 50.71 (12)°. The two terminal benzene rings are oriented at dihedral angles of 37.59 (11) and 20.12 (11)° to their bonded thiophene rings.

Related literature

For the synthesis of the precursor, see: Irie *et al.* (2000). For applications of photochromic molecules, see: Irie *et al.* (2001). For diarylethenes with four different bridging units, see: Peters *et al.* (2003); Yamaguchi *et al.* (1997); Lucas *et al.* (1998); Chen & Zeng (2004). For ring-closure reactions, see: Ramamurthy & Venkatesan (1987). For a related structure, see: Pu *et al.* (2005).



Experimental

Crystal data

$C_{28}H_{22}S_2$
M_r = 422.58
Triclinic, $P\overline{1}$
a = 10.0934 (12) Å
b = 10.0945 (12) Å
c = 11.9565 (15) Å
α = 83.803 (1)°
β = 67.769 (1)°
γ = 86.362 (1)°
V = 1120.7 (2) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.25 mm^{-1}
T = 296 K
0.40 × 0.24 × 0.15 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.907, T_{max} = 0.964
8610 measured reflections
4136 independent reflections
2920 reflections with $I > 2\sigma(I)$
R_{int} = 0.021

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.108
S = 1.02
4136 reflections
273 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL* software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU2660).

References

Bruker (1997). *SMART* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Chen, Y. & Zeng, D. X. (2004). *J. Org. Chem.* **69**, 5037–5040.
Irie, M., Kobatake, S. & Horichim, M. (2001). *Science*, **291**, 1769–1772.
Irie, M., Lifka, T., Kobatake, S. & Kato, N. (2000). *J. Am. Chem. Soc.* **122**, 4871–4876.
Lucas, L. N., Esch, J. V., Kellogg, R. M. & Feringa, B. L. (1998). *Chem. Commun.* pp. 2313–2314.
Peters, N., Vitols, C., McDonald, R. & Branda, N. R. (2003). *Org. Lett.* **5**, 1183-1186.
Pu, S.-Z., Liu, G., Chen, B. & Wang, R.-J. (2005). *Acta Cryst.* C**61**, o599–o601.
Ramamurthy, V. & Venkatesan, K. (1987). *Chem. Rev.* **87**, 433–481.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Yamaguchi, T., Uchida, K. & Irie, M. (1997). *J. Am. Chem. Soc.* **119**, 6066–6071.

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1,2-Bis(2-methyl-5-phenyl-3-thienyl)benzene

Wen-Juan Miao, Liang-Hua Li, Shan Lu, Gang Liu and Cong-Bin Fan

S1. Comment

The design and synthesis of photochromic molecules is an area of intense research because of the widespread use in photonic device applications such as memory media and optical switching (Irie *et al.* 2001). To date, four kinds of diarylethenes with different bridge units have been reported, that is diarylethenes with a perfluorocyclopentene moiety (Peters *et al.* 2003), diarylethenes with maleic anhydride and maleimide moieties (Yamaguchi *et al.* 1997), diarylethenes with a cyclopentene moiety (Lucas *et al.* 1998), and diarylethenes with a 2,5-dihydrothiphene moiety (Chen & Zeng, 2004). One of our research goals is to develop a novel diarylethene derivative with the inexpensive benzene ring as bridge unit. In this paper, the *ORTEP* drawing of the single-crystal shows the title compound, *i.e.* 1,2-(2-methyl-5-phenyl-3-thienyl)benzene, packed in a parallel conformation which is very rare in other diarylethene system. The two independent planar thiophene ring systems have essentially identical geometries, and the dihedral angles between the central benzene-ring and these of the two thiophene rings, S1/C7—C10, and S2/ C18—C21 are 71.6 (4)° and 50.5 (7)°. The two thiophene groups are linked by the central benzene-ring, with both of them attached to the ethylene group *via* the 2-position. The distance between the two C atoms (C8···C19) is 4.06 (7) Å, which is short enough, theoretically, for the ring-closure reaction to take place in the crystalline phase (Ramamurthy & Venkatesan, 1987), but the crystals of the title compound is parallel thiophene-ring, so, the crystals cannot show photochromism.

