Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2-Chloro-5-nitropyrimidine

Jun-Tao Kang, Zhi-Gang Li, Jing-Wei Xu* and Yang Wei

National Analytical Research Center of Electrochemistry and Spectroscopy, Changchun Institute of Applied Chemistry, Chinese Academy of Sciences, Changchun 130022, People's Republic of China
Correspondence e-mail: jwxu@ciac.jl.cn

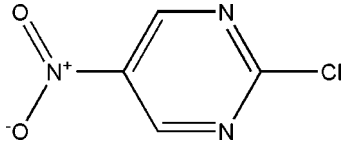
Received 6 November 2007; accepted 13 November 2007

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.029; wR factor = 0.067; data-to-parameter ratio = 12.8.

The crystal structure of the title compound, $C_4H_2ClN_3O_2$, is stabilized by a C—H···O hydrogen bond and a Cl···O halogen bond [Br···O = 3.270 (2) Å]. The molecule is planar.

Related literature

For studies in chemotherapy, see: Roblin *et al.* (1942). For the synthesis of chloropyrimidines, see: Hurst (1984). For related literature, see: Politzer *et al.* (2007).



Experimental

Crystal data

$C_4H_2ClN_3O_2$
M_r = 159.54
Orthorhombic, $Pna2_1$
a = 7.812 (3) Å
b = 13.649 (5) Å
c = 5.711 (2) Å
V = 608.9 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.56 mm^{-1}
T = 293 (2) K
0.34 × 0.29 × 0.15 mm

Data collection

Bruker APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SAINT-Plus*; Bruker, 2003)
T_{min} = 0.833, T_{max} = 0.923
3197 measured reflections
1169 independent reflections
1096 reflections with $I > 2\sigma(I)$
R_{int} = 0.021

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.029
$wR(F^2)$ = 0.067
S = 1.08
1169 reflections
91 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.15 e Å^{-3}
$\Delta\rho_{min}$ = −0.14 e Å^{-3}
Absolute structure: Flack (1983), 502 Friedel pairs
Flack parameter: 0.06 (10)

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

D—H···A	D—H	H···A	D···A	D—H···A
C3—H3···O2^{i}	0.93	2.47	3.390 (3)	174

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

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1998); software used to prepare material for publication: *SHELXTL*.

This work is supported by the National Analytical Research Center of Electrochemistry and Spectroscopy, Changchun Institute of Applied Chemistry, Changchun, China.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LX2031).

References

Bruker (1998). *SMART*, *SAINT* and *SHELXTL*. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2003). *SAINT-Plus*. Version 6. Bruker AXS, Inc., Madison, Wisconsion, USA.
Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
Hurst, D. T. (1984). *Heterocycles*, **22**, 79–84.
Politzer, P., Lane, P., Concha, M. C., Ma, Y. & Murray, J. S. (2007). *J. Mol. Model.* **13**, 305–311.
Roblin, O. R. Jr, Winnek, S. P. & English, J. P. (1942). *J. Am. Chem. Soc.* **64**, 567–570.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.

supplementary materials

Acta Cryst. (2007). E**63**, o4815 [**doi:10.1107/S1600536807058795**]

2-Chloro-5-nitropyrimidine

J.-T. Kang, Z.-G. Li, J.-W. Xu and Y. Wei

Comment

The chloropyrimidine derivatives are important intermediates in the synthesis of sulfur drugs (Roblin*et al.*, 1942). Herein we report the molecular and crystal structure of the title compound, 2-chloro-5-nitropyrimidine (Fig. 1).

The molecular packing (Fig. 2) is stabilized by a C—H···O hydrogen bond (Table 1 and Fig. 2), between a pyrimidine H and the nitro group, *i.e.* C3—H3···O2^{i}. Further stability comes from a weak Cl···O interation of halogen bond (Fig. 2) (Politzer *et al.*, 2007), between the Cl atom and the oxygen of a neighbouring NO_2 group, with a Cl···O2^{ii} distance of 3.270 (2) Å (Symmetry codes as in Fig. 2) and a nearly linear C—Cl···O^{ii} angle of 172.5 (2) °.

