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2-(Naphthalen-2-yloxy)-5-nitropyridine

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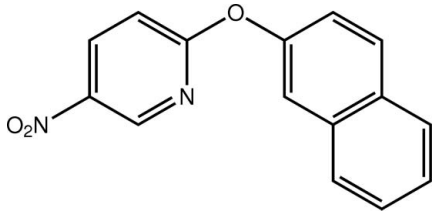
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.054; wR factor = 0.193; data-to-parameter ratio = 14.1.

A nearly orthogonal relationship is found for the ring systems in the title compound, $C_{15}H_{10}N_2O_3$, with the dihedral angle between the rings being 86.13 (11)°. The nitro group is approximately coplanar with the pyridine ring to which it is connected [the O—N—C—C torsion angle = −1.8 (4)°]. This coplanarity allows for the close approach of these residues in the crystal structure enabling the formation of N—O···π(pyridine) interactions [3.547 (4) Å]. Further consolidation of the crystal packing is afforded by weak π–π interactions [centroid–centroid distances = 3.9576 (16) and 3.9822 (16) Å].

Related literature

For the structure of a related nitropyridine derivative, see: Nasir *et al.* (2010). For discussion on nitro-O···π interactions, see: Huang *et al.* (2008).



Experimental

Crystal data

$C_{15}H_{10}N_2O_3$
M_r = 266.25
Monoclinic, $P2_1/c$
a = 6.7389 (12) Å
b = 8.9182 (16) Å
c = 21.072 (4) Å
β = 94.289 (3)°
V = 1262.9 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 293 K
0.25 × 0.20 × 0.15 mm

Data collection

Bruker SMART APEX diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.976, T_{max} = 0.985
6512 measured reflections
2224 independent reflections
1052 reflections with $I > 2\sigma(I)$
R_{int} = 0.052

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.054
$wR(F^2)$ = 0.193
S = 0.94
2224 reflections
158 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.26 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HG5118).

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supplementary materials

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2-(Naphthalen-2-yloxy)-5-nitropyridine

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Comment

In continuation of structural studies of nitro-pyridine derivatives (Nasir *et al.*, 2010), the title compound was synthesized and characterized crystallographically. The molecule of (I), Fig. 1, is highly twisted as seen in the near orthogonal relationship between the two ring systems with the dihedral angle formed between the nitro-pyridine ring and naphthalyl ring being 86.13 (11)°. The nitro group is co-planar with the pyridyl ring to which it is attached with the O2—N2—C4—C3 torsion angle being -1.8 (4)°.

The most prominent feature of the crystal packing appears to be N—O···π interactions (Huang *et al.*, 2008). The distance between O3···π(pyridyl) = 3.547 (4) Å, with the N2—O3···ring centroid(pyridyl)^{i} angle = 81.9 (2)° for symmetry operation *i*: 1 - *x*, 1 - *y*, 1 - *z*. Similar interactions were reported in the crystal structure of 2-(4-methoxyphenoxy)-3-nitropyridine (Nasir *et al.*, 2010). In (I), the N—O···π interactions along with weak π–π interactions, whereby both rings of the naphthalyl residue interact with the pyridyl ring, consolidate the crystal packing. The parameters associated with the π–π interactions are ring centroid(pyridyl)···ring centroid(C6–C11) and (C10–C15) = 3.9822 (16) and 3.9576 (16) Å, respectively, for *ii*: 1 - *x*, -1/2 + *y*, 3/2 - *z*. A view of the crystal packing is shown in Fig. 2.

Experimental

2-Naphthol (2.88 g, 20 mmol) and sodium hydroxide (0.80 g, 20 mmol) were dissolved in water (50 ml) and to the solution was added 2-chloro-5-nitropyridine (3.17 g, 20 mmol) dissolved in THF (50 ml). The mixture was heated for 7 h. Water was added and the organic phase extracted with chloroform. The chloroform solution was dried over sodium sulfate; slow evaporation led to the formation of colourless crystals.

