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3-Nitrophenyl pyrimidin-2-yl ether

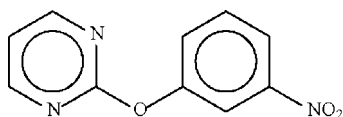
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Key indicators: single-crystal X-ray study; $T = 118$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å;
 R factor = 0.037; wR factor = 0.102; data-to-parameter ratio = 15.5.In the title compound, $\text{C}_{10}\text{H}_7\text{N}_3\text{O}_3$, the dihedral angle between the two aromatic rings is $87.5(1)^\circ$; their *ipso*-C atoms subtend an angle of $117.4(1)^\circ$ at the ether O atom.

Related literature

For the structure of phenyl pyrimidin-2-yl ether, see: Shah Bakhtiar *et al.* (2009).

Experimental

Crystal data

 $\text{C}_{10}\text{H}_7\text{N}_3\text{O}_3$ $M_r = 217.19$ Orthorhombic, *Pbcn* $a = 18.1360(3)$ Å
 $b = 7.3355(1)$ Å
 $c = 14.5986(3)$ Å
 $V = 1942.15(6)$ Å³ $Z = 8$ Mo $K\alpha$ radiation $\mu = 0.11$ mm⁻¹ $T = 118$ K $0.40 \times 0.20 \times 0.15$ mm

Data collection

Bruker SMART APEX CCD
diffractometer
Absorption correction: none
12785 measured reflections2242 independent reflections
1890 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.029$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.037$
 $wR(F^2) = 0.102$
 $S = 1.02$
2242 reflections145 parameters
H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.27$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.29$ e Å⁻³Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2922).

References

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 Shah Bakhtiar, N., Abdullah, Z. & Ng, S. W. (2009). *Acta Cryst.* **E65**, o114.
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supplementary materials

Acta Cryst. (2009). E65, o704 [doi:10.1107/S1600536809007697]

3-Nitrophenyl pyrimidin-2-yl ether

N. Shah Bakhtiar, Z. Abdullah and S. W. Ng

Experimental

3-Nitrophenol (2.78 g, 20 mmol) was mixed with sodium hydroxide (0.08 g, 20 mmol) in several drops of water. The water was then evaporated. The paste was heated with 2-chloropyrimidine (2.30 g, 20 mmol) at 423–433 K for 6 h. The product was dissolved in water and the solution extracted with chloroform. The chloroform phase was dried over sodium sulfate; the evaporation of the solvent gave well shaped very pale brown blocks of (I) 40% yield along with some unidentified brown material.

Refinement

The H-atoms were placed in calculated positions (C—H 0.95 Å) and refined as riding with $U(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

Figures

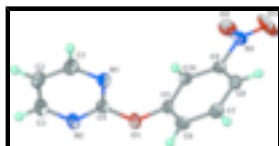


Fig. 1. The molecular structure of (I) with displacement ellipsoids drawn at the 70% probability level. Hydrogen atoms are drawn as spheres of arbitrary radius.

3-Nitrophenyl pyrimidin-2-yl ether

Crystal data

$\text{C}_{10}\text{H}_7\text{N}_3\text{O}_3$

$M_r = 217.19$

Orthorhombic, *Pbcn*

Hall symbol: -P 2n 2ab

$a = 18.1360$ (3) Å

$b = 7.3355$ (1) Å

$c = 14.5986$ (3) Å

$V = 1942.15$ (6) Å³

$Z = 8$

$F_{000} = 896$

$D_x = 1.486$ Mg m⁻³

Mo $K\alpha$ radiation

$\lambda = 0.71073$ Å

Cell parameters from 4130 reflections

$\theta = 2.8$ – 28.2°

$\mu = 0.11$ mm⁻¹

$T = 118$ K

Block, faint brown

$0.40 \times 0.20 \times 0.15$ mm

Data collection

Bruker SMART APEX CCD
diffractometer

Radiation source: fine-focus sealed tube

1890 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.029$

supplementary materials

Monochromator: graphite $\theta_{\max} = 27.5^\circ$
 $T = 120$ K $\theta_{\min} = 2.3^\circ$
 ω scans $h = -23 \rightarrow 23$
Absorption correction: None $k = -9 \rightarrow 9$
12785 measured reflections $l = -18 \rightarrow 18$
2242 independent reflections

