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8-Hydroxy-2-methylquinoline

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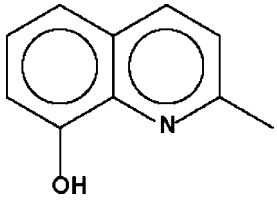
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.003 Å; R factor = 0.053; wR factor = 0.188; data-to-parameter ratio = 16.5.

The asymmetric unit of the title compound, $C_{10}H_9NO$, contains two independent molecules which are linked by a pair of O—H···N hydrogen bonds into a hydrogen-bonded dimer.

Related literature

Aluminium derivatives of 2-methyl-8-hydroxyquinoline are light-emitting compounds. For their crystal structures, see: Iijima & Yamamoto (2006); Kushi & Fernando (1970); Rajeswaran *et al.* (2007); Toulokhonova *et al.* (2002); Yamaguchi *et al.* (2002*a*,*b*); Yuchi *et al.* (2003).



Experimental

Crystal data

$C_{10}H_9NO$
M_r = 159.18
Orthorhombic, *Pbca*
a = 12.6542 (5) Å
b = 10.9976 (6) Å
c = 23.6264 (10) Å
V = 3288.0 (3) Å^3
Z = 16
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 295 (2) K
0.30 × 0.25 × 0.25 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.975, T_{max} = 0.979
30335 measured reflections
3769 independent reflections
2055 reflections with $I > 2\sigma(I)$
R_{int} = 0.047

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.053
$wR(F^2)$ = 0.188
S = 1.10
3769 reflections
228 parameters
2 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1O···N2	0.86 (3)	2.17 (2)	2.884 (2)	140 (3)
O2—H2O···N1	0.85 (3)	2.19 (2)	2.912 (2)	142 (3)

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2007).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2524).

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S1. Comment

The asymmetric unit of the title compound contains two molecules; the corresponding bond lengths and angles of these two molecules agree with each other. In the solid state, the two independent molecules exist as O—H···N hydrogen-bonded dimer; the mean planes through the non-hydrogen atoms of the two molecules form a dihedral angle of 77.98 (5)°.

S2. Experimental

Commercially available 2-methyl-8-hydroxyquinoline was recrystallized from diethyl ether.

S3. Refinement

Carbon- and oxygen-bound H atoms were placed in calculated positions [C—H 0.93–0.96 Å and U_{iso}(H) = 1.2–1.5U_{eq}(C)], and were included in the refinement in the riding-model approximation. The hydroxyl H-atoms were located in a difference Fourier map, and were refined with a O—H distance restraint of 0.85 (1) Å.

