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Key indicators

Single-crystal X-ray study
 $T = 293$ K
Mean $\sigma(\text{C}-\text{C}) = 0.003$ Å
 R factor = 0.040
 wR factor = 0.113
Data-to-parameter ratio = 12.4For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.

2-Benzyloxy-3-nitropyridine

The molecule of the title compound, $\text{C}_{12}\text{H}_{10}\text{N}_2\text{O}_3$, is non-planar. The nitro group is twisted out of the pyridine ring plane by 31.0 (1) $^\circ$. Inversion-related molecules are arranged in layers.

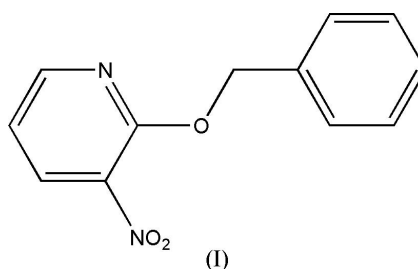
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Comment

We report here the crystal structure of the title compound, (I), which is one of a series of *ortho*-nitroalkoxy pyridines prepared for a study of their photochemical properties.



The bond lengths and angles in (I) are normal (Fig. 1). Atoms O3 and C6 are almost coplanar with the pyridine ring plane, the deviation of atom C6 from the ring plane being only 0.129 (3) Å. In addition, the O3—C6—C7—C12 torsion angle is only 2.5 (2) $^\circ$. The pyridine and benzene ring planes are therefore almost coplanar, with a small dihedral angle of 3.9 (1) $^\circ$.

As observed in many *ortho*-substituted aromatic nitro compounds (Hu *et al.*, 1992; De Ridder *et al.*, 1993; Shiro *et al.*, 1977; Trotter, 1959; Vande Velde *et al.*, 2004; Yeap *et al.*, 1992), the nitro group is twisted out of the pyridine ring plane, in this case by 31.0 (1) $^\circ$, in order to minimize the steric hindrance between atoms O2 and O3. The pyridine and phenyl rings of the centrosymmetrically related molecules are stacked with their centroids 3.736 (2) Å apart, indicating weak π - π stacking

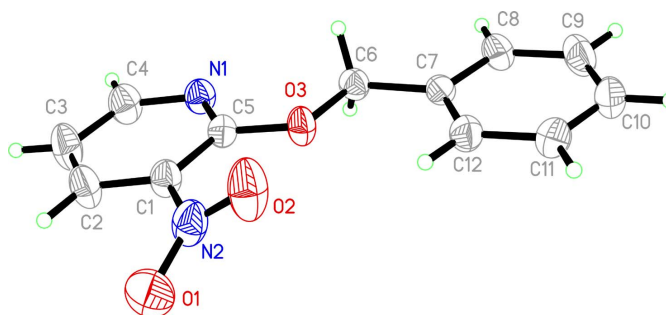


Figure 1

The molecular structure of (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme.

interactions (Fig. 2); the perpendicular distance between the two rings is 3.525 (3) Å. These centrosymmetric molecular pairs are further assembled into layers in the overall crystal packing, as shown in Fig. 3.

Experimental

A solution of benzyl alcohol (55 mmol, 5.940 g) in 50% aqueous NaOH was added to a solution of 2-chloro-3-nitropyridine (50 mmol, 7.925 g) in dichloromethane (150 ml). Tetrabutylammonium bromide (2.5 mmol, 0.378 g) was then added. The mixture was stirred for 10 h at room temperature. Water (150 ml) was then added and the dichloromethane layer was concentrated. The crude product was further purified chromatographically (light petroleum/ethyl ether 3:1) to yield pale-yellow crystals of the title compound (6.763 g, 58.8%, m.p. 315–316 K). IR (KBr, ν cm⁻¹): 3087 (w), 3070 (w), 2930 (w), 2865 (w), 1604 (s), 1518 (s), 1354 (s), 1306 (s), 1250 (s), 1014 (ms), 731 (ms). Mass spectrum: 154 (1.6%), 124 (64.4%), 91 (100%), 65 (17.4%).

