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2-Chloro-3-nitropyridine

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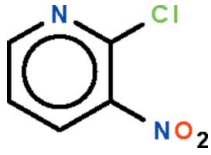
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.037; wR factor = 0.108; data-to-parameter ratio = 14.0.

In the title compound, $C_5H_3ClN_2O_2$, the nitro group is twisted by 38.5 (2)° with respect to the pyridine ring. In the crystal, adjacent molecules are linked by non-classical C—H···N and C—H···O hydrogen bonds, forming a layer motif.

Related literature

For the crystal structure of isostructural 2-iodo-3-nitropyridine, see: Mao & Chen (2009). For the crystal structure of 2-chloro-5-nitropyridine, see: Ng (2010).



Experimental

Crystal data

$C_5H_3ClN_2O_2$
M_r = 158.54
Monoclinic, $P2_1/n$
a = 7.613 (1) Å
b = 12.232 (2) Å
c = 7.716 (1) Å
β = 118.485 (2)°
V = 631.5 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.53 mm^{-1}
T = 293 K
0.30 × 0.20 × 0.05 mm

Data collection

Bruker SMART APEX diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.771, T_{max} = 0.862
5889 measured reflections
1445 independent reflections
1061 reflections with $I > 2\sigma(I)$
R_{int} = 0.040

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.108
S = 1.02
1445 reflections
103 parameters
3 restraints
All H-atom parameters refined
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.29 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C3—H3···N1^{i}	0.93 (1)	2.53 (1)	3.430 (3)	166 (2)
C4—H4···O1^{ii}	0.93 (1)	2.64 (2)	3.327 (3)	132 (2)

Symmetry codes: (i) $-x+\frac{3}{2}, y+\frac{1}{2}, -z+\frac{1}{2}$; (ii) $x, y, z-1$.

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: IM2183).

References

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Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
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supporting information

Acta Cryst. (2010). E**66**, o1020 [https://doi.org/10.1107/S1600536810011955]

2-Chloro-3-nitropyridine

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S1. Comment

According to a recent report on the crystal structure of 2-chloro-5-nitropyridine the respective molecule is planar (maximum r.m.s. deviation of non-hydrogen atoms is 0.090 Å). This molecule has the electron withdrawing substituents *para* to each other. The substituents interact through a short Cl···O contact of 3.068 (4) Å to generate a chain motif (Ng, 2010).

In the title compound 2-chloro-3-nitropyridine with the nitro group *ortho* to the chlorine substituent (Scheme I, Fig. 1), a similar Cl···O contact is also observed but the nitro group is twisted to avoid repulsion. Adjacent molecules are linked by non-classical C–H···N and C–H···O hydrogen bonds to form a layer motif (Fig. 2, Table 1). The C–H···N interaction is almost linear (Table 1).

2-Chloro-3-nitropyridine is isostructural with the iodo analog. In the iodo compound, the I···O contact is necessarily longer (Mao & Chen, 2009).

S2. Experimental

2-Chloro-3-nitropyridine was obtained from the Aldrich Chemical Company, and was recrystallized from ethyl acetate.

S3. Refinement

Carbon bound H-atoms were located in a difference Fourier map. They were refined with a distance restraint of C–H 0.93±0.01 Å; their temperature factors were refined without constraints.

