Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2,3,5-Trichloropyridine

Hong-Fei Ma,* Hong-Sheng Jia, Yi Qian, Fan Wen and Bin-Lin Chen

Department of Applied Chemistry, College of Science, Nanjing University of Technology, Nanjing 210009, People's Republic of China

Correspondence e-mail: mhf2356@njut.edu.cn

Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.005 Å
R factor = 0.046
wR factor = 0.131
Data-to-parameter ratio = 16.0

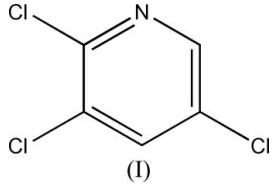
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

The molecule of the title compound, $C_5H_2Cl_3N$, is essentially planar. In the crystal structure, molecules are stacked along the short *a* axis and form a layer structure parallel to the $(\bar{1}02)$ plane. No π–π stacking interactions or hydrogen bonds are observed.

Received 8 December 2006
Accepted 10 December 2006

Comment

2,3,5-Trichloropyridine is a valuable intermediate for producing herbicidally active α-[4-(3′,5′-dichloropyrid-2-yloxy)-phenoxy]alkanecarboxylic acids and their derivatives (Fah & Grieder, 1981). We report here the crystal structure of the title compound, (I).



(I)

The molecular structure of (I) is shown in Fig. 1. Bond lengths and angles (Table 1) are within normal ranges (Allen *et al.*, 1987). The molecule is essentially planar. In the crystal structure, the molecules are stacked along the short *a* axis without any π–π interactions (Fig. 2). The stacking results in the formation of layers parallel to the $(\bar{1}02)$ plane. No hydrogen bonds are observed in the crystal structure.

Experimental

Compound (I) was prepared according to the literature method of Fah & Grieder (1981). Single crystals were obtained by dissolving

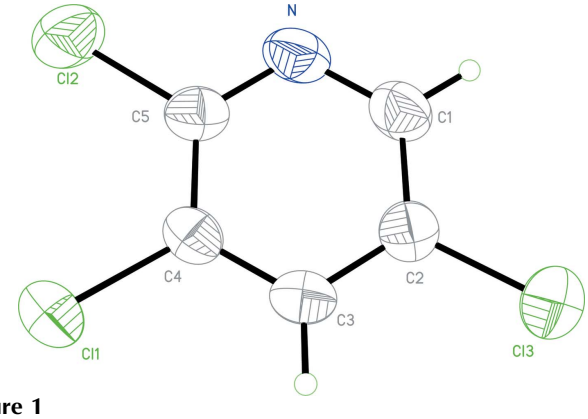


Figure 1
The molecular structure of (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

compound (I) (0.2 g) in methanol (30 ml) and evaporating the solvent slowly at room temperature for about 7 d.

Crystal data

$C_5H_2Cl_3N$
M_r = 182.43
Monoclinic, $P2_1/c$
a = 3.8860 (8) Å
b = 16.144 (3) Å
c = 10.959 (2) Å
β = 97.61 (3)°
V = 681.5 (2) Å^3
Z = 4
D_x = 1.788 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 1.24 mm^{-1}
T = 298 (2) K
Block, colorless
0.40 × 0.20 × 0.20 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.637, T_{max} = 0.790
1525 measured reflections
1328 independent reflections
953 reflections with $I > 2\sigma(I)$
R_{int} = 0.043
θ_{max} = 25.9°
3 standard reflections
every 200 reflections
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.131
S = 1.02
1328 reflections
83 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.075P)^2 + 0.0336P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.34 e Å^{-3}
$\Delta\rho_{min}$ = −0.37 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.050 (6)

Table 1
Selected geometric parameters (Å, °).

Cl1—C4	1.722 (3)	N—C5	1.315 (4)
Cl2—C5	1.717 (3)	N—C1	1.332 (4)
Cl3—C2	1.729 (4)		
C5—N—C1	118.4 (3)	C5—C4—Cl1	120.9 (3)
N—C1—C2	122.1 (3)	N—C5—C4	122.8 (3)
C3—C2—Cl3	120.6 (3)	N—C5—Cl2	116.0 (2)
C1—C2—Cl3	119.6 (3)	C4—C5—Cl2	121.2 (3)
C3—C4—Cl1	120.2 (2)		

H atoms were positioned geometrically, with C—H = 0.93 Å, and constrained to ride on their parent atoms, with U_{iso}(H) = 1.2U_{eq}(C).

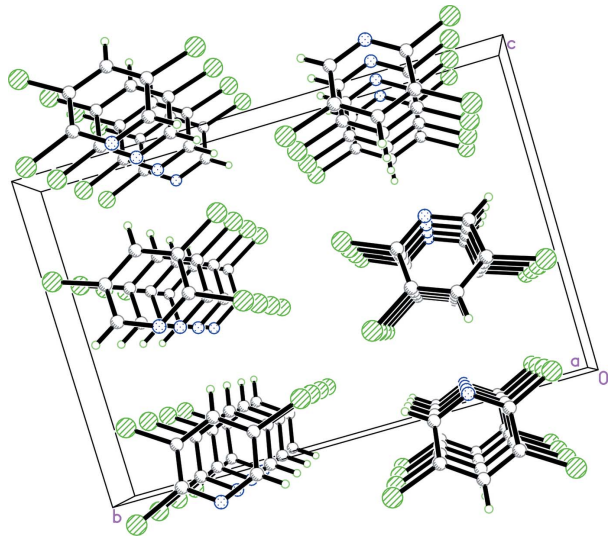


Figure 2
A packing diagram of (I).

Data collection: *CAD-4 Software* (Enraf–Nonius, 1985); cell refinement: *CAD-4 Software*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2000); software used to prepare material for publication: *SHELXTL*.

The authors thank the Center for Testing and Analysis, Nanjing University, for support.

References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
Bruker (2000). *SHELXTL*. Bruker AXS Inc., Madison, Wisconsin, USA.
Enraf–Nonius (1985). *CAD-4 Software*. Version 5.0. Enraf–Nonius, Delft, The Netherlands.
Fah, H. & Grieder, A. (1981). US Patent No. 4 287 347.
Harms, K. & Wocadlo, S. (1995). *XCAD4*. University of Marburg, Germany.
North, A. C. T., Phillips, D. C. & Mathews, F. S. (1968). *Acta Cryst.* A**24**, 351–359.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.