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4,4′-Bis(prop-2-ynyloxy)biphenyl

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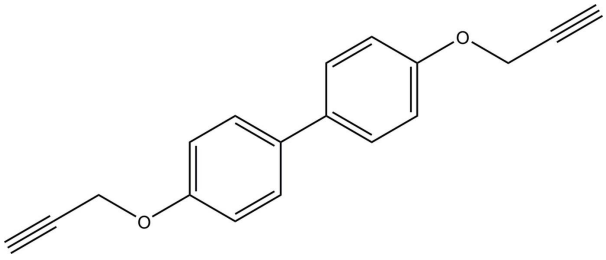
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.002 Å; R factor = 0.051; wR factor = 0.116; data-to-parameter ratio = 15.3.

The title compound, $C_{18}H_{14}O_2$, crystallizes with one half-molecule in the asymmetric unit. The molecule lies on an inversion center, located at the mid-point of the central C—C bond. As a result, the benzene rings are coplanar. No classical hydrogen bonds or stacking interactions are observed in the crystal structure.

Related literature

The title molecule was obtained unintentionally during an attempt at the synthesis of a Co^{II} complex, carried out following a published work (Burchell *et al.*, 2006).



Experimental

Crystal data

$C_{18}H_{14}O_2$
M_r = 262.29
Orthorhombic, *Pbca*
a = 7.5881 (16) Å
b = 8.2061 (18) Å
c = 22.873 (5) Å
V = 1424.3 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 293 (2) K
0.20 × 0.17 × 0.15 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: none
7569 measured reflections
1392 independent reflections
1037 reflections with $I > 2\sigma(I)$
R_{int} = 0.040

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.051
$wR(F^2)$ = 0.116
S = 1.08
1392 reflections
91 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.16 e Å^{-3}
$\Delta\rho_{min}$ = −0.14 e Å^{-3}

Data collection: *APEX2* (Bruker, 2005); cell refinement: *APEX2*; data reduction: *APEX2*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2005) and *DIAMOND* (Brandenburg, 1998); 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: BH2156).

References

Brandenburg, K. (1998). *DIAMOND*. Version 2.0. University of Bonn, Germany.
Bruker (2005). *APEX2* (Version 1.27) and *SHELXTL* (Version 6.12). Bruker AXS Inc., Madison, Wisconsin, USA.
Burchell, T. J., Jennings, M. C. & Puddephatt, R. J. (2006). *Inorg. Chim. Acta*, **359**, 2812–2818.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.

supplementary materials

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Comment

The title compound has been X-ray characterized (Fig. 1). The molecule lies on an inversion center, placed at the midpoint of the central C—C bond. As a result, all non-H atoms are almost coplanar, with a mean deviation from the least-squares plane of 0.0318 (13) Å. The bond lengths and angles show normal values. The crystal structure is characterized by zigzag chains (Fig. 2 and 3) formed along [100].

Experimental

The title compound was obtained unintentionally as the product of an attempted synthesis of a network complex (Burchell *et al.*, 2006) based on Co^{II} and 4,4'-bis(prop-2-ynyloxy)biphenyl, by evaporation of a methyl alcohol and acetone solution of $CoCl_2$, NaN_3 and the title molecule, at 298 K.

Refinement

All H atoms were included in calculated positions, with C—H distances fixed to 0.93 (aromatic CH) or 0.97 Å (methylene CH_2) and were refined in the riding-model approximation, with $U_{iso}(H) = 1.2U_{eq}$(carrier C).

Figures

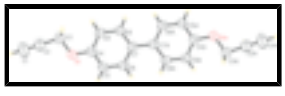

Fig. 1. The molecular structure of the title molecule, showing the atom-labeling scheme. Displacement ellipsoids are drawn at the 50% probability level. 'A' labeled atoms are generated by symmetry code −*x*, −*y*, −*z*.

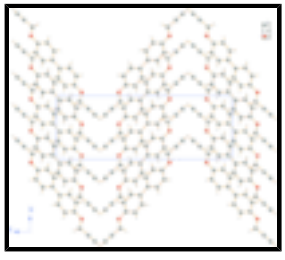

Fig. 2. The molecular packing of the title compound, viewed along the *a* axis.

Fig. 3. The molecular packing of the title compound, viewed along the *b* axis.

