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2,2′-[(1*E*,1′*E*)-2,2′-(2,5-Dibutoxy-1,4-phenylene)bis(ethene-2,1-diyl)]-dipyridine

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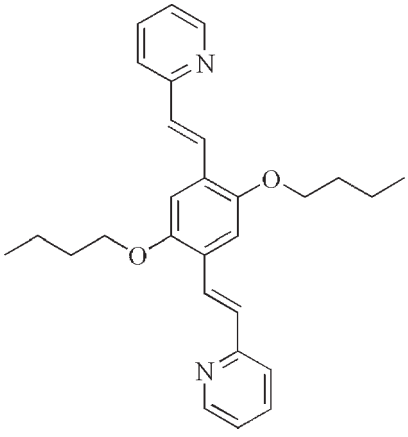
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.003 Å; R factor = 0.049; wR factor = 0.154; data-to-parameter ratio = 14.8.

The centrosymmetric title molecule, $C_{28}H_{32}N_2O_2$, has a central benzene ring subsituted in the 1- and 4-positions by (ethene-2,1-diyl)pyridine groups, and in the 2- and 5-positions by butoxy groups. The whole molecule is X-shaped and relatively flat, the dihedral angle between the pyridine and the central benzene ring being 11.29 (10)°. In the crystal, neighboring molecules are linked by weak C—H···N interactions, forming a two-dimensional undulating network.

Related literature

For information on pyridine-based photo-refractive materials, see: Naumov *et al.* (2002); Liu *et al.* (2008).



Experimental

Crystal data

$C_{28}H_{32}N_2O_2$
M_r = 428.56
Monoclinic, $P2_1/c$
a = 8.882 (5) Å
b = 13.892 (5) Å
c = 10.387 (5) Å
β = 107.392 (5)°
V = 1223.0 (10) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.07 mm^{-1}
T = 298 K
0.50 × 0.30 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.964, T_{max} = 0.986
8512 measured reflections
2162 independent reflections
1385 reflections with $I > 2\sigma(I)$
R_{int} = 0.040

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.154
S = 1.03
2162 reflections
146 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.16 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C5—H5···N1^{i}	0.93	2.70	3.446 (3)	138

Symmetry code: (i) $x, -y+\frac{3}{2}, z-\frac{1}{2}$.

Data collection: *SMART* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg & Putz, 2008); 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: SU2172).

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supporting information

Acta Cryst. (2010). E**66**, o1877 [doi:10.1107/S1600536810013656]

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S1. Comment

Pyridine based materials have been investigated for their electrical and optical properties. The introduction of substituents in the 2- and 4-positions of pyridine represents a possible approach for designing pyridine-based photo-refractive materials (Naumov *et al.*, 2002; Liu *et al.*, 2008).

In the title molecule (Fig. 1), which is centrosymmetric, there are two pyridine rings and a central benzene ring. The dihedral angle between the pyridine and the central benzene ring is 11.29 (10) °.

In the crystal structure of the title compound there exist C5—H5···N1^{i} interactions between neighboring molecules [see Fig. 2 and Table 1]. This leads to the formation of a two-dimensional network lieing parallel to the *bc*-plane.

S2. Experimental

The title compound was prepared by firstly placing t-BuOK (8.98 g, 0.080 mol) in a dry motar and milling it to give very small particles. Then 2,5-Dibutoxy-1,4-bis(triphenylphosphonium)benzene dischloride (8.45 g, 0.010 mol) and picolinaldehyde (4.28 g, 0.040 mol) were added. The mixture was then milled vigorously for about 10 min. After the reaction was completed (monitored by TLC), the mixture was dispersed in 50 ml of H_2O. The solution was extracted three times with 50 ml dichloromethane. The dichloromethane solution was dried for 12 h and concentrated. The concentrated solution was passed over a silica gel column and eluted with peroleum ether/ethyl acetate (8:1). By slow evaporation of the solvent yellow block-like crystals were obtained in 75% yield.

S3. Refinement

The H-atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms: C—H = 0.93, 0.96 and 0.97 Å for CH, CH_3 and CH_2 H-atoms, respectively, with U_{iso}(H) = k × U_{eq}(parent C-atom), where k = 1.2 for CH and CH_2 H-atoms and = 1.5 for CH_3 H-atoms.

