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2,2′-Bis(prop-2-ynyloxy)-1,1′-binaphthyl

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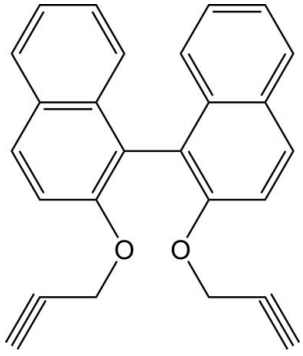
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.002 Å; R factor = 0.052; wR factor = 0.139; data-to-parameter ratio = 18.1.

In the title compound, $C_{26}H_{18}O_2$, the molecule is located on a twofold rotation axis. The two naphthyl ring planes in the molecule are nearly perpendicular to each other [dihedral angle = 82.42 (1)°. No classical hydrogen bonds or aromatic π–π stacking interactions were observed.

Related literature

For related literature, see: Burchell *et al.* (2006); Steed & Atwood (2000); Wang & Kong (2007).



Experimental

Crystal data

$C_{26}H_{18}O_2$
M_r = 362.40
Monoclinic, $C2/c$
a = 13.866 (2) Å
b = 8.8591 (14) Å
c = 15.255 (2) Å
β = 96.317 (3)°
V = 1862.6 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 293 (2) K
0.22 × 0.18 × 0.16 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: none
6053 measured reflections
2298 independent reflections
1321 reflections with $I > 2\sigma(I)$
R_{int} = 0.058

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.052
$wR(F^2)$ = 0.139
S = 0.95
2298 reflections
127 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}

Data collection: *APEX2* (Bruker, 2005); cell refinement: *APEX2*; data reduction: *SAINT* (Bruker, 2005); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2005); 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: RK2069).

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supporting information

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2,2′-Bis(prop-2-ynyloxy)-1,1′-binaphthyl

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S1. Comment

The title compound, $C_{26}H_{18}O_2$, was obtained unintentionally as the product of an attempted synthesis of a network complex of cobalt(II) with 2,2′-bis(prop-2-ynyloxy)-1,1′-binaphthyl.

The title compound has two naphthyl rings. The bond lengths and angles show normal values. The dihedral angle between the two naphthyl rings of the molecule is 82.42 (1) °.

It seems like that the π-π stacking interaction is a normal interaction found in aromatics (Wang & Kong, 2007). But in the structure of the title complex, the minimal distance between ring centroids is 3.795 (1) Å. So there is no π-π stacking interactions (Steed & Atwood, 2000). The classic hydrogen bonds are not observed.

S2. Experimental

The title compound was obtained unintentionally as the product of an attempted synthesis of a network complex (Burchell *et al.*, 2006) of cobalt(II) with 2,2′-bis(prop-2-ynyloxy)-1,1′-binaphthyl, vapouring an methyl alcohol and acetone solution of cobalt(II) chloride, sodium azide and the title compound at room temperature.

S3. Refinement

All H atoms were placed in calculated positions with C–H distances 0.93 and 0.97 Å and refined in the riding-model approximation with U_{iso}(H) = 1.2U_{eq}(C).

