Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

S-Phenyl benzothioate

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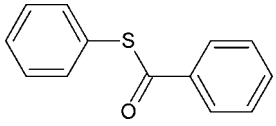
Received 22 August 2012; accepted 28 August 2012

Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.002 Å; R factor = 0.032; wR factor = 0.082; data-to-parameter ratio = 12.9.

In the title compound, $C_{13}H_{10}OS$, the phenyl rings are inclined to one another by 51.12 (8)°. There is a short C—H···S contact in the molecule.In the crystal, molecules are linked *via* C—H···O hydrogen bonds forming chains along the *a* axis. Molecules are also linked by C—H···π and weak π–π interactions [centroid–centroid distance = 3.9543 (10) Å].

Related literature

The title compound was obtained by the reaction of thiophenolyate and benzoyl chloride in an alkaline medium. For background to the title compound, see: Reddy *et al.* (2010); Katritzky *et al.* (2007). For details of the Cambridge Structural Database, see: Allen (2002).



Experimental

Crystal data

$C_{13}H_{10}OS$
M_r = 214.27
Monoclinic, $P2_1/c$
a = 5.7203 (1) Å
b = 15.1315 (3) Å
c = 12.0606 (3) Å
β = 96.867 (1)°
V = 1036.44 (4) Å^3
Z = 4
Cu $K\alpha$ radiation
μ = 2.49 mm^{-1}
T = 100 K
0.25 × 0.12 × 0.12 mm

Data collection

Bruker APEX DUO 4K-CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2008)
T_{min} = 0.575, T_{max} = 0.754
9164 measured reflections
1759 independent reflections
1702 reflections with $I > 2\sigma(I)$
R_{int} = 0.022

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.082
S = 1.04
1759 reflections
136 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.35 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}

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

*Cg*1 and *Cg*2 are the centroids of the C2–C7 and C8–C13 rings, respectively.

D—H···A	D—H	H···A	D···A	D—H···A
C7—H7···S1	0.95	2.52	2.9592 (16)	109
C13—H13···O1^{i}	0.95	2.56	3.4889 (18)	167
C10—H10···*Cg*1^{ii}	0.95	2.97	3.506 (2)	117
C5—H5···*Cg*2^{iii}	0.95	2.73	3.5915 (19)	152

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

Data collection: *APEX2* (Bruker, 2011); cell refinement: *SAINT* (Bruker, 2008); data reduction: *SAINT* and *XPREP* (Bruker, 2008); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg & Putz, 2005); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

Research funds of the University of Johannesburg and the Research Center for Synthesis and Catalysis are gratefully acknowledged. Mrs Z. H. Phasha is thanked for the data collection.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: DS2217).

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supporting information

Acta Cryst. (2012). E**68**, o2825 [https://doi.org/10.1107/S1600536812037142]

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S1. Comment

Reaction of thiophenolyate and benzyol chloride in alkaline medium was described previously by Reddy *et al.*, 2010. We have repeated the preparation of this compound to be used as starting material in some of our research. Benzoylation of thiophenol afforded colorless crystals of the title compound (see scheme and Figure 1) suitable for single crystal X-ray analysis of which the structure is reported herein. Molecules of the title compound crystalizes in the $P2_1/c$ (Z=4) space group. All bond lengths are within their normal ranges (Allen, 2002). In the crystal packing several C—H···O/S/π interactions (see table 1, Fig. 2) as well as π-π stacking are observed (centroid to centroid distance = 3.9543 (10) Å, ring slippage = 1.366 Å).

S2. Experimental

A mixture of sodium hydroxide (344 mg, 8.61 mmol) and thiophenol (0.9 ml, 8.61 mmol) were dissolved in methanol (22 ml) for about 10 minutes. Benzoyl chloride (1 ml) was added to it. The reaction mixture was stirred overnight and then poured into ice-cold water. Afterwards it was filtered and dried to afford the title compound as white crystals in 63% yield.

