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Crystal structure of phenyl(pyridin-2-yl)-methanol

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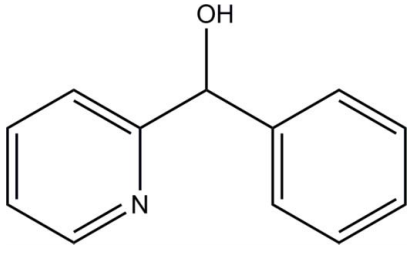
In the title compound, $C_{12}H_{11}NO$, the pyridine and phenyl rings are inclined to each other by 71.42 (10)°. In the crystal, O—H···N hydrogen bonds link the molecules into helical chains extending along the *c*-axis direction.

Keywords: crystal structure; phenyl(pyridin-2-yl)methanol; hydrogen bonding.

CCDC reference: 1015307

1. Related literature

For the synthesis of the title compound and some derivatives, see: Frassoldati *et al.* (2013); Tao *et al.* (2012). For its use in synthesis, see: Miyamura *et al.* (2008); Lucchesi *et al.* (2008); Lash *et al.* (2007); Szajna *et al.* (2004).



2. Experimental

2.1. Crystal data

$C_{12}H_{11}NO$
M_r = 185.22
Orthorhombic, $Pna2_1$
a = 7.4385 (8) Å
b = 14.3429 (16) Å
c = 9.2255 (10) Å
V = 984.27 (19) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 296 K
0.3 × 0.26 × 0.18 mm

2.2. Data collection

Bruker SMART CCD area-detector diffractometer
7290 measured reflections
2245 independent reflections
1190 reflections with $I > 2\sigma(I)$
R_{int} = 0.055

2.3. Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.084
S = 0.81
2245 reflections
131 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.09 e Å^{-3}
$\Delta\rho_{min}$ = −0.12 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O8—H8···N1^{i}	0.98 (5)	1.85 (5)	2.809 (4)	166 (4)

Symmetry code: (i) $-x+1, -y+1, z-\frac{1}{2}$.

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS2013* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2013* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012); software used to prepare material for publication: *WinGX* (Farrugia, 2012).

Acknowledgements

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Supporting information for this paper is available from the IUCr electronic archives (Reference: SU2760).

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supporting information

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Crystal structure of phenyl(pyridin-2-yl)methanol

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S1. Experimental

To a solution of 2-benzoylpyridine (5.0 g, 0.027 mol) in EtOH (60 ml) was added $NaBH_4$ (3.13 g, 0.083 mol) slowly at room temperature. The solution was stirred gently for 1 h. After adding 60 ml H_2O, this solution was heated at 363 K for 15 min. After cooling, the product was extracted with AcOEt (50 ml). The solvent was evaporated under reduced pressure to leave a pale green oil. Colourless crystals of the title compound were obtained by slow evaporation of a solution in EtOH at room temperature.

S2. Refinement

Atom H8 of the OH group was located in a difference Fourier map and freely refined. C-bound H atoms were positioned geometrically and refined using a riding model: C—H = 0.93 - 0.98 Å with U_{iso}(H) = 1.2U_{eq}(C).

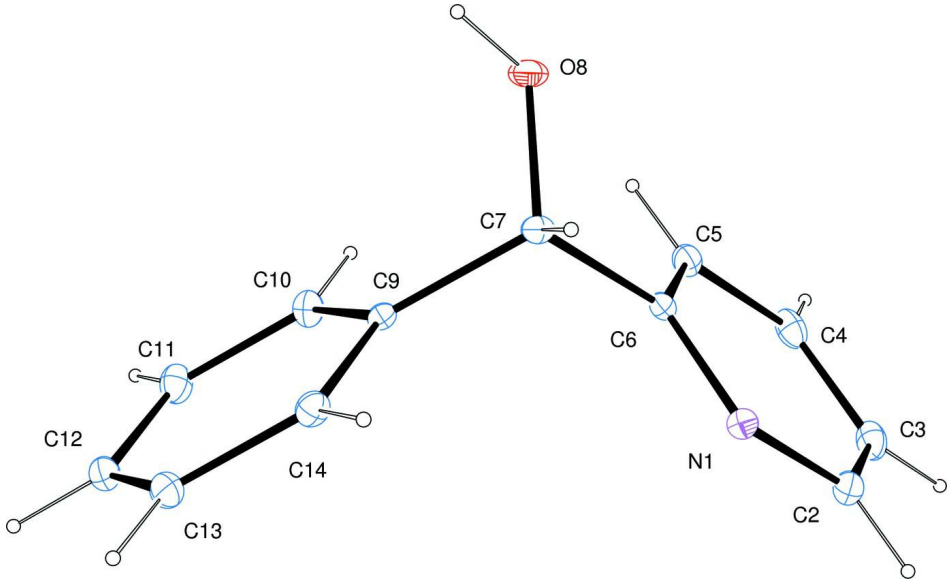

Figure 1

Molecular structure of the title molecule, with atom labelling. The displacement ellipsoids are drawn at the 30% probability level.

