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# 5-Chloropyrimidin-2-amine

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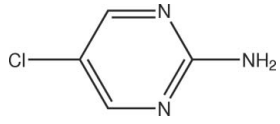
Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(C–C) = 0.002 Å; $R$ factor = 0.033; $wR$ factor = 0.116; data-to-parameter ratio = 12.1.

The complete molecule of the title compound, $C_4H_3ClN_3$, is generated by crystallographic mirror symmetry, with the Cl atom, one N atom and two C atoms lying on the reflecting plane. In the crystal structure, intermolecular N—H···N hydrogen bonds link the molecules into chains propagating in [100].

## Related literature

For general background, see: Hannouta & Johnson (1982). For bond-length data, see: Allen *et al.* (1987).




## Experimental

### Crystal data

$C_4H_4ClN_3$
$M_r$ = 129.55
Orthorhombic, *Cmca*
$a$ = 7.6380 (15) Å
$b$ = 8.2240 (16) Å
$c$ = 17.100 (3) Å
$V$ = 1074.1 (4) Å$^3$
$Z$ = 8
Mo $K\alpha$ radiation
$\mu$ = 0.59 mm$^{-1}$
$T$ = 293 K
0.30 × 0.20 × 0.10 mm

### Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: $\psi$ scan (North *et al.*, 1968)
$T_{min}$ = 0.844, $T_{max}$ = 0.944
1047 measured reflections
534 independent reflections
462 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.020
3 standard reflections
every 200 reflections
intensity decay: 1%

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.116
$S$ = 0.92
534 reflections
44 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.20 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.22 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N2—H2$A$···N1$^{i}$ | 0.90 | 2.22 | 3.087 (2) | 161 |

Symmetry code: (i) $-x+\frac{3}{2}, -y-\frac{1}{2}, -z+1$.

Data collection: *CAD-4 EXPRESS* (Enraf–Nonius, 1994); cell refinement: *CAD-4 EXPRESS*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *PLATON* (Spek, 2009).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB5158).

## References

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# supporting information

*Acta Cryst.* (2009). E**65**, o2863 [https://doi.org/10.1107/S1600536809043645]

## 5-Chloropyrimidin-2-amine

**Bin Wang, Ran-Zhe Lu, Lu-Na Han, Wen-Bin Wei and Hai-Bo Wang**

### S1. Experimental

Guanidine (20 g) and 2-chloromalonaldehyde (16 g) were added to concentrated $H_2SO_4$ (50g) with cooling; the mixture was allowed to stand for two hours at room temperature, the product poured into ice water, neutralized with $NH_4OH$, the precipitated filtered, made strongly alkaline with $NH_4OH$, and the precipitate was recrystallized from alcohol or sublimed to give the title compound. Colourless blocks of (I) were obtained by slow evaporation of an methanol solution.

### S2. Refinement

H atoms were positioned geometrically (N—H = 0.86 Å, C—H = 0.93–0.98Å) and refined as riding with $U_{iso}$(H) = 1.2$U_{eq}$(C,N) or 1.5$U_{eq}$(methyl C).

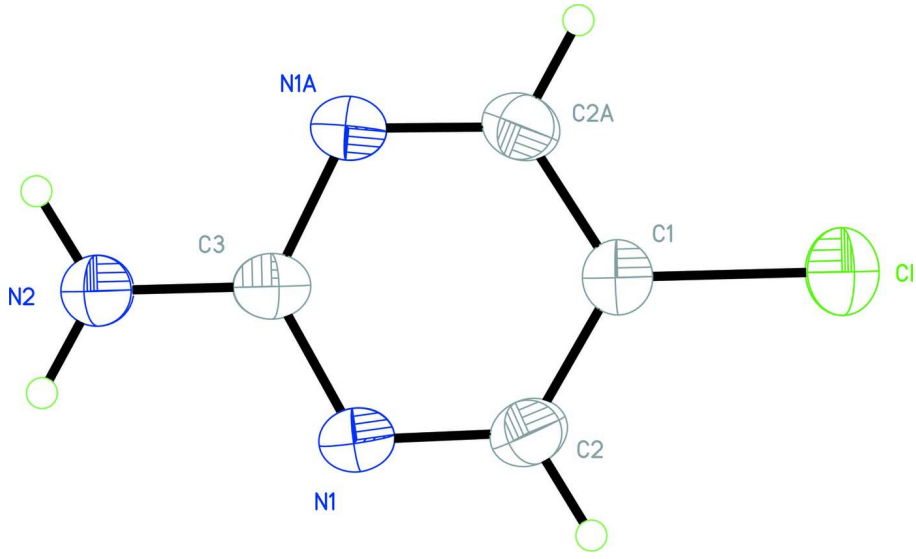


**Figure 1**

The molecular structure of (I) showing 50% displacement ellipsoids.

