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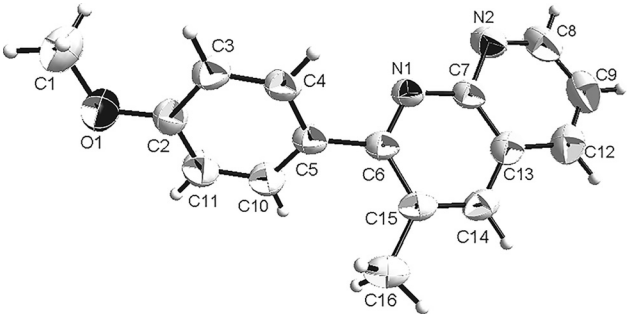
Crystal structure of 2-(4-methoxyphenyl)-3-methyl-1,8-naphthyridine, $C_{16}H_{14}N_2O$



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Abstract

$C_{16}H_{14}N_2O$, monoclinic, $P2_1/c$ (no. 14), a = 6.903(2) Å, b = 7.217(2) Å, c = 26.071(8) Å, β = 93.023(4)°, V = 1296.9(7) Å^3, Z = 4, $R_{gt}(F)$ = 0.0474, $wR_{ref}(F^2)$ = 0.1423, 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.

Table 1: Data collection and handling.

Crystal:	Colourless block
Size:	0.26 × 0.24 × 0.20 mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ:	0.08 mm^{-1}
Diffractometer, scan mode:	Bruker APEX-II, φ and ω
θ_{max}, completeness:	27.7°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	14,057, 2953, 0.047
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 2227
$N(param)_{refined}$:	174
Programs:	Bruker [1], SHELX [2], Olex2 [3]

Source of material

Under N_2 a atmosphere, *t*-BuOK (50 mol%), Xantphos (3 mol%), $Ru_3(CO)_{12}$ (1 mol%), (2-aminopyridin-3-yl)methanol (0.5 mmol), and 1-(4-methoxyphenyl)propan-1-one (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 8 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 2-(4-methoxyphenyl)-3-methyl-1,8-naphthyridine as a colourless blocks.

Experimental details

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

Comment

The 1,8-naphthyridine ring system is an attractive structural motif owing to its wide distribution in bioactive molecules and pharmaceuticals, which include a potent $\alpha_v\beta_3$ receptor antagonist **A**, antibacterial agents **B**, and CETP inhibitor **C** [4]. Recently, some articles describe the synthesis of 1,8-naphthyridines by the hydrogen transfer strategy [5–8]. We here describe the one-pot facile synthesis of 2-(4-methoxyphenyl)-3-methyl-1,8-naphthyridine. However, the crystal structure of 2-(4-methoxyphenyl)-3-methyl-1,8-naphthyridine has not been reported until now. The title compound is described to enrich the structural chemistry of this class of compounds [9, 10].

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

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
O1	0.52135 (17)	0.38716 (16)	0.679694)	0.0696 (3)
N1	0.60958 (15)	0.27562 (16)	0.91744 (4)	0.0496 (3)
N2	0.78826 (18)	0.18212 (19)	0.98981 (5)	0.0634 (4)
C1	0.6785 (3)	0.4878 (3)	0.66002 (7)	0.0755 (5)
H1A	0.673780	0.614090	0.671463	0.113*
H1B	0.668814	0.484442	0.623163	0.113*
H1C	0.798972	0.432771	0.672171	0.113*
C2	0.5072 (2)	0.38309 (19)	0.73184 (5)	0.0519 (3)
C3	0.6282 (2)	0.47898 (19)	0.76663 (6)	0.0536 (4)
H3	0.726756	0.553504	0.755023	0.064*
C4	0.60204 (18)	0.4635 (2)	0.81861 (5)	0.0512 (3)
H4	0.685012	0.527362	0.841646	0.061*
C5	0.45521 (18)	0.35511 (18)	0.83752 (5)	0.0481 (3)
C6	0.44447 (18)	0.32837 (18)	0.89397 (5)	0.0466 (3)
C7	0.61425 (19)	0.24222 (18)	0.96883 (5)	0.0491 (3)
C8	0.7955 (3)	0.1449 (2)	1.03926 (7)	0.0715 (5)
H8	0.912813	0.102215	1.053988	0.086*
C9	0.6409 (3)	0.1643 (2)	1.07152 (6)	0.0727 (5)
H9	0.656644	0.136853	1.106337	0.087*
C10	0.3348 (2)	0.2614 (2)	0.80179 (6)	0.0606 (4)
H10	0.234689	0.188570	0.813228	0.073*
C11	0.360 (2)	0.2739 (2)	0.74981 (6)	0.0632 (4)
H11	0.278687	0.208816	0.726730	0.076*
C12	0.4679 (3)	0.2241 (2)	1.05084 (6)	0.0655 (4)
H12	0.362742	0.238703	1.071351	0.079*
C13	0.4490 (2)	0.26407 (18)	0.99778 (5)	0.0511 (3)
C14	0.2765 (2)	0.3246 (2)	0.97152 (5)	0.0547 (4)
H14	0.165700	0.342120	0.989730	0.066*
C15	0.26912 (18)	0.35771 (18)	0.92006 (5)	0.0503 (3)
C16	0.0860 (2)	0.4292 (2)	0.89283 (6)	0.0672 (4)
H16A	0.029890	0.333618	0.871175	0.101*
H16B	0.116138	0.534625	0.872259	0.101*
H16C	−0.004595	0.464874	0.917732	0.101*

Thedre is one molecule in the asymmetric unit (see the figure). The crystal structure verifies that all bond lengths are in normal ranges [10].

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Conflict of interest statement: The authors declare no conflicts of interest regarding this article.

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