Refinement

Refinement on F^2 Secondary atom site location: difference Fourier map
Least-squares matrix: full Hydrogen site location: inferred from neighbouring sites
 $R[F^2 > 2\sigma(F^2)] = 0.037$ H-atom parameters constrained
 $wR(F^2) = 0.102$ $w = 1/[\sigma^2(F_o^2) + (0.0556P)^2 + 0.7122P]$
where $P = (F_o^2 + 2F_c^2)/3$
 $S = 1.02$ $(\Delta/\sigma)_{\max} = 0.001$
2242 reflections $\Delta\rho_{\max} = 0.27 \text{ e } \text{\AA}^{-3}$
145 parameters $\Delta\rho_{\min} = -0.29 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods Extinction correction: none

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

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	0.46423 (5)	0.52259 (12)	0.36904 (6)	0.0222 (2)
O2	0.34305 (5)	0.73218 (14)	0.08352 (6)	0.0291 (2)
O3	0.22956 (6)	0.7828 (2)	0.12079 (7)	0.0467 (3)
N1	0.42087 (6)	0.22878 (14)	0.35641 (8)	0.0228 (2)
N2	0.54579 (6)	0.29874 (15)	0.39501 (8)	0.0234 (3)
N3	0.29278 (6)	0.73707 (16)	0.13953 (7)	0.0238 (3)
C1	0.43734 (8)	0.05109 (18)	0.36142 (10)	0.0280 (3)
H1	0.3994	-0.0355	0.3502	0.034*
C2	0.50707 (8)	-0.01134 (18)	0.38219 (10)	0.0284 (3)
H2	0.5182	-0.1378	0.3850	0.034*
C3	0.56002 (7)	0.12058 (19)	0.39866 (10)	0.0267 (3)
H3	0.6087	0.0824	0.4132	0.032*
C4	0.47660 (7)	0.33980 (16)	0.37377 (8)	0.0180 (3)
C5	0.39288 (6)	0.58007 (15)	0.34572 (8)	0.0179 (3)
C6	0.34150 (7)	0.60883 (16)	0.41443 (8)	0.0205 (3)
H6	0.3532	0.5820	0.4764	0.025*
C7	0.27269 (7)	0.67742 (17)	0.39132 (9)	0.0218 (3)
H7	0.2369	0.6965	0.4378	0.026*
C8	0.25564 (7)	0.71852 (17)	0.30078 (8)	0.0202 (3)
H8	0.2086	0.7655	0.2845	0.024*
C9	0.30919 (7)	0.68896 (16)	0.23527 (8)	0.0181 (3)
C10	0.37846 (6)	0.61910 (15)	0.25487 (8)	0.0180 (2)
H10	0.4141	0.5991	0.2083	0.022*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0150 (4)	0.0171 (4)	0.0344 (5)	-0.0013 (3)	-0.0053 (4)	0.0031 (4)
O2	0.0272 (5)	0.0406 (6)	0.0196 (5)	-0.0023 (4)	0.0039 (4)	0.0012 (4)
O3	0.0262 (6)	0.0873 (10)	0.0266 (6)	0.0152 (6)	-0.0062 (4)	0.0083 (6)
N1	0.0197 (5)	0.0192 (5)	0.0295 (6)	-0.0015 (4)	-0.0035 (4)	-0.0006 (4)
N2	0.0175 (5)	0.0233 (6)	0.0294 (6)	0.0008 (4)	-0.0015 (4)	0.0036 (4)
N3	0.0215 (5)	0.0300 (6)	0.0199 (5)	0.0000 (4)	-0.0019 (4)	0.0000 (4)
C1	0.0278 (7)	0.0187 (6)	0.0375 (8)	-0.0030 (5)	-0.0046 (6)	-0.0024 (5)
C2	0.0300 (7)	0.0199 (6)	0.0352 (7)	0.0038 (5)	-0.0011 (6)	-0.0005 (5)
C3	0.0209 (6)	0.0265 (7)	0.0326 (7)	0.0050 (5)	-0.0013 (5)	0.0033 (5)
C4	0.0183 (6)	0.0186 (6)	0.0173 (6)	-0.0010 (4)	0.0003 (4)	0.0019 (4)
C5	0.0150 (5)	0.0133 (5)	0.0255 (6)	-0.0016 (4)	-0.0025 (5)	0.0005 (4)
C6	0.0237 (6)	0.0193 (6)	0.0186 (6)	-0.0031 (5)	-0.0010 (5)	0.0015 (4)
C7	0.0215 (6)	0.0224 (6)	0.0214 (6)	0.0007 (5)	0.0046 (5)	-0.0013 (5)
C8	0.0154 (5)	0.0213 (6)	0.0240 (6)	0.0022 (4)	0.0007 (5)	-0.0010 (5)
C9	0.0185 (6)	0.0182 (5)	0.0175 (6)	-0.0013 (4)	-0.0012 (4)	-0.0005 (4)
C10	0.0152 (5)	0.0173 (5)	0.0214 (6)	-0.0010 (4)	0.0023 (4)	-0.0021 (4)

