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6-Chloro-*N*′-(2-hydroxy-1-naphthylmethylene)nicotinohydrazide

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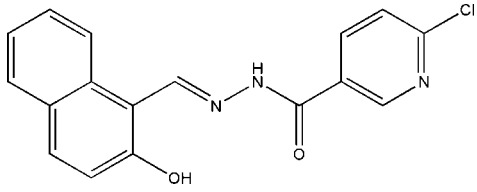
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.006 Å; R factor = 0.056; wR factor = 0.109; data-to-parameter ratio = 14.1.

The title compound, $C_{17}H_{12}ClN_3O_2$, was synthesized by the Schiff base condensation reaction of 2-hydroxy-1-naphthaldehyde with 6-chloronicotinic acid hydrazide in a methanol solution. The molecule displays a *trans* configuration with respect to the C=N and C—N bonds. The dihedral angle between the naphthyl ring system and the pyridine ring is 7.6 (4)°. There is an intramolecular O—H···N hydrogen bond. The crystal structure is stabilized by intermolecular N—H···O and C—H···O hydrogen bonds, forming chains running along the *b* axis.

Related literature

For related literature, see: Allen *et al.* (1987); Chen *et al.* (1997); Fan *et al.* (2007); Kim *et al.* (2005); Nimitsiriwat *et al.* (2004); Ren *et al.* (2002).



Experimental

Crystal data

$C_{17}H_{12}ClN_3O_2$
M_r = 325.75
Monoclinic, *Pc*
a = 4.7450 (9) Å
b = 6.0420 (12) Å
c = 25.752 (5) Å
β = 91.93 (3)°
V = 737.9 (2) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.27 mm^{-1}
T = 293 (2) K
0.23 × 0.20 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.937, T_{max} = 0.940
5692 measured reflections
2980 independent reflections
1948 reflections with $I > 2\sigma(I)$
R_{int} = 0.043

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.057
$wR(F^2)$ = 0.110
S = 0.99
2980 reflections
212 parameters
3 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.15 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}
Absolute structure: Flack (1983), 1447 Friedel pairs
Flack parameter: 0.11 (10)

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2···N3	0.82	1.84	2.559 (4)	146
N2—H2B···O1^{i}	0.900 (10)	2.05 (2)	2.862 (4)	150 (4)
C2—H2A···O1^{ii}	0.93	2.50	3.396 (4)	161

Symmetry codes: (i) $x+1, y, z$; (ii) $x+1, y+1, z$.

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

Financial support from the Third Affiliated Hospital of Suzhou University is acknowledged.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BV2083).

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supporting information

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S1. Comment

Schiff base compounds have been widely investigated over a century (Fan *et al.*, 2007; Kim *et al.*, 2005; Nimitsiriwat *et al.*, 2004). Some of the compounds have been found to have pharmacological and antibacterial activity (Chen *et al.*, 1997; Ren *et al.*, 2002). In this paper, the crystal structure of a new Schiff base compound derived from the condensation reaction of 2-hydroxy-1-naphthaldehyde with 6-chloronicotinic acid hydrazide is reported.

The Schiff base molecule of the compound displays a *trans* configuration with respect to the C?N and C—N bonds (Fig. 1). The dihedral angle between the C8—C17 naphthyl ring and the C1—C5/N1 pyridine ring is 7.6 (4)°. All the bond lengths are within normal ranges (Allen *et al.*, 1987). There is an intramolecular O–H···N hydrogen bond in the molecule (Table 1). The crystal structure is stabilized by intermolecular N–H···O and C–H···O hydrogen bonds (Table 1), forming chains running along the *b* axis (Fig. 2).

S2. Experimental

2-Hydroxy-1-naphthaldehyde (0.1 mmol, 17.2 mg) and 6-chloronicotinic acid hydrazide (0.1 mmol, 17.1 mg) were dissolved in a methanol solution (10 ml). The mixture was stirred at room temperature to give a clear yellow solution. Crystals of the title compound were formed by gradual evaporation of the solvent for two days at room temperature.

