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2,2′-Bis(allyloxy)-1,1′-binaphthyl

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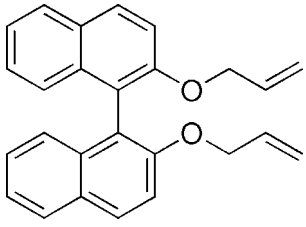
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.004 Å; R factor = 0.037; wR factor = 0.095; data-to-parameter ratio = 8.1.

The complete molecule of the title compound, $C_{26}H_{22}O_2$, is generated by a crystallographic twofold rotation axis. The dihedral angle between the planes of the two symmetry-related naphthalene ring systems is 69.05 (4)°, while that between the naphthalene ring system and the allyl plane is 13.7 (2)°. No hydrogen bonds or aromatic π–π stacking interactions are observed.

Related literature

For related structures, see: Fu & Zhao (2007); Zhang *et al.* (2008).



Experimental

Crystal data

$C_{26}H_{22}O_2$
M_r = 366.46
Tetragonal, $I4_1$
a = 11.7167 (9) Å
c = 14.583 (2) Å
V = 2001.9 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 298 K
0.20 × 0.18 × 0.14 mm

Data collection

Rigaku SCXmini diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
T_{min} = 0.892, T_{max} = 0.990
5346 measured reflections
1024 independent reflections
806 reflections with $I > 2\sigma(I)$
R_{int} = 0.045

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.095
S = 1.02
1024 reflections
127 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.14 e Å^{-3}
$\Delta\rho_{min}$ = −0.12 e Å^{-3}

Data collection: *CrystalClear* (Rigaku, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; 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: CI2788).

References

Fu, D.-W. & Zhao, H. (2007). *Acta Cryst.* E**63**, o3206.
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supporting information

Acta Cryst. (2009). E**65**, o1179 [doi:10.1107/S1600536809015815]

2,2′-Bis(allyloxy)-1,1′-binaphthyl

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S1. Comment

The molecule is located on a twofold rotation axis. The dihedral angle between the two naphthalene ring systems is 69.05 (4)° while that between the naphthalene ring and allyl plane is 13.7 (2)°. The molecule is twisted around the central C1—C1A bond with a torsion angle C2—C1—C1A—C2A of -66.6 (3)°. There are no remarkable short intermolecular interactions observed in the structure.

S2. Experimental

Racemic 1,1′-binaphthyl-2,2′-diol (2.86 g, 10 mmol) and allyl bromide (2.42 g, 20 mmol) were dissolved in acetone (50 ml) in the presence of K_2CO_3 (1.38 g, 10 mmol) and refluxed for 24 h. After the mixture was cooled to room temperature, the solution was filtered and rotated in vacuum. The title compound was purified by column chromatography with dichloromethane as eluent and was recrystallized from dichloromethane. Colorless single crystals of the title compound suitable for X-ray diffraction were obtained from an ethanol solution after a week.

S3. Refinement

H atoms were positioned geometrically and were allowed to ride on the C atoms to which they are bonded, with C-H = 0.93-0.97 Å and U_{iso}(H) = 1.2U_{eq}(C). In the absence of significant anomalous scattering, Friedel pairs were merged prior to the final refinement.