Refinement

Hydrogen atoms were placed at calculated positions (C—H 0.93 Å) and were treated as riding on their parent carbon atoms, with U(H) set to 1.2U_{eq}(C). The naphthalene fused-ring was refined as two fused hexagons with C⋯C distances fixed at 1.39 Å.

Figures

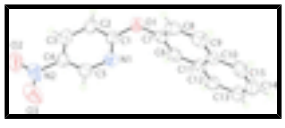

Fig. 1. The molecular structure of (I) showing the atom-labelling scheme and displacement ellipsoids at the 35% probability level.

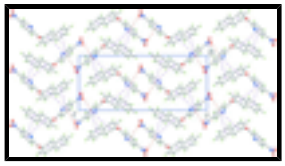

Fig. 2. Unit-cell contents for (I) shown in projection down the *a* axis. The N—O···π and π–π interactions are shown as orange and purple dashed lines, respectively.

2-(Naphthalen-2-yloxy)-5-nitropyridine

Crystal data

$C_{15}H_{10}N_2O_3$	$F(000) = 552$
$M_r = 266.25$	$D_x = 1.400$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: -P 2ybc	Cell parameters from 1499 reflections
$a = 6.7389$ (12) Å	$\theta = 2.5$–$21.3°$
$b = 8.9182$ (16) Å	$\mu = 0.10$ mm^{-1}
$c = 21.072$ (4) Å	$T = 293$ K
$\beta = 94.289$ (3)°	Block, colourless
$V = 1262.9$ (4) Å^3	0.25 × 0.20 × 0.15 mm
$Z = 4$	

Data collection

Bruker SMART APEX diffractometer	2224 independent reflections
Radiation source: fine-focus sealed tube	1052 reflections with $I > 2\sigma(I)$
graphite	$R_{int} = 0.052$
ω scans	$\theta_{max} = 25.0°$, $\theta_{min} = 1.9°$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	$h = -8 \rightarrow 7$
$T_{min} = 0.976$, $T_{max} = 0.985$	$k = -9 \rightarrow 10$
6512 measured reflections	$l = -23 \rightarrow 25$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.054$	H-atom parameters constrained
$wR(F^2) = 0.193$	$w = 1/[\sigma^2(F_o^2) + (0.1P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.94$	$(\Delta/\sigma)_{max} = 0.001$
2224 reflections	$\Delta\rho_{max} = 0.26$ e Å^{-3}
158 parameters	$\Delta\rho_{min} = -0.18$ e Å^{-3}
0 restraints	Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$

Primary atom site location: structure-invariant direct methods

Extinction coefficient: 0.024 (5)