S2. Experimental

2-Methyl-5-phenylthiophen-3-yl-3-boronic acid, (2) in Fig 2, was obtained in the presence of compound 3-bromo-2-methyl-5-phenylthiophene, (1), (Irie *et al.*, 2000) (2.53 g, 10.00 mmol) in a n-BuLi/hexane solution (2.50 mol/*L*, 12.00 mmol) and tri-n-butylborate (2.76 g, 12.00 mmol) at 195 K under a nitrogen atmosphere.

The title compound was prepared by adding compound (2) (0.88 g, 4.05 mmol) with Na_2CO_3 (2.00 mol/*L*, 60.00 mmol) to a stirred THF solution (50 ml) containing 1,2-dibromobenzene (0.48 g, 2.03 mmol) and $Pd(PPh_3)_4$ (0.27 g) at 293 K under a nitrogen atmosphere. After reflux for 16 h, the reaction mixture was extracted with ether, evaporated *in vacuo* and purified by column chromatography on SiO_2 using petroleum ether as the eluent to obtain the title compound. Single crystals of the title compound (1a) were grown from a chloroform solution by slow evaporation (m.p. 404.8–405.2 K).

S3. Refinement

H atoms were placed in calculated positions and treated as riding with C—H = 0.96 Å (methyl) or 0.93 Å (aromatic), U_{iso}(H) = 1.5U_{eq}(C) for methyl H atoms and U_{iso}(H) = 1.2U_{eq}(C) for the others.

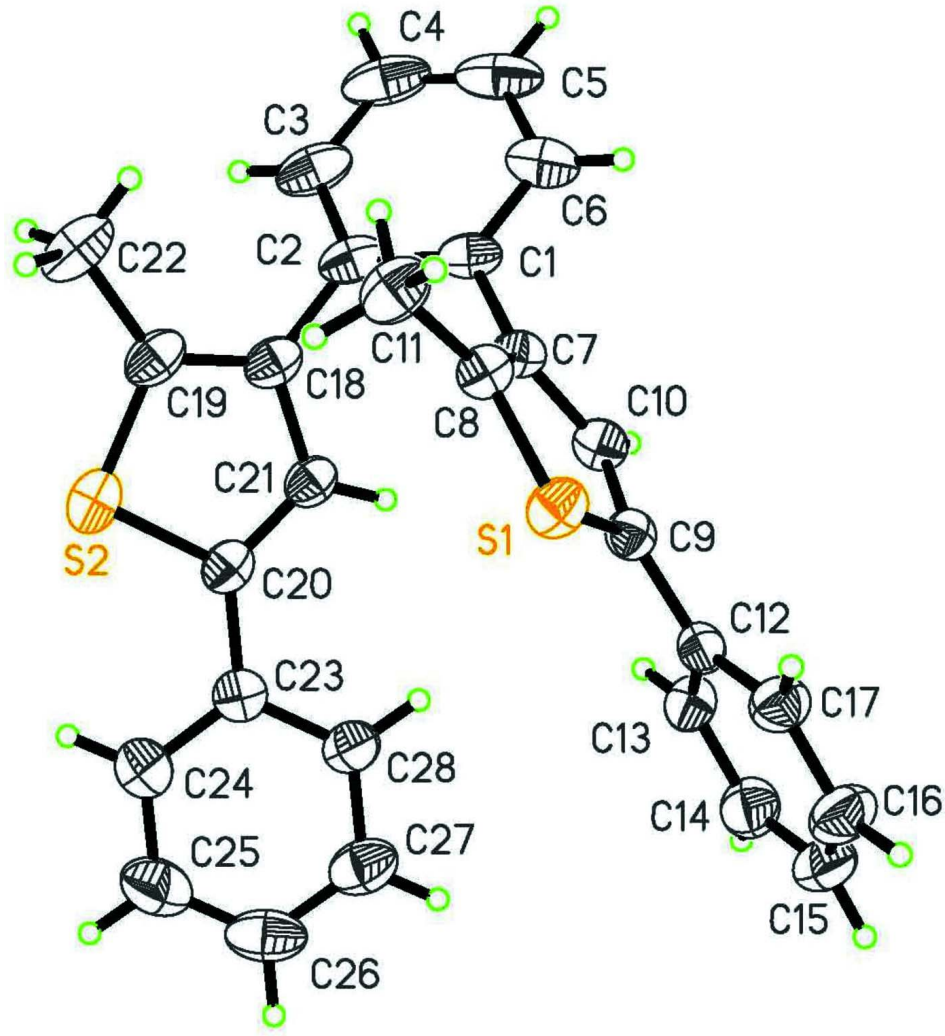

Figure 1

Molecular view the atom-labeling scheme. Ellipsoids are drawn at the 30% probability level. H atoms are represented as small spheres of arbitrary radii.

