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4-Chloro-*N*-(pyrimidin-2-yl)aniline

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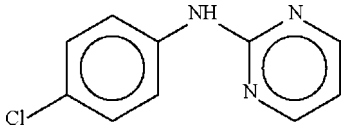
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.002 Å; R factor = 0.031; wR factor = 0.080; data-to-parameter ratio = 15.5.

The two aromatic rings in the title compound, $C_{10}H_8ClN_3$, open the angle at the planar N atom to 128.00 (12)°. The amino N atom of one molecule forms a hydrogen bond to the 1-N atom of an adjacent pyrimidyl ring, generating a hydrogen-bonded dimer.

Related literature

For other 4-chloroanilino substituted *N*-heterocycles, see: Fairuz *et al.* (2008); Idris *et al.* (2008).



Experimental

Crystal data

$C_{10}H_8ClN_3$
M_r = 205.64
Triclinic, $P\overline{1}$
a = 3.7750 (1) Å
b = 10.0589 (3) Å
c = 12.0116 (3) Å
α = 89.237 (1)°
β = 89.037 (1)°
γ = 89.399 (2)°
V = 455.98 (2) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.38 mm^{-1}
T = 100 (2) K
0.35 × 0.15 × 0.05 mm

Data collection

Bruker SMART APEX diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.880, T_{max} = 0.982
3625 measured reflections
2032 independent reflections
1757 reflections with $I > 2\sigma(I)$
R_{int} = 0.014

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.080
S = 1.02
2032 reflections
131 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.34 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 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}	0.85 (2)	2.18 (2)	3.028 (2)	174 (2)

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

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); 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: TK2341).

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supplementary materials

Acta Cryst. (2009). E**65**, o94 [**doi:10.1107/S1600536808041184**]

4-Chloro-*N*-(pyrimidin-2-yl)aniline

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Experimental

2-Chloropyrimidine (2.88 g, 2.5 mmol) and 4-chloroaniline (3.20 g, 25 mmol) were mixed with ethanol (2 ml) and the mixture was heated at 423–433 K for 8 h. The product was dissolved in water and the solution extracted with ether. The ether phase was dried over sodium sulfate; the evaporation of the solvent gave well shaped crystals along with some unidentified brown material.

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) set to 1.2*U*eq(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; its temperature factors were freely refined.

Figures

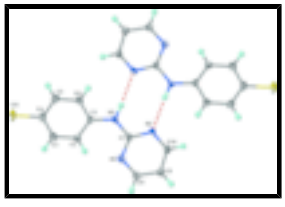

Fig. 1. Thermal ellipsoid plot (Barbour, 2001) of hydrogen-bonded dimeric structure of $C_{10}H_8ClN_3$ at the 70% probability level. Hydrogen atoms are drawn as spheres of arbitrary radius. Hydrogen bonds are shown as red dashed lines.

4-Chloro-*N*-(pyrimidin-2-yl)aniline

Crystal data

$C_{10}H_8ClN_3$	$Z = 2$
$M_r = 205.64$	$F_{000} = 212$
Triclinic, $P\bar{1}$	$D_x = 1.498$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 3.7750$ (1) Å	Cell parameters from 2160 reflections
$b = 10.0589$ (3) Å	$\theta = 2.6$–$28.2°$
$c = 12.0116$ (3) Å	$\mu = 0.38$ mm^{-1}
$\alpha = 89.237$ (1)°	$T = 100$ (2) K
$\beta = 89.037$ (1)°	Plate, yellow
$\gamma = 89.399$ (2)°	0.35 × 0.15 × 0.05 mm
$V = 455.98$ (2) Å^3	