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

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.5816 (3)	0.6709 (3)	0.69203 (11)	0.0864 (8)
O2	0.8327 (5)	0.2782 (3)	0.47200 (13)	0.1210 (11)
O3	0.5363 (6)	0.1958 (4)	0.48260 (14)	0.1319 (12)
N1	0.4532 (4)	0.4809 (3)	0.62772 (12)	0.0709 (8)
N2	0.6776 (7)	0.2766 (4)	0.49811 (14)	0.0929 (10)
C1	0.6029 (5)	0.5686 (4)	0.64546 (14)	0.0662 (8)
C2	0.7856 (5)	0.5678 (4)	0.61964 (15)	0.0796 (10)
H2	0.8868	0.6323	0.6347	0.096*
C3	0.8131 (5)	0.4702 (4)	0.57165 (15)	0.0804 (10)
H3	0.9339	0.4653	0.5531	0.097*
C4	0.6578 (6)	0.3793 (3)	0.55143 (13)	0.0663 (9)
C5	0.4845 (6)	0.3863 (3)	0.58025 (15)	0.0747 (10)
H5	0.3819	0.3219	0.5662	0.090*
C6	0.41265 (19)	0.58487 (18)	0.78172 (8)	0.0638 (8)
H6	0.5213	0.5246	0.7941	0.077*
C7	0.4128 (2)	0.6695 (2)	0.72633 (7)	0.0638 (8)
C8	0.2505 (3)	0.75959 (18)	0.70776 (6)	0.0727 (9)
H8	0.2506	0.8162	0.6707	0.087*
C9	0.0879 (2)	0.76505 (16)	0.74459 (7)	0.0740 (9)
H9	−0.0208	0.8253	0.7322	0.089*
C10	0.08767 (17)	0.68042 (13)	0.79997 (6)	0.0565 (8)
C11	0.25006 (17)	0.59033 (13)	0.81854 (6)	0.0521 (7)
C12	0.2499 (3)	0.50569 (17)	0.87393 (7)	0.0714 (9)
H12	0.3585	0.4454	0.8863	0.086*
C13	0.0873 (3)	0.5111 (2)	0.91075 (7)	0.0822 (10)
H13	0.0872	0.4545	0.9478	0.099*
C14	−0.0751 (3)	0.6012 (2)	0.89219 (8)	0.0864 (11)
H14	−0.1839	0.6049	0.9168	0.104*
C15	−0.07492 (19)	0.6859 (2)	0.83680 (9)	0.0745 (10)
H15	−0.1836	0.7461	0.8244	0.089*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0829 (16)	0.0914 (17)	0.0898 (16)	−0.0342 (13)	0.0385 (13)	−0.0301 (14)
O2	0.158 (3)	0.121 (2)	0.089 (2)	0.032 (2)	0.0437 (19)	−0.0121 (16)
O3	0.164 (3)	0.118 (2)	0.110 (2)	−0.007 (2)	−0.016 (2)	−0.0479 (19)
N1	0.0775 (18)	0.0660 (17)	0.0704 (17)	−0.0159 (14)	0.0136 (14)	−0.0087 (14)
N2	0.133 (3)	0.083 (2)	0.062 (2)	0.023 (2)	0.000 (2)	−0.0026 (18)
C1	0.074 (2)	0.067 (2)	0.0588 (19)	−0.0110 (17)	0.0132 (16)	−0.0046 (16)
C2	0.073 (2)	0.094 (2)	0.074 (2)	−0.0240 (19)	0.0173 (18)	−0.012 (2)
C3	0.085 (3)	0.095 (3)	0.063 (2)	0.000 (2)	0.0180 (19)	0.003 (2)
C4	0.089 (3)	0.063 (2)	0.0475 (18)	0.0060 (18)	0.0089 (17)	0.0015 (15)

C5	0.092 (3)	0.065 (2)	0.067 (2)	−0.0149 (18)	0.0039 (19)	−0.0038 (17)
C6	0.0594 (19)	0.0561 (18)	0.075 (2)	0.0043 (14)	0.0001 (16)	−0.0062 (16)
C7	0.068 (2)	0.0581 (19)	0.066 (2)	−0.0146 (15)	0.0123 (16)	−0.0168 (16)
C8	0.090 (2)	0.061 (2)	0.064 (2)	−0.0162 (18)	−0.0125 (18)	0.0053 (16)
C9	0.064 (2)	0.069 (2)	0.086 (2)	0.0077 (16)	−0.0115 (18)	0.0010 (18)
C10	0.0562 (18)	0.0519 (17)	0.0608 (18)	0.0013 (14)	0.0011 (15)	−0.0056 (14)
C11	0.0529 (17)	0.0497 (16)	0.0535 (17)	0.0008 (13)	0.0023 (13)	−0.0044 (14)
C12	0.083 (2)	0.065 (2)	0.066 (2)	0.0065 (16)	0.0013 (18)	0.0028 (16)
C13	0.114 (3)	0.073 (2)	0.061 (2)	−0.008 (2)	0.016 (2)	0.0011 (17)
C14	0.077 (3)	0.094 (3)	0.092 (3)	−0.009 (2)	0.026 (2)	−0.022 (2)
C15	0.062 (2)	0.077 (2)	0.085 (2)	0.0101 (16)	0.0050 (18)	−0.0151 (19)

