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2,4-Dichloropyrimidine

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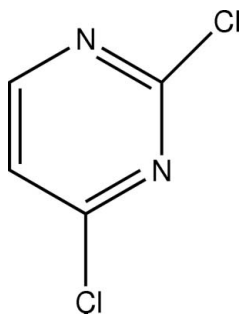
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Key indicators: single-crystal X-ray study; $T = 294$ K; mean $\sigma(\text{C}-\text{C}) = 0.008$ Å; R factor = 0.069; wR factor = 0.180; data-to-parameter ratio = 15.6.

The molecule of the title compound, $\text{C}_4\text{H}_2\text{Cl}_2\text{N}_2$, is almost planar [maximum deviation = 0.013 (3) Å for a Cl atom]. In the crystal structure, intermolecular $\text{C}-\text{H}\cdots\text{N}$ interactions link the molecules into chains.

Related literature

For a related structure, see: Bhasin *et al.* (2009). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$\text{C}_4\text{H}_2\text{Cl}_2\text{N}_2$
 $M_r = 148.98$
Monoclinic, $P2_1/c$
 $a = 7.5090$ (15) Å

$b = 10.776$ (2) Å
 $c = 7.1980$ (14) Å
 $\beta = 92.92$ (3)°
 $V = 581.7$ (2) Å³

$Z = 4$
Mo $K\alpha$ radiation
 $\mu = 0.99$ mm⁻¹

$T = 294$ K
 $0.30 \times 0.20 \times 0.20$ mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: ψ scan (North *et al.*, 1968)
 $T_{\min} = 0.755$, $T_{\max} = 0.826$
1223 measured reflections

1139 independent reflections
733 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.084$
3 standard reflections
frequency: 120 min
intensity decay: 1%

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.069$
 $wR(F^2) = 0.180$
 $S = 1.01$
1139 reflections

73 parameters
H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.39$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.32$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{C}1-\text{H}1\text{B}\cdots\text{N}2^i$	0.93	2.62	3.548 (7)	174

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

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; 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: *ORTEP-3 for Windows* (Farrugia, 1997) and *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HK2698).

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supplementary materials

Acta Cryst. (2009). E65, o1438 [doi:10.1107/S1600536809019667]

2,4-Dichloropyrimidine

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Comment

Some derivatives of pyrimidine are important chemical materials. We report herein the crystal structure of the title compound.

In the molecule of the title compound (Fig 1), the bond lengths (Allen *et al.*, 1987) and angles are within normal ranges. Ring A (N1/N2/C1-C4) is, of course, planar. Atoms C11 and C12 are 0.012 (3) and 0.013 (3) Å away from the ring plane, respectively. So, the molecule is planar.

In the crystal structure, intermolecular C-H...N interactions (Table 1) link the molecules into chains (Fig. 2), in which they may be effective in the stabilization of the structure.

Experimental

For the preparation of the title compound, uracil (100 g, 0.82 mol) was dissolved in phosphorous oxychloride (400 ml) in a two-necked round-bottom flask (500 ml) equipped with a condenser. The solution was refluxed with stirring for 3.5 h at 383 K. The residual phosphorous oxychloride was removed in vacuo at 323 K, and the remaining oil was poured into ice (50 g) followed by extraction with chloroform (3 × 50 ml). The combined organic extract was washed with dilute sodium carbonate solution and dried over anhydrous sodium sulfate. The title compound was obtained by evaporation of solvent (Bhasin *et al.*, 2009). Crystals suitable for X-ray analysis were obtained by slow evaporation of a methanol solution.

Refinement

H atoms were positioned geometrically, with C-H = 0.93 Å for aromatic H and constrained to ride on their parent atoms, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

Figures

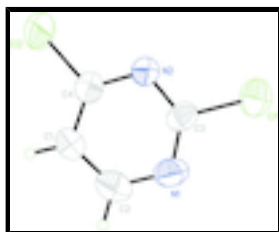


Fig. 1. The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids at the 30% probability level.

