Guo-Kai Jia, Chen Xiu-Wen, Lv Jing-Kun and Xiao-Ming Chen*

Crystal structure of 2-(naphthalen-2-yl)-1,8-naphthyridine, C₁₈H₁₂N₂

<https://doi.org/10.1515/ncrs-2019-0061>

Received January 19, 2019; accepted March 5, 2019; available online May 22, 2019

Abstract

C₁₈H₁₂N₂, monoclinic, $P2_1/c$ (no. 14), $a = 27.514(5)$ Å, $b = 6.3231(11)$ Å, $c = 7.4175(13)$ Å, $\beta = 95.805(2)^\circ$, $V = 1283.8(4)$ Å³, $Z = 4$, $R_{\text{gt}}(F) = 0.0439$, $wR_{\text{ref}}(F^2) = 0.1233$, $T = 296(2)$ K.

CCDC no.: 1901187

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

Under N₂ atmosphere, *t*-BuOK (50 mol%), xantphos (3 mol%), Ru₃(CO)₁₂ (1 mol%), (2-aminopyridin-3-yl) methanol (0.5 mmol), 1-(naphthalen-2-yl)ethan-1-one (0.5 mmol) and *t*-amyl alcohol (1.0 mL) were introduced in

Table 1: Data collection and handling.

Crystal:	Yellow block
Size:	0.36 × 0.30 × 0.24 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	0.08 mm ⁻¹
Diffractometer, scan mode:	Bruker APEX-II, φ and ω
θ_{max} , completeness:	27.3°, >99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	13579, 2862, 0.020
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 2245
$N(\text{param})_{\text{refined}}$:	181
Programs:	Bruker [1], SHELX [2], Olex2 [3]

a Schlenk tube (25 mL), successively. Then, the Schlenk tube was closed and the resulting mixture was stirred at 403 K for 5 h. After cooling to room temperature, the reaction mixture was concentrated under vacuum, and the residue was purified by preparative TLC on silica, eluting with petroleum ether (333–363 K): ethyl acetate (5:1, v/v) to give 2-(naphthalen-2-yl)-1,8-naphthyridine as a yellow solid (103.7 mg, 81% yield).

Experimental details

Hydrogen atoms were placed in their geometrically idealized positions and constrained to ride on their parent atoms.

Comment

1,8-Naphthyridine and their derivatives are both structure moieties commonly found in bioactive compounds and versatile synthetic intermediates for the preparation of drug-like molecules [4–7]. The syntheses of these compounds have attracted much attention in industrial and academic research due to their biological and pharmaceutical properties. 1,8-Naphthyridines and naphthalene [8] are common substructures in natural products. To synthesize and/or introduce these simple structures to complex molecules would not only have significant potential biological applications but also represent a significant contribution to synthetic methodologies. However, the crystal structure of 2-(naphthalen-2-yl)-1,8-naphthyridine has not been reported before only a related complex is known [9].

As in our previous study [10, 11], the title compound, built up by the C₁₈H₁₂N₂ molecules, has been synthesized.

*Corresponding author: Xiao-Ming Chen, Department of Biology and Chemistry, Hunan University of Science and Engineering, Yongzhou Hunan 425199, People's Republic of China; and Hunan HengWei Pharmaceutical Co., Ltd, Yongzhou Hunan 425199, People's Republic of China, e-mail: 45737620@qq.com

Guo-Kai Jia: Department of Biology and Chemistry, Hunan University of Science and Engineering, Yongzhou Hunan 425199, People's Republic of China; and Hunan Key Laboratory of Comprehensive Utilization of Advantage Plants Resources of Hunan South, Hunan University of Science and Engineering, Yongzhou Hunan 425199, People's Republic of China

Chen Xiu-Wen: School of Biotechnology and Health Sciences, Wuyi University, Jiangmen 529020, People's Republic of China

Lv Jing-Kun: Hunan HengWei Pharmaceutical Co., Ltd, Yongzhou Hunan 425199, People's Republic of China

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

Atom	x	y	z	<i>U</i> _{iso} [*] / <i>U</i> _{eq}
N1	0.10055(4)	0.46526(19)	0.74640(16)	0.0535(3)
N2	0.17913(4)	0.52998(16)	0.87154(14)	0.0417(3)
C1	0.04647(5)	0.7524(3)	0.6512(2)	0.0594(4)
H1	0.0158	0.7931	0.5982	0.071*
C2	0.05829(5)	0.5394(3)	0.6747(2)	0.0585(4)
H2	0.0343	0.4412	0.6365	0.070*
C3	0.13559(4)	0.6105(2)	0.80191(16)	0.0407(3)
C4	0.21444(4)	0.66502(19)	0.92501(15)	0.0379(3)
C5	0.26233(4)	0.57577(19)	0.99495(15)	0.0381(3)
C6	0.26498(5)	0.3769(2)	1.08411(16)	0.0428(3)
H6	0.2363	0.3044	1.1002	0.051*
C7	0.30872(5)	0.2907(2)	1.14623(17)	0.0472(3)
H7	0.3095	0.1606	1.2049	0.057*
C8	0.35313(5)	0.3952(2)	1.12336(16)	0.0451(3)
C9	0.39936(5)	0.3098(3)	1.18509(19)	0.0588(4)
H9	0.4013	0.1795	1.2435	0.071*
C10	0.44096(6)	0.4166(3)	1.1597(2)	0.0693(5)
H10	0.4711	0.3585	1.2011	0.083*
C11	0.20791(5)	0.8865(2)	0.91738(18)	0.0452(3)
H11	0.2334	0.9758	0.9599	0.054*
C12	0.16456(5)	0.9687(2)	0.84820(18)	0.0478(3)
H12	0.1600	1.1144	0.8424	0.057*
C13	0.12665(4)	0.8308(2)	0.78540(16)	0.0430(3)
C14	0.08064(5)	0.8994(2)	0.70737(19)	0.0539(4)
H14	0.0737	1.0429	0.6945	0.065*
C15	0.30521(4)	0.6807(2)	0.97272(16)	0.0408(3)
H15	0.3038	0.8115	0.9150	0.049*
C16	0.35106(4)	0.5952(2)	1.03508(16)	0.0426(3)
C17	0.43908(5)	0.6128(3)	1.0719(2)	0.0653(4)
H17	0.4679	0.6834	1.0549	0.078*
C18	0.39533(5)	0.7010(3)	1.01124(19)	0.0540(4)
H18	0.3945	0.8318	0.9537	0.065*

The single crystal structure verifies that all bond lengths are in normal ranges. The angles between the best planes of the naphthalene unit and the naphthyridine is 31.18(3)° (see the figure).

Acknowledgements: The work was supported by the opening project of key laboratory of comprehensive utilization of advantage plants resources in Hunan south, Hunan university of science and engineering (XNZW17C05); Foundation for

Young Talents (Construction of *N*-Biheteroarenes by hydrogen transfer strategy and its antitumor activity); The Planned Science and Technology Project of Hunan YongZhou, China (NO. 2018ZD15); The major development project of Hunan Province, China (NO.2017SK2204).

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