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2-(3-Chloroanilino)pyridine

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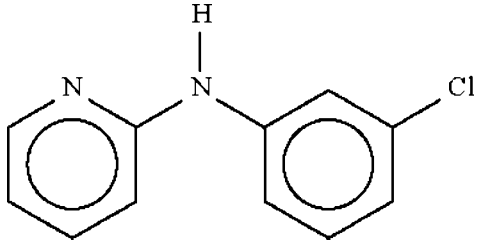
Key indicators: single-crystal X-ray study; T = 119 K; mean σ(C–C) = 0.003 Å; R factor = 0.047; wR factor = 0.133; data-to-parameter ratio = 15.8.

In the title compound, $C_{11}H_9ClN$, the dihedral angle between the aromatic ring planes is 44.2 (1)° and the bridging C—N—C bond angle is 127.60 (19)°. The amino N—H grouping makes a hydrogen bond to the pyridyl N atom of an adjacent molecule across a center of inversion, generating a hydrogen-bonded dimer.

Related literature

For the crystal structure of the 4-chloro derivative, see: Fairuz *et al.* (2008).



Experimental

Crystal data

$C_{11}H_9ClN_2$
M_r = 204.65
Triclinic, $P\overline{1}$
a = 3.8954 (1) Å
b = 10.7804 (4) Å
c = 12.4548 (4) Å
α = 64.932 (2)°
β = 88.004 (2)°
γ = 88.240 (2)°
V = 473.40 (3) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.36 mm^{-1}
T = 119 K
0.40 × 0.05 × 0.02 mm

Data collection

Bruker SMART APEX diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.870, T_{max} = 0.993
5923 measured reflections
2064 independent reflections
1807 reflections with $I > 2\sigma(I)$
R_{int} = 0.019

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.133
S = 1.07
2064 reflections
131 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.37 e Å^{-3}
$\Delta\rho_{min}$ = −0.29 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···N2^{i}	0.88 (1)	2.18 (1)	3.042 (3)	167 (3)

Symmetry code: (i) $-x+1, -y+1, -z+1$.

Data collection: *APEX2* (Bruker, 2008); cell refinement: *SAINT* (Bruker, 2008); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: TK2464).

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supporting information

Acta Cryst. (2009). E**65**, o1449 [doi:10.1107/S1600536809019941]

2-(3-Chloroanilino)pyridine

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S1. Experimental

2-Chloropyridine (0.5 ml, 5.28 mmol) and 3-chloroaniline (0.67 g, 5.28 mmol) were heated at 423–433 K for 3 h. The solid was dissolved in water and extracted with ether. The ether extract was dried over sodium sulfate. The solvent was evaporated and the product recrystallized from ethanol to yield pale-purple crystals.

S2. Refinement

Carbon-bound H-atoms were placed in calculated positions (C—H 0.95 Å) and were included in the refinement in the riding model approximation with *U*(H) fixed at 1.2*U*(C). The amino H-atom was located in a difference Fourier map and was refined with a distance restraint of N–H 0.88±0.01 Å; the isotropic temperature factor were refined.

