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2-(2-Naphthyloxy)pyrimidine

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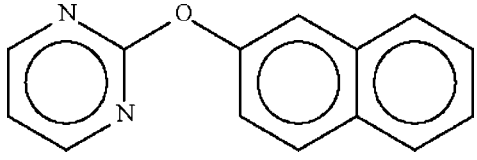
Key indicators: single-crystal X-ray study; T = 120 K; mean σ(C–C) = 0.003 Å; R factor = 0.029; wR factor = 0.081; data-to-parameter ratio = 8.9.

In the title compound, $C_{14}H_{10}N_2O$, the organic rings are inclined at an angle of 86.1 (1)°. The angle at the ether O atom is widened to 117.18 (14)°.

Related literature

For 2-phenoxypyrimidine, see: Shah Bakhtiar *et al.* (2009).



Experimental

Crystal data

$C_{14}H_{10}N_2O$
M_r = 222.24
Orthorhombic, $Aba2$
a = 13.0119 (3) Å
b = 22.4944 (5) Å
c = 7.5355 (2) Å
V = 2205.60 (9) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 120 K
0.35 × 0.25 × 0.15 mm

Data collection

Bruker SMART APEX diffractometer
Absorption correction: none
7375 measured reflections
1366 independent reflections
1271 reflections with $I > 2\sigma(I)$
R_{int} = 0.026

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.029
$wR(F^2)$ = 0.081
S = 1.03
1366 reflections
154 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

Data collection: *APEX2* (Bruker, 2008); cell refinement: *SAINT* (Bruker, 2008); 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: BT2997).

References

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supporting information

Acta Cryst. (2009). E**65**, o1881 [doi:10.1107/S1600536809026592]

2-(2-Naphthyloxy)pyrimidine

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S1. 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-chloropyridimidine (2.60 g, 20 mmol) dissolved in THF (50 ml). The mixture was heated for 4 h. Water was added and the organic phase was extracted with chloroform. The chloroform solution was dried over sodium sulfate; slow evaporation led to the formation of colorless crystals.

S2. Refinement

H-atoms were placed in calculated positions (C—H 0.95 Å) and were included in the refinement in the riding model approximation, with U(H) set to 1.2U(C).

In the absence of anomalous scatterers, 1111 Friedel pairs were merged and the absolute structure was arbitrarily set.

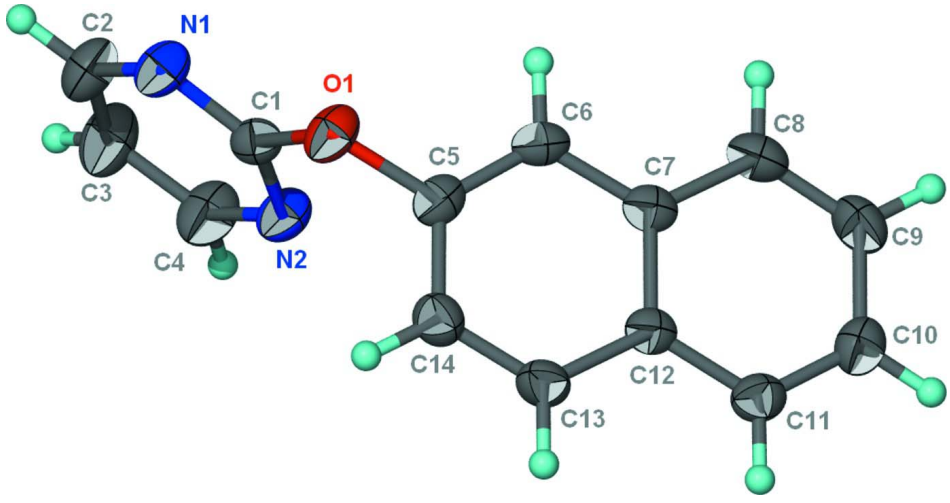

Figure 1

Anisotropic displacement ellipsoid plot (Barbour, 2001) of $C_{14}H_{10}N_2O$ at the 70% probability level; hydrogen atoms are drawn as spheres of arbitrary radius.

2-(2-Naphthyloxy)pyrimidine

Crystal data

$C_{14}H_{10}N_2O$
M_r = 222.24
Orthorhombic, *Aba*2
Hall symbol: A 2 -2ac
a = 13.0119 (3) Å
b = 22.4944 (5) Å
c = 7.5355 (2) Å
V = 2205.60 (9) Å^3
Z = 8
F(000) = 928
D_x = 1.339 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å

Cell parameters from 3105 reflections
θ = 2.4–28.0°
μ = 0.09 mm^{-1}
T = 120 K
Block, colorless
0.35 × 0.25 × 0.15 mm

