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(2-Chloropyridin-3-yl)(4-nitrobenzylidene)amine

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Key indicators

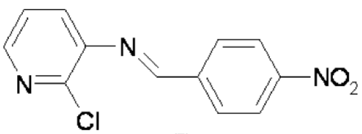
Single-crystal X-ray study
T = 296 K
Mean σ(C–C) = 0.003 Å
R factor = 0.040
wR factor = 0.079
Data-to-parameter ratio = 14.0

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

In the title compound, $C_{12}H_8ClN_3O_2$, the dihedral angle between the least-squares planes of the pyridine and benzene rings is 20.8 (1)°. In the crystal structure, molecules pack nearly parallel along the *a* axis, with some π stacking interactions.

Comment

Schiff bases are reported to show a variety of biological activities, such as antibacterial (Pandeya *et al.*, 1999; El-masry *et al.*, 2000; Kabeer *et al.*, 2001), anticancer (Phatak *et al.*, 2000; Desai *et al.*, 2001), antifungal (Singh & Dash, 1988; More *et al.*, 2001) and herbicidal (Samadhiya & Halve, 2001). Pyridinium compounds have biological activities (Sepcic, 2000) such as antibacterial (Sliwa & Mianowska, 1989; Druta *et al.*, 2000) and antifungal (Sliwa & Mianowska, 1989). The presence of a chloro substituent in different types of compounds causes them to exhibit pesticidal activity (Samadhiya & Halve, 2001). Therefore, we synthesized (2-chloropyridin-3-yl)(4-nitrobenzylidene)amine, (I), and now report its crystal stucture.



(I)

The molecular structure of (I) is shown in Fig. 1 with the atom-numbering scheme. All geometric parameters are comparable to the values for similar structures reported in the literature (Allen *et al.*, 1987). The dihedral angle between the least-squares planes of the pyridine and benzene rings is 20.8 (1)°. The C2—N2—C6—C7 torsion angle is 177.0 (2)°. In the crystal packing, an overlapped arrangement of the molecules is observed along the *a* axis (Figs 2 and 3). The pyridine

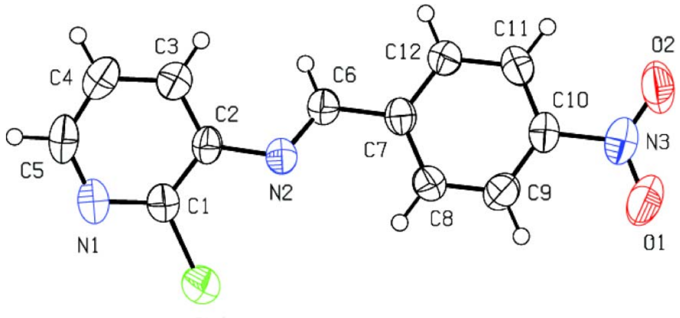


Figure 1
An *ORTEP-3* plot (Farrugia, 1997) of (I), with the atom-numbering scheme and 50% probability displacement ellipsoids.

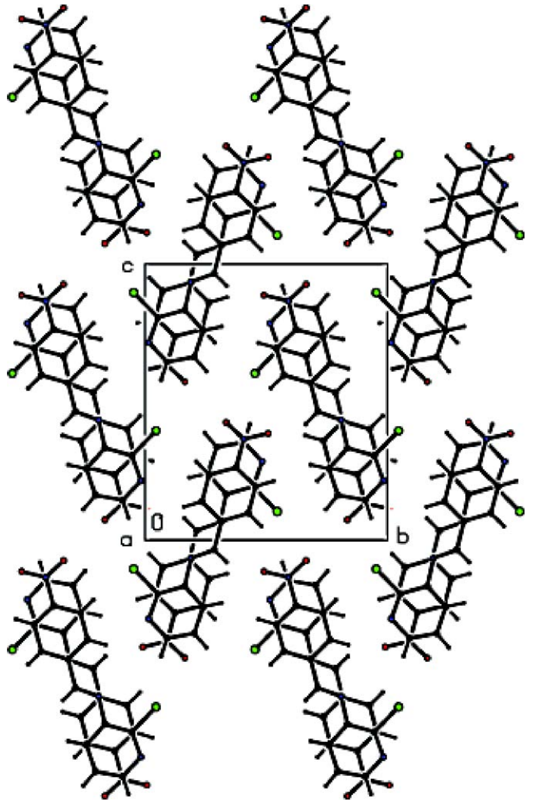


Figure 2
Packing diagram for (I), viewed along the *a* axis.