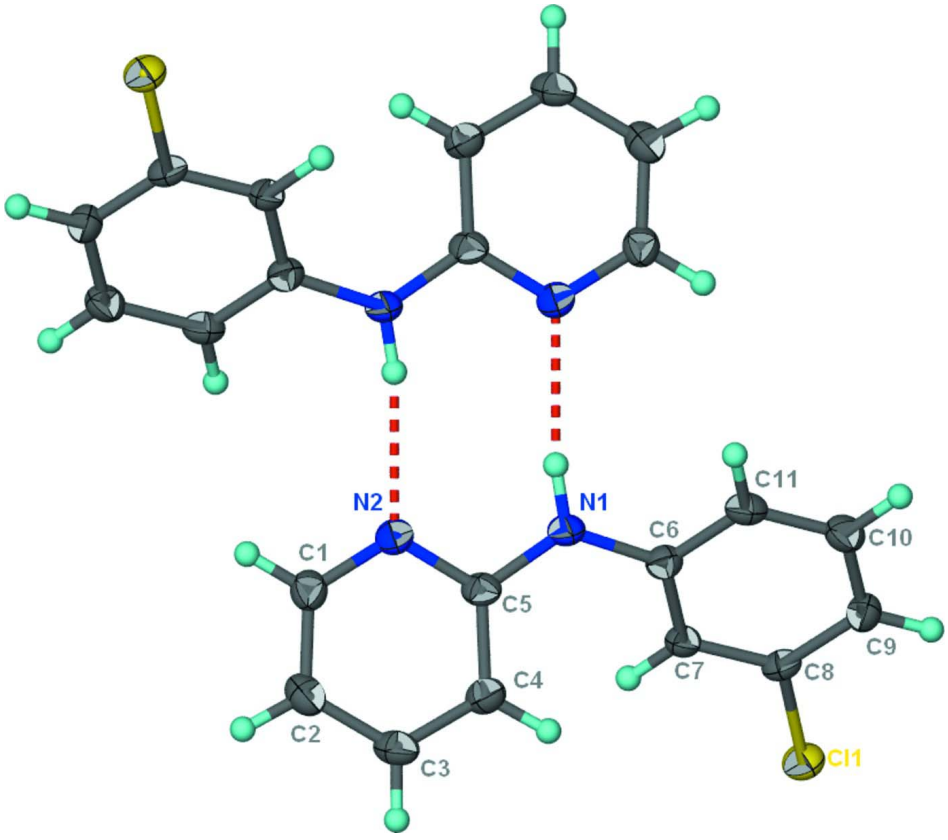

Figure 1

Thermal ellipsoid plot (Barbour, 2001) of the hydrogen-bonded (dashed lines) centrosymmetric dimer $\{C_{11}H_9ClN_2\}_2$ with molecules drawn at the 70% probability level; hydrogen atoms are drawn as spheres of arbitrary radius.

2-(3-Chloroanilino)pyridine

Crystal data

$C_{11}H_9ClN_2$
$M_r = 204.65$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 3.8954$ (1) Å
$b = 10.7804$ (4) Å
$c = 12.4548$ (4) Å
$\alpha = 64.932$ (2)°
$\beta = 88.004$ (2)°
$\gamma = 88.240$ (2)°
$V = 473.40$ (3) Å^3
$Z = 2$
$F(000) = 212$
$D_x = 1.436$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1691 reflections
$\theta = 3.2$–$27.7°$
$\mu = 0.36$ mm^{-1}
$T = 119$ K
Prism, pale purple
0.40 × 0.05 × 0.02 mm

Data collection

Bruker SMART APEX diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.870$, $T_{max} = 0.993$
5923 measured reflections
2064 independent reflections
1807 reflections with $I > 2\sigma(I)$
$R_{int} = 0.019$
$\theta_{max} = 27.5°$, $\theta_{min} = 1.8°$
$h = -5 \rightarrow 5$
$k = -13 \rightarrow 14$
$l = -16 \rightarrow 16$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.047$
$wR(F^2) = 0.133$
$S = 1.07$
2064 reflections
131 parameters
1 restraint
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
$w = 1/[\sigma^2(F_o^2) + (0.0578P)^2 + 0.8P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.37$ e Å^{-3}
$\Delta\rho_{min} = -0.29$ e Å^{-3}

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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl1	0.67761 (16)	−0.15289 (6)	0.94724 (5)	0.0242 (2)
N1	0.7040 (6)	0.3450 (2)	0.62528 (17)	0.0224 (5)
H1	0.654 (8)	0.390 (3)	0.5500 (11)	0.024 (7)*
N2	0.5081 (5)	0.5439 (2)	0.63195 (17)	0.0207 (4)
C1	0.4688 (6)	0.6248 (2)	0.6895 (2)	0.0215 (5)
H1A	0.3597	0.7118	0.6492	0.026*

C2	0.5768 (7)	0.5897 (3)	0.8032 (2)	0.0237 (5)
H2	0.5413	0.6501	0.8404	0.028*
C3	0.7401 (7)	0.4624 (2)	0.8620 (2)	0.0230 (5)
H3	0.8192	0.4351	0.9402	0.028*
C4	0.7861 (6)	0.3767 (2)	0.8060 (2)	0.0206 (5)
H4	0.8982	0.2901	0.8443	0.025*
C5	0.6623 (6)	0.4211 (2)	0.69013 (19)	0.0186 (5)
C6	0.8088 (6)	0.2076 (2)	0.6660 (2)	0.0185 (5)
C7	0.7102 (6)	0.1066 (2)	0.77788 (19)	0.0179 (5)
H7	0.5747	0.1306	0.8314	0.022*
C8	0.8122 (6)	−0.0275 (2)	0.80912 (19)	0.0179 (5)
C9	1.0038 (6)	−0.0685 (2)	0.7336 (2)	0.0209 (5)
H9	1.0677	−0.1619	0.7565	0.025*
C10	1.0995 (6)	0.0324 (3)	0.6223 (2)	0.0225 (5)
H10	1.2316	0.0075	0.5687	0.027*
C11	1.0045 (6)	0.1685 (2)	0.5891 (2)	0.0201 (5)
H11	1.0731	0.2357	0.5132	0.024*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0325 (4)	0.0186 (3)	0.0169 (3)	−0.0002 (2)	−0.0003 (2)	−0.0032 (2)
N1	0.0351 (12)	0.0172 (10)	0.0128 (9)	0.0037 (8)	−0.0029 (8)	−0.0044 (8)
N2	0.0263 (11)	0.0173 (9)	0.0156 (9)	0.0010 (8)	0.0006 (8)	−0.0043 (7)
C1	0.0234 (12)	0.0194 (11)	0.0205 (11)	0.0009 (9)	0.0027 (9)	−0.0076 (9)
C2	0.0287 (13)	0.0228 (12)	0.0222 (12)	−0.0034 (10)	0.0036 (10)	−0.0119 (10)
C3	0.0297 (13)	0.0224 (12)	0.0158 (11)	−0.0051 (10)	−0.0008 (9)	−0.0069 (9)
C4	0.0225 (12)	0.0183 (11)	0.0194 (11)	−0.0007 (9)	−0.0038 (9)	−0.0061 (9)
C5	0.0227 (12)	0.0169 (11)	0.0135 (10)	−0.0034 (9)	0.0011 (8)	−0.0038 (8)
C6	0.0192 (11)	0.0185 (11)	0.0173 (11)	0.0007 (9)	−0.0028 (8)	−0.0071 (9)
C7	0.0191 (11)	0.0204 (11)	0.0139 (10)	0.0021 (9)	−0.0005 (8)	−0.0070 (9)
C8	0.0198 (11)	0.0166 (10)	0.0139 (10)	−0.0013 (8)	−0.0022 (8)	−0.0029 (8)
C9	0.0227 (12)	0.0180 (11)	0.0224 (11)	0.0032 (9)	−0.0038 (9)	−0.0091 (9)
C10	0.0209 (12)	0.0286 (13)	0.0201 (11)	0.0026 (9)	−0.0002 (9)	−0.0126 (10)
C11	0.0202 (12)	0.0244 (12)	0.0145 (10)	−0.0011 (9)	−0.0004 (8)	−0.0071 (9)

