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(2*E*)-3-(Biphenyl-4-yl)-1-(3-bromo-2-thienyl)prop-2-en-1-one

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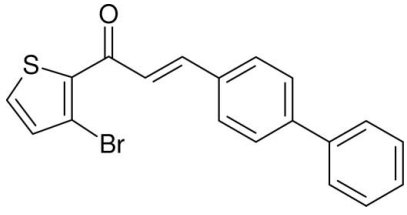
Key indicators: single-crystal X-ray study; T = 291 K; mean σ(C–C) = 0.005 Å; R factor = 0.046; wR factor = 0.139; data-to-parameter ratio = 15.6.

In the title compound, $C_{19}H_{13}BrOS$, the dihedral angles between the enone fragment and its adjacent thienyl (th) and phenylene (bz) rings are 8.0 (2) and 12.8 (2)°, respectively. The dihedral angle between the th and bz rings is 19.9 (2)° and that between the two rings of the biphenyl fragment is 28.49 (18)°. A C—H···O interaction may help to consolidate the crystal packing.

Related literature

For general background, see: Uchida *et al.* (1998); Dimmock *et al.* (1999). For related structures, see: Butcher *et al.* (2007); Harrison *et al.* (2006). For reference structural data, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{19}H_{13}BrOS$
M_r = 369.26
Monoclinic, $P2_1/c$
a = 8.8345 (5) Å
b = 11.7429 (6) Å
c = 15.2162 (8) Å
β = 92.817 (1)°
V = 1576.66 (15) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 2.74 mm^{-1}
T = 291 (2) K
0.51 × 0.40 × 0.40 mm

Data collection

Bruker SMART 1000 CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1999)
T_{min} = 0.336, T_{max} = 0.409
(expected range = 0.275–0.334)
9060 measured reflections
3101 independent reflections
2252 reflections with $I > 2\sigma(I)$
R_{int} = 0.021

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.139
S = 1.06
3101 reflections
199 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.63 e Å^{-3}
$\Delta\rho_{min}$ = −0.61 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C10—H10···O1^{i}	0.93	2.54	3.321 (5)	142

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

Data collection: *SMART* (Bruker, 1999); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); 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: NG2313).

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supplementary materials

Acta Cryst. (2007). E**63**, o3898 [**doi:10.1107/S1600536807041141**]

(2*E*)-3-(Biphenyl-4-yl)-1-(3-bromo-2-thienyl)prop-2-en-1-one

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Comment

The title compound, (I), (Fig. 1), was prepared as part of our ongoing studies (Harrison *et al.*, 2006; Butcher *et al.*, 2007) of the non-linear optical (NLO) properties (Uchida *et al.*, 1998) and crystal structures of chalcone derivatives. Chalcones also display a wide variety of pharmacological effects (Dimmock *et al.*, 1999). Compound (I) is centrosymmetric, thus its second harmonic generation (SHG) response is zero.

The geometrical parameters for (I) mostly fall within their expected ranges (Allen *et al.*, 1995). The C4—C3—Br1 angle of 127.0 (3)° is somewhat obtuse, perhaps due to steric repulsion between Br1 and H6 (H···Br = 2.69 Å). The dihedral angles between the enone (C5/C6/C7/O1) fragment and its adjacent thienyl (C1–C4/S1) and benzne (C8–C13) rings are 8.0 (2)° and 12.8 (2)°, respectively. The dihedral angle between the thienyl and C8—C13 benzne ring systems is 19.9 (2)° and the dihedral angle between the two benzene ring planes (C8–C13 and C14–C19) of the biphenyl fragment is 28.49 (18)°. A possible weak intermolecular C—H···O interaction (Table 1) resulting in [001] chains of molecules may help to establish the crystal packing in (I).

