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1,4-Bis(4-nitrostyryl)benzene

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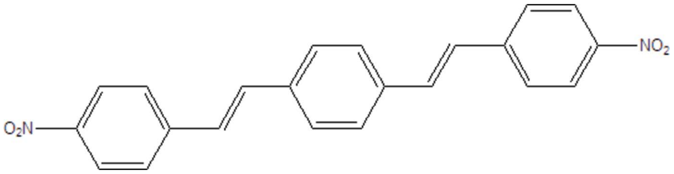
Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.002 Å; R factor = 0.038; wR factor = 0.116; data-to-parameter ratio = 12.6.

The complete molecule of the title compound, $C_{22}H_{16}N_2O_4$, is generated by a crystallographic centre of inversion. The plane of the central aromatic ring is tilted by 11.85 (4)° with respect to the outer aromatic ring. The crystal packing is determined by van der Waals interactions, with stair-like stacking between adjacent aromatic rings. The stacks are staggered and each layer is approximately 3.8 Å from the next. The closest intermolecular contact (approximately 2.42 Å) is between an O atom and a vinyl H atom.

Related literature

For background information on photonic materials, see: He *et al.* (2008). For stilbenes, see: Moreno-Fuquen *et al.* (2008, 2009). For the synthesis, see: Borsche (1912); Nakatsuji *et al.* (1991). For a related structure, see: Bazan *et al.* (2000).



Experimental

Crystal data

$C_{22}H_{16}N_2O_4$
M_r = 372.37
Monoclinic, $P2_1/c$
a = 7.4689 (12) Å
b = 16.615 (3) Å
c = 7.3917 (12) Å
β = 108.824 (3)°
V = 868.2 (2) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 173 K
0.40 × 0.18 × 0.12 mm

Data collection

Bruker SMART Platform CCD diffractometer
Absorption correction: none
10088 measured reflections
2001 independent reflections
1486 reflections with $I > 2\sigma(I)$
$R_{\rm int}$ = 0.041

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.116
S = 1.02
2001 reflections
159 parameters
All H-atom parameters refined
$\Delta\rho_{\max}$ = 0.30 e Å^{-3}
$\Delta\rho_{\min}$ = −0.18 e Å^{-3}

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; 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: *publCIF* (Westrip, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NG2592).

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supplementary materials

Acta Cryst. (2009). E**65**, o1806 [**doi:10.1107/S1600536809024751**]

1,4-Bis(4-nitrostyryl)benzene

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Comment

Distyrylbenzene derivatives have been studied as laser dyes, components of organic light-emitting diodes, and as model compounds for the study of conductivity and molecular properties in substituted *p*-phenylenevinylene (PPV) polymers. For background information on photonic materials, see: He *et al.* (2008). For related systems of stilbene, see: Moreno-Fuquen *et al.* (2008, 2009). For literature related to the synthesis, see: Borsche (1912).

Experimental

Synthesis was carried out following literature procedures (Nakatsuj) by standard Wittig synthesis. To a mixture of *p*-phenylenedimethylene- bis(tripheny1phosphonium chloride) (1.00 g, 1.43 mmol) and *p*-nitrobenzaldehyde (0.432 g 2.86 mmol) in EtOH (10 ml) was added 0.2 mol/*L* EtOLi(20 ml, 4.0 mmol) and the mixture was stirred overnight. The resulting reaction mixture was poured into water to give a yellow precipitate (0.4 g, 75%) which was filtered off, washed with EtOH, dried under reduced pressure, m.p. 289–290. Crystallization attempts from various solvents yielded only powders. Yellowish orange crystals however were grown by sublimation.

Refinement

All hydrogen atoms were placed in ideal positions and refined as riding atoms with relative isotropic displacement parameters.

Figures

Fig. 1. The molecular structure of 1,4-di(4-nitrostyryl)benzene with atom lables.

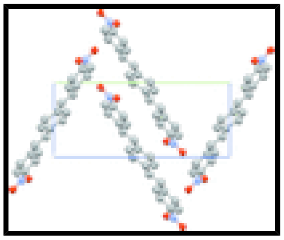


Fig. 2. Crystal packing viewed along the *a* axis.

1,4-Bis(4-nitrostyryl)benzene

Crystal data

$C_{22}H_{16}N_2O_4$	$F_{000} = 388$
$M_r = 372.37$	$D_x = 1.424$ Mg m^{-3}

Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 7.4689$ (12) Å
$b = 16.615$ (3) Å
$c = 7.3917$ (12) Å
$\beta = 108.824$ (3)°
$V = 868.2$ (2) Å^3
$Z = 2$

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 851 reflections
$\theta = 2.5–27.5$°
$\mu = 0.10$ mm^{-1}
$T = 173$ K
Needle, yellow
0.40 × 0.18 × 0.12 mm