Crystal data

C ₁₂ H ₁₀ N ₂ O ₃	Z = 2
M _r = 230.22	D _x = 1.394 Mg m ⁻³
Triclinic, P $\bar{1}$	Mo K α radiation
a = 7.374 (2) Å	Cell parameters from 662 reflections
b = 7.707 (2) Å	θ = 3.0–22.4°
c = 10.928 (3) Å	μ = 0.10 mm ⁻¹
α = 83.340 (4)°	T = 293 (2) K
β = 82.215 (4)°	Block, colourless
γ = 63.269 (3)°	0.28 × 0.20 × 0.14 mm
V = 548.5 (3) Å ³	

Data collection

Bruker SMART CCD area-detector diffractometer	1909 independent reflections
φ and ω scans	1229 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	R _{int} = 0.018
T _{min} = 0.972, T _{max} = 0.986	θ_{max} = 25.0°
2991 measured reflections	h = -7 → 8
	k = -8 → 9
	l = -13 → 11

Refinement

Refinement on F ²	H-atom parameters constrained
R[F ² > 2 σ (F ²)] = 0.040	w = 1/[$\sigma^2(F_o^2) + (0.062P)^2$]
wR(F ²) = 0.113	where P = (F _o ² + 2F _c ²)/3
S = 1.02	(Δ/σ) _{max} < 0.001
1909 reflections	$\Delta\rho_{max}$ = 0.12 e Å ⁻³
154 parameters	$\Delta\rho_{min}$ = -0.19 e Å ⁻³

Table 1

Selected geometric parameters (Å, °).

O1–N2	1.2208 (19)	O3–C6	1.4349 (18)
O2–N2	1.2169 (19)	C6–C7	1.500 (2)
O3–C5	1.3334 (17)		
C5–O3–C6	117.68 (11)	O2–N2–C1	119.16 (16)
C5–N1–C4	117.48 (15)	O1–N2–C1	117.27 (17)
O2–N2–O1	123.53 (17)	O3–C6–C7	107.78 (13)
O2–N2–C1–C2	-148.20 (18)	C5–O3–C6–C7	-176.92 (12)
O1–N2–C1–C2	29.5 (2)	O3–C6–C7–C12	2.5 (2)
C6–O3–C5–C1	176.02 (13)		

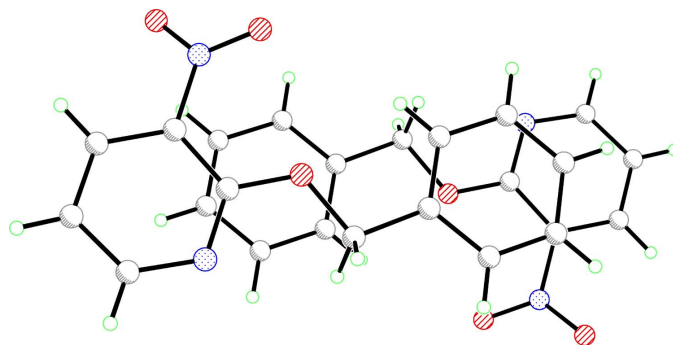


Figure 2

A view of the weak π – π stacking interactions in (I).

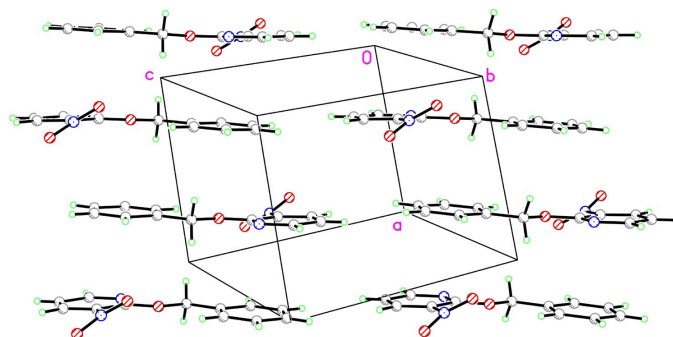


Figure 3

The crystal packing of (I).

H atoms were placed in calculated positions (C–H = 0.93–0.97 Å) and allowed to ride on the parent atoms, with U_{iso} values constrained to be 1.2 U_{eq} of the parent atom.

Data collection: SMART (Bruker, 1997); cell refinement: SAINT (Bruker, 1997); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL (Bruker, 1997); software used to prepare material for publication: SHELXTL.

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