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Crystal structure of 2-(2-(6-methylpyridin-2-yl)naphthalen-1-yl)pyrimidine, C₂₀H₁₅N₃

Table 1: Data collection and handling.

Crystal:	Colourless prism
Size:	0.25 × 0.21 × 0.20 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	0.08 mm ⁻¹
Diffractometer, scan mode:	Xcalibur, ω
$\theta_{\max}$, completeness:	26.4°, >99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	8875, 3209, 0.029
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 2347
$N(\text{param})_{\text{refined}}$:	209
Programs:	SHELX [1], CrysAlis ^{PRO} [2]

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

Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} */ <i>U</i> _{eq}
C1	−0.19379(16)	0.56128(13)	0.20289(9)	0.0593(5)
H1	−0.1931	0.5983	0.2401	0.071*
C2	−0.27880(17)	0.58019(14)	0.15845(10)	0.0659(5)
H2	−0.3361	0.6295	0.1653	0.079*
C3	−0.28046(16)	0.52534(14)	0.10216(9)	0.0629(5)
H3	−0.3401	0.5377	0.0721	0.075*
C4	−0.19588(14)	0.45402(13)	0.09089(8)	0.0530(4)
H4	−0.1975	0.4195	0.0528	0.064*
C5	−0.10513(12)	0.43163(11)	0.13655(7)	0.0413(4)
C6	−0.10589(13)	0.48648(11)	0.19413(7)	0.0458(4)
C7	−0.01786(14)	0.46511(13)	0.24054(7)	0.0519(4)
H7	−0.0174	0.5007	0.2783	0.062*
C8	0.06620(14)	0.39345(12)	0.23098(7)	0.0487(4)
H8	0.1221	0.3798	0.2627	0.058*
C9	0.07072(12)	0.33889(10)	0.17365(7)	0.0403(4)
C10	−0.01337(11)	0.35911(10)	0.12634(7)	0.0371(3)
C11	−0.00324(11)	0.30969(10)	0.06321(7)	0.0366(3)
C12	−0.08204(13)	0.20918(13)	−0.01149(8)	0.0531(4)
H12	−0.1451	0.1704	−0.0268	0.064*
C13	0.02105(14)	0.21744(13)	−0.04707(8)	0.0537(4)
H13	0.0314	0.1823	−0.0846	0.064*
C14	0.10793(13)	0.28010(13)	−0.02450(8)	0.0528(4)
H14	0.1775	0.2896	−0.0485	0.063*
C15	0.16500(12)	0.26159(11)	0.16536(7)	0.0410(4)
C16	0.28196(13)	0.27394(13)	0.18914(8)	0.0517(4)
H16	0.3024	0.3304	0.2121	0.062*
C17	0.36596(14)	0.20157(15)	0.17812(9)	0.0599(5)
H17	0.4441	0.2081	0.1939	0.072*
C18	0.33442(14)	0.11936(14)	0.14368(8)	0.0567(5)
H18	0.3914	0.0707	0.1346	0.068*
C19	0.21613(14)	0.11007(12)	0.12260(7)	0.0479(4)

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Abstract

C₂₀H₁₅N₃, orthorhombic, *Pbca* (no. 61), *a* = 11.0487(4) Å, *b* = 13.5000(6) Å, *c* = 21.1032(10) Å, *V* = 3147.7(2) Å³, *Z* = 8, *R*_{gt}(*F*) = 0.0448, *wR*_{ref}(*F*²) = 0.1136, *T* = 293(2) K.

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The molecular structure is shown in the figure. Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

Source of material

The title compound was obtained from the ruthenium-catalyzed C–H arylation of 2-(1-naphthyl)pyrimidine and 2-chloro-4-methylpyridine as described in literature [3]. The product was recrystallized from dichloromethane/petroleum ether solution at room temperature to give the desired crystals suitable for single-crystal X-ray diffraction.

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Table 2 (continued)

Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} [*] / <i>U</i> _{eq}
C20	0.17532(17)	0.02074(13)	0.08638(9)	0.0676(5)
H20A	0.1286	−0.0214	0.1137	0.101*
H20B	0.2447	−0.0148	0.0712	0.101*
H20C	0.1265	0.0412	0.0511	0.101*
N1	−0.09573(10)	0.25429(9)	0.04400(6)	0.0459(3)
N2	0.09761(10)	0.32820(10)	0.03034(6)	0.0451(3)
N3	0.13268(11)	0.17967(9)	0.13382(6)	0.0437(3)

Experimental details

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

Comment

The pyrimidyl moiety is an important component of several key biomolecules, has been employed in pharmaceuticals [4–6]. Some pyrimidines are also used in supramolecular chemistry and organometallic chemistry as ligands [7–9]. Consequently, numerous approaches to their synthesis have been reported [10, 11]. Recently, metal-catalyzed C–H activation of arylpyrimidines has received extensive attention [3, 12, 13].

A view of the molecular structure of the title compound is given in the figure. The molecule is not planar, the dihedral angle (62.3°) between the pyrimidyl and naphthalene ring is larger than that between the pyridine and naphthalene ring (35.4°). The pyrimidyl and pyridine ring are not coplanar too (50.0°). Owing to the CH/π interaction between CH of a methyl group and pyrimidyl ring [14], the methyl and nitrogen atom of pyridine ring are oriented toward the pyrimidyl ring. In the crystal there exist weak intermolecular C–H⋯N hydrogen bonds [15] (H⋯N = 2.576 Å) between a nitrogen atom and the adjacent CH group of pyrimidine, while the nitrogen atom of pyrimidine does not participate in hydrogen bonding in related arylpyrimidines [16, 17].

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