Data collection

Bruker SMART APEX diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
7375 measured reflections
1366 independent reflections
1271 reflections with $I > 2\sigma(I)$
R_{int} = 0.026
θ_{max} = 27.5°, θ_{min} = 1.8°
h = −16→16
k = −29→29
l = −9→9

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.029
$wR(F^2)$ = 0.081
S = 1.03
1366 reflections
154 parameters
1 restraint
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
$w = 1/[\sigma^2(F_o^2) + (0.0476P)^2 + 0.7203P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

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

	x	y	z	U_{iso}*/U_{eq}
O1	0.05750 (10)	0.07574 (6)	0.49878 (19)	0.0292 (3)
N1	0.15301 (12)	0.04684 (7)	0.7306 (2)	0.0289 (4)
N2	−0.00893 (12)	0.09426 (7)	0.7772 (2)	0.0282 (3)
C1	0.06580 (13)	0.07234 (7)	0.6787 (2)	0.0225 (4)
C2	0.16628 (15)	0.04528 (9)	0.9060 (3)	0.0343 (5)
H2	0.2275	0.0280	0.9513	0.041*
C3	0.09591 (17)	0.06737 (10)	1.0241 (3)	0.0394 (5)
H3	0.1074	0.0663	1.1486	0.047*
C4	0.00719 (16)	0.09122 (10)	0.9522 (3)	0.0362 (5)
H4	−0.0442	0.1060	1.0302	0.043*
C5	−0.02862 (13)	0.10606 (8)	0.4298 (2)	0.0247 (4)
C6	−0.01790 (13)	0.16416 (8)	0.3824 (3)	0.0246 (4)
H6	0.0460	0.1839	0.3985	0.030*
C7	−0.10287 (13)	0.19501 (7)	0.3090 (2)	0.0233 (4)
C8	−0.09853 (15)	0.25595 (8)	0.2640 (3)	0.0306 (4)
H8	−0.0356	0.2770	0.2763	0.037*
C9	−0.18366 (15)	0.28497 (8)	0.2030 (3)	0.0326 (4)
H9	−0.1795	0.3260	0.1747	0.039*
C10	−0.27770 (14)	0.25454 (8)	0.1818 (3)	0.0292 (4)
H10	−0.3367	0.2753	0.1407	0.035*
C11	−0.28390 (13)	0.19533 (8)	0.2202 (3)	0.0266 (4)
H11	−0.3471	0.1749	0.2032	0.032*
C12	−0.19730 (13)	0.16397 (7)	0.2850 (2)	0.0226 (3)

C13	−0.20239 (14)	0.10272 (8)	0.3295 (3)	0.0271 (4)
H13	−0.2641	0.0813	0.3086	0.033*
C14	−0.11979 (14)	0.07416 (7)	0.4021 (3)	0.0277 (4)
H14	−0.1241	0.0333	0.4333	0.033*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0250 (6)	0.0400 (7)	0.0225 (6)	0.0093 (5)	0.0003 (5)	−0.0022 (6)
N1	0.0250 (7)	0.0328 (8)	0.0290 (9)	0.0070 (6)	−0.0002 (6)	−0.0046 (7)
N2	0.0237 (7)	0.0350 (8)	0.0260 (8)	0.0053 (6)	0.0005 (7)	−0.0019 (7)
C1	0.0219 (8)	0.0222 (7)	0.0235 (9)	−0.0017 (6)	−0.0003 (7)	−0.0034 (7)
C2	0.0309 (10)	0.0381 (10)	0.0339 (12)	0.0091 (8)	−0.0079 (9)	−0.0034 (8)
C3	0.0435 (12)	0.0513 (13)	0.0234 (11)	0.0129 (10)	−0.0051 (9)	−0.0014 (9)
C4	0.0331 (10)	0.0500 (12)	0.0255 (11)	0.0115 (9)	0.0047 (9)	−0.0026 (9)
C5	0.0227 (8)	0.0335 (9)	0.0180 (8)	0.0034 (7)	0.0001 (7)	−0.0016 (7)
C6	0.0198 (8)	0.0323 (8)	0.0218 (9)	−0.0040 (6)	0.0013 (7)	−0.0037 (7)
C7	0.0245 (8)	0.0275 (8)	0.0177 (8)	−0.0040 (7)	0.0020 (7)	−0.0029 (7)
C8	0.0296 (9)	0.0299 (9)	0.0322 (10)	−0.0082 (7)	0.0042 (8)	−0.0005 (8)
C9	0.0380 (10)	0.0240 (8)	0.0358 (11)	−0.0032 (7)	0.0041 (10)	0.0029 (8)
C10	0.0300 (9)	0.0314 (8)	0.0263 (10)	0.0050 (7)	−0.0013 (8)	0.0007 (8)
C11	0.0236 (8)	0.0318 (8)	0.0243 (9)	−0.0029 (6)	−0.0013 (7)	−0.0005 (7)
C12	0.0231 (8)	0.0261 (8)	0.0186 (8)	−0.0032 (6)	0.0007 (7)	−0.0011 (7)
C13	0.0254 (8)	0.0275 (8)	0.0285 (10)	−0.0066 (7)	−0.0034 (8)	0.0012 (7)
C14	0.0293 (9)	0.0236 (8)	0.0303 (11)	−0.0007 (7)	0.0006 (9)	0.0009 (7)

