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2-[(5-Chloropyridin-2-ylimino)methyl]phenol

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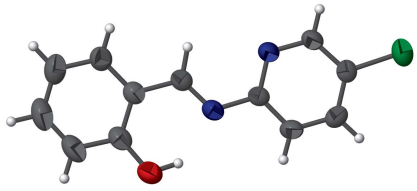
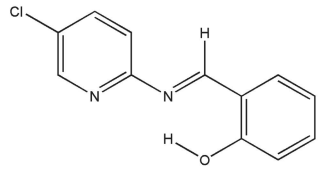
In the title compound, $C_{12}H_9ClN_2O$, the dihedral angle between the aromatic rings is 1.78 (4)° and an intramolecular O—H···N hydrogen bond closes an $S(6)$ ring. In the crystal, C—H···O and C—H···N hydrogen bonds connect the molecules into [001] chains.

3D view



Chemical scheme



Structure description

The dihedral angle between the N1/C2–C6 pyridine ring and C7–C12 benzene ring is 1.78 (4)° and an intramolecular O—H···N hydrogen bond closes an $S(6)$ ring. The disposition of the aromatic rings is *trans* as indicated by the C2—N2—C13—C7 torsion angle of −179.7 (2)° (Fig. 1). In the crystal, centrosymmetric dimers linked by pairs of weak C6—H6···N1 hydrogen bonds (Table 1) generate $R_2^2(6)$ loops. These dimers are linked by two pairs of C3—H3···O1 hydrogen bonds to form $R_6^6(42)$ loops (Fig. 2). These alternating loops lead to wave-like supramolecular strands propagating along [001]. Intermolecular Cl···Cl [3.476 (4)] and Cl···π [3.528 (4) Å] contacts slightly shorter than van der Waals separations are also observed (Fig. 3).

For the pharmaceutical behavior of Schiff bases, see: Mounika *et al.* (2010); Miri *et al.* (2013); Aboul-Fadl *et al.* (2003); Wei *et al.* (2006). For ring-opening reactions of pyrroles, see: Mannaert *et al.* (1997); . For halogen–halogen reactions, see: Pedireddi *et al.* (1994) and for halogen···π reactions, see: Rahman *et al.* (2003).

Synthesis and crystallization

2-Amino-5-chloropyridine (1 mmol) and 2-hydroxy benzaldehyde (1.2 mmol) were mixed in 20 ml of absolute ethanol with the addition of few drops of piperidine as catalyst. The mixture was refluxed for 5 h at 60–70°C. Colourless blocks of the title compound were obtained from the mother solution on cooling.

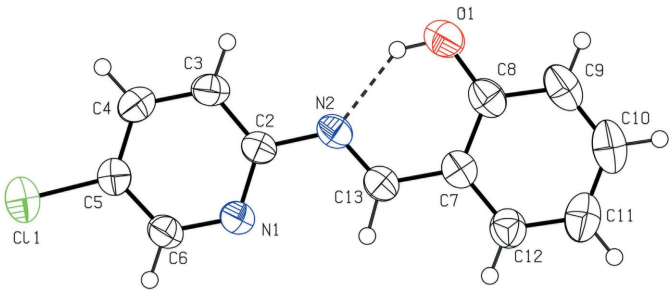


Figure 1
The molecular structure of the title compound with displacement ellipsoids drawn at the 50% probability level. The O—H···N hydrogen bond is indicated by a dashed line.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Acknowledgements

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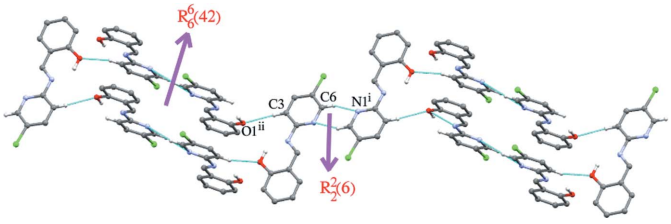

Figure 2
Supramolecular strands formed by weak C—H···N and C—H···O hydrogen bonds. Symmetry codes: (i) $1-x, 1-y, -z$; (ii) $\frac{1}{2}-x, -\frac{1}{2}+y, \frac{1}{2}-z$.

