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2,7-Bis(prop-2-yn-1-yloxy)naphthalene

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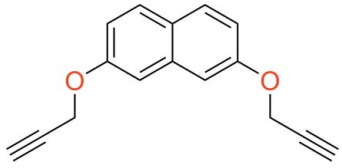
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.003 Å; R factor = 0.063; wR factor = 0.146; data-to-parameter ratio = 17.3.

The title compound, $C_{16}H_{12}O_2$, was synthesized from naphthalene-2,7-diol and prop-2-ynyl 4-methylbenzenesulfonate in the presence of sodium hydride. The crystal packing exhibits intermolecular non-classical C—H···O hydrogen bonds and C—H···π interactions.

Related literature

For the preparation of the title compound, see: Srinivasan *et al.* (2006).



Experimental

Crystal data

$C_{16}H_{12}O_2$
M_r = 236.26
Orthorhombic, *Pbca*
a = 11.3742 (12) Å
b = 8.1364 (9) Å
c = 26.880 (3) Å
V = 2487.6 (5) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 298 K
0.16 × 0.12 × 0.04 mm

Data collection

Bruker SMART 1000 diffractometer
8492 measured reflections
2812 independent reflections
1807 reflections with $I > 2\sigma(I)$
R_{int} = 0.070

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.063
$wR(F^2)$ = 0.146
S = 1.02
2812 reflections
163 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}

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

*Cg*2 is the centroid of the C4–C9 benzene ring.

D—H···A	D—H	H···A	D···A	D—H···A
C13—H13···O2^{i}	0.93	2.54	3.465 (3)	172
C14—H14B···O1^{ii}	0.97	2.57	3.533 (3)	173
C11—H11A···*Cg*2^{ii}	0.97	2.67	3.526 (3)	148

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

Data collection: *SMART* (Bruker, 1999); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

The authors are grateful to Xianggao Meng for the data collection.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: OM2339).

References

Bruker (1999). *SMART* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Srinivasan, R., Uttamchandani, M. & Yao, S. Q. (2006). *Org. Lett.* **8**, 713–716.

supporting information

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S1. Comment

Naphthalene derivatives have manifested applications in many fields, for example, as a colorant, explosive, disinfectant, insecticide and plant hormone auxin. The reaction which between hydroxybenzene and prop-2-yn-1-yl 4-methylbenzene-sulfonate gives rise to the product with rapid reaction rates by the introduction of sodium hydride (Srinivasan *et al.*, 2006;).

Here we report the crystal structure of the title compound (Fig. 1). The crystal packing exhibits non-classical C—H···O hydrogen bonds and C—H···π interaction (Table 1).

S2. Experimental

The title compound was synthesized according to the literature procedure of Srinivasan *et al.* (2006). Single crystals suitable for X-ray diffraction were prepared by slow evaporation of a solution of the title compound in chloroform : methanol (10:1) at room temperature.

S3. Refinement

All H atoms were initially located in a difference map, but were constrained to an idealized geometry. Constrained bond lengths and isotropic displacement parameters: (C—H = 0.97 Å) and U_{iso}(H) = 1.2 U_{eq}(C) for methylene, (C—H = 0.93 Å) and U_{iso}(H) =1.2U_{eq}(C) for aromatic H atoms, and (C—H = 0.93 Å) and U_{iso}(H) = 1.2U_{eq}(C) for alkynyl aromatic H atoms.