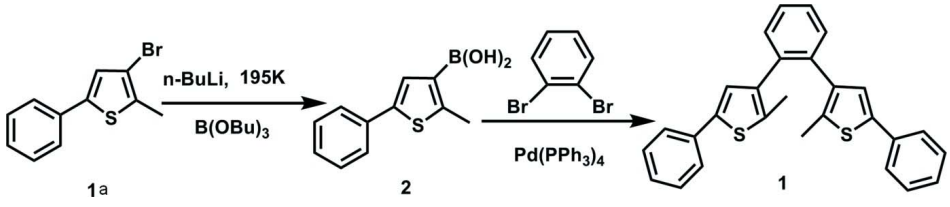

Figure 2

The preparation of the title compound.

1,2-Bis(2-methyl-5-phenyl-3-thienyl)benzene

Crystal data

$C_{28}H_{22}S_2$
$M_r = 422.58$

Triclinic, $P\overline{1}$
Hall symbol: -P 1

a = 10.0934 (12) Å
b = 10.0945 (12) Å
c = 11.9565 (15) Å
α = 83.803 (1)°
β = 67.769 (1)°
γ = 86.362 (1)°
V = 1120.7 (2) Å^3
Z = 2
F(000) = 444

D_x = 1.252 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 2224 reflections
θ = 2.6–22.8°
μ = 0.25 mm^{-1}
T = 296 K
Block, colourless
0.40 × 0.24 × 0.15 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.907, T_{max} = 0.964

8610 measured reflections
4136 independent reflections
2920 reflections with $I > 2\sigma(I)$
R_{int} = 0.021
θ_{max} = 25.5°, θ_{min} = 2.3°
h = −12→12
k = −12→12
l = −14→14

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.108
S = 1.02
4136 reflections
273 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
$w = 1/[\sigma^2(F_o^2) + (0.0442P)^2 + 0.2296P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.006
$\Delta\rho_{max}$ = 0.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

Special details

Experimental. ^{1}HNMR (400 MHz, $CDCl_3$, TMS): δ 2.17 (s, 3H, -CH_3), 6.92 (s, 1H, thienyl-H), 7.20 (t, 1H, J=7.2 Hz,phenyl-H), 7.29 (t, 2H, J=7.4 Hz, phenyl-H), 7.42–7.44 (m, 4H, phenyl-H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 13.93, 125.51, 126.00, 127.00, 127.26, 128.76, 130.61, 134.60, 135.03, 136.09, 139.01, 139.45. IR (KBr, cm^{-1}): 756, 766, 849, 908, 946, 1001, 1029, 1073, 1153, 1184, 1227, 1377, 1462, 1479, 1505, 1596, 1629, 2854, 2924, 3014, 3053, 3254, 3443, 3529, 3676.

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	0.8690 (3)	0.1761 (2)	0.33341 (19)	0.0593 (6)
C2	1.0178 (3)	0.1571 (2)	0.27841 (19)	0.0632 (6)
C3	1.0724 (3)	0.0279 (3)	0.2524 (2)	0.0837 (8)
H3	1.1708	0.0137	0.2160	0.100*