S3. Refinement

All hydrogen atoms were positioned in geometrically idealized positions with C—H = 0.95 Å and were allowed to ride on their parent atoms with U_{iso}(H) = 1.2U_{eq}. A discrepant reflection (1 3 2) was removed in the final stages of refinement

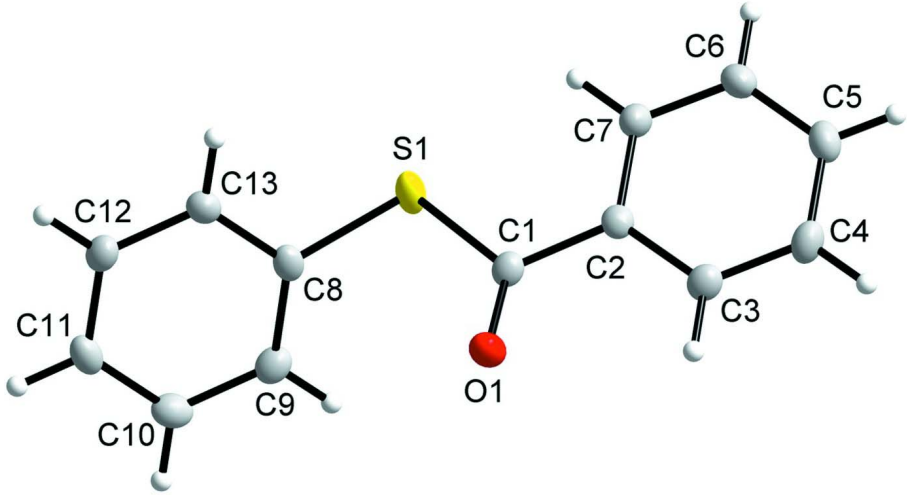

Figure 1

A view of (1). Displacement ellipsoids are drawn at the 50% probability level.

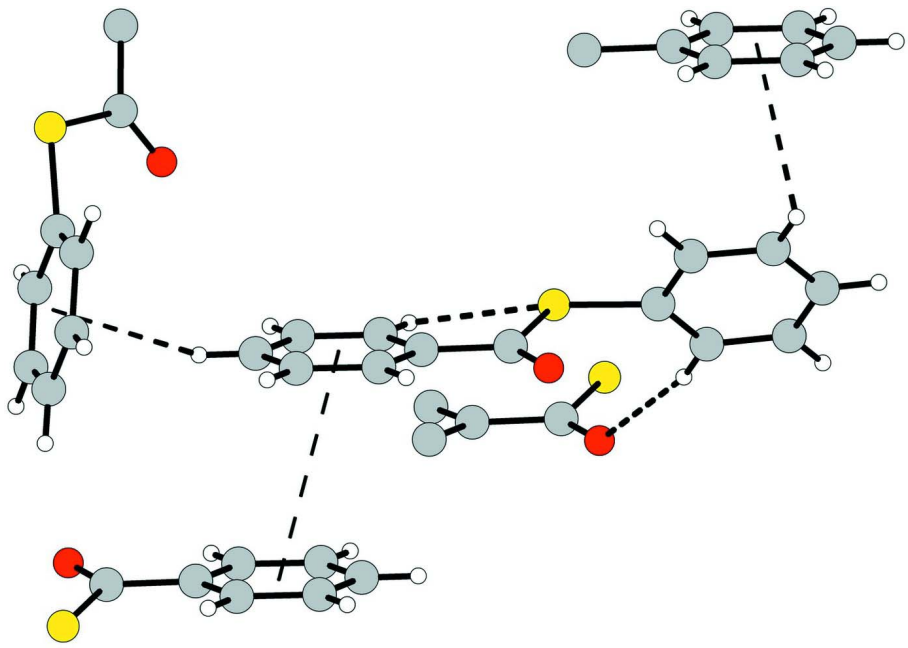

Figure 2

Packing diagram of (1) showing the C—H···O/S/π interactions as well as the π-π stacking.

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Crystal data

$C_{13}H_{10}OS$
M_r = 214.27
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
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b = 15.1315 (3) Å
c = 12.0606 (3) Å
β = 96.867 (1)°
V = 1036.44 (4) Å^3
Z = 4
F(000) = 448
D_x = 1.373 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54178 Å
Cell parameters from 6683 reflections
θ = 4.7–65.8°
μ = 2.49 mm^{-1}
T = 100 K
Rectangular, colourless
0.25 × 0.12 × 0.12 mm

Data collection

Bruker APEX DUO 4K-CCD diffractometer
Radiation source: Incoatec IμS microfocus X-ray source
Incoatec Quazar Multilayer Mirror monochromator
Detector resolution: 8.4 pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2008)
T_{min} = 0.575, T_{max} = 0.754
9164 measured reflections
1759 independent reflections
1702 reflections with $I > 2\sigma(I)$
R_{int} = 0.022
θ_{max} = 66.4°, θ_{min} = 4.7°
h = −2→6
k = −17→17
l = −14→13

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.032$
$wR(F^2) = 0.082$
$S = 1.04$
1759 reflections
136 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
$w = 1/[\sigma^2(F_o^2) + (0.0364P)^2 + 0.7558P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.35$ e Å^{-3}
$\Delta\rho_{min} = -0.26$ e Å^{-3}