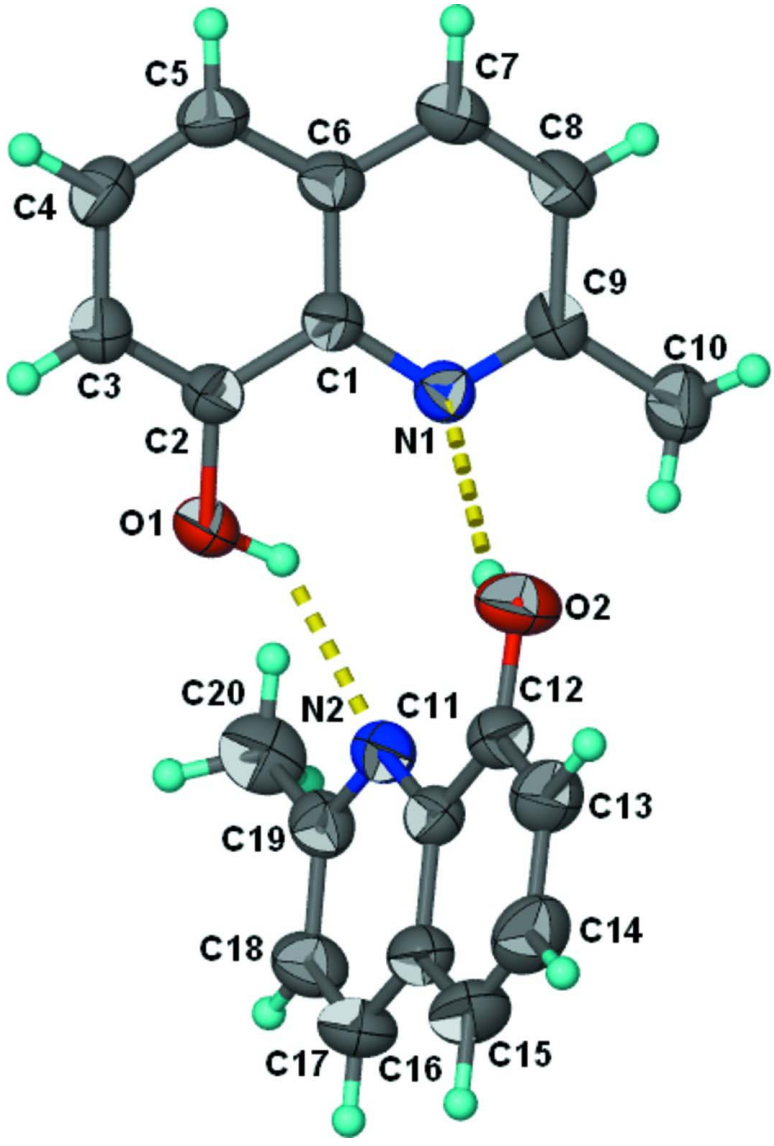

Figure 1

The asymmetric unit of the title compound, showing the hydrogen-bonded dimeric structure. Displacement ellipsoids are drawn at the 50% probability level.

8-Hydroxy-2-methylquinoline

Crystal data

$C_{10}H_9NO$
$M_r = 159.18$
Orthorhombic, *Pbca*
Hall symbol: -P 2ac 2ab
$a = 12.6542\ (5)$ Å
$b = 10.9976\ (6)$ Å
$c = 23.6264\ (10)$ Å
$V = 3288.0\ (3)$ Å^3
$Z = 16$
$F(000) = 1344$
$D_x = 1.286$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 15421 reflections
$\theta = 3.0–27.5°$
$\mu = 0.08$ mm^{-1}
$T = 295$ K
Block, colourless
0.30 × 0.25 × 0.25 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 10.000 pixels mm^{-1}
ω–scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.975, T_{max} = 0.979
30335 measured reflections
3769 independent reflections
2055 reflections with $I > 2\sigma(I)$
R_{int} = 0.047
θ_{max} = 27.5°, θ_{min} = 3.0°
h = −16→16
k = −14→14
l = −30→26

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.053
$wR(F^2)$ = 0.188
S = 1.10
3769 reflections
228 parameters
2 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.1035P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}
Extinction correction: *SHELXL*, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0065 (13)

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.75378 (11)	0.58979 (15)	0.60707 (6)	0.0612 (4)
H1O	0.712 (2)	0.644 (2)	0.6204 (12)	0.117 (11)*
O2	0.49093 (12)	0.60686 (17)	0.66008 (6)	0.0703 (5)
H2O	0.534 (2)	0.650 (3)	0.6411 (12)	0.127 (12)*
N1	0.58151 (11)	0.69189 (15)	0.55393 (6)	0.0467 (4)
N2	0.66746 (12)	0.72562 (15)	0.70068 (7)	0.0501 (4)
C1	0.64032 (13)	0.60751 (17)	0.52540 (7)	0.0440 (4)
C2	0.72545 (14)	0.55220 (19)	0.55461 (8)	0.0474 (5)
C3	0.78109 (15)	0.4604 (2)	0.52974 (9)	0.0544 (5)
H3	0.8351	0.4222	0.5496	0.065*
C4	0.75763 (16)	0.4235 (2)	0.47477 (9)	0.0580 (6)
H4	0.7958	0.3601	0.4586	0.070*
C5	0.67994 (15)	0.4782 (2)	0.44415 (8)	0.0563 (5)
H5	0.6671	0.4546	0.4070	0.068*
C6	0.61901 (14)	0.57120 (19)	0.46936 (8)	0.0483 (5)
C7	0.53480 (15)	0.6315 (2)	0.44188 (8)	0.0574 (6)
H7	0.5183	0.6126	0.4046	0.069*
C8	0.47827 (16)	0.7167 (2)	0.46992 (9)	0.0577 (6)
H8	0.4236	0.7573	0.4517	0.069*
C9	0.50225 (14)	0.74416 (19)	0.52701 (8)	0.0511 (5)
C10	0.43762 (18)	0.8347 (2)	0.55908 (10)	0.0708 (7)
H10A	0.4510	0.8260	0.5989	0.106*
H10B	0.3640	0.8208	0.5517	0.106*