Geometric parameters (Å, º)

O1—C1	1.362 (2)	C7—C8	1.413 (2)
O1—C5	1.411 (2)	C7—C12	1.425 (2)
N1—C1	1.330 (2)	C8—C9	1.365 (3)
N1—C2	1.334 (3)	C8—H8	0.9500
N2—C1	1.319 (2)	C9—C10	1.411 (3)
N2—C4	1.337 (3)	C9—H9	0.9500
C2—C3	1.370 (3)	C10—C11	1.365 (3)
C2—H2	0.9500	C10—H10	0.9500
C3—C4	1.383 (3)	C11—C12	1.416 (2)
C3—H3	0.9500	C11—H11	0.9500
C4—H4	0.9500	C12—C13	1.420 (2)
C5—C6	1.362 (2)	C13—C14	1.366 (3)
C5—C14	1.402 (2)	C13—H13	0.9500
C6—C7	1.418 (2)	C14—H14	0.9500
C6—H6	0.9500		
C1—O1—C5	117.18 (14)	C6—C7—C12	118.81 (14)
C1—N1—C2	114.41 (16)	C9—C8—C7	120.79 (16)
C1—N2—C4	114.86 (16)	C9—C8—H8	119.6
N2—C1—N1	128.65 (17)	C7—C8—H8	119.6

N2—C1—O1	118.73 (15)	C8—C9—C10	120.66 (16)
N1—C1—O1	112.61 (15)	C8—C9—H9	119.7
N1—C2—C3	123.22 (19)	C10—C9—H9	119.7
N1—C2—H2	118.4	C11—C10—C9	120.02 (17)
C3—C2—H2	118.4	C11—C10—H10	120.0
C2—C3—C4	116.4 (2)	C9—C10—H10	120.0
C2—C3—H3	121.8	C10—C11—C12	120.80 (16)
C4—C3—H3	121.8	C10—C11—H11	119.6
N2—C4—C3	122.46 (19)	C12—C11—H11	119.6
N2—C4—H4	118.8	C11—C12—C13	121.86 (16)
C3—C4—H4	118.8	C11—C12—C7	119.05 (14)
C6—C5—C14	122.60 (16)	C13—C12—C7	119.08 (16)
C6—C5—O1	118.62 (16)	C14—C13—C12	120.94 (16)
C14—C5—O1	118.65 (15)	C14—C13—H13	119.5
C5—C6—C7	119.48 (15)	C12—C13—H13	119.5
C5—C6—H6	120.3	C13—C14—C5	118.99 (15)
C7—C6—H6	120.3	C13—C14—H14	120.5
C8—C7—C6	122.49 (15)	C5—C14—H14	120.5
C8—C7—C12	118.66 (16)		

C4—N2—C1—N1	1.5 (3)	C6—C7—C8—C9	−176.20 (19)
C4—N2—C1—O1	−177.46 (18)	C12—C7—C8—C9	1.6 (3)
C2—N1—C1—N2	−2.1 (3)	C7—C8—C9—C10	−0.7 (3)
C2—N1—C1—O1	176.91 (17)	C8—C9—C10—C11	−0.8 (3)
C5—O1—C1—N2	3.8 (2)	C9—C10—C11—C12	1.3 (3)
C5—O1—C1—N1	−175.36 (14)	C10—C11—C12—C13	178.62 (19)
C1—N1—C2—C3	0.7 (3)	C10—C11—C12—C7	−0.3 (3)
N1—C2—C3—C4	1.0 (3)	C8—C7—C12—C11	−1.1 (3)
C1—N2—C4—C3	0.5 (3)	C6—C7—C12—C11	176.80 (17)
C2—C3—C4—N2	−1.7 (4)	C8—C7—C12—C13	179.90 (17)
C1—O1—C5—C6	96.5 (2)	C6—C7—C12—C13	−2.2 (3)
C1—O1—C5—C14	−87.6 (2)	C11—C12—C13—C14	−175.94 (19)
C14—C5—C6—C7	2.8 (3)	C7—C12—C13—C14	3.0 (3)
O1—C5—C6—C7	178.52 (16)	C12—C13—C14—C5	−1.0 (3)
C5—C6—C7—C8	177.22 (18)	C6—C5—C14—C13	−2.0 (3)
C5—C6—C7—C12	−0.6 (3)	O1—C5—C14—C13	−177.73 (17)