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5-[(*E*)-2-Phenylethen-1-yl]quinolin-8-ol

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Key indicators

Single-crystal X-ray study
T = 150 K
Mean σ(C–C) = 0.002 Å
R factor = 0.052
wR factor = 0.142
Data-to-parameter ratio = 20.5

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

The title compound, $C_{17}H_{13}NO$, dimerizes through O—H···N hydrogen bonds with H···N in the range 2.00–2.27 Å. These dimers form an extended structure through π–π stacking and C—H···π interactions.

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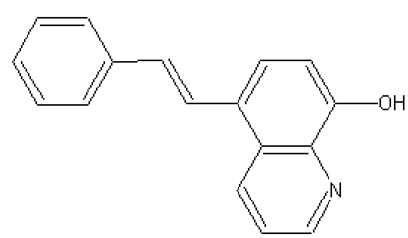
Comment

Due to their luminescence, quinolin-8-olate complexes have been widely used in organic light-emitting diodes and much work has gone into tuning the exact wavelengths produced. In a recent publication, the substituents in the 4′ position of 5-phenylazoquinolin-8-ol, (II), have been varied systematically and the free quinolin-8-ols have been structurally characterized. Their Zn^{II} and Al^{III} complexes [Zn(II)$_2$, Al(II)$_3$] have also been investigated (La Deda *et al.*, 2004). We report here the carbon analogue of La Deda's parent compound, *viz.* 5-[(*E*)-2-phenylethen-1-yl]-quinolin-8-ol, (I).



(I)

Compound (I) crystallizes in the space group $P2_1/c$ with three molecules in the asymmetric unit. They are each essentially planar with modest twists around the ethylene group of 179.51 (12), 177.63 (12) and 176.97 (12)° for molecules *A*, *B* and *C*, respectively, but do show significant twists of the phenylethenyl group relative to the quinoline [8.1 (2), 17.3 (2) and 8.1 (2)°, respectively]. The configuration is *E* and the phenyl group and the pyridine ring in the quinoline take an *anti* conformation in relation to one another. This is the same conformation found in (II) and can be rationalized as the one that ensures minimal interaction between the H atoms on the ethylene and the pyridine.

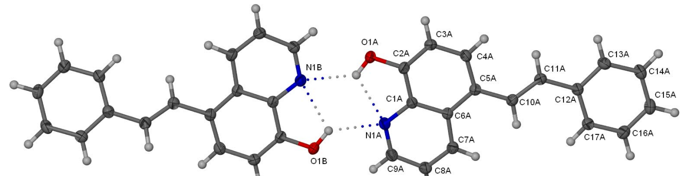


Figure 1
View of molecules *A* and *B* of (I) (50% probability displacement ellipsoids). Dotted lines indicate hydrogen bonds.

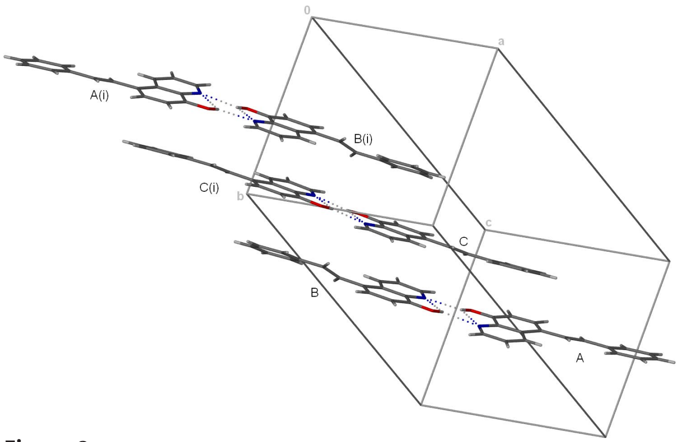


Figure 2
Side view of the π–π stacking along [021] [symmetry code: (i) $1-x$, $2-y$, $-z$].

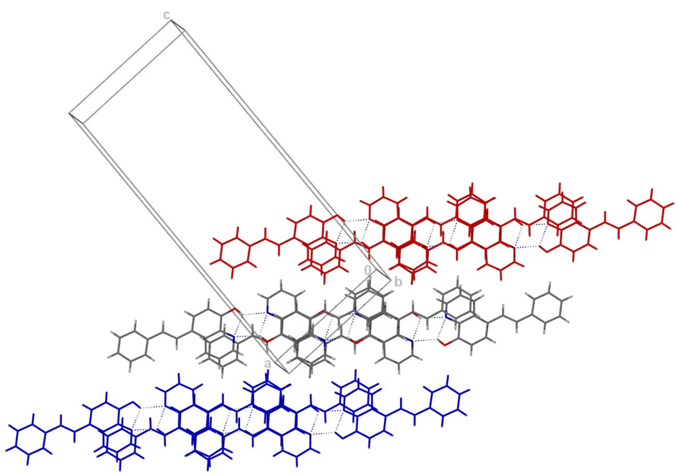


Figure 3
Parallel hexamers viewed along [021].

