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2-Phenoxypyrimidine

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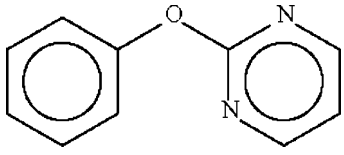
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.002 Å; R factor = 0.037; wR factor = 0.102; data-to-parameter ratio = 16.6.

There are two molecules in the asymmetric unit of, $C_{10}H_8N_2O$, with dihedral angles between the aromatic ring planes of 75.9 (1) and 79.3 (1)°.

Related literature

For other phenoxy-substituted *N*-heterocycles, see: Abdullah & Ng (2008); Hassan *et al.* (2008); Idris *et al.* (2009).



Experimental

Crystal data

$C_{10}H_8N_2O$ M_r = 172.18
Monoclinic, $P2_1/c$
a = 10.859 (1) Å
b = 20.181 (2) Å
c = 8.1339 (8) Å
β = 106.637 (2)°
V = 1707.8 (3) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 100 (2) K
0.25 × 0.20 × 0.15 mm

Data collection

Bruker SMART APEX diffractometer
Absorption correction: none
9752 measured reflections
3901 independent reflections
3026 reflections with $I > 2\sigma(I)$
R_{int} = 0.024

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.102
S = 1.03
3901 reflections
235 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}

Data 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).

We thank the University of Malaya for supporting this study (FS358/2008 A).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: TK2342).

References

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supplementary materials

Acta Cryst. (2009). E**65**, o114 [**doi:10.1107/S1600536808041196**]

2-Phenoxypyrimidine

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

Comment

(type here to add)

Experimental

Phenol (1.88 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 ether. The ether phase was dried over sodium sulfate; the evaporation of the solvent gave well shaped colorless crystals along with some unidentified brown material.

Refinement

Carbon-bound 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_{eq}(C).

Figures

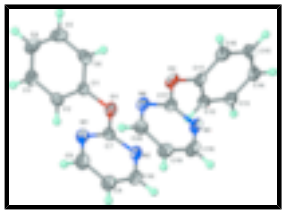


Fig. 1. Thermal ellipsoid plot (Barbour, 2001) of the two independent molecules of $C_{10}H_8N_2O$ at the 70% probability level. Hydrogen atoms are drawn as spheres of arbitrary radius.

2-Phenoxypyrimidine

Crystal data

$C_{10}H_8N_2O$	F_{000} = 720
M_r = 172.18	D_x = 1.339 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 2782 reflections
a = 10.859 (1) Å	θ = 2.2–28.2°
b = 20.181 (2) Å	μ = 0.09 mm^{-1}
c = 8.1339 (8) Å	T = 100 (2) K
β = 106.637 (2)°	Block, colorless
V = 1707.8 (3) Å^3	0.25 × 0.20 × 0.15 mm

$Z = 8$

Data collection

Bruker SMART APEX diffractometer	3026 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	$R_{int} = 0.024$
Monochromator: graphite	$\theta_{max} = 27.5^{o}$
$T = 100(2)$ K	$\theta_{min} = 2.0^{o}$
ω scans	$h = -11 \rightarrow 14$
Absorption correction: None	$k = -26 \rightarrow 26$
9752 measured reflections	$l = -10 \rightarrow 10$
3901 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
$wR(F^2) = 0.102$	$w = 1/[\sigma^2(F_o^2) + (0.0497P)^2 + 0.2571P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.03$	$(\Delta/\sigma)_{max} = 0.001$
3901 reflections	$\Delta\rho_{max} = 0.18$ e Å^{-3}
235 parameters	$\Delta\rho_{min} = -0.22$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.69295 (8)	0.58216 (5)	0.51546 (11)	0.0274 (2)
O2	0.97744 (9)	0.67233 (5)	0.77250 (11)	0.0281 (2)
N1	0.59037 (10)	0.60351 (5)	0.72195 (13)	0.0245 (2)
N2	0.77301 (10)	0.53229 (5)	0.76936 (14)	0.0253 (2)
N3	1.05326 (11)	0.62385 (5)	1.03911 (13)	0.0264 (3)
N4	0.87443 (10)	0.69812 (5)	0.96601 (13)	0.0247 (2)
C1	0.59965 (12)	0.62116 (6)	0.40077 (16)	0.0213 (3)
C2	0.48239 (12)	0.59386 (6)	0.31580 (17)	0.0256 (3)
H2	0.4617	0.5500	0.3408	0.031*
C3	0.39513 (13)	0.63124 (7)	0.19343 (18)	0.0297 (3)
H3	0.3136	0.6133	0.1346	0.036*
C4	0.42700 (14)	0.69480 (7)	0.15706 (17)	0.0311 (3)
H4	0.3671	0.7204	0.0729	0.037*
C5	0.54526 (14)	0.72141 (6)	0.24218 (18)	0.0314 (3)
H15A	0.5666	0.7650	0.2161	0.038*
C6	0.63298 (13)	0.68443 (6)	0.36592 (17)	0.0263 (3)
H6B	0.7144	0.7024	0.4254	0.032*