Geometric parameters (Å, °)

O1—C1	1.355 (3)	C6—H6	0.9300
O1—C7	1.393 (2)	C7—C8	1.3900
O2—N2	1.217 (4)	C8—C9	1.3900
O3—N2	1.219 (4)	C8—H8	0.9300
N1—C1	1.309 (4)	C9—C10	1.3900
N1—C5	1.337 (4)	C9—H9	0.9300
N2—C4	1.463 (4)	C10—C11	1.3900
C1—C2	1.383 (4)	C10—C15	1.3900
C2—C3	1.358 (4)	C11—C12	1.3900
C2—H2	0.9300	C12—C13	1.3900
C3—C4	1.366 (4)	C12—H12	0.9300
C3—H3	0.9300	C13—C14	1.3900
C4—C5	1.358 (4)	C13—H13	0.9300
C5—H5	0.9300	C14—C15	1.3900
C6—C7	1.3900	C14—H14	0.9300
C6—C11	1.3900	C15—H15	0.9300
C1—O1—C7	120.3 (2)	C8—C7—O1	120.35 (16)
C1—N1—C5	115.4 (3)	C7—C8—C9	120.0
O2—N2—O3	124.5 (4)	C7—C8—H8	120.0
O2—N2—C4	118.0 (4)	C9—C8—H8	120.0
O3—N2—C4	117.5 (4)	C10—C9—C8	120.0
N1—C1—O1	119.2 (3)	C10—C9—H9	120.0
N1—C1—C2	125.1 (3)	C8—C9—H9	120.0
O1—C1—C2	115.7 (3)	C9—C10—C11	120.0
C3—C2—C1	118.1 (3)	C9—C10—C15	120.0
C3—C2—H2	120.9	C11—C10—C15	120.0
C1—C2—H2	120.9	C12—C11—C10	120.0
C2—C3—C4	118.0 (3)	C12—C11—C6	120.0
C2—C3—H3	121.0	C10—C11—C6	120.0
C4—C3—H3	121.0	C13—C12—C11	120.0
C5—C4—C3	119.8 (3)	C13—C12—H12	120.0
C5—C4—N2	120.2 (4)	C11—C12—H12	120.0
C3—C4—N2	119.9 (3)	C12—C13—C14	120.0
N1—C5—C4	123.6 (3)	C12—C13—H13	120.0
N1—C5—H5	118.2	C14—C13—H13	120.0

C4—C5—H5	118.2	C15—C14—C13	120.0
C7—C6—C11	120.0	C15—C14—H14	120.0
C7—C6—H6	120.0	C13—C14—H14	120.0
C11—C6—H6	120.0	C14—C15—C10	120.0
C6—C7—C8	120.0	C14—C15—H15	120.0
C6—C7—O1	119.52 (16)	C10—C15—H15	120.0
C5—N1—C1—O1	178.1 (3)	C1—O1—C7—C8	−94.2 (3)
C5—N1—C1—C2	−1.0 (5)	C6—C7—C8—C9	0.0
C7—O1—C1—N1	8.4 (4)	O1—C7—C8—C9	−175.77 (15)
C7—O1—C1—C2	−172.4 (3)	C7—C8—C9—C10	0.0
N1—C1—C2—C3	0.8 (5)	C8—C9—C10—C11	0.0
O1—C1—C2—C3	−178.3 (3)	C8—C9—C10—C15	180.0
C1—C2—C3—C4	0.5 (5)	C9—C10—C11—C12	180.0
C2—C3—C4—C5	−1.4 (5)	C15—C10—C11—C12	0.0
C2—C3—C4—N2	177.5 (3)	C9—C10—C11—C6	0.0
O2—N2—C4—C5	177.1 (3)	C15—C10—C11—C6	180.0
O3—N2—C4—C5	−2.4 (5)	C7—C6—C11—C12	180.0
O2—N2—C4—C3	−1.8 (4)	C7—C6—C11—C10	0.0
O3—N2—C4—C3	178.7 (3)	C10—C11—C12—C13	0.0
C1—N1—C5—C4	−0.1 (5)	C6—C11—C12—C13	180.0
C3—C4—C5—N1	1.3 (5)	C11—C12—C13—C14	0.0
N2—C4—C5—N1	−177.6 (3)	C12—C13—C14—C15	0.0
C11—C6—C7—C8	0.0	C13—C14—C15—C10	0.0
C11—C6—C7—O1	175.81 (15)	C9—C10—C15—C14	180.0
C1—O1—C7—C6	90.0 (3)	C11—C10—C15—C14	0.0

