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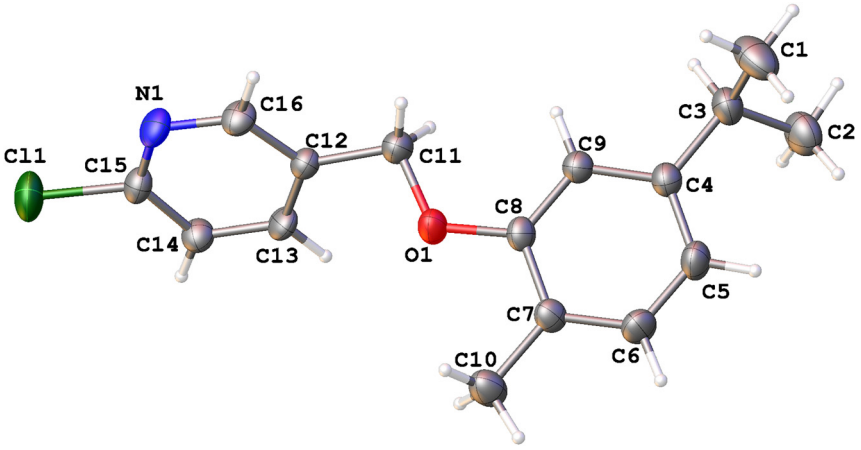
Crystal structure of 2-chloro-5-((5-isopropyl-2-methylphenoxy)methyl)pyridine, $C_{16}H_{18}ClNO$



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Abstract

$C_{16}H_{18}ClNO$, monoclinic, *C*2/*c*, a = 18.6281(16) Å, b = 6.1621(4) Å, c = 27.621(3) Å, β = 108.167(2)°, V = 3012.6(5) Å^3, Z = 8, $R_{gt}(F)$ = 0.0491, w$R_{ref}(F^2)$ = 0.1168, T = 296.15 K.

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The molecular structure is shown in the figure. Table 1 contains the crystallographic data and the list of the atoms including atomic coordinates and displacement parameters can be found in the cif-file attached to this article.

Table 1: Data collection and handling.

Crystal:	Colourless block
Size:	0.50 × 0.40 × 0.30 mm
Wavelength:	MoKα radiation (0.71073 Å)
μ:	0.25 mm^{-1}
Diffractometer, scan mode:	Bruker APEX-II, φ and ω scans
θ_{max}, completeness:	25.1°, 99 %
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	16546, 2667, 0.048
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 1727
$N(param)_{refined}$:	175
Programs:	Bruker,[1] Olex2,[2] SHELX[3,4]

1 Source of material

Carvacrol (300.4 mg, 2.00 mmol), 2-chloro-5-(chloromethyl) pyridine (486.0 mg, 3.00 mmol) and 10.0 mL of *N*,*N*-dimethylformamide were added into a 50 mL three-necked flask, and the reaction was stirred at room temperature. After the completion of the reaction was monitored by TLC (petroleum ether:ethyl acetate = 10:1), the reaction mixture was poured into 100 mL of water. The aqueous layer was extracted with 10 mL of ethyl acetate for three times, and the organic layers were combined, dried over anhydrous sodium sulfate, and then concentrated under reduced pressure to remove the solvent. The obtained substance was separated by column chromatography, and then naturally volatilized in a mixed solvent (petroleum ether:ethyl acetate = 10:1) at room temperature. Colorless block crystals of the title compound were obtained after three days.

2 Experimental details

Hydrogen atoms were added using riding models. Their U_{iso} values were set to 1.2U_{eq} of the parent atoms. The structure

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was solved with the ShelXT[3] structure solution program and refined with the ShelXL.[4]

3 Comment

Monoterpenes are natural products containing 10 carbon atoms, which are polymerized from two isoprene units and exhibit a wide range of biological activities, such as antioxidant,[5] antibacterial[6] and insecticidal[7] activities. To further enhance the insecticidal activity of carvacrol, our group designed and synthesized a series of compounds using an active splicing strategy, among which the title compound represents one.

The crystal structure of the title compound crystallizes in the monoclinic system with the space group *C*2/*c*. In the asymmetric unit, there is one complete 2-chloro-5-((5-isopropyl-2-methylphenoxy)methyl)pyridine molecule. The molecular structure features a monoterpene carvacrol moiety linked to a chloropyridinemethyl moiety *via* an oxygen bridge. The carvacrol framework is characterized by its aromatic ring (C4–C5–C6–C7–C8–C9) with bond lengths of C4–C5 [1.375(3) Å], C5–C6 [1.378(3) Å], C6–C7 [1.379(3) Å], C7–C8 [1.390(3) Å], and C8–C9 [1.383(3) Å]. These bond lengths are comparable to the corresponding bond lengths of the reported carvacrol molecule.[8,9] The phenolic oxygen (O1) in carvacrol forms a covalent bond with C8 [O1–C8 = 1.376(2) Å] and bridges to C11 [O1–C11 = 1.424(3) Å]; the bond angle C8–O1–C11 [118.39(17)°] indicates a bent configuration typical of ether linkages. In the reported analogous structure, the corresponding bond lengths and bond angle are 1.375(3) Å, 1.413(4) Å and 119.0(2)°, respectively.[10] The carvacrol moiety is connected *via* O1–C11 to the chloropyridinemethyl moiety, which constitutes the second aromatic system. This segment includes a pyridine ring (C12–C13–C14–C15–N1–C16) where C12 is linked to C11 [1.494(3) Å]. A chlorine atom is substituted at C15 [Cl1–C15 = 1.744(2) Å], contributing to the molecular polarity. All bond distances are within the normal range. Intermolecular stabilization is provided by an unconventional very weak hydrogen bond between the aromatic C13–H13 and the nitrogen atom N1 of an adjacent molecule [d(C···N) = 3.411(3) Å, ∠C–H···N = 173.8°].

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