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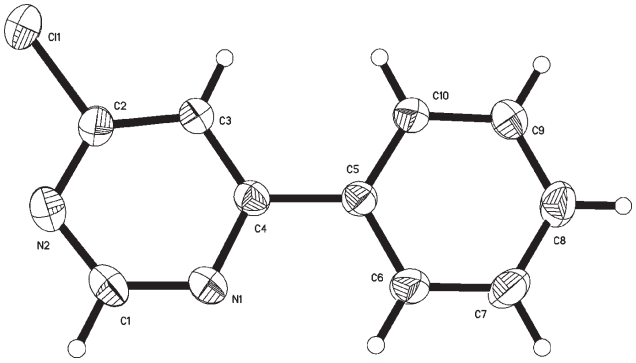
Crystal structure of 4-chloro-6-phenylpyrimidine, $C_{10}H_7ClN_2$



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Abstract

$C_{10}H_7ClN_2$, monoclinic, $P2_1/n$ (no. 14), $a = 7.582(5)$ Å, $b = 11.059(8)$ Å, $c = 10.734(8)$ Å, $\beta = 99.661(8)°$, $V = 887.3(11)$ Å^3, $Z = 4$, $R_{gt}(F) = 0.0331$, $wR_{ref}(F^2) = 0.0951$, $T = 296(2)$ K.

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The crystal structure is shown in the figure. Tables 1 and 2 contain details on crystal structure and measurement conditions and a list of the atoms including atomic coordinates and displacement parameters.

Source of material

The title compound was prepared by the coupling reaction of 4,6-dichloropyrimidine and phenyl boronic acid as described in literature [3]. The raw product was recrystallized from dichloromethane/petroleum ether solution at room temperature to give crystals suitable for single-crystal X-ray diffraction.

Table 1: Data collection and handling.

Crystal:	Colourless block
Size:	0.48 × 0.28 × 0.14 mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ:	3.8 cm^{-1}
Diffractometer, scan mode:	Bruker SMART, φ and ω
$2\theta_{max}$, completeness:	51°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	6589, 1654, 0.023
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 1325
$N(param)_{refined}$:	118
Programs:	Bruker programs [1], SHELX [2]

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2).

Atom	x	y	z	U_{iso}*/U_{eq}
C1	0.0611(2)	0.61529(16)	−0.22174(16)	0.0619(5)
H1	−0.0085	0.5956	−0.2989	0.074*
C2	0.1863(2)	0.75619(15)	−0.08883(15)	0.0518(4)
C3	0.2578(2)	0.66938(14)	−0.00256(14)	0.0480(4)
H3	0.3268	0.6902	0.0745	0.058*
C4	0.22202(18)	0.54966(14)	−0.03622(13)	0.0419(3)
C5	0.28960(18)	0.44590(13)	0.04577(13)	0.0419(3)
C6	0.2602(2)	0.32838(15)	0.00023(16)	0.0580(4)
H6	0.2017	0.3160	−0.0821	0.070*
C7	0.3169(2)	0.22981(15)	0.07593(19)	0.0684(5)
H7	0.2945	0.1519	0.0446	0.082*
C8	0.4060(2)	0.24633(15)	0.19720(18)	0.0612(5)
H8	0.4436	0.1800	0.2481	0.073*
C9	0.4390(2)	0.36141(16)	0.24243(16)	0.0581(4)
H9	0.5007	0.3728	0.3241	0.070*
C10	0.3818(2)	0.46126(14)	0.16814(14)	0.0508(4)
H10	0.4052	0.5388	0.2003	0.061*
Cl1	0.22598(8)	0.90829(4)	−0.05308(5)	0.0840(2)
N1	0.12071(18)	0.52285(12)	−0.14841(12)	0.0546(4)
N2	0.08773(19)	0.73314(13)	−0.19951(13)	0.0583(4)

Experimental details

Hydrogen atoms were placed in calculated positions and were included in the refinement using the riding model approximation, with U_{iso}(H) set to 1.2U_{eq}(C).

Discussion

The pyrimidyl heterocycle is a common subunit in many natural products, pharmaceuticals and agrochemicals [4, 5]. In

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addition, some pyrimidines are also used in supramolecular chemistry and organometallic catalysis [6–8]. Therefore, the syntheses of pyrimidines have received a great deal of attention. Compared to conventional methods [9, 10], the direct coupling of halopyrimidine is an alternative approach which does not involve the preparation of product-specific intermediates [11–13]. Here we report the crystal structure of the title compound, derived from the coupling reaction of 4,6-dichloropyrimidine and phenyl boronic acid.

The molecular structure of the title compound is shown in the figure. The pyrimidyl and phenyl ring are approximately coplanar, making a dihedral angle of 5.6°. In the crystal may exist very weak intermolecular C–H$\cdots$Cl (H$\cdots$Cl = 2.906 Å) and π-π interactions between the pyrimidyl and phenyl ring (the interplane distances are about 3.822 Å), which construct the lamellar structure.

All geometric parameters are in the expected ranges.

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