C7	0.68331 (12)	0.57302 (6)	0.67684 (16)	0.0208 (3)
C8	0.58755 (14)	0.59106 (7)	0.88258 (17)	0.0303 (3)
H8	0.5227	0.6115	0.9225	0.036*
C9	0.67458 (14)	0.54993 (7)	0.99239 (17)	0.0295 (3)
H9	0.6711	0.5416	1.1059	0.035*
C10	0.76711 (13)	0.52151 (6)	0.92888 (17)	0.0267 (3)
H10	0.8291	0.4931	1.0015	0.032*
C11	1.07433 (12)	0.63814 (6)	0.72453 (15)	0.0235 (3)
C12	1.05906 (12)	0.57148 (6)	0.68472 (15)	0.0235 (3)
H12	0.9859	0.5480	0.6954	0.028*
C13	1.15275 (12)	0.53963 (6)	0.62894 (15)	0.0239 (3)
H13	1.1439	0.4939	0.6007	0.029*
C14	1.25931 (13)	0.57413 (7)	0.61407 (16)	0.0258 (3)
H14	1.3239	0.5518	0.5773	0.031*
C15	1.27177 (13)	0.64082 (7)	0.65256 (18)	0.0298 (3)
H15	1.3445	0.6644	0.6409	0.036*
C16	1.17853 (13)	0.67363 (6)	0.70825 (17)	0.0284 (3)
H16	1.1865	0.7196	0.7345	0.034*
C17	0.96950 (12)	0.66360 (6)	0.93451 (15)	0.0214 (3)
C18	1.03893 (14)	0.61819 (7)	1.19692 (17)	0.0302 (3)
H18	1.0957	0.5900	1.2774	0.036*
C19	0.94557 (14)	0.65152 (7)	1.24657 (16)	0.0293 (3)
H19	0.9368	0.6472	1.3590	0.035*
C20	0.86503 (13)	0.69161 (6)	1.12499 (17)	0.0271 (3)
H20	0.7999	0.7157	1.1560	0.033*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0224 (5)	0.0355 (5)	0.0264 (5)	0.0089 (4)	0.0102 (4)	0.0033 (4)
O2	0.0304 (5)	0.0329 (5)	0.0221 (5)	0.0140 (4)	0.0092 (4)	0.0064 (4)
N1	0.0230 (6)	0.0253 (5)	0.0255 (6)	0.0043 (4)	0.0075 (5)	−0.0019 (4)
N2	0.0205 (6)	0.0237 (5)	0.0302 (6)	0.0025 (4)	0.0050 (5)	−0.0001 (4)
N3	0.0246 (6)	0.0298 (6)	0.0219 (5)	0.0066 (5)	0.0018 (4)	0.0021 (4)
N4	0.0242 (6)	0.0241 (5)	0.0261 (6)	0.0051 (4)	0.0079 (5)	0.0030 (4)
C1	0.0202 (6)	0.0238 (6)	0.0221 (6)	0.0030 (5)	0.0097 (5)	−0.0010 (5)
C2	0.0237 (7)	0.0206 (6)	0.0340 (7)	−0.0018 (5)	0.0107 (6)	0.0004 (5)
C3	0.0232 (7)	0.0314 (7)	0.0326 (7)	0.0008 (5)	0.0052 (6)	−0.0040 (6)
C4	0.0389 (8)	0.0280 (7)	0.0260 (7)	0.0102 (6)	0.0084 (6)	0.0020 (5)
C5	0.0441 (9)	0.0198 (6)	0.0346 (7)	−0.0002 (6)	0.0181 (7)	0.0007 (5)
C6	0.0262 (7)	0.0263 (6)	0.0291 (7)	−0.0069 (5)	0.0121 (6)	−0.0077 (5)
C7	0.0192 (6)	0.0181 (5)	0.0248 (6)	−0.0026 (5)	0.0059 (5)	−0.0031 (5)
C8	0.0297 (7)	0.0349 (7)	0.0285 (7)	0.0062 (6)	0.0118 (6)	−0.0031 (6)
C9	0.0321 (8)	0.0323 (7)	0.0231 (6)	0.0014 (6)	0.0059 (6)	0.0008 (5)
C10	0.0239 (7)	0.0236 (6)	0.0288 (7)	0.0007 (5)	0.0015 (5)	0.0012 (5)
C11	0.0232 (7)	0.0282 (6)	0.0175 (6)	0.0075 (5)	0.0034 (5)	0.0034 (5)
C12	0.0213 (6)	0.0276 (6)	0.0209 (6)	0.0000 (5)	0.0052 (5)	0.0034 (5)
C13	0.0246 (7)	0.0248 (6)	0.0205 (6)	0.0010 (5)	0.0037 (5)	−0.0004 (5)

