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Crystal structure of fenclorim

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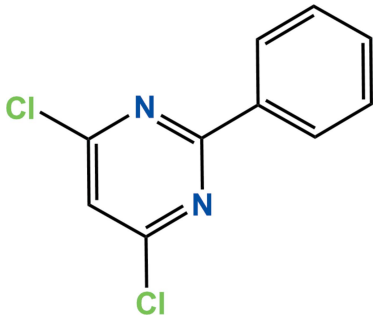
In the title compound, $C_{10}H_6Cl_2N_2$ (systematic name: 4,6-dichloro-2-phenylpyrimidine), which is used commercially as the herbicide safener, fenclorim, the dihedral angle between the dichloropyrimidyl and phenyl rings is 9.45 (10)°. In the crystal, C—H···N hydrogen bonds link adjacent molecules, forming chains along the *c*-axis direction. In addition, weak intermolecular C—Cl···π [3.6185 (10) Å] and π–π [3.8796 (11) Å] interactions are present, forming a three-dimensional network.

Keywords: crystal structure; herbicide; fenclorim; pyrimidine; C—Cl···π interactions; π–π interactions; hydrogen bonding.

CCDC reference: 1421258

1. Related literature

For information on the herbicidal properties of the title compound, see: Wu *et al.* (1999). For a related crystal structure, see: Leban & Polanc (1992).



2. Experimental

2.1. Crystal data

$C_{10}H_6Cl_2N_2$
M_r = 225.07
Monoclinic, $P2_1/c$
a = 5.6210 (6) Å
b = 17.0659 (18) Å
c = 10.2582 (12) Å
β = 99.690 (6)°
V = 970.00 (19) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.62 mm^{-1}
T = 173 K
0.16 × 0.06 × 0.04 mm

2.2. Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2013)
T_{min} = 0.690, T_{max} = 0.746
9071 measured reflections
2212 independent reflections
1750 reflections with $I > 2\sigma(I)$
R_{int} = 0.034

2.3. Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.077
S = 1.07
2212 reflections
127 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.28 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C2—H2···N2^{i}	0.95	2.46	3.317 (2)	151

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

Data collection: *APEX2* (Bruker, 2013); cell refinement: *SAINT* (Bruker, 2013); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2013* (Sheldrick, 2015); molecular graphics: *DIAMOND* (Brandenburg, 2010); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

Acknowledgements

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Supporting information for this paper is available from the IUCr electronic archives (Reference: SJ5469).

References

Brandenburg, K. (2010). *DIAMOND*. Crystal Impact GbR, Bonn, Germany.
Bruker (2013). *APEX2*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Leban, I. & Polanc, S. (1992). *Acta Cryst.* C**48**, 2227–2229.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Sheldrick, G. M. (2015). *Acta Cryst.* C**71**, 3–8.
Wu, J., Cramer, C. L. & Hatzios, K. K. (1999). *Physiol. Plant.* **105**, 102–108.

supporting information

Acta Cryst. (2015). E**71**, o714 [doi:10.1107/S2056989015016187]

Crystal structure of fenclorim

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S1. Comment

Fenclorim [systematic name: 4,6-dichloro-2-phenylpyrimidine] is a herbicide safener that is used in many rice-producing countries to protect rice plants from damage likely to be caused by the chloroacetanilide herbicide pretilachlor. (Wu *et al.*, 1999). The dihedral angle between the dichloropyrimidyl and phenyl rings is 9.45 (10)°. All bond lengths and bond angles are normal and comparable to those observed in a similar crystal structure (Leban & Polanc, 1992).

In the crystal structure (Fig. 2), C–H···N hydrogen bonds (Table 1) link adjacent molecules, forming a one-dimensional chains along the *c*-axis. In addition, weak intermolecular C3–Cl2···*Cg*2^{iii} [Cl2···Cg2 = 3.6185 (10) Å] (*Cg2* is the centroid of the C5–C10 ring) and *Cg*1···*Cg*2^{iv} [Cg1···Cg2 = 3.8796 (11) Å] interactions are present (Cg1 is the centroid of the N1,N2,C1–C4 ring), forming a three-dimensional network [symmetry codes: (ii), *x* - 1, *y*, *z*; (iii), *x* - 1, -*y* + 1/2, *z* - 1/2; (iv), -*x* + 1, -*y* + 1, -*z*].

S2. Experimental

The title compound was purchased from the Dr. Ehrenstorfer GmbH Company. Slow evaporation of a solution in CH_2Cl_2 gave single crystals suitable for X-ray analysis.

S3. Refinement

All H-atoms were positioned geometrically and refined using a riding model with d(C—H) = 0.95 Å, U_{iso} = 1.2U_{eq}(C) for the aromatic C—H.

