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Crystal structure of 2-(4-bromobenzyloxy)-6-chloropyridine, C₁₂H₉BrClNO

Table 1: Data collection and handling.

Crystal:	Colorless block
Size:	0.28 × 0.27 × 0.25 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	3.69 mm ⁻¹
Diffractometer, scan mode:	XtaLAB Synergy, ω
$\theta_{\max}$, completeness:	29.6°, >99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	8608, 2921, 0.059
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 1526
$N(\text{param})_{\text{refined}}$:	145
Programs:	CrysAlis ^{PRO} [1], SHELX [2], Olex2 [3]

<https://doi.org/10.1515/ncrs-2022-0026>

Received January 17, 2022; accepted February 21, 2022;
published online March 7, 2022

Abstract

C₁₂H₉BrClNO, monoclinic, $P2_1/n$ (no. 14), $a = 4.3665(3)$ Å, $b = 22.5576(17)$ Å, $c = 12.1286(10)$ Å, $\beta = 99.028(7)^\circ$, $V = 1179.84(16)$ Å³, $Z = 4$, $R_{\text{gt}}(F) = 0.0595$, $wR_{\text{ref}}(F^2) = 0.1451$, $T = 293$ K.

CCDC no.: 2133175

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 prepared according to the synthetic method reported previously [4]. The crude product was recrystallized from ethanol to afford colorless crystals.

Experimental details

The hydrogen atoms were assigned with isotropic displacement factors $U_{\text{iso}}(\text{H}) = 1.2$ times $U_{\text{eq}}(\text{C, aromatic ring})$, $U_{\text{iso}}(\text{H}) = 1.2$ times $U_{\text{eq}}(\text{CH}_2)$. The final refinement were furnished using geometrical restraints, with C–H = 0.93 Å (aromatic ring), C–H = 0.97 Å (CH₂).

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Comment

Both O-alkylation and N-alkylation of 2-pyridone are important making the resulting molecules to be different in their biological or pharmaceutical properties [5–7].

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

Atom	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Br1	−0.32031 (11)	0.55891 (2)	0.14854 (5)	0.0803 (3)
Cl1	1.2510 (3)	0.18517 (5)	0.45230 (12)	0.0791 (4)
O1	0.6109 (7)	0.36343 (13)	0.4736 (2)	0.0671 (8)
N1	0.9196 (8)	0.28001 (16)	0.4700 (3)	0.0583 (9)
C1	0.8132 (10)	0.3236 (2)	0.5270 (4)	0.0588 (11)
C2	0.8987 (11)	0.3315 (2)	0.6426 (4)	0.0701 (13)
H2	0.8183	0.3625	0.6799	0.084*
C3	1.1051 (11)	0.2919 (3)	0.6984 (4)	0.0773 (14)
H3	1.1686	0.2957	0.7749	0.093*
C4	1.2188 (10)	0.2460 (2)	0.6404 (4)	0.0698 (13)
H4	1.3595	0.2186	0.6762	0.084*
C5	1.1153 (10)	0.2430 (2)	0.5290 (4)	0.0605 (11)
C6	0.5219 (10)	0.35531 (19)	0.3559 (3)	0.0587 (11)
H6A	0.4156	0.3177	0.3414	0.070*
H6B	0.7048	0.3549	0.3197	0.070*
C7	0.3116 (9)	0.40504 (18)	0.3099 (4)	0.0551 (10)
C8	0.2212 (10)	0.4505 (2)	0.3749 (4)	0.0654 (12)
H8	0.2889	0.4504	0.4515	0.079*
C9	0.0346 (10)	0.4956 (2)	0.3284 (4)	0.0701 (13)
H9	−0.0206	0.5261	0.3729	0.084*
C10	−0.0711 (9)	0.49553 (18)	0.2153 (4)	0.0606 (11)
C11	0.0116 (10)	0.45080 (19)	0.1480 (4)	0.0641 (12)
H11	−0.0602	0.4508	0.0717	0.077*
C12	0.2030 (10)	0.4062 (2)	0.1966 (4)	0.0636 (11)
H12	0.2606	0.3760	0.1517	0.076*

There are many kinds of methods for achieving the useful motif. Due to the behavior of proton shuttling and tautomer transformation in those enolizable 2-pyridones itself, often results in an ambident reactivity and these compounds are very sophisticated to handle [8]. Up to now, to set up a regio- or chemo-selective alkylation is a challenge, and the controllable and regioselective synthesis of the N-alkylation and O-alkylation are still intrigued task for many decades.

The asymmetric unit of the title structure contains one molecule (see the figure). All bond lengths and angles are in the expected ranges. The dihedral angle between the phenyl ring and the pyridine ring is 3.8 °C, indicating the slightly twisted molecular conformation.

Author contributions: The author has accepted responsibility for the entire content of this submitted manuscript and approved submission.

Research funding: We thank financial support from Natural Science Foundation of Henan Province (212300410374).

Conflict of interest statement: The author declares no conflicts of interest regarding this article.

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