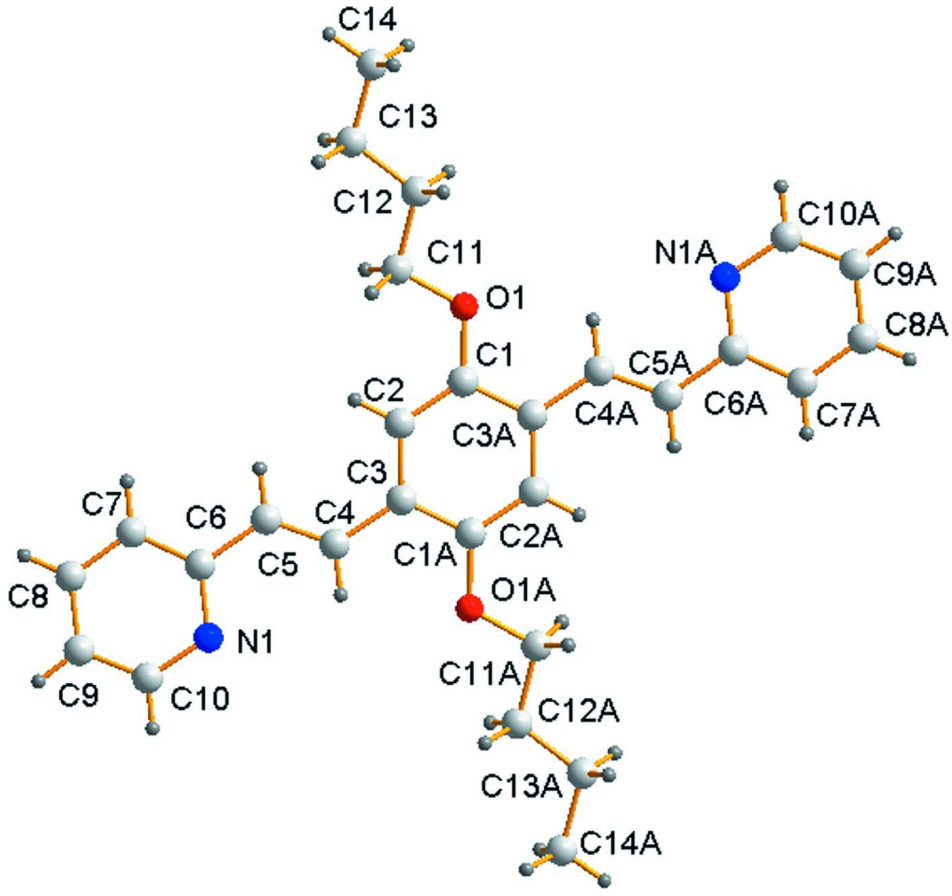

Figure 1

The molecular structure of the title molecule.

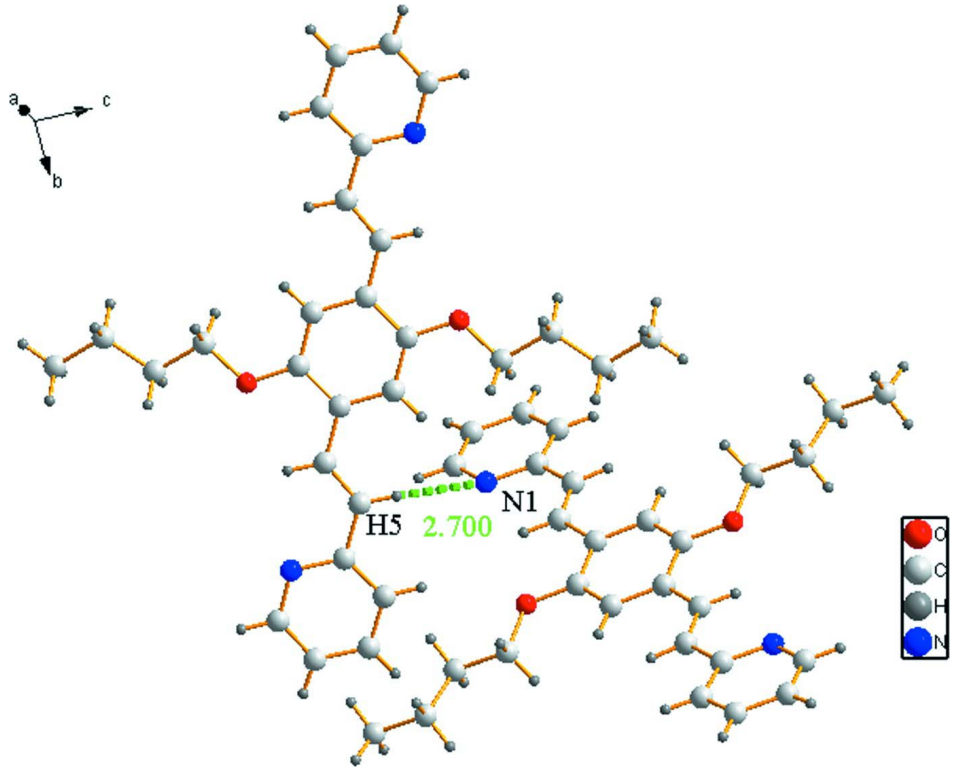

Figure 2

A view of the intermolecular C-H···N interactions (dashed lines) in the crystal structure of the title compound.