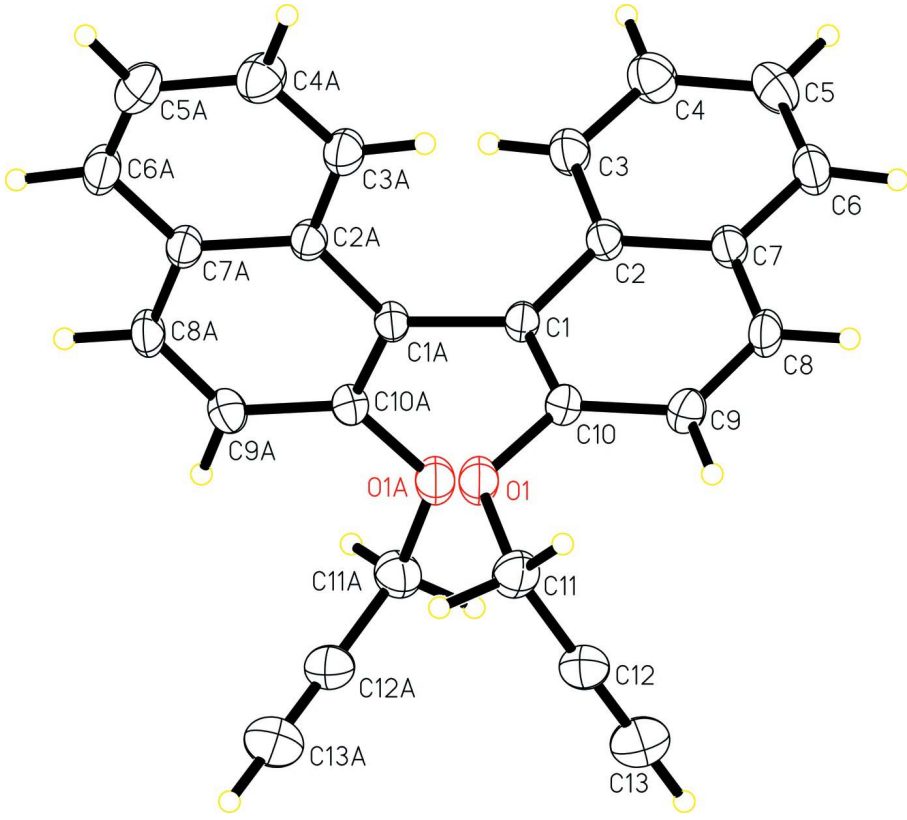

Figure 1

The molecular structure of the title complound with the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms are presented as small spheres of arbitrary radius.

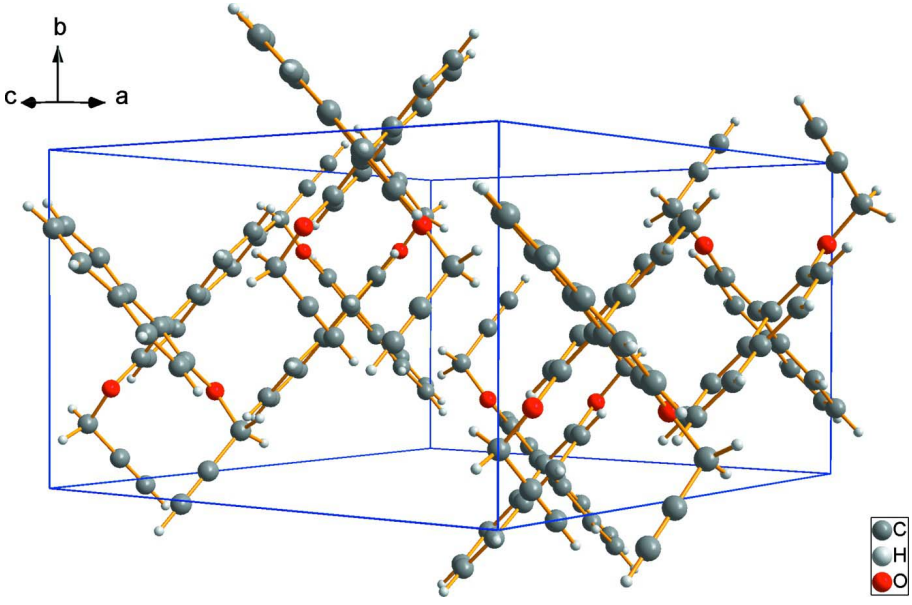

Figure 2

The molecular packing of the title compound.

2,2′-Bis(prop-2-ynyloxy)-1,1′-binaphthyl

Crystal data

$C_{26}H_{18}O_2$
$M_r = 362.40$
Monoclinic, $C2/c$
Hall symbol: -C 2yc
$a = 13.866$ (2) Å
$b = 8.8591$ (14) Å
$c = 15.255$ (2) Å
$\beta = 96.317$ (3)°
$V = 1862.6$ (5) Å^3
$Z = 4$
$F(000) = 760$
$D_x = 1.292$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1326 reflections
$\theta = 5.4$–$55.7°$
$\mu = 0.08$ mm^{-1}
$T = 293$ K
Block, colourless
0.22 × 0.18 × 0.16 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ– and ω–scans
6053 measured reflections
2298 independent reflections
1321 reflections with $I > 2\sigma(I)$
$R_{int} = 0.058$
$\theta_{max} = 28.3°$, $\theta_{min} = 2.7°$
$h = -18 \rightarrow 13$
$k = -11 \rightarrow 11$
$l = -19 \rightarrow 20$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.052$
$wR(F^2) = 0.139$
$S = 0.95$
2298 reflections
127 parameters
0 restraints
0 constraints
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
$w = 1/[\sigma^2(F_o^2) + (0.068P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.29$ e Å^{-3}
$\Delta\rho_{min} = -0.17$ e Å^{-3}

