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3,3′-Oxybi[isobenzofuran-1(3*H*)-one]

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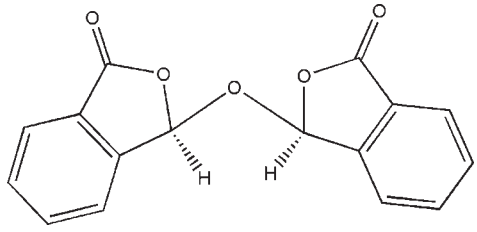
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.005 Å; R factor = 0.031; wR factor = 0.078; data-to-parameter ratio = 6.0.

The title compound, $C_{16}H_{10}O_5$, consists of two isobenzofuran-1(3*H*)-one moieties which are linked by a bridging O atom. The two halves of the molecule display approximate non-crystallographic mirror symmetry. The dihedral angle between the two isobenzofuran-1(3*H*)-one ring systems is 53.18 (6) Å. Two chiral carbon centres are observed in the compound, but their absolute configurations could not be determined. In the crystal structure, intermolecular C—H···O hydrogen bonds link molecules into zigzag chains along *c*. Additional C—H···O interactions connect adjacent chains.

Related literature

For general background to isobenzofuran-1(3*H*)-ones, see: Landge *et al.* (2008); Mukhopadhyay & Kundu (2001); Paradkar *et al.* (1998).



Experimental

Crystal data

$C_{16}H_{10}O_5$
M_r = 282.24
Monoclinic, *Pn*
a = 4.4449 (6) Å
b = 6.4937 (8) Å
c = 22.222 (2) Å
β = 91.334 (1)°
V = 641.25 (13) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.11 mm^{-1}
T = 298 K
0.44 × 0.29 × 0.11 mm

Data collection

Siemens SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.953, T_{max} = 0.988
3081 measured reflections
1139 independent reflections
972 reflections with $I > 2\sigma(I)$
R_{int} = 0.025

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.078
S = 1.01
1139 reflections
190 parameters
2 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.13 e Å^{-3}
$\Delta\rho_{min}$ = −0.13 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C6—H6···O5^{i}	0.93	2.68	3.407 (4)	136
C1—H1···O3^{ii}	0.98	2.61	3.337 (4)	131

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

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); 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: SJ2658).

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supporting information

Acta Cryst. (2009). E**65**, o2577 [doi:10.1107/S1600536809038914]

3,3′-Oxybi[isobenzofuran-1(3*H*)-one]

Wenkuan Li, Handong Yin, Liyuan Wen, Kang Li and Weidong Fan

S1. Comment

Isobenzofuran-1(3*H*)-ones represent an important class of natural products that possess significant biological properties (Landge *et al.*, 2008). A number of isobenzofuran derivatives have been reported in the literature (Paradkar *et al.*, 1998; Mukhopadhyay & Kundu, 2001). Herein, the crystal structure of the title compound is presented.

The title compound (Fig. 1) is composed of two isobenzofuran-1(3*H*) -one moieties which are linked together by a bridging O1 atom. The two moieties display approximate mirror symmetry. The two isobenzofuran-1(3*H*)-one ring systems are not coplanar and are twisted from each other by a dihedral angle of 53.18 (6)Å. The title compound is a chiral compound with two chiral centers at C_1 and C_9 but the absolute configuration could not be determined. In the crystal structure, C6—H6···O5 hydrogen bonds link molecules into zig-zag chains along *c*. Additional C1—H1···O3 interactions connect adjacent chains (Fig. 2).

S2. Experimental

The product was obtained by a simple synthetic method: A mixture of triphenylantimony (3.00 mmol) and phthalic acid (3.00 mmol) in a stoppered flask was heated to 383 K. The mixture was shaken for 2.5 h. The product was crytallized from a solution of dichloromethane/petroleum ether (1:1), and to afford the title compound unexpectedly.

S3. Refinement

In the absence of significant anomalous scattering effects, 1139 Friedel pairs were merged. H atoms were positioned geometrically, and constrained to ride on their parent atoms, with C—H = 0.93 and 0.98 Å for aromatic and methine H atoms, respectively. and with U_{iso}(H) = 1.2U_{eq}(C).