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Crystal data

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$a = 8.882$ (5) Å
$b = 13.892$ (5) Å
$c = 10.387$ (5) Å
$\beta = 107.392$ (5)°
$V = 1223.0$ (10) Å^3
$Z = 2$
$F(000) = 460$
$D_x = 1.164$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71069$ Å
Cell parameters from 1446 reflections
$\theta = 2.5$–21.8°
$\mu = 0.07$ mm^{-1}
$T = 298$ K
Block, yellow
0.50 × 0.30 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
phi and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.964$, $T_{max} = 0.986$
8512 measured reflections
2162 independent reflections
1385 reflections with $I > 2\sigma(I)$
$R_{int} = 0.040$
$\theta_{max} = 25.0°$, $\theta_{min} = 2.4°$
$h = -10 \rightarrow 10$
$k = -16 \rightarrow 16$
$l = -11 \rightarrow 12$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.049$
$wR(F^2) = 0.154$
$S = 1.03$
2162 reflections
146 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
$w = 1/[\sigma^2(F_o^2) + (0.0821P)^2 + 0.0525P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.16$ e Å^{-3}
$\Delta\rho_{min} = -0.16$ 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	−0.10160 (17)	0.50961 (9)	0.22161 (12)	0.0589 (4)
C2	0.0431 (2)	0.57863 (13)	0.43825 (17)	0.0477 (5)
H2	0.0725	0.6313	0.3960	0.057*
C1	−0.0472 (2)	0.50707 (13)	0.36022 (17)	0.0458 (5)
C5	0.2548 (2)	0.72369 (13)	0.61936 (18)	0.0491 (5)
H5	0.2324	0.7310	0.5265	0.059*
C4	0.1898 (2)	0.64922 (13)	0.66286 (18)	0.0487 (5)
H4	0.2083	0.6442	0.7556	0.058*
C6	0.3587 (2)	0.79507 (14)	0.70512 (19)	0.0500 (5)
C3	0.0919 (2)	0.57414 (13)	0.57915 (17)	0.0447 (5)
N1	0.3841 (2)	0.78919 (14)	0.83829 (17)	0.0781 (6)
C7	0.4305 (3)	0.86549 (15)	0.6486 (2)	0.0617 (6)
H7	0.4106	0.8689	0.5556	0.074*
C11	−0.0751 (3)	0.59382 (15)	0.15295 (19)	0.0620 (6)
H11A	0.0359	0.5996	0.1601	0.074*
H11B	−0.1069	0.6507	0.1922	0.074*
C12	−0.1717 (3)	0.58404 (16)	0.00746 (18)	0.0639 (6)
H12A	−0.1503	0.5217	−0.0253	0.077*
H12B	−0.2826	0.5857	0.0020	0.077*
C8	0.5312 (3)	0.93013 (17)	0.7318 (3)	0.0770 (7)
H8	0.5797	0.9780	0.6957	0.092*
C10	0.4832 (3)	0.8533 (2)	0.9145 (2)	0.0988 (10)
H10	0.5018	0.8498	1.0074	0.119*
C9	0.5588 (3)	0.9232 (2)	0.8671 (3)	0.0907 (9)
H9	0.6277	0.9652	0.9258	0.109*

C13	−0.1405 (4)	0.6606 (2)	−0.0831 (2)	0.0963 (9)
H13A	−0.0302	0.6582	−0.0795	0.116*
H13B	−0.1603	0.7231	−0.0499	0.116*
C14	−0.2407 (4)	0.6502 (2)	−0.2276 (2)	0.0996 (10)
H14A	−0.2273	0.5868	−0.2594	0.149*
H14B	−0.2092	0.6972	−0.2822	0.149*
H14C	−0.3496	0.6599	−0.2335	0.149*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0777 (10)	0.0571 (9)	0.0353 (8)	−0.0123 (7)	0.0069 (7)	−0.0006 (6)
C2	0.0541 (12)	0.0462 (10)	0.0408 (11)	−0.0014 (9)	0.0111 (9)	−0.0001 (8)
C1	0.0492 (11)	0.0514 (11)	0.0330 (10)	0.0032 (9)	0.0066 (9)	−0.0017 (8)
C5	0.0514 (12)	0.0543 (12)	0.0386 (11)	0.0007 (9)	0.0090 (9)	−0.0031 (9)
C4	0.0550 (12)	0.0529 (11)	0.0346 (11)	−0.0021 (9)	0.0081 (9)	−0.0050 (8)
C6	0.0510 (12)	0.0529 (12)	0.0467 (12)	−0.0029 (9)	0.0155 (10)	−0.0073 (9)
C3	0.0466 (11)	0.0463 (11)	0.0387 (10)	0.0006 (8)	0.0090 (9)	−0.0034 (8)
N1	0.0928 (15)	0.0965 (15)	0.0456 (11)	−0.0454 (12)	0.0215 (10)	−0.0188 (10)
C7	0.0672 (14)	0.0618 (13)	0.0568 (13)	−0.0111 (11)	0.0194 (11)	−0.0026 (10)
C11	0.0807 (16)	0.0550 (13)	0.0478 (12)	−0.0075 (11)	0.0154 (11)	0.0028 (10)
C12	0.0770 (16)	0.0679 (14)	0.0421 (12)	−0.0073 (11)	0.0107 (11)	0.0048 (10)
C8	0.0811 (17)	0.0685 (15)	0.0898 (19)	−0.0262 (13)	0.0385 (14)	−0.0114 (13)
C10	0.115 (2)	0.129 (2)	0.0536 (15)	−0.067 (2)	0.0270 (15)	−0.0310 (15)
C9	0.0903 (19)	0.105 (2)	0.0823 (19)	−0.0484 (16)	0.0338 (15)	−0.0386 (16)
C13	0.131 (2)	0.0873 (18)	0.0572 (16)	−0.0271 (17)	0.0078 (16)	0.0158 (13)
C14	0.125 (3)	0.108 (2)	0.0532 (15)	−0.0132 (18)	0.0064 (15)	0.0242 (14)