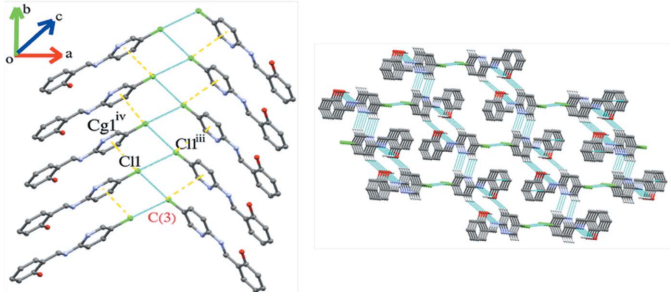

Figure 3
Left: Supramolecular chain arising from Cl···Cl and C—Cl···π contacts. [Symmetry code: (iii) $\frac{3}{2}-x, -\frac{1}{2}+y, 1/2-z$; (iv) $x, -1+y, z$]. Right: Honeycomb architecture formed by the weak non-covalent interactions.

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H8···N2	0.89 (5)	1.89 (5)	2.627 (4)	140 (4)
C3—H3···O1^{i}	0.93	2.50	3.361 (5)	154
C6—H6···N1^{ii}	0.93	2.59	3.365 (5)	141

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{12}H_9ClN_2O$
M_r	232.66
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	294
a, b, c (Å)	14.753 (12), 4.639 (3), 16.379 (16)
β (°)	105.35 (4)
V (Å^3)	1081.0 (16)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.33
Crystal size (mm)	0.14 × 0.12 × 0.09
Data collection	
Diffractometer	Bruker Kappa APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2004)
T_{min}, T_{max}	0.955, 0.971
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	22920, 3033, 1878
R_{int}	0.060
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.695
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.071, 0.219, 1.12
No. of reflections	3033
No. of parameters	154
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.36, −0.38

Computer programs: *APEX2* and *SAINT* (Bruker, 2004), *SHELXS97* and *SHELXL97* (Sheldrick, 2008), *Mercury* (Macrae *et al.*, 2008), *POV-RAY* (Cason, 2004), *PLATON* (Spek, 2020) and *publCIF* (Westrip, 2010).

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full crystallographic data

IUCrData (2020). **5**, x200011 [https://doi.org/10.1107/S2414314620000115]

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2-[(5-Chloropyridin-2-ylimino)methyl]phenol

Crystal data

$C_{12}H_9ClN_2O$
M_r = 232.66
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
a = 14.753 (12) Å
b = 4.639 (3) Å
c = 16.379 (16) Å
β = 105.35 (4)°
V = 1081.0 (16) Å^3
Z = 4
$F(000)$ = 480
D_x = 1.430 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71076 Å
Cell parameters from 3033 reflections
θ = 2.9–29.6°
μ = 0.33 mm^{-1}
T = 294 K
Block, colourless
0.14 × 0.12 × 0.09 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω and φ scan
Absorption correction: multi-scan (SADABS; Bruker, 2004)
T_{min} = 0.955, T_{max} = 0.971
22920 measured reflections
3033 independent reflections
1878 reflections with $I > 2\sigma(I)$
R_{int} = 0.060
θ_{max} = 29.6°, θ_{min} = 2.9°
h = −20→20
k = −6→6
l = −22→22

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.071
$wR(F^2)$ = 0.219
S = 1.12
3033 reflections
154 parameters
0 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
$w = 1/[\sigma^2(F_o^2) + (0.0991P)^2 + 0.6777P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.36 e Å^{-3}
$\Delta\rho_{min}$ = −0.38 e Å^{-3}
Extinction correction: shelxl, $FC^*=KFC[1+0.001XFC^2\Lambda^3/SIN(2\Theta)]^{-1/4}$
Extinction coefficient: 0.096 (14)