H10C	0.4563	0.9154	0.5473	0.106*
C11	0.60152 (14)	0.66840 (18)	0.73818 (8)	0.0482 (5)
C12	0.51288 (15)	0.6056 (2)	0.71618 (8)	0.0540 (5)
C13	0.44816 (16)	0.5426 (2)	0.75192 (9)	0.0651 (6)
H13	0.3903	0.5008	0.7374	0.078*
C14	0.4678 (2)	0.5401 (3)	0.81019 (10)	0.0758 (7)
H14	0.4230	0.4963	0.8338	0.091*
C15	0.5506 (2)	0.6003 (3)	0.83250 (9)	0.0727 (7)
H15	0.5624	0.5981	0.8713	0.087*
C16	0.61957 (15)	0.6667 (2)	0.79724 (8)	0.0563 (5)
C17	0.70723 (18)	0.7335 (2)	0.81663 (9)	0.0686 (7)
H17	0.7214	0.7378	0.8552	0.082*
C18	0.77087 (17)	0.7914 (2)	0.77952 (9)	0.0663 (6)
H18	0.8283	0.8360	0.7926	0.080*
C19	0.75035 (15)	0.7842 (2)	0.72081 (9)	0.0548 (5)
C20	0.82399 (19)	0.8427 (2)	0.67981 (10)	0.0756 (7)
H20A	0.8021	0.8239	0.6419	0.113*
H20B	0.8943	0.8126	0.6859	0.113*
H20C	0.8230	0.9292	0.6852	0.113*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0610 (8)	0.0722 (11)	0.0505 (8)	0.0135 (7)	−0.0151 (7)	−0.0101 (7)
O2	0.0653 (9)	0.0976 (14)	0.0480 (8)	−0.0233 (9)	−0.0058 (7)	−0.0011 (8)
N1	0.0446 (8)	0.0474 (10)	0.0480 (9)	−0.0003 (7)	−0.0025 (7)	−0.0011 (7)
N2	0.0519 (9)	0.0510 (10)	0.0472 (9)	0.0005 (7)	−0.0025 (7)	0.0006 (7)
C1	0.0424 (9)	0.0459 (11)	0.0436 (10)	−0.0044 (8)	0.0001 (8)	0.0012 (8)
C2	0.0453 (10)	0.0522 (13)	0.0447 (10)	−0.0002 (8)	−0.0032 (8)	−0.0014 (9)
C3	0.0496 (10)	0.0569 (14)	0.0569 (12)	0.0058 (9)	−0.0013 (9)	−0.0021 (10)
C4	0.0551 (11)	0.0561 (13)	0.0629 (13)	0.0015 (10)	0.0084 (10)	−0.0107 (10)
C5	0.0572 (11)	0.0649 (15)	0.0468 (11)	−0.0067 (10)	0.0012 (9)	−0.0092 (10)
C6	0.0469 (10)	0.0535 (12)	0.0444 (10)	−0.0077 (9)	−0.0015 (8)	0.0006 (8)
C7	0.0580 (11)	0.0683 (15)	0.0457 (11)	−0.0061 (10)	−0.0076 (9)	0.0024 (10)
C8	0.0523 (11)	0.0643 (14)	0.0565 (12)	0.0021 (10)	−0.0112 (9)	0.0088 (11)
C9	0.0456 (10)	0.0498 (12)	0.0580 (12)	−0.0007 (9)	−0.0035 (9)	0.0054 (9)
C10	0.0630 (12)	0.0677 (17)	0.0816 (16)	0.0154 (11)	−0.0038 (11)	−0.0077 (13)
C11	0.0507 (10)	0.0497 (12)	0.0443 (10)	0.0064 (9)	0.0006 (8)	−0.0018 (8)
C12	0.0521 (10)	0.0619 (14)	0.0482 (11)	−0.0001 (9)	0.0016 (9)	−0.0026 (9)
C13	0.0565 (12)	0.0762 (17)	0.0625 (14)	−0.0072 (11)	0.0075 (10)	0.0017 (12)
C14	0.0747 (15)	0.087 (2)	0.0660 (15)	0.0006 (13)	0.0227 (12)	0.0095 (13)
C15	0.0825 (16)	0.090 (2)	0.0458 (12)	0.0035 (14)	0.0082 (11)	0.0029 (12)
C16	0.0632 (12)	0.0614 (14)	0.0441 (10)	0.0094 (10)	−0.0013 (9)	−0.0026 (10)
C17	0.0759 (14)	0.0834 (18)	0.0465 (12)	0.0016 (13)	−0.0129 (11)	−0.0078 (11)
C18	0.0664 (13)	0.0716 (17)	0.0608 (13)	−0.0041 (12)	−0.0157 (11)	−0.0100 (11)
C19	0.0539 (11)	0.0508 (13)	0.0595 (12)	0.0017 (9)	−0.0057 (10)	−0.0016 (10)
C20	0.0762 (15)	0.0700 (17)	0.0804 (16)	−0.0200 (12)	−0.0057 (12)	0.0064 (13)