Experimental

Biphenyl-4-carbaldehyde (1.82 g, 0.01 mol) in ethanol (30 ml) was mixed with 1-(3-bromo-2-thienyl)ethanone (2.05 ml, 0.01 mol) and the mixture was treated with 7 ml of 10% aqueous KOH and stirred for 8 h. The precipitate obtained was filtered, washed with ethanol and dried. Colourless chunks of (I) were recrystallized from ethyl acetate (m.p.: 404–406 K). Analysis for $C_{19}H_{13}BrOS$: Found (calculated): C 61.71 (61.80); H 3.49 (3.55); S 8.61% (8.68%).

Refinement

The rather large, anisotropic displacement ellipsoids of C1, C2 and S1 are suggestive of disorder, but attempts to model this were not successful. The hydrogen atoms were geometrically placed (C—H = 0.93 Å) and refined as riding with U_{iso}(H) = 1.2U_{eq}(carrier).

Figures

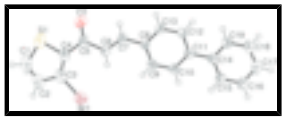


Fig. 1. View of the molecular structure of (I) showing 50% displacement ellipsoids (arbitrary spheres for the H atoms).

(2E)-3-(Biphenyl-4-yl)-1-(3-bromo-2-thienyl)prop-2-en-1-one

Crystal data

$C_{19}H_{13}BrOS$	F_{000} = 744
M_r = 369.26	D_x = 1.556 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 3780 reflections
a = 8.8345 (5) Å	θ = 2.3–26.0º
b = 11.7429 (6) Å	μ = 2.74 mm^{-1}
c = 15.2162 (8) Å	T = 291 (2) K
β = 92.817 (1)º	Chunk, colourless
V = 1576.66 (15) Å^3	0.51 × 0.40 × 0.40 mm
Z = 4	

Data collection

Bruker SMART1000 CCD diffractometer	3101 independent reflections
Radiation source: fine-focus sealed tube	2252 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.021
T = 291(2) K	θ_{max} = 26.0º
ω scans	θ_{min} = 2.2º
Absorption correction: multi-scan (SADABS; Bruker, 1999)	h = −10→10
T_{min} = 0.336, T_{max} = 0.409	k = −13→14
9060 measured reflections	l = −18→18

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.046	H-atom parameters constrained
$wR(F^2)$ = 0.139	$w = 1/[\sigma^2(F_o^2) + (0.0796P)^2 + 0.7492P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.06	$(\Delta/\sigma)_{max} < 0.001$
3101 reflections	$\Delta\rho_{max}$ = 1.63 e Å^{-3}
199 parameters	$\Delta\rho_{min}$ = −0.61 e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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 $F^2 > 2\text{sigma}(F^2)$ 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 ($Å^2$)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.2215 (7)	−0.1259 (4)	0.3559 (4)	0.0859 (18)
H1	0.1736	−0.1909	0.3334	0.103*
C2	0.1833 (5)	−0.0763 (4)	0.4308 (4)	0.0673 (13)
H2	0.1066	−0.1015	0.4658	0.081*
C3	0.2759 (4)	0.0202 (3)	0.4495 (3)	0.0528 (10)
C4	0.3794 (4)	0.0426 (3)	0.3897 (3)	0.0470 (9)
C5	0.4951 (4)	0.1313 (3)	0.3766 (3)	0.0456 (9)
C6	0.5326 (4)	0.2158 (3)	0.4463 (2)	0.0437 (8)
H6	0.4967	0.2059	0.5023	0.052*
C7	0.6174 (4)	0.3059 (3)	0.4292 (2)	0.0431 (8)
H7	0.6468	0.3120	0.3715	0.052*
C8	0.6705 (4)	0.3961 (3)	0.4883 (2)	0.0382 (7)
C9	0.6416 (4)	0.4009 (3)	0.5778 (2)	0.0413 (8)
H9	0.5830	0.3443	0.6021	0.050*
C10	0.6981 (4)	0.4878 (3)	0.6306 (2)	0.0401 (8)
H10	0.6769	0.4885	0.6899	0.048*
C11	0.7865 (4)	0.5750 (3)	0.5974 (2)	0.0360 (7)
C12	0.8154 (5)	0.5704 (3)	0.5082 (2)	0.0448 (8)
H12	0.8736	0.6271	0.4837	0.054*
C13	0.7589 (4)	0.4833 (3)	0.4558 (2)	0.0470 (9)
H13	0.7804	0.4826	0.3966	0.056*
C14	0.8449 (4)	0.6702 (3)	0.6537 (2)	0.0372 (7)
C15	0.7666 (5)	0.7065 (3)	0.7262 (2)	0.0466 (9)
H15	0.6784	0.6689	0.7404	0.056*
C16	0.8182 (5)	0.7973 (4)	0.7770 (3)	0.0554 (10)
H16	0.7641	0.8204	0.8248	0.066*
C17	0.9485 (5)	0.8537 (4)	0.7576 (3)	0.0567 (10)
H17	0.9829	0.9145	0.7922	0.068*
C18	1.0277 (5)	0.8198 (3)	0.6869 (3)	0.0556 (10)
H18	1.1160	0.8578	0.6735	0.067*
C19	0.9766 (4)	0.7292 (3)	0.6353 (3)	0.0482 (9)
H19	1.0313	0.7072	0.5875	0.058*
O1	0.5569 (4)	0.1320 (3)	0.3065 (2)	0.0685 (9)

