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4,4′-[1,1′-Binaphthalene-2,2′-diyldi(oxymethylene)]benzonitrile

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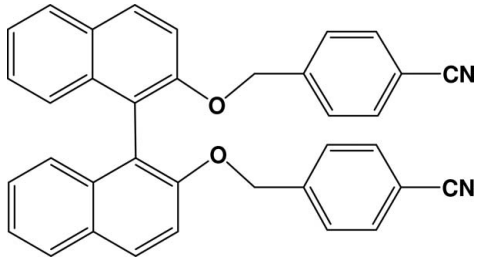
Key indicators: single-crystal X-ray study; T = 291 K; mean σ(C–C) = 0.003 Å; R factor = 0.053; wR factor = 0.112; data-to-parameter ratio = 14.7.

In the title compound, $C_{36}H_{24}N_2O_2$, the two naphthyl systems are approximately perpendicular to each other and the two 4-cyanobenzyloxy rings are almost parallel to each other. There are strong π–π interactions [3.835 (3) Å] between neighbouring molecules. The face-to-face π–π interactions between the benzene rings of neighbouring molecules stabilize the crystal structure to form a one-dimensional chain structure along the a axis.

Related literature

For related literature, see: Hiroshi *et al.* (2005); Minatti & Dötz (2005); Pu (1998).



Experimental

Crystal data

$C_{36}H_{24}N_2O_2$
M_r = 516.57
Triclinic, $P\overline{1}$
a = 7.835 (1) Å
b = 10.112 (1) Å
c = 17.864 (2) Å
α = 104.696 (2)°
β = 91.999 (2)°
γ = 98.995 (3)°
V = 1348.0 (3) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 291 (2) K
0.30 × 0.26 × 0.24 mm

Data collection

Bruker SMART APEX CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.97, T_{max} = 0.98
12114 measured reflections
5312 independent reflections
4098 reflections with $I > 2\sigma(I)$
R_{int} = 0.033

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.053
$wR(F^2)$ = 0.112
S = 1.07
5312 reflections
361 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.13 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Bruker, 2000); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; 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: IM2019).

References

Bruker (2000). *SMART* (Version 5.625), *SAINT* (Version 6.22), *SHELXTL* (Version 6.10) and *SADABS* (Version 2.03). Bruker AXS Inc., Madison, Wisconsin, USA.
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Pu, L. (1998). *Chem. Rev.* **98**, 2405–2494.

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supplementary materials

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4,4'-[1,1'-Binaphthalene-2,2'-diyldi(oxymethylene)]benzonitrile

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Comment

Because of their highly stable chiral configuration, the 2,2-substituted 1,1-binaphthyls have been extensively used to control many asymmetric processes and have demonstrated outstanding chiral discrimination properties (Pu, 1998). Most 1,1-binaphthyl molecules are *C*2 symmetric with two identical naphthyl units. The rigid structure and the *C*2 symmetry of the chiral binaphthyl molecules play an important role in chiral induction (Minatti & Dötz, 2005; Hiroshi, *et al.*, 2005). Herein we report the 1,1'-binaphthyl derivative shown below (I) and its crystal structure.

The crystal data show that in the title compound, $C_{36}H_{24}N_2O_2$, the two naphthyl rings are approximately perpendicular to each other and the dihedral angle is 86.68 (3)°. Nevertheless, the two 4-cyanobenzyloxy rings are almost parallel with respect to each other with a dihedral angle of 10.33 (8)°. In Fig. 2, *Cg*1 and *Cg*2 are the centroids of ring A (C30—C35) and ring B (C22—C27), respectively. The centroid distance for *Cg*1—*Cg*2^{ii} is 3.835 (3) Å, indicating quite strong π-π interactions between the neighbouring molecules. The face to face π-π interactions between the phenyl rings of neighbouring molecules play a very important function in stabilizing the crystal structure. The one-dimensional chain structure is formed by stacking of molecules showing the same absolute configuration *via* π-π interactions along the *a* axis. (symmetry code: (i) 1 + *x*,*y*,*z*; (ii) −1 + *x*,*y*,*z*)

Experimental

Racemic 1,1'-binaphthyl-2,2'-diol (0.286 g, 1 mmol) and 4-(bromomethyl)benzonitrile (0.392 g, 2 mmol) were dissolved in acetone (25 ml) in the presence of K_2CO_3 (0.138 g, 1 mmol) and refluxed for 3 days. After the mixture was cooled to room temperature, the solution was filtered and rotated in vacuum affording a white precipitate of compound (I). Colourless crystals of the title compound suitable for X-ray diffraction were obtained from a solution of 100 mg (I) in 15 ml diethylether after 3 weeks.