Special details

Geometry. All s.u.'s (except the s.u.'s in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'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 $F^2 > 2\sigma(F^2)$ 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	0.53783 (11)	0.02688 (17)	0.28936 (9)	0.0337 (4)
C2	0.53225 (11)	−0.07606 (18)	0.36043 (9)	0.0351 (4)
C3	0.45901 (12)	−0.18646 (19)	0.36016 (11)	0.0445 (4)
H3	0.4137	−0.1965	0.3108	0.053*
C4	0.45339 (14)	−0.2796 (2)	0.43149 (12)	0.0541 (5)

H4	0.4044	−0.3516	0.4299	0.065*
C5	0.52108 (14)	−0.2670 (2)	0.50676 (12)	0.0548 (5)
H5	0.5161	−0.3290	0.5552	0.066*
C6	0.59366 (13)	−0.1641 (2)	0.50849 (10)	0.0483 (5)
H6	0.6385	−0.1570	0.5584	0.058*
C7	0.60280 (12)	−0.06741 (18)	0.43620 (10)	0.0378 (4)
C8	0.67634 (12)	0.04140 (19)	0.43727 (10)	0.0422 (4)
H8	0.7230	0.0469	0.4859	0.051*
C9	0.68140 (12)	0.13914 (19)	0.36920 (10)	0.0416 (4)
H9	0.7308	0.2105	0.3716	0.050*
C10	0.61115 (12)	0.13157 (18)	0.29481 (9)	0.0364 (4)
O1	0.61167 (9)	0.22689 (14)	0.22387 (7)	0.0499 (4)
C11	0.68206 (13)	0.3446 (2)	0.22703 (11)	0.0506 (5)
H11A	0.6807	0.3895	0.1689	0.061*
H11B	0.7460	0.3014	0.2421	0.061*
C12	0.66649 (14)	0.4617 (2)	0.29005 (12)	0.0520 (5)
C13	0.65408 (17)	0.5555 (3)	0.34144 (16)	0.0713 (6)
H13	0.6442	0.6302	0.3823	0.086*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0369 (9)	0.0350 (9)	0.0278 (7)	0.0026 (7)	−0.0028 (6)	−0.0025 (7)
C2	0.0364 (9)	0.0369 (9)	0.0309 (8)	0.0056 (7)	−0.0007 (6)	−0.0006 (7)
C3	0.0424 (10)	0.0470 (10)	0.0422 (9)	−0.0026 (8)	−0.0040 (7)	0.0048 (8)
C4	0.0505 (12)	0.0554 (12)	0.0560 (11)	−0.0054 (9)	0.0044 (9)	0.0092 (9)
C5	0.0629 (13)	0.0583 (12)	0.0433 (10)	0.0080 (10)	0.0060 (9)	0.0155 (9)
C6	0.0547 (11)	0.0561 (12)	0.0320 (9)	0.0080 (9)	−0.0045 (7)	0.0042 (8)
C7	0.0420 (10)	0.0394 (9)	0.0305 (8)	0.0089 (7)	−0.0027 (7)	−0.0010 (7)
C8	0.0411 (10)	0.0492 (10)	0.0330 (8)	0.0055 (8)	−0.0112 (7)	−0.0040 (8)
C9	0.0393 (9)	0.0441 (10)	0.0394 (9)	−0.0039 (8)	−0.0052 (7)	−0.0047 (8)
C10	0.0424 (9)	0.0363 (9)	0.0295 (8)	0.0007 (7)	−0.0002 (7)	−0.0022 (7)
O1	0.0598 (8)	0.0502 (8)	0.0370 (6)	−0.0170 (6)	−0.0072 (5)	0.0071 (5)
C11	0.0564 (12)	0.0485 (11)	0.0465 (10)	−0.0137 (9)	0.0045 (8)	0.0027 (9)
C12	0.0570 (12)	0.0418 (11)	0.0563 (11)	−0.0049 (9)	0.0032 (9)	0.0027 (10)
C13	0.0842 (17)	0.0549 (14)	0.0746 (14)	0.0047 (11)	0.0083 (12)	−0.0089 (12)

