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2,2′-(1,4-Phenylenedivinylene)diquinolin-8-ol

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Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.003 Å
R factor = 0.044
wR factor = 0.118
Data-to-parameter ratio = 14.4

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

The title compound, $C_{28}H_{20}N_2O_2$, has a crystallographic inversion centre, and an intramolecular O—H···N hydrogen bond may have an effect on some bond lengths and angles.

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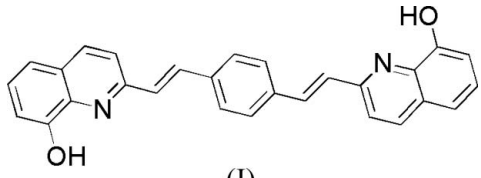
Comment

The electroluminescent properties of the title compound, (I), together with its Al^{III} and Zn^{II} complexes, were reported previously (Kim *et al.*, 2002; Cui & Kim, 2004).



(I)

The molecular structure of (I) is illustrated in Fig. 1. The asymmetric unit contains one half-molecule; the other half is generated by a centre of inversion, which lies at the centre of the benzene ring. The intramolecular O—H···N hydrogen bond (Table 2) may have an effect on some bond lengths and angles. A view of the molecular packing is shown in Fig. 2.

Experimental

The title compound was synthesized according to the method of Diakoumakos & Mikroyannidis (1993). Single crystals of (I) suitable for an X-ray diffraction study were obtained by recrystallization from a dimethylformamide solution.

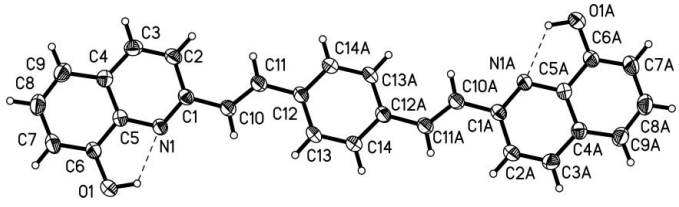


Figure 1
A drawing of the molecule of (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 35% probability level. The broken lines indicate hydrogen bonds. Atoms labelled with the suffix 'A' are at the symmetry position (−*x*, −*y*, −*z*).

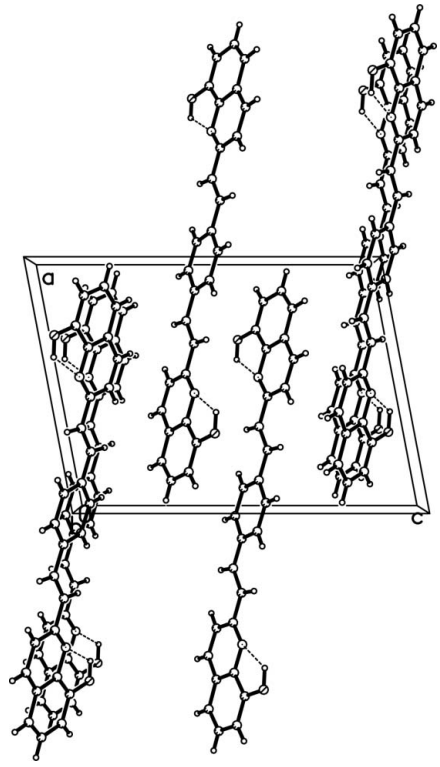


Figure 2
A packing diagram for (I). Dashed lines indicate hydrogen bonds..

Crystal data

$C_{28}H_{20}N_2O_2$
M_r = 416.46
Monoclinic, $P2_1/c$
a = 11.648 (6) Å
b = 5.777 (3) Å
c = 15.852 (8) Å
β = 100.740 (9)°
V = 1047.9 (10) Å^3
Z = 2
D_x = 1.320 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1827 reflections
θ = 2.6–26.4°
μ = 0.08 mm^{-1}
T = 294 (2) K
Prism, yellow
0.22 × 0.20 × 0.10 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2002)
T_{min} = 0.980, T_{max} = 0.992
5549 measured reflections
2142 independent reflections
1323 reflections with $I > 2\sigma(I)$
R_{int} = 0.023
θ_{max} = 26.4°
$h = -14 \rightarrow 10$
$k = -7 \rightarrow 6$
$l = -16 \rightarrow 19$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.118
S = 1.02
2142 reflections
149 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0519P)^2 + 0.0516P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.15 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

N1—C1	1.330 (2)	C4—C5	1.417 (2)
N1—C5	1.370 (2)	C5—C6	1.413 (2)
O1—C6	1.368 (2)	C6—C7	1.369 (2)
C1—N1—C5	118.34 (15)	C6—C5—C4	118.88 (15)
N1—C1—C2	121.21 (16)	O1—C6—C7	121.09 (17)
N1—C5—C6	117.15 (16)	O1—C6—C5	118.62 (15)
N1—C5—C4	123.96 (16)		

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N1	0.96 (2)	2.06 (2)	2.694 (2)	122 (2)

Atom H1 was located in a difference synthesis and refined freely [O—H = 0.96 (2) Å]. The remaining H atoms were positioned geometrically at distances of 0.93 Å from their parent C atoms, and a riding model was used during the refinement process, with the U_{iso}(H) values constrained to 1.2 times U_{eq} of the carrier atom.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

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