Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

5-Chloropyrimidin-2-amine

Bin Wang,[a,b] Ran-Zhe Lu,[a,b] Lu-Na Han,[a,b] Wen-Bin Wei[a,b] and Hai-Bo Wang[a]*

[a]College of Food Science and Light Industry, Nanjing University of Technology, Xinmofan Road No. 5 Nanjing, Nanjing 210009, People's Republic of China, and [b]College of Science, Nanjing University of Technology, Xinmofan Road No. 5 Nanjing, Nanjing 210009, People's Republic of China
Correspondence e-mail: wanghaibo@njut.edu.cn

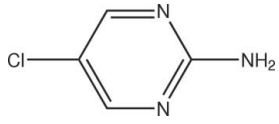
Received 19 October 2009; accepted 22 October 2009

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(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
μ = 0.59 mm^{-1}
T = 293 K
0.30 × 0.20 × 0.10 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: ψ 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—H2A···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

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
Enraf–Nonius (1994). *CAD-4 EXPRESS*. Enraf–Nonius, Delft, The Netherlands.
Hannouta, I. B. & Johnson, A. (1982). *Dyes Pigments*, **3**, 173–182.
Harms, K. & Wocadlo, S. (1995). *XCAD4*. University of Marburg, Germany.
North, A. C. T., Phillips, D. C. & Mathews, F. S. (1968). *Acta Cryst.* A**24**, 351–359.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.

supplementary materials

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

5-Chloropyrimidin-2-amine

B. Wang, R.-Z. Lu, L.-N. Han, W.-B. Wei and H.-B. Wang

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.

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) = 1.2U_{eq}(C,N) or 1.5U_{eq}(methyl C).

Figures

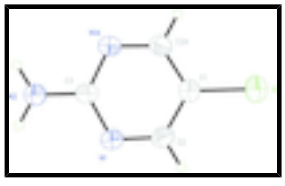


Fig. 1. The molecular structure of (I) showing 50% displacement ellipsoids.

5-Chloropyrimidin-2-amine

Crystal data

$C_4H_4ClN_3$	D_x = 1.602 Mg m^{-3}
M_r = 129.55	Melting point: 506 K
Orthorhombic, *Cmca*	Mo *K*α radiation, λ = 0.71073 Å
Hall symbol: -C 2bc 2	Cell parameters from 25 reflections
a = 7.6380 (15) Å	θ = 10–13°
b = 8.2240 (16) Å	μ = 0.59 mm^{-1}
c = 17.100 (3) Å	*T* = 293 K
V = 1074.1 (4) Å^3	Block, colourless
Z = 8	0.30 × 0.20 × 0.10 mm
F(000) = 528	

Data collection

Enraf–Nonius CAD-4 diffractometer	462 reflections with $I > 2^{-}I$)

Radiation source: fine-focus sealed tube	$R_{int} = 0.020$
graphite	$\theta_{max} = 25.3°$, $\theta_{min} = 2.4°$
ω/2θ scans	$h = 0 \rightarrow 9$
Absorption correction: ψ scan (North *et al.*, 1968)	$k = 0 \rightarrow 9$
$T_{min} = 0.844$, $T_{max} = 0.944$	$l = -20 \rightarrow 20$
1047 measured reflections	3 standard reflections every 200 reflections
534 independent reflections	intensity decay: 1%

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.033$	H-atom parameters constrained
$wR(F^2) = 0.116$	$w = 1/[\sigma^2(F_o^2) + (0.1P)^2 + 0.2P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.92$	$(\Delta/\sigma)_{max} < 0.001$
534 reflections	$\Delta\rho_{max} = 0.20$ e Å^{-3}
44 parameters	$\Delta\rho_{min} = -0.22$ e Å^{-3}
0 restraints	Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	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 (Å^2)

	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, °)

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 codes: (i) −*x*+1, *y*, *z*.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2A···N1^{ii}	0.90	2.22	3.087 (2)	161

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

Fig. 1