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

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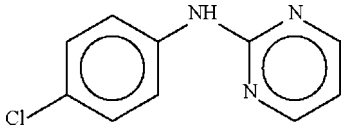
Key indicators: single-crystal X-ray study; $T$ = 100 K; mean $\sigma$(C–C) = 0.002 Å; $R$ factor = 0.031; $wR$ factor = 0.080; data-to-parameter ratio = 15.5.

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
$\alpha$ = 89.237 (1)°
$\beta$ = 89.037 (1)°
$\gamma$ = 89.399 (2)°
$V$ = 455.98 (2) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 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).

We thank the University of Malaya for supporting this study (PS077/2007 C).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: TK2341).

## References

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# supporting information

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

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

**A. Bakar Maizathul Akmam, Zanariah Abdullah and Seik Weng Ng**

### S1. 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.

### 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) 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.

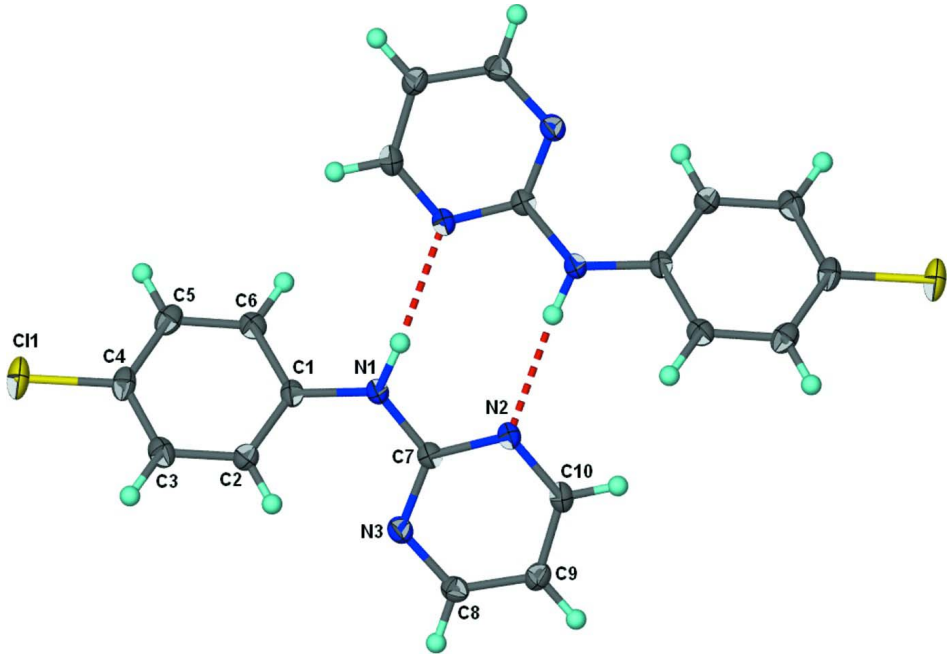


**Figure 1**

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*

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

*Data collection*

Bruker SMART APEX diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega$ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.880$, $T_{max} = 0.982$
3625 measured reflections
2032 independent reflections
1757 reflections with $I > 2\sigma(I)$
$R_{int} = 0.014$
$\theta_{max} = 27.5°$, $\theta_{min} = 2.0°$
$h = -4\rightarrow4$
$k = -13\rightarrow13$
$l = -14\rightarrow15$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.031$
$wR(F^2) = 0.080$
$S = 1.02$
2032 reflections
131 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
$w = 1/[\sigma^2(F_o^2) + (0.0319P)^2 + 0.3201P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.34$ e Å$^{-3}$
$\Delta\rho_{min} = -0.24$ e Å$^{-3}$

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

| | *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 (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| 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, º)*

| | | | |
|---|---|---|---|
| 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, º)*

| *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.