C4	0.9833 (5)	−0.0781 (3)	0.2798 (3)	0.1002 (11)
H4	1.0217	−0.1633	0.2634	0.120*
C5	0.8382 (5)	−0.0587 (3)	0.3312 (3)	0.0994 (11)
H5	0.7780	−0.1303	0.3478	0.119*
C6	0.7806 (3)	0.0679 (2)	0.3587 (2)	0.0803 (7)
H6	0.6819	0.0803	0.3944	0.096*
C7	0.8057 (2)	0.3112 (2)	0.36380 (18)	0.0534 (5)
C8	0.8183 (2)	0.3757 (2)	0.45372 (19)	0.0564 (5)
C9	0.6907 (2)	0.5132 (2)	0.33745 (18)	0.0517 (5)
C10	0.7318 (2)	0.3902 (2)	0.29899 (19)	0.0563 (5)
H10	0.7133	0.3602	0.2357	0.068*
C11	0.8878 (3)	0.3254 (3)	0.5415 (2)	0.0791 (7)
H11A	0.9079	0.2315	0.5370	0.119*
H11B	0.8245	0.3414	0.6223	0.119*
H11C	0.9755	0.3712	0.5214	0.119*
C12	0.6259 (2)	0.6253 (2)	0.28537 (19)	0.0535 (5)
C13	0.6640 (2)	0.6476 (2)	0.1601 (2)	0.0626 (6)
H13	0.7277	0.5890	0.1095	0.075*
C14	0.6079 (3)	0.7558 (3)	0.1111 (3)	0.0798 (7)
H14	0.6339	0.7703	0.0274	0.096*
C15	0.5132 (3)	0.8426 (3)	0.1857 (3)	0.0821 (8)
H15	0.4765	0.9163	0.1523	0.099*
C16	0.4735 (3)	0.8211 (3)	0.3071 (3)	0.0855 (8)
H16	0.4077	0.8791	0.3568	0.103*
C17	0.5293 (2)	0.7141 (2)	0.3585 (2)	0.0692 (6)
H17	0.5022	0.7013	0.4424	0.083*
C18	1.1146 (2)	0.2710 (2)	0.24104 (19)	0.0586 (6)
C19	1.2360 (3)	0.2804 (2)	0.2660 (2)	0.0659 (6)
C20	1.1898 (2)	0.4834 (2)	0.14581 (18)	0.0552 (5)
C21	1.0915 (2)	0.3879 (2)	0.17170 (18)	0.0554 (5)
H21	1.0148	0.3978	0.1462	0.066*
C22	1.2975 (3)	0.1831 (3)	0.3393 (3)	0.0933 (9)
H22A	1.2255	0.1213	0.3891	0.140*
H22B	1.3286	0.2306	0.3899	0.140*
H22C	1.3775	0.1354	0.2855	0.140*
C23	1.1947 (2)	0.6143 (2)	0.07776 (19)	0.0567 (5)
C24	1.3183 (3)	0.6851 (3)	0.0253 (3)	0.0844 (8)
H24	1.4020	0.6492	0.0327	0.101*
C25	1.3216 (4)	0.8071 (3)	−0.0376 (3)	0.1023 (10)
H25	1.4068	0.8529	−0.0719	0.123*
C26	1.2003 (4)	0.8618 (3)	−0.0504 (2)	0.0908 (9)
H26	1.2025	0.9452	−0.0926	0.109*
C27	1.0761 (4)	0.7937 (3)	−0.0010 (2)	0.0833 (8)
H27	0.9936	0.8298	−0.0108	0.100*
C28	1.0726 (3)	0.6706 (2)	0.0638 (2)	0.0664 (6)
H28	0.9871	0.6252	0.0984	0.080*
S1	0.74075 (6)	0.53246 (6)	0.45767 (5)	0.06329 (19)
S2	1.31728 (6)	0.43038 (7)	0.20603 (6)	0.0720 (2)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0884 (17)	0.0445 (12)	0.0466 (12)	−0.0012 (11)	−0.0277 (12)	−0.0017 (9)