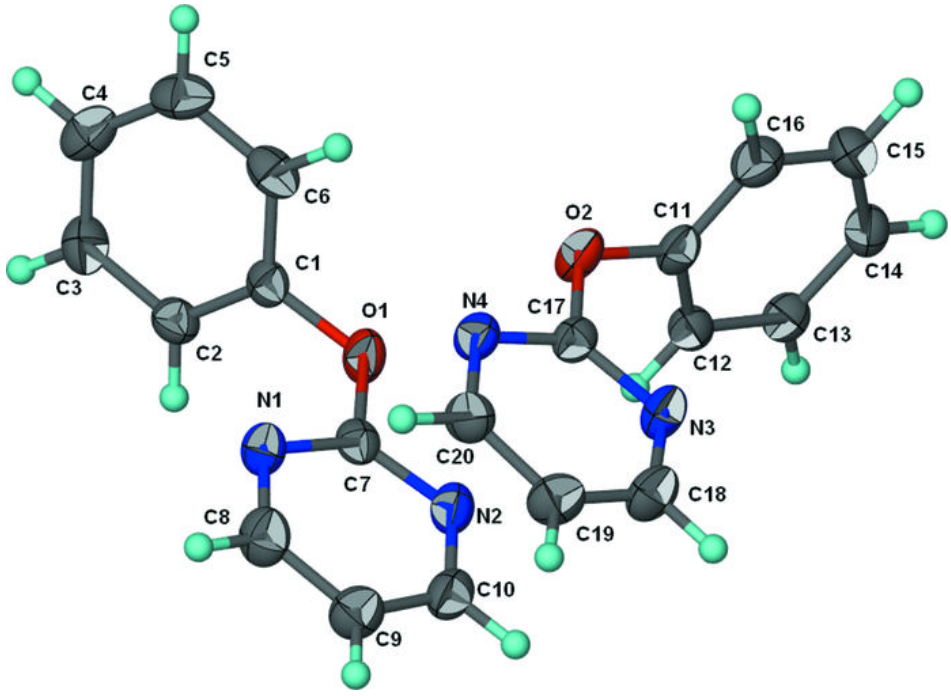
C14	0.0218 (7)	0.0313 (7)	0.0240 (6)	0.0039 (5)	0.0064 (5)	0.0011 (5)
C15	0.0226 (7)	0.0320 (7)	0.0345 (7)	−0.0030 (6)	0.0077 (6)	0.0028 (6)
C16	0.0298 (7)	0.0234 (6)	0.0292 (7)	0.0006 (5)	0.0039 (6)	0.0005 (5)
C17	0.0218 (6)	0.0202 (6)	0.0204 (6)	0.0007 (5)	0.0031 (5)	0.0000 (5)
C18	0.0308 (8)	0.0343 (7)	0.0210 (6)	0.0057 (6)	0.0001 (6)	0.0038 (5)
C19	0.0357 (8)	0.0316 (7)	0.0200 (6)	0.0016 (6)	0.0069 (6)	0.0015 (5)
C20	0.0275 (7)	0.0268 (6)	0.0291 (7)	0.0024 (5)	0.0113 (6)	0.0007 (5)

Geometric parameters (Å, °)

O1—C7	1.3590 (15)	C6—H6B	0.9500
O1—C1	1.4053 (15)	C8—C9	1.3771 (19)
O2—C17	1.3565 (14)	C8—H8	0.9500
O2—C11	1.4037 (15)	C9—C10	1.3793 (19)
N1—C7	1.3205 (16)	C9—H9	0.9500
N1—C8	1.3394 (17)	C10—H10	0.9500
N2—C7	1.3307 (16)	C11—C16	1.3772 (19)
N2—C10	1.3352 (17)	C11—C12	1.3824 (18)
N3—C17	1.3235 (16)	C12—C13	1.3850 (17)
N3—C18	1.3414 (17)	C12—H12	0.9500
N4—C17	1.3297 (16)	C13—C14	1.3851 (18)
N4—C20	1.3324 (16)	C13—H13	0.9500
C1—C2	1.3780 (18)	C14—C15	1.3797 (18)
C1—C6	1.3785 (17)	C14—H14	0.9500
C2—C3	1.3848 (19)	C15—C16	1.3897 (19)
C2—H2	0.9500	C15—H15	0.9500
C3—C4	1.3824 (19)	C16—H16	0.9500
C3—H3	0.9500	C18—C19	1.3703 (19)
C4—C5	1.381 (2)	C18—H18	0.9500
C4—H4	0.9500	C19—C20	1.3792 (18)
C5—C6	1.389 (2)	C19—H19	0.9500
C5—H15A	0.9500	C20—H20	0.9500
C7—O1—C1	118.48 (9)	N2—C10—C9	122.61 (12)
C17—O2—C11	117.86 (9)	N2—C10—H10	118.7
C7—N1—C8	114.61 (11)	C9—C10—H10	118.7
C7—N2—C10	114.78 (11)	C16—C11—C12	122.03 (12)
C17—N3—C18	114.85 (11)	C16—C11—O2	118.22 (11)
C17—N4—C20	114.51 (11)	C12—C11—O2	119.62 (12)
C2—C1—C6	121.77 (12)	C11—C12—C13	118.57 (12)
C2—C1—O1	119.74 (11)	C11—C12—H12	120.7
C6—C1—O1	118.26 (11)	C13—C12—H12	120.7
C1—C2—C3	119.11 (12)	C12—C13—C14	120.38 (12)
C1—C2—H2	120.4	C12—C13—H13	119.8
C3—C2—H2	120.4	C14—C13—H13	119.8
C4—C3—C2	119.85 (13)	C15—C14—C13	120.04 (12)
C4—C3—H3	120.1	C15—C14—H14	120.0
C2—C3—H3	120.1	C13—C14—H14	120.0
C5—C4—C3	120.48 (13)	C14—C15—C16	120.37 (12)
C5—C4—H4	119.8	C14—C15—H15	119.8