Fig. 1

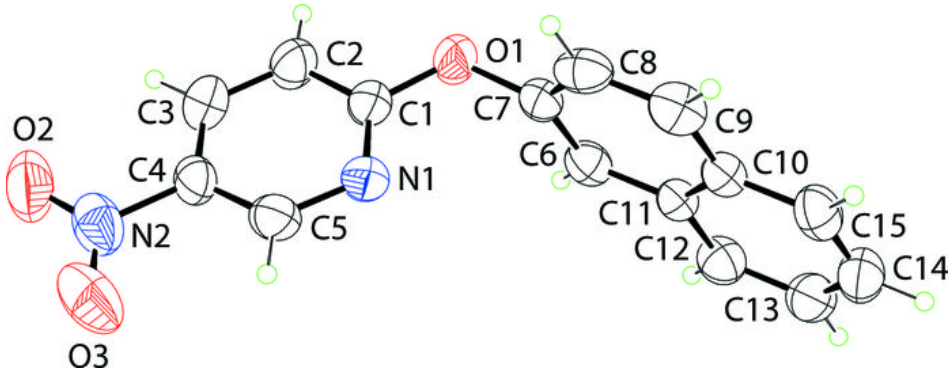
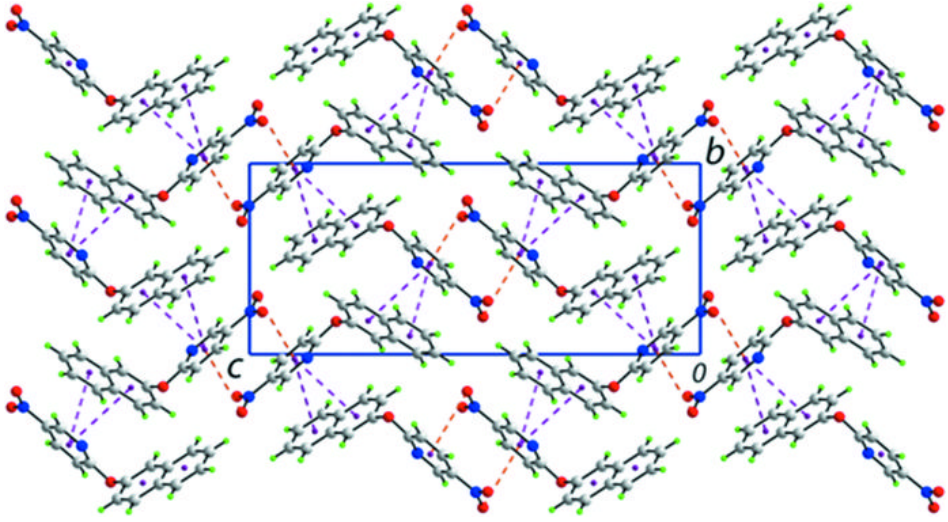
Fig. 2