Experimental

The title compund is synthesized according to previous reported literature (Hurst, 1984). Single crystals suitable for X-ray diffraction were obtained by slow evaporation of a solution of the title compound in dichloromethane at room temperature.

Refinement

H atoms were placed geometrically and refined with fixed individual displacement parameters [U_{iso}(H) = 1.2U_{eq}(C)], using a riding model, with C—H distances of 0.93 Å.

Figures

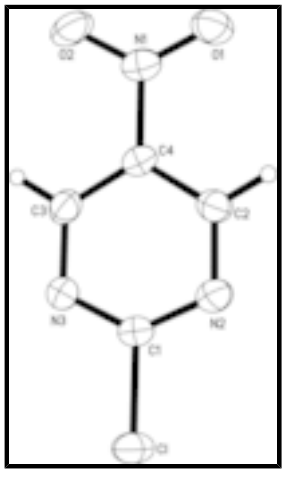


Fig. 1. The molecular structure of the title compound. Showing displacement ellipsoides drawn at the 30% probability level.

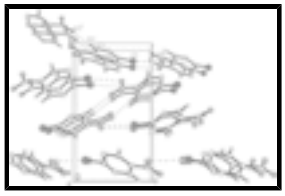


Fig. 2. C—H···O hydrogen bond and Cl···O halogen bond interaction (dotted lines) in the title compound. [Symmetry code: (i) −*x*, −*y* + 2, *z* − 1/2; (ii) *x* + 1, *y*, *z* − 1.]

2-Chloro-5-nitropyrimidine

Crystal data

$C_4H_2ClN_3O_2$	F_{000} = 320
M_r = 159.54	D_x = 1.740 Mg m^{-3}
Orthorhombic, *Pna*2(1)	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: P 2c -2n	Cell parameters from 1404 reflections
a = 7.812 (3) Å	θ = 3.0–25.2º
b = 13.649 (5) Å	μ = 0.56 mm^{-1}
c = 5.711 (2) Å	*T* = 293 (2) K
V = 608.9 (4) Å^3	Block, white
Z = 4	0.34 × 0.29 × 0.15 mm

Data collection

Bruker APEX CCD area detector diffractometer	1169 independent reflections
Radiation source: fine-focus sealed tube	1096 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.021
Detector resolution: 10.0 pixels mm^{-1}	θ_{max} = 26.1º
T = 293(2) K	θ_{min} = 3.0º
φ and ω scans	*h* = −5→9
Absorption correction: multi-scan (SAINT-Plus; Bruker, 2003)	*k* = −15→16
T_{min} = 0.833, T_{max} = 0.923	*l* = −7→6
3197 measured reflections	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.029	$w = 1/[\sigma^2(F_o^2) + (0.0313P)^2 + 0.0657P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.067	$(\Delta/\sigma)_{max}$ = <0.001
S = 1.08	$\Delta\rho_{max}$ = 0.15 e Å^{-3}
1169 reflections	$\Delta\rho_{min}$ = −0.14 e Å^{-3}
91 parameters	Extinction correction: none
1 restraint	Absolute structure: Flack (1983), 502 Friedel pairs

Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Flack parameter: 0.06 (10)

