Acta Crystallographica Section E
Structure Reports
Online
ISSN 1600-5368

(*E*)-Quinoline-4-carbaldehyde oxime

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Received 7 December 2006
Accepted 10 December 2006

The title compound, $C_{10}H_8N_2O$, exists as the *E* isomer. The crystal packing is stabilized by intermolecular O—H···N and C—H···N hydrogen bonds, as well as π–π stacking.

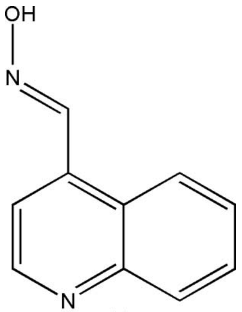
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.002 Å
R factor = 0.047
wR factor = 0.134
Data-to-parameter ratio = 14.1

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

Comment

The title compound, (I), was synthesized to support our ongoing drug development program. Its structure is shown in Fig. 1. The molecule exists as the *E* isomer.



(I)

In the structure there are two kinds of intermolecular hydrogen bonds, namely O—H···N and C—H···N (Table 1). These generate a dimeric $R_2^2(7)$ motif (Bernstein *et al.*, 1995), and assemble these dimers into one-dimensional supramolecular chains (Fig. 2). The chains are arranged in an antiparallel fashion and are stabilized by π–π stacking interactions between the quinoline rings at (x, y, z) and (x + 1.272, y + 0.321, z + 3.342) with centroid-to-centroid distances of 3.590 (2) Å.

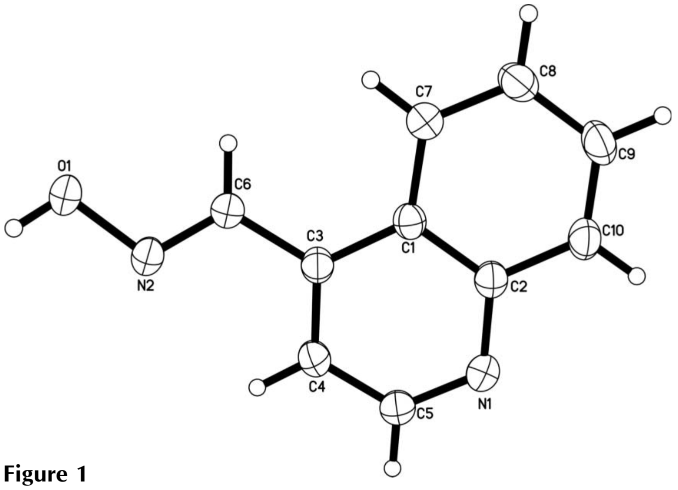


Figure 1
The molecular structure of (I) with 30% probability displacement ellipsoids (arbitrary spheres for H atoms).

Experimental

Compound (I) was prepared according to a known procedure (Ginsburg & Wilson, 1957). Single crystals suitable for X-ray diffraction were obtained by slow evaporation of a methanol solution at room temperature.

Crystal data

$C_{10}H_8N_2O$
$M_r = 172.18$
Monoclinic, $P2_1/c$
$a = 8.161$ (2) Å
$b = 15.746$ (4) Å
$c = 7.1509$ (18) Å
$\beta = 110.826$ (4)°
$V = 858.8$ (4) Å^3
$Z = 4$
$D_x = 1.332$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.09$ mm^{-1}
$T = 293$ (2) K
Prism, colorless
0.25 × 0.15 × 0.10 mm

Data collection

Bruker SMART APEX diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.978$, $T_{max} = 0.991$
4737 measured reflections
1688 independent reflections
1441 reflections with $I > 2\sigma(I)$
$R_{int} = 0.015$
$\theta_{max} = 26.1°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.047$
$wR(F^2) = 0.134$
$S = 1.04$
1688 reflections
120 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0805P)^2 + 0.1178P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.17$ e Å^{-3}
$\Delta\rho_{min} = -0.22$ e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.051 (7)

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N1^{i}	0.82	1.97	2.782 (2)	171
C10—H10···N2^{ii}	0.93	2.56	3.377 (3)	146

Symmetry codes: (i) $-x+1, y-\frac{1}{2}, -z+\frac{1}{2}$; (ii) $-x+1, y+\frac{1}{2}, -z+\frac{1}{2}$.

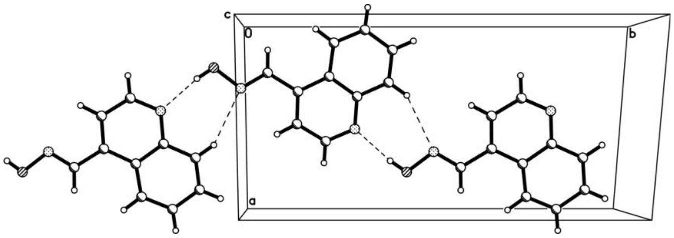


Figure 2
Perspective view along the *c* axis, of the hydrogen bonding (dashed lines) of (I).

The hydroxy H atom was located in a difference Fourier map and refined as riding in its as-found relative position, with $U_{iso}(H) = 1.5U_{eq}(O)$, while other H atoms were placed in calculated positions (C—H = 0.93 Å) and refined in riding mode, with $U_{iso}(H) = 1.2U_{eq}(C)$

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 2003); 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*.

This work is supported by the National Analytical Research Center of Electrochemistry and Spectroscopy, Changchun Institute of Applied Chemistry, Changchun, China.

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