Refinement

All the C—H hydrogen atoms were generated geometrically and with C—H distances ranging from 0.93 to 0.97 Å and included in the refinement in riding motion approximation with $U_{iso} = 1.2U_{eq}$ of the carrier atom.

Figures

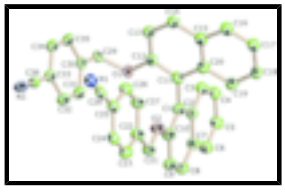

Fig. 1. The molecular structure of the *R*-enantiomer of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

Fig. 2. View of the 1-D chain structure along *a* axis. (symmetry code: (i) 1 + *x*,*y*,*z*; (ii) −1 + *x*,*y*,*z*)

4,4'-[1,1'-Binaphthalene-2,2'-diyldi(oxymethylene)]benzonitrile

Crystal data

$C_{36}H_{24}N_2O_2$	$Z = 2$
$M_r = 516.57$	$F_{000} = 540$
Triclinic, $P\bar{1}$	$D_x = 1.273$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 7.835$ (1) Å	Cell parameters from 3754 reflections
$b = 10.112$ (1) Å	$\theta = 2.1$–22.0º
$c = 17.864$ (2) Å	$\mu = 0.08$ mm^{-1}
$\alpha = 104.696$ (2)º	$T = 291$ (2) K
$\beta = 91.999$ (2)º	Block, colourless
$\gamma = 98.995$ (3)º	0.30 × 0.26 × 0.24 mm
$V = 1348.0$ (3) Å^3	

Data collection

Bruker SMART APEX CCD diffractometer	5312 independent reflections
Radiation source: sealed tube	4098 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.033$
$T = 291$(2) K	$\theta_{max} = 26.0$º
φ and ω scans	$\theta_{min} = 1.2$º
Absorption correction: multi-scan (SADABS; Bruker, 2000)	$h = -9 \rightarrow 9$
$T_{min} = 0.97$, $T_{max} = 0.98$	$k = -12 \rightarrow 12$
12114 measured reflections	$l = -22 \rightarrow 22$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.053$	H-atom parameters constrained
$wR(F^2) = 0.112$	$w = 1/[\sigma^2(F_o^2) + (0.04P)^2 + 0.33P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.07$	$(\Delta/\sigma)_{max} < 0.001$
5312 reflections	$\Delta\rho_{max} = 0.13$ e Å^{-3}
361 parameters	$\Delta\rho_{min} = -0.16$ e Å^{-3}

Primary atom site location: structure-invariant direct methods

Extinction correction: none

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.

Least-squares planes (*x*,*y*,*z* in crystal coordinates) and deviations from them (* indicates atom used to define plane)

7.1647 (0.0015) *x* − 3.8763 (0.0051) *y* + 6.1389 (0.0071) *z* = 2.8650 (0.0046)

* 0.0056 (0.0016) C1 * −0.0023 (0.0017) C2 * −0.0187 (0.0015) C3 * −0.0022 (0.0015) C4 * 0.0187 (0.0015) C5 * 0.0019 (0.0016) C6 * −0.0008 (0.0018) C7 * −0.0149 (0.0016) C8 * −0.0050 (0.0016) C9 * 0.0177 (0.0016) C10

Rms deviation of fitted atoms = 0.0114

− 3.5151 (0.0024) *x* − 6.1219 (0.0043) *y* + 13.3947 (0.0063) *z* = 3.2425 (0.0024)

Angle to previous plane (with approximate e.s.d.) = 86.68 (0.03)

* −0.0245 (0.0015) C11 * 0.0118 (0.0015) C12 * 0.0277 (0.0016) C13 * −0.0005 (0.0016) C14 * −0.0134 (0.0018) C15 * −0.0233 (0.0015) C16 * 0.0078 (0.0015) C17 * 0.0303 (0.0015) C18 * 0.0004 (0.0015) C19 * −0.0164 (0.0017) C20