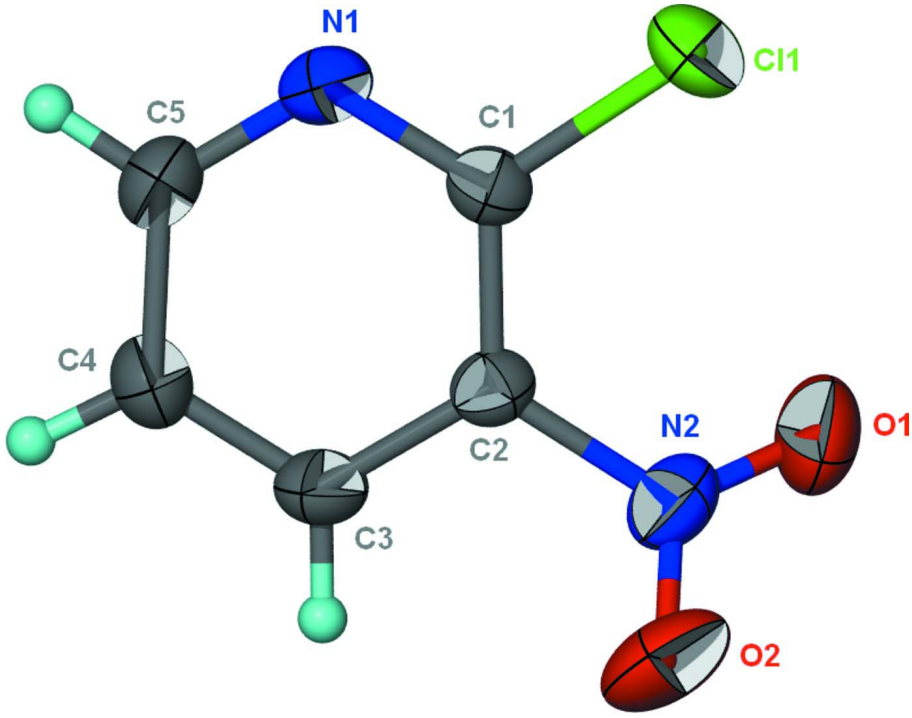

Figure 1

Thermal ellipsoid plot (Barbour, 2001) of $C_5H_3ClNO_2$ at the 50% probability level; hydrogen atoms are drawn as spheres of arbitrary radius.

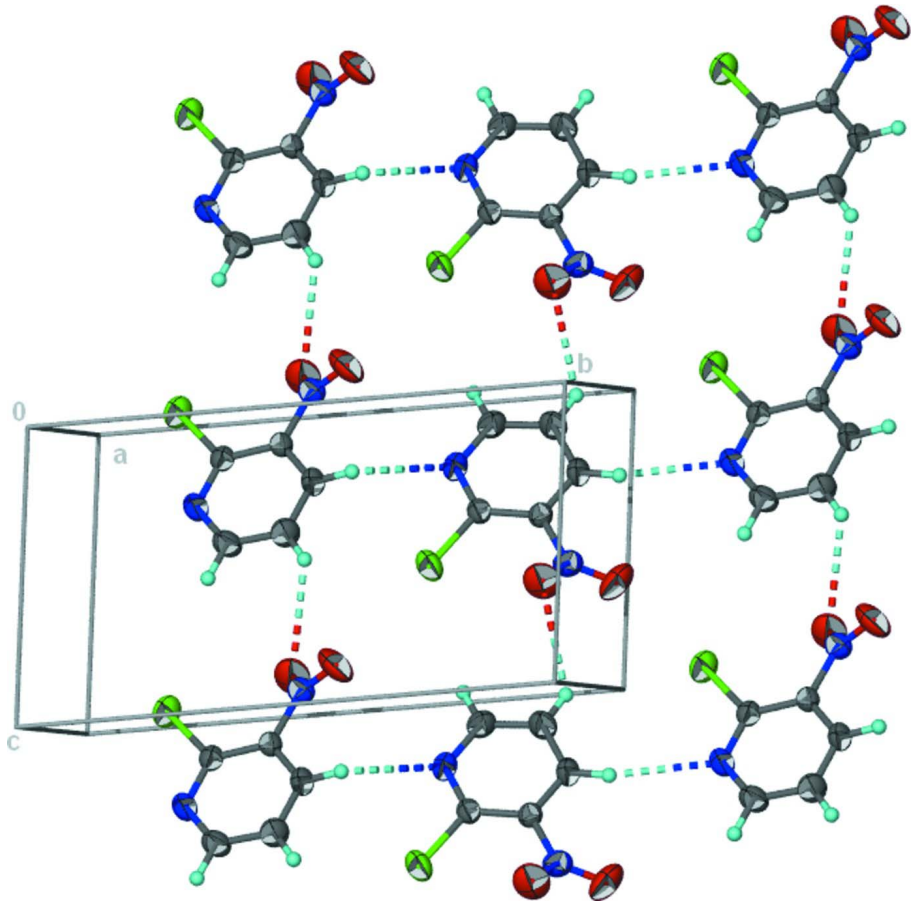

Figure 2

Non-classical hydrogen-bonded layer motif.

2-chloro-3-nitropyridine

Crystal data

$C_5H_3ClN_2O_2$
$M_r = 158.54$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 7.613$ (1) Å
$b = 12.232$ (2) Å
$c = 7.716$ (1) Å
$\beta = 118.485$ (2)°
$V = 631.5$ (2) Å^3
$Z = 4$
$F(000) = 320$
$D_x = 1.668$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1393 reflections
$\theta = 3.3$–24.8°
$\mu = 0.53$ mm^{-1}
$T = 293$ K
Block, faint yellow
0.30 × 0.20 × 0.05 mm

Data collection

Bruker SMART APEX diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.771$, $T_{max} = 0.862$
5889 measured reflections
1445 independent reflections
1061 reflections with $I > 2\sigma(I)$

R_{int} = 0.040
θ_{max} = 27.5°, θ_{min} = 3.1°
h = −9→9
k = −15→15
l = −9→10

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.108
S = 1.02
1445 reflections
103 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
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0539P)^2 + 0.1169P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.29 e Å^{-3}

