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Crystal structure of 5-bromo-2-(naphthalen-6-yl)pyridine, C₁₅H₁₀BrN

Table 1: Data collection and handling.

Crystal:	Colourless prism
Size:	0.20 × 0.18 × 0.15 mm
Wavelength:	Cu K α radiation (1.54184 Å)
μ :	4.56 mm ⁻¹
Diffractometer, scan mode:	Xcalibur, ω
$\theta_{\max}$, completeness:	67.1°, >99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	4263, 2078, 0.026
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 1651
$N(\text{param})_{\text{refined}}$:	154
Programs:	SHELX [1], CrysAlis ^{PRO} [2]

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Abstract

C₁₅H₁₀BrN, monoclinic, $P2_1/c$ (no. 14), $a = 14.6998(9)$ Å, $b = 5.9337(4)$ Å, $c = 14.6275(11)$ Å, $\beta = 113.542(8)^\circ$, $V = 1169.67(15)$ Å³, $Z = 4$, $R_{\text{gt}}(F) = 0.0396$, $wR_{\text{ref}}(F^2) = 0.1103$, $T = 293(2)$ 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 obtained from the palladium-catalyzed Suzuki coupling of naphthalen-2-yl-2-boronic acid and 2,5-dibromopyridine, which were prepared according to the published procedures [3]. The product was recrystallized from dichloromethane/petroleum ether at room temperature to give the desired crystals suitable for single-crystal X-ray diffraction.

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

Atom	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Br1	0.55224(3)	0.57982(9)	0.68324(3)	0.0684(2)
C1	1.3067(2)	0.2805(6)	1.0306(2)	0.0460(8)
H1	1.3278	0.1460	1.0653	0.055*
C2	1.3753(2)	0.4336(7)	1.0287(3)	0.0498(9)
H2	1.4427	0.4024	1.0617	0.060*
C3	1.3449(3)	0.6360(6)	0.9776(3)	0.0497(9)
H3	1.3923	0.7385	0.9764	0.060*
C4	1.2463(2)	0.6867(6)	0.9288(3)	0.0439(8)
H4	1.2274	0.8235	0.8955	0.053*
C5	1.1730(2)	0.5323(5)	0.9289(2)	0.0369(7)
C6	1.2036(2)	0.3242(6)	0.9803(2)	0.0373(7)
C7	1.1299(2)	0.1704(6)	0.9792(2)	0.0414(8)
H7	1.1486	0.0340	1.0129	0.050*
C8	1.0318(2)	0.2190(5)	0.9296(2)	0.0391(7)
H8	0.9849	0.1136	0.9294	0.047*
C9	0.9991(2)	0.4255(5)	0.8784(2)	0.0333(7)
C10	1.0703(2)	0.5777(5)	0.8789(2)	0.0364(7)
H10	1.0502	0.7140	0.8456	0.044*
C11	0.8910(2)	0.4740(5)	0.8288(2)	0.0350(7)
C12	0.8538(2)	0.6739(6)	0.7784(3)	0.0436(8)
H12	0.8971	0.7836	0.7741	0.052*
C13	0.7527(2)	0.7101(6)	0.7346(3)	0.0451(8)
H13	0.7267	0.8430	0.7005	0.054*
C14	0.6917(2)	0.5428(6)	0.7432(2)	0.0435(8)
C15	0.7324(2)	0.3472(6)	0.7938(3)	0.0476(9)
H15	0.6900	0.2357	0.7986	0.057*
N1	0.8298(2)	0.3115(5)	0.8360(2)	0.0440(7)

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Experimental details

Hydrogen atoms were added using the riding models implemented in the SHELX system.

Comment

Pyridines are an important class of *N*-containing heterocyclic compounds for natural products, pharmaceuticals [4]. Moreover, some aryl-pyridines are used in functional materials, supramolecular chemistry and organometallic catalysis [5–8]. Among several methods for their synthesis, the Suzuki coupling has become an extremely useful method for the formation of carbon-carbon [9–12]. It is known that the 2-pyridyl boronic acid was not stable [10]. Thus we prepared the title compound from the Suzuki coupling of naphthalen-2-yl-2-boronic acid and 2,5-dibromopyridine (the ratio of 1:1).

A view of the molecular structure of the title compound is given in the figure. The pyridine ring and naphthalene ring are coplanar, which is similar to those of related aryl-*N*-heterocyclic derivatives [13, 14]. The bromine and nitrogen atom in pyrimidine ring do not participate in hydrogen bonds.

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