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4,4′-Bis[2-(3,4-dibutyl-2-thienylethynyl)]biphenyl

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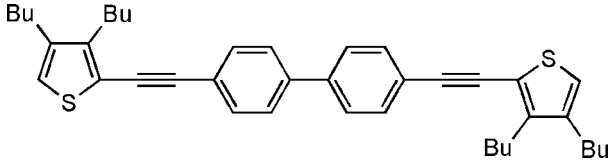
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.067; wR factor = 0.241; data-to-parameter ratio = 18.9.

The molecule of the title compound, $C_{40}H_{46}S_2$, reveals C_i symmetry. An inversion centre is located at the mid-point of the C—C bond of the biphenyl unit; the asymmetric unit comprises one-half of the molecule. The conjugated backbone is nearly planar, with a mean deviation of 0.041 Å.

Related literature

For general background, see: Brad Wan *et al.* (2000); Cornil *et al.* (2001); Grosshenny *et al.* (1997); Huang & Tour (1998); Tour (1996). For related structures, see: Baudour (1972); Charbonneau & Delugeard (1977); Domenicano *et al.* (1975); Robertson (1961). For the synthesis, see: Liu *et al.* (2005).



Experimental

Crystal data

$C_{40}H_{46}S_2$
M_r = 590.89
Triclinic, $P\overline{1}$
a = 9.2040 (18) Å
b = 9.3640 (19) Å
c = 10.582 (2) Å
α = 85.69 (3)°
β = 85.18 (3)°
γ = 69.41 (3)°
V = 849.7 (3) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 0.18 mm^{-1}
T = 293 (2) K
0.62 × 0.40 × 0.07 mm

Data collection

Rigaku R-AXIS RAPID IP diffractometer
Absorption correction: empirical (using intensity measurements) (*ABSCOR*; Higashi, 1995)
T_{min} = 0.805, T_{max} = 0.992
3595 measured reflections
3595 independent reflections
2287 reflections with $I > 2\sigma(I)$

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.067
$wR(F^2)$ = 0.241
S = 1.07
3595 reflections
190 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.44 e Å^{-3}
$\Delta\rho_{min}$ = −0.42 e Å^{-3}

Data collection: *RAPID-AUTO* (Rigaku, 2001); cell refinement: *RAPID-AUTO*; data reduction: *RAPID-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); 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: KP2189).

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supporting information

Acta Cryst. (2008). E**64**, o2306 [doi:10.1107/S1600536808036143]

4,4′-Bis[2-(3,4-dibutyl-2-thienylethynyl)]biphenyl

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S1. Comment

The synthesis and characterization of nanometer-sized conjugated molecules of precise length and constitution are of widespread interest, which is due to their electroconductive, magnetic, and optical properties (Tour, 1996; Huang & Tour, 1998; Grosshenny *et al.*, 1997; Brad Wan *et al.*, 2000). Generally, crystal structure of a molecule is important for better understanding of its properties. Therefore, structures of oligothiophene single crystals have been reported. The field of molecular organic semiconductors is being revolutionized by the availability of ultrahigh purity single crystals that have allowed the demonstration of phenomena long thought to be restricted to inorganic semiconductors (Cornil *et al.*, 2001).

The molecule of the title compound (Fig. 1) is centrosymmetric. An asymmetric unit comprises a half on the molecule. The inversion centre is located in the middle of C3—C3i bond. Conjugated molecular skeleton is nearly planar; mean deviation from the best least-square plane is 0.041 Å. The endocyclic bond angles on the long molecular axis are less than the normal 120° value (they vary from 116.42–117.52°) whereas that situated out of this long molecular axis are greater than 120° (in the range 120.73–122.43°). This result agrees with those obtained for polyphenyls (Robertson, 1961; Baudour, 1972; Domenicano *et al.*, 1975; Charbonneau & Delugeard, 1977). The two thiophene rings, phenyl rings and C≡C are coplanar. The crystal packing is dominated by van der Waals interactions.

S2. Experimental

The synthesis of 4,4′-bis-[2-(3,4-dibutyl-2-thienylethynyl)]biphenyl was performed as previously described (Liu *et al.*, 2005).