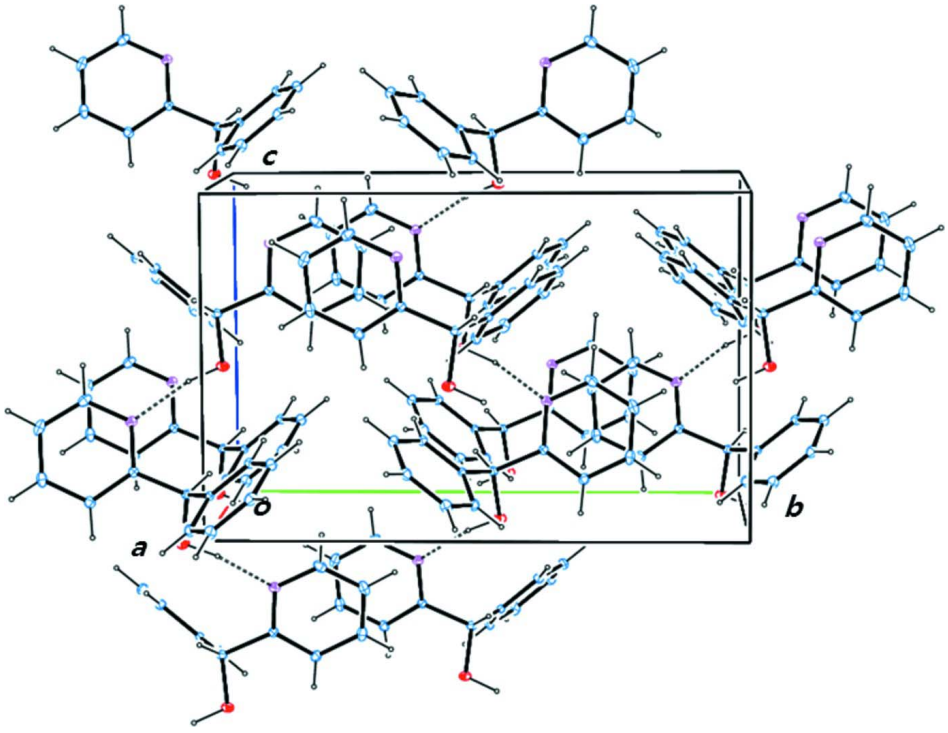

Figure 2

A view along the a axis of the crystal packing of the title compound, showing molecules linked by O—H···N hydrogen bonds (dashed lines; see Table 1 for details).

Phenyl(pyridin-2-yl)methanol

Crystal data

$C_{12}H_{11}NO$
$M_r = 185.22$
Orthorhombic, $Pna2_1$
Hall symbol: P 2c -2n
$a = 7.4385$ (8) Å
$b = 14.3429$ (16) Å
$c = 9.2255$ (10) Å
$V = 984.27$ (19) Å^3
$Z = 4$
$F(000) = 392$
$D_x = 1.25$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 973 reflections
$\theta = 2.6$–19.7°
$\mu = 0.08$ mm^{-1}
$T = 296$ K
Block, colourless
0.3 × 0.26 × 0.18 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
φ and ω scans
7290 measured reflections
2245 independent reflections
1190 reflections with $I > 2\sigma(I)$
$R_{int} = 0.055$
$\theta_{max} = 27.5°$, $\theta_{min} = 2.6°$
$h = -7 \rightarrow 9$
$k = -18 \rightarrow 18$
$l = -11 \rightarrow 11$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.039$
$wR(F^2) = 0.084$
$S = 0.81$
2245 reflections
131 parameters
1 restraint

Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0303P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.09$ e Å^{-3}
$\Delta\rho_{min} = -0.12$ e Å^{-3}

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
N1	0.4374 (3)	0.37463 (19)	0.8538 (3)	0.0544 (7)
C2	0.4309 (5)	0.2902 (3)	0.9150 (5)	0.0738 (12)
H2	0.4616	0.2851	1.0124	0.089*
C3	0.3819 (5)	0.2112 (3)	0.8433 (6)	0.0773 (12)
H3	0.3794	0.154	0.8907	0.093*
C4	0.3365 (4)	0.2177 (2)	0.7004 (5)	0.0733 (12)
H4	0.302	0.1651	0.6485	0.088*
C5	0.3426 (4)	0.3039 (2)	0.6344 (4)	0.0582 (9)
H5	0.3119	0.3104	0.5372	0.07*
C6	0.3949 (4)	0.3804 (2)	0.7141 (3)	0.0434 (7)
C7	0.4046 (4)	0.4769 (2)	0.6482 (3)	0.0501 (8)
H7	0.5021	0.5116	0.6949	0.06*
O8	0.4471 (3)	0.46457 (19)	0.5006 (3)	0.0700 (7)
H8	0.474 (5)	0.526 (3)	0.460 (5)	0.111 (16)*
C9	0.2299 (3)	0.52994 (18)	0.6693 (3)	0.0409 (7)
C10	0.0771 (4)	0.5047 (2)	0.5952 (4)	0.0587 (9)
H10	0.0817	0.4549	0.5307	0.07*
C11	−0.0819 (4)	0.5515 (3)	0.6146 (4)	0.0715 (11)
H11	−0.1837	0.5334	0.5633	0.086*
C12	−0.0908 (5)	0.6244 (3)	0.7087 (4)	0.0679 (10)
H12	−0.1989	0.6557	0.7224	0.081*
C13	0.0579 (5)	0.6514 (2)	0.7824 (4)	0.0697 (10)
H13	0.0515	0.7017	0.8459	0.084*
C14	0.2204 (4)	0.6043 (2)	0.7639 (4)	0.0570 (8)
H14	0.3219	0.623	0.8151	0.068*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0530 (17)	0.061 (2)	0.0488 (19)	0.0047 (13)	0.0014 (14)	0.0027 (15)
C2	0.066 (3)	0.084 (3)	0.071 (3)	0.019 (2)	0.008 (2)	0.024 (2)
C3	0.059 (2)	0.059 (3)	0.114 (4)	0.006 (2)	0.015 (2)	0.029 (3)
C4	0.059 (2)	0.049 (2)	0.112 (4)	0.0045 (17)	0.006 (3)	−0.008 (2)
C5	0.056 (2)	0.057 (2)	0.062 (2)	0.0079 (16)	0.0005 (17)	−0.0047 (19)