Geometric parameters (\AA , $^\circ$)

O1—C4	1.3613 (15)	C2—H2	0.9500
O1—C5	1.4029 (14)	C3—H3	0.9500
O2—N3	1.2252 (14)	C5—C10	1.3819 (17)
O3—N3	1.2256 (15)	C5—C6	1.3852 (17)
N1—C4	1.3225 (16)	C6—C7	1.3872 (18)
N1—C1	1.3392 (17)	C6—H6	0.9500
N2—C4	1.3273 (16)	C7—C8	1.3907 (18)
N2—C3	1.3332 (17)	C7—H7	0.9500
N3—C9	1.4720 (16)	C8—C9	1.3801 (17)
C1—C2	1.379 (2)	C8—H8	0.9500
C1—H1	0.9500	C9—C10	1.3867 (17)
C2—C3	1.384 (2)	C10—H10	0.9500
C4—O1—C5	117.41 (9)	C10—C5—C6	122.42 (11)
C4—N1—C1	114.73 (11)	C10—C5—O1	118.01 (10)
C4—N2—C3	114.50 (11)	C6—C5—O1	119.37 (11)
O2—N3—O3	123.73 (11)	C5—C6—C7	118.97 (11)
O2—N3—C9	118.44 (11)	C5—C6—H6	120.5
O3—N3—C9	117.82 (11)	C7—C6—H6	120.5
N1—C1—C2	122.68 (13)	C6—C7—C8	120.65 (11)
N1—C1—H1	118.7	C6—C7—H7	119.7
C2—C1—H1	118.7	C8—C7—H7	119.7
C1—C2—C3	116.25 (12)	C9—C8—C7	117.91 (11)
C1—C2—H2	121.9	C9—C8—H8	121.0
C3—C2—H2	121.9	C7—C8—H8	121.0
N2—C3—C2	122.96 (12)	C8—C9—C10	123.55 (11)

supplementary materials

N2—C3—H3	118.5	C8—C9—N3	118.55 (11)
C2—C3—H3	118.5	C10—C9—N3	117.88 (11)
N1—C4—N2	128.87 (12)	C5—C10—C9	116.49 (11)
N1—C4—O1	118.10 (11)	C5—C10—H10	121.8
N2—C4—O1	113.03 (10)	C9—C10—H10	121.8
C4—N1—C1—C2	-0.6 (2)	O1—C5—C6—C7	175.68 (10)
N1—C1—C2—C3	0.5 (2)	C5—C6—C7—C8	-0.65 (18)
C4—N2—C3—C2	-0.3 (2)	C6—C7—C8—C9	-0.02 (18)
C1—C2—C3—N2	0.0 (2)	C7—C8—C9—C10	0.66 (18)
C1—N1—C4—N2	0.2 (2)	C7—C8—C9—N3	-178.15 (11)
C1—N1—C4—O1	179.32 (11)	O2—N3—C9—C8	171.09 (11)
C3—N2—C4—N1	0.3 (2)	O3—N3—C9—C8	-7.71 (18)
C3—N2—C4—O1	-178.92 (11)	O2—N3—C9—C10	-7.78 (17)
C5—O1—C4—N1	-0.16 (16)	O3—N3—C9—C10	173.41 (13)
C5—O1—C4—N2	179.13 (10)	C6—C5—C10—C9	-0.15 (17)
C4—O1—C5—C10	-94.96 (13)	O1—C5—C10—C9	-175.15 (10)
C4—O1—C5—C6	89.88 (13)	C8—C9—C10—C5	-0.57 (18)
C10—C5—C6—C7	0.74 (18)	N3—C9—C10—C5	178.25 (10)

Fig. 1