Yellow needles were grown from an ethanol/hexane solution by slow evaporation.

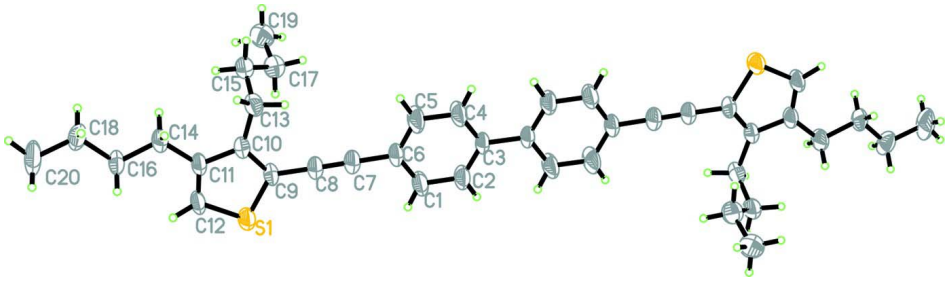

Figure 1

View of the title compound, showing the atom-labelling scheme and displacement ellipsoids at the 50% probability. To generate the molecule symmetry code -*x*, -*y*, -*z* + 2 is applied.

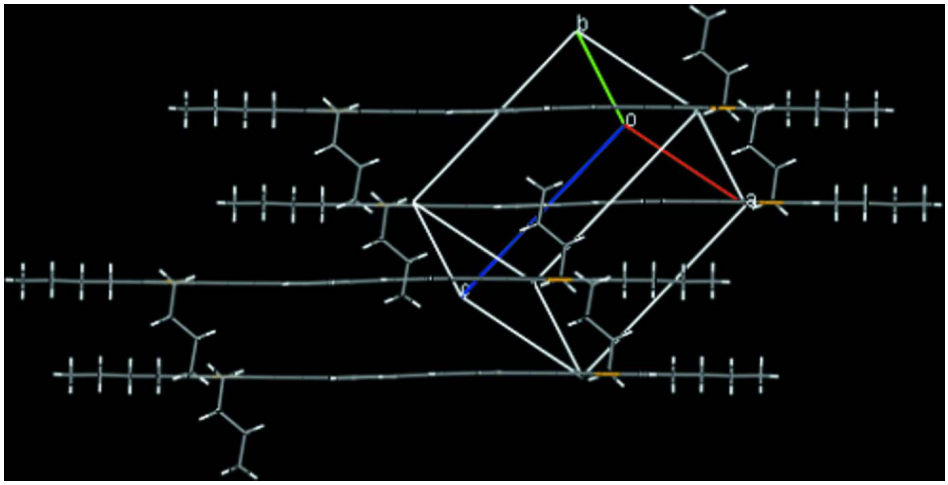

Figure 2

View of the packing mode along *a* axis of (I).

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$\beta = 85.18$ (3)°
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$V = 849.7$ (3) Å^3
$Z = 1$
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Needle, yellow
0.62 × 0.40 × 0.07 mm

