Crystal structure of 2-(2-chlorophenylamino)pyridine, $C_{11}H_9ClN_2$

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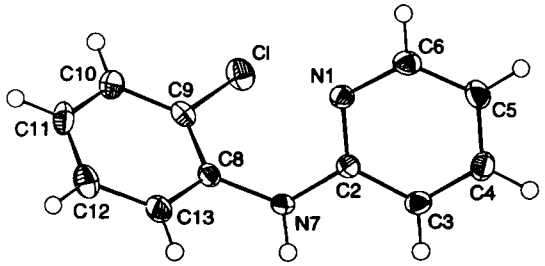

Abstract

$C_{11}H_9ClN_2$, monoclinic, $P12_1/c1$ (no. 14), $a = 14.061(3)$ Å, $b = 7.732(2)$ Å, $c = 9.161(4)$ Å, $\beta = 106.85(2)°$, $V = 953.2$ Å^3, $Z = 4$, $R_{gt}(F) = 0.040$, $wR_{ref}(F^2) = 0.096$, $T = 173$ K.

Source of material

The title compound was obtained in a one-step procedure [1,2]. 2-Chloropyridine and 2-chloroaniline hydrochloride were heated at 180 °C for 90 minutes. The hydrochlorous raw product was suspended to aqueous sodium carbonate and then extracted with dichloromethane. The dichloromethane solution was dried over anhydrous sodium sulfate and then filtered. Colorless crystals were obtained overnight. Recrystallization from dichloromethane/pentane yielded suitable crystals for X-ray measurement.

Experimental details

The H7 atom found in the fourier map was refined freely to comment the hydrogen bonding pattern.

Discussion

The outline of the structure obtained is similar to 2-(2,6-difluorophenylamino)pyridine reported earlier [3]. 2-(2-Chlorophenylamino)pyridine crystallizes with N7–H7···N1′ interactions that form a zig-zag chain structure along the *c*-axis, instead of the usual centrosymmetric dimeric structure. N7–H7···N1′ angle is 162(2)°, where the N1···H7′ distance is fairly long 2.26(2) Å and this leads to the donor-acceptor distance of 3.093(3) Å.

Table 1. Data collection and handling.

Crystal:	colorless needle, size 0.10 × 0.12 × 0.30 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	3.56 cm^{-1}
Diffractometer, scan mode:	Nonius 95 mm KappaCCD, φ/ω
$2\theta_{max}$:	55.12°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	13450, 2193
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 1675
$N(param)_{refined}$:	131
Programs:	SHELXS-97 [4], SHELXL-97 [5], SHELXTL [6]

Table 2. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	*x*	*y*	*z*	U_{iso}
H(3)	4*e*	0.1612	0.0332	0.5548	0.025
H(4)	4*e*	0.0471	−0.1714	0.5892	0.030
H(5)	4*e*	0.0112	−0.1845	0.8255	0.031
H(6)	4*e*	0.0908	0.0057	1.0153	0.027
H(7)	4*e*	0.243(1)	0.294(3)	0.650(2)	0.019(5)
H(10)	4*e*	0.4556	0.4479	1.1934	0.029
H(11)	4*e*	0.4096	0.7379	1.1435	0.033
H(12)	4*e*	0.2979	0.8155	0.9093	0.036
H(13)	4*e*	0.2259	0.6025	0.7313	0.029

Table 3. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	*x*	*y*	*z*	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Cl	4*e*	0.40912(3)	0.14176(6)	1.02644(6)	0.0255(2)	0.0183(2)	0.0354(3)	0.0048(2)	0.0059(2)	0.0038(2)
N(1)	4*e*	0.1700(1)	0.1344(2)	0.9038(2)	0.0185(7)	0.0199(8)	0.0179(8)	−0.0005(6)	0.0065(6)	−0.0002(7)
C(2)	4*e*	0.1882(1)	0.1419(2)	0.7682(2)	0.0175(8)	0.0134(8)	0.0181(9)	0.0033(7)	0.0045(7)	0.0009(7)
C(3)	4*e*	0.1449(1)	0.0272(2)	0.6483(2)	0.0275(9)	0.019(1)	0.0175(9)	0.0024(8)	0.0081(8)	−0.0005(8)
C(4)	4*e*	0.0783(1)	−0.0939(2)	0.6692(2)	0.027(1)	0.020(1)	0.024(1)	−0.0024(8)	0.0022(9)	−0.0036(8)
C(5)	4*e*	0.0571(1)	−0.1023(3)	0.8084(2)	0.0229(9)	0.026(1)	0.028(1)	−0.0080(8)	0.0042(9)	0.0032(8)
C(6)	4*e*	0.1046(1)	0.0123(3)	0.9199(2)	0.0200(9)	0.029(1)	0.021(1)	−0.0017(8)	0.0089(8)	0.0021(8)
N(7)	4*e*	0.2516(1)	0.2689(2)	0.7451(2)	0.0281(8)	0.0182(8)	0.0151(8)	−0.0035(6)	0.0088(7)	−0.0001(7)
C(8)	4*e*	0.2965(1)	0.3962(2)	0.8544(2)	0.0208(8)	0.0156(9)	0.0198(9)	−0.0029(7)	0.0097(8)	−0.0010(7)
C(9)	4*e*	0.3679(1)	0.3541(2)	0.9905(2)	0.0182(8)	0.0156(9)	0.024(1)	0.0010(7)	0.0089(8)	0.0031(8)
C(10)	4*e*	0.4092(1)	0.4796(3)	1.0994(2)	0.0212(9)	0.025(1)	0.025(1)	−0.0041(8)	0.0042(8)	−0.0018(9)
C(11)	4*e*	0.3821(2)	0.6516(3)	1.0694(2)	0.030(1)	0.021(1)	0.033(1)	−0.0074(8)	0.0100(9)	−0.0091(9)
C(12)	4*e*	0.3148(2)	0.6975(3)	0.9313(3)	0.035(1)	0.0149(9)	0.039(1)	−0.0013(8)	0.011(1)	−0.0006(9)
C(13)	4*e*	0.2723(1)	0.5703(2)	0.8253(2)	0.028(1)	0.0175(9)	0.026(1)	0.0007(8)	0.0048(9)	0.0042(8)

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