Data collection

Bruker SMART APEX diffractometer	2032 independent reflections
Radiation source: fine-focus sealed tube	1757 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.014$
$T = 100(2)$ K	$\theta_{max} = 27.5^o$
ω scans	$\theta_{min} = 2.0^o$
Absorption correction: Multi-scan (SADABS; Sheldrick, 1996)	$h = -4\rightarrow4$
$T_{min} = 0.880$, $T_{max} = 0.982$	$k = -13\rightarrow13$
3625 measured reflections	$l = -14\rightarrow15$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.031$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.080$	$w = 1/[\sigma^2(F_o^2) + (0.0319P)^2 + 0.3201P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.02$	$(\Delta/\sigma)_{max} = 0.001$
2032 reflections	$\Delta\rho_{max} = 0.34$ e Å^{-3}
131 parameters	$\Delta\rho_{min} = -0.24$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl1	1.12780 (11)	0.77439 (4)	1.04792 (3)	0.02641 (13)
N1	0.6990 (3)	0.63747 (13)	0.59185 (10)	0.0156 (3)
H1	0.642 (5)	0.556 (2)	0.5875 (16)	0.028 (5)*
N2	0.5390 (3)	0.64905 (12)	0.40908 (10)	0.0150 (3)
N3	0.7907 (3)	0.83808 (12)	0.49717 (10)	0.0156 (3)
C1	0.8101 (4)	0.67719 (14)	0.69743 (11)	0.0136 (3)
C2	0.7505 (4)	0.80454 (15)	0.73923 (11)	0.0156 (3)
H2	0.6416	0.8710	0.6941	0.019*
C3	0.8504 (4)	0.83405 (15)	0.84683 (12)	0.0178 (3)
H3	0.8117	0.9208	0.8752	0.021*
C4	1.0064 (4)	0.73655 (16)	0.91245 (11)	0.0172 (3)
C5	1.0687 (4)	0.60984 (15)	0.87278 (12)	0.0175 (3)
H5	1.1767	0.5436	0.9184	0.021*
C6	0.9703 (4)	0.58131 (15)	0.76498 (12)	0.0156 (3)
H6	1.0131	0.4947	0.7368	0.019*
C7	0.6752 (4)	0.71254 (14)	0.49723 (11)	0.0132 (3)

C8	0.7695 (4)	0.90471 (14)	0.40058 (12)	0.0156 (3)
H8	0.8469	0.9943	0.3975	0.019*
C9	0.6401 (4)	0.84960 (15)	0.30478 (12)	0.0165 (3)
H9	0.6296	0.8981	0.2365	0.020*
C10	0.5268 (4)	0.71961 (15)	0.31431 (11)	0.0159 (3)
H10	0.4358	0.6785	0.2502	0.019*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0288 (2)	0.0384 (2)	0.01228 (18)	−0.00173 (17)	−0.00450 (14)	−0.00490 (15)
N1	0.0213 (7)	0.0124 (6)	0.0133 (6)	−0.0040 (5)	−0.0022 (5)	−0.0008 (5)
N2	0.0171 (6)	0.0139 (6)	0.0141 (6)	−0.0007 (5)	−0.0017 (5)	−0.0020 (4)
N3	0.0169 (6)	0.0151 (6)	0.0146 (6)	−0.0028 (5)	0.0002 (5)	−0.0010 (5)
C1	0.0129 (6)	0.0158 (7)	0.0121 (6)	−0.0037 (5)	0.0005 (5)	−0.0004 (5)
C2	0.0173 (7)	0.0159 (7)	0.0136 (6)	−0.0006 (5)	0.0002 (5)	0.0005 (5)
C3	0.0184 (7)	0.0185 (7)	0.0164 (7)	−0.0019 (6)	0.0022 (5)	−0.0043 (5)
C4	0.0152 (7)	0.0260 (8)	0.0103 (6)	−0.0035 (6)	0.0003 (5)	−0.0020 (5)
C5	0.0141 (7)	0.0224 (8)	0.0158 (7)	−0.0005 (6)	0.0003 (5)	0.0030 (6)
C6	0.0153 (7)	0.0154 (7)	0.0162 (7)	−0.0012 (5)	0.0016 (5)	−0.0009 (5)
C7	0.0118 (6)	0.0145 (7)	0.0133 (6)	0.0001 (5)	0.0007 (5)	−0.0018 (5)
C8	0.0159 (7)	0.0138 (7)	0.0170 (7)	−0.0013 (5)	0.0017 (5)	−0.0001 (5)
C9	0.0182 (7)	0.0177 (7)	0.0135 (6)	0.0008 (6)	0.0004 (5)	0.0012 (5)
C10	0.0161 (7)	0.0180 (7)	0.0136 (6)	0.0010 (5)	−0.0019 (5)	−0.0030 (5)