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Rigaku R-AXIS RAPID IP diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 0.76 pixels mm^{-1}
Oscillation scans
Absorption correction: empirical (using intensity measurements) (*ABSCOR*; Higashi, 1995)
$T_{min} = 0.805$, $T_{max} = 0.992$
3595 measured reflections
3595 independent reflections
2287 reflections with $I > 2\sigma(I)$
$R_{int} = 0.000$
$\theta_{max} = 27.5°$, $\theta_{min} = 2.3°$
$h = 0 \rightarrow 11$
$k = -10 \rightarrow 12$
$l = -13 \rightarrow 13$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.067$
$wR(F^2) = 0.241$
$S = 1.07$
3595 reflections
190 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
$w = 1/[\sigma^2(F_o^2) + (0.1672P)^2 + 0.1626P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.44$ e Å^{-3}
$\Delta\rho_{min} = -0.42$ 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.34733 (8)	0.37884 (8)	0.02833 (7)	0.0512 (3)
C1	−0.2000 (4)	0.5223 (4)	0.3588 (3)	0.0657 (9)
H1A	−0.1334	0.5778	0.3558	0.079*
C2	−0.3290 (4)	0.5588 (4)	0.4443 (3)	0.0615 (8)
H2A	−0.3467	0.6388	0.4973	0.074*
C3	−0.4314 (3)	0.4808 (3)	0.4534 (2)	0.0393 (5)
C4	−0.4016 (4)	0.3655 (4)	0.3702 (4)	0.0750 (12)
H4A	−0.4696	0.3116	0.3721	0.090*
C5	−0.2733 (4)	0.3276 (5)	0.2840 (4)	0.0816 (13)
H5A	−0.2573	0.2494	0.2295	0.098*
C6	−0.1694 (3)	0.4041 (3)	0.2779 (2)	0.0439 (6)
C7	−0.0335 (3)	0.3631 (3)	0.1922 (3)	0.0476 (6)
C8	0.0798 (3)	0.3289 (3)	0.1211 (2)	0.0440 (6)
C9	0.2138 (3)	0.2853 (3)	0.0369 (2)	0.0415 (6)
C10	0.2565 (3)	0.1695 (3)	−0.0473 (2)	0.0387 (5)
C11	0.3994 (3)	0.1568 (3)	−0.1180 (2)	0.0419 (6)
C12	0.4587 (3)	0.2635 (3)	−0.0862 (3)	0.0497 (7)
H12	0.5507	0.2720	−0.1235	0.060*
C13	0.1620 (3)	0.0701 (3)	−0.0634 (3)	0.0463 (6)
H13A	0.0948	0.0719	0.0126	0.056*
H13B	0.2317	−0.0344	−0.0728	0.056*
C14	0.4717 (3)	0.0371 (3)	−0.2152 (3)	0.0515 (7)
H14A	0.4910	−0.0630	−0.1731	0.062*
H14B	0.3969	0.0498	−0.2784	0.062*
C15	0.0618 (3)	0.1215 (3)	−0.1791 (3)	0.0503 (6)
H15A	0.1267	0.1352	−0.2527	0.060*
H15B	0.0233	0.0412	−0.1960	0.060*
C16	0.6214 (3)	0.0406 (3)	−0.2825 (3)	0.0498 (7)
H16A	0.6965	0.0293	−0.2201	0.060*
H16B	0.6025	0.1390	−0.3274	0.060*
C17	−0.0748 (3)	0.2680 (4)	−0.1618 (3)	0.0575 (7)
H17A	−0.0376	0.3445	−0.1336	0.069*
H17B	−0.1465	0.2501	−0.0953	0.069*
C18	0.6894 (3)	−0.0855 (4)	−0.3767 (3)	0.0604 (8)
H18A	0.7095	−0.1838	−0.3314	0.073*