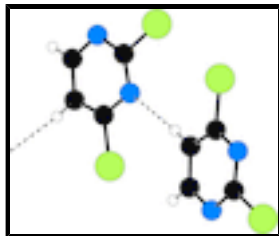


Fig. 2. A partial packing diagram of the title compound. Hydrogen bonds are shown as dashed lines.

2,4-Dichloropyrimidine

Crystal data

$C_4H_2Cl_2N_2$

$M_r = 148.98$

Monoclinic, $P2_1/c$

Hall symbol: -P 2ybc

$a = 7.5090$ (15) Å

$b = 10.776$ (2) Å

$c = 7.1980$ (14) Å

$\beta = 92.92$ (3)°

$V = 581.7$ (2) Å³

$Z = 4$

$F_{000} = 296$

$D_x = 1.701$ Mg m⁻³

Mo $K\alpha$ radiation

$\lambda = 0.71073$ Å

Cell parameters from 25 reflections

$\theta = 10\text{--}13^\circ$

$\mu = 0.99$ mm⁻¹

$T = 294$ K

Block, colorless

$0.30 \times 0.20 \times 0.20$ mm

Data collection

Enraf-Nonius CAD-4
diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 294$ K

$\omega/2\theta$ scans

Absorption correction: ψ scan
(North *et al.*, 1968)

$T_{\min} = 0.755$, $T_{\max} = 0.826$

1223 measured reflections

1139 independent reflections

733 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.084$

$\theta_{\max} = 26.0^\circ$

$\theta_{\min} = 2.7^\circ$

$h = -9 \rightarrow 0$

$k = 0 \rightarrow 13$

$l = -8 \rightarrow 8$

3 standard reflections

every 120 min

intensity decay: 1%

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.069$

$wR(F^2) = 0.180$

$S = 1.01$

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.07P)^2 + 1.45P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} < 0.001$

1139 reflections $\Delta\rho_{\max} = 0.39 \text{ e \AA}^{-3}$
 73 parameters $\Delta\rho_{\min} = -0.32 \text{ e \AA}^{-3}$
 Primary atom site location: structure-invariant direct methods Extinction correction: none

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.

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 $F^2 > \sigma(F^2)$ 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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Cl1	0.5768 (2)	0.63809 (14)	0.0975 (2)	0.0762 (6)
Cl2	1.1679 (2)	0.83010 (16)	0.3510 (3)	0.0862 (7)
N1	0.6273 (6)	0.8744 (4)	0.0912 (7)	0.0612 (12)
N2	0.8628 (5)	0.7492 (4)	0.2211 (6)	0.0555 (11)
C1	0.8975 (7)	0.9681 (5)	0.2072 (8)	0.0652 (15)
H1B	0.9665	1.0384	0.2321	0.078*
C2	0.7272 (8)	0.9751 (5)	0.1252 (9)	0.0689 (16)
H2B	0.6808	1.0526	0.0927	0.083*
C3	0.7027 (6)	0.7699 (5)	0.1403 (7)	0.0485 (12)
C4	0.9577 (7)	0.8520 (5)	0.2490 (8)	0.0562 (14)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0693 (9)	0.0670 (10)	0.0897 (12)	-0.0184 (7)	-0.0222 (8)	-0.0065 (8)
Cl2	0.0581 (9)	0.0731 (11)	0.1233 (15)	-0.0074 (7)	-0.0370 (9)	-0.0038 (10)
N1	0.055 (3)	0.059 (3)	0.068 (3)	0.013 (2)	-0.009 (2)	0.002 (2)
N2	0.052 (2)	0.042 (2)	0.071 (3)	-0.0014 (18)	-0.017 (2)	-0.002 (2)
C1	0.070 (4)	0.042 (3)	0.081 (4)	0.000 (2)	-0.013 (3)	-0.007 (3)
C2	0.079 (4)	0.047 (3)	0.081 (4)	0.006 (3)	0.000 (3)	0.007 (3)
C3	0.045 (2)	0.056 (3)	0.044 (3)	0.005 (2)	-0.006 (2)	-0.007 (2)
C4	0.051 (3)	0.052 (3)	0.064 (3)	-0.002 (2)	-0.008 (3)	-0.005 (3)

Geometric parameters (\AA , $^\circ$)