Rms deviation of fitted atoms = 0.0187

− 7.0702 (0.0028) *x* + 5.5597 (0.0069) *y* − 3.4434 (0.0131) *z* = 1.4634 (0.0020)

Angle to previous plane (with approximate e.s.d.) = 86.97 (0.04)

* 0.0025 (0.0013) C30 * 0.0009 (0.0013) C31 * −0.0039 (0.0014) C32 * 0.0034 (0.0013) C33 * 0.0000 (0.0014) C34 * −0.0030 (0.0013) C35

Rms deviation of fitted atoms = 0.0027

7.1892 (0.0026) *x* − 4.4575 (0.0072) *y* + 5.3099 (0.0132) *z* = 2.6051 (0.0034)

Angle to previous plane (with approximate e.s.d.) = 10.33 (0.08)

* −0.0098 (0.0014) C22 * 0.0074 (0.0014) C23 * 0.0030 (0.0013) C24 * −0.0110 (0.0013) C25 * 0.0087 (0.0013) C26 * 0.0017 (0.0014) C27

Rms deviation of fitted atoms = 0.0077

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 $F^2 > 2\text{sigma}(F^2)$ 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	0.2017 (3)	0.29019 (19)	0.41549 (11)	0.0433 (4)
C2	0.1441 (2)	0.30558 (19)	0.49104 (11)	0.0426 (4)
C3	0.0597 (2)	0.19262 (19)	0.51564 (11)	0.0411 (4)
H3	0.0386	0.1048	0.4811	0.049*
C4	0.0081 (2)	0.20905 (19)	0.58890 (10)	0.0389 (4)
H4	−0.0466	0.1326	0.6041	0.047*
C5	0.0369 (2)	0.33958 (19)	0.64112 (11)	0.0398 (4)
H5	0.0030	0.3500	0.6914	0.048*
C6	0.1142 (2)	0.4520 (2)	0.61907 (11)	0.0451 (4)
H6	0.1300	0.5391	0.6541	0.054*
C7	0.1709 (3)	0.4387 (2)	0.54415 (12)	0.0455 (4)
C8	0.2511 (2)	0.5520 (2)	0.51978 (12)	0.0465 (5)
H8	0.2671	0.6401	0.5540	0.056*
C9	0.3061 (3)	0.5372 (2)	0.44789 (11)	0.0467 (5)
H9	0.3594	0.6142	0.4328	0.056*
C10	0.2822 (3)	0.4056 (2)	0.39633 (11)	0.0462 (5)
C11	0.1844 (2)	0.15117 (19)	0.35772 (10)	0.0398 (4)
C12	0.0469 (2)	0.10386 (19)	0.30272 (10)	0.0399 (4)
C13	0.0371 (2)	−0.01979 (19)	0.24483 (11)	0.0432 (4)
H13	−0.0579	−0.0499	0.2084	0.052*
C14	0.1651 (2)	−0.0958 (2)	0.24160 (11)	0.0432 (4)
H14	0.1586	−0.1768	0.2020	0.052*
C15	0.3073 (2)	−0.0546 (2)	0.29676 (11)	0.0441 (4)
C16	0.4430 (2)	−0.1339 (2)	0.29537 (11)	0.0442 (4)
H16	0.4398	−0.2143	0.2557	0.053*
C17	0.5746 (2)	−0.0945 (2)	0.35025 (11)	0.0434 (4)
H17	0.6609	−0.1485	0.3487	0.052*
C18	0.5836 (2)	0.0262 (2)	0.40949 (11)	0.0425 (4)
H18	0.6751	0.0515	0.4477	0.051*
C19	0.4591 (2)	0.1089 (2)	0.41237 (11)	0.0437 (4)
H19	0.4689	0.1908	0.4516	0.052*
C20	0.3159 (2)	0.0704 (2)	0.35593 (11)	0.0430 (4)
C21	0.4282 (2)	0.47657 (19)	0.29425 (11)	0.0413 (4)
H21A	0.5379	0.5130	0.3250	0.050*
H21B	0.3654	0.5527	0.2964	0.050*
C22	0.4599 (3)	0.4117 (2)	0.21174 (11)	0.0450 (4)
C23	0.5443 (2)	0.4935 (2)	0.16926 (11)	0.0448 (4)
H23	0.5869	0.5866	0.1925	0.054*
C24	0.5663 (2)	0.43691 (19)	0.09120 (10)	0.0387 (4)
H24	0.6232	0.4930	0.0626	0.046*
C25	0.5052 (2)	0.29965 (18)	0.05614 (10)	0.0373 (4)
C26	0.4246 (2)	0.2174 (2)	0.09994 (11)	0.0420 (4)
H26	0.3855	0.1235	0.0774	0.050*
C27	0.4018 (2)	0.27383 (19)	0.17680 (10)	0.0408 (4)
H27	0.3461	0.2175	0.2055	0.049*