C2	0.0946 (18)	0.0483 (13)	0.0484 (12)	0.0156 (12)	−0.0301 (12)	−0.0083 (10)
C3	0.131 (2)	0.0569 (16)	0.0672 (16)	0.0299 (16)	−0.0444 (16)	−0.0162 (13)
C4	0.188 (4)	0.0461 (16)	0.081 (2)	0.021 (2)	−0.068 (2)	−0.0143 (14)
C5	0.184 (4)	0.0475 (16)	0.080 (2)	−0.023 (2)	−0.066 (2)	0.0057 (14)
C6	0.118 (2)	0.0591 (16)	0.0649 (16)	−0.0183 (15)	−0.0345 (15)	0.0021 (12)
C7	0.0589 (13)	0.0478 (12)	0.0491 (12)	−0.0035 (10)	−0.0159 (10)	−0.0009 (9)
C8	0.0610 (13)	0.0558 (13)	0.0527 (12)	0.0030 (10)	−0.0217 (10)	−0.0075 (10)
C9	0.0501 (11)	0.0513 (12)	0.0501 (12)	−0.0015 (9)	−0.0141 (9)	−0.0067 (10)
C10	0.0634 (13)	0.0543 (13)	0.0525 (12)	−0.0050 (10)	−0.0219 (11)	−0.0085 (10)
C11	0.0984 (19)	0.0797 (17)	0.0720 (16)	0.0163 (15)	−0.0466 (15)	−0.0164 (13)
C12	0.0456 (11)	0.0528 (12)	0.0599 (13)	−0.0046 (9)	−0.0166 (10)	−0.0054 (10)
C13	0.0586 (13)	0.0684 (15)	0.0603 (14)	0.0055 (11)	−0.0224 (11)	−0.0072 (11)
C14	0.0778 (17)	0.0892 (19)	0.0730 (17)	−0.0020 (15)	−0.0326 (14)	0.0068 (15)
C15	0.0871 (19)	0.0654 (16)	0.090 (2)	0.0093 (14)	−0.0358 (16)	0.0098 (15)
C16	0.0881 (19)	0.0652 (17)	0.091 (2)	0.0222 (14)	−0.0230 (16)	−0.0115 (15)
C17	0.0703 (15)	0.0608 (15)	0.0668 (15)	0.0054 (12)	−0.0164 (12)	−0.0032 (12)
C18	0.0679 (14)	0.0547 (13)	0.0486 (12)	0.0163 (11)	−0.0177 (11)	−0.0113 (10)
C19	0.0751 (15)	0.0671 (15)	0.0543 (13)	0.0249 (12)	−0.0247 (12)	−0.0144 (11)
C20	0.0573 (13)	0.0598 (13)	0.0472 (12)	0.0106 (11)	−0.0181 (10)	−0.0116 (10)
C21	0.0596 (13)	0.0561 (13)	0.0490 (12)	0.0106 (11)	−0.0195 (10)	−0.0081 (10)
C22	0.115 (2)	0.0891 (19)	0.0877 (19)	0.0411 (17)	−0.0562 (18)	−0.0157 (15)
C23	0.0633 (14)	0.0582 (13)	0.0478 (12)	0.0019 (11)	−0.0185 (11)	−0.0124 (10)
C24	0.0715 (17)	0.0837 (19)	0.092 (2)	−0.0104 (14)	−0.0261 (15)	0.0034 (16)
C25	0.107 (2)	0.086 (2)	0.100 (2)	−0.0264 (19)	−0.025 (2)	0.0139 (18)
C26	0.149 (3)	0.0630 (17)	0.0606 (16)	−0.011 (2)	−0.0398 (19)	0.0025 (13)
C27	0.114 (2)	0.0696 (17)	0.0803 (18)	0.0118 (17)	−0.0540 (18)	−0.0101 (14)
C28	0.0756 (16)	0.0585 (14)	0.0708 (15)	0.0037 (12)	−0.0347 (13)	−0.0059 (12)
S1	0.0722 (4)	0.0584 (4)	0.0657 (4)	0.0089 (3)	−0.0312 (3)	−0.0185 (3)
S2	0.0651 (4)	0.0846 (5)	0.0711 (4)	0.0146 (3)	−0.0318 (3)	−0.0135 (3)