S1	0.36513 (15)	−0.06020 (11)	0.30495 (8)	0.0698 (4)
Br1	0.24246 (5)	0.10336 (4)	0.55286 (3)	0.0651 (2)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.084 (4)	0.046 (3)	0.124 (5)	−0.013 (2)	−0.048 (3)	−0.003 (3)
C2	0.058 (3)	0.050 (3)	0.092 (4)	−0.014 (2)	−0.021 (2)	0.008 (3)
C3	0.045 (2)	0.043 (2)	0.069 (3)	0.0021 (17)	−0.0107 (18)	0.0043 (19)
C4	0.043 (2)	0.034 (2)	0.062 (2)	0.0016 (15)	−0.0115 (17)	−0.0055 (17)
C5	0.040 (2)	0.038 (2)	0.057 (2)	0.0045 (15)	−0.0042 (16)	−0.0086 (16)
C6	0.0443 (19)	0.044 (2)	0.0432 (18)	−0.0037 (16)	0.0030 (15)	−0.0050 (16)
C7	0.051 (2)	0.0366 (19)	0.0422 (18)	0.0025 (16)	0.0033 (15)	−0.0012 (15)
C8	0.0426 (19)	0.0294 (17)	0.0425 (18)	0.0002 (14)	0.0022 (14)	0.0017 (14)
C9	0.0446 (19)	0.0345 (19)	0.0455 (19)	−0.0039 (15)	0.0081 (15)	0.0050 (15)
C10	0.0459 (19)	0.0381 (19)	0.0370 (17)	−0.0006 (15)	0.0073 (14)	0.0029 (15)
C11	0.0393 (18)	0.0284 (16)	0.0403 (17)	0.0036 (13)	0.0008 (14)	0.0045 (13)
C12	0.061 (2)	0.0329 (18)	0.0415 (18)	−0.0087 (16)	0.0099 (16)	0.0048 (15)
C13	0.067 (2)	0.038 (2)	0.0363 (18)	−0.0060 (18)	0.0109 (16)	0.0004 (15)
C14	0.0434 (19)	0.0310 (18)	0.0366 (17)	0.0037 (14)	−0.0023 (14)	0.0032 (13)
C15	0.052 (2)	0.044 (2)	0.0435 (19)	−0.0034 (17)	0.0026 (16)	−0.0032 (16)
C16	0.070 (3)	0.052 (2)	0.044 (2)	0.001 (2)	0.0022 (18)	−0.0101 (18)
C17	0.067 (3)	0.041 (2)	0.060 (2)	0.000 (2)	−0.016 (2)	−0.0087 (19)
C18	0.050 (2)	0.045 (2)	0.071 (3)	−0.0093 (18)	−0.0031 (19)	−0.0020 (19)
C19	0.047 (2)	0.042 (2)	0.056 (2)	−0.0022 (17)	0.0067 (16)	−0.0041 (17)
O1	0.074 (2)	0.069 (2)	0.0636 (18)	−0.0089 (16)	0.0186 (16)	−0.0273 (15)
S1	0.0722 (8)	0.0585 (7)	0.0765 (8)	0.0023 (6)	−0.0177 (6)	−0.0149 (6)
Br1	0.0550 (3)	0.0701 (3)	0.0708 (3)	−0.0029 (2)	0.0100 (2)	0.0002 (2)