C28	0.5283 (2)	0.24323 (19)	−0.02306 (10)	0.0374 (4)
C29	−0.2123 (2)	0.15527 (18)	0.24646 (10)	0.0373 (4)
H29A	−0.3047	0.2070	0.2630	0.045*
H29B	−0.2607	0.0572	0.2339	0.045*
C30	−0.1420 (2)	0.19107 (19)	0.17444 (10)	0.0392 (4)
C31	−0.0440 (2)	0.3190 (2)	0.18004 (11)	0.0426 (4)
H31	−0.0178	0.3826	0.2283	0.051*
C32	0.0161 (2)	0.3539 (2)	0.11436 (11)	0.0448 (4)
H32	0.0831	0.4404	0.1191	0.054*
C33	−0.0220 (2)	0.26212 (19)	0.04243 (11)	0.0407 (4)
C34	−0.1196 (2)	0.1337 (2)	0.03658 (12)	0.0451 (5)
H34	−0.1462	0.0701	−0.0117	0.054*
C35	−0.1781 (2)	0.0996 (2)	0.10237 (11)	0.0442 (4)
H35	−0.2435	0.0124	0.0977	0.053*
C36	0.0382 (2)	0.29689 (18)	−0.02469 (11)	0.0400 (4)
N1	0.5449 (2)	0.19579 (17)	−0.08698 (9)	0.0439 (4)
N2	0.0847 (2)	0.32188 (16)	−0.08039 (9)	0.0445 (4)
O1	−0.07884 (15)	0.18709 (13)	0.30920 (7)	0.0389 (3)
O2	0.33595 (18)	0.38044 (13)	0.32265 (7)	0.0471 (3)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0440 (10)	0.0398 (10)	0.0434 (10)	0.0031 (8)	0.0030 (8)	0.0087 (8)
C2	0.0454 (10)	0.0367 (9)	0.0446 (11)	0.0094 (8)	0.0047 (8)	0.0073 (8)
C3	0.0424 (10)	0.0422 (10)	0.0401 (10)	0.0133 (8)	0.0141 (8)	0.0083 (8)
C4	0.0397 (9)	0.0431 (10)	0.0386 (9)	0.0126 (8)	0.0180 (7)	0.0138 (8)
C5	0.0382 (9)	0.0442 (10)	0.0398 (10)	0.0152 (8)	0.0226 (8)	0.0088 (8)
C6	0.0414 (10)	0.0412 (10)	0.0494 (11)	0.0102 (8)	0.0146 (8)	0.0029 (8)
C7	0.0477 (11)	0.0373 (10)	0.0481 (11)	0.0087 (8)	0.0060 (8)	0.0036 (8)
C8	0.0438 (10)	0.0374 (10)	0.0520 (12)	0.0035 (8)	0.0054 (9)	0.0020 (8)
C9	0.0473 (11)	0.0384 (10)	0.0496 (11)	−0.0026 (8)	0.0036 (9)	0.0087 (8)
C10	0.0486 (11)	0.0419 (10)	0.0431 (11)	−0.0035 (8)	0.0080 (8)	0.0082 (8)
C11	0.0402 (10)	0.0414 (10)	0.0389 (10)	0.0067 (8)	0.0097 (8)	0.0115 (8)
C12	0.0379 (10)	0.0437 (10)	0.0396 (10)	0.0129 (8)	0.0048 (8)	0.0100 (8)
C13	0.0430 (10)	0.0427 (10)	0.0406 (10)	0.0121 (8)	0.0022 (8)	0.0024 (8)
C14	0.0426 (10)	0.0428 (10)	0.0431 (10)	0.0132 (8)	0.0068 (8)	0.0053 (8)
C15	0.0433 (10)	0.0484 (11)	0.0430 (10)	0.0147 (9)	0.0115 (8)	0.0110 (8)
C16	0.0417 (10)	0.0500 (11)	0.0456 (11)	0.0190 (9)	0.0168 (8)	0.0124 (9)
C17	0.0443 (10)	0.0474 (11)	0.0416 (10)	0.0144 (8)	0.0128 (8)	0.0122 (8)
C18	0.0427 (10)	0.0466 (11)	0.0403 (10)	0.0083 (8)	0.0019 (8)	0.0148 (8)
C19	0.0388 (10)	0.0486 (11)	0.0432 (10)	0.0040 (8)	0.0047 (8)	0.0132 (8)
C20	0.0400 (10)	0.0452 (10)	0.0445 (10)	0.0064 (8)	0.0095 (8)	0.0128 (8)
C21	0.0437 (10)	0.0380 (10)	0.0423 (10)	0.0001 (8)	0.0125 (8)	0.0137 (8)
C22	0.0477 (11)	0.0413 (10)	0.0444 (11)	0.0014 (8)	0.0122 (8)	0.0110 (8)
C23	0.0415 (10)	0.0478 (11)	0.0435 (10)	0.0055 (8)	0.0132 (8)	0.0092 (8)
C24	0.0381 (9)	0.0427 (10)	0.0412 (10)	0.0144 (8)	0.0169 (7)	0.0153 (8)
C25	0.0403 (9)	0.0396 (9)	0.0372 (9)	0.0169 (8)	0.0174 (7)	0.0117 (7)