H18B	0.6131	−0.0752	−0.4380	0.073*
C19	−0.1626 (4)	0.3311 (4)	−0.2807 (3)	0.0680 (9)
H19A	−0.2477	0.4233	−0.2623	0.102*
H19B	−0.2019	0.2571	−0.3085	0.102*
H19C	−0.0936	0.3526	−0.3464	0.102*
C20	0.8373 (5)	−0.0823 (6)	−0.4465 (4)	0.0866 (13)
H20A	0.8747	−0.1641	−0.5037	0.130*
H20B	0.9140	−0.0944	−0.3866	0.130*
H20C	0.8177	0.0135	−0.4937	0.130*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0432 (4)	0.0556 (4)	0.0568 (5)	−0.0203 (3)	0.0164 (3)	−0.0206 (3)
C1	0.0576 (17)	0.080 (2)	0.070 (2)	−0.0398 (16)	0.0352 (15)	−0.0323 (17)
C2	0.0596 (17)	0.0696 (18)	0.0622 (18)	−0.0334 (15)	0.0336 (14)	−0.0329 (15)
C3	0.0314 (11)	0.0457 (12)	0.0341 (11)	−0.0071 (9)	0.0110 (9)	−0.0058 (9)
C4	0.0615 (18)	0.088 (2)	0.090 (2)	−0.0447 (18)	0.0481 (18)	−0.055 (2)
C5	0.068 (2)	0.090 (2)	0.097 (3)	−0.0424 (19)	0.054 (2)	−0.062 (2)
C6	0.0326 (11)	0.0505 (14)	0.0415 (13)	−0.0084 (10)	0.0130 (10)	−0.0066 (10)
C7	0.0395 (13)	0.0532 (14)	0.0433 (14)	−0.0099 (11)	0.0122 (11)	−0.0087 (11)
C8	0.0372 (12)	0.0506 (14)	0.0393 (13)	−0.0113 (11)	0.0109 (10)	−0.0059 (10)
C9	0.0326 (11)	0.0477 (13)	0.0404 (12)	−0.0116 (10)	0.0126 (10)	−0.0065 (10)
C10	0.0321 (11)	0.0443 (12)	0.0366 (12)	−0.0116 (9)	0.0080 (9)	−0.0025 (9)
C11	0.0315 (11)	0.0488 (13)	0.0406 (13)	−0.0098 (10)	0.0118 (9)	−0.0082 (10)
C12	0.0360 (12)	0.0596 (15)	0.0526 (15)	−0.0182 (11)	0.0201 (11)	−0.0148 (12)
C13	0.0430 (13)	0.0452 (13)	0.0514 (14)	−0.0190 (11)	0.0110 (11)	−0.0048 (11)
C14	0.0385 (13)	0.0582 (16)	0.0552 (16)	−0.0142 (12)	0.0173 (11)	−0.0212 (13)
C15	0.0452 (13)	0.0580 (15)	0.0509 (15)	−0.0225 (12)	0.0100 (11)	−0.0140 (12)
C16	0.0374 (13)	0.0617 (16)	0.0442 (14)	−0.0113 (12)	0.0149 (11)	−0.0129 (12)
C17	0.0475 (15)	0.0641 (18)	0.0589 (17)	−0.0165 (13)	0.0028 (13)	−0.0116 (14)
C18	0.0478 (15)	0.077 (2)	0.0428 (15)	−0.0039 (14)	0.0070 (12)	−0.0187 (14)
C19	0.0546 (18)	0.080 (2)	0.068 (2)	−0.0214 (17)	−0.0071 (15)	−0.0038 (17)
C20	0.063 (2)	0.111 (3)	0.061 (2)	−0.003 (2)	0.0313 (17)	−0.018 (2)

Geometric parameters (Å, º)

S1—C12	1.702 (3)	C13—H13A	0.9700
S1—C9	1.735 (3)	C13—H13B	0.9700
C1—C6	1.385 (4)	C14—C16	1.507 (3)
C1—C2	1.387 (4)	C14—H14A	0.9700
C1—H1A	0.9300	C14—H14B	0.9700
C2—C3	1.375 (4)	C15—C17	1.511 (4)
C2—H2A	0.9300	C15—H15A	0.9700
C3—C4	1.382 (4)	C15—H15B	0.9700
C3—C3^{i}	1.490 (4)	C16—C18	1.527 (4)
C4—C5	1.387 (4)	C16—H16A	0.9700
C4—H4A	0.9300	C16—H16B	0.9700

C5—C6	1.377 (4)	C17—C19	1.519 (5)
C5—H5A	0.9300	C17—H17A	0.9700
C6—C7	1.435 (3)	C17—H17B	0.9700
C7—C8	1.193 (3)	C18—C20	1.502 (5)
C8—C9	1.414 (3)	C18—H18A	0.9700
C9—C10	1.382 (3)	C18—H18B	0.9700
C10—C11	1.428 (3)	C19—H19A	0.9600
C10—C13	1.507 (4)	C19—H19B	0.9600
C11—C12	1.369 (4)	C19—H19C	0.9600
C11—C14	1.514 (3)	C20—H20A	0.9600
C12—H12	0.9300	C20—H20B	0.9600
C13—C15	1.539 (4)	C20—H20C	0.9600