Geometric parameters (Å, º)

O1—C1	1.375 (2)	C11—C12	1.504 (3)
O1—C11	1.426 (2)	C11—H11A	0.9700
C2—C1	1.379 (3)	C11—H11B	0.9700
C2—C3	1.398 (2)	C12—C13	1.499 (3)
C2—H2	0.9300	C12—H12A	0.9700
C1—C3^{i}	1.406 (3)	C12—H12B	0.9700
C5—C4	1.328 (3)	C8—C9	1.356 (3)
C5—C6	1.462 (3)	C8—H8	0.9300
C5—H5	0.9300	C10—C9	1.353 (3)
C4—C3	1.466 (3)	C10—H10	0.9300
C4—H4	0.9300	C9—H9	0.9300
C6—N1	1.336 (2)	C13—C14	1.506 (3)
C6—C7	1.390 (3)	C13—H13A	0.9700
C3—C1^{i}	1.406 (3)	C13—H13B	0.9700
N1—C10	1.334 (3)	C14—H14A	0.9600
C7—C8	1.375 (3)	C14—H14B	0.9600
C7—H7	0.9300	C14—H14C	0.9600

C1—O1—C11	119.07 (14)	H11A—C11—H11B	108.5
C1—C2—C3	121.80 (18)	C13—C12—C11	114.19 (19)
C1—C2—H2	119.1	C13—C12—H12A	108.7
C3—C2—H2	119.1	C11—C12—H12A	108.7
O1—C1—C2	123.88 (17)	C13—C12—H12B	108.7
O1—C1—C3^{i}	115.58 (15)	C11—C12—H12B	108.7
C2—C1—C3^{i}	120.53 (17)	H12A—C12—H12B	107.6
C4—C5—C6	125.48 (18)	C9—C8—C7	119.1 (2)
C4—C5—H5	117.3	C9—C8—H8	120.4
C6—C5—H5	117.3	C7—C8—H8	120.4
C5—C4—C3	126.43 (18)	N1—C10—C9	125.0 (2)
C5—C4—H4	116.8	N1—C10—H10	117.5
C3—C4—H4	116.8	C9—C10—H10	117.5
N1—C6—C7	121.57 (18)	C10—C9—C8	118.2 (2)
N1—C6—C5	118.03 (18)	C10—C9—H9	120.9
C7—C6—C5	120.38 (18)	C8—C9—H9	120.9
C2—C3—C1^{i}	117.66 (16)	C12—C13—C14	113.1 (2)
C2—C3—C4	122.17 (17)	C12—C13—H13A	109.0
C1^{i}—C3—C4	120.15 (16)	C14—C13—H13A	109.0
C10—N1—C6	116.8 (2)	C12—C13—H13B	109.0
C8—C7—C6	119.3 (2)	C14—C13—H13B	109.0
C8—C7—H7	120.4	H13A—C13—H13B	107.8
C6—C7—H7	120.4	C13—C14—H14A	109.5
O1—C11—C12	107.37 (16)	C13—C14—H14B	109.5
O1—C11—H11A	110.2	H14A—C14—H14B	109.5
C12—C11—H11A	110.2	C13—C14—H14C	109.5
O1—C11—H11B	110.2	H14A—C14—H14C	109.5
C12—C11—H11B	110.2	H14B—C14—H14C	109.5

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C5—H5···N1^{ii}	0.93	2.70	3.446 (3)	138

Symmetry code: (ii) $x, -y+3/2, z-1/2$.