Special details

Geometry. Bond distances, angles etc. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell esds are taken into account in the estimation of distances, angles and torsion angles

Refinement. Refinement on F^2 for ALL reflections except those flagged by the user for potential systematic errors. Weighted R-factors wR and all goodnesses 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 observed criterion of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating -R-factor-obs 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl1	0.66137 (5)	0.10505 (17)	0.21103 (5)	0.0569 (3)
O1	0.22420 (18)	1.2528 (6)	0.17721 (15)	0.0632 (9)
N1	0.46749 (16)	0.6578 (5)	0.09207 (14)	0.0458 (7)
N2	0.35223 (15)	0.9377 (5)	0.13429 (14)	0.0407 (7)
C2	0.42598 (17)	0.7322 (5)	0.15259 (16)	0.0372 (8)
C3	0.4511 (2)	0.6134 (6)	0.23285 (18)	0.0455 (9)
C4	0.5240 (2)	0.4173 (6)	0.25253 (18)	0.0478 (9)
C5	0.56824 (18)	0.3459 (6)	0.19071 (17)	0.0405 (8)
C6	0.5382 (2)	0.4667 (7)	0.11164 (18)	0.0463 (9)
C7	0.25370 (18)	1.2702 (6)	0.03971 (17)	0.0417 (8)
C8	0.2054 (2)	1.3599 (6)	0.0985 (2)	0.0476 (9)
C9	0.1342 (2)	1.5664 (7)	0.0744 (3)	0.0614 (13)
C10	0.1122 (2)	1.6815 (8)	−0.0058 (3)	0.0657 (13)
C11	0.1594 (2)	1.5959 (7)	−0.0644 (2)	0.0625 (11)
C12	0.2300 (2)	1.3929 (6)	−0.04133 (19)	0.0505 (9)
C13	0.32852 (19)	1.0574 (6)	0.06114 (18)	0.0413 (8)
H3	0.41950	0.66460	0.27280	0.0550*
H4	0.54300	0.33510	0.30610	0.0570*
H6	0.56780	0.41440	0.07030	0.0560*
H8	0.266 (3)	1.111 (10)	0.186 (3)	0.091 (15)*
H9	0.10170	1.62620	0.11280	0.0740*
H10	0.06480	1.81910	−0.02100	0.0790*
H11	0.14380	1.67410	−0.11860	0.0750*
H12	0.26230	1.33660	−0.08030	0.0610*
H13	0.358 (2)	1.009 (7)	0.015 (2)	0.047 (8)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0455 (5)	0.0518 (5)	0.0695 (6)	0.0066 (3)	0.0084 (3)	0.0004 (3)
O1	0.0711 (15)	0.0624 (15)	0.0660 (15)	0.0137 (12)	0.0356 (12)	0.0063 (12)
N1	0.0448 (12)	0.0539 (14)	0.0402 (12)	0.0083 (11)	0.0138 (10)	−0.0007 (10)
N2	0.0410 (12)	0.0376 (11)	0.0460 (13)	−0.0020 (9)	0.0158 (10)	−0.0057 (9)
C2	0.0376 (13)	0.0363 (13)	0.0387 (13)	−0.0046 (10)	0.0118 (10)	−0.0065 (10)
C3	0.0542 (16)	0.0452 (15)	0.0414 (14)	−0.0010 (12)	0.0202 (12)	−0.0029 (12)
C4	0.0560 (16)	0.0466 (15)	0.0396 (14)	−0.0020 (13)	0.0107 (12)	0.0037 (12)