Special details

Experimental. The intensity data was collected on a Bruker Apex DUO 4 K CCD diffractometer using an exposure time of 5 s/frame. A total of 2274 frames were collected with a frame width of 1° covering up to $\theta = 66.38°$ with 96.3% completeness accomplished.
Analytical data: mp: 53–55 °C (Lit. 54–55 °C; Katritzky *et al.*, 2007); ^{1}H NMR ($CDCl_3$, 400 MHz): d 8.03 (d, $J = 0.8$ Hz, 1H), 8.01(d, $J = 1.2$ Hz, 1H), 7.62–7.58 (m, 1H), 7.52–7.44 (m, 7H), ^{13}C NMR ($CDCl_3$, 400 MHz): d 190.1, 136.6, 135.1, 133.6, 129.5, 129.2, 128.7, 127.5, 127.3.

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}
S1	0.66521 (7)	0.44609 (2)	0.09450 (3)	0.02499 (16)
O1	1.05856 (19)	0.36323 (7)	0.17500 (9)	0.0242 (3)
C1	0.9304 (3)	0.42516 (10)	0.18525 (12)	0.0180 (3)
C2	0.9751 (3)	0.49420 (10)	0.27395 (12)	0.0174 (3)
C3	1.1950 (3)	0.49605 (10)	0.33797 (13)	0.0210 (3)
H3	1.3106	0.4531	0.3262	0.025*
C4	1.2443 (3)	0.56059 (11)	0.41871 (14)	0.0237 (4)
H4	1.3943	0.5619	0.462	0.028*
C5	1.0767 (3)	0.62332 (11)	0.43703 (13)	0.0234 (3)
H5	1.1117	0.6673	0.4928	0.028*
C6	0.8580 (3)	0.62174 (11)	0.37383 (13)	0.0239 (4)
H6	0.7429	0.6647	0.3863	0.029*
C7	0.8067 (3)	0.55781 (11)	0.29258 (13)	0.0214 (3)
H7	0.6566	0.5571	0.2493	0.026*
C8	0.6486 (3)	0.35922 (10)	−0.00504 (12)	0.0182 (3)
C9	0.8130 (3)	0.35150 (10)	−0.08087 (13)	0.0211 (3)
H9	0.9497	0.3877	−0.0737	0.025*
C10	0.7749 (3)	0.29047 (11)	−0.16688 (13)	0.0231 (4)
H10	0.8871	0.2843	−0.2184	0.028*
C11	0.5735 (3)	0.23835 (10)	−0.17811 (13)	0.0221 (3)

H11	0.5472	0.1972	−0.2378	0.027*
C12	0.4107 (3)	0.24634 (10)	−0.10217 (13)	0.0210 (3)
H12	0.2734	0.2105	−0.1097	0.025*
C13	0.4483 (3)	0.30674 (10)	−0.01499 (12)	0.0192 (3)
H13	0.3376	0.312	0.0374	0.023*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0287 (3)	0.0191 (2)	0.0243 (2)	0.00622 (15)	−0.00893 (16)	−0.00571 (15)
O1	0.0236 (6)	0.0242 (6)	0.0242 (6)	0.0056 (5)	0.0007 (4)	−0.0028 (5)
C1	0.0190 (7)	0.0164 (7)	0.0181 (8)	−0.0014 (6)	0.0004 (6)	0.0032 (6)
C2	0.0203 (7)	0.0174 (8)	0.0146 (7)	−0.0018 (6)	0.0027 (6)	0.0027 (6)
C3	0.0211 (8)	0.0189 (8)	0.0224 (8)	0.0007 (6)	0.0002 (6)	0.0032 (6)
C4	0.0235 (8)	0.0246 (8)	0.0215 (8)	−0.0034 (6)	−0.0043 (6)	0.0024 (6)
C5	0.0298 (8)	0.0226 (8)	0.0174 (7)	−0.0044 (6)	0.0015 (6)	−0.0019 (6)
C6	0.0245 (8)	0.0247 (8)	0.0233 (8)	0.0008 (6)	0.0055 (6)	−0.0040 (7)
C7	0.0188 (8)	0.0259 (9)	0.0191 (8)	0.0003 (6)	0.0010 (6)	−0.0019 (6)
C8	0.0223 (8)	0.0148 (7)	0.0161 (7)	0.0031 (6)	−0.0030 (6)	0.0010 (6)
C9	0.0203 (8)	0.0205 (8)	0.0220 (8)	−0.0013 (6)	0.0006 (6)	0.0060 (6)
C10	0.0248 (8)	0.0272 (9)	0.0181 (8)	0.0047 (6)	0.0054 (6)	0.0048 (6)
C11	0.0285 (8)	0.0196 (8)	0.0171 (8)	0.0045 (6)	−0.0021 (6)	−0.0021 (6)
C12	0.0195 (7)	0.0187 (8)	0.0242 (8)	−0.0010 (6)	−0.0005 (6)	−0.0006 (6)
C13	0.0202 (8)	0.0191 (8)	0.0184 (7)	0.0030 (6)	0.0024 (6)	0.0010 (6)