Geometric parameters (Å, º)

O1—C2	1.355 (2)	C9—C10	1.494 (3)
O1—H1O	0.86 (3)	C10—H10A	0.96
O2—C12	1.354 (2)	C10—H10B	0.96
O2—H2O	0.85 (3)	C10—H10C	0.96
N1—C9	1.319 (2)	C11—C16	1.414 (3)
N1—C1	1.367 (2)	C11—C12	1.416 (3)
N2—C19	1.320 (2)	C12—C13	1.365 (3)
N2—C11	1.370 (2)	C13—C14	1.399 (3)
C1—C6	1.409 (2)	C13—H13	0.93
C1—C2	1.417 (2)	C14—C15	1.348 (3)
C2—C3	1.364 (3)	C14—H14	0.93
C3—C4	1.393 (3)	C15—C16	1.410 (3)
C3—H3	0.93	C15—H15	0.93
C4—C5	1.361 (3)	C16—C17	1.407 (3)
C4—H4	0.93	C17—C18	1.350 (3)
C5—C6	1.412 (3)	C17—H17	0.930
C5—H5	0.93	C18—C19	1.413 (3)
C6—C7	1.413 (3)	C18—H18	0.93
C7—C8	1.352 (3)	C19—C20	1.490 (3)
C7—H7	0.93	C20—H20A	0.96
C8—C9	1.415 (3)	C20—H20B	0.96
C8—H8	0.93	C20—H20C	0.96
C2—O1—H1O	113 (2)	H10A—C10—H10C	109.5
C12—O2—H2O	113 (2)	H10B—C10—H10C	109.5
C9—N1—C1	118.15 (16)	N2—C11—C16	123.07 (17)
C19—N2—C11	118.38 (17)	N2—C11—C12	117.97 (17)
N1—C1—C6	123.48 (16)	C16—C11—C12	118.93 (18)
N1—C1—C2	117.72 (16)	O2—C12—C13	119.17 (19)
C6—C1—C2	118.79 (17)	O2—C12—C11	121.11 (18)
O1—C2—C3	118.90 (17)	C13—C12—C11	119.72 (19)
O1—C2—C1	121.06 (17)	C12—C13—C14	120.8 (2)
C3—C2—C1	120.04 (18)	C12—C13—H13	119.6
C2—C3—C4	120.50 (18)	C14—C13—H13	119.6
C2—C3—H3	119.8	C15—C14—C13	120.9 (2)
C4—C3—H3	119.8	C15—C14—H14	119.6
C5—C4—C3	121.4 (2)	C13—C14—H14	119.6
C5—C4—H4	119.3	C14—C15—C16	120.3 (2)
C3—C4—H4	119.3	C14—C15—H15	119.8
C4—C5—C6	119.38 (19)	C16—C15—H15	119.8
C4—C5—H5	120.3	C17—C16—C15	124.4 (2)
C6—C5—H5	120.3	C17—C16—C11	116.22 (19)
C1—C6—C5	119.80 (17)	C15—C16—C11	119.33 (19)
C1—C6—C7	116.30 (18)	C18—C17—C16	120.33 (19)
C5—C6—C7	123.90 (19)	C18—C17—H17	119.8
C8—C7—C6	119.93 (19)	C16—C17—H17	119.8