Geometric parameters (Å, º)

C1—C10	1.372 (2)	C7—C8	1.402 (2)
C1—C2	1.425 (2)	C8—C9	1.360 (2)
C1—C1^{i}	1.505 (3)	C8—H8	0.9300
C2—C3	1.410 (2)	C9—C10	1.413 (2)
C2—C7	1.432 (2)	C9—H9	0.9300
C3—C4	1.375 (2)	C10—O1	1.3734 (18)
C3—H3	0.9300	O1—C11	1.425 (2)
C4—C5	1.405 (3)	C11—C12	1.447 (2)
C4—H4	0.9300	C11—H11A	0.9700

C5—C6	1.356 (3)	C11—H11B	0.9700
C5—H5	0.9300	C12—C13	1.168 (3)
C6—C7	1.413 (2)	C13—H13	0.9300
C6—H6	0.9300		

C10—C1—C2	119.23 (13)	C6—C7—C2	119.05 (16)
C10—C1—C1^{i}	119.68 (13)	C9—C8—C7	121.84 (14)
C2—C1—C1^{i}	121.03 (13)	C9—C8—H8	119.1
C3—C2—C1	122.77 (14)	C7—C8—H8	119.1
C3—C2—C7	117.86 (14)	C8—C9—C10	119.60 (15)
C1—C2—C7	119.37 (14)	C8—C9—H9	120.2
C4—C3—C2	121.19 (15)	C10—C9—H9	120.2
C4—C3—H3	119.4	C1—C10—O1	115.85 (13)
C2—C3—H3	119.4	C1—C10—C9	121.43 (14)
C3—C4—C5	120.53 (17)	O1—C10—C9	122.72 (14)
C3—C4—H4	119.7	C10—O1—C11	119.09 (12)
C5—C4—H4	119.7	O1—C11—C12	113.29 (15)
C6—C5—C4	119.80 (17)	O1—C11—H11A	108.9
C6—C5—H5	120.1	C12—C11—H11A	108.9
C4—C5—H5	120.1	O1—C11—H11B	108.9
C5—C6—C7	121.50 (16)	C12—C11—H11B	108.9
C5—C6—H6	119.3	H11A—C11—H11B	107.7
C7—C6—H6	119.3	C13—C12—C11	179.5 (2)
C8—C7—C6	122.37 (15)	C12—C13—H13	180.0
C8—C7—C2	118.53 (14)		

C10—C1—C2—C3	179.70 (15)	C1—C2—C7—C6	176.48 (15)
C1^{i}—C1—C2—C3	2.5 (2)	C6—C7—C8—C9	−176.48 (15)
C10—C1—C2—C7	0.4 (2)	C2—C7—C8—C9	0.9 (2)
C1^{i}—C1—C2—C7	−176.80 (14)	C7—C8—C9—C10	−0.2 (2)
C1—C2—C3—C4	−177.15 (16)	C2—C1—C10—O1	−179.93 (13)
C7—C2—C3—C4	2.1 (2)	C1^{i}—C1—C10—O1	−2.7 (2)
C2—C3—C4—C5	−0.1 (3)	C2—C1—C10—C9	0.2 (2)
C3—C4—C5—C6	−1.3 (3)	C1^{i}—C1—C10—C9	177.49 (15)
C4—C5—C6—C7	0.5 (3)	C8—C9—C10—C1	−0.4 (2)
C5—C6—C7—C8	178.90 (17)	C8—C9—C10—O1	179.83 (15)
C5—C6—C7—C2	1.6 (3)	C1—C10—O1—C11	176.21 (15)
C3—C2—C7—C8	179.73 (15)	C9—C10—O1—C11	−4.0 (2)
C1—C2—C7—C8	−0.9 (2)	C10—O1—C11—C12	−68.9 (2)
C3—C2—C7—C6	−2.8 (2)		

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