



Crystal structure of 4,6-dichloro-5-methylpyrimidine

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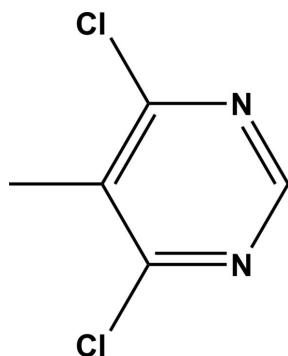
The title compound, C₅H₄Cl₂N₂, is essentially planar with an r.m.s. deviation for all non-H atoms of 0.009 Å. The largest deviation from the mean plane is 0.016 (4) Å for an N atom. In the crystal, molecules are linked by pairs of C—H...N hydrogen bonds, forming inversion dimers, enclosing an R₂²(6) ring motif.

Keywords: crystal structure; pyrimidine; inversion dimers; C—H...N hydrogen bonding.

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1. Related literature

For the applications of pyrimidine derivatives as pesticides and pharmaceutical agents, see: Condon *et al.* (1993); as agrochemicals, see: Maeno *et al.* (1990); as antiviral agents, see: Gilchrist (1997); as herbicides, see: Selby *et al.* (2002); Zhu *et al.* (2007); and for applications of organoselenide compounds, see: Ip *et al.* (1997). For the crystal structure of 5-methylpyrimidine, see: Furberg *et al.* (1979).



2. Experimental

2.1. Crystal data

C ₅ H ₄ Cl ₂ N ₂	<i>V</i> = 687.6 (7) Å ³
<i>M_r</i> = 163.00	<i>Z</i> = 4
Monoclinic, <i>P</i> 2 ₁ / <i>n</i>	Mo <i>K</i> α radiation
<i>a</i> = 7.463 (5) Å	<i>μ</i> = 0.85 mm ⁻¹
<i>b</i> = 7.827 (5) Å	<i>T</i> = 293 K
<i>c</i> = 11.790 (5) Å	0.11 × 0.10 × 0.08 mm
<i>β</i> = 93.233 (5)°	

2.2. Data collection

Oxford Diffraction Xcalibur, Eos diffractometer	2347 measured reflections
Absorption correction: multi-scan (<i>CrysAlis PRO</i> ; Oxford Diffraction, 2013)	1228 independent reflections
<i>T</i> _{min} = 0.922, <i>T</i> _{max} = 0.934	791 reflections with <i>I</i> > 2σ(<i>I</i>)
	<i>R</i> _{int} = 0.099

2.3. Refinement

<i>R</i> [<i>F</i> ² > 2σ(<i>F</i> ²)] = 0.068	83 parameters
<i>wR</i> (<i>F</i> ²) = 0.173	H-atom parameters constrained
<i>S</i> = 1.01	Δρ _{max} = 0.39 e Å ⁻³
1228 reflections	Δρ _{min} = -0.38 e Å ⁻³

Table 1

Hydrogen-bond geometry (Å, °).

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
C2—H2...N3 ⁱ	0.93	2.66	3.468 (6)	146

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

Data collection: *CrysAlis PRO* (Oxford Diffraction, 2013); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL2014/6* (Sheldrick, 2015); molecular graphics: *PLATON* (Spek, 2009) and *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *SHELXL2014/6* and *PLATON*.

Acknowledgements

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Supporting information for this paper is available from the IUCr electronic archives (Reference: SU5261).

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supporting information

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Crystal structure of 4,6-dichloro-5-methylpyrimidine

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S1. Comments

Pyrimidines have interesting biological properties with applications as pesticides, pharmaceutical agents (Condon *et al.*, 1993; Maeno *et al.*, 1990) and are also interesting from a biochemical point of view and applications of organoselenide compounds (Ip *et al.*, 1997). Pyrimidine derivatives have been developed as antiviral agents, such as AZT, which is the anti-AIDS drug most widely used (Gilchrist, 1997). Recently, a new series of highly substituted pyrimidine herbicides have been reported (Selby *et al.*, 2002; Zhu *et al.*, 2007). In the present study, we were interested in examining a derivative of pyrimidine with a methyl substituent surrounded by two chlorine atoms.

The molecular structure of the title compound is shown in Fig. 1. The molecule is planar, as is typical in benzenes substituted by halogen atoms and methyl groups, with an r.m.s. deviation for all non-H atoms of 0.009 Å. The largest deviation from the mean plane is 0.016 (4) Å for atom N3. The bond distances and bond angles in the molecule are similar to those reported for 5-methylpyrimidine (Furberg *et al.*, 1979).

