

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

Haneol Kim and Sung Kwon Kang\*

Department of Chemistry, Chungnam National University, Daejeon 305-764, Republic of Korea. \*Correspondence e-mail: [skkang@cnu.ac.kr](mailto:skkang@cnu.ac.kr)

Received 19 July 2014; accepted 21 July 2014

Edited by H. Stoeckli-Evans, University of Neuchâtel, Switzerland

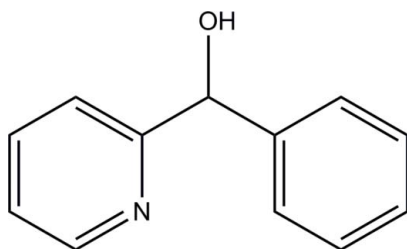
In the title compound, C<sub>12</sub>H<sub>11</sub>NO, the pyridine and phenyl rings are inclined to each other by 71.42 (10)°. In the crystal, O—H···N hydrogen bonds link the molecules into helical chains extending along the *c*-axis direction.

**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<sub>12</sub>H<sub>11</sub>NO  
*M<sub>r</sub>* = 185.22  
 Orthorhombic, *Pna*2<sub>1</sub>  
*a* = 7.4385 (8) Å

*b* = 14.3429 (16) Å  
*c* = 9.2255 (10) Å  
*V* = 984.27 (19) Å<sup>3</sup>  
*Z* = 4

Mo *K*α radiation  
 $\mu = 0.08 \text{ mm}^{-1}$

*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* > 2σ(*I*)  
*R*<sub>int</sub> = 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  
 $\Delta\rho_{\text{max}} = 0.09 \text{ e \AA}^{-3}$   
 $\Delta\rho_{\text{min}} = -0.12 \text{ e \AA}^{-3}$

Table 1

Hydrogen-bond geometry (Å, °).

<i>D</i> —H··· <i>A</i>	<i>D</i> —H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> —H··· <i>A</i>
O8—H8···N1 <sup>1</sup>	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: *SAINTE* (Bruker, 2002); data reduction: *SAINTE*; 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

This work was supported by research funding of Chungnam National University.

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

## References

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## supporting information

*Acta Cryst.* (2014). E70, o947 [doi:10.1107/S1600536814016857]

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

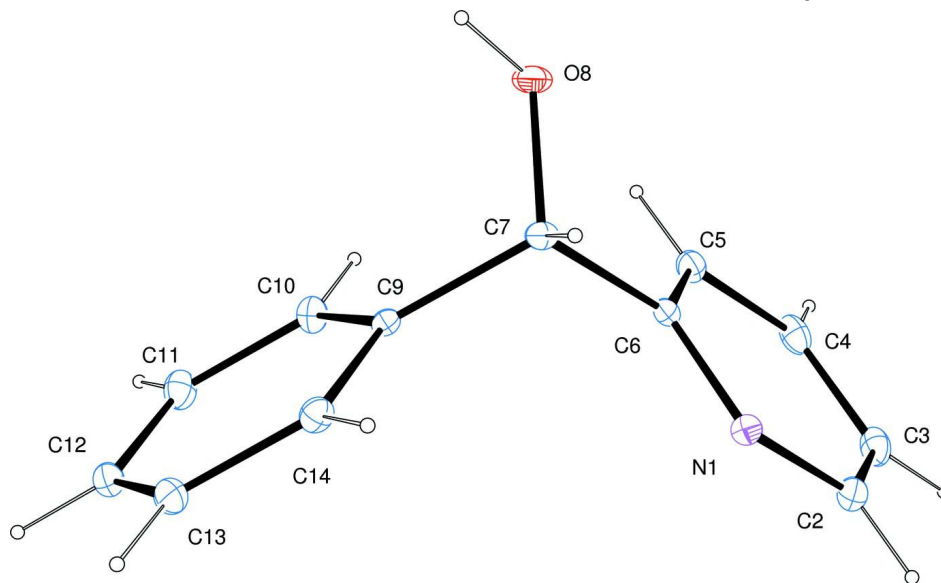
Haneol Kim and Sung Kwon Kang

### S1. Experimental

To a solution of 2-benzoylpyridine (5.0 g, 0.027 mol) in EtOH (60 ml) was added NaBH<sub>4</sub> (3.13 g, 0.083 mol) slowly at room temperature. The solution was stirred gently for 1 h. After adding 60 ml H<sub>2</sub>O, 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.

