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2,3-Dichloropyridine

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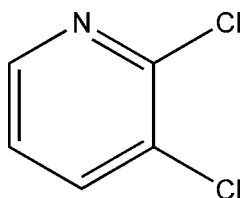
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Key indicators: single-crystal X-ray study; $T = 113$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; disorder in main residue; R factor = 0.025; wR factor = 0.054; data-to-parameter ratio = 15.7.

The complete molecule of the title compound, $\text{C}_5\text{H}_3\text{Cl}_2\text{N}$, is generated by crystallographic twofold symmetry, which forces the pyridine N atom and the opposite C–H group to be statistically disordered. In the crystal, weak aromatic π – π stacking [centroid–centroid separation = $3.805(4)$ Å and slippage = 1.704 Å] leads to [100] stacks of molecules. Short Cl...Cl contacts [$3.334(3)$ Å] are also observed.

Related literature

For the biological activity of related compounds, see: Liu *et al.* (2011). For related structures, see: Ma *et al.* (2007), Liu & Liu (2011).



Experimental

Crystal data

$\text{C}_5\text{H}_3\text{Cl}_2\text{N}$	$V = 572.3(9)$ Å ³
$M_r = 147.98$	$Z = 4$
Monoclinic, $C2/c$	Mo $K\alpha$ radiation
$a = 3.805(3)$ Å	$\mu = 1.00$ mm ⁻¹
$b = 14.196(12)$ Å	$T = 113$ K
$c = 10.68(1)$ Å	$0.36 \times 0.04 \times 0.04$ mm
$\beta = 97.221(14)^\circ$	

Data collection

Rigaku Saturn CCD diffractometer	2936 measured reflections
Absorption correction: multi-scan (<i>CrystalClear</i> ; Rigaku/MSC, 2005)	675 independent reflections
$T_{\min} = 0.714$, $T_{\max} = 0.961$	541 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.044$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.025$	2 restraints
$wR(F^2) = 0.054$	All H-atom parameters refined
$S = 1.01$	$\Delta\rho_{\max} = 0.31$ e Å ⁻³
675 reflections	$\Delta\rho_{\min} = -0.19$ e Å ⁻³
43 parameters	

Data collection: *CrystalClear* (Rigaku/MSC, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *CrystalStructure* (Rigaku/MSC, 2005).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB5953).

References

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supporting information

Acta Cryst. (2011). E67, o2211 [doi:10.1107/S1600536811030261]

2,3-Dichloropyridine

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S1. Comment

Pyridine derivatives are valuable intermediates and various biological activities. the structure of 2,3-dichloropyridine was confirmed by X-ray crstallography. For biological activities of related compounds, see: Liu *et al.* (2011). For related structure, see: Ma *et al.* (2007), Liu *et al.* & Liu (2011);

Single-crystal X-ray diffraction analysis reveals that the title compound crystallizes in the monoclinic space group $C2/c$. As shown in Fig. 1, the pyridine ring is nearly planar [mean deviation = 0.003 Å]. As shown in Fig. 2, the crystal structure is stabilized by van der Waals' interactions.

S2. Experimental

2,3-dichloropyridine is commercially available. Colourless prisms were grown from ethanol.

S3. Refinement

All the H atoms were positioned geometrically (C—H = 0.93Å) and refined as riding with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$