Cl1—C3	1.725 (5)	N2—C4	1.327 (6)
Cl2—C4	1.723 (5)	C1—C2	1.383 (8)
N1—C2	1.334 (7)	C1—C4	1.358 (7)

supplementary materials

N1—C3	1.302 (6)	C1—H1B	0.9300
N2—C3	1.327 (6)	C2—H2B	0.9300
C3—N1—C2	114.9 (5)	C1—C2—H2B	118.9
C4—N2—C3	113.2 (4)	N1—C3—N2	129.5 (5)
C4—C1—C2	115.8 (5)	N1—C3—C11	115.9 (4)
C4—C1—H1B	122.1	N2—C3—C11	114.6 (4)
C2—C1—H1B	122.1	N2—C4—C1	124.4 (5)
N1—C2—C1	122.2 (5)	N2—C4—C12	115.0 (4)
N1—C2—H2B	118.9	C1—C4—C12	120.5 (4)
C3—N1—C2—C1	-0.2 (9)	C4—N2—C3—C11	178.8 (4)
C4—C1—C2—N1	0.7 (10)	C3—N2—C4—C1	2.5 (9)
C2—N1—C3—N2	1.0 (9)	C3—N2—C4—C12	-179.2 (4)
C2—N1—C3—C11	-179.9 (4)	C2—C1—C4—N2	-2.0 (10)
C4—N2—C3—N1	-2.0 (9)	C2—C1—C4—C12	179.8 (5)

Hydrogen-bond geometry (Å, °)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
C1—H1B \cdots N2 ⁱ	0.93	2.62	3.548 (7)	174

Symmetry codes: (i) $-x+2, y+1/2, -z+1/2$.

Fig. 1

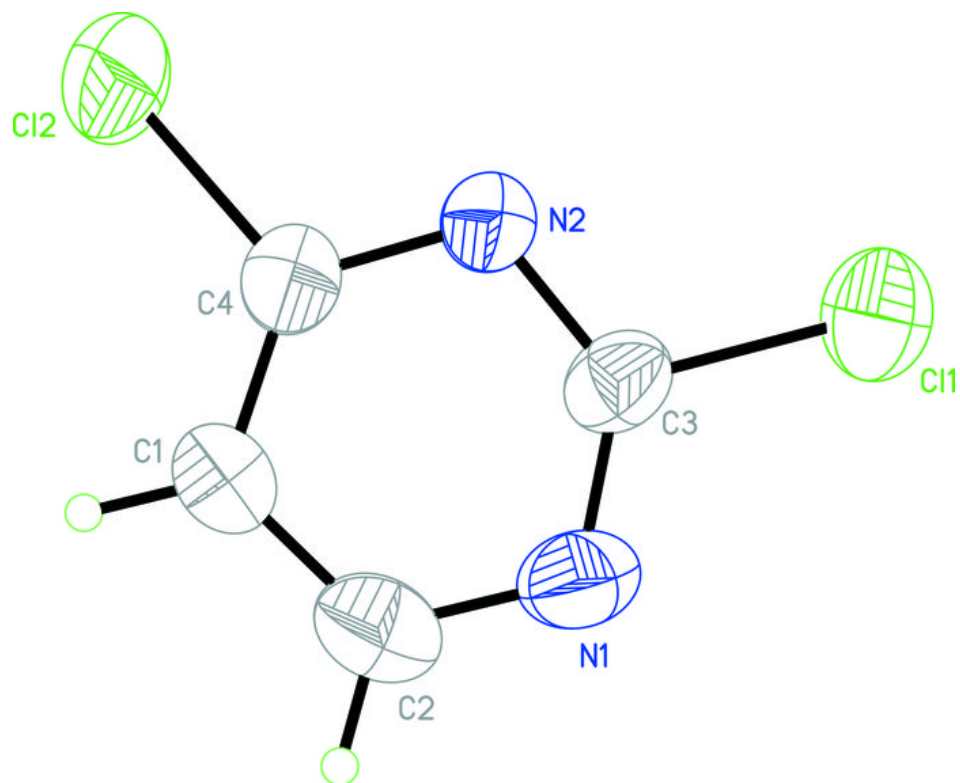


Fig. 2