Data collection

Bruker SMART Platform CCD diffractometer
Radiation source: normal-focus sealed tube
Monochromator: graphite
$T = 173$ K
ω scans
Absorption correction: None
10088 measured reflections
2001 independent reflections

1486 reflections with $I > 2\sigma(I)$
$R_{\text{int}} = 0.041$
$\theta_{\text{max}} = 27.5$°
$\theta_{\text{min}} = 2.5$°
$h = -9 \rightarrow 9$
$k = -21 \rightarrow 21$
$l = -9 \rightarrow 9$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.038$
$wR(F^2) = 0.116$
$S = 1.02$
2001 reflections
159 parameters
Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0595P)^2 + 0.1981P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\text{max}} < 0.001$
$\Delta\rho_{\text{max}} = 0.30$ e Å^{-3}
$\Delta\rho_{\text{min}} = -0.18$ e Å^{-3}
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.

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 (Å^2)

	x	y	z	U_{iso}*/U_{eq}
N1	−0.18351 (16)	0.18081 (7)	−0.31257 (17)	0.0314 (3)
O1	−0.31485 (14)	0.14204 (7)	−0.29133 (16)	0.0424 (3)
O2	−0.20374 (14)	0.23244 (7)	−0.43745 (15)	0.0415 (3)
C1	0.00888 (18)	0.16483 (8)	−0.18509 (19)	0.0268 (3)
C2	0.03516 (19)	0.10424 (8)	−0.0511 (2)	0.0293 (3)
H2	−0.068 (2)	0.0758 (9)	−0.037 (2)	0.034 (4)*
C3	0.2169 (2)	0.08605 (8)	0.0623 (2)	0.0299 (3)
H3	0.234 (2)	0.0439 (10)	0.154 (2)	0.036 (4)*
C4	0.37281 (19)	0.12795 (8)	0.04412 (18)	0.0274 (3)
C5	0.3394 (2)	0.19080 (9)	−0.0888 (2)	0.0309 (3)
H5	0.440 (2)	0.2209 (9)	−0.102 (2)	0.032 (4)*
C6	0.1573 (2)	0.20926 (9)	−0.2043 (2)	0.0302 (3)
H6	0.137 (2)	0.2519 (10)	−0.294 (2)	0.037 (4)*
C7	0.56766 (19)	0.10807 (9)	0.1593 (2)	0.0304 (3)
H7	0.659 (2)	0.1468 (9)	0.145 (2)	0.036 (4)*
C8	0.62118 (19)	0.04369 (9)	0.27155 (19)	0.0296 (3)
H8	0.530 (2)	0.0058 (9)	0.282 (2)	0.027 (4)*
C9	0.81506 (18)	0.02312 (8)	0.38677 (18)	0.0270 (3)
C10	0.9717 (2)	0.07130 (9)	0.39725 (19)	0.0291 (3)
H10	0.959 (2)	0.1202 (10)	0.333 (2)	0.040 (4)*
C11	0.8479 (2)	−0.04871 (9)	0.49188 (19)	0.0295 (3)
H11	0.740 (2)	−0.0827 (10)	0.482 (2)	0.039 (4)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0255 (6)	0.0340 (7)	0.0330 (6)	0.0040 (5)	0.0072 (5)	−0.0046 (5)
O1	0.0245 (5)	0.0545 (7)	0.0467 (7)	−0.0036 (5)	0.0091 (5)	−0.0009 (5)
O2	0.0348 (6)	0.0417 (6)	0.0426 (6)	0.0100 (5)	0.0050 (5)	0.0105 (5)
C1	0.0224 (6)	0.0296 (7)	0.0267 (7)	0.0041 (5)	0.0054 (5)	−0.0038 (5)
C2	0.0261 (7)	0.0292 (7)	0.0330 (7)	−0.0030 (5)	0.0103 (6)	−0.0011 (6)
C3	0.0309 (7)	0.0280 (7)	0.0299 (7)	−0.0001 (5)	0.0087 (6)	0.0026 (6)
C4	0.0267 (7)	0.0279 (7)	0.0260 (7)	0.0015 (5)	0.0064 (5)	−0.0017 (5)
C5	0.0246 (7)	0.0322 (7)	0.0355 (8)	−0.0021 (5)	0.0093 (6)	0.0031 (6)
C6	0.0295 (7)	0.0293 (7)	0.0312 (7)	0.0027 (5)	0.0089 (6)	0.0056 (6)
C7	0.0244 (7)	0.0331 (8)	0.0314 (7)	−0.0010 (6)	0.0059 (6)	−0.0005 (6)
C8	0.0260 (7)	0.0312 (7)	0.0300 (7)	0.0002 (6)	0.0071 (5)	−0.0017 (6)
C9	0.0278 (7)	0.0301 (7)	0.0221 (6)	0.0037 (5)	0.0066 (5)	−0.0032 (5)
C10	0.0313 (7)	0.0283 (7)	0.0268 (7)	0.0034 (5)	0.0082 (5)	0.0026 (5)
C11	0.0270 (7)	0.0313 (7)	0.0294 (7)	−0.0008 (5)	0.0082 (5)	−0.0011 (6)

