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# Bis(2-iodothiophen-3-yl)methanone

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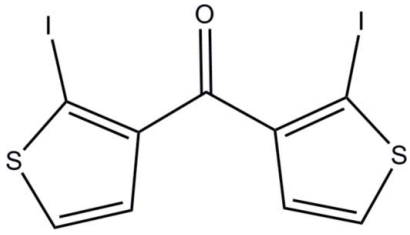
Key indicators: single-crystal X-ray study; $T$ = 298 K; mean $\sigma$(C–C) = 0.007 Å; $R$ factor = 0.043; $wR$ factor = 0.103; data-to-parameter ratio = 23.6.

In the title molecule, $C_9H_4I_2OS_2$, the two five-membered rings form a dihedral angle of 64.2 (2)°. In the crystal, weak intermolecular C—H···O hydrogen bonds link the molecules into layers parallel to the *ab* plane. The crystal packing exhibits short C···I contacts of 3.442 (5) Å between the molecules of adjacent layers.

## Related literature

For general background to the synthesis of thiophene-based conjugated polymers, see: Cheng *et al.* (2009). For the synthesis of the title compound, see: Brzezinski & Reynolds (2002).



## Experimental

### Crystal data

$C_9H_4I_2OS_2$
$M_r$ = 446.04
Monoclinic, $P2_1/n$
$a$ = 10.1908 (9) Å
$b$ = 11.4832 (10) Å
$c$ = 10.9083 (10) Å
$\beta$ = 107.600 (1)°
$V$ = 1216.77 (19) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 5.48 mm$^{-1}$
$T$ = 298 K
0.16 × 0.12 × 0.10 mm

### Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.474, $T_{max}$ = 0.610
8022 measured reflections
3003 independent reflections
2541 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.084

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.103
$S$ = 1.11
3003 reflections
127 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.08 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.67 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C4—H4···O1$^{i}$ | 0.93 | 2.51 | 3.233 (7) | 135 |
| C8—H8···O1$^{ii}$ | 0.93 | 2.40 | 3.324 (6) | 172 |

Symmetry codes: (i) $-x+\frac{3}{2}, y-\frac{1}{2}, -z+\frac{3}{2}$; (ii) $-x+\frac{1}{2}, y-\frac{1}{2}, -z+\frac{3}{2}$.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; 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: CV5050).

## References

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# supplementary materials

*Acta Cryst.* (2011). E**67**, o691 [ **doi:10.1107/S1600536811005472** ]

# Bis(2-iodothiophen-3-yl)methanone

**H. Cheng**

## Comment

The title compound, (I), is an important organic intermediate for the synthesis of conjugated polymers for organic solar cell applications (Brzezinski & Reynolds, 2002; Cheng *et al.*, 2009). In (I) (Fig. 1), two five-membered rings form a dihedral angle of 64.2 (2)°. Weak intermolecular C—H···O hydrogen bonds link the molecules into layers parallel to *ab* plane. The crystal packing exhibits short C···I contacts of 3.442 (5) Å between the molecules from the neighbouring layers.

## Experimental

The title compound was synthesized according to the reported method by Brzezinski & Reynolds (2002). After being dissolved in the mixture of MeOH-Hexane (1:3) for seversal days, colourless crystals suitable for single-crystal X-ray diffraction were obtained.

## Refinement

All hydrogen atoms were positioned geometrically (C—H = 0.93 Å) and allowed to ride on their parent atoms, with $U_{iso}$(H) = 1.2 $U_{eq}$(C).

## Figures

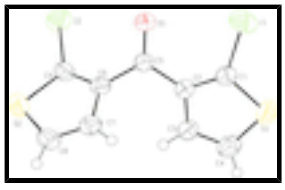

Fig. 1. The title molecule with the atom-numbering scheme. The displacement ellipsoids are drawn at the 50% probability level.

## Bis(2-iodothiophen-3-yl)methanone

*Crystal data*

| | |
|---|---|
| $C_9H_4I_2OS_2$ | $F(000)$ = 816 |
| $M_r$ = 446.04 | $D_x$ = 2.435 Mg m$^{-3}$ |
| Monoclinic, $P2_1/n$ | Mo $K\alpha$ radiation, λ = 0.71073 Å |
| Hall symbol: -P 2yn | Cell parameters from 2906 reflections |
| $a$ = 10.1908 (9) Å | θ = 2.4–26.9° |
| $b$ = 11.4832 (10) Å | μ = 5.48 mm$^{-1}$ |
| $c$ = 10.9083 (10) Å | $T$ = 298 K |
| β = 107.600 (1)° | Block, colourless |

