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Crystal structure of 6-chloro-*N*-methylpyrimidin-4-amine, C₅H₆ClN₃

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Abstract

C₅H₆ClN₃, monoclinic, $P2_1/c$ (no. 14), $a = 3.8335(2)$ Å, $b = 11.1158(7)$ Å, $c = 15.4294(7)$ Å, $\beta = 94.901(5)^\circ$, $V = 655.07(6)$ Å³, $Z = 4$, $R_{\text{gt}}(F) = 0.0388$, $wR_{\text{ref}}(F^2) = 0.0960$, $T = 293$ K.

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The asymmetric unit of the title 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 purchased from a commercial source. Colorless needle crystals of the title compound were obtained through solvent evaporation method dichloromethane at room temperature.

Experimental details

The data were collected on a Rigaku Saturn 724 CCD diffractometer at temperature of 293 K. All hydrogen atoms were added using the corresponding AFIX options of the SHELX system [16].

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Table 1: Data collection and handling.

Crystal:	Colourless block
Size:	0.28 × 0.24 × 0.21 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	0.49 mm ⁻¹
Diffractometer, scan mode:	SuperNova, ω
θ_{max} , completeness:	25.5°, 99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	3522, 1208, 0.020
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 982
$N(\text{param})_{\text{refined}}$:	83
Programs:	CrysAlisPro [16], Olex2 [17], SHELX [18]

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²).

Atom	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Cl1	0.51357(17)	0.54368(6)	0.86351(3)	0.0636(3)
N1	0.8816(5)	0.44206(15)	0.60916(11)	0.0469(4)
N2	0.7316(5)	0.39042(16)	0.75215(11)	0.0525(5)
N3	0.8242(5)	0.63451(16)	0.55638(10)	0.0509(5)
H3	0.9070	0.6071	0.5102	0.061*
C1	0.8454(6)	0.3676(2)	0.67434(14)	0.0523(6)
H1	0.9078	0.2881	0.6648	0.063*
C2	0.6483(5)	0.5060(2)	0.76228(13)	0.0454(5)
C3	0.6649(5)	0.59374(18)	0.70129(12)	0.0435(5)
H3A	0.5985	0.6726	0.7116	0.052*
C4	0.7879(5)	0.55855(18)	0.62193(12)	0.0414(5)
C5	0.7318(7)	0.7604(2)	0.55876(15)	0.0613(6)
H5A	0.7848	0.7983	0.5055	0.092*
H5B	0.8633	0.7985	0.6069	0.092*
H5C	0.4861	0.7681	0.5654	0.092*

Comment

Pyrimidine is a key structural component of a variety of important biological molecules [1–3]. A large number of pyrimidine derivatives have been reported to exhibit a variety of biological activities, including antibacterial [4–6], antiviral [7, 8], antioxidant [9, 10], anti-proliferative [11], anti-inflammatory [12], antiplasmodial [13] and anticancer [14, 15].

Geometric parameters of the title molecule are in the expected ranges. Adjacent molecules pairwise form a dimer due to intermolecular N3–H3...N1 hydrogen bonds. The bond length of H3...N1 is 2.15 Å typical for weak NH...N hydrogen bond. On the other hand, there is no C–H...Cl

hydrogen bond due to weak π - π stacking interactions and the steric hindrance of $-\text{CH}_3$.

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