Geometric parameters (Å, º)

Cl1—C8	1.752 (2)	C4—C5	1.411 (3)
N1—C5	1.376 (3)	C4—H4	0.9500
N1—C6	1.400 (3)	C6—C11	1.396 (3)
N1—H1	0.880 (10)	C6—C7	1.406 (3)
N2—C5	1.345 (3)	C7—C8	1.378 (3)
N2—C1	1.346 (3)	C7—H7	0.9500
C1—C2	1.380 (3)	C8—C9	1.386 (3)
C1—H1A	0.9500	C9—C10	1.398 (3)
C2—C3	1.397 (3)	C9—H9	0.9500
C2—H2	0.9500	C10—C11	1.386 (3)

C3—C4	1.378 (3)	C10—H10	0.9500
C3—H3	0.9500	C11—H11	0.9500
C5—N1—C6	127.60 (19)	N1—C6—C11	118.1 (2)
C5—N1—H1	114.3 (19)	N1—C6—C7	123.0 (2)
C6—N1—H1	118.1 (19)	C11—C6—C7	118.8 (2)
C5—N2—C1	117.3 (2)	C8—C7—C6	119.3 (2)
N2—C1—C2	124.2 (2)	C8—C7—H7	120.4
N2—C1—H1A	117.9	C6—C7—H7	120.4
C2—C1—H1A	117.9	C7—C8—C9	122.7 (2)
C1—C2—C3	117.8 (2)	C7—C8—Cl1	118.76 (18)
C1—C2—H2	121.1	C9—C8—Cl1	118.48 (17)
C3—C2—H2	121.1	C8—C9—C10	117.6 (2)
C4—C3—C2	119.7 (2)	C8—C9—H9	121.2
C4—C3—H3	120.1	C10—C9—H9	121.2
C2—C3—H3	120.1	C11—C10—C9	121.0 (2)
C3—C4—C5	118.2 (2)	C11—C10—H10	119.5
C3—C4—H4	120.9	C9—C10—H10	119.5
C5—C4—H4	120.9	C10—C11—C6	120.6 (2)
N2—C5—N1	114.4 (2)	C10—C11—H11	119.7
N2—C5—C4	122.7 (2)	C6—C11—H11	119.7
N1—C5—C4	122.8 (2)		
C5—N2—C1—C2	0.2 (4)	C5—N1—C6—C7	37.1 (4)
N2—C1—C2—C3	0.6 (4)	N1—C6—C7—C8	177.1 (2)
C1—C2—C3—C4	−0.4 (4)	C11—C6—C7—C8	0.8 (3)
C2—C3—C4—C5	−0.5 (4)	C6—C7—C8—C9	−1.4 (4)
C1—N2—C5—N1	−178.1 (2)	C6—C7—C8—Cl1	−178.31 (17)
C1—N2—C5—C4	−1.1 (4)	C7—C8—C9—C10	1.1 (4)
C6—N1—C5—N2	−170.1 (2)	Cl1—C8—C9—C10	178.04 (18)
C6—N1—C5—C4	12.9 (4)	C8—C9—C10—C11	−0.2 (4)
C3—C4—C5—N2	1.3 (4)	C9—C10—C11—C6	−0.3 (4)
C3—C4—C5—N1	178.1 (2)	N1—C6—C11—C10	−176.5 (2)
C5—N1—C6—C11	−146.5 (2)	C7—C6—C11—C10	0.1 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···N2^{i}	0.88 (1)	2.18 (1)	3.042 (3)	167 (3)

Symmetry code: (i) −*x*+1, −*y*+1, −*z*+1.