Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

A 1:1 cocrystal of 8-hydroxyquinoline and 5-methyl-1*H*-imidazole

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Received 10 February 2006
Accepted 2 March 2006

Key indicators

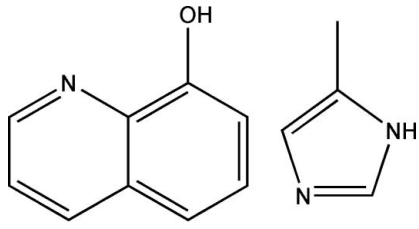
Single-crystal X-ray study
T = 292 K
Mean σ(C–C) = 0.006 Å
R factor = 0.059
wR factor = 0.129
Data-to-parameter ratio = 9.9

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

In the title compound, $C_9H_7NO{\cdot}C_4H_6N_2$, the imidazole ring is twisted away from the quinoline ring system with a dihedral angle of 60.8 (1)°. The crystal packing is stabilized by N—H···O, N—H···N, O—H···N hydrogen bonds and C—H···π interactions.

Comment

In contrast to covalent synthesis, supramolecular synthesis has not reached anywhere near the same level of sophistication despite much recent progress (Aakeröy & Salmon, 2005; Hosseini, 2005). In order to further understand molecular recognition occurring in solution, we have recently prepared cocrystals of the title compound, (I), whose crystal structure is reported here.



(I)

In the asymmetric unit of (I), the imidazole ring is twisted away from the quinoline ring system with a dihedral angle of 60.8 (1)° (Fig. 1). The bond lengths and angles are unremarkable.

In the crystal packing, hydroxy atom O1 of the molecule at (*x*, *y*, *z*) acts as a hydrogen-bond donor, *via* H1, to imidazole atom N3 of the molecule at $(\frac{1}{2}+x, \frac{1}{2}-y, -z)$, while atom N2 of the molecule at $(\frac{1}{2}+y, \frac{1}{2}-y, -z)$ likewise acts as donor to O1 and N1 at $(2-x, \frac{1}{2}+y, -\frac{1}{2}+z)$, producing a bifurcated hydrogen bond. By a combination of the O—H···N and the three-center hydrogen bonds (Table 1), the molecules are linked into chains along the *b* axis (Fig. 2). Adjacent chains are linked into sheets parallel to the *ac* plane by means of C—H···π interactions (Table 1 and Fig. 3). Analysis of the atomic coordinates using *PLATON* (Spek, 2003) shows that no π–π interactions are present in the crystal structure.

Experimental

The title compound was synthesized by dissolving 8-hydroxyquinoline (0.14 g, 1 mmol) and 4(5)-methylimidazole (0.08 g, 1 mmol) in methanol (35 ml). The resulting solution was stirred at 333 K for 30 min. Single crystals of (I) suitable for X-ray diffraction were

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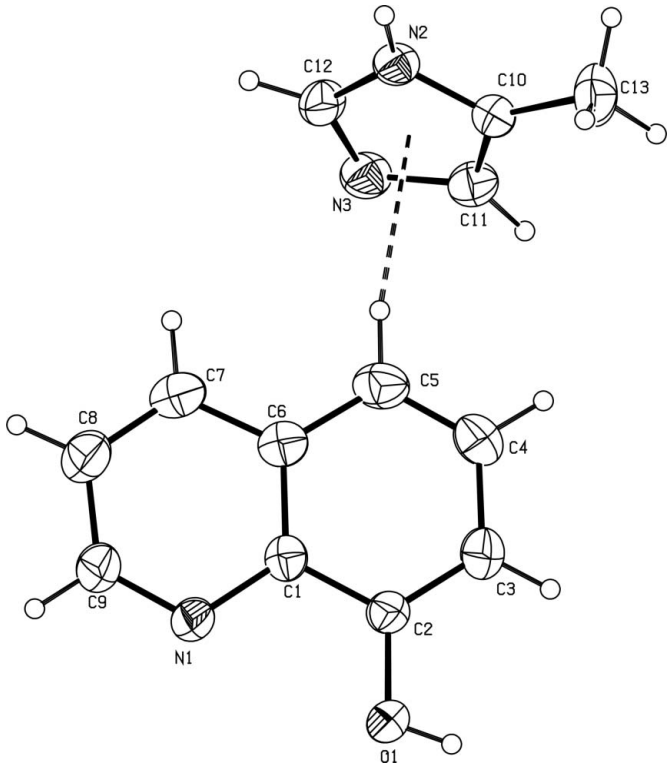

Figure 1
The molecular structure of (I), showing 50% probability displacement ellipsoids. The C—H···π interaction is shown as a dashed line.

obtained by slow evaporation of the clear methanol solution at room temperature.

Crystal data

$C_9H_7NO{\cdot}C_4H_6N_2$	Mo $K\alpha$ radiation
M_r = 227.26	Cell parameters from 878 reflections
Orthorhombic, $P2_12_12_1$	θ = 3.0–15.9°
a = 7.259 (3) Å	μ = 0.08 mm^{-1}
b = 9.109 (3) Å	T = 292 (2) K
c = 18.334 (7) Å	Plate, colourless
V = 1212.3 (8) Å^3	0.20 × 0.10 × 0.02 mm
Z = 4	
D_x = 1.245 Mg m^{-3}	

Data collection

Bruker SMART APEX CCD area-detector diffractometer	1537 independent reflections
	900 reflections with $I > 2\sigma(I)$
ω scans	R_{int} = 0.100
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)	θ_{max} = 27.0°
	$h = -9 \rightarrow 9$
T_{min} = 0.984, T_{max} = 0.998	$k = -11 \rightarrow 10$
10211 measured reflections	$l = -23 \rightarrow 23$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0561P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.059	
$wR(F^2)$ = 0.129	$(\Delta/\sigma)_{max}$ = 0.003
S = 1.00	$\Delta\rho_{max}$ = 0.12 e Å^{-3}
1537 reflections	$\Delta\rho_{min}$ = −0.16 e Å^{-3}
156 parameters	Extinction correction: *SHELXL97*
H-atom parameters constrained	Extinction coefficient: 0.011 (4)

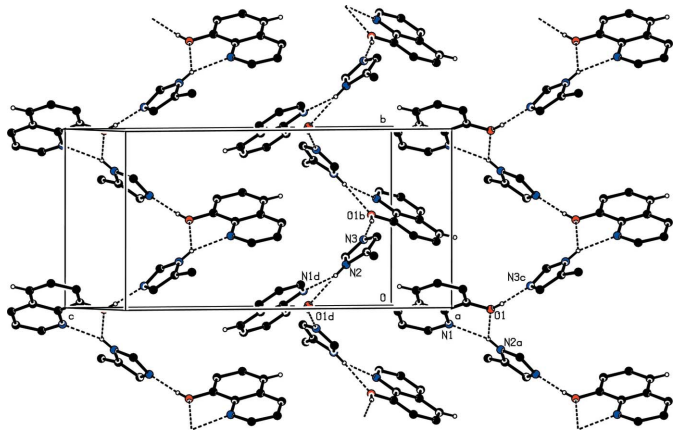

Figure 2
Part of the crystal structure of (I), showing the chains of molecules along the b axis formed by intermolecular hydrogen bonds (dashed lines). For clarity, H atoms not involved in hydrogen bonding have been omitted. [Symmetry codes: (*a*) $\frac{3}{2} - x, -y, -\frac{1}{2} + z$; (*b*) $-\frac{1}{2} + x, -\frac{1}{2} - y, -z$; (*c*) $\frac{1}{2} + x, \frac{1}{2} - y, -z$; (*d*) $\frac{3}{2} - x, -y, \frac{1}{2} + z$.]

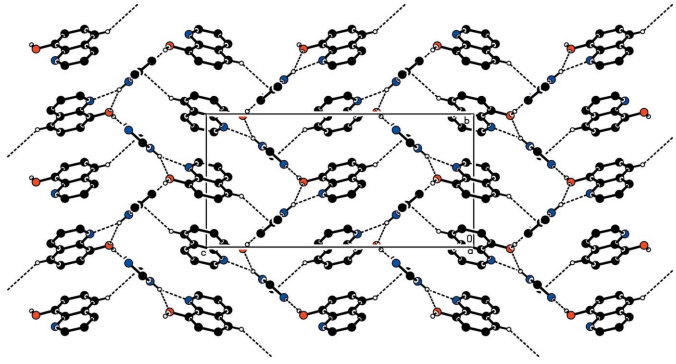

Figure 3
Part of the crystal structure of (I), showing the formation of layers parallel to the *ac* plane *via* hydrogen bonds and C—H···π interactions (dashed lines). For clarity, H atoms not involved in hydrogen bonding have been omitted.

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

D—H···A	D—H	H···A	D···A	D—H···A
C5—H5···$Cg1$	0.93	2.80	3.649 (6)	151
O1—H1···N3^{i}	0.82	1.86	2.654 (4)	162
N2—H2···O1^{ii}	0.86	2.45	2.989 (4)	121
N2—H2···N1^{ii}	0.86	2.20	3.022 (4)	160

Cg is the centroid of the imidazole ring. Symmetry codes: (i) $x + \frac{1}{2}, -y + \frac{1}{2}, -z + 2$; (ii) $-x + \frac{1}{2}, -y + 1, z - \frac{1}{2}$.

All H atoms were positioned geometrically (methyl C—H = 0.96 Å, aromatic C—H = 0.93 Å, N—H = 0.86 Å and O—H = 0.82 Å) and included in the refinement in the riding model approximation, with U_{iso}(H) = 1.2U_{eq}(N and aromatic C) or 1.5U_{eq}(O and methyl C). In the absence of significant anomalous dispersion effects, Friedel pairs were averaged.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics:

PLATON (Spek, 2003); software used to prepare material for publication: *PLATON*.

The authors are grateful to the Central China Normal University, the National Natural Science Foundation of China (grant No. 20472022) and the Hubei Province Natural Science Fund (grant Nos. 2004ABA085 and 2004ABC002) for financial support.

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