C5	0.0360 (12)	0.0377 (13)	0.0451 (15)	−0.0032 (10)	0.0060 (11)	−0.0027 (11)
C6	0.0453 (15)	0.0528 (16)	0.0426 (15)	0.0070 (12)	0.0147 (12)	−0.0052 (12)
C7	0.0391 (13)	0.0357 (13)	0.0499 (15)	−0.0057 (11)	0.0110 (11)	−0.0058 (11)
C8	0.0404 (14)	0.0424 (15)	0.0636 (18)	−0.0047 (11)	0.0200 (13)	−0.0048 (13)
C9	0.0480 (16)	0.0505 (17)	0.092 (3)	0.0043 (14)	0.0296 (16)	−0.0033 (17)
C10	0.0445 (16)	0.0496 (17)	0.097 (3)	0.0057 (14)	0.0080 (17)	0.0017 (18)
C11	0.0592 (19)	0.0510 (17)	0.066 (2)	0.0043 (15)	−0.0034 (16)	0.0012 (15)
C12	0.0520 (16)	0.0459 (15)	0.0513 (16)	0.0032 (13)	0.0095 (13)	−0.0043 (13)
C13	0.0405 (13)	0.0388 (13)	0.0453 (15)	−0.0025 (11)	0.0125 (11)	−0.0055 (11)

Geometric parameters (Å, º)

Cl1—C5	1.733 (3)	C7—C8	1.404 (4)
O1—C8	1.340 (4)	C8—C9	1.399 (5)
O1—H8	0.89 (5)	C9—C10	1.375 (7)
N1—C6	1.342 (4)	C10—C11	1.385 (5)
N1—C2	1.341 (4)	C11—C12	1.381 (5)
N2—C13	1.282 (4)	C3—H3	0.9300
N2—C2	1.418 (4)	C4—H4	0.9300
C2—C3	1.383 (4)	C6—H6	0.9300
C3—C4	1.380 (4)	C9—H9	0.9300
C4—C5	1.382 (4)	C10—H10	0.9300
C5—C6	1.373 (4)	C11—H11	0.9300
C7—C12	1.401 (4)	C12—H12	0.9300
C7—C13	1.453 (4)	C13—H13	0.99 (3)
Cl1···C6^{i}	3.627 (5)	C8···N2^{vi}	3.398 (5)
Cl1···Cl1^{ii}	3.476 (4)	C8···C2^{vi}	3.582 (5)
Cl1···H11^{iii}	3.1500	C10···C13^{vi}	3.546 (6)
O1···N2	2.627 (4)	C10···C7^{vi}	3.398 (6)
O1···C3^{iv}	3.361 (5)	C11···C13^{vi}	3.510 (5)
O1···H3^{iv}	2.5000	C13···N1^{vi}	3.416 (5)
O1···H8^{iv}	2.76 (5)	C13···C6^{vi}	3.536 (5)
N1···C13^{i}	3.416 (5)	C13···C10^{i}	3.546 (6)
N1···C6^{v}	3.365 (5)	C13···C11^{i}	3.510 (5)
N2···O1	2.627 (4)	C4···H11^{viii}	3.0300
N2···C8^{i}	3.398 (5)	C6···H6^{v}	3.0300
N1···H6^{v}	2.5900	C11···H4^{ix}	3.0800
N1···H13	2.40 (3)	C13···H8	2.47 (5)
N2···H8	1.89 (5)	H3···O1^{vii}	2.5000
C2···C5^{vi}	3.494 (5)	H4···C11^{iii}	3.0800
C2···C7^{i}	3.462 (5)	H6···N1^{v}	2.5900
C2···C8^{i}	3.582 (5)	H6···C6^{v}	3.0300
C3···O1^{vii}	3.361 (5)	H8···N2	1.89 (5)
C5···C2^{i}	3.494 (5)	H8···C13	2.47 (5)
C6···C13^{i}	3.536 (5)	H8···O1^{vii}	2.76 (5)
C6···Cl1^{vi}	3.627 (5)	H11···Cl1^{ix}	3.1500
C6···N1^{v}	3.365 (5)	H11···C4^{x}	3.0300