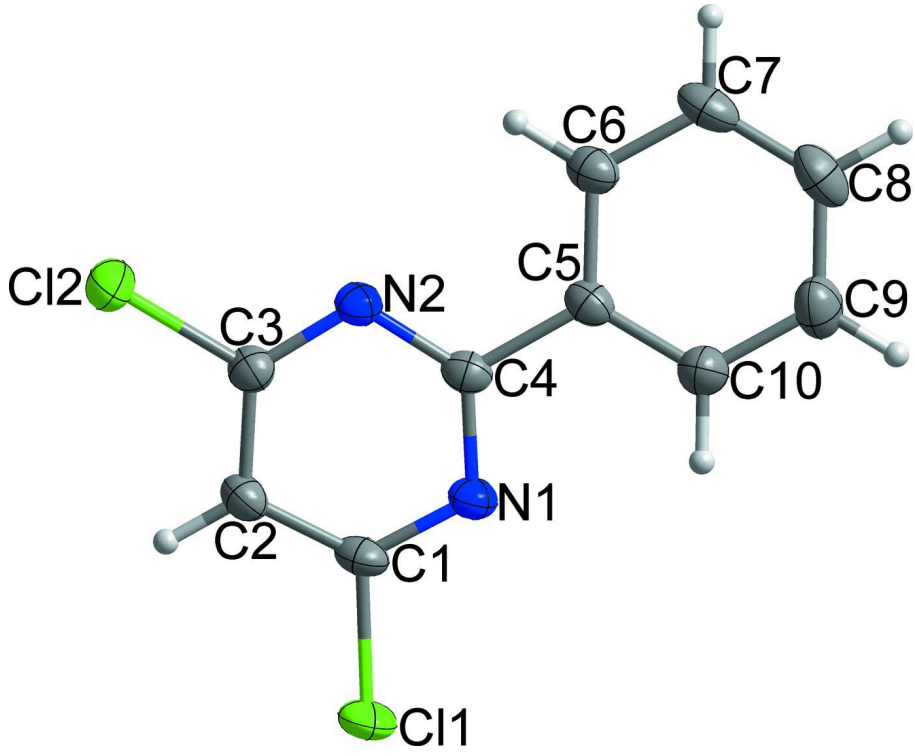

Figure 1

The asymmetric unit of the title compound with the atom numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are shown as small spheres of arbitrary radius.