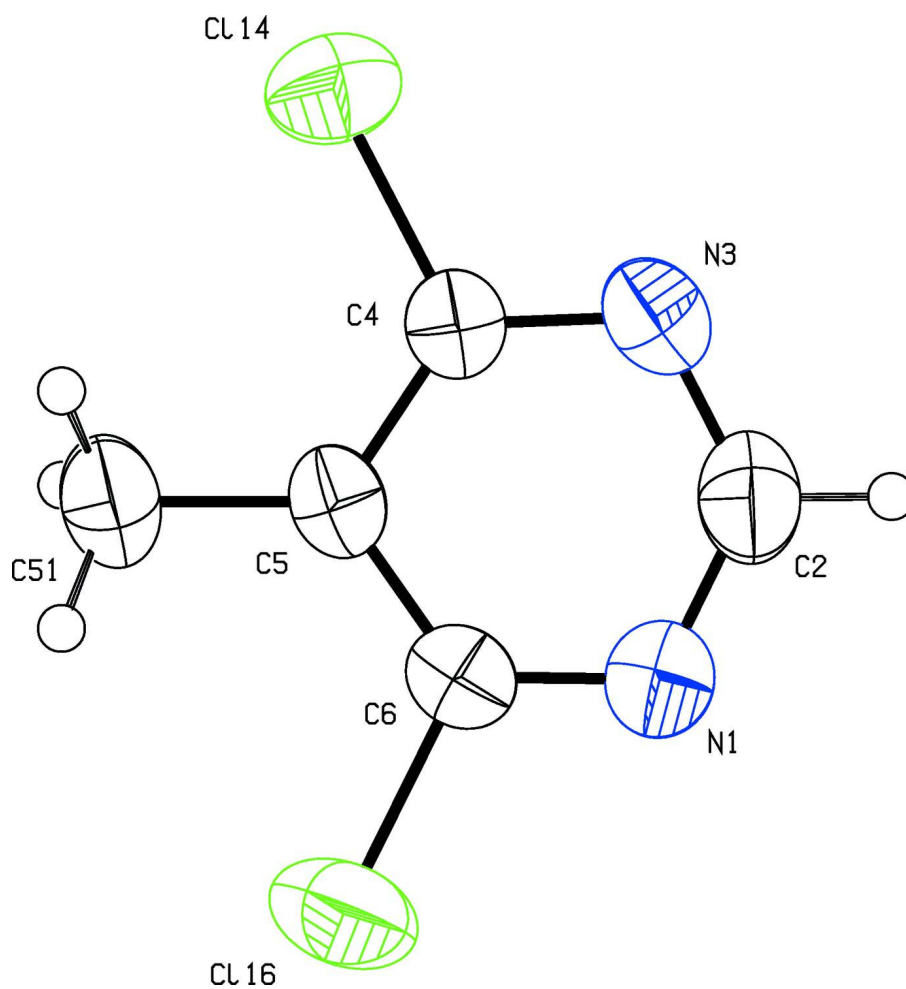
In the crystal, molecules are linked by a pair of C—H $\cdots$ N hydrogen bonds forming inversion dimers (Table 1 and Fig. 2), enclosing an R²₂(6) ring motif.

S2. Synthesis and crystallization

The commercially available title compound (Sigma-Aldrich) was recrystallized from ethanol giving colourless prismatic crystals.

S3. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. All H atoms were localized in a difference Fourier map but introduced in calculated positions and treated as riding: C—H = 0.93–0.96 Å with $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C-methyl})$ and $1.2U_{\text{eq}}(\text{C})$ for other H atoms.

**Figure 1**

The molecular structure of the title compound, with atom labelling. Displacement ellipsoids drawn at the 50% probability level.

