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N-(3,5-Dichloro-2-pyridyl)formamide

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Key indicators

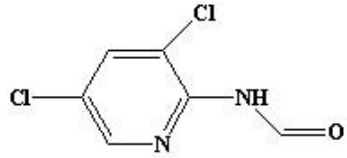
Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.004 Å
R factor = 0.041
wR factor = 0.130
Data-to-parameter ratio = 26.1

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

The molecule of the title compound, $C_6H_4Cl_2N_2O$, is essentially planar.

Comment

There is only one crystal structure of a 2-pyridylformamide found in the literature to date, *viz.* dimeric 2-pyridylformamide (Bock *et al.*, 1996). In the monomeric title compound, (I), atom Cl31 forces the formamide group to be *trans*, thus preventing the hydrogen bonding which forms the dimer in the unchlorinated compound through the equivalents of N1 and N21. The torsion angle for N1—C2—C21—C22 is −5.3 (7)°.



(I)

Experimental

The synthesis of (I) from 6,8-dichlorotetrazolo[1,5-*a*]pyridine and dialkylamines has been reported previously (Reisinger *et al.*, 2004; Reisinger & Wentrup, 2005).

Crystal data

$C_6H_4Cl_2N_2O$
M_r = 191.01
Monoclinic, $C2/c$
a = 28.869 (7) Å
b = 3.760 (1) Å
c = 15.403 (6) Å
β = 118.04 (3)°
V = 1475.7 (9) Å^3
Z = 8
D_x = 1.719 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
θ = 10.0–12.5°
μ = 0.81 mm^{-1}
T = 298 (2) K
Thick plate, colourless
0.3 × 0.2 × 0.1 mm

Data collection

Enraf-Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.827, T_{max} = 0.922
2614 measured reflections
2614 independent reflections
1665 reflections with $I > 2\sigma(I)$
θ_{max} = 25.0°
$h = -34 \rightarrow 34$
$k = -4 \rightarrow 0$
$l = -18 \rightarrow 18$
3 standard reflections
frequency: 120 min
intensity decay: 4%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.130
S = 0.87
2614 reflections
100 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0852P)^2 + 1.7332P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.32 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

N1—C2	1.334 (3)	N21—C22	1.350 (3)
N1—C6	1.336 (3)	C3—C4	1.370 (3)
C2—N21	1.394 (3)	C4—C5	1.379 (4)
C2—C3	1.394 (3)	C5—C6	1.374 (4)
N1—C2—N21	117.3 (2)	O23—C22—N21	123.7 (2)
C22—N21—C2	124.2 (2)		
N1—C2—N21—C22	−5.4 (4)		

Table 2
Hydrogen-bond geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N21—H21···O23^{i}	0.86	2.11	2.942 (3)	164

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

All H atoms were refined using a riding model, with N—H = 0.86 Å and U_{iso}(H) = 1.2U_{eq}(N), and C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C) for sp^2 C atoms.

Data collection: *SDP* (Frenz, 1985); cell refinement: *SDP*; data reduction: *WinGX* (Farrugia, 1999); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON98* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

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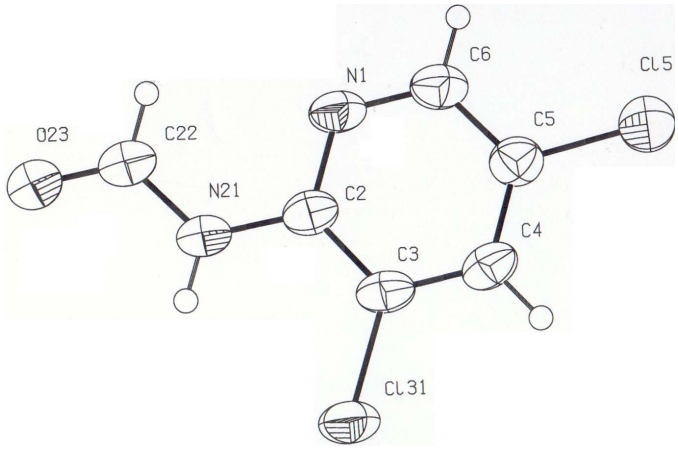

Figure 1
The molecular structure of (I), showing displacement ellipsoids at the 50% probability level.

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