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2-Chloro-5-nitropyridine

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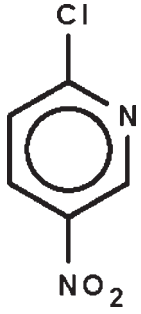
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.009 Å; R factor = 0.056; wR factor = 0.143; data-to-parameter ratio = 12.2.

The non-H atoms of the title compound, $C_5H_3ClN_2O_2$, almost lie in a common plane (r.m.s. deviation = 0.090 Å). In the crystal, adjacent molecules feature a short Cl···O contact [3.068 (4) Å], forming a chain; these chains are consolidated into a layer structure by non-classical C—H···O interactions.

Related literature

For the mechanism of the reaction between 2-chloro-5-nitropyridine and aryloxide ions, see: El-Bardan (1999); Haynes & Pett (2007); Zeller *et al.* (2007).



Experimental

Crystal data

$C_5H_3ClN_2O_2$
M_r = 158.54
Triclinic, $P\overline{1}$
a = 3.7599 (8) Å
b = 5.8641 (13) Å
c = 7.0189 (15) Å
α = 84.687 (3)°
β = 89.668 (3)°
γ = 76.020 (3)°
V = 149.50 (6) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 0.56 mm^{-1}
T = 100 K
0.45 × 0.15 × 0.03 mm

Data collection

Bruker SMART APEX diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.786, T_{max} = 0.983
1379 measured reflections
1114 independent reflections
1071 reflections with $I > 2\sigma(I)$
R_{int} = 0.022

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.056
$wR(F^2)$ = 0.143
S = 1.17
1114 reflections
91 parameters
3 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.63 e Å^{-3}
$\Delta\rho_{min}$ = −0.59 e Å^{-3}
Absolute structure: Flack (1983), 449 Friedel pairs
Flack parameter: −0.05 (14)

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

D—H···A	D—H	H···A	D···A	D—H···A
C2—H2···O1^{i}	0.95	2.50	3.361 (7)	151

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

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2010).

I thank the University of Malaya for supporting this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT5214).

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supporting information

Acta Cryst. (2010). E**66**, o848 [doi:10.1107/S1600536810008974]

2-Chloro-5-nitropyridine

Seik Weng Ng

S1. Comment

We have synthesized some nitropyridyl aryl ethers by the reaction of the aryloxide ion with the chlorine-substituted nitropyridine. The mechanism of this reaction has been reported (El-Bardan, 1999). With 2-chloro-5-nitropyridine, additional hydroxide base should not be used as the compound undergoes ring opening (Haynes & Pett, 2007; Zeller *et al.*, 2007).

2-Chloro-5-nitropyridine (Scheme I, Fig. 1) is a flat molecule; the non-hydrogen atoms all lie in a common plane (r.m.s. deviation 0.090 Å). Adjacent molecules interact by a Cl···O contact [3.068 (4) Å] to form a chain. The chains are consolidated into a layer structure by a non-classical C–H···O interaction; this interaction involves the second oxygen atom of the nitro group.

S2. Experimental

2-Chloro-5-nitropyridine as supplied by Aldrich Chemical Company is crystalline.

S3. Refinement

H-atoms were placed in calculated positions (C—H 0.95 Å) and were included in the refinement in the riding model approximation, with U(H) set to 1.2U(C).

The checking program *PLATON* detects some pseudo symmetry. However, as the Flack parameter refined to nearly zero, the non-centric space group must be the correct one. Nevertheless, an attempt was made to treat the structure as a whole-molecule-disordered structure but this gave a model with bad bond dimensions.