Geometric parameters (Å, °)

C1—C2	1.339 (8)	C10—C11	1.397 (5)
C1—S1	1.703 (7)	C10—H10	0.9300
C1—H1	0.9300	C11—C12	1.395 (5)
C2—C3	1.418 (6)	C11—C14	1.484 (5)
C2—H2	0.9300	C12—C13	1.376 (5)
C3—C4	1.348 (6)	C12—H12	0.9300
C3—Br1	1.887 (4)	C13—H13	0.9300
C4—C5	1.480 (5)	C14—C19	1.395 (5)
C4—S1	1.766 (4)	C14—C15	1.397 (5)
C5—O1	1.222 (5)	C15—C16	1.381 (5)
C5—C6	1.478 (5)	C15—H15	0.9300
C6—C7	1.330 (5)	C16—C17	1.373 (6)
C6—H6	0.9300	C16—H16	0.9300
C7—C8	1.452 (5)	C17—C18	1.371 (6)
C7—H7	0.9300	C17—H17	0.9300
C8—C13	1.393 (5)	C18—C19	1.384 (5)
C8—C9	1.399 (5)	C18—H18	0.9300
C9—C10	1.378 (5)	C19—H19	0.9300

C9—H9	0.9300		
C2—C1—S1	114.5 (4)	C11—C10—H10	119.1
C2—C1—H1	122.7	C12—C11—C10	117.1 (3)
S1—C1—H1	122.7	C12—C11—C14	121.1 (3)
C1—C2—C3	110.6 (5)	C10—C11—C14	121.8 (3)
C1—C2—H2	124.7	C13—C12—C11	121.0 (3)
C3—C2—H2	124.7	C13—C12—H12	119.5
C4—C3—C2	115.1 (4)	C11—C12—H12	119.5
C4—C3—Br1	127.0 (3)	C12—C13—C8	122.3 (3)
C2—C3—Br1	117.9 (4)	C12—C13—H13	118.8
C3—C4—C5	136.4 (4)	C8—C13—H13	118.8
C3—C4—S1	109.5 (3)	C19—C14—C15	117.2 (3)
C5—C4—S1	114.1 (3)	C19—C14—C11	121.9 (3)
O1—C5—C6	121.9 (4)	C15—C14—C11	120.9 (3)
O1—C5—C4	117.6 (3)	C16—C15—C14	121.0 (4)
C6—C5—C4	120.5 (3)	C16—C15—H15	119.5
C7—C6—C5	120.1 (3)	C14—C15—H15	119.5
C7—C6—H6	119.9	C17—C16—C15	120.6 (4)
C5—C6—H6	119.9	C17—C16—H16	119.7
C6—C7—C8	128.8 (3)	C15—C16—H16	119.7
C6—C7—H7	115.6	C18—C17—C16	119.6 (4)
C8—C7—H7	115.6	C18—C17—H17	120.2
C13—C8—C9	116.6 (3)	C16—C17—H17	120.2
C13—C8—C7	119.1 (3)	C17—C18—C19	120.2 (4)
C9—C8—C7	124.3 (3)	C17—C18—H18	119.9
C10—C9—C8	121.3 (3)	C19—C18—H18	119.9
C10—C9—H9	119.4	C18—C19—C14	121.4 (4)
C8—C9—H9	119.4	C18—C19—H19	119.3
C9—C10—C11	121.7 (3)	C14—C19—H19	119.3
C9—C10—H10	119.1	C1—S1—C4	90.3 (2)
S1—C1—C2—C3	−0.7 (5)	C10—C11—C12—C13	−0.1 (5)
C1—C2—C3—C4	0.7 (6)	C14—C11—C12—C13	−178.8 (3)
C1—C2—C3—Br1	−179.7 (3)	C11—C12—C13—C8	0.2 (6)
C2—C3—C4—C5	177.4 (4)	C9—C8—C13—C12	−0.1 (6)
Br1—C3—C4—C5	−2.1 (7)	C7—C8—C13—C12	−178.9 (4)
C2—C3—C4—S1	−0.4 (4)	C12—C11—C14—C19	−28.0 (5)
Br1—C3—C4—S1	−179.9 (2)	C10—C11—C14—C19	153.3 (3)
C3—C4—C5—O1	−170.5 (4)	C12—C11—C14—C15	150.0 (4)
S1—C4—C5—O1	7.2 (5)	C10—C11—C14—C15	−28.6 (5)
C3—C4—C5—C6	9.1 (7)	C19—C14—C15—C16	0.1 (5)
S1—C4—C5—C6	−173.2 (3)	C11—C14—C15—C16	−178.0 (3)
O1—C5—C6—C7	10.7 (6)	C14—C15—C16—C17	−0.3 (6)
C4—C5—C6—C7	−169.0 (3)	C15—C16—C17—C18	0.3 (6)
C5—C6—C7—C8	−178.0 (3)	C16—C17—C18—C19	0.0 (6)
C6—C7—C8—C13	−179.9 (4)	C17—C18—C19—C14	−0.2 (6)
C6—C7—C8—C9	1.5 (6)	C15—C14—C19—C18	0.1 (5)
C13—C8—C9—C10	0.0 (5)	C11—C14—C19—C18	178.2 (3)
C7—C8—C9—C10	178.6 (3)	C2—C1—S1—C4	0.4 (4)