$V$ = 1216.77 (19) Å$^3$
$Z$ = 4

0.16 × 0.12 × 0.10 mm

*Data collection*

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
graphite
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.474, $T_{max}$ = 0.610
8022 measured reflections

3003 independent reflections
2541 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.084
$\theta_{max}$ = 28.2°, $\theta_{min}$ = 2.4°
$h = -13 \rightarrow 7$
$k = -15 \rightarrow 12$
$l = -14 \rightarrow 14$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.103
$S$ = 1.11
3003 reflections
127 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
$w = 1/[\sigma^2(F_o^2) + (0.0342P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 1.08 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.67 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* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| C1 | 0.7428 (5) | 0.3871 (4) | 0.9017 (5) | 0.0377 (10) |
| C2 | 0.6198 (5) | 0.3657 (4) | 0.8086 (4) | 0.0328 (9) |
| C3 | 0.6258 (5) | 0.2588 (4) | 0.7431 (5) | 0.0392 (11) |
| H3 | 0.5515 | 0.2291 | 0.6783 | 0.047* |

| | | | | |
|---|---|---|---|---|
| C4 | 0.7482 (6) | 0.2053 (5) | 0.7835 (5) | 0.0486 (13) |
| H4 | 0.7688 | 0.1359 | 0.7495 | 0.058* |
| C5 | 0.5029 (5) | 0.4469 (4) | 0.7705 (5) | 0.0349 (10) |
| C6 | 0.3643 (5) | 0.3977 (4) | 0.7066 (5) | 0.0350 (10) |
| C7 | 0.3112 (6) | 0.2950 (4) | 0.7492 (5) | 0.0438 (12) |
| H7 | 0.3628 | 0.2488 | 0.8166 | 0.053* |
| C8 | 0.1801 (6) | 0.2717 (5) | 0.6827 (6) | 0.0499 (13) |
| H8 | 0.1300 | 0.2093 | 0.6996 | 0.060* |
| C9 | 0.2680 (5) | 0.4481 (4) | 0.6055 (5) | 0.0372 (10) |
| I1 | 0.79608 (5) | 0.51950 (4) | 1.03536 (4) | 0.05838 (16) |
| I2 | 0.28839 (4) | 0.58784 (3) | 0.49276 (4) | 0.05046 (14) |
| O1 | 0.5191 (4) | 0.5512 (3) | 0.7870 (5) | 0.0569 (10) |
| S1 | 0.86152 (15) | 0.28059 (13) | 0.90534 (14) | 0.0517 (4) |
| S2 | 0.11662 (14) | 0.37150 (14) | 0.56270 (15) | 0.0512 (3) |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C1 | 0.043 (3) | 0.035 (3) | 0.034 (2) | 0.002 (2) | 0.012 (2) | 0.0020 (19) |
| C2 | 0.036 (3) | 0.033 (2) | 0.030 (2) | 0.0025 (19) | 0.011 (2) | 0.0009 (18) |
| C3 | 0.043 (3) | 0.037 (3) | 0.034 (2) | 0.004 (2) | 0.006 (2) | −0.003 (2) |
| C4 | 0.059 (4) | 0.044 (3) | 0.042 (3) | 0.010 (2) | 0.012 (3) | −0.006 (2) |
| C5 | 0.034 (2) | 0.030 (2) | 0.043 (3) | 0.0002 (18) | 0.014 (2) | 0.000 (2) |
| C6 | 0.039 (3) | 0.028 (2) | 0.042 (2) | 0.0007 (18) | 0.018 (2) | −0.0017 (19) |
| C7 | 0.049 (3) | 0.036 (3) | 0.047 (3) | −0.002 (2) | 0.014 (2) | 0.006 (2) |
| C8 | 0.048 (3) | 0.040 (3) | 0.066 (4) | −0.011 (2) | 0.023 (3) | 0.003 (3) |
| C9 | 0.035 (3) | 0.035 (2) | 0.043 (3) | −0.0045 (19) | 0.014 (2) | −0.002 (2) |
| I1 | 0.0753 (3) | 0.0496 (2) | 0.0436 (2) | −0.01260 (18) | 0.0080 (2) | −0.01168 (16) |
| I2 | 0.0553 (3) | 0.0435 (2) | 0.0549 (2) | 0.00141 (15) | 0.02021 (19) | 0.01160 (16) |
| O1 | 0.041 (2) | 0.0288 (18) | 0.094 (3) | 0.0001 (15) | 0.011 (2) | −0.005 (2) |
| S1 | 0.0430 (8) | 0.0537 (9) | 0.0501 (8) | 0.0140 (6) | 0.0018 (6) | 0.0014 (6) |
| S2 | 0.0357 (7) | 0.0542 (8) | 0.0600 (8) | −0.0072 (6) | 0.0092 (6) | 0.0008 (7) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| C1—C2 | 1.376 (7) | C5—C6 | 1.485 (7) |
| C1—S1 | 1.712 (5) | C6—C9 | 1.364 (7) |
| C1—I1 | 2.063 (5) | C6—C7 | 1.433 (6) |
| C2—C3 | 1.431 (7) | C7—C8 | 1.339 (8) |
| C2—C5 | 1.471 (7) | C7—H7 | 0.9300 |
| C3—C4 | 1.339 (8) | C8—S2 | 1.713 (6) |
| C3—H3 | 0.9300 | C8—H8 | 0.9300 |
| C4—S1 | 1.709 (6) | C9—S2 | 1.714 (5) |
| C4—H4 | 0.9300 | C9—I2 | 2.070 (5) |
| C5—O1 | 1.215 (6) | | |
| C2—C1—S1 | 111.7 (4) | C9—C6—C7 | 111.2 (4) |
| C2—C1—I1 | 129.8 (4) | C9—C6—C5 | 124.6 (4) |
| S1—C1—I1 | 118.5 (3) | C7—C6—C5 | 124.1 (4) |