Geometric parameters (Å, °)

N1—O1	1.2253 (16)	C5—H5	0.932 (16)
N1—O2	1.2332 (15)	C6—H6	0.950 (16)

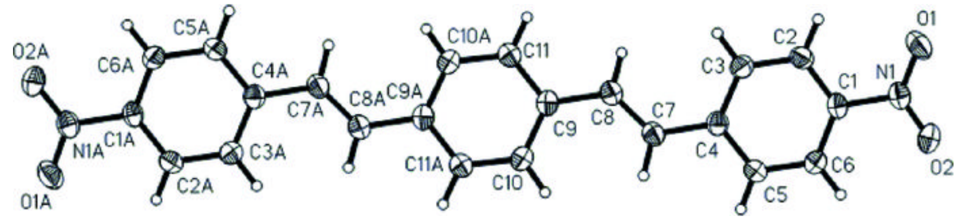
N1—C1	1.4661 (17)	C7—C8	1.334 (2)
C1—C6	1.3765 (19)	C7—H7	0.969 (16)
C1—C2	1.381 (2)	C8—C9	1.4640 (19)
C2—C3	1.379 (2)	C8—H8	0.951 (15)
C2—H2	0.940 (16)	C9—C10	1.399 (2)
C3—C4	1.4001 (19)	C9—C11	1.4020 (19)
C3—H3	0.953 (16)	C10—C11^{i}	1.384 (2)
C4—C5	1.3999 (19)	C10—H10	0.930 (17)
C4—C7	1.4670 (19)	C11—C10^{i}	1.384 (2)
C5—C6	1.3868 (19)	C11—H11	0.968 (17)

O1—N1—O2	123.49 (12)	C1—C6—C5	118.71 (13)
O1—N1—C1	118.79 (12)	C1—C6—H6	121.2 (10)
O2—N1—C1	117.71 (11)	C5—C6—H6	120.1 (10)
C6—C1—C2	122.13 (12)	C8—C7—C4	125.71 (13)
C6—C1—N1	119.44 (12)	C8—C7—H7	121.2 (9)
C2—C1—N1	118.42 (12)	C4—C7—H7	113.1 (9)
C3—C2—C1	118.68 (13)	C7—C8—C9	126.21 (14)
C3—C2—H2	120.4 (9)	C7—C8—H8	120.2 (9)
C1—C2—H2	120.9 (9)	C9—C8—H8	113.6 (9)
C2—C3—C4	121.26 (13)	C10—C9—C11	117.57 (12)
C2—C3—H3	118.2 (9)	C10—C9—C8	123.46 (13)
C4—C3—H3	120.6 (9)	C11—C9—C8	118.97 (13)
C5—C4—C3	118.20 (12)	C11^{i}—C10—C9	120.98 (13)
C5—C4—C7	119.61 (13)	C11^{i}—C10—H10	117.5 (10)
C3—C4—C7	122.18 (13)	C9—C10—H10	121.5 (10)
C6—C5—C4	120.96 (13)	C10^{i}—C11—C9	121.45 (13)
C6—C5—H5	118.6 (9)	C10^{i}—C11—H11	121.0 (9)
C4—C5—H5	120.5 (9)	C9—C11—H11	117.6 (9)

O1—N1—C1—C6	−178.44 (12)	N1—C1—C6—C5	−176.92 (12)
O2—N1—C1—C6	2.28 (19)	C4—C5—C6—C1	0.4 (2)
O1—N1—C1—C2	2.67 (19)	C5—C4—C7—C8	−170.57 (14)
O2—N1—C1—C2	−176.61 (12)	C3—C4—C7—C8	9.5 (2)
C6—C1—C2—C3	−2.3 (2)	C4—C7—C8—C9	179.87 (13)
N1—C1—C2—C3	176.57 (12)	C7—C8—C9—C10	1.9 (2)
C1—C2—C3—C4	0.3 (2)	C7—C8—C9—C11	−177.62 (13)
C2—C3—C4—C5	1.9 (2)	C11—C9—C10—C11^{i}	−0.2 (2)
C2—C3—C4—C7	−178.18 (13)	C8—C9—C10—C11^{i}	−179.77 (13)
C3—C4—C5—C6	−2.3 (2)	C10—C9—C11—C10^{i}	0.2 (2)
C7—C4—C5—C6	177.80 (13)	C8—C9—C11—C10^{i}	179.80 (13)
C2—C1—C6—C5	1.9 (2)		

Symmetry codes: (i) $-x+2, -y, -z+1$.

Fig. 1


O2A
C6A
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C9
C8
C7
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C1
N1
O1
O2
C6
C5
C4
C10
C11A
C3A
C2A
C1A
N1A
O1A

Fig. 2