Geometric parameters (Å, º)

C1—C6	1.389 (3)	C14—H14	0.9300
C1—C2	1.403 (3)	C15—C16	1.348 (4)
C1—C7	1.490 (3)	C15—H15	0.9300
C2—C3	1.403 (3)	C16—C17	1.380 (3)
C2—C18	1.475 (3)	C16—H16	0.9300
C3—C4	1.373 (4)	C17—H17	0.9300
C3—H3	0.9300	C18—C19	1.377 (3)
C4—C5	1.367 (4)	C18—C21	1.427 (3)
C4—H4	0.9300	C19—C22	1.505 (3)
C5—C6	1.390 (4)	C19—S2	1.720 (3)
C5—H5	0.9300	C20—C21	1.354 (3)
C6—H6	0.9300	C20—C23	1.468 (3)

C7—C8	1.364 (3)	C20—S2	1.730 (2)
C7—C10	1.422 (3)	C21—H21	0.9300
C8—C11	1.500 (3)	C22—H22A	0.9600
C8—S1	1.718 (2)	C22—H22B	0.9600
C9—C10	1.356 (3)	C22—H22C	0.9600
C9—C12	1.469 (3)	C23—C24	1.373 (3)
C9—S1	1.727 (2)	C23—C28	1.384 (3)
C10—H10	0.9300	C24—C25	1.367 (4)
C11—H11A	0.9600	C24—H24	0.9300
C11—H11B	0.9600	C25—C26	1.366 (4)
C11—H11C	0.9600	C25—H25	0.9300
C12—C17	1.390 (3)	C26—C27	1.362 (4)
C12—C13	1.394 (3)	C26—H26	0.9300
C13—C14	1.375 (3)	C27—C28	1.388 (3)
C13—H13	0.9300	C27—H27	0.9300
C14—C15	1.376 (4)	C28—H28	0.9300

C6—C1—C2	119.4 (2)	C16—C15—H15	119.9
C6—C1—C7	120.1 (2)	C14—C15—H15	119.9
C2—C1—C7	120.50 (19)	C15—C16—C17	120.8 (2)
C1—C2—C3	118.4 (2)	C15—C16—H16	119.6
C1—C2—C18	121.09 (18)	C17—C16—H16	119.6
C3—C2—C18	120.4 (2)	C16—C17—C12	120.1 (2)
C4—C3—C2	121.2 (3)	C16—C17—H17	119.9
C4—C3—H3	119.4	C12—C17—H17	119.9
C2—C3—H3	119.4	C19—C18—C21	111.2 (2)
C5—C4—C3	120.2 (3)	C19—C18—C2	126.3 (2)
C5—C4—H4	119.9	C21—C18—C2	122.4 (2)
C3—C4—H4	119.9	C18—C19—C22	129.2 (2)
C4—C5—C6	120.1 (3)	C18—C19—S2	111.29 (17)
C4—C5—H5	120.0	C22—C19—S2	119.5 (2)
C6—C5—H5	120.0	C21—C20—C23	127.9 (2)
C1—C6—C5	120.7 (3)	C21—C20—S2	109.85 (16)
C1—C6—H6	119.7	C23—C20—S2	122.28 (18)
C5—C6—H6	119.7	C20—C21—C18	114.9 (2)
C8—C7—C10	112.25 (19)	C20—C21—H21	122.5
C8—C7—C1	123.57 (19)	C18—C21—H21	122.5
C10—C7—C1	124.11 (19)	C19—C22—H22A	109.5
C7—C8—C11	128.1 (2)	C19—C22—H22B	109.5
C7—C8—S1	110.85 (16)	H22A—C22—H22B	109.5
C11—C8—S1	121.04 (16)	C19—C22—H22C	109.5
C10—C9—C12	129.5 (2)	H22A—C22—H22C	109.5
C10—C9—S1	109.77 (16)	H22B—C22—H22C	109.5
C12—C9—S1	120.54 (15)	C24—C23—C28	117.4 (2)
C9—C10—C7	114.25 (19)	C24—C23—C20	122.3 (2)
C9—C10—H10	122.9	C28—C23—C20	120.3 (2)
C7—C10—H10	122.9	C25—C24—C23	121.8 (3)
C8—C11—H11A	109.5	C25—C24—H24	119.1