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 $F^2 > 2\text{sigma}(F^2)$ 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	0.75367 (8)	0.85258 (4)	0.34560 (17)	0.05833 (18)
N1	0.1234 (2)	0.89202 (14)	0.8681 (4)	0.0484 (4)
N2	0.5619 (2)	0.81848 (14)	0.7062 (4)	0.0534 (5)
N3	0.4484 (2)	0.92123 (13)	0.4046 (3)	0.0490 (5)
O1	0.1184 (2)	0.85840 (12)	1.0650 (3)	0.0640 (5)
O2	0.0021 (2)	0.93094 (14)	0.7696 (3)	0.0674 (5)
C1	0.5650 (3)	0.86551 (15)	0.5040 (4)	0.0422 (5)
C2	0.4157 (3)	0.82858 (15)	0.8238 (5)	0.0504 (5)
H2	0.4031	0.7973	0.9675	0.061*
C3	0.3035 (3)	0.92896 (17)	0.5257 (4)	0.0493 (5)
H3	0.2139	0.9658	0.4648	0.059*
C4	0.2836 (3)	0.88393 (14)	0.7380 (4)	0.0399 (5)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl	0.0457 (3)	0.0646 (3)	0.0648 (4)	0.0038 (2)	0.0151 (2)	−0.0001 (3)
N1	0.0424 (10)	0.0470 (9)	0.0557 (13)	−0.0028 (7)	0.0050 (10)	−0.0133 (10)
N2	0.0443 (11)	0.0585 (11)	0.0576 (12)	0.0109 (9)	0.0063 (9)	0.0079 (10)
N3	0.0449 (10)	0.0574 (10)	0.0446 (12)	0.0075 (8)	0.0009 (9)	0.0050 (8)
O1	0.0587 (11)	0.0789 (13)	0.0543 (12)	−0.0009 (8)	0.0135 (9)	−0.0041 (9)
O2	0.0389 (9)	0.0829 (11)	0.0803 (14)	0.0144 (8)	0.0019 (8)	−0.0077 (10)
C1	0.0370 (11)	0.0421 (11)	0.0476 (13)	−0.0006 (9)	0.0044 (10)	−0.0046 (10)
C2	0.0483 (13)	0.0530 (12)	0.0500 (12)	0.0048 (9)	0.0105 (12)	0.0082 (11)
C3	0.0426 (11)	0.0550 (13)	0.0504 (13)	0.0091 (10)	−0.0051 (11)	−0.0016 (11)
C4	0.0340 (11)	0.0369 (10)	0.0490 (13)	0.0000 (8)	0.0000 (9)	−0.0072 (10)

Geometric parameters (Å, °)

Cl—O1^{i}	3.270 (2)	N3—C1	1.315 (3)

Cl—C1	1.738 (2)	N3—C3	1.330 (3)
N1—O1	1.215 (3)	C2—C4	1.370 (3)
N1—O2	1.223 (2)	C2—H2	0.9300
N1—C4	1.459 (3)	C3—C4	1.368 (3)
N2—C1	1.322 (3)	C3—H3	0.9300
N2—C2	1.332 (3)		
C1—Cl—O1^{i}	172.5 (2)	N2—C2—C4	121.5 (2)
O1—N1—O2	124.40 (19)	N2—C2—H2	119.2
O1—N1—C4	118.04 (19)	C4—C2—H2	119.2
O2—N1—C4	117.5 (2)	N3—C3—C4	121.5 (2)
C1—N2—C2	114.0 (2)	N3—C3—H3	119.3
C1—N3—C3	114.23 (18)	C4—C3—H3	119.3
N3—C1—N2	130.2 (2)	C3—C4—C2	118.6 (2)
N3—C1—Cl	114.91 (17)	C3—C4—N1	121.0 (2)
N2—C1—Cl	114.89 (17)	C2—C4—N1	120.4 (2)
C3—N3—C1—N2	−1.8 (3)	N3—C3—C4—N1	−179.3 (2)
C3—N3—C1—Cl	178.81 (16)	N2—C2—C4—C3	0.4 (3)
C2—N2—C1—N3	1.2 (4)	N2—C2—C4—N1	178.66 (19)
C2—N2—C1—Cl	−179.42 (16)	O1—N1—C4—C3	−173.2 (2)
C1—N2—C2—C4	−0.4 (3)	O2—N1—C4—C3	8.0 (3)
C1—N3—C3—C4	1.6 (3)	O1—N1—C4—C2	8.6 (3)
N3—C3—C4—C2	−1.1 (3)	O2—N1—C4—C2	−170.2 (2)

