Hong-Mei Li*, Hao-Feng Wang, Bei-Jing Sun and Xin-Hua Lou

Crystal structure of 5-bromo-2-(naphthalen-6-yl)pyridine, C_{15}H_{10}BrN

Abstract

C_{15}H_{10}BrN, monoclinic, P2_1/c (no. 14), a = 14.6998(9) Å, b = 5.9337(4) Å, c = 14.6275(11) Å, β = 113.542(8)°, V = 1169.67(15) Å³, Z = 4, R_{gt}(F) = 0.0396, wR_{ref}(F²) = 0.1103, T = 293(2) K.

CCDC no.: 1848649

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 1: Data collection and handling.

<table>
<thead>
<tr>
<th>Atom</th>
<th>x</th>
<th>y</th>
<th>z</th>
<th>U_{iso}/U_{eq}</th>
</tr>
</thead>
<tbody>
<tr>
<td>Br1</td>
<td>0.55224(3)</td>
<td>0.57982(9)</td>
<td>0.68324(3)</td>
<td>0.0684(2)</td>
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<tr>
<td>C1</td>
<td>1.3067(2)</td>
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<td>1.0306(2)</td>
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<tr>
<td>H1</td>
<td>1.3278</td>
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<td>1.0653</td>
<td>0.055*</td>
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<tr>
<td>C2</td>
<td>1.3753(2)</td>
<td>0.4336(7)</td>
<td>1.0287(3)</td>
<td>0.0498(9)</td>
</tr>
<tr>
<td>H2</td>
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<td>1.0617</td>
<td>0.060*</td>
</tr>
<tr>
<td>C3</td>
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<td>0.6360(6)</td>
<td>0.9776(3)</td>
<td>0.0497(9)</td>
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<tr>
<td>H3</td>
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<td>0.9764</td>
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<td>C4</td>
<td>1.2463(2)</td>
<td>0.6867(6)</td>
<td>0.9288(3)</td>
<td>0.0439(8)</td>
</tr>
<tr>
<td>H4</td>
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<td>0.8235</td>
<td>0.9855</td>
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<td>C5</td>
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<td>0.0369(7)</td>
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<td>0.9803(2)</td>
<td>0.0373(7)</td>
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<td>0.9792(2)</td>
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<tr>
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<td>1.0129</td>
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</tr>
<tr>
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<tr>
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<td>0.9294</td>
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<td>0.7005</td>
<td>0.054*</td>
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<td>0.0476(9)</td>
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</tr>
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<td>0.8360(2)</td>
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</table>

*Corresponding author: Hong-Mei Li, College of Chemistry and Chemical Engineering, and Henan Key Laboratory of Function-Oriented Porous Materials, Luoyang Normal University, Luoyang 471022, China, e-mail: lhm11197@163.com

Experimental details

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

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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 naphthaline 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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References