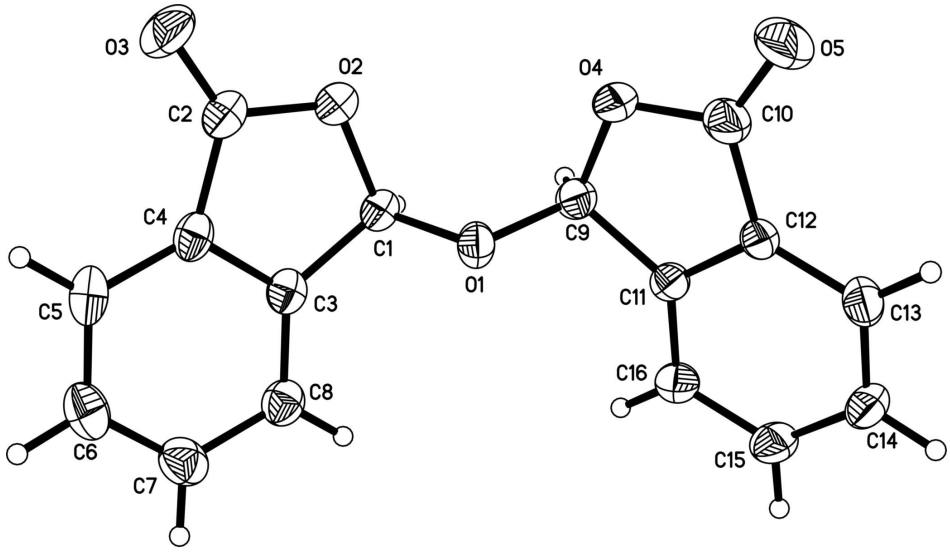

Figure 1

The asymmetric unit of the title compound, showing 50% probability displacement ellipsoids.

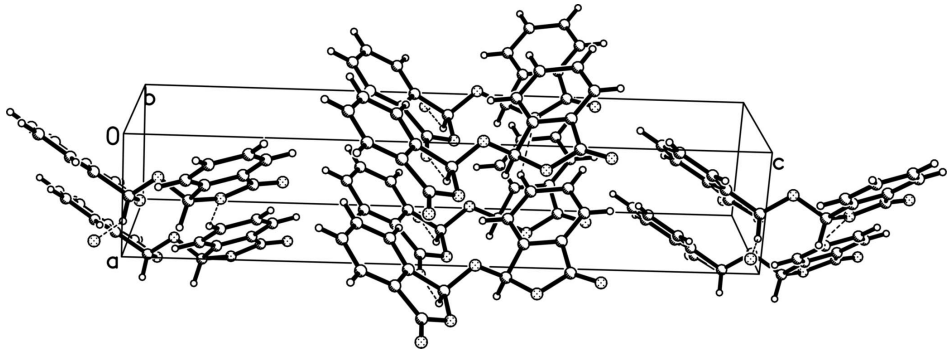

Figure 2

Packing diagram of the title compound viewed approximately along the *b* axis. H atoms are omitted for clarity.

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Crystal data

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c = 22.222 (2) Å
β = 91.334 (1)°
V = 641.25 (13) Å^3
Z = 2
F(000) = 292
D_x = 1.462 Mg m^{-3}
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 1280 reflections
θ = 2.8–23.0°
μ = 0.11 mm^{-1}
T = 298 K
Block, colorless
0.44 × 0.29 × 0.11 mm

Data collection

Siemens 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} = 0.953, T_{max} = 0.988
3081 measured reflections
1139 independent reflections
972 reflections with $I > 2\sigma(I)$