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl1	0.67770 (9)	0.67094 (4)	0.54558 (9)	0.0583 (2)
O1	0.5971 (3)	0.89254 (15)	0.6322 (3)	0.0793 (6)
O2	0.8242 (3)	1.00241 (15)	0.6464 (3)	0.0804 (6)
N1	0.6852 (3)	0.71189 (13)	0.2214 (3)	0.0471 (4)
N2	0.7123 (3)	0.92525 (15)	0.5760 (3)	0.0514 (5)
C1	0.6891 (3)	0.75880 (14)	0.3767 (3)	0.0381 (4)
C2	0.7109 (3)	0.87120 (14)	0.4062 (3)	0.0375 (4)
C3	0.7322 (3)	0.93592 (16)	0.2719 (3)	0.0468 (5)
C4	0.7252 (4)	0.88674 (18)	0.1090 (3)	0.0522 (5)
C5	0.7011 (3)	0.77541 (19)	0.0896 (3)	0.0516 (5)
H3	0.751 (3)	1.0104 (9)	0.294 (3)	0.060 (7)*
H4	0.740 (3)	0.9261 (17)	0.013 (3)	0.061 (7)*
H5	0.693 (3)	0.7407 (18)	−0.021 (2)	0.060 (7)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0742 (4)	0.0455 (3)	0.0605 (4)	−0.0024 (2)	0.0366 (3)	0.0121 (2)
O1	0.1151 (16)	0.0782 (12)	0.0759 (13)	0.0077 (11)	0.0709 (13)	−0.0011 (9)
O2	0.0855 (13)	0.0709 (11)	0.0755 (12)	−0.0105 (10)	0.0308 (11)	−0.0382 (10)
N1	0.0558 (11)	0.0367 (8)	0.0490 (10)	−0.0028 (7)	0.0252 (9)	−0.0068 (7)
N2	0.0605 (12)	0.0499 (10)	0.0427 (10)	0.0115 (8)	0.0236 (9)	−0.0031 (8)
C1	0.0370 (10)	0.0354 (9)	0.0399 (10)	0.0002 (7)	0.0168 (8)	0.0023 (7)
C2	0.0385 (10)	0.0340 (8)	0.0378 (10)	0.0031 (7)	0.0164 (8)	−0.0014 (7)
C3	0.0585 (13)	0.0324 (9)	0.0497 (12)	−0.0014 (8)	0.0260 (10)	−0.0009 (8)
C4	0.0671 (14)	0.0491 (12)	0.0507 (13)	−0.0024 (10)	0.0366 (11)	0.0038 (9)
C5	0.0640 (14)	0.0520 (12)	0.0447 (12)	−0.0029 (10)	0.0307 (11)	−0.0083 (9)

Geometric parameters (Å, º)

Cl1—C1	1.7226 (18)	C2—C3	1.374 (3)
O1—N2	1.217 (2)	C3—C4	1.371 (3)
O2—N2	1.213 (2)	C3—H3	0.925 (9)
N1—C1	1.317 (2)	C4—C5	1.373 (3)
N1—C5	1.330 (3)	C4—H4	0.930 (10)
N2—C2	1.462 (2)	C5—H5	0.929 (10)
C1—C2	1.391 (3)		
C1—N1—C5	118.07 (17)	C4—C3—C2	118.15 (18)
O2—N2—O1	124.60 (19)	C4—C3—H3	122.2 (15)
O2—N2—C2	117.20 (19)	C2—C3—H3	119.7 (15)
O1—N2—C2	118.15 (18)	C3—C4—C5	118.67 (19)
N1—C1—C2	121.95 (16)	C3—C4—H4	122.2 (15)
N1—C1—Cl1	115.43 (14)	C5—C4—H4	119.2 (15)
C2—C1—Cl1	122.55 (14)	N1—C5—C4	123.54 (18)
C3—C2—C1	119.58 (17)	N1—C5—H5	116.5 (15)
C3—C2—N2	117.52 (16)	C4—C5—H5	120.0 (15)
C1—C2—N2	122.90 (17)		
C5—N1—C1—C2	−0.5 (3)	O2—N2—C2—C1	143.2 (2)
C5—N1—C1—Cl1	−177.56 (15)	O1—N2—C2—C1	−39.3 (3)
N1—C1—C2—C3	−1.1 (3)	C1—C2—C3—C4	1.9 (3)
Cl1—C1—C2—C3	175.72 (15)	N2—C2—C3—C4	−178.09 (19)
N1—C1—C2—N2	178.96 (18)	C2—C3—C4—C5	−1.2 (3)
Cl1—C1—C2—N2	−4.2 (3)	C1—N1—C5—C4	1.3 (3)
O2—N2—C2—C3	−36.8 (3)	C3—C4—C5—N1	−0.4 (4)
O1—N2—C2—C3	140.7 (2)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3—H3···N1^{i}	0.93 (1)	2.53 (1)	3.430 (3)	166 (2)
C4—H4···O1^{ii}	0.93 (1)	2.64 (2)	3.327 (3)	132 (2)

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