S3. Refinement

Atom H2B was located from a difference Fourier map and refined isotropically, with N–H distance restrained to 0.90 (1) Å. Other H atoms were constrained to ideal geometries, with C–H = 0.93 Å, O–H = 0.82 Å, and with U_{iso}(H) set to 1.2U_{eq}(C) and 1.5U_{eq}(O).

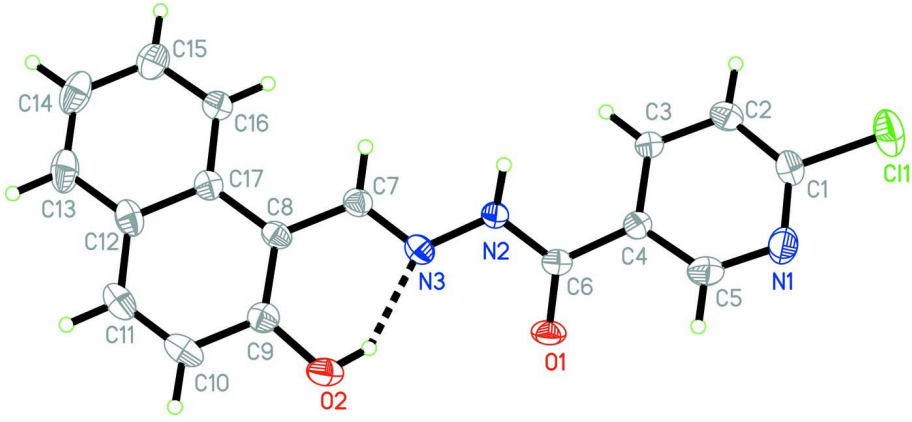

Figure 1

The structure of (I) at the 30% probability level.

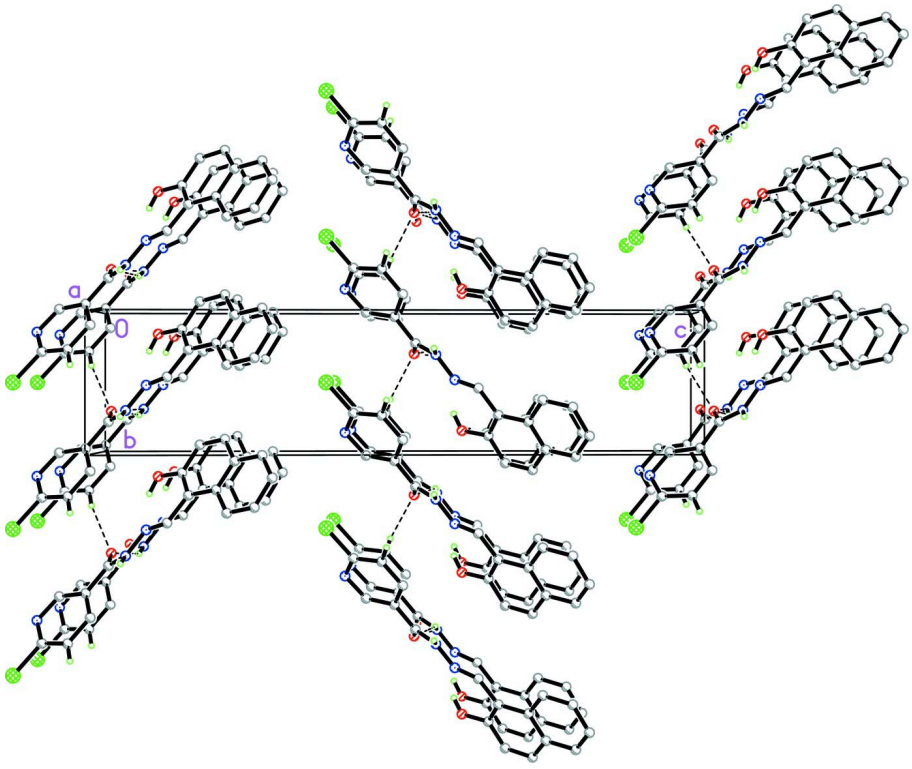

Figure 2

Molecular packing of (I), viewed along the *a* axis. Intermolecular hydrogen bonds are shown as dashed lines.