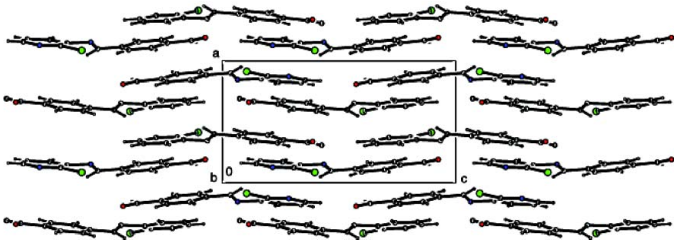


Figure 3
Packing diagram for (I), viewed along the *b* axis.

ring and the benzene ring of an adjacent molecule at ($\frac{1}{2}+x$, $\frac{3}{2}-y$, $1-z$) are nearly parallel [dihedral angle = 3.83 (8)°], with a separation of about 3.68 Å, indicating the presence of some π stacking interaction.

Experimental

Treatment of 3-amino-2-chloropyridine with 4-nitrobenzeldehyde gave the title Schiff base, (I). The title compound was recrystallized from ethanol to give yellow lath-shaped crystals. The IR spectrum showed absorption bands at 1340.4 and 1517.9 (NO_2), 1600.0 (Schiff base C═N) and 1633.6 cm^{-1} (C═N pyridine ring). The ^{1}H NMR spectrum showed ArH at 7.23–8.38 p.p.m. and the imino proton at 8.54 p.p.m. The ^{13}C NMR showed the C═N at 161.41 p.p.m. The experimental and spectroscopic details of (I) have already been published (Jarrahpour *et al.*, 2004).

Crystal data

$C_{12}H_8ClN_3O_2$
$M_r = 261.66$
Orthorhombic, $P2_12_12_1$
$a = 7.1404$ (6) Å
$b = 11.9642$ (11) Å
$c = 13.6188$ (16) Å
$V = 1163.4$ (2) Å^3
$Z = 4$
$D_x = 1.494$ Mg m^{-3}

Mo Kα radiation
Cell parameters from 1966 reflections
$\theta = 2.3$–$29.0°$
$\mu = 0.33$ mm^{-1}
$T = 296$ K
Lath, yellow
0.72 × 0.32 × 0.11 mm

Data collection

Stoe IPDS-II diffractometer
ω scans
Absorption correction: by integration *X-RED32* (Stoe & Cie, 2002)
$T_{\rm min} = 0.800$, $T_{\rm max} = 0.965$
11 387 measured reflections

2280 independent reflections
1887 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.048$
$\theta_{\rm max} = 26.0°$
$h = -9 \rightarrow 9$
$k = -16 \rightarrow 16$
$l = -18 \rightarrow 18$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.040$
$wR(F^2) = 0.079$
$S = 1.06$
2280 reflections
163 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0274P)^2 + 0.1715P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} < 0.001$
$\Delta\rho_{\rm max} = 0.10$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.18$ e Å^{-3}
Absolute structure: Flack (1983), 943 Friedel pairs
Flack parameter = 0.23 (8)

Table 1
Selected geometric parameters (Å, °).

Cl1—C1	1.734 (2)	N1—C5	1.329 (3)
O1—N3	1.209 (3)	N2—C2	1.418 (3)
O2—N3	1.226 (3)	N2—C6	1.270 (3)
N1—C1	1.318 (3)	N3—C10	1.472 (3)
C1—N1—C5	116.3 (2)	N1—C1—C2	125.4 (2)
C2—N2—C6	119.96 (19)	N2—C2—C1	118.59 (19)
O1—N3—O2	123.6 (2)	N2—C2—C3	124.7 (2)
O1—N3—C10	118.3 (2)	N1—C5—C4	123.8 (2)
O2—N3—C10	118.1 (2)	N2—C6—C7	120.59 (19)
Cl1—C1—N1	115.58 (18)	N3—C10—C9	118.7 (2)
Cl1—C1—C2	119.03 (17)	N3—C10—C11	118.7 (2)

All H atoms were positioned geometrically and refined with a riding model at distances of 0.93 Å, with isotropic displacement parameters of $1.2U_{\rm eq}$(C).

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED32* (Stoe & Cie, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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