All three molecules dimerize through O—H···N hydrogen bonds [*A* with *B* and *C* with C^{i}; symmetry code: (i) $1-x$, $2-y$, $-z$; details given in Table 1]. This motif is seen for about 20% of the *ca* 120 quinolin-8-ols in the Cambridge Structural Database (Version 5.25, November 2003 with three updates, the latest being July 2004; Allen, 2002). Half of these, however, are twisted out of planarity compared to (I). The dimers stack through π–π interactions evident in Fig. 2. The quinoline in molecule *C* lies over that in *B* in a head-to-tail fashion (separation 3.49 Å), with the phenylethenyl group above the quinoline in *A* (3.52 Å). Similarly, the phenylethenyl group in *B* is below the quinoline in C^{i} (3.61 Å). This head-to-tail stacking and additional interaction through the phenyl is identical to the packing observed in both substituted examples of (II), but while the stacking continues throughout the structure in both of these, it is finite in (I). Molecules *A*, *B* and *C*, together with their symmetry equivalents [related by symmetry code (i)], form a basic six-molecule building block for the structure. This block then interacts weakly with symmetry-related blocks in a parallel but slightly offset position along *c* (Fig. 3). Furthermore, stronger C—H···π interactions are found to blocks that are tilted and displaced along *b* (Fig. 4). Both these latter interactions are also observed in (II), but again in an infinite form. Finally there are two C—H···O interactions to consider: C16*A*—H16*A*···O1*A*($1+x$, y, z) = 2.71 Å and C16*B*—H16*B*···O1*B*($x-1$, y, z) = 2.67 Å. The latter is particularly short and this is consistent with the observation that *B* is the molecule with the largest deviation from planarity of the phenylethenyl and quinoline groups.

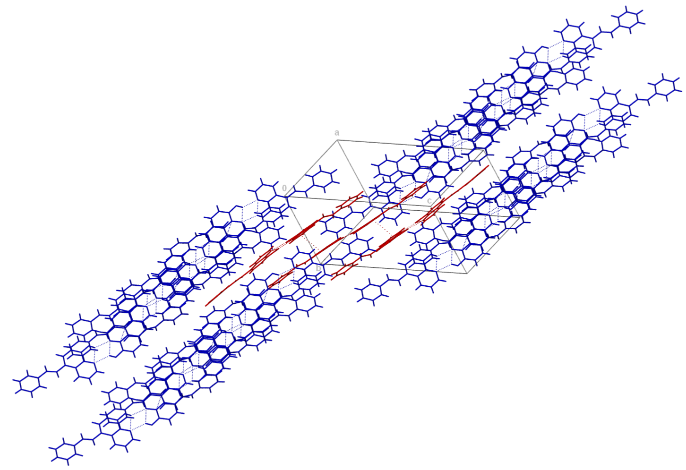


Figure 4
Central hexamer with C—H···π interactions to other hexamers.

Experimental

The title compound was synthesized *via* a Wittig reaction (Friedrich & Henning, 1959). Single crystals of (I) were produced by leaving a 3:1 mixture of (I) and $AlCl_3$ dissolved in methanol to evaporate to dryness.

Crystal data

$C_{17}H_{13}NO$
$M_r = 247.28$
Monoclinic, $P2_1/c$
$a = 11.9280$ (1) Å
$b = 11.0120$ (1) Å
$c = 28.1700$ (3) Å
$\beta = 92.654$ (1)°
$V = 3696.19$ (6) Å^3
$Z = 12$
$D_x = 1.333$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 54 542 reflections
$\theta = 2.9$–30.0°
$\mu = 0.08$ mm^{-1}
$T = 150$ (2) K
Prism, translucent yellow
0.38 × 0.20 × 0.05 mm

Data collection

Nonius KappaCCD diffractometer
φ and ω scans
Absorption correction: multi-scan (*SORTAV*; Blessing, 1995)
$T_{min} = 0.922$, $T_{max} = 0.997$
65 180 measured reflections
10 796 independent reflections
6893 reflections with $I > 2\sigma(I)$
$R_{int} = 0.061$
$\theta_{max} = 30.0°$
$h = -16 \rightarrow 16$
$k = -15 \rightarrow 15$
$l = -39 \rightarrow 39$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.052$
$wR(F^2) = 0.142$
$S = 1.04$
10 796 reflections
526 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0688P)^2 + 0.3349P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.29$ e Å^{-3}
$\Delta\rho_{min} = -0.27$ e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1A—H1A···N1B	0.88 (2)	2.15 (2)	2.8177 (16)	132.9 (17)
O1B—H1B···N1A	0.90 (2)	2.20 (2)	2.9173 (16)	135.6 (17)
O1C—H1C···N1C^{i}	0.94 (2)	2.00 (2)	2.7519 (15)	135.9 (16)

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

H atoms in C—H bonds were constrained with C—H = 0.95 Å and U_{iso}(H) = 1.2U_{eq}(C). Hydroxyl H atoms were located in a difference map and refined freely.

Data collection: *COLLECT* (Nonius, 1997–2000); cell refinement: *HKL SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *HKL SCALEPACK* and *DENZO* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SIR*97 (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *X-Seed* (Barbour, 2001); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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