C8—C7—H7	120.0	C17—C18—C19	120.1 (2)
C6—C7—H7	120.0	C17—C18—H18	119.9
C7—C8—C9	120.10 (18)	C19—C18—H18	119.9
C7—C8—H8	120.0	N2—C19—C18	121.8 (2)
C9—C8—H8	120.0	N2—C19—C20	118.26 (18)
N1—C9—C8	121.96 (19)	C18—C19—C20	119.95 (19)
N1—C9—C10	117.50 (18)	C19—C20—H20A	109.5
C8—C9—C10	120.53 (18)	C19—C20—H20B	109.5
C9—C10—H10A	109.5	H20A—C20—H20B	109.5
C9—C10—H10B	109.5	C19—C20—H20C	109.5
H10A—C10—H10B	109.5	H20A—C20—H20C	109.5
C9—C10—H10C	109.5	H20B—C20—H20C	109.5

C9—N1—C1—C6	−1.7 (3)	C19—N2—C11—C16	−1.6 (3)
C9—N1—C1—C2	179.80 (17)	C19—N2—C11—C12	−179.91 (18)
N1—C1—C2—O1	−6.1 (3)	N2—C11—C12—O2	−3.1 (3)
C6—C1—C2—O1	175.38 (17)	C16—C11—C12—O2	178.49 (19)
N1—C1—C2—C3	174.58 (17)	N2—C11—C12—C13	176.9 (2)
C6—C1—C2—C3	−3.9 (3)	C16—C11—C12—C13	−1.5 (3)
O1—C2—C3—C4	−176.79 (19)	O2—C12—C13—C14	−179.4 (2)
C1—C2—C3—C4	2.5 (3)	C11—C12—C13—C14	0.6 (4)
C2—C3—C4—C5	0.7 (3)	C12—C13—C14—C15	0.4 (4)
C3—C4—C5—C6	−2.5 (3)	C13—C14—C15—C16	−0.3 (4)
N1—C1—C6—C5	−176.28 (17)	C14—C15—C16—C17	179.2 (2)
C2—C1—C6—C5	2.2 (3)	C14—C15—C16—C11	−0.7 (4)
N1—C1—C6—C7	3.0 (3)	N2—C11—C16—C17	3.4 (3)
C2—C1—C6—C7	−178.55 (17)	C12—C11—C16—C17	−178.32 (19)
C4—C5—C6—C1	1.0 (3)	N2—C11—C16—C15	−176.7 (2)
C4—C5—C6—C7	−178.21 (19)	C12—C11—C16—C15	1.6 (3)
C1—C6—C7—C8	−1.5 (3)	C15—C16—C17—C18	177.9 (2)
C5—C6—C7—C8	177.73 (19)	C11—C16—C17—C18	−2.2 (3)
C6—C7—C8—C9	−1.0 (3)	C16—C17—C18—C19	−0.6 (4)
C1—N1—C9—C8	−1.0 (3)	C11—N2—C19—C18	−1.4 (3)
C1—N1—C9—C10	179.00 (17)	C11—N2—C19—C20	177.9 (2)
C7—C8—C9—N1	2.4 (3)	C17—C18—C19—N2	2.5 (4)
C7—C8—C9—C10	−177.6 (2)	C17—C18—C19—C20	−176.7 (2)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*O*···N2	0.86 (3)	2.17 (2)	2.884 (2)	140 (3)
O2—H2*O*···N1	0.85 (3)	2.19 (2)	2.912 (2)	142 (3)