Geometric parameters (Å, º)

S1—C8	1.7751 (15)	C6—H6	0.95
S1—C1	1.7894 (15)	C7—H7	0.95
O1—C1	1.2054 (19)	C8—C13	1.387 (2)
C1—C2	1.495 (2)	C8—C9	1.393 (2)
C2—C3	1.395 (2)	C9—C10	1.386 (2)
C2—C7	1.399 (2)	C9—H9	0.95
C3—C4	1.384 (2)	C10—C11	1.390 (2)
C3—H3	0.95	C10—H10	0.95
C4—C5	1.385 (2)	C11—C12	1.387 (2)
C4—H4	0.95	C11—H11	0.95
C5—C6	1.385 (2)	C12—C13	1.390 (2)
C5—H5	0.95	C12—H12	0.95
C6—C7	1.383 (2)	C13—H13	0.95
C8—S1—C1	104.81 (7)	C6—C7—H7	119.9
O1—C1—C2	124.23 (13)	C2—C7—H7	119.9
O1—C1—S1	123.81 (12)	C13—C8—C9	120.70 (14)
C2—C1—S1	111.96 (10)	C13—C8—S1	117.35 (12)
C3—C2—C7	119.34 (14)	C9—C8—S1	121.36 (12)
C3—C2—C1	118.40 (13)	C10—C9—C8	119.29 (14)
C7—C2—C1	122.24 (13)	C10—C9—H9	120.4

C4—C3—C2	119.85 (15)	C8—C9—H9	120.4
C4—C3—H3	120.1	C9—C10—C11	120.34 (14)
C2—C3—H3	120.1	C9—C10—H10	119.8
C3—C4—C5	120.60 (15)	C11—C10—H10	119.8
C3—C4—H4	119.7	C12—C11—C10	120.02 (15)
C5—C4—H4	119.7	C12—C11—H11	120
C6—C5—C4	119.80 (15)	C10—C11—H11	120
C6—C5—H5	120.1	C11—C12—C13	120.09 (14)
C4—C5—H5	120.1	C11—C12—H12	120
C7—C6—C5	120.21 (15)	C13—C12—H12	120
C7—C6—H6	119.9	C8—C13—C12	119.54 (14)
C5—C6—H6	119.9	C8—C13—H13	120.2
C6—C7—C2	120.20 (14)	C12—C13—H13	120.2

C8—S1—C1—O1	−0.46 (15)	C3—C2—C7—C6	−0.1 (2)
C8—S1—C1—C2	178.75 (10)	C1—C2—C7—C6	−178.42 (14)
O1—C1—C2—C3	10.8 (2)	C1—S1—C8—C13	122.78 (12)
S1—C1—C2—C3	−168.42 (11)	C1—S1—C8—C9	−66.00 (14)
O1—C1—C2—C7	−170.86 (15)	C13—C8—C9—C10	−0.1 (2)
S1—C1—C2—C7	9.93 (18)	S1—C8—C9—C10	−171.00 (11)
C7—C2—C3—C4	−0.1 (2)	C8—C9—C10—C11	0.8 (2)
C1—C2—C3—C4	178.26 (14)	C9—C10—C11—C12	−0.9 (2)
C2—C3—C4—C5	0.3 (2)	C10—C11—C12—C13	0.3 (2)
C3—C4—C5—C6	−0.2 (2)	C9—C8—C13—C12	−0.5 (2)
C4—C5—C6—C7	0.0 (2)	S1—C8—C13—C12	170.75 (11)
C5—C6—C7—C2	0.2 (2)	C11—C12—C13—C8	0.4 (2)

Hydrogen-bond geometry (Å, º)

*Cg*1 and *Cg*2 are the centroids of the C2–C7 and C8–C13 rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C7—H7···S1	0.95	2.52	2.9592 (16)	109
C13—H13···O1^{i}	0.95	2.56	3.4889 (18)	167
C10—H10···*Cg*1^{ii}	0.95	2.97	3.506 (2)	117
C5—H5···*Cg*2^{iii}	0.95	2.73	3.5915 (19)	152

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