C12—S1—C9	91.29 (12)	C11—C14—H14A	108.5
C6—C1—C2	120.7 (3)	C16—C14—H14B	108.5
C6—C1—H1A	119.7	C11—C14—H14B	108.5
C2—C1—H1A	119.7	H14A—C14—H14B	107.5
C3—C2—C1	122.4 (3)	C17—C15—C13	113.7 (2)
C3—C2—H2A	118.8	C17—C15—H15A	108.8
C1—C2—H2A	118.8	C13—C15—H15A	108.8
C2—C3—C4	116.4 (2)	C17—C15—H15B	108.8
C2—C3—C3^{i}	122.1 (3)	C13—C15—H15B	108.8
C4—C3—C3^{i}	121.5 (3)	H15A—C15—H15B	107.7
C3—C4—C5	122.0 (3)	C14—C16—C18	112.4 (2)
C3—C4—H4A	119.0	C14—C16—H16A	109.1
C5—C4—H4A	119.0	C18—C16—H16A	109.1
C6—C5—C4	121.1 (3)	C14—C16—H16B	109.1
C6—C5—H5A	119.5	C18—C16—H16B	109.1
C4—C5—H5A	119.5	H16A—C16—H16B	107.9
C5—C6—C1	117.5 (2)	C15—C17—C19	114.3 (3)
C5—C6—C7	121.7 (2)	C15—C17—H17A	108.7
C1—C6—C7	120.8 (2)	C19—C17—H17A	108.7
C8—C7—C6	179.8 (4)	C15—C17—H17B	108.7
C7—C8—C9	178.8 (3)	C19—C17—H17B	108.7
C10—C9—C8	126.9 (2)	H17A—C17—H17B	107.6
C10—C9—S1	111.52 (17)	C20—C18—C16	113.2 (3)
C8—C9—S1	121.6 (2)	C20—C18—H18A	108.9
C9—C10—C11	112.0 (2)	C16—C18—H18A	108.9
C9—C10—C13	123.8 (2)	C20—C18—H18B	108.9
C11—C10—C13	124.2 (2)	C16—C18—H18B	108.9
C12—C11—C10	111.9 (2)	H18A—C18—H18B	107.7
C12—C11—C14	126.0 (2)	C17—C19—H19A	109.5
C10—C11—C14	122.0 (2)	C17—C19—H19B	109.5
C11—C12—S1	113.24 (18)	H19A—C19—H19B	109.5
C11—C12—H12	123.4	C17—C19—H19C	109.5
S1—C12—H12	123.4	H19A—C19—H19C	109.5
C10—C13—C15	112.8 (2)	H19B—C19—H19C	109.5
C10—C13—H13A	109.0	C18—C20—H20A	109.5

C15—C13—H13A	109.0	C18—C20—H20B	109.5
C10—C13—H13B	109.0	H20A—C20—H20B	109.5
C15—C13—H13B	109.0	C18—C20—H20C	109.5
H13A—C13—H13B	107.8	H20A—C20—H20C	109.5
C16—C14—C11	115.3 (2)	H20B—C20—H20C	109.5
C16—C14—H14A	108.5		

C12—C11—C10—C9	−0.6 (4)	C4—C5—C6—C1	−1.5 (1)
C12—S1—C9—C10	0.1 (8)	C1—C2—C3—C4	−1.6 (1)
C10—C11—C12—S1	0.5 (1)	C5—C4—C3—C2	1.5 (1)
C11—C12—S1—C9	−0.2 (1)	C5—C6—C1—C2	1.4 (2)
C11—C10—C9—S1	0.4 (9)	C9—C8—C7—C6	93.5 (2)
C11—C10—C9—C8	−179.9 (8)	C10—C9—C8—C7	24.6 (9)
C12—S1—C9—C8	−179.7 (4)	S1—C9—C8—C7	−155.8 (2)
C7—C6—C5—C4	177.9 (5)	C5—C6—C7—C8	−117.5 (4)
C7—C6—C1—C2	−178.0 (5)	C1—C6—C7—C8	61.9 (1)
C6—C5—C4—C3	0.0 (4)	C4—C3—C3—C4	90.0 (1)
C6—C1—C2—C3	0.1 (5)		

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