4,4'-Bis(prop-2-ynyloxy)biphenyl

Crystal data

$C_{18}H_{14}O_2$	F_{000} = 552
M_r = 262.29	D_x = 1.223 Mg m^{-3}
Orthorhombic, *Pbca*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -P 2ac 2ab	Cell parameters from 1896 reflections
a = 7.5881 (16) Å	θ = 5.4–55.8º
b = 8.2061 (18) Å	μ = 0.08 mm^{-1}
c = 22.873 (5) Å	*T* = 293 (2) K
V = 1424.3 (5) Å^3	Block, colourless
Z = 4	0.20 × 0.17 × 0.15 mm

Data collection

Bruker APEXII CCD area-detector diffractometer	1037 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	R_{int} = 0.040
Monochromator: graphite	θ_{max} = 26.0º
T = 293(2) K	θ_{min} = 3.2º
φ and ω scans	*h* = −9→8
Absorption correction: none	*k* = −9→10
7569 measured reflections	*l* = −28→26
1392 independent reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.051	H-atom parameters constrained
$wR(F^2)$ = 0.116	$w = 1/[\sigma^2(F_o^2) + (0.0448P)^2 + 0.3393P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.08	$(\Delta/\sigma)_{max} < 0.001$
1392 reflections	$\Delta\rho_{max}$ = 0.16 e Å^{-3}
91 parameters	$\Delta\rho_{min}$ = −0.14 e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.0440 (4)	0.7955 (3)	0.21976 (10)	0.0956 (9)
H1	0.0256	0.8708	0.2495	0.115*

C2	0.0669 (3)	0.7021 (2)	0.18279 (8)	0.0636 (5)
C3	0.0975 (3)	0.5881 (2)	0.13510 (8)	0.0587 (5)
H3A	0.0660	0.6382	0.0981	0.070*
H3B	0.2212	0.5586	0.1336	0.070*
C4	0.0023 (2)	0.32626 (19)	0.10298 (7)	0.0408 (4)
C5	−0.0877 (2)	0.1838 (2)	0.11486 (7)	0.0474 (4)
H5A	−0.1484	0.1728	0.1500	0.057*
C6	−0.0879 (2)	0.0580 (2)	0.07515 (7)	0.0465 (4)
H6A	−0.1493	−0.0369	0.0842	0.056*
C7	0.0007 (2)	0.06755 (18)	0.02165 (6)	0.0381 (4)
C8	0.0918 (2)	0.2113 (2)	0.01155 (7)	0.0483 (5)
H8A	0.1545	0.2222	−0.0232	0.058*
C9	0.0934 (2)	0.3391 (2)	0.05092 (7)	0.0493 (5)
H9A	0.1558	0.4337	0.0424	0.059*
O1	−0.00711 (15)	0.44653 (14)	0.14459 (5)	0.0507 (4)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.139 (3)	0.0774 (17)	0.0706 (14)	−0.0022 (17)	0.0079 (14)	−0.0255 (13)
C2	0.0802 (14)	0.0552 (12)	0.0554 (11)	−0.0051 (11)	0.0010 (10)	−0.0046 (10)
C3	0.0691 (13)	0.0485 (11)	0.0586 (11)	−0.0098 (10)	0.0079 (10)	−0.0049 (9)
C4	0.0390 (9)	0.0414 (9)	0.0421 (8)	0.0028 (8)	−0.0008 (7)	0.0011 (7)
C5	0.0483 (10)	0.0518 (11)	0.0421 (9)	−0.0054 (8)	0.0082 (8)	0.0036 (8)
C6	0.0485 (10)	0.0439 (10)	0.0470 (9)	−0.0094 (8)	0.0049 (8)	0.0042 (8)
C7	0.0323 (8)	0.0388 (9)	0.0431 (8)	0.0033 (7)	−0.0009 (7)	0.0052 (7)
C8	0.0523 (10)	0.0459 (10)	0.0468 (9)	−0.0057 (8)	0.0132 (8)	0.0021 (8)
C9	0.0541 (11)	0.0407 (10)	0.0531 (10)	−0.0093 (8)	0.0111 (8)	0.0018 (8)
O1	0.0577 (8)	0.0463 (7)	0.0480 (6)	−0.0062 (6)	0.0081 (6)	−0.0044 (6)

Geometric parameters (Å, °)

C1—C2	1.155 (3)	C5—C6	1.375 (2)
C1—H1	0.9300	C5—H5A	0.9300
C2—C3	1.456 (3)	C6—C7	1.399 (2)
C3—O1	1.424 (2)	C6—H6A	0.9300
C3—H3A	0.9700	C7—C8	1.386 (2)
C3—H3B	0.9700	C7—C7^{i}	1.487 (3)
C4—O1	1.3729 (19)	C8—C9	1.382 (2)
C4—C5	1.381 (2)	C8—H8A	0.9300
C4—C9	1.381 (2)	C9—H9A	0.9300
C2—C1—H1	180.0	C5—C6—C7	122.35 (15)
C1—C2—C3	178.3 (2)	C5—C6—H6A	118.8
O1—C3—C2	108.71 (15)	C7—C6—H6A	118.8
O1—C3—H3A	109.9	C8—C7—C6	115.68 (14)
C2—C3—H3A	109.9	C8—C7—C7^{i}	121.82 (17)
O1—C3—H3B	109.9	C6—C7—C7^{i}	122.50 (17)
C2—C3—H3B	109.9	C9—C8—C7	122.78 (15)