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$C_{17}H_{12}ClN_3O_2$
$M_r = 325.75$
Monoclinic, *Pc*
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$b = 6.0420\ (12)$ Å
$c = 25.752\ (5)$ Å
$\beta = 91.93\ (3)°$
$V = 737.9\ (2)$ Å^3
$Z = 2$
$F(000) = 336$
$D_x = 1.466$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 790 reflections
$\theta = 2.4–24.3°$
$\mu = 0.27$ mm^{-1}
$T = 293$ K
Block, yellow
0.23 × 0.20 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scan
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.937$, $T_{max} = 0.940$
5692 measured reflections
2980 independent reflections
1948 reflections with $I > 2\sigma(I)$
$R_{int} = 0.043$
$\theta_{max} = 26.5°$, $\theta_{min} = 1.6°$
$h = -5\rightarrow5$
$k = -7\rightarrow7$
$l = -32\rightarrow32$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.057$
$wR(F^2) = 0.110$
$S = 0.99$
2980 reflections
212 parameters
3 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
$w = 1/[\sigma^2(F_o^2) + (0.0375P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.15$ e Å^{-3}
$\Delta\rho_{min} = -0.18$ e Å^{-3}
Absolute structure: Flack (1983), 1447 Friedel pairs
Absolute structure parameter: 0.11 (10)

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl1	0.0611 (3)	1.5001 (2)	−0.11216 (6)	0.0788 (4)
O1	−0.4774 (5)	0.7030 (4)	0.02688 (11)	0.0494 (7)
O2	−0.3951 (6)	0.1598 (5)	0.10628 (11)	0.0515 (7)
H2	−0.3567	0.2788	0.0929	0.077*
N1	−0.2165 (8)	1.1504 (6)	−0.08492 (13)	0.0577 (10)
N2	−0.0394 (6)	0.6927 (6)	0.06381 (12)	0.0380 (8)
N3	−0.1179 (6)	0.5186 (5)	0.09455 (13)	0.0416 (8)
C1	−0.0145 (9)	1.2884 (7)	−0.06934 (16)	0.0484 (11)
C2	0.1344 (8)	1.2758 (6)	−0.02279 (15)	0.0472 (10)
H2A	0.2741	1.3785	−0.0141	0.057*
C3	0.0704 (8)	1.1058 (6)	0.01076 (16)	0.0390 (9)
H3	0.1677	1.0913	0.0425	0.047*
C4	−0.1420 (8)	0.9566 (6)	−0.00370 (16)	0.0375 (10)
C5	−0.2731 (9)	0.9895 (7)	−0.05108 (17)	0.0525 (12)
H5	−0.4155	0.8905	−0.0608	0.063*
C6	−0.2328 (8)	0.7734 (6)	0.02998 (14)	0.0367 (9)
C7	0.0501 (10)	0.4617 (6)	0.13256 (18)	0.0401 (9)
H7	0.2148	0.5417	0.1391	0.048*
C8	−0.0149 (7)	0.2745 (6)	0.16510 (15)	0.0376 (9)
C9	−0.2276 (8)	0.1283 (7)	0.14941 (16)	0.0432 (10)
C10	−0.2774 (9)	−0.0650 (7)	0.17726 (19)	0.0555 (13)
H10	−0.4147	−0.1643	0.1654	0.067*
C11	−0.1272 (9)	−0.1079 (7)	0.22124 (18)	0.0569 (13)