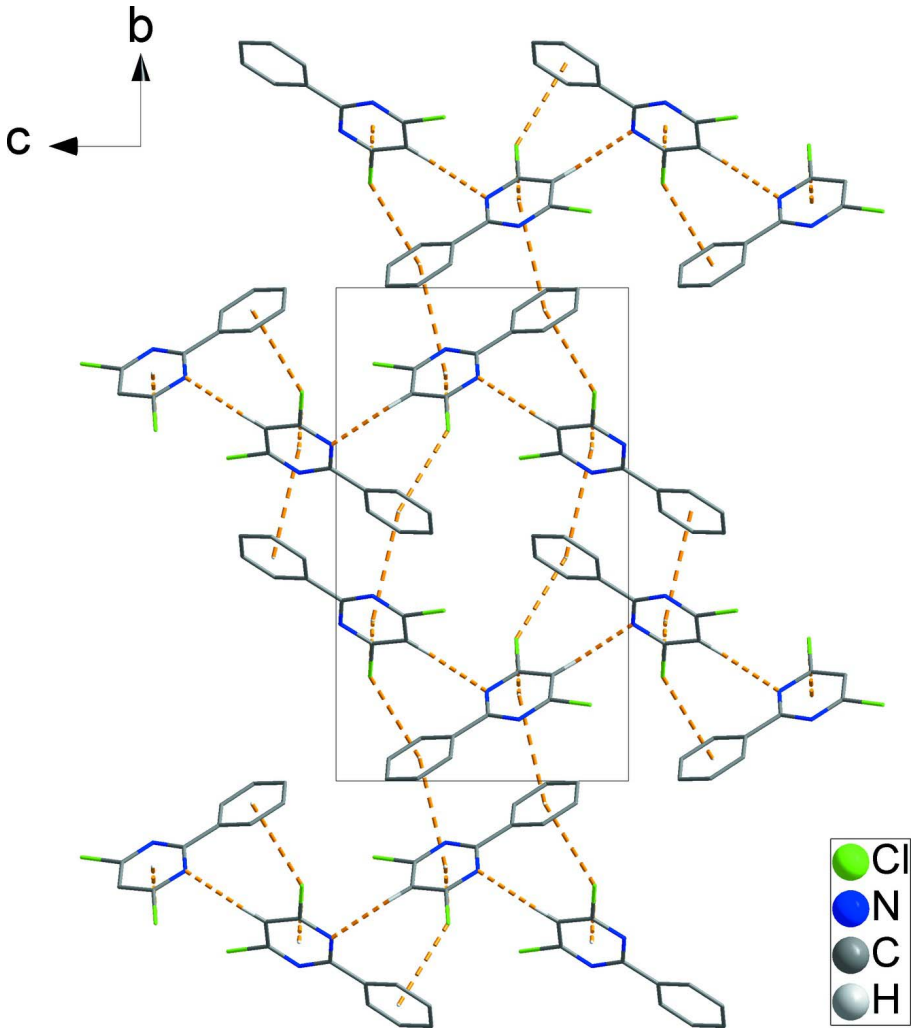

Figure 2

Crystal packing viewed along the *a* axis. The intermolecular interactions are shown as dashed lines.

4,6-Dichloro-2-phenylpyrimidine

Crystal data

$C_{10}H_6Cl_2N_2$
$M_r = 225.07$
Monoclinic, $P2_1/c$
$a = 5.6210\ (6)$ Å
$b = 17.0659\ (18)$ Å
$c = 10.2582\ (12)$ Å
$\beta = 99.690\ (6)°$
$V = 970.00\ (19)$ Å^3
$Z = 4$

$F(000) = 456$
$D_x = 1.541$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2286 reflections
$\theta = 2.3–25.9°$
$\mu = 0.62$ mm^{-1}
$T = 173$ K
Plate, colourless
0.16 × 0.06 × 0.04 mm

Data collection

Bruker APEXII CCD diffractometer
φ and ω scans

Absorption correction: multi-scan (*SADABS*; Bruker, 2013)
$T_{min} = 0.690$, $T_{max} = 0.746$

9071 measured reflections
2212 independent reflections
1750 reflections with $I > 2\sigma(I)$
$R_{int} = 0.034$
$\theta_{max} = 27.5°$, $\theta_{min} = 2.3°$
$h = -6 \rightarrow 7$
$k = -19 \rightarrow 22$
$l = -13 \rightarrow 9$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.034$
$wR(F^2) = 0.077$
$S = 1.07$
2212 reflections
127 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0277P)^2 + 0.269P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.28$ e Å^{-3}
$\Delta\rho_{min} = -0.23$ e Å^{-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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl1	0.65642 (9)	0.34546 (3)	−0.36827 (4)	0.04016 (15)
Cl2	0.00001 (9)	0.21187 (3)	−0.11631 (4)	0.03800 (15)
N1	0.6078 (2)	0.37521 (8)	−0.12511 (13)	0.0265 (3)
N2	0.3094 (2)	0.31826 (8)	−0.01497 (13)	0.0251 (3)
C1	0.5151 (3)	0.33485 (10)	−0.23126 (16)	0.0266 (4)
C2	0.3205 (3)	0.28518 (10)	−0.24028 (16)	0.0274 (4)
H2	0.2551	0.2580	−0.3190	0.033*
C3	0.2296 (3)	0.27863 (10)	−0.12406 (16)	0.0258 (4)
C4	0.4978 (3)	0.36583 (9)	−0.01979 (15)	0.0239 (4)
C5	0.5944 (3)	0.41068 (10)	0.10104 (15)	0.0248 (4)
C6	0.4715 (3)	0.41288 (10)	0.20807 (16)	0.0294 (4)
H6	0.3240	0.3851	0.2044	0.035*
C7	0.5644 (4)	0.45554 (11)	0.31979 (17)	0.0355 (4)
H7	0.4809	0.4566	0.3929	0.043*
C8	0.7773 (4)	0.49654 (12)	0.32573 (18)	0.0381 (5)
H8	0.8395	0.5259	0.4026	0.046*
C9	0.9000 (3)	0.49498 (12)	0.22019 (19)	0.0391 (5)
H9	1.0460	0.5236	0.2239	0.047*
C10	0.8099 (3)	0.45159 (11)	0.10867 (18)	0.0332 (4)
H10	0.8964	0.4498	0.0367	0.040*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0519 (3)	0.0482 (3)	0.0248 (2)	−0.0100 (2)	0.0192 (2)	−0.0056 (2)
Cl2	0.0424 (3)	0.0384 (3)	0.0344 (3)	−0.0145 (2)	0.0099 (2)	−0.00277 (19)

