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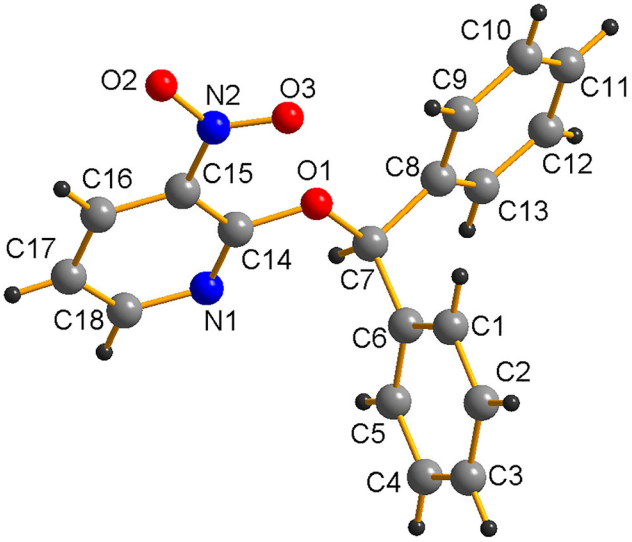
The crystal structure of 2-(benzhydryloxy)-3-nitropyridine, $C_{18}H_{14}N_2O_3$



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Abstract

$C_{18}H_{14}N_2O_3$, monoclinic, $P2_1/n$ (no. 14), a = 8.1644(3) Å, b = 14.5766(6) Å, c = 12.9462(4) Å, β = 91.902(3)°, V = 1539.87(10) Å^3, Z = 4, $R_{gt}(F)$ = 0.0456, $\omega R_{ref}(F^2)$ = 0.1400, T = 293(2) K.

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The crystal 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 materials

The title compound was prepared according to the synthetic method reported in the previous literature [4]. The crude product was recrystallized from ethanol to afford crystals suitable for single crystal X-ray diffraction.

Table 1: Data collection and handling.

Crystal:	Colorless block
Size:	0.25 × 0.22 × 0.16 mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ:	0.09 mm^{-1}
Diffractometer, scan mode:	Bruker SMART, φ and ω-scans
θ_{max}, completeness:	29.6°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	11,916, 3825, 0.027
Criterion for I_{obs}, $N(hkl)_{gt}$:	I_{obs} > 2 σ(I_{obs}), 2796
$N(param)_{refined}$:	208
Programs:	SHELX [1, 2], OLEX2 [3]

Experimental details

The hydrogen atoms were assigned with common isotropic displacement factors U_{iso}(H) = 1.2 times U_{eq}(C, aromatic ring), U_{iso}(H) = 1.2 times U_{eq}(CH). The final refinement was performed using geometrical restraints, with C–H = 0.93 Å (aromatic ring), C–H = 0.98 Å (CH).

Comment

Both O-alkylation and N-alkylation of 2-pyridone are all an important molecular scaffold for there biological and pharmaceutical properties [5–7]. However, based on the Hard–Soft Acid–Base theory, the softer nitrogen atom will tends to bond the softer carbon atom than oxygen. And, the N-alkylation compound is more thermodynamic stable than O-alkylation products. Thus, there are many methods for the N-alkylation of the 2-pyridone moiety, but the absolute selective synthesis of O-alkylated products is even rarer. We have reported the syntheses and the structures of some related compounds [4, 8]. In this paper, we reported the synthesis and structure of the compound 2-(benzhydryloxy)-3-nitropyridine.

The asymmetric unit of the title structure contains one molecule (see the figure). All bond lengths and

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

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.22413 (12)	0.34883 (7)	0.70184 (7)	0.0457 (3)
O2	−0.0318 (3)	0.19323 (19)	0.49957 (14)	0.1493 (10)
O3	0.1047 (2)	0.31363 (16)	0.51760 (10)	0.1089 (7)
N1	0.08023 (17)	0.28975 (9)	0.83617 (9)	0.0503 (3)
N2	0.0288 (2)	0.25240 (13)	0.55302 (11)	0.0702 (5)
C1	0.1894 (2)	0.54946 (11)	0.72630 (12)	0.0515 (4)
H1	0.212180	0.536690	0.657881	0.062*
C2	0.1072 (2)	0.62952 (13)	0.75029 (15)	0.0616 (4)
H2	0.074514	0.670071	0.698113	0.074*
C3	0.0740 (2)	0.64882 (13)	0.85182 (17)	0.0686 (5)
H3	0.018591	0.702364	0.868110	0.082*
C4	0.1226 (3)	0.58936 (14)	0.92843 (15)	0.0709 (5)
H4	0.101048	0.602974	0.996837	0.085*
C5	0.2035 (2)	0.50909 (12)	0.90499 (11)	0.0572 (4)
H5	0.235152	0.468795	0.957659	0.069*
C6	0.23792 (17)	0.48823 (10)	0.80342 (10)	0.0414 (3)
C7	0.32383 (17)	0.39987 (10)	0.77740 (9)	0.0410 (3)
H7	0.339421	0.362967	0.840231	0.049*
C8	0.48808 (17)	0.41507 (10)	0.72895 (11)	0.0438 (3)
C9	0.5069 (2)	0.41189 (12)	0.62327 (12)	0.0565 (4)
H9	0.417345	0.399296	0.579276	0.068*
C10	0.6607 (2)	0.42764 (14)	0.58288 (15)	0.0686 (5)
H10	0.673387	0.424743	0.511830	0.082*
C11	0.7935 (2)	0.44736 (13)	0.64680 (17)	0.0668 (5)
H11	0.895335	0.458300	0.619117	0.080*
C12	0.7755 (2)	0.45088 (13)	0.75159 (16)	0.0636 (5)
H12	0.865197	0.464389	0.795059	0.076*
C13	0.6237 (2)	0.43433 (12)	0.79300 (13)	0.0539 (4)
H13	0.612638	0.436143	0.864237	0.065*
C14	0.10411 (17)	0.29552 (10)	0.73592 (10)	0.0407 (3)
C15	0.00814 (19)	0.24509 (11)	0.66414 (12)	0.0506 (4)
C16	−0.1113 (2)	0.18736 (14)	0.69954 (17)	0.0719 (5)
H16	−0.174327	0.152218	0.653296	0.086*
C17	−0.1365 (3)	0.18224 (14)	0.80361 (18)	0.0793 (6)
H17	−0.217925	0.144893	0.829401	0.095*
C18	−0.0382 (3)	0.23360 (12)	0.86785 (14)	0.0658 (5)
H18	−0.054295	0.229518	0.938483	0.079*

angles are in the expected ranges. The dihedral angle between the phenyl ring (C1/C2/C3/C4/C5/C6), the phenyl ring (C8/C9/C10/C11/C12/C13) and the pyridine ring (C14/C15/C16/C17/C18/N2) are 73.8 °, 77.2 °, and 29.1 °, respectively.

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

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