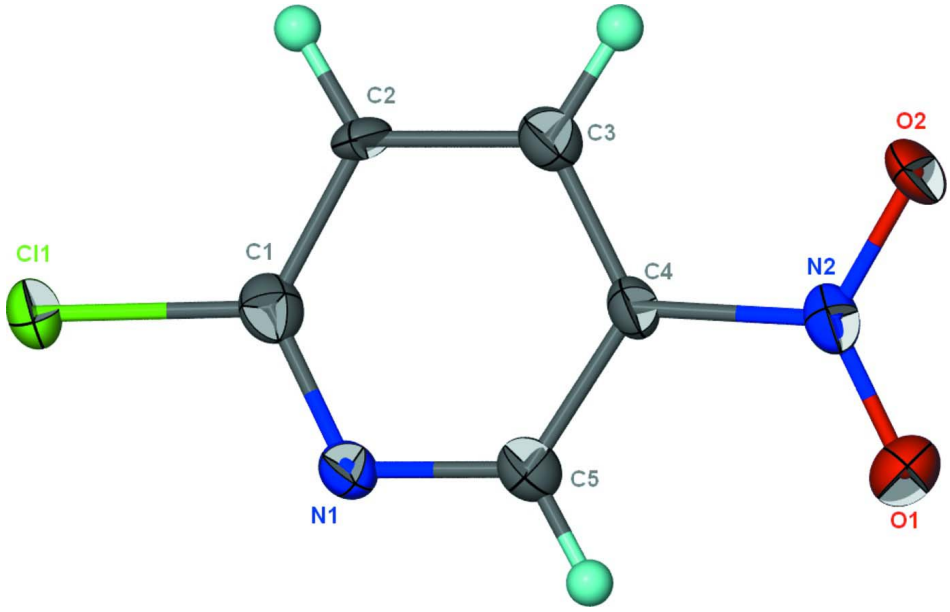

Figure 1

Anisotropic displacement ellipsoid plot (Barbour, 2001) of 2-chloro-5-nitropyridine at the 70% probability level; hydrogen atoms are drawn as spheres of arbitrary radius.

2-Chloro-5-nitropyridine

Crystal data

$C_5H_3ClN_2O_2$
$M_r = 158.54$
Triclinic, $P\overline{1}$
Hall symbol: P -1
$a = 3.7599\ (8)$ Å
$b = 5.8641\ (13)$ Å
$c = 7.0189\ (15)$ Å
$\alpha = 84.687\ (3)°$
$\beta = 89.668\ (3)°$
$\gamma = 76.020\ (3)°$
$V = 149.50\ (6)$ Å^3
$Z = 1$
$F(000) = 80$
$D_x = 1.761$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 637 reflections
$\theta = 2.9–28.2°$
$\mu = 0.56$ mm^{-1}
$T = 100$ K
Plate, colorless
0.45 × 0.15 × 0.03 mm

Data collection

Bruker SMART APEX diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.786$, $T_{max} = 0.983$
1379 measured reflections
1114 independent reflections
1071 reflections with $I > 2\sigma(I)$
$R_{int} = 0.022$
$\theta_{max} = 27.5°$, $\theta_{min} = 2.9°$
$h = -4\rightarrow4$
$k = -7\rightarrow7$
$l = -9\rightarrow9$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.056$
$wR(F^2) = 0.143$
$S = 1.17$
1114 reflections
91 parameters
3 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
$w = 1/[\sigma^2(F_o^2) + (0.070P)^2 + 0.2047P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.63$ e Å^{-3}
$\Delta\rho_{min} = -0.59$ e Å^{-3}
Absolute structure: Flack (1983), 449 Friedel pairs
Absolute structure parameter: −0.05 (14)