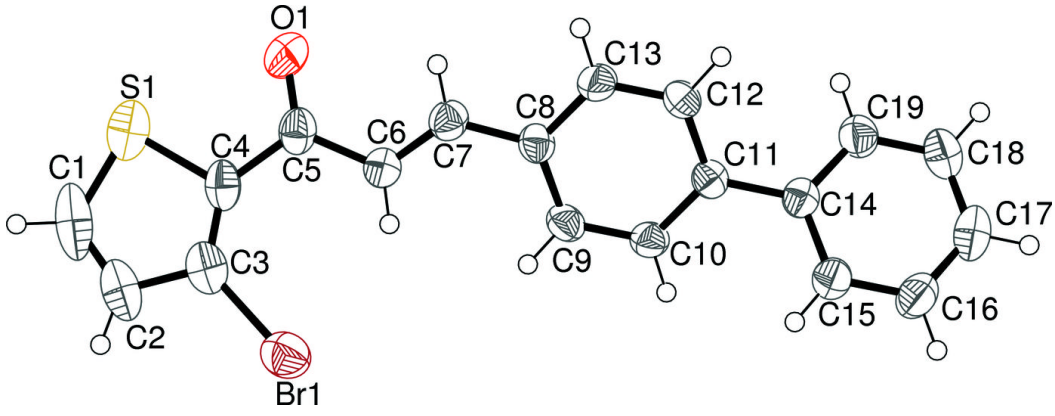
C8—C9—C10—C11	0.1 (5)	C3—C4—S1—C1	0.0 (3)
C9—C10—C11—C12	0.0 (5)	C5—C4—S1—C1	−178.3 (3)
C9—C10—C11—C14	178.7 (3)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C10—H10···O1^{i}	0.93	2.54	3.321 (5)	142

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

Fig. 1


O1
S1
C13
C12
C19
C8
C6
C7
C4
C5
C1
C11
C18
C14
C17
C3
C9
C10
C15
C16
C2
Br1