C6	0.0362 (15)	0.0463 (19)	0.0476 (19)	0.0058 (13)	0.0045 (15)	−0.0004 (15)
C7	0.0500 (18)	0.0578 (19)	0.0426 (19)	−0.0030 (15)	0.0052 (15)	−0.0001 (16)
O8	0.0827 (17)	0.0741 (18)	0.0530 (15)	0.0020 (14)	0.0260 (13)	0.0028 (13)
C9	0.0452 (16)	0.0391 (15)	0.0383 (15)	−0.0036 (14)	0.0017 (14)	0.0062 (14)
C10	0.059 (2)	0.047 (2)	0.069 (2)	−0.0019 (17)	−0.0103 (18)	−0.0040 (17)
C11	0.052 (2)	0.072 (2)	0.090 (3)	0.0003 (19)	−0.009 (2)	0.010 (2)
C12	0.061 (2)	0.071 (2)	0.072 (3)	0.016 (2)	0.011 (2)	0.014 (2)
C13	0.091 (3)	0.057 (2)	0.061 (2)	0.018 (2)	0.004 (2)	−0.005 (2)
C14	0.066 (2)	0.0535 (18)	0.0512 (19)	−0.0022 (16)	−0.0088 (18)	−0.0012 (17)

Geometric parameters (Å, º)

N1—C6	1.329 (4)	C7—H7	0.98
N1—C2	1.338 (4)	O8—H8	0.98 (5)
C2—C3	1.362 (5)	C9—C10	1.374 (4)
C2—H2	0.93	C9—C14	1.380 (4)
C3—C4	1.364 (5)	C10—C11	1.372 (4)
C3—H3	0.93	C10—H10	0.93
C4—C5	1.379 (5)	C11—C12	1.361 (5)
C4—H4	0.93	C11—H11	0.93
C5—C6	1.376 (4)	C12—C13	1.354 (5)
C5—H5	0.93	C12—H12	0.93
C6—C7	1.514 (4)	C13—C14	1.395 (4)
C7—O8	1.408 (4)	C13—H13	0.93
C7—C9	1.518 (4)	C14—H14	0.93
C6—N1—C2	117.2 (3)	C9—C7—H7	108.8
N1—C2—C3	123.9 (4)	C7—O8—H8	108 (3)
N1—C2—H2	118.1	C10—C9—C14	118.4 (3)
C3—C2—H2	118.1	C10—C9—C7	120.8 (3)
C2—C3—C4	118.6 (4)	C14—C9—C7	120.8 (3)
C2—C3—H3	120.7	C11—C10—C9	121.3 (3)
C4—C3—H3	120.7	C11—C10—H10	119.4
C3—C4—C5	118.7 (4)	C9—C10—H10	119.4
C3—C4—H4	120.7	C12—C11—C10	120.1 (4)
C5—C4—H4	120.7	C12—C11—H11	120
C6—C5—C4	119.2 (3)	C10—C11—H11	120
C6—C5—H5	120.4	C13—C12—C11	120.0 (3)
C4—C5—H5	120.4	C13—C12—H12	120
N1—C6—C5	122.4 (3)	C11—C12—H12	120
N1—C6—C7	115.8 (3)	C12—C13—C14	120.5 (3)
C5—C6—C7	121.8 (3)	C12—C13—H13	119.8
O8—C7—C6	106.5 (3)	C14—C13—H13	119.8
O8—C7—C9	112.3 (2)	C9—C14—C13	119.8 (3)
C6—C7—C9	111.4 (2)	C9—C14—H14	120.1
O8—C7—H7	108.8	C13—C14—H14	120.1
C6—C7—H7	108.8		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O8—H8···N1^{i}	0.98 (5)	1.85 (5)	2.809 (4)	166 (4)

Symmetry code: (i) −*x*+1, −*y*+1, *z*−1/2.