R_{int} = 0.025
θ_{max} = 25.0°, θ_{min} = 1.8°
$h = -3 \rightarrow 5$
$k = -7 \rightarrow 7$
$l = -26 \rightarrow 26$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.078
S = 1.01
1139 reflections
190 parameters
2 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
$w = 1/[\sigma^2(F_o^2) + (0.0502P)^2 + 0.0032P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.13 e Å^{-3}
$\Delta\rho_{min}$ = −0.13 e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.4119 (4)	0.1516 (3)	0.04946 (8)	0.0445 (5)
O2	0.7298 (5)	0.4086 (3)	0.01338 (9)	0.0511 (6)
O3	0.7306 (7)	0.7164 (3)	−0.03192 (13)	0.0742 (8)
O4	0.6010 (5)	0.2116 (3)	0.14674 (10)	0.0581 (6)
O5	0.4721 (8)	0.2569 (4)	0.24282 (12)	0.0859 (9)
C1	0.6000 (7)	0.2076 (5)	0.00288 (13)	0.0401 (7)
H1	0.7583	0.1044	−0.0022	0.048*
C2	0.6456 (7)	0.5423 (5)	−0.03175 (14)	0.0494 (8)
C3	0.4189 (7)	0.2325 (4)	−0.05400 (13)	0.0414 (7)
C4	0.4482 (7)	0.4308 (5)	−0.07433 (13)	0.0445 (7)
C5	0.3011 (8)	0.4956 (6)	−0.12687 (14)	0.0555 (9)
H5	0.3231	0.6295	−0.1409	0.067*
C6	0.1225 (9)	0.3563 (6)	−0.15739 (15)	0.0620 (10)
H6	0.0207	0.3965	−0.1925	0.074*
C7	0.0922 (9)	0.1584 (6)	−0.13675 (16)	0.0598 (9)
H7	−0.0305	0.0669	−0.1582	0.072*
C8	0.2407 (7)	0.0915 (5)	−0.08456 (14)	0.0499 (8)
H8	0.2207	−0.0430	−0.0708	0.060*
C9	0.5534 (7)	0.0616 (5)	0.10002 (14)	0.0443 (7)
H9	0.7448	−0.0014	0.0890	0.053*
C10	0.4522 (8)	0.1563 (5)	0.19777 (15)	0.0561 (9)
C11	0.3520 (6)	−0.0951 (4)	0.12751 (13)	0.0383 (7)
C12	0.2908 (6)	−0.0361 (5)	0.18517 (12)	0.0398 (7)
C13	0.1088 (8)	−0.1539 (6)	0.22104 (14)	0.0527 (8)
H13	0.0671	−0.1132	0.2601	0.063*
C14	−0.0088 (8)	−0.3326 (5)	0.19756 (16)	0.0567 (9)
H14	−0.1309	−0.4152	0.2209	0.068*
C15	0.0531 (8)	−0.3905 (5)	0.13930 (15)	0.0565 (9)

H15	−0.0294	−0.5119	0.1240	0.068*
C16	0.2336 (7)	−0.2733 (5)	0.10336 (14)	0.0475 (8)
H16	0.2740	−0.3131	0.0642	0.057*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0407 (11)	0.0523 (13)	0.0405 (11)	0.0026 (9)	0.0024 (9)	0.0118 (10)
O2	0.0571 (13)	0.0440 (13)	0.0520 (12)	−0.0096 (11)	−0.0019 (10)	0.0043 (11)
O3	0.097 (2)	0.0396 (14)	0.0862 (17)	−0.0174 (15)	0.0044 (15)	0.0040 (13)
O4	0.0705 (15)	0.0480 (13)	0.0551 (14)	−0.0231 (12)	−0.0137 (11)	0.0084 (11)
O5	0.132 (3)	0.0649 (18)	0.0596 (15)	−0.0248 (17)	−0.0195 (16)	−0.0118 (14)
C1	0.0425 (17)	0.0349 (15)	0.0430 (16)	−0.0007 (13)	0.0061 (13)	0.0023 (13)
C2	0.055 (2)	0.0401 (19)	0.0534 (18)	−0.0032 (15)	0.0119 (16)	0.0017 (16)
C3	0.0455 (17)	0.0412 (17)	0.0382 (15)	0.0043 (15)	0.0114 (13)	−0.0021 (14)
C4	0.0517 (18)	0.0407 (17)	0.0416 (16)	0.0028 (15)	0.0144 (14)	0.0031 (14)
C5	0.070 (2)	0.0505 (19)	0.0468 (18)	0.0112 (18)	0.0135 (17)	0.0141 (17)
C6	0.068 (2)	0.076 (3)	0.0421 (19)	0.012 (2)	0.0024 (17)	0.0031 (18)
C7	0.060 (2)	0.073 (3)	0.0467 (18)	−0.0015 (18)	0.0011 (16)	−0.0067 (19)
C8	0.056 (2)	0.0453 (19)	0.0483 (18)	−0.0011 (16)	0.0072 (15)	−0.0006 (15)
C9	0.0421 (16)	0.0425 (18)	0.0479 (17)	−0.0022 (14)	−0.0052 (13)	0.0075 (14)
C10	0.072 (2)	0.0447 (19)	0.051 (2)	−0.0063 (17)	−0.0157 (18)	0.0046 (17)
C11	0.0325 (14)	0.0384 (17)	0.0437 (16)	0.0012 (13)	−0.0046 (12)	0.0066 (13)
C12	0.0415 (15)	0.0410 (17)	0.0367 (15)	−0.0018 (14)	−0.0058 (12)	0.0053 (13)
C13	0.0552 (19)	0.064 (2)	0.0389 (16)	−0.0008 (18)	−0.0001 (14)	0.0066 (16)
C14	0.054 (2)	0.056 (2)	0.060 (2)	−0.0156 (17)	0.0015 (17)	0.0150 (17)
C15	0.062 (2)	0.0431 (18)	0.064 (2)	−0.0142 (17)	−0.0052 (17)	0.0016 (17)
C16	0.0485 (19)	0.0449 (18)	0.0490 (18)	−0.0032 (15)	−0.0011 (15)	−0.0036 (15)