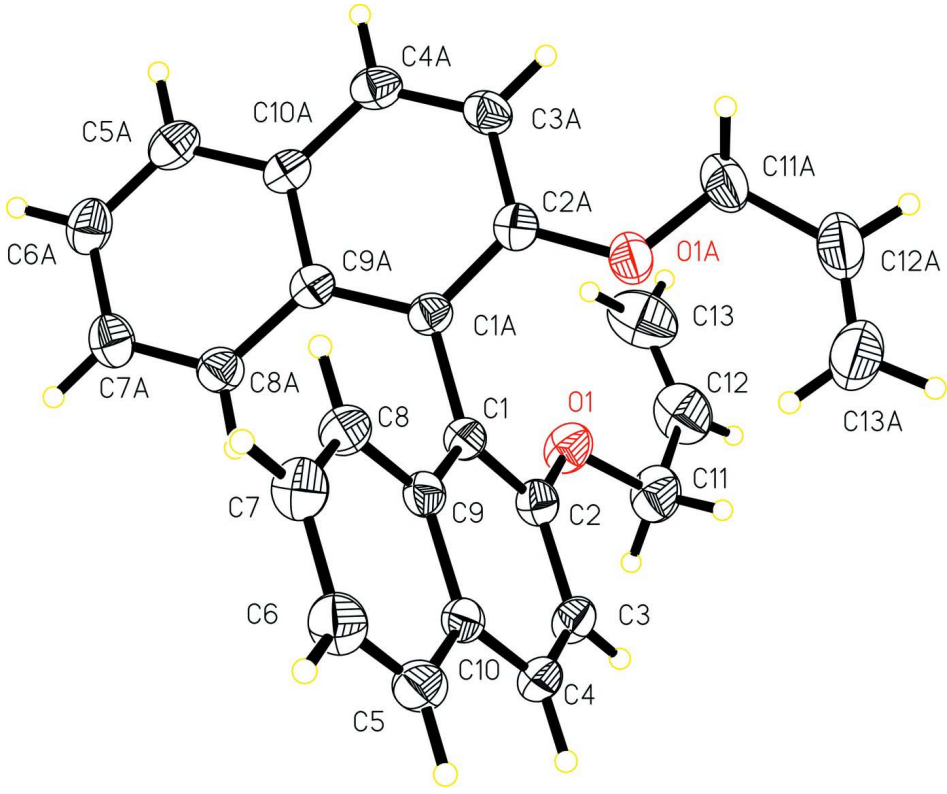

Figure 1

The molecular structure of the compound, with the atomic numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. Atoms labelled with the suffix A are generated by the symmetry operation (1-x, -y, z).

2,2′-Bis(allyloxy)-1,1′-binaphthyl

Crystal data

$C_{26}H_{22}O_2$
$M_r = 366.46$
Tetragonal, $I4_1$
Hall symbol: I 4bw
$a = 11.7167\ (9)$ Å
$c = 14.583\ (2)$ Å
$V = 2001.9\ (4)$ Å^3
$Z = 4$
$F(000) = 776$
$D_x = 1.216$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1024 reflections
$\theta = 2.0$–$27.5°$
$\mu = 0.08$ mm^{-1}
$T = 298$ K
Prism, colourless
0.20 × 0.18 × 0.14 mm

Data collection

Rigaku SCXmini diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 13.6612 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
$T_{min} = 0.892$, $T_{max} = 0.990$
5346 measured reflections
1024 independent reflections
806 reflections with $I > 2\sigma(I)$
$R_{int} = 0.045$
$\theta_{max} = 26.0°$, $\theta_{min} = 2.2°$
$h = -6\rightarrow14$
$k = -14\rightarrow14$
$l = -17\rightarrow17$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.037$
$wR(F^2) = 0.095$
$S = 1.02$
1024 reflections
127 parameters
1 restraint
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
$w = 1/[\sigma^2(F_o^2) + (0.0479P)^2 + 0.119P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.14$ e Å^{-3}
$\Delta\rho_{min} = -0.12$ e Å^{-3}