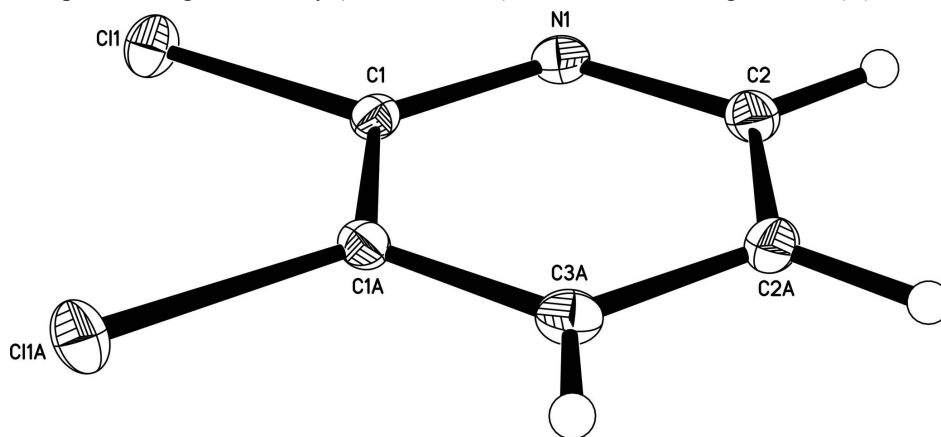
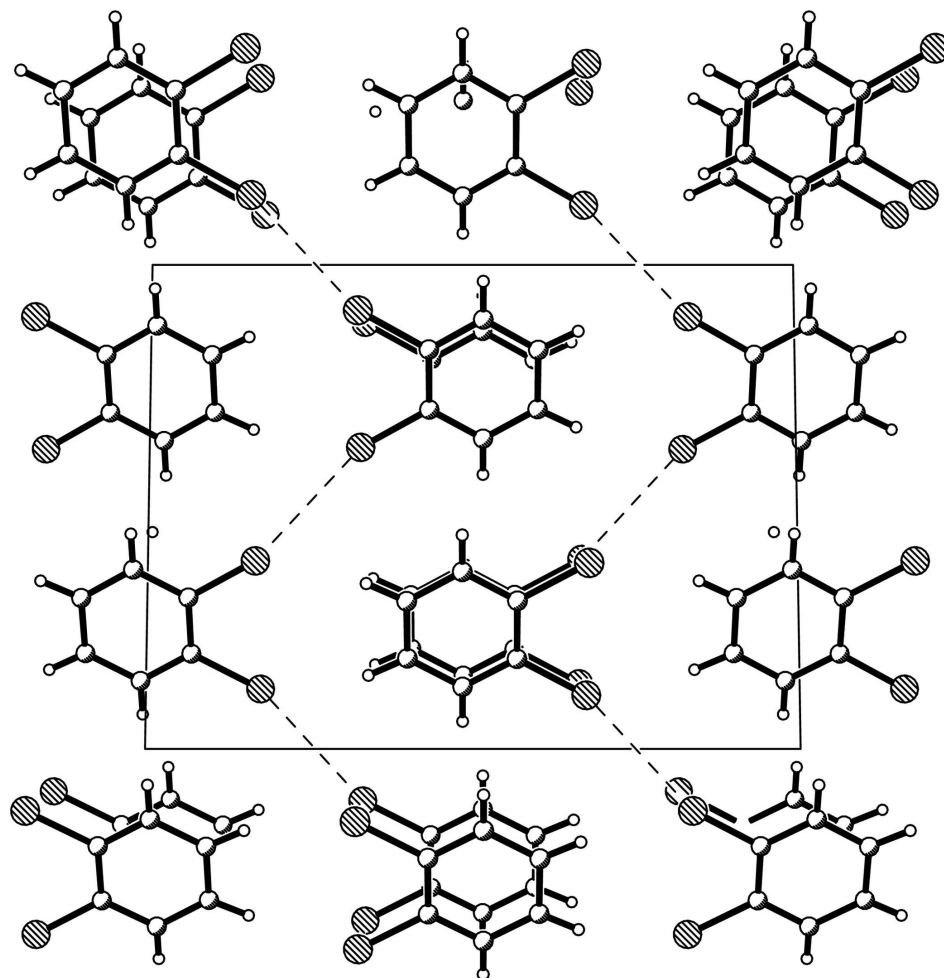


Figure 1

The molecular structure of (I). Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as small spheres of arbitrary radii. Atoms with suffix A are generated by $(1-x, y, 3/2-z)$. Just one orientation of N1 and C3 is shown.

**Figure 2**

The crystal packing for (I) with short Cl...Cl contacts indicated by dashed lines.