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3—H3···O2^{ii}	0.93	2.47	3.390 (3)	174

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

Fig. 1

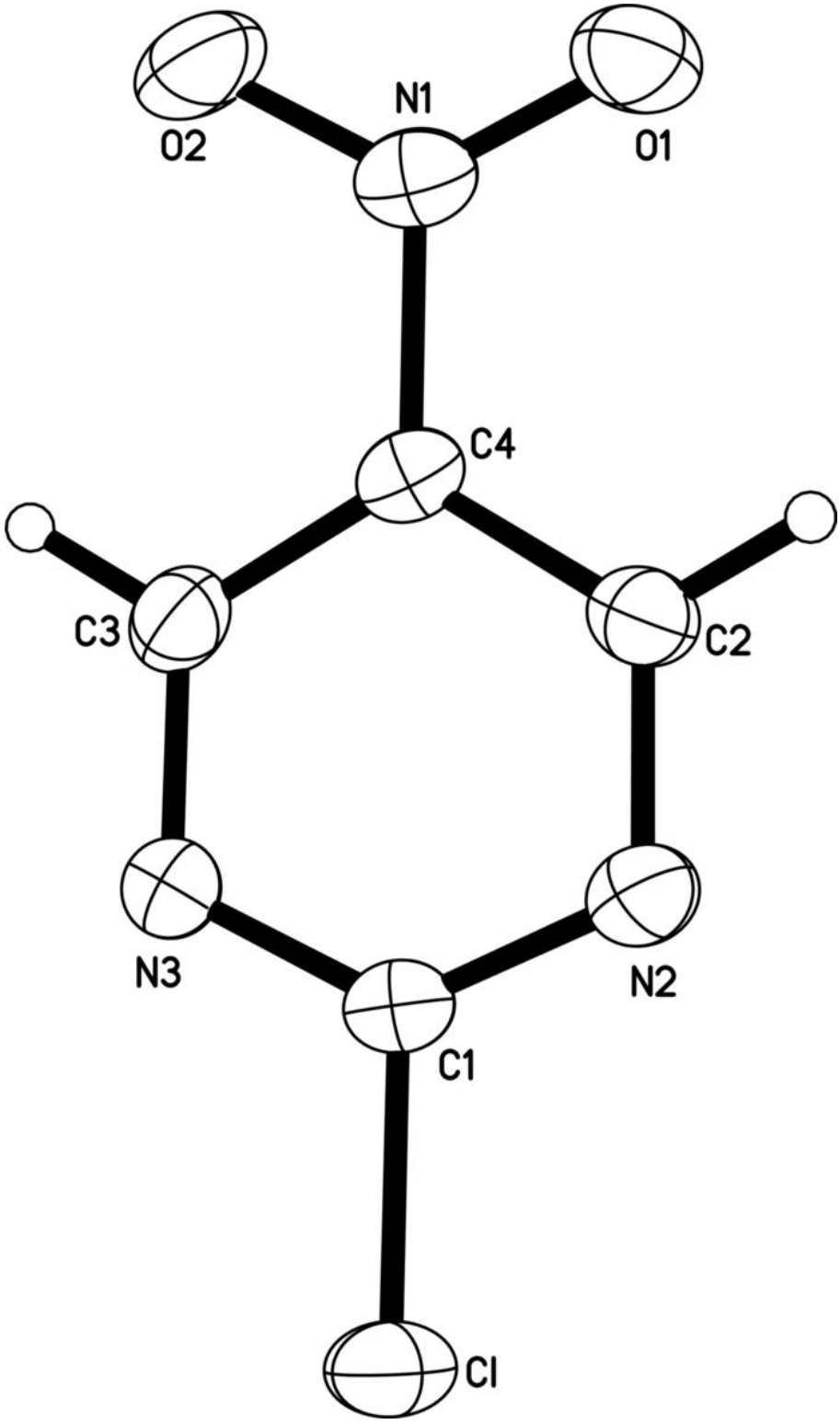


Fig. 2