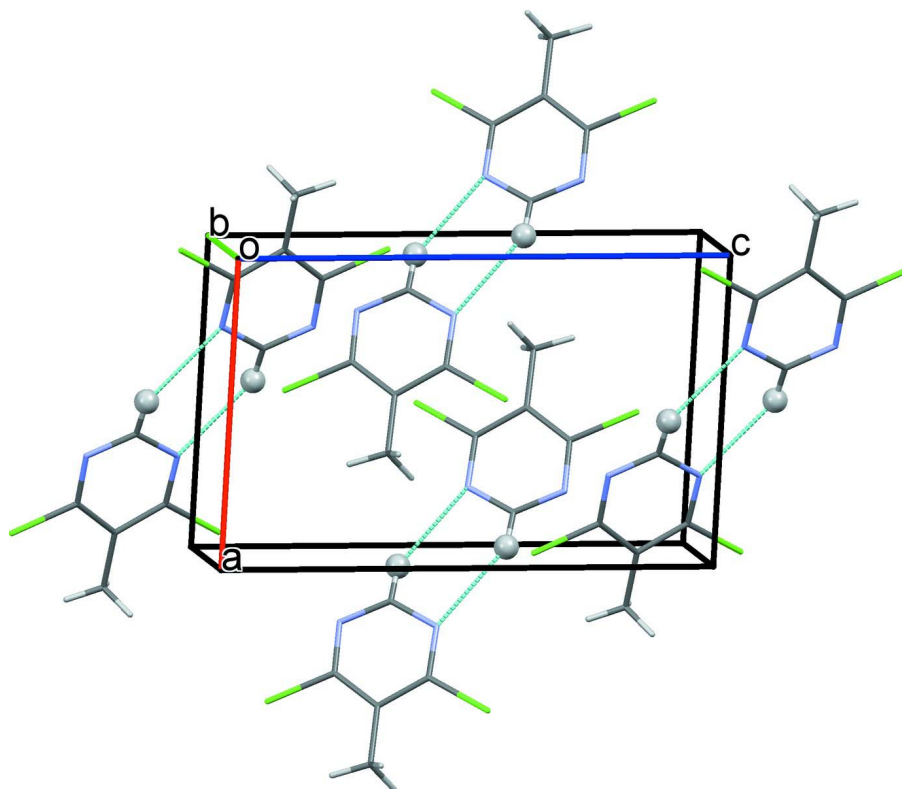


Figure 2

The crystal packing of the title compound, viewed along the *b* axis. Hydrogen bonds are shown as dashed lines (see Table 1).

4,6-Dichloro-5-methylpyrimidine

Crystal data

$C_5H_4Cl_2N_2$

$M_r = 163.00$

Monoclinic, $P2_1/n$

$a = 7.463 (5) \text{ \AA}$

$b = 7.827 (5) \text{ \AA}$

$c = 11.790 (5) \text{ \AA}$

$\beta = 93.233 (5)^\circ$

$V = 687.6 (7) \text{ \AA}^3$

$Z = 4$

$F(000) = 328$

$D_x = 1.575 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$

Cell parameters from 776 reflections

$\theta = 4.2\text{--}27.8^\circ$

$\mu = 0.85 \text{ mm}^{-1}$

$T = 293 \text{ K}$

Prism, colourless

$0.11 \times 0.10 \times 0.08 \text{ mm}$

Data collection

Oxford Diffraction Xcalibur, Eos
diffractometer

Radiation source: Enhance (Mo) X-ray Source
Graphite monochromator

CCD rotation images, thin slices ω scans

Absorption correction: multi-scan

(*CrysAlis PRO*; Oxford Diffraction, 2013)

$T_{\min} = 0.922$, $T_{\max} = 0.934$

2347 measured reflections

1228 independent reflections

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

$R_{\text{int}} = 0.099$

$\theta_{\max} = 25.2^\circ$, $\theta_{\min} = 3.1^\circ$

$h = -8 \rightarrow 8$

$k = -9 \rightarrow 4$

$l = -14 \rightarrow 10$

*Refinement*Refinement on F^2

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.068$ $wR(F^2) = 0.173$ $S = 1.01$

1228 reflections

83 parameters

0 restraints

Primary atom site location: structure-invariant
direct methodsSecondary atom site location: difference Fourier
mapHydrogen site location: inferred from
neighbouring sites