Special details

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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
C9	0.3589 (2)	0.0005 (2)	0.65091 (16)	0.0410 (6)
C1	0.4419 (2)	−0.0269 (2)	0.71920 (16)	0.0406 (6)
C10	0.2494 (2)	−0.0516 (2)	0.65478 (17)	0.0419 (6)
O1	0.49556 (16)	−0.12473 (17)	0.85183 (13)	0.0557 (5)
C7	0.2987 (2)	0.1036 (2)	0.51508 (19)	0.0571 (8)
H7A	0.3147	0.1559	0.4688	0.068*
C2	0.4132 (2)	−0.1021 (2)	0.78793 (19)	0.0451 (6)
C4	0.2253 (2)	−0.1283 (2)	0.72628 (18)	0.0490 (6)
H4A	0.1537	−0.1624	0.7293	0.059*
C8	0.3794 (2)	0.0793 (2)	0.57953 (19)	0.0486 (6)
H8A	0.4499	0.1155	0.5764	0.058*
C3	0.3047 (2)	−0.1536 (2)	0.79115 (19)	0.0499 (7)
H3A	0.2873	−0.2049	0.8377	0.060*
C5	0.1674 (2)	−0.0254 (3)	0.5868 (2)	0.0540 (7)
H5A	0.0961	−0.0602	0.5888	0.065*
C6	0.1911 (2)	0.0498 (3)	0.5184 (2)	0.0597 (8)
H6A	0.1366	0.0658	0.4738	0.072*
C11	0.4636 (3)	−0.1789 (3)	0.9343 (2)	0.0687 (9)
H11A	0.4433	−0.2578	0.9224	0.082*
H11B	0.3979	−0.1408	0.9607	0.082*
C12	0.5612 (4)	−0.1738 (3)	0.9988 (3)	0.0834 (11)
H12A	0.5519	−0.2102	1.0550	0.100*
C13	0.6573 (4)	−0.1243 (4)	0.9849 (3)	0.0976 (13)
H13C	0.6709	−0.0868	0.9298	0.117*
H13A	0.7135	−0.1259	1.0300	0.117*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C9	0.0387 (14)	0.0427 (14)	0.0415 (14)	0.0017 (11)	0.0029 (11)	−0.0071 (12)
C1	0.0377 (13)	0.0424 (14)	0.0419 (13)	−0.0010 (11)	0.0017 (12)	−0.0031 (12)
C10	0.0335 (14)	0.0452 (14)	0.0470 (14)	0.0019 (12)	0.0042 (12)	−0.0120 (12)
O1	0.0517 (11)	0.0685 (13)	0.0468 (10)	−0.0008 (10)	−0.0022 (9)	0.0134 (10)
C7	0.0595 (18)	0.0593 (18)	0.0524 (17)	0.0089 (15)	−0.0030 (14)	0.0075 (14)
C2	0.0455 (14)	0.0467 (14)	0.0430 (13)	0.0033 (12)	0.0010 (13)	−0.0022 (12)
C4	0.0389 (14)	0.0541 (15)	0.0539 (15)	−0.0053 (13)	0.0104 (13)	−0.0073 (13)
C8	0.0422 (15)	0.0506 (15)	0.0529 (15)	0.0006 (12)	0.0003 (13)	0.0025 (13)
C3	0.0504 (15)	0.0525 (15)	0.0468 (14)	−0.0058 (13)	0.0108 (14)	0.0037 (13)
C5	0.0372 (15)	0.0618 (17)	0.0630 (18)	0.0028 (13)	−0.0016 (14)	−0.0109 (16)
C6	0.0495 (17)	0.074 (2)	0.0556 (17)	0.0094 (15)	−0.0096 (15)	−0.0009 (16)
C11	0.085 (2)	0.073 (2)	0.0484 (17)	−0.0002 (18)	0.0014 (17)	0.0169 (16)
C12	0.106 (3)	0.085 (3)	0.0588 (19)	0.004 (2)	−0.020 (2)	0.0141 (19)
C13	0.106 (3)	0.089 (3)	0.098 (3)	0.001 (3)	−0.044 (3)	0.005 (3)

Geometric parameters (Å, º)