H11	−0.1638	−0.2377	0.2392	0.068*
C12	0.0845 (9)	0.0363 (7)	0.24135 (17)	0.0485 (12)
C13	0.2286 (11)	−0.0050 (10)	0.28798 (17)	0.0631 (15)
H13	0.1877	−0.1323	0.3066	0.076*
C14	0.4314 (10)	0.1389 (9)	0.30741 (18)	0.0651 (14)
H14	0.5319	0.1062	0.3381	0.078*
C15	0.4840 (9)	0.3345 (8)	0.28043 (16)	0.0596 (13)
H15	0.6164	0.4348	0.2938	0.072*
C16	0.3413 (8)	0.3798 (7)	0.23432 (15)	0.0460 (10)
H16	0.3789	0.5106	0.2168	0.055*
C17	0.1391 (8)	0.2315 (7)	0.21308 (15)	0.0384 (10)
H2B	0.142 (3)	0.733 (7)	0.0613 (17)	0.080*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.1123 (10)	0.0589 (7)	0.0659 (7)	−0.0054 (7)	0.0137 (6)	0.0212 (6)
O1	0.0287 (14)	0.0529 (18)	0.0662 (19)	−0.0089 (14)	−0.0033 (13)	0.0008 (15)
O2	0.0416 (15)	0.057 (2)	0.0557 (18)	−0.0132 (14)	0.0021 (14)	−0.0051 (15)
N1	0.073 (3)	0.055 (3)	0.044 (2)	−0.001 (2)	−0.005 (2)	0.0076 (19)
N2	0.0300 (17)	0.0427 (19)	0.0414 (18)	−0.0028 (15)	0.0004 (16)	0.0072 (16)
N3	0.040 (2)	0.041 (2)	0.0444 (19)	−0.0037 (17)	0.0083 (16)	0.0022 (17)
C1	0.059 (3)	0.043 (3)	0.044 (3)	−0.002 (2)	0.010 (2)	0.005 (2)
C2	0.046 (2)	0.042 (3)	0.053 (3)	−0.006 (2)	0.004 (2)	−0.005 (2)
C3	0.037 (2)	0.040 (2)	0.040 (2)	−0.004 (2)	−0.0024 (18)	0.000 (2)
C4	0.036 (2)	0.041 (3)	0.036 (2)	0.0013 (19)	0.0026 (18)	−0.0020 (19)
C5	0.048 (3)	0.053 (3)	0.056 (3)	−0.007 (2)	−0.001 (2)	−0.011 (2)
C6	0.033 (2)	0.039 (2)	0.038 (2)	−0.0016 (19)	0.0035 (18)	−0.0067 (18)
C7	0.035 (2)	0.041 (2)	0.045 (2)	0.000 (2)	0.0052 (17)	0.003 (2)
C8	0.033 (2)	0.035 (2)	0.045 (2)	−0.0019 (18)	0.0092 (18)	−0.0023 (18)
C9	0.038 (2)	0.045 (3)	0.047 (3)	0.002 (2)	0.006 (2)	−0.002 (2)
C10	0.055 (3)	0.042 (3)	0.071 (3)	−0.014 (2)	0.019 (3)	−0.010 (3)
C11	0.063 (3)	0.041 (3)	0.068 (3)	−0.007 (2)	0.016 (3)	0.007 (2)
C12	0.056 (3)	0.037 (3)	0.053 (3)	0.007 (2)	0.016 (2)	0.006 (2)
C13	0.076 (4)	0.071 (4)	0.043 (3)	0.016 (3)	0.014 (3)	0.022 (3)
C14	0.068 (3)	0.088 (4)	0.040 (3)	0.028 (3)	0.006 (2)	0.010 (3)
C15	0.066 (3)	0.065 (3)	0.047 (3)	0.005 (3)	−0.002 (2)	0.002 (2)
C16	0.043 (3)	0.046 (3)	0.049 (3)	−0.003 (2)	0.002 (2)	0.003 (2)
C17	0.038 (2)	0.039 (3)	0.038 (2)	0.0033 (19)	0.0086 (19)	−0.0006 (19)