C26	0.0419 (10)	0.0416 (10)	0.0409 (10)	0.0074 (8)	0.0158 (8)	0.0061 (8)
C27	0.0442 (10)	0.0375 (9)	0.0412 (10)	0.0000 (8)	0.0173 (8)	0.0136 (8)
C28	0.0417 (10)	0.0419 (10)	0.0386 (10)	0.0210 (8)	0.0202 (8)	0.0182 (8)
C29	0.0388 (9)	0.0365 (9)	0.0387 (9)	0.0106 (7)	−0.0032 (7)	0.0119 (7)
C30	0.0368 (9)	0.0406 (10)	0.0395 (10)	0.0100 (8)	−0.0065 (7)	0.0086 (8)
C31	0.0394 (10)	0.0425 (10)	0.0422 (10)	0.0056 (8)	−0.0018 (8)	0.0056 (8)
C32	0.0423 (10)	0.0420 (10)	0.0444 (11)	−0.0030 (8)	0.0023 (8)	0.0074 (8)
C33	0.0386 (10)	0.0398 (10)	0.0442 (10)	0.0037 (8)	0.0014 (8)	0.0140 (8)
C34	0.0411 (10)	0.0424 (10)	0.0466 (11)	0.0018 (8)	−0.0051 (8)	0.0067 (8)
C35	0.0402 (10)	0.0454 (10)	0.0413 (10)	−0.0023 (8)	−0.0061 (8)	0.0078 (8)
C36	0.0389 (10)	0.0361 (9)	0.0451 (11)	−0.0039 (7)	−0.0013 (8)	0.0176 (8)
N1	0.0424 (9)	0.0483 (9)	0.0435 (9)	0.0137 (7)	0.0145 (7)	0.0116 (7)
N2	0.0427 (9)	0.0409 (8)	0.0438 (9)	−0.0164 (7)	0.0056 (7)	0.0139 (7)
O1	0.0371 (7)	0.0419 (7)	0.0385 (7)	0.0158 (5)	−0.0031 (5)	0.0074 (5)
O2	0.0547 (8)	0.0389 (7)	0.0438 (7)	−0.0111 (6)	0.0130 (6)	0.0139 (6)

Geometric parameters (Å, °)