Geometric parameters (Å, °)

Cl1—C4	1.7458 (14)	C3—C4	1.383 (2)
N1—C7	1.3599 (18)	C3—H3	0.9500
N1—C1	1.4067 (17)	C4—C5	1.383 (2)
N1—H1	0.85 (2)	C5—C6	1.3875 (19)
N2—C10	1.3346 (18)	C5—H5	0.9500
N2—C7	1.3552 (17)	C6—H6	0.9500
N3—C8	1.3353 (18)	C8—C9	1.383 (2)
N3—C7	1.3404 (18)	C8—H8	0.9500
C1—C6	1.392 (2)	C9—C10	1.383 (2)
C1—C2	1.397 (2)	C9—H9	0.9500
C2—C3	1.3890 (19)	C10—H10	0.9500
C2—H2	0.9500		
C7—N1—C1	128.00 (12)	C4—C5—H5	120.7
C7—N1—H1	116.9 (14)	C6—C5—H5	120.7
C1—N1—H1	115.1 (14)	C5—C6—C1	121.22 (13)
C10—N2—C7	115.63 (12)	C5—C6—H6	119.4
C8—N3—C7	116.05 (12)	C1—C6—H6	119.4
C6—C1—C2	119.06 (13)	N3—C7—N2	125.91 (13)
C6—C1—N1	117.44 (13)	N3—C7—N1	119.22 (12)
C2—C1—N1	123.41 (13)	N2—C7—N1	114.85 (12)
C3—C2—C1	120.03 (14)	N3—C8—C9	123.14 (13)

C3—C2—H2	120.0	N3—C8—H8	118.4
C1—C2—H2	120.0	C9—C8—H8	118.4
C4—C3—C2	119.69 (14)	C10—C9—C8	115.99 (13)
C4—C3—H3	120.2	C10—C9—H9	122.0
C2—C3—H3	120.2	C8—C9—H9	122.0
C5—C4—C3	121.30 (13)	N2—C10—C9	123.27 (13)
C5—C4—Cl1	119.40 (12)	N2—C10—H10	118.4
C3—C4—Cl1	119.31 (12)	C9—C10—H10	118.4
C4—C5—C6	118.70 (14)		
C7—N1—C1—C6	−150.50 (14)	N1—C1—C6—C5	−176.11 (13)
C7—N1—C1—C2	33.1 (2)	C8—N3—C7—N2	−0.4 (2)
C6—C1—C2—C3	−0.1 (2)	C8—N3—C7—N1	178.01 (13)
N1—C1—C2—C3	176.32 (13)	C10—N2—C7—N3	1.0 (2)
C1—C2—C3—C4	−0.5 (2)	C10—N2—C7—N1	−177.43 (13)
C2—C3—C4—C5	0.6 (2)	C1—N1—C7—N3	5.1 (2)
C2—C3—C4—Cl1	−179.51 (11)	C1—N1—C7—N2	−176.27 (13)
C3—C4—C5—C6	−0.2 (2)	C7—N3—C8—C9	−0.6 (2)
Cl1—C4—C5—C6	179.93 (11)	N3—C8—C9—C10	0.8 (2)
C4—C5—C6—C1	−0.4 (2)	C7—N2—C10—C9	−0.7 (2)
C2—C1—C6—C5	0.5 (2)	C8—C9—C10—N2	−0.1 (2)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···N2^{i}	0.85 (2)	2.18 (2)	3.028 (2)	174 (2)

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

Fig. 1