C8—C11—H11B	109.5	C23—C24—H24	119.1
H11A—C11—H11B	109.5	C26—C25—C24	120.3 (3)
C8—C11—H11C	109.5	C26—C25—H25	119.9
H11A—C11—H11C	109.5	C24—C25—H25	119.9
H11B—C11—H11C	109.5	C27—C26—C25	119.6 (3)
C17—C12—C13	118.3 (2)	C27—C26—H26	120.2
C17—C12—C9	121.3 (2)	C25—C26—H26	120.2
C13—C12—C9	120.39 (19)	C26—C27—C28	120.0 (3)
C14—C13—C12	120.4 (2)	C26—C27—H27	120.0
C14—C13—H13	119.8	C28—C27—H27	120.0
C12—C13—H13	119.8	C23—C28—C27	120.9 (2)
C13—C14—C15	120.0 (2)	C23—C28—H28	119.6
C13—C14—H14	120.0	C27—C28—H28	119.6
C15—C14—H14	120.0	C8—S1—C9	92.87 (10)
C16—C15—C14	120.3 (2)	C19—S2—C20	92.73 (11)

C6—C1—C2—C3	−1.0 (3)	C9—C12—C17—C16	177.9 (2)
C7—C1—C2—C3	179.48 (19)	C1—C2—C18—C19	131.3 (2)
C6—C1—C2—C18	175.0 (2)	C3—C2—C18—C19	−52.8 (3)
C7—C1—C2—C18	−4.6 (3)	C1—C2—C18—C21	−48.9 (3)
C1—C2—C3—C4	0.0 (3)	C3—C2—C18—C21	126.9 (2)
C18—C2—C3—C4	−176.0 (2)	C21—C18—C19—C22	177.8 (2)
C2—C3—C4—C5	1.3 (4)	C2—C18—C19—C22	−2.4 (4)
C3—C4—C5—C6	−1.6 (4)	C21—C18—C19—S2	0.5 (2)
C2—C1—C6—C5	0.7 (3)	C2—C18—C19—S2	−179.78 (16)
C7—C1—C6—C5	−179.8 (2)	C23—C20—C21—C18	−179.37 (19)
C4—C5—C6—C1	0.6 (4)	S2—C20—C21—C18	0.6 (2)
C6—C1—C7—C8	110.3 (3)	C19—C18—C21—C20	−0.7 (3)
C2—C1—C7—C8	−70.1 (3)	C2—C18—C21—C20	179.54 (18)
C6—C1—C7—C10	−73.0 (3)	C21—C20—C23—C24	−159.5 (2)
C2—C1—C7—C10	106.6 (2)	S2—C20—C23—C24	20.6 (3)
C10—C7—C8—C11	179.6 (2)	C21—C20—C23—C28	20.2 (3)
C1—C7—C8—C11	−3.3 (4)	S2—C20—C23—C28	−159.79 (17)
C10—C7—C8—S1	−0.4 (2)	C28—C23—C24—C25	0.5 (4)
C1—C7—C8—S1	176.70 (17)	C20—C23—C24—C25	−179.8 (3)
C12—C9—C10—C7	173.27 (19)	C23—C24—C25—C26	−0.3 (5)
S1—C9—C10—C7	−1.0 (2)	C24—C25—C26—C27	−0.6 (5)
C8—C7—C10—C9	0.9 (3)	C25—C26—C27—C28	1.2 (4)
C1—C7—C10—C9	−176.1 (2)	C24—C23—C28—C27	0.1 (3)
C10—C9—C12—C17	147.8 (2)	C20—C23—C28—C27	−179.5 (2)
S1—C9—C12—C17	−38.5 (3)	C26—C27—C28—C23	−1.0 (4)
C10—C9—C12—C13	−34.4 (3)	C7—C8—S1—C9	−0.15 (17)
S1—C9—C12—C13	139.39 (18)	C11—C8—S1—C9	179.88 (19)
C17—C12—C13—C14	0.7 (3)	C10—C9—S1—C8	0.66 (17)
C9—C12—C13—C14	−177.3 (2)	C12—C9—S1—C8	−174.21 (17)
C12—C13—C14—C15	−0.2 (4)	C18—C19—S2—C20	−0.12 (17)
C13—C14—C15—C16	−0.9 (4)	C22—C19—S2—C20	−177.74 (19)
C14—C15—C16—C17	1.6 (4)	C21—C20—S2—C19	−0.27 (16)

C15—C16—C17—C12	−1.1 (4)	C23—C20—S2—C19	179.69 (17)
C13—C12—C17—C16	0.0 (3)		