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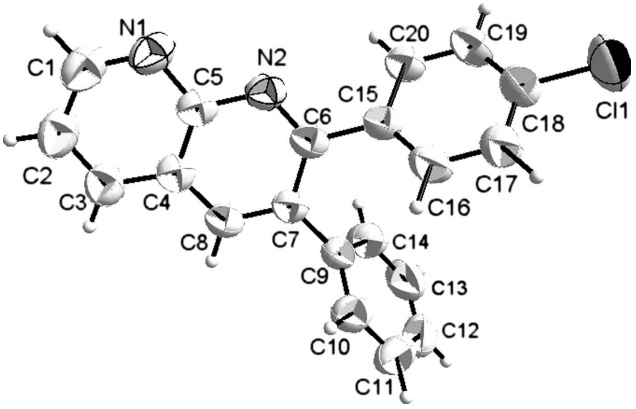
Crystal structure of 2-(4-chlorophenyl)-3-phenyl-1,8-naphthyridine, $C_{20}H_{13}N_2Cl$



https://doi.org/10.1515/ncrs-2018-0275
Received July 30, 2018; accepted October 7, 2018; available online October 15, 2018

Abstract

$C_{20}H_{13}N_2Cl$, monoclinic, $P2_1/n$ (no. 14), $a = 6.179(4)$ Å, $b = 11.666(8)$ Å, $c = 22.460(15)$ Å, $\beta = 95.837°$, $V = 1610.6(19)$ Å^3, $Z = 4$, $R_{gt}(F) = 0.0507$, $wR_{ref}(F^2) = 0.1599$, $T = 296(2)$ K.

CCDC no.: 1843849

The 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

Under N_2 atmosphere, *tert.*-BuOK (50 mol%), Xantphos (3 mol%), $Ru_3(CO)_{12}$ (1 mol%), (2-aminopyridin-3-yl) methanol (0.5 mmol), 1-(4-chlorophenyl)-2-phenylethan-1-ol (0.5 mmol) and *tert.*-amyl alcohol (1.0 mL) were introduced in 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 by removing the solvent under vacuum,

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Table 1: Data collection and handling.

Crystal:	Colorless block
Size:	0.32 × 0.27 × 0.24 mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ:	0.24 mm^{-1}
Diffractometer, scan mode:	Bruker APEX-II, φ and ω-scans
θ_{max}, completeness:	25.5°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	12531, 3334, 0.033
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 2062
$N(param)_{refined}$:	208
Programs:	Bruker programs [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}
Cl1	−0.11456(12)	0.32015(7)	0.44569(3)	0.1187(4)
N1	0.7453(3)	0.51981(14)	0.17572(8)	0.0758(5)
N2	0.5456(3)	0.52907(13)	0.25657(7)	0.0610(4)
C1	0.9010(5)	0.5622(2)	0.14642(10)	0.0852(7)
H1	0.936922	0.521921	0.113051	0.102*
C2	1.0160(4)	0.6620(2)	0.16131(10)	0.0829(7)
H2	1.124782	0.686891	0.138660	0.099*
C3	0.9663(4)	0.72223(19)	0.20942(9)	0.0719(6)
H3	1.038856	0.790201	0.220039	0.086*
C4	0.8038(3)	0.68094(15)	0.24322(8)	0.0584(5)
C5	0.6985(3)	0.57806(16)	0.22508(8)	0.0604(5)
C6	0.4945(3)	0.58075(16)	0.30515(8)	0.0567(5)
C7	0.5828(3)	0.68933(15)	0.32489(8)	0.0562(5)
C8	0.7369(3)	0.73620(16)	0.29356(8)	0.0592(5)
H8	0.799135	0.806063	0.305676	0.071*
C9	0.5032(3)	0.75243(16)	0.37566(8)	0.0602(5)
C10	0.6345(4)	0.76961(19)	0.42816(9)	0.0750(6)
H10	0.775786	0.741038	0.432299	0.090*
C11	0.5567(6)	0.8294(2)	0.47487(11)	0.0950(8)
H11	0.644985	0.839069	0.510578	0.114*
C12	0.3521(6)	0.8742(2)	0.46896(14)	0.1008(9)
H12	0.301837	0.914567	0.500487	0.121*
C13	0.2216(4)	0.8599(2)	0.41720(15)	0.1007(9)
H13	0.082487	0.891201	0.412951	0.121*
C14	0.2960(4)	0.7990(2)	0.37112(11)	0.0830(7)
H14	0.204910	0.788798	0.335938	0.100*
C15	0.3398(3)	0.51849(15)	0.34029(8)	0.0578(5)
C16	0.3816(4)	0.5040(2)	0.40085(10)	0.0827(7)
H16	0.506759	0.536065	0.420588	0.099*

Table 2 (continued)

Atom	x	y	z	U_{iso}*/U_{eq}
C17	0.2435(4)	0.4433(2)	0.43311(10)	0.0896(8)
H17	0.275308	0.434177	0.474199	0.108*
C18	0.0596(4)	0.39664(19)	0.40461(11)	0.0751(6)
C19	0.0141(3)	0.40930(19)	0.34424(11)	0.0766(6)
H19	−0.112417	0.377764	0.324951	0.092*
C20	0.1545(3)	0.46851(17)	0.31188(9)	0.0650(5)
H20	0.124743	0.474992	0.270592	0.078*

and the residue was purified by preparative TLC on silica, eluting with petroleum ether (333–363 K): ethyl acetate (6:1, *v*/*v*) to give 2-(4-chlorophenyl)-3-phenyl-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.

Discussion

1,8-Naphthyridine ring systems are attractive structural motifs because of their wide distribution in bioactive molecules and pharmaceuticals [4, 5]. Hence, there is considerable interest in the development of effective methods for the synthesis of 1,8-naphthyridine and its analogues [6, 7]. However, the crystal structure of 2-(4-chlorophenyl)-3-phenyl-1,8-naphthyridine has not been reported before. Herein the crystal structure of the title compound is described to enrich the related crystal structures of 2-(4-chlorophenyl)-3-phenyl-1,8-naphthyridine.

As in our previous study [8], the title compound, built up by the $C_{20}H_{13}N_2Cl$ molecules, has been synthesized. The single crystal structure verifies that all bond lengths are in normal ranges [8, 9].

Acknowledgements: The work was supported by the Foundation of the Department of Education of Guangdong Province (2016KTSCX144, 2017KZDXM085) and the High-level Scientific Research Foundation for the introduction of talent (AL2018008).

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