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## (3-Phenylisoxazol-5-yl)methanol

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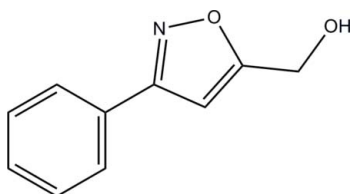
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Received 25 January 2010; accepted 27 January 2010

Key indicators: single-crystal X-ray study;  $T = 298$  K; mean  $\sigma(\text{C}-\text{C}) = 0.003$  Å;  $R$  factor = 0.054;  $wR$  factor = 0.119; data-to-parameter ratio = 12.7.

In the title compound,  $\text{C}_{10}\text{H}_9\text{NO}_2$ , the isoxazole and phenyl rings form a dihedral angle of  $25.82(3)^\circ$ . In the crystal, intermolecular  $\text{O}-\text{H}\cdots\text{O}$  hydrogen bonds link the molecules into ribbons propagating along  $[001]$ . The crystal packing is further stabilized by weak  $\text{C}-\text{H}\cdots\text{O}$  and  $\text{C}-\text{H}\cdots\text{N}$  interactions.

## Related literature

For related structures, see: Tian & Li (2006); Tang *et al.* (2006).

## Experimental

## Crystal data

 $\text{C}_{10}\text{H}_9\text{NO}_2$  $M_r = 175.18$ 

Monoclinic,  $C2/c$   
 $a = 41.03(4)$  Å  
 $b = 5.694(5)$  Å  
 $c = 7.348(7)$  Å  
 $\beta = 98.51(2)^\circ$   
 $V = 1698(3)$  Å<sup>3</sup>

$Z = 8$   
 Mo  $K\alpha$  radiation  
 $\mu = 0.10$  mm<sup>-1</sup>  
 $T = 298$  K  
 $0.55 \times 0.45 \times 0.02$  mm

## Data collection

Bruker SMART APEX  
 diffractometer  
 3328 measured reflections

1500 independent reflections  
 1182 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.059$

## Refinement

$R[F^2 > 2\sigma(F^2)] = 0.054$   
 $wR(F^2) = 0.119$   
 $S = 1.05$   
 1500 reflections

118 parameters  
 H-atom parameters constrained  
 $\Delta\rho_{\text{max}} = 0.16$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.23$  e Å<sup>-3</sup>

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{O2}-\text{H2B}\cdots\text{O2}^{\text{i}}$	0.86	1.89	2.669 (4)	151
$\text{O2}-\text{H2A}\cdots\text{O2}^{\text{ii}}$	0.88	2.09	2.677 (5)	124
$\text{C8}-\text{H8}\cdots\text{N1}^{\text{iii}}$	0.93	2.61	3.542 (4)	177
$\text{C10}-\text{H10B}\cdots\text{O2}^{\text{iv}}$	0.97	2.58	3.352 (4)	137

Symmetry codes: (i)  $-x, -y + 1, -z + 1$ ; (ii)  $-x, y, -z + \frac{1}{2}$ ; (iii)  $x, y + 1, z$ ; (iv)  $-x, -y + 2, -z + 1$ .

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

The authors express sincere gratitude to Xi-Zhao Wang for valuable discussions on the preparation of this manuscript.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV2692).

## References

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## supporting information

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**(3-Phenylisoxazol-5-yl)methanol**

Ling Yin, Gui-Long Zhao, Jiong Jia, Qing-Yang Meng and Jian-wu Wang

**S1. Comment**

In continuation of our study of isoxazole derivatives (Tang *et al.*, 2006), we present here the crystal structure of the title compound, (I).