| | | | |
|---|---|---|---|
| C1—C2—C3 | 110.8 (4) | C8—C7—C6 | 113.7 (5) |
| C1—C2—C5 | 125.1 (4) | C8—C7—H7 | 123.2 |
| C3—C2—C5 | 123.8 (4) | C6—C7—H7 | 123.2 |
| C4—C3—C2 | 113.9 (5) | C7—C8—S2 | 111.4 (4) |
| C4—C3—H3 | 123.1 | C7—C8—H8 | 124.3 |
| C2—C3—H3 | 123.1 | S2—C8—H8 | 124.3 |
| C3—C4—S1 | 111.6 (4) | C6—C9—S2 | 111.8 (4) |
| C3—C4—H4 | 124.2 | C6—C9—I2 | 129.3 (4) |
| S1—C4—H4 | 124.2 | S2—C9—I2 | 118.7 (3) |
| O1—C5—C2 | 121.4 (4) | C4—S1—C1 | 92.1 (3) |
| O1—C5—C6 | 120.8 (4) | C8—S2—C9 | 92.0 (3) |
| C2—C5—C6 | 117.8 (4) | | |
| S1—C1—C2—C3 | 1.2 (5) | C2—C5—C6—C7 | 44.7 (7) |
| I1—C1—C2—C3 | −175.7 (4) | C9—C6—C7—C8 | −0.8 (6) |
| S1—C1—C2—C5 | −172.4 (4) | C5—C6—C7—C8 | 175.3 (5) |
| I1—C1—C2—C5 | 10.6 (7) | C6—C7—C8—S2 | 1.6 (6) |
| C1—C2—C3—C4 | −1.6 (6) | C7—C6—C9—S2 | −0.3 (5) |
| C5—C2—C3—C4 | 172.2 (5) | C5—C6—C9—S2 | −176.4 (4) |
| C2—C3—C4—S1 | 1.2 (6) | C7—C6—C9—I2 | −173.7 (4) |
| C1—C2—C5—O1 | 24.2 (7) | C5—C6—C9—I2 | 10.1 (7) |
| C3—C2—C5—O1 | −148.6 (5) | C3—C4—S1—C1 | −0.4 (5) |
| C1—C2—C5—C6 | −158.0 (5) | C2—C1—S1—C4 | −0.5 (4) |
| C3—C2—C5—C6 | 29.2 (7) | I1—C1—S1—C4 | 176.8 (3) |
| O1—C5—C6—C9 | 38.0 (7) | C7—C8—S2—C9 | −1.5 (5) |
| C2—C5—C6—C9 | −139.7 (5) | C6—C9—S2—C8 | 1.0 (4) |
| O1—C5—C6—C7 | −137.6 (5) | I2—C9—S2—C8 | 175.2 (3) |

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C4—H4···O1$^{i}$ | 0.93 | 2.51 | 3.233 (7) | 135 |
| C8—H8···O1$^{ii}$ | 0.93 | 2.40 | 3.324 (6) | 172 |

Symmetry codes: (i) −*x*+3/2, *y*−1/2, −*z*+3/2; (ii) −*x*+1/2, *y*−1/2, −*z*+3/2.

**Fig. 1**