2,3-Dichloropyridine

Crystal data

$C_5H_3Cl_2N$

$M_r = 147.98$

Monoclinic, $C2/c$

Hall symbol: $-C 2yc$

$a = 3.805 (3) \text{ \AA}$

$b = 14.196 (12) \text{ \AA}$

$c = 10.68 (1) \text{ \AA}$

$\beta = 97.221 (14)^\circ$

$V = 572.3 (9) \text{ \AA}^3$

$Z = 4$

$F(000) = 296$

$D_x = 1.717 \text{ Mg m}^{-3}$

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

Cell parameters from 985 reflections

$\theta = 1.9\text{--}27.8^\circ$

$\mu = 1.00 \text{ mm}^{-1}$

$T = 113 \text{ K}$

Prism, colorless

$0.36 \times 0.04 \times 0.04 \text{ mm}$

Data collection

Rigaku Saturn CCD
diffractometer

Radiation source: rotating anode
Multilayer monochromator

Detector resolution: $14.63 \text{ pixels mm}^{-1}$

ω and φ scans

Absorption correction: multi-scan

(*CrystalClear*; Rigaku/MS, 2005)

$T_{\min} = 0.714$, $T_{\max} = 0.961$
 2936 measured reflections
 675 independent reflections
 541 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.044$

$\theta_{\max} = 27.8^\circ$, $\theta_{\min} = 2.9^\circ$
 $h = -4 \rightarrow 4$
 $k = -18 \rightarrow 18$
 $l = -13 \rightarrow 13$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.025$
 $wR(F^2) = 0.054$
 $S = 1.01$
 675 reflections
 43 parameters
 2 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
 $w = 1/[\sigma^2(F_o^2) + (0.022P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$
 $\Delta\rho_{\max} = 0.31 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.19 \text{ e } \text{\AA}^{-3}$

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>	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
C11	0.26918 (10)	0.32961 (3)	0.61537 (4)	0.02346 (14)	
C1	0.3983 (4)	0.43421 (10)	0.69098 (13)	0.0154 (3)	
C2	0.2951 (3)	0.51548 (10)	0.63275 (12)	0.0182 (3)	0.50
H2	0.138 (6)	0.514 (2)	0.5570 (16)	0.022*	0.50
N1	0.2951 (3)	0.51548 (10)	0.63275 (12)	0.0182 (3)	0.50
C3	0.3971 (4)	0.59762 (10)	0.69191 (15)	0.0214 (4)	
H3	0.312 (4)	0.6559 (8)	0.6561 (15)	0.026*	

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C11	0.0279 (3)	0.0201 (2)	0.0216 (2)	-0.00436 (16)	0.00026 (17)	-0.00631 (16)
C1	0.0142 (8)	0.0163 (7)	0.0160 (7)	-0.0009 (6)	0.0031 (6)	-0.0027 (6)
C2	0.0158 (8)	0.0235 (7)	0.0149 (7)	-0.0009 (6)	0.0008 (6)	0.0016 (6)
N1	0.0158 (8)	0.0235 (7)	0.0149 (7)	-0.0009 (6)	0.0008 (6)	0.0016 (6)
C3	0.0184 (9)	0.0185 (8)	0.0269 (9)	0.0015 (6)	0.0012 (7)	0.0073 (7)

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

C11—C1	1.7317 (18)	C2—H2	0.943 (10)
C1—C2	1.346 (2)	C3—C3 ⁱ	1.382 (3)

C1—C1 ⁱ	1.394 (3)	C3—H3	0.951 (9)
C2—C3	1.359 (2)		
C2—C1—C1 ⁱ	120.97 (9)	C3—C2—H2	122.4 (18)
C2—C1—C11	118.07 (12)	C2—C3—C3 ⁱ	120.92 (9)
C1 ⁱ —C1—C11	120.96 (6)	C2—C3—H3	119.8 (10)
C1—C2—C3	118.10 (14)	C3 ⁱ —C3—H3	119.1 (10)
C1—C2—H2	119.2 (18)		
C1 ⁱ —C1—C2—C3	0.5 (3)	C1—C2—C3—C3 ⁱ	0.5 (3)
C11—C1—C2—C3	-179.84 (12)		

Symmetry code: (i) $-x+1, y, -z+3/2$.