C6···C6^{v}	3.544 (5)	H12···H13	2.3600
C7···C2^{vi}	3.462 (5)	H13···N1	2.40 (3)
C7···C10^{i}	3.398 (6)	H13···H12	2.3600
C8—O1—H8	113 (3)	C10—C11—C12	119.2 (3)
C2—N1—C6	118.2 (2)	C7—C12—C11	121.2 (3)
C2—N2—C13	119.5 (2)	N2—C13—C7	121.5 (3)
N1—C2—N2	119.5 (2)	C2—C3—H3	121.00
N1—C2—C3	122.7 (2)	C4—C3—H3	121.00
N2—C2—C3	117.8 (2)	C3—C4—H4	121.00
C2—C3—C4	118.8 (3)	C5—C4—H4	121.00
C3—C4—C5	118.5 (3)	N1—C6—H6	119.00
Cl1—C5—C6	119.1 (2)	C5—C6—H6	119.00
C4—C5—C6	119.8 (3)	C8—C9—H9	120.00
Cl1—C5—C4	121.2 (2)	C10—C9—H9	120.00
N1—C6—C5	122.1 (3)	C9—C10—H10	120.00
C8—C7—C12	119.0 (3)	C11—C10—H10	119.00
C12—C7—C13	119.2 (3)	C10—C11—H11	120.00
C8—C7—C13	121.8 (3)	C12—C11—H11	120.00
O1—C8—C7	122.4 (3)	C7—C12—H12	119.00
C7—C8—C9	119.3 (3)	C11—C12—H12	119.00
O1—C8—C9	118.3 (3)	N2—C13—H13	123.2 (19)
C8—C9—C10	120.4 (3)	C7—C13—H13	115.3 (19)
C9—C10—C11	121.1 (3)		
C6—N1—C2—N2	178.8 (2)	C12—C7—C8—O1	−179.9 (3)
C6—N1—C2—C3	−2.1 (4)	C12—C7—C8—C9	0.8 (4)
C2—N1—C6—C5	0.4 (4)	C13—C7—C8—O1	−0.9 (4)
C13—N2—C2—N1	−2.5 (4)	C13—C7—C8—C9	179.8 (3)
C13—N2—C2—C3	178.4 (3)	C8—C7—C12—C11	−1.0 (4)
C2—N2—C13—C7	−179.7 (2)	C13—C7—C12—C11	−180.0 (3)
N1—C2—C3—C4	2.2 (4)	C8—C7—C13—N2	1.5 (4)
N2—C2—C3—C4	−178.7 (3)	C12—C7—C13—N2	−179.5 (3)
C2—C3—C4—C5	−0.6 (4)	O1—C8—C9—C10	−179.7 (3)
C3—C4—C5—Cl1	179.1 (2)	C7—C8—C9—C10	−0.4 (5)
C3—C4—C5—C6	−1.0 (4)	C8—C9—C10—C11	0.2 (5)
Cl1—C5—C6—N1	−179.0 (2)	C9—C10—C11—C12	−0.4 (5)
C4—C5—C6—N1	1.1 (5)	C10—C11—C12—C7	0.8 (5)

Symmetry codes: (i) *x*, *y*−1, *z*; (ii) −*x*+3/2, *y*+1/2, −*z*+1/2; (iii) *x*+1/2, −*y*+3/2, *z*+1/2; (iv) −*x*+1/2, *y*+1/2, −*z*+1/2; (v) −*x*+1, −*y*+1, −*z*; (vi) *x*, *y*+1, *z*; (vii) −*x*+1/2, *y*−1/2, −*z*+1/2; (viii) *x*+1/2, −*y*+5/2, *z*+1/2; (ix) *x*−1/2, −*y*+3/2, *z*−1/2; (x) *x*−1/2, −*y*+5/2, *z*−1/2.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H8···N2	0.89 (5)	1.89 (5)	2.627 (4)	140 (4)

C3—H3···O1^{vii}	0.93	2.50	3.361 (5)	154
C6—H6···N1^{v}	0.93	2.59	3.365 (5)	141

Symmetry codes: (v) $-x+1, -y+1, -z$; (vii) $-x+1/2, y-1/2, -z+1/2$.