### 5-Chloropyrimidin-2-amine

*Crystal data*

$C_4H_4ClN_3$
$M_r$ = 129.55
Orthorhombic, *Cmca*
Hall symbol: -C 2bc 2
*a* = 7.6380 (15) Å
*b* = 8.2240 (16) Å
*c* = 17.100 (3) Å
*V* = 1074.1 (4) Å$^3$
*Z* = 8
*F*(000) = 528
$D_x$ = 1.602 Mg m$^{-3}$
Melting point: 506 K
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 25 reflections

$\theta$ = 10–13°
$\mu$ = 0.59 mm$^{-1}$
$T$ = 293 K

Block, colourless
0.30 × 0.20 × 0.10 mm

*Data collection*

Enraf–Nonius CAD-4 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega/2\theta$ scans
Absorption correction: $\psi$ scan (North *et al.*, 1968)
$T_{min}$ = 0.844, $T_{max}$ = 0.944
1047 measured reflections

534 independent reflections
462 reflections with $I > 2^{\sim}I$)
$R_{int}$ = 0.020
$\theta_{max}$ = 25.3°, $\theta_{min}$ = 2.4°
$h$ = 0→9
$k$ = 0→9
$l$ = −20→20
3 standard reflections every 200 reflections
intensity decay: 1%

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.116
$S$ = 0.92
534 reflections
44 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-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1P)^2 + 0.2P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.20 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.22 e Å$^{-3}$
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.025 (4)

*Special details*

**Geometry**. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

**Refinement**. Refinement of $F^2$ against ALL reflections. The weighted R-factor wR and goodness of fit S are based on $F^2$, conventional R-factors R are based on F, with F set to zero for negative $F^2$. The threshold expression of $F^2 > 2$sigma($F^2$) is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on $F^2$ are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

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

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Cl | 0.5000 | 0.22728 (9) | 0.27440 (4) | 0.0527 (4) |
| N1 | 0.65713 (16) | −0.11849 (18) | 0.41923 (8) | 0.0360 (5) |
| C3 | 0.5000 | −0.1761 (3) | 0.44284 (14) | 0.0319 (6) |
| N2 | 0.5000 | −0.3014 (3) | 0.49308 (15) | 0.0432 (7) |
| H2A | 0.6021 | −0.3434 | 0.5099 | 0.052* |
| C2 | 0.6542 (2) | 0.0027 (2) | 0.36821 (10) | 0.0364 (5) |
| H2C | 0.7598 | 0.0457 | 0.3507 | 0.044* |
| C1 | 0.5000 | 0.0674 (3) | 0.34019 (13) | 0.0347 (6) |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Cl | 0.0488 (6) | 0.0514 (6) | 0.0580 (6) | 0.000 | 0.000 | 0.0225 (3) |
| N1 | 0.0258 (9) | 0.0398 (9) | 0.0424 (9) | −0.0007 (6) | 0.0004 (5) | 0.0045 (6) |
| C3 | 0.0278 (12) | 0.0325 (13) | 0.0354 (12) | 0.000 | 0.000 | −0.0039 (11) |
| N2 | 0.0288 (11) | 0.0450 (13) | 0.0559 (14) | 0.000 | 0.000 | 0.0179 (11) |
| C2 | 0.0296 (10) | 0.0379 (10) | 0.0418 (9) | −0.0033 (7) | 0.0032 (7) | 0.0013 (7) |
| C1 | 0.0353 (13) | 0.0328 (13) | 0.0359 (13) | 0.000 | 0.000 | 0.0026 (10) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Cl—C1 | 1.730 (2) | N2—H2A | 0.9000 |
| N1—C2 | 1.325 (2) | C2—C1 | 1.378 (2) |
| N1—C3 | 1.3519 (18) | C2—H2C | 0.9300 |
| C3—N2 | 1.341 (4) | C1—C2$^{i}$ | 1.378 (2) |
| C3—N1$^{i}$ | 1.3519 (18) | | |
| | | | |
| C2—N1—C3 | 116.44 (14) | N1—C2—H2C | 118.9 |
| N2—C3—N1$^{i}$ | 117.41 (11) | C1—C2—H2C | 118.9 |
| N2—C3—N1 | 117.41 (11) | C2—C1—C2$^{i}$ | 117.4 (2) |
| N1$^{i}$—C3—N1 | 125.2 (2) | C2—C1—Cl | 121.28 (11) |
| C3—N2—H2A | 120.0 | C2$^{i}$—C1—Cl | 121.28 (11) |
| N1—C2—C1 | 122.25 (15) | | |
| | | | |
| C2—N1—C3—N2 | 178.5 (2) | N1—C2—C1—C2$^{i}$ | 1.0 (4) |
| C2—N1—C3—N1$^{i}$ | −0.8 (4) | N1—C2—C1—Cl | 179.28 (14) |
| C3—N1—C2—C1 | −0.1 (3) | | |

Symmetry code: (i) −*x*+1, *y*, *z*.

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N2—H2*A*···N1$^{ii}$ | 0.90 | 2.22 | 3.087 (2) | 161 |

Symmetry code: (ii) −*x*+3/2, −*y*−1/2, −*z*+1.