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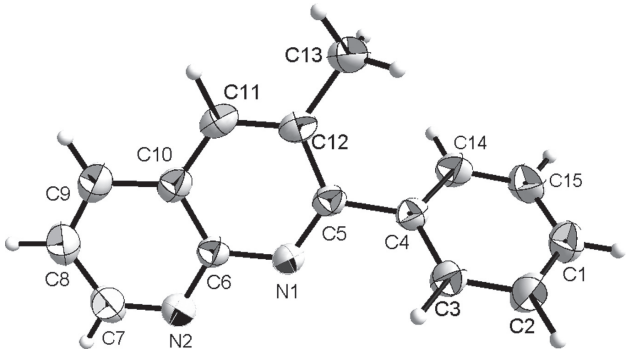
# Crystal structure of 3-methyl-2-phenyl-1,8-naphthyridine, $C_{15}H_{12}N_2$

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**Abstract**

$C_{15}H_{12}N_2$, monoclinic, $P2_1/c$ (no. 14), $a = 7.323(4)$ Å, $b = 6.975(3)$ Å, $c = 22.411(11)$ Å, $\beta = 93.195(5)°$, $V = 1143.0(10)$ Å$^3$, $Z = 4$, $R_{gt}(F) = 0.0457$, $wR_{ref}(F^2) = 0.1324$, $T = 296(2)$ 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

Under $N_2$ atmosphere, *t*-BuOK (50 mol%), Xantphos (3 mol%), $Ru_3(CO)_{12}$ (1 mol%), (2-aminopyridin-3-yl)methanol (0.5 mmol), and propiophenone (0.5 mmol) were introduced in a Schlenk tube (25 mL), successively. Then, the Schlenk tube was closed and the resulting mixture was stirred in *t*-amyl alcohol (1.0 mL) at 383 K for 5 h. When the reaction was completed (monitored by TLC), the mixture was cooled to room temperature, the reaction mixture was concentrated by removing the solvent under vacuum, and the residue was purified by preparative TLC on silica, eluting with petroleum ether (333–363 K): ethyl acetate (4:1, *v*/*v*) to give 3-methyl-2-phenyl-1,8-naphthyridine as a colourless blocks.

**Table 1:** Data collection and handling.

| | |
|---|---|
| Crystal: | Colourless block |
| Size: | 0.28 × 0.24 × 0.22 mm |
| Wavelength: | Mo *Kα* radiation (0.71073 Å) |
| $\mu$: | 0.08 mm$^{-1}$ |
| Diffractometer, scan mode: | Bruker APEX-II, $\varphi$ and $\omega$ |
| $\theta_{max}$, completeness: | 27.4°, >99% |
| $N(hkl)_{measured}$, $N(hkl)_{unique}$, $R_{int}$: | 12343, 2569, 0.042 |
| Criterion for $I_{obs}$, $N(hkl)_{gt}$: | $I_{obs} > 2\ \sigma(I_{obs})$, 2075 |
| $N(param)_{refined}$: | 155 |
| Programs: | Bruker [1], SHELX [2], Olex2 [3] |

**Table 2:** Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å$^2$).

| Atom | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| N1 | 0.81060(13) | 0.60304(13) | 0.09694(4) | 0.0393(3) |
| N2 | 0.68573(15) | 0.78064(15) | 0.01798(5) | 0.0480(3) |
| C1 | 1.0526(2) | 0.4692(2) | 0.30428(6) | 0.0540(4) |
| H1 | 1.094656 | 0.475351 | 0.344165 | 0.065* |
| C2 | 1.11924(19) | 0.5951(2) | 0.26334(6) | 0.0529(4) |
| H2 | 1.205705 | 0.686573 | 0.275685 | 0.063* |
| C3 | 1.05791(18) | 0.58562(18) | 0.20409(5) | 0.0446(3) |
| H3 | 1.101189 | 0.673068 | 0.176917 | 0.054* |
| C4 | 0.93197(16) | 0.44665(16) | 0.18451(5) | 0.0379(3) |
| C5 | 0.87055(15) | 0.43850(16) | 0.12004(5) | 0.0361(3) |
| C6 | 0.75318(15) | 0.60854(16) | 0.03818(5) | 0.0376(3) |
| C7 | 0.62649(19) | 0.7893(2) | −0.03841(6) | 0.0522(3) |
| H7 | 0.578624 | 0.905328 | −0.052447 | 0.063* |
| C8 | 0.63013(19) | 0.6363(2) | −0.07897(6) | 0.0537(4) |
| H8 | 0.587550 | 0.652134 | −0.118539 | 0.064* |
| C9 | 0.69723(18) | 0.4646(2) | −0.05923(5) | 0.0489(3) |
| H9 | 0.701037 | 0.360759 | −0.085175 | 0.059* |
| C10 | 0.76095(15) | 0.44558(17) | 0.00099(5) | 0.0395(3) |
| C11 | 0.82862(16) | 0.27386(18) | 0.02707(5) | 0.0421(3) |
| H11 | 0.836139 | 0.164719 | 0.003496 | 0.050* |
| C12 | 0.88319(15) | 0.26472(16) | 0.08613(5) | 0.0392(3) |
| C13 | 0.95794(19) | 0.08056(18) | 0.11286(6) | 0.0521(4) |
| H13A | 0.862860 | 0.014456 | 0.132323 | 0.078* |
| H13B | 1.056642 | 0.108915 | 0.141492 | 0.078* |
| H13C | 1.001940 | 0.001026 | 0.081785 | 0.078* |
| C14 | 0.86522(18) | 0.32221(19) | 0.22652(6) | 0.0484(3) |
| H14 | 0.779938 | 0.229246 | 0.214439 | 0.058* |
| C15 | 0.9243(2) | 0.3350(2) | 0.28623(6) | 0.0549(4) |
| H15 | 0.876860 | 0.252574 | 0.314064 | 0.066* |

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## Experimental details

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

## Comment

Nitrogen-containing heterocycles are of great importance in the pharmaceutical and agrochemical industries. Functionalized, nitrogen-containing heterocycles constitute a widespread structural motif in biologically active compounds [4, 5]. In particular, 1,8-naphthyridines are common structural motifs in important compounds. Consequently, the selective construction of such compounds is of significant importance. As part of our continuous research interest in construction of *N*-heterocycles by hydrogen transfer strategy [6–8], we report here a one-pot facile synthesis of 3-methyl-2-phenyl-1,8-naphthyridine. The crystal structure of 3-methyl-2-phenyl-1,8-naphthyridine has not been reported until now. Herein the crystal structure of the title compound is described to enrich the related crystal structures of 3-methyl-2-phenyl-1,8-naphthyridine.

As in our previous study [9, 10], the compound, built up by the $C_{15}H_{12}N_2$ molecules, has been synthesized. The single crystal structure verifies that all bond lengths are in normal ranges. As expected, the naphthyridinyl moiety and the phenyl group are not coplanar (*cf*. the figure).

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