H3A—C3—H3B	108.3	C9—C8—H8A	118.6
O1—C4—C5	116.53 (14)	C7—C8—H8A	118.6
O1—C4—C9	124.67 (15)	C4—C9—C8	119.95 (15)
C5—C4—C9	118.80 (15)	C4—C9—H9A	120.0
C6—C5—C4	120.43 (15)	C8—C9—H9A	120.0
C6—C5—H5A	119.8	C4—O1—C3	116.87 (12)
C4—C5—H5A	119.8		
O1—C4—C5—C6	178.87 (15)	O1—C4—C9—C8	−178.91 (16)
C9—C4—C5—C6	−0.8 (2)	C5—C4—C9—C8	0.7 (3)
C4—C5—C6—C7	−0.1 (3)	C7—C8—C9—C4	0.3 (3)
C5—C6—C7—C8	1.1 (2)	C5—C4—O1—C3	174.67 (16)
C5—C6—C7—C7^{i}	−179.38 (18)	C9—C4—O1—C3	−5.7 (2)
C6—C7—C8—C9	−1.2 (2)	C2—C3—O1—C4	178.71 (15)
C7^{i}—C7—C8—C9	179.30 (18)		

Symmetry codes: (i) −*x*, −*y*, −*z*.

Fig. 1

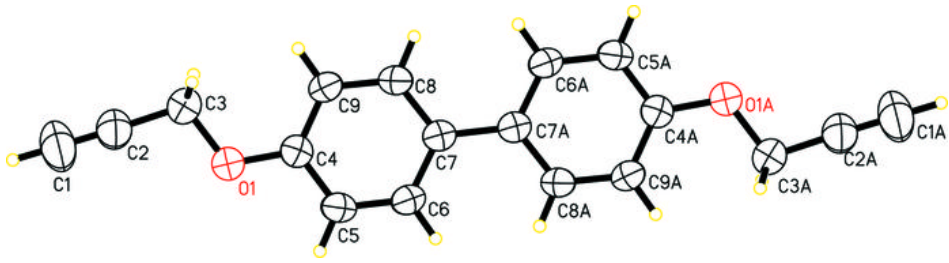
C1
C2
C3
O1
C4
C5
C6
C7
C8
C9
C7A
C8A
C9A
C4A
C5A
C6A
O1A
C3A
C2A
C1A

Fig. 2

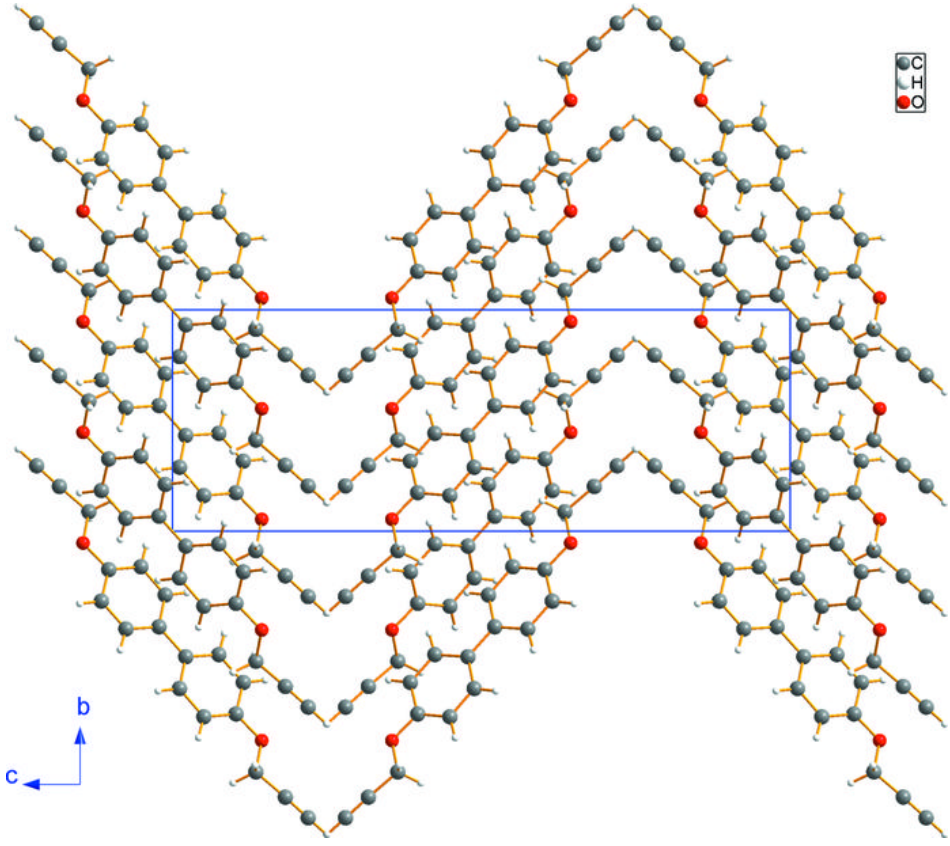

Fig. 3