Geometric parameters (Å, º)

Cl1—C1	1.734 (4)	C7—H7	0.9300
O1—C6	1.236 (4)	C8—C9	1.391 (5)
O2—C9	1.357 (4)	C8—C17	1.438 (5)
O2—H2	0.8200	C9—C10	1.395 (6)
N1—C1	1.323 (5)	C10—C11	1.343 (6)
N1—C5	1.339 (5)	C10—H10	0.9300

N2—C6	1.336 (4)	C11—C12	1.415 (6)
N2—N3	1.375 (4)	C11—H11	0.9300
N2—H2B	0.900 (10)	C12—C13	1.385 (6)
N3—C7	1.288 (5)	C12—C17	1.414 (5)
C1—C2	1.373 (5)	C13—C14	1.378 (7)
C2—C3	1.382 (5)	C13—H13	0.9300
C2—H2A	0.9300	C14—C15	1.398 (6)
C3—C4	1.393 (5)	C14—H14	0.9300
C3—H3	0.9300	C15—C16	1.374 (5)
C4—C5	1.365 (5)	C15—H15	0.9300
C4—C6	1.479 (5)	C16—C17	1.410 (5)
C5—H5	0.9300	C16—H16	0.9300
C7—C8	1.447 (5)		

C9—O2—H2	109.5	C17—C8—C7	121.8 (4)
C1—N1—C5	114.8 (4)	O2—C9—C8	123.2 (4)
C6—N2—N3	117.5 (3)	O2—C9—C10	115.7 (4)
C6—N2—H2B	120 (3)	C8—C9—C10	121.1 (4)
N3—N2—H2B	122 (3)	C11—C10—C9	120.1 (4)
C7—N3—N2	118.0 (3)	C11—C10—H10	120.0
N1—C1—C2	125.2 (4)	C9—C10—H10	120.0
N1—C1—Cl1	115.8 (3)	C10—C11—C12	122.7 (4)
C2—C1—Cl1	119.0 (3)	C10—C11—H11	118.7
C1—C2—C3	118.0 (4)	C12—C11—H11	118.7
C1—C2—H2A	121.0	C13—C12—C17	120.2 (4)
C3—C2—H2A	121.0	C13—C12—C11	122.0 (4)
C2—C3—C4	119.0 (4)	C17—C12—C11	117.7 (4)
C2—C3—H3	120.5	C14—C13—C12	121.3 (5)
C4—C3—H3	120.5	C14—C13—H13	119.3
C5—C4—C3	116.7 (4)	C12—C13—H13	119.3
C5—C4—C6	120.0 (4)	C13—C14—C15	119.1 (5)
C3—C4—C6	123.3 (4)	C13—C14—H14	120.4
N1—C5—C4	126.3 (4)	C15—C14—H14	120.4
N1—C5—H5	116.9	C16—C15—C14	120.4 (5)
C4—C5—H5	116.9	C16—C15—H15	119.8
O1—C6—N2	122.6 (3)	C14—C15—H15	119.8
O1—C6—C4	120.7 (4)	C15—C16—C17	121.2 (4)
N2—C6—C4	116.6 (3)	C15—C16—H16	119.4
N3—C7—C8	120.7 (4)	C17—C16—H16	119.4
N3—C7—H7	119.7	C16—C17—C12	117.7 (4)
C8—C7—H7	119.7	C16—C17—C8	122.6 (3)
C9—C8—C17	118.5 (3)	C12—C17—C8	119.8 (4)
C9—C8—C7	119.6 (4)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2···N3	0.82	1.84	2.559 (4)	146

N2—H2*B*···O1^{i}	0.90 (1)	2.05 (2)	2.862 (4)	150 (4)
C2—H2*A*···O1^{ii}	0.93	2.50	3.396 (4)	161

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