C1—C10	1.365 (3)	C19—C20	1.419 (3)
C1—C2	1.417 (3)	C19—H19	0.9300
C1—C11	1.501 (3)	C21—O2	1.334 (2)
C2—C3	1.405 (3)	C21—C22	1.500 (3)
C2—C7	1.416 (3)	C21—H21A	0.9700
C3—C4	1.361 (2)	C21—H21B	0.9700
C3—H3	0.9300	C22—C27	1.371 (3)
C4—C5	1.390 (3)	C22—C23	1.371 (3)
C4—H4	0.9300	C23—C24	1.394 (3)
C5—C6	1.357 (3)	C23—H23	0.9300
C5—H5	0.9300	C24—C25	1.371 (3)
C6—C7	1.405 (3)	C24—H24	0.9300
C6—H6	0.9300	C25—C26	1.379 (2)
C7—C8	1.395 (3)	C25—C28	1.414 (2)
C8—C9	1.348 (3)	C26—C27	1.376 (2)
C8—H8	0.9300	C26—H26	0.9300
C9—C10	1.394 (3)	C27—H27	0.9300
C9—H9	0.9300	C28—N1	1.141 (2)
C10—O2	1.370 (2)	C29—O1	1.443 (2)
C11—C12	1.372 (3)	C29—C30	1.521 (3)
C11—C20	1.407 (3)	C29—H29A	0.9700
C12—O1	1.382 (2)	C29—H29B	0.9700
C12—C13	1.395 (3)	C30—C35	1.372 (3)
C13—C14	1.350 (3)	C30—C31	1.375 (3)
C13—H13	0.9300	C31—C32	1.385 (3)
C14—C15	1.399 (3)	C31—H31	0.9300
C14—H14	0.9300	C32—C33	1.372 (3)
C15—C20	1.418 (3)	C32—H32	0.9300
C15—C16	1.425 (3)	C33—C34	1.377 (3)
C16—C17	1.337 (3)	C33—C36	1.409 (3)
C16—H16	0.9300	C34—C35	1.380 (3)

C17—C18	1.389 (3)	C34—H34	0.9300
C17—H17	0.9300	C35—H35	0.9300
C18—C19	1.374 (3)	C36—N2	1.145 (2)
C18—H18	0.9300		
C10—C1—C2	118.37 (17)	C20—C19—H19	119.7
C10—C1—C11	119.35 (17)	C11—C20—C15	120.10 (17)
C2—C1—C11	122.22 (17)	C11—C20—C19	122.19 (18)
C3—C2—C7	118.16 (17)	C15—C20—C19	117.71 (18)
C3—C2—C1	122.21 (17)	O2—C21—C22	108.83 (15)
C7—C2—C1	119.63 (17)	O2—C21—H21A	109.9
C4—C3—C2	121.36 (18)	C22—C21—H21A	109.9
C4—C3—H3	119.3	O2—C21—H21B	109.9
C2—C3—H3	119.3	C22—C21—H21B	109.9
C3—C4—C5	120.23 (17)	H21A—C21—H21B	108.3
C3—C4—H4	119.9	C27—C22—C23	119.03 (18)
C5—C4—H4	119.9	C27—C22—C21	121.88 (16)
C6—C5—C4	120.26 (16)	C23—C22—C21	119.06 (17)
C6—C5—H5	119.9	C22—C23—C24	119.97 (18)
C4—C5—H5	119.9	C22—C23—H23	120.0
C5—C6—C7	121.08 (17)	C24—C23—H23	120.0
C5—C6—H6	119.5	C25—C24—C23	120.77 (17)
C7—C6—H6	119.5	C25—C24—H24	119.6
C8—C7—C6	122.47 (17)	C23—C24—H24	119.6
C8—C7—C2	118.64 (18)	C24—C25—C26	118.77 (16)
C6—C7—C2	118.89 (18)	C24—C25—C28	120.34 (16)
C9—C8—C7	121.66 (18)	C26—C25—C28	120.87 (17)
C9—C8—H8	119.2	C27—C26—C25	120.30 (17)
C7—C8—H8	119.2	C27—C26—H26	119.9
C8—C9—C10	119.44 (19)	C25—C26—H26	119.9
C8—C9—H9	120.3	C22—C27—C26	121.12 (17)
C10—C9—H9	120.3	C22—C27—H27	119.4
C1—C10—O2	114.29 (16)	C26—C27—H27	119.4
C1—C10—C9	122.25 (18)	N1—C28—C25	178.8 (2)
O2—C10—C9	123.46 (17)	O1—C29—C30	111.64 (14)
C12—C11—C20	118.51 (17)	O1—C29—H29A	109.3
C12—C11—C1	121.18 (17)	C30—C29—H29A	109.3
C20—C11—C1	120.18 (17)	O1—C29—H29B	109.3
C11—C12—O1	115.20 (16)	C30—C29—H29B	109.3
C11—C12—C13	121.56 (17)	H29A—C29—H29B	108.0
O1—C12—C13	123.23 (16)	C35—C30—C31	118.23 (18)
C14—C13—C12	120.16 (18)	C35—C30—C29	121.50 (17)
C14—C13—H13	119.9	C31—C30—C29	120.24 (16)
C12—C13—H13	119.9	C30—C31—C32	120.57 (17)
C13—C14—C15	121.11 (18)	C30—C31—H31	119.7
C13—C14—H14	119.4	C32—C31—H31	119.7
C15—C14—H14	119.4	C33—C32—C31	120.76 (18)
C14—C15—C20	118.51 (17)	C33—C32—H32	119.6
C14—C15—C16	122.26 (18)	C31—C32—H32	119.6
C20—C15—C16	119.23 (18)	C32—C33—C34	118.87 (18)

