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

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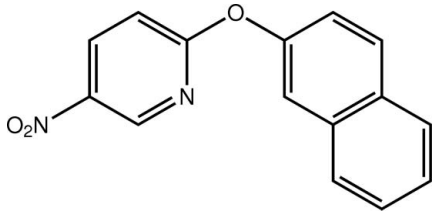
Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(C–C) = 0.003 Å; $R$ factor = 0.054; $wR$ factor = 0.193; data-to-parameter ratio = 14.1.

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···$\pi$(pyridine) interactions [3.547 (4) Å]. Further consolidation of the crystal packing is afforded by weak $\pi$–$\pi$ 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···$\pi$ 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
$\beta$ = 94.289 (3)°
$V$ = 1262.9 (4) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 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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# supporting information

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

**Shah Bakhtiar Nasir, Zainal Abidin Fairuz, Zanariah Abdullah, Seik Weng Ng and Edward R. T. Tiekink**

### S1. 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···$\pi$ interactions (Huang *et al.*, 2008). The distance between O3···$\pi$(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-nitro-pyridine (Nasir *et al.*, 2010). In (I), the N—O···$\pi$ interactions along with weak $\pi$–$\pi$ interactions, whereby both rings of the naphthalyl residue interact with the pyridyl ring, consolidate the crystal packing. The parameters associated with the $\pi$–$\pi$ 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.

### S2. 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.

### S3. 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 1.2$U_{eq}$(C). The naphthalene fused-ring was refined as two fused hexagons with C⋯C distances fixed at 1.39 Å.

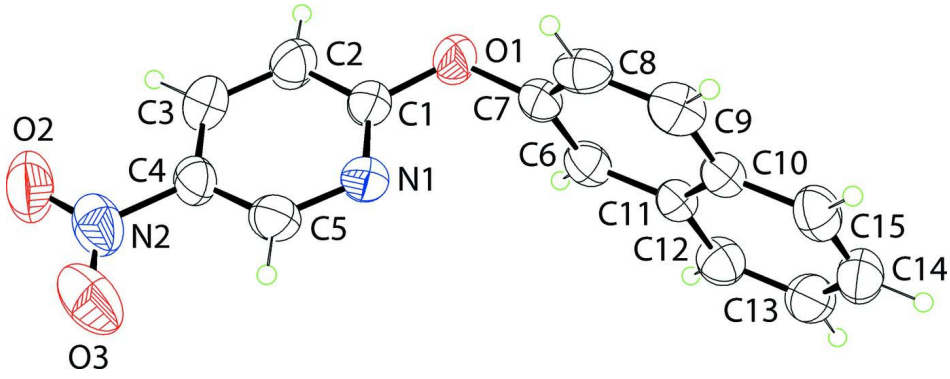


**Figure 1**

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

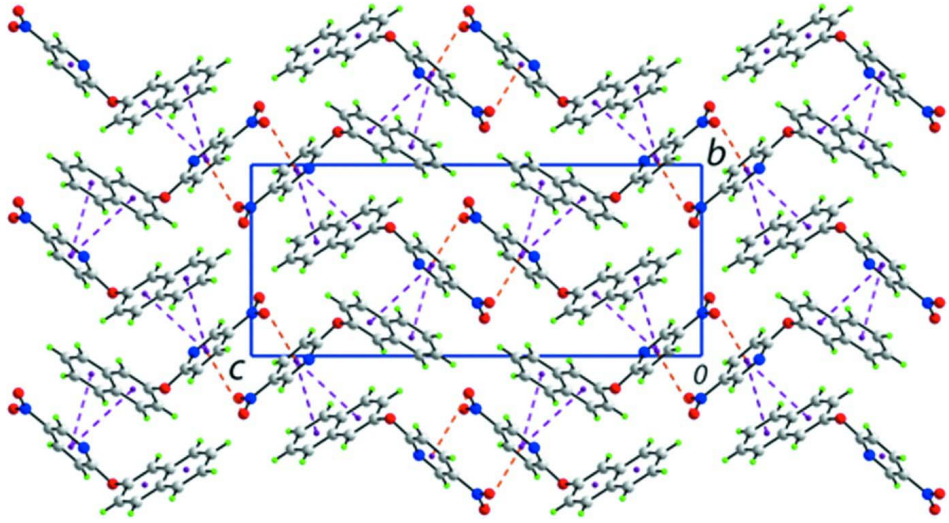


**Figure 2**

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

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*Crystal data*

$C_{15}H_{10}N_2O_3$
$M_r$ = 266.25
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a$ = 6.7389 (12) Å
$b$ = 8.9182 (16) Å
$c$ = 21.072 (4) Å
$\beta$ = 94.289 (3)°
$V$ = 1262.9 (4) Å$^3$
$Z$ = 4

$F(000)$ = 552
$D_x$ = 1.400 Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å
Cell parameters from 1499 reflections
$\theta$ = 2.5–21.3°
$\mu$ = 0.10 mm$^{-1}$
$T$ = 293 K
Block, colourless
0.25 × 0.20 × 0.15 mm

*Data collection*

Bruker SMART APEX diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega$ scans
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
$\theta_{max}$ = 25.0°, $\theta_{min}$ = 1.9°
$h$ = −8→7
$k$ = −9→10
$l$ = −23→25

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.054
$wR(F^2)$ = 0.193
$S$ = 0.94
2224 reflections
158 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.26 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.18 e Å$^{-3}$
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
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 (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| 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, º)*

| | | | |
|---|---|---|---|
| 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 |