N1	0.0314 (8)	0.0280 (8)	0.0213 (7)	−0.0007 (7)	0.0077 (6)	−0.0002 (6)
N2	0.0290 (8)	0.0250 (8)	0.0217 (7)	−0.0008 (6)	0.0056 (6)	0.0012 (6)
C1	0.0352 (10)	0.0268 (9)	0.0194 (8)	0.0042 (8)	0.0095 (7)	0.0021 (7)
C2	0.0346 (10)	0.0265 (9)	0.0210 (8)	−0.0003 (8)	0.0042 (7)	−0.0027 (7)
C3	0.0296 (9)	0.0234 (9)	0.0244 (8)	−0.0008 (7)	0.0043 (7)	0.0021 (7)
C4	0.0278 (9)	0.0240 (9)	0.0200 (8)	0.0047 (7)	0.0046 (7)	0.0033 (6)
C5	0.0307 (9)	0.0226 (9)	0.0209 (8)	0.0032 (7)	0.0035 (7)	0.0011 (6)
C6	0.0375 (10)	0.0264 (9)	0.0253 (9)	0.0013 (8)	0.0080 (7)	0.0005 (7)
C7	0.0500 (12)	0.0366 (11)	0.0206 (9)	0.0080 (9)	0.0078 (8)	−0.0013 (7)
C8	0.0442 (12)	0.0383 (11)	0.0276 (9)	0.0086 (10)	−0.0063 (8)	−0.0079 (8)
C9	0.0323 (10)	0.0415 (12)	0.0406 (11)	−0.0028 (9)	−0.0019 (8)	−0.0081 (9)
C10	0.0316 (10)	0.0375 (11)	0.0311 (9)	−0.0021 (8)	0.0073 (8)	−0.0037 (8)

Geometric parameters (Å, º)

Cl1—C1	1.7362 (17)	C5—C6	1.393 (2)
Cl2—C3	1.7333 (17)	C6—C7	1.384 (2)
N1—C1	1.319 (2)	C6—H6	0.9500
N1—C4	1.342 (2)	C7—C8	1.379 (3)
N2—C3	1.320 (2)	C7—H7	0.9500
N2—C4	1.342 (2)	C8—C9	1.378 (3)
C1—C2	1.375 (2)	C8—H8	0.9500
C2—C3	1.379 (2)	C9—C10	1.385 (2)
C2—H2	0.9500	C9—H9	0.9500
C4—C5	1.480 (2)	C10—H10	0.9500
C5—C10	1.389 (2)		
C1—N1—C4	115.52 (14)	C6—C5—C4	120.90 (15)
C3—N2—C4	115.88 (14)	C7—C6—C5	119.93 (17)
N1—C1—C2	125.22 (15)	C7—C6—H6	120.0
N1—C1—Cl1	116.28 (13)	C5—C6—H6	120.0
C2—C1—Cl1	118.49 (13)	C8—C7—C6	120.49 (17)
C1—C2—C3	113.49 (15)	C8—C7—H7	119.8
C1—C2—H2	123.3	C6—C7—H7	119.8
C3—C2—H2	123.3	C9—C8—C7	120.06 (17)
N2—C3—C2	124.69 (16)	C9—C8—H8	120.0
N2—C3—Cl2	116.58 (13)	C7—C8—H8	120.0
C2—C3—Cl2	118.70 (13)	C8—C9—C10	119.83 (18)
N1—C4—N2	125.13 (15)	C8—C9—H9	120.1
N1—C4—C5	117.31 (15)	C10—C9—H9	120.1
N2—C4—C5	117.55 (14)	C9—C10—C5	120.63 (17)
C10—C5—C6	119.06 (16)	C9—C10—H10	119.7
C10—C5—C4	120.04 (15)	C5—C10—H10	119.7
C4—N1—C1—C2	−0.4 (2)	N1—C4—C5—C10	−8.8 (2)
C4—N1—C1—Cl1	−179.46 (12)	N2—C4—C5—C10	170.39 (16)
N1—C1—C2—C3	−1.8 (3)	N1—C4—C5—C6	170.99 (15)
Cl1—C1—C2—C3	177.25 (12)	N2—C4—C5—C6	−9.9 (2)

C4—N2—C3—C2	−2.3 (2)	C10—C5—C6—C7	0.1 (3)
C4—N2—C3—Cl2	175.70 (12)	C4—C5—C6—C7	−179.64 (15)
C1—C2—C3—N2	3.2 (3)	C5—C6—C7—C8	0.5 (3)
C1—C2—C3—Cl2	−174.72 (13)	C6—C7—C8—C9	−0.3 (3)
C1—N1—C4—N2	1.6 (2)	C7—C8—C9—C10	−0.6 (3)
C1—N1—C4—C5	−179.38 (14)	C8—C9—C10—C5	1.2 (3)
C3—N2—C4—N1	−0.3 (2)	C6—C5—C10—C9	−1.0 (3)
C3—N2—C4—C5	−179.36 (14)	C4—C5—C10—C9	178.79 (16)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2···N2^{i}	0.95	2.46	3.317 (2)	151

Symmetry code: (i) *x*, −*y*+1/2, *z*−1/2.