C3—C4—H4	119.8	C16—C15—H15	119.8
C4—C5—C6	120.05 (12)	C11—C16—C15	118.61 (12)
C4—C5—H15A	120.0	C11—C16—H16	120.7
C6—C5—H15A	120.0	C15—C16—H16	120.7
C1—C6—C5	118.74 (12)	N3—C17—N4	128.48 (11)
C1—C6—H6B	120.6	N3—C17—O2	118.70 (11)
C5—C6—H6B	120.6	N4—C17—O2	112.82 (10)
N1—C7—N2	128.65 (11)	N3—C18—C19	122.58 (12)
N1—C7—O1	118.78 (11)	N3—C18—H18	118.7
N2—C7—O1	112.56 (10)	C19—C18—H18	118.7
N1—C8—C9	122.86 (12)	C18—C19—C20	116.58 (12)
N1—C8—H8	118.6	C18—C19—H19	121.7
C9—C8—H8	118.6	C20—C19—H19	121.7
C8—C9—C10	116.48 (12)	N4—C20—C19	123.00 (12)
C8—C9—H9	121.8	N4—C20—H20	118.5
C10—C9—H9	121.8	C19—C20—H20	118.5
C7—O1—C1—C2	−80.80 (14)	C17—O2—C11—C16	−106.60 (13)
C7—O1—C1—C6	104.66 (13)	C17—O2—C11—C12	77.48 (15)
C6—C1—C2—C3	−0.72 (19)	C16—C11—C12—C13	0.84 (19)
O1—C1—C2—C3	−175.06 (11)	O2—C11—C12—C13	176.60 (10)
C1—C2—C3—C4	0.64 (19)	C11—C12—C13—C14	0.14 (18)
C2—C3—C4—C5	−0.1 (2)	C12—C13—C14—C15	−0.92 (19)
C3—C4—C5—C6	−0.3 (2)	C13—C14—C15—C16	0.7 (2)
C2—C1—C6—C5	0.28 (18)	C12—C11—C16—C15	−1.03 (19)
O1—C1—C6—C5	174.70 (11)	O2—C11—C16—C15	−176.84 (11)
C4—C5—C6—C1	0.24 (19)	C14—C15—C16—C11	0.23 (19)
C8—N1—C7—N2	−0.11 (19)	C18—N3—C17—N4	0.05 (19)
C8—N1—C7—O1	179.36 (11)	C18—N3—C17—O2	179.77 (11)
C10—N2—C7—N1	−0.22 (19)	C20—N4—C17—N3	0.79 (19)
C10—N2—C7—O1	−179.71 (10)	C20—N4—C17—O2	−178.94 (11)
C1—O1—C7—N1	−3.06 (16)	C11—O2—C17—N3	0.36 (17)
C1—O1—C7—N2	176.49 (10)	C11—O2—C17—N4	−179.88 (10)
C7—N1—C8—C9	0.14 (19)	C17—N3—C18—C19	−0.63 (19)
N1—C8—C9—C10	0.1 (2)	N3—C18—C19—C20	0.3 (2)
C7—N2—C10—C9	0.52 (18)	C17—N4—C20—C19	−1.10 (19)
C8—C9—C10—N2	−0.5 (2)	C18—C19—C20—N4	0.6 (2)

Fig. 1


C5
C4
C6
C1
C3
C2
O1
N1
C7
N2
C8
C10
C9
N4
C17
O2
C11
C16
C15
C14
C13
C12
N3
C20
C18
C19