C9—C8	1.411 (4)	C4—H4A	0.93
C9—C10	1.422 (3)	C8—H8A	0.93
C9—C1	1.428 (3)	C3—H3A	0.93
C1—C2	1.376 (3)	C5—C6	1.360 (4)
C1—C1^{i}	1.500 (5)	C5—H5A	0.93
C10—C4	1.405 (4)	C6—H6A	0.93
C10—C5	1.415 (4)	C11—C12	1.482 (5)
O1—C2	1.368 (3)	C11—H11A	0.97
O1—C11	1.411 (4)	C11—H11B	0.97
C7—C8	1.363 (4)	C12—C13	1.282 (5)
C7—C6	1.410 (4)	C12—H12A	0.93
C7—H7A	0.93	C13—H13C	0.93
C2—C3	1.408 (4)	C13—H13A	0.93
C4—C3	1.359 (4)		
C8—C9—C10	117.6 (2)	C4—C3—C2	120.1 (3)
C8—C9—C1	123.1 (2)	C4—C3—H3A	120.0
C10—C9—C1	119.3 (2)	C2—C3—H3A	120.0
C2—C1—C9	119.0 (2)	C6—C5—C10	121.0 (3)
C2—C1—C1^{i}	119.4 (2)	C6—C5—H5A	119.5
C9—C1—C1^{i}	121.6 (2)	C10—C5—H5A	119.5
C4—C10—C5	121.5 (2)	C5—C6—C7	119.8 (3)
C4—C10—C9	119.0 (2)	C5—C6—H6A	120.1
C5—C10—C9	119.5 (2)	C7—C6—H6A	120.1
C2—O1—C11	118.8 (2)	O1—C11—C12	108.6 (3)
C8—C7—C6	120.2 (3)	O1—C11—H11A	110.0
C8—C7—H7A	119.9	C12—C11—H11A	110.0
C6—C7—H7A	119.9	O1—C11—H11B	110.0

O1—C2—C1	116.6 (2)	C12—C11—H11B	110.0
O1—C2—C3	122.1 (2)	H11A—C11—H11B	108.4
C1—C2—C3	121.3 (2)	C13—C12—C11	126.6 (4)
C3—C4—C10	121.2 (2)	C13—C12—H12A	116.7
C3—C4—H4A	119.4	C11—C12—H12A	116.7
C10—C4—H4A	119.4	C12—C13—H13C	120.0
C7—C8—C9	121.8 (3)	C12—C13—H13A	120.0
C7—C8—H8A	119.1	H13C—C13—H13A	120.0
C9—C8—H8A	119.1		

C8—C9—C1—C2	178.0 (2)	C5—C10—C4—C3	179.6 (2)
C10—C9—C1—C2	−0.9 (3)	C9—C10—C4—C3	−0.2 (4)
C8—C9—C1—C1^{i}	−0.2 (4)	C6—C7—C8—C9	0.0 (4)
C10—C9—C1—C1^{i}	−179.1 (2)	C10—C9—C8—C7	−1.3 (4)
C8—C9—C10—C4	−178.5 (2)	C1—C9—C8—C7	179.8 (2)
C1—C9—C10—C4	0.4 (3)	C10—C4—C3—C2	0.4 (4)
C8—C9—C10—C5	1.7 (3)	O1—C2—C3—C4	179.8 (2)
C1—C9—C10—C5	−179.4 (2)	C1—C2—C3—C4	−0.9 (4)
C11—O1—C2—C1	165.4 (2)	C4—C10—C5—C6	179.3 (3)
C11—O1—C2—C3	−15.3 (4)	C9—C10—C5—C6	−0.8 (4)
C9—C1—C2—O1	−179.6 (2)	C10—C5—C6—C7	−0.5 (4)
C1^{i}—C1—C2—O1	−1.4 (4)	C8—C7—C6—C5	0.9 (4)
C9—C1—C2—C3	1.1 (3)	C2—O1—C11—C12	−169.1 (2)
C1^{i}—C1—C2—C3	179.3 (3)	O1—C11—C12—C13	3.0 (5)

Symmetry code: (i) $-x+1, -y, z$.