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl1	0.5000 (2)	0.50003 (18)	0.49998 (17)	0.0193 (3)
O1	0.8088 (11)	0.9486 (7)	1.2731 (6)	0.0254 (9)
O2	0.3611 (12)	1.2366 (7)	1.1607 (7)	0.0259 (10)
N1	0.7126 (12)	0.5558 (8)	0.8407 (7)	0.0161 (10)
N2	0.5729 (13)	1.0408 (10)	1.1526 (7)	0.0170 (11)
C1	0.5156 (14)	0.6688 (11)	0.6894 (8)	0.0180 (11)
C2	0.3197 (14)	0.9038 (9)	0.6723 (8)	0.0137 (11)
H2	0.1837	0.9735	0.5592	0.016*
C3	0.3320 (17)	1.0316 (12)	0.8277 (10)	0.0182 (13)
H3	0.2017	1.1922	0.8260	0.022*
C4	0.5415 (15)	0.9162 (10)	0.9860 (8)	0.0146 (11)
C5	0.7254 (14)	0.6800 (10)	0.9887 (8)	0.0173 (11)
H5	0.8644	0.6050	1.0995	0.021*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0220 (6)	0.0165 (6)	0.0198 (6)	−0.0033 (4)	−0.0008 (4)	−0.0072 (4)
O1	0.028 (2)	0.024 (2)	0.023 (2)	−0.0037 (17)	−0.0085 (18)	−0.0027 (18)
O2	0.034 (2)	0.015 (2)	0.024 (2)	0.0062 (16)	−0.0050 (17)	−0.0097 (17)
N1	0.015 (2)	0.014 (2)	0.019 (2)	−0.0011 (18)	−0.0014 (18)	−0.0041 (18)
N2	0.018 (2)	0.016 (3)	0.018 (3)	−0.005 (2)	0.002 (2)	−0.006 (2)
C1	0.016 (2)	0.019 (3)	0.020 (3)	−0.004 (2)	0.003 (2)	−0.005 (2)
C2	0.013 (2)	0.014 (2)	0.013 (3)	0.001 (2)	−0.0043 (18)	0.001 (2)
C3	0.017 (3)	0.016 (3)	0.021 (3)	−0.002 (2)	0.000 (2)	−0.004 (2)
C4	0.015 (2)	0.013 (2)	0.016 (3)	−0.003 (2)	0.0011 (19)	−0.005 (2)
C5	0.017 (2)	0.015 (3)	0.018 (3)	−0.003 (2)	0.001 (2)	−0.003 (2)

Geometric parameters (Å, º)

Cl1—C1	1.739 (6)	C2—C3	1.387 (9)
O1—N2	1.219 (7)	C2—H2	0.9500
O2—N2	1.235 (7)	C3—C4	1.387 (9)

N1—C1	1.325 (7)	C3—H3	0.9500
N1—C5	1.330 (7)	C4—C5	1.389 (8)
N2—C4	1.455 (8)	C5—H5	0.9500
C1—C2	1.391 (7)		
C1—N1—C5	116.7 (5)	C2—C3—C4	117.6 (6)
O1—N2—O2	124.1 (6)	C2—C3—H3	121.2
O1—N2—C4	118.4 (6)	C4—C3—H3	121.2
O2—N2—C4	117.4 (5)	C3—C4—C5	120.8 (5)
N1—C1—C2	126.0 (5)	C3—C4—N2	120.5 (5)
N1—C1—Cl1	115.4 (4)	C5—C4—N2	118.7 (5)
C2—C1—Cl1	118.6 (4)	N1—C5—C4	122.0 (5)
C3—C2—C1	117.0 (5)	N1—C5—H5	119.0
C3—C2—H2	121.5	C4—C5—H5	119.0
C1—C2—H2	121.5		
C5—N1—C1—C2	−0.6 (7)	O1—N2—C4—C3	−166.8 (5)
C5—N1—C1—Cl1	−179.2 (4)	O2—N2—C4—C3	11.9 (9)
N1—C1—C2—C3	0.1 (8)	O1—N2—C4—C5	13.1 (8)
Cl1—C1—C2—C3	178.6 (4)	O2—N2—C4—C5	−168.1 (5)
C1—C2—C3—C4	0.8 (8)	C1—N1—C5—C4	0.1 (8)
C2—C3—C4—C5	−1.2 (8)	C3—C4—C5—N1	0.8 (8)
C2—C3—C4—N2	178.7 (4)	N2—C4—C5—N1	−179.2 (5)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2···O1^{i}	0.95	2.50	3.361 (7)	151

Symmetry code: (i) *x*−1, *y*, *z*−1.