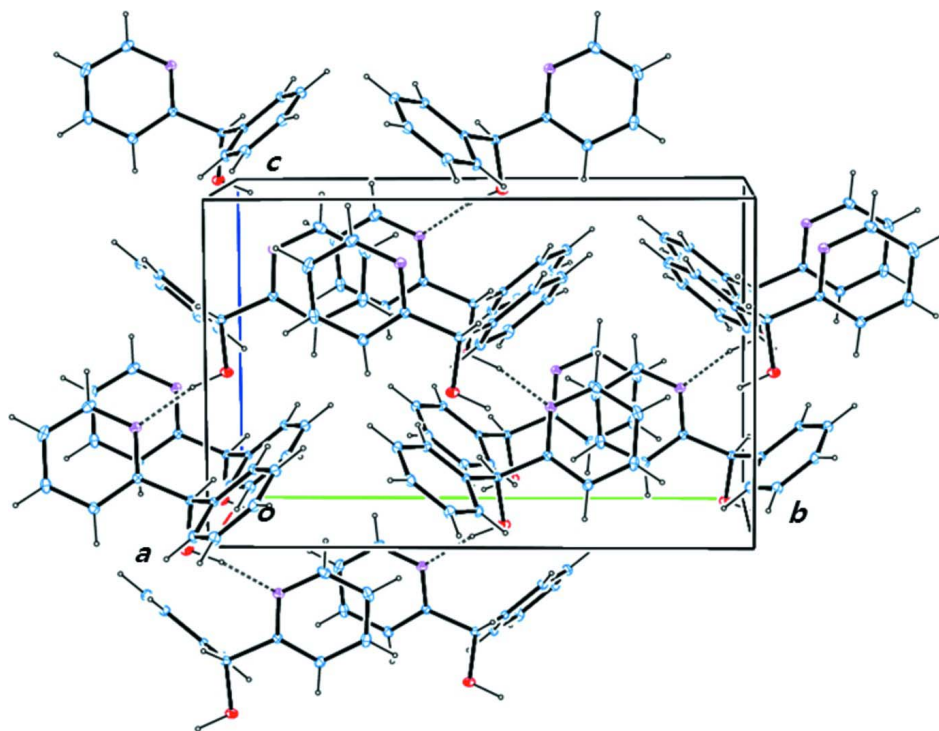
### S2. Refinement

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  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ .



**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:  $P\ 2c\ -2n$

$a = 7.4385\ (8)\ \text{\AA}$

$b = 14.3429\ (16)\ \text{\AA}$

$c = 9.2255\ (10)\ \text{\AA}$

$V = 984.27\ (19)\ \text{\AA}^3$

$Z = 4$

$F(000) = 392$

$D_x = 1.25\ \text{Mg m}^{-3}$

Mo  $K\alpha$  radiation,  $\lambda = 0.71073\ \text{\AA}$

Cell parameters from 973 reflections

$\theta = 2.6\text{--}19.7^\circ$

$\mu = 0.08\ \text{mm}^{-1}$

$T = 296\ \text{K}$

Block, colourless

$0.3 \times 0.26 \times 0.18\ \text{mm}$

#### Data collection

Bruker SMART CCD area-detector  
diffractometer

Radiation source: fine-focus sealed tube  
 $\varphi$  and  $\omega$  scans

7290 measured reflections

2245 independent reflections

1190 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.055$

$\theta_{\text{max}} = 27.5^\circ$ ,  $\theta_{\text{min}} = 2.6^\circ$

$h = -7 \rightarrow 9$

$k = -18 \rightarrow 18$

$l = -11 \rightarrow 11$

#### 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  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} < 0.001$   
 $\Delta\rho_{\max} = 0.09 \text{ e } \text{\AA}^{-3}$   
 $\Delta\rho_{\min} = -0.12 \text{ e } \text{\AA}^{-3}$

### 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 ( $\text{\AA}^2$ )

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
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 ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
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, °)*

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, °)*

<i>D</i> —H $\cdots$ <i>A</i>	<i>D</i> —H	H $\cdots$ <i>A</i>	<i>D</i> $\cdots$ <i>A</i>	<i>D</i> —H $\cdots$ <i>A</i>
O8—H8 $\cdots$ N1 <sup>i</sup>	0.98 (5)	1.85 (5)	2.809 (4)	166 (4)

Symmetry code: (i)  $-x+1, -y+1, z-1/2$ .