H-atom parameters constrained

 $w = 1/[\sigma^2(F_o^2) + (0.0729P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$ $(\Delta/\sigma)_{\max} < 0.001$ $\Delta\rho_{\max} = 0.39 \text{ e } \text{\AA}^{-3}$ $\Delta\rho_{\min} = -0.38 \text{ e } \text{\AA}^{-3}$ *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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($\text{\AA}^2$)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Cl14	0.47393 (16)	0.21816 (17)	0.57181 (8)	0.0686 (5)
Cl16	0.45631 (17)	0.4430 (2)	0.13763 (9)	0.0853 (6)
N1	0.2066 (5)	0.4832 (6)	0.2775 (3)	0.0604 (11)
N3	0.2153 (5)	0.3882 (5)	0.4695 (3)	0.0579 (10)
C2	0.1383 (6)	0.4657 (7)	0.3784 (4)	0.0661 (14)
H2	0.0251	0.5123	0.3865	0.079*
C4	0.3744 (5)	0.3225 (5)	0.4544 (3)	0.0458 (10)
C5	0.4659 (5)	0.3309 (6)	0.3546 (3)	0.0458 (10)
C6	0.3650 (6)	0.4175 (6)	0.2685 (3)	0.0514 (11)
C51	0.6464 (6)	0.2553 (7)	0.3426 (4)	0.0666 (14)
H51A	0.7041	0.3121	0.2823	0.100*
H51B	0.6344	0.1359	0.3252	0.100*
H51C	0.7175	0.2692	0.4124	0.100*

Atomic displacement parameters ($\text{\AA}^2$)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl14	0.0846 (9)	0.0601 (9)	0.0604 (6)	−0.0009 (7)	−0.0019 (6)	0.0089 (5)
Cl16	0.0934 (11)	0.1053 (14)	0.0592 (7)	−0.0109 (9)	0.0219 (6)	0.0116 (6)
N1	0.057 (2)	0.061 (3)	0.063 (2)	0.005 (2)	0.0033 (16)	0.0012 (19)
N3	0.057 (2)	0.057 (3)	0.0602 (19)	0.000 (2)	0.0160 (15)	−0.0040 (17)
C2	0.050 (2)	0.074 (4)	0.075 (3)	0.008 (3)	0.005 (2)	−0.008 (3)
C4	0.045 (2)	0.039 (3)	0.0537 (19)	−0.003 (2)	0.0041 (16)	−0.0034 (18)
C5	0.042 (2)	0.039 (3)	0.057 (2)	−0.005 (2)	0.0089 (16)	−0.0056 (17)
C6	0.054 (2)	0.053 (3)	0.0475 (18)	−0.004 (2)	0.0070 (16)	−0.0023 (18)
C51	0.051 (3)	0.070 (4)	0.081 (3)	0.007 (3)	0.016 (2)	−0.002 (2)

Geometric parameters (Å, °)

Cl14—C4	1.737 (4)	C4—C5	1.395 (5)
Cl16—C6	1.733 (4)	C5—C6	1.403 (6)
N1—C6	1.299 (6)	C5—C51	1.486 (6)
N1—C2	1.327 (5)	C51—H51A	0.9600
N3—C4	1.315 (5)	C51—H51B	0.9600
N3—C2	1.335 (5)	C51—H51C	0.9600
C2—H2	0.9300		
C6—N1—C2	115.4 (3)	C6—C5—C51	125.2 (4)
C4—N3—C2	114.8 (3)	N1—C6—C5	125.9 (3)
N1—C2—N3	126.8 (4)	N1—C6—Cl16	115.6 (3)
N1—C2—H2	116.6	C5—C6—Cl16	118.5 (3)
N3—C2—H2	116.6	C5—C51—H51A	109.5
N3—C4—C5	125.7 (4)	C5—C51—H51B	109.5
N3—C4—Cl14	115.1 (3)	H51A—C51—H51B	109.5
C5—C4—Cl14	119.2 (3)	C5—C51—H51C	109.5
C4—C5—C6	111.4 (4)	H51A—C51—H51C	109.5
C4—C5—C51	123.4 (4)	H51B—C51—H51C	109.5
C6—N1—C2—N3	−0.2 (8)	Cl14—C4—C5—C51	−0.2 (6)
C4—N3—C2—N1	−0.7 (8)	C2—N1—C6—C5	0.5 (8)
C2—N3—C4—C5	1.3 (7)	C2—N1—C6—Cl16	−179.0 (4)
C2—N3—C4—Cl14	−178.9 (4)	C4—C5—C6—N1	0.1 (7)
N3—C4—C5—C6	−1.1 (6)	C51—C5—C6—N1	179.5 (5)
Cl14—C4—C5—C6	179.2 (3)	C4—C5—C6—Cl16	179.6 (3)
N3—C4—C5—C51	179.5 (4)	C51—C5—C6—Cl16	−1.0 (7)

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>
C2—H2 $\cdots$ N3 ⁱ	0.93	2.66	3.468 (6)	146

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