Geometric parameters (Å, º)

O1—C1	1.394 (3)	C6—H6	0.9300
O1—C9	1.403 (4)	C7—C8	1.391 (5)
O2—C2	1.372 (4)	C7—H7	0.9300
O2—C1	1.444 (4)	C8—H8	0.9300
O3—C2	1.192 (4)	C9—C11	1.495 (4)
O4—C10	1.374 (4)	C9—H9	0.9800
O4—C9	1.436 (4)	C10—C12	1.465 (5)
O5—C10	1.197 (4)	C11—C12	1.371 (4)
C1—C3	1.491 (4)	C11—C16	1.375 (4)
C1—H1	0.9800	C12—C13	1.380 (4)
C2—C4	1.467 (4)	C13—C14	1.371 (5)
C3—C4	1.372 (4)	C13—H13	0.9300
C3—C8	1.379 (4)	C14—C15	1.382 (5)
C4—C5	1.390 (4)	C14—H14	0.9300
C5—C6	1.373 (5)	C15—C16	1.375 (4)
C5—H5	0.9300	C15—H15	0.9300
C6—C7	1.372 (5)	C16—H16	0.9300

C1—O1—C9	116.0 (2)	C7—C8—H8	121.3
C2—O2—C1	110.6 (2)	O1—C9—O4	110.6 (2)
C10—O4—C9	110.7 (2)	O1—C9—C11	110.4 (2)
O1—C1—O2	111.1 (2)	O4—C9—C11	104.2 (2)
O1—C1—C3	109.6 (2)	O1—C9—H9	110.5
O2—C1—C3	104.2 (2)	O4—C9—H9	110.5
O1—C1—H1	110.6	C11—C9—H9	110.5
O2—C1—H1	110.6	O5—C10—O4	121.4 (3)
C3—C1—H1	110.6	O5—C10—C12	130.7 (3)
O3—C2—O2	121.4 (3)	O4—C10—C12	107.9 (3)
O3—C2—C4	130.6 (3)	C12—C11—C16	121.1 (3)
O2—C2—C4	108.0 (2)	C12—C11—C9	109.0 (3)
C4—C3—C8	121.3 (3)	C16—C11—C9	129.8 (3)
C4—C3—C1	109.1 (3)	C11—C12—C13	121.1 (3)
C8—C3—C1	129.6 (3)	C11—C12—C10	108.1 (3)
C3—C4—C5	120.9 (3)	C13—C12—C10	130.8 (3)
C3—C4—C2	108.1 (3)	C14—C13—C12	118.2 (3)
C5—C4—C2	130.9 (3)	C14—C13—H13	120.9
C6—C5—C4	118.1 (3)	C12—C13—H13	120.9
C6—C5—H5	121.0	C13—C14—C15	120.3 (3)
C4—C5—H5	121.0	C13—C14—H14	119.9
C7—C6—C5	120.8 (3)	C15—C14—H14	119.9
C7—C6—H6	119.6	C16—C15—C14	121.7 (3)
C5—C6—H6	119.6	C16—C15—H15	119.2
C6—C7—C8	121.5 (4)	C14—C15—H15	119.2
C6—C7—H7	119.2	C11—C16—C15	117.5 (3)
C8—C7—H7	119.2	C11—C16—H16	121.2
C3—C8—C7	117.3 (3)	C15—C16—H16	121.2
C3—C8—H8	121.3		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C6—H6···O5^{i}	0.93	2.68	3.407 (4)	136
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