C17—C16—C15	121.02 (18)	C32—C33—C36	121.13 (17)
C17—C16—H16	119.5	C34—C33—C36	119.99 (17)
C15—C16—H16	119.5	C33—C34—C35	119.96 (18)
C16—C17—C18	120.58 (18)	C33—C34—H34	120.0
C16—C17—H17	119.7	C35—C34—H34	120.0
C18—C17—H17	119.7	C30—C35—C34	121.60 (18)
C19—C18—C17	120.86 (18)	C30—C35—H35	119.2
C19—C18—H18	119.6	C34—C35—H35	119.2
C17—C18—H18	119.6	N2—C36—C33	178.20 (19)
C18—C19—C20	120.55 (18)	C12—O1—C29	117.85 (13)
C18—C19—H19	119.7	C21—O2—C10	124.00 (15)

Fig. 1

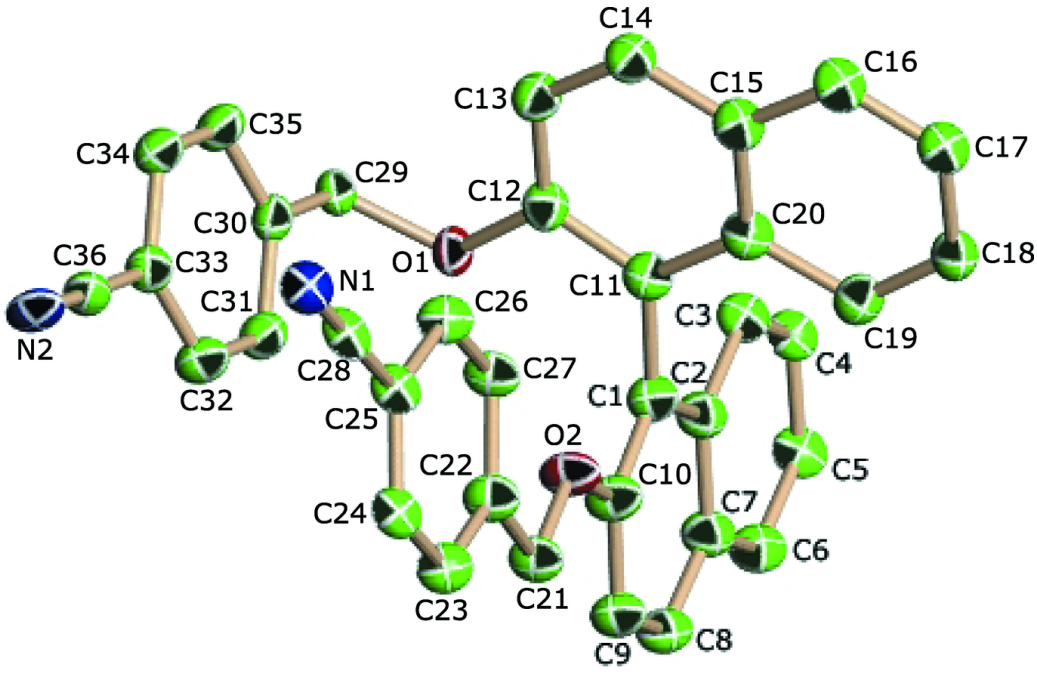
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Fig. 2