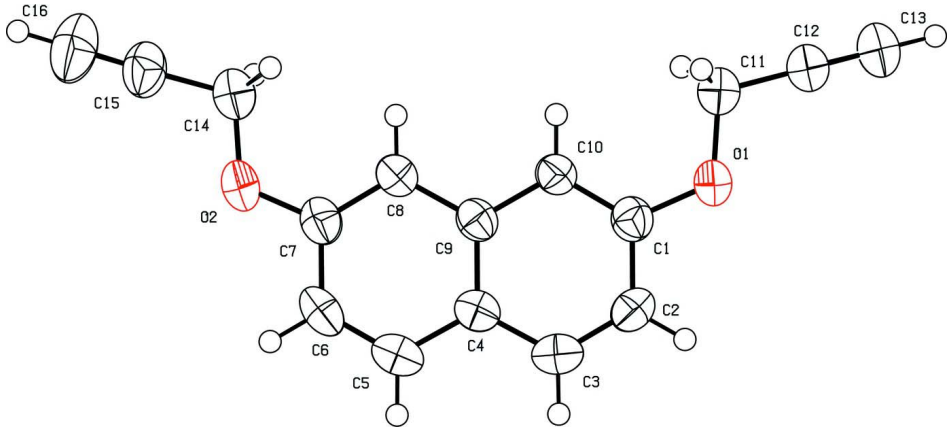

Figure 1

View of the title compound showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms are represented by spheres of arbitrary radius.

2,7-Bis(prop-2-yn-1-yloxy)naphthalene

Crystal data

$C_{16}H_{12}O_2$
$M_r = 236.26$
Orthorhombic, *Pbca*
Hall symbol: -P 2ac 2ab
$a = 11.3742\ (12)$ Å
$b = 8.1364\ (9)$ Å
$c = 26.880\ (3)$ Å
$V = 2487.6\ (5)$ Å^3
$Z = 8$
$F(000) = 992$
$D_x = 1.262$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1273 reflections
$\theta = 3.0–22.2°$
$\mu = 0.08$ mm^{-1}
$T = 298$ K
Plate, colorless
0.16 × 0.12 × 0.04 mm

Data collection

Bruker SMART 1000 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
8492 measured reflections
2812 independent reflections
1807 reflections with $I > 2\sigma(I)$
$R_{int} = 0.070$
$\theta_{max} = 27.5°$, $\theta_{min} = 2.4°$
$h = -14\rightarrow12$
$k = -9\rightarrow10$
$l = -11\rightarrow34$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.063$
$wR(F^2) = 0.146$
$S = 1.02$
2812 reflections
163 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
$w = 1/[\sigma^2(F_o^2) + (0.0571P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.17$ e Å^{-3}
$\Delta\rho_{min} = -0.23$ e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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	0.88182 (18)	0.2124 (2)	0.28194 (7)	0.0385 (5)
C2	0.78099 (18)	0.1252 (3)	0.26709 (8)	0.0441 (5)
H2	0.7296	0.0839	0.2909	0.053*
C3	0.75854 (19)	0.1013 (3)	0.21809 (8)	0.0462 (6)
H3	0.6915	0.0437	0.2087	0.055*
C4	0.83522 (18)	0.1623 (2)	0.18105 (7)	0.0373 (5)

C5	0.8135 (2)	0.1425 (3)	0.12958 (8)	0.0479 (6)
H5	0.7458	0.0881	0.1192	0.057*
C6	0.8896 (2)	0.2014 (3)	0.09503 (8)	0.0486 (6)
H6	0.8733	0.1879	0.0614	0.058*
C7	0.99257 (19)	0.2824 (2)	0.10979 (7)	0.0410 (5)
C8	1.01698 (18)	0.3049 (2)	0.15926 (7)	0.0386 (5)
H8	1.0857	0.3584	0.1688	0.046*
C9	0.93755 (18)	0.2466 (2)	0.19607 (7)	0.0349 (5)
C10	0.95915 (17)	0.2723 (2)	0.24742 (7)	0.0356 (5)
H10	1.0256	0.3296	0.2576	0.043*
C11	0.9945 (2)	0.3094 (3)	0.35131 (8)	0.0511 (6)
H11A	0.9876	0.4270	0.3460	0.061*
H11B	1.0642	0.2707	0.3342	0.061*
C12	1.0032 (2)	0.2742 (3)	0.40422 (8)	0.0538 (6)
C13	1.0111 (2)	0.2413 (3)	0.44607 (10)	0.0777 (9)
H13	1.0173	0.2149	0.4796	0.093*
C14	1.1715 (2)	0.4069 (3)	0.08303 (7)	0.0486 (6)
H14A	1.2248	0.3255	0.0967	0.058*
H14B	1.1602	0.4926	0.1077	0.058*
C15	1.2208 (2)	0.4766 (3)	0.03774 (8)	0.0512 (6)
C16	1.2596 (2)	0.5391 (3)	0.00261 (10)	0.0727 (8)
H16	1.2907	0.5892	−0.0256	0.087*
O1	0.89297 (13)	0.22760 (17)	0.33268 (5)	0.0490 (4)
O2	1.06171 (14)	0.33243 (19)	0.07121 (5)	0.0513 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0421 (13)	0.0378 (11)	0.0356 (11)	0.0007 (10)	−0.0013 (9)	0.0027 (9)
C2	0.0396 (13)	0.0481 (13)	0.0448 (13)	−0.0091 (10)	0.0048 (10)	0.0058 (10)
C3	0.0381 (13)	0.0467 (13)	0.0540 (14)	−0.0078 (10)	−0.0041 (10)	−0.0019 (11)
C4	0.0371 (13)	0.0350 (11)	0.0398 (11)	0.0014 (9)	−0.0048 (9)	−0.0021 (9)
C5	0.0450 (14)	0.0507 (13)	0.0479 (13)	−0.0044 (11)	−0.0123 (11)	−0.0066 (11)
C6	0.0592 (16)	0.0554 (14)	0.0312 (11)	0.0003 (12)	−0.0104 (10)	−0.0058 (10)
C7	0.0487 (14)	0.0408 (12)	0.0335 (11)	0.0012 (10)	−0.0006 (10)	−0.0022 (9)
C8	0.0406 (13)	0.0422 (12)	0.0329 (11)	−0.0031 (10)	−0.0035 (9)	−0.0013 (9)
C9	0.0390 (12)	0.0324 (10)	0.0331 (10)	0.0024 (9)	−0.0026 (9)	−0.0015 (8)
C10	0.0357 (12)	0.0377 (11)	0.0333 (10)	−0.0018 (9)	−0.0032 (8)	0.0012 (8)
C11	0.0502 (15)	0.0653 (15)	0.0377 (12)	−0.0113 (12)	0.0010 (10)	0.0041 (10)
C12	0.0550 (16)	0.0705 (16)	0.0358 (12)	−0.0158 (13)	0.0011 (11)	−0.0001 (11)
C13	0.078 (2)	0.119 (2)	0.0368 (14)	−0.0317 (17)	−0.0031 (13)	0.0089 (14)
C14	0.0537 (15)	0.0559 (14)	0.0361 (11)	−0.0011 (12)	0.0023 (10)	−0.0015 (10)
C15	0.0618 (16)	0.0499 (14)	0.0420 (13)	0.0013 (12)	0.0130 (11)	−0.0047 (11)
C16	0.092 (2)	0.0675 (17)	0.0582 (17)	−0.0010 (15)	0.0295 (15)	0.0021 (14)
O1	0.0529 (10)	0.0647 (10)	0.0295 (8)	−0.0162 (8)	0.0016 (7)	0.0032 (7)
O2	0.0597 (10)	0.0663 (10)	0.0278 (8)	−0.0085 (9)	0.0018 (7)	−0.0025 (7)

Geometric parameters (Å, º)

C1—C10	1.368 (3)	C8—H8	0.9300
C1—O1	1.375 (2)	C9—C10	1.417 (3)
C1—C2	1.406 (3)	C10—H10	0.9300
C2—C3	1.356 (3)	C11—O1	1.424 (2)
C2—H2	0.9300	C11—C12	1.454 (3)
C3—C4	1.414 (3)	C11—H11A	0.9700
C3—H3	0.9300	C11—H11B	0.9700
C4—C9	1.410 (3)	C12—C13	1.160 (3)
C4—C5	1.415 (3)	C13—H13	0.9300
C5—C6	1.357 (3)	C14—O2	1.424 (3)
C5—H5	0.9300	C14—C15	1.455 (3)
C6—C7	1.401 (3)	C14—H14A	0.9700
C6—H6	0.9300	C14—H14B	0.9700
C7—O2	1.364 (2)	C15—C16	1.160 (3)
C7—C8	1.371 (3)	C16—H16	0.9300
C8—C9	1.421 (3)		
C10—C1—O1	125.53 (18)	C4—C9—C10	119.59 (18)
C10—C1—C2	120.75 (19)	C4—C9—C8	119.19 (17)
O1—C1—C2	113.71 (17)	C10—C9—C8	121.22 (19)
C3—C2—C1	120.12 (19)	C1—C10—C9	119.76 (19)
C3—C2—H2	119.9	C1—C10—H10	120.1
C1—C2—H2	119.9	C9—C10—H10	120.1
C2—C3—C4	121.2 (2)	O1—C11—C12	107.91 (17)
C2—C3—H3	119.4	O1—C11—H11A	110.1
C4—C3—H3	119.4	C12—C11—H11A	110.1
C9—C4—C3	118.59 (18)	O1—C11—H11B	110.1
C9—C4—C5	118.69 (18)	C12—C11—H11B	110.1
C3—C4—C5	122.72 (19)	H11A—C11—H11B	108.4
C6—C5—C4	121.1 (2)	C13—C12—C11	177.9 (3)
C6—C5—H5	119.4	C12—C13—H13	180.0
C4—C5—H5	119.4	O2—C14—C15	108.50 (17)
C5—C6—C7	120.38 (19)	O2—C14—H14A	110.0
C5—C6—H6	119.8	C15—C14—H14A	110.0
C7—C6—H6	119.8	O2—C14—H14B	110.0
O2—C7—C8	125.5 (2)	C15—C14—H14B	110.0
O2—C7—C6	114.03 (18)	H14A—C14—H14B	108.4
C8—C7—C6	120.45 (19)	C16—C15—C14	176.9 (3)
C7—C8—C9	120.13 (19)	C15—C16—H16	180.0
C7—C8—H8	119.9	C1—O1—C11	117.76 (15)
C9—C8—H8	119.9	C7—O2—C14	117.59 (15)
C10—C1—C2—C3	−0.8 (3)	C3—C4—C9—C8	178.38 (18)
O1—C1—C2—C3	179.76 (19)	C5—C4—C9—C8	−1.7 (3)
C1—C2—C3—C4	0.2 (3)	C7—C8—C9—C4	1.5 (3)
C2—C3—C4—C9	1.2 (3)	C7—C8—C9—C10	−178.24 (18)

C2—C3—C4—C5	−178.8 (2)	O1—C1—C10—C9	179.43 (17)
C9—C4—C5—C6	0.7 (3)	C2—C1—C10—C9	0.1 (3)
C3—C4—C5—C6	−179.4 (2)	C4—C9—C10—C1	1.3 (3)
C4—C5—C6—C7	0.6 (3)	C8—C9—C10—C1	−179.01 (18)
C5—C6—C7—O2	178.94 (19)	C10—C1—O1—C11	−1.4 (3)
C5—C6—C7—C8	−0.8 (3)	C2—C1—O1—C11	178.01 (17)
O2—C7—C8—C9	−179.92 (18)	C12—C11—O1—C1	−165.49 (18)
C6—C7—C8—C9	−0.2 (3)	C8—C7—O2—C14	3.4 (3)
C3—C4—C9—C10	−1.9 (3)	C6—C7—O2—C14	−176.27 (18)
C5—C4—C9—C10	178.05 (18)	C15—C14—O2—C7	−170.02 (17)

Hydrogen-bond geometry (Å, º)

Cg2 is the centroid of the C4–C9 benzene ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C13—H13···O2^{i}	0.93	2.54	3.465 (3)	172
C14—H14*B*···O1^{ii}	0.97	2.57	3.533 (3)	173
C11—H11*A*···*Cg*2^{ii}	0.97	2.67	3.526 (3)	148

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