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Key indicators

Single-crystal X-ray study T = 93 K Mean σ (C–C) = 0.004 Å R factor = 0.037 wR factor = 0.107 Data-to-parameter ratio = 7.7

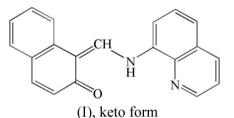
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

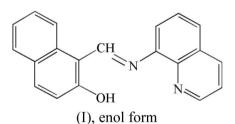
1-(8-Quinolylaminomethylene)naphthalen-2(1H)-one

The title hydroxynaphthalene derivative, $C_{20}H_{14}N_2O$, crystallizes in the keto form. Intramolecular N-H···O/N hydrogen bonds stabilize the planar conformation of the molecule. Received 17 May 2006 Accepted 1 June 2006

Comment

The title compound, (I), has been reported as a fluorescent reagent for molybdenum (Jiang *et al.*, 2001) and beryllium (Jiang & He, 2003). The structure of (I) has not been reported, although the structures of the mononuclear complexes of technetium (Tisato *et al.*, 1990) and vanadium (Asgedom *et al.*, 1996) containing (I) as ligand have been determined. The molecule of (I) may show tautomerism, and keto and enol forms are possible. The present study reveals that the molecule adopts the keto form in the crystal structure.





In (I), all the atoms are located almost in the same plane (Fig. 1). Selected bond distances and angles are listed in Table 1. The O1-C1 distance is shorter than the O-C bond of phenol (1.372 Å; Zavodnik *et al.*, 1987), indicating double-bond character. There exist intramolecular N1-H1...O1/N2 hydrogen bonds (Table 2), forming six- and five-membered rings. The hydrogen bonds and the multiple bond character of C10-C11, C11-N1 and N1-C12 stabilize the planar

Experimental

conformation of the molecule.

Compound (I) was synthesized according to the method of Jiang *et al.* (2001). For recrystallization, compound (I) (100 mg) in ethanol (30 ml) was refluxed for 1 h (353 K). The solution was filtered quickly and cooled to ambient temperature to obtain crystals suitable for X-ray analysis.

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Crystal data

 $\begin{array}{l} C_{20}H_{14}N_{2}O\\ M_{r}=298.34\\ Monoclinic, Pc\\ a=11.7365~(19)~\text{\AA}\\ b=5.8687~(5)~\text{\AA}\\ c=14.251~(2)~\text{\AA}\\ \beta=134.496~(4)^{\circ}\\ V=700.15~(17)~\text{\AA}^{3} \end{array}$

Data collection

Rigaku Mercury diffractometer ω scans Absorption correction: multi-scan (Jacobson, 1998) $T_{\min} = 0.933, T_{\max} = 0.996$

Refinement

 Refinement on F^2 $w = 1/[\sigma^2(F_o^2) + (0.0746P)^2 + 0.0816P]$
 $R[F^2 > 2\sigma(F^2)] = 0.037$ $w = 1/[\sigma^2(F_o^2) + (0.0746P)^2 + 0.0816P]$
 $wR(F^2) = 0.107$ where $P = (F_o^2 + 2F_c^2)/3$

 S = 1.08 $(\Delta/\sigma)_{max} < 0.001$

 1610 reflections
 $\Delta\rho_{max} = 0.32$ e Å⁻³

 209 parameters
 $\Delta\rho_{min} = -0.22$ e Å⁻³

 H-atom parameters not refined
 $\Delta\rho_{min} = -0.22$ e Å⁻³

Z = 2

 $D_x = 1.415 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation

 $\mu = 0.09 \text{ mm}^{-1}$

Needle, orange

 $0.55 \times 0.10 \times 0.05 \text{ mm}$

6503 measured reflections

1610 independent reflections 1521 reflections with $F^2 > 2\sigma(F^2)$

T = 93.1 K

 $R_{\rm int} = 0.014$

 $\theta_{\rm max} = 27.5^\circ$

Table 1

Selected geometric parameters (Å, °).

O1-C1	1.256 (3)	C1-C2	1.453 (3)
N1-C11	1.334 (3)	C1-C10	1.461 (5)
N1-C12	1.407 (2)	C10-C11	1.381 (2)
C11-N1-C12	124.6 (2)	C1-C10-C11	119.8 (2)
O1-C1-C2	120.8 (3)	N1-C11-C10	125.3 (3)
O1-C1-C10	122.1 (2)		
C11-N1-C12-C13	1.3 (2)	C8-C9-C10-C11	5.4 (2)
C12-N1-C11-C10	179.11 (17)	C1-C10-C11-N1	1.4 (2)
O1-C1-C10-C11	-4.1 (2)	N1-C12-C20-N2	-3.9 (2)

Table 2

Hydrogen-bond geometry (Å, °).

$D - H \cdots A$	<i>D</i> -H	H···A	$D \cdots A$	$D - \mathbf{H} \cdot \cdot \cdot A$
$\begin{array}{c} N1 - H1 \cdots O1 \\ N1 - H1 \cdots N2 \end{array}$	0.92	1.94	2.624 (3)	131
	0.92	2.29	2.698 (3)	107

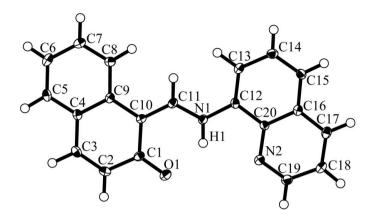


Figure 1

The molecular structure of (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

All H atoms were located in difference maps, and their positional parameters were fixed with $U_{iso}(H) = 1.2U_{eq}(C,N)$. In the absence of significant anomalous scattering effects, Friedel pairs were averaged.

Data collection: *CrystalClear* (Rigaku, 1999); cell refinement: *CrystalClear*; data reduction: *CrystalStructure* (Rigaku/MSC, 2005); program(s) used to solve structure: *SIR2002* (Burla *et al.*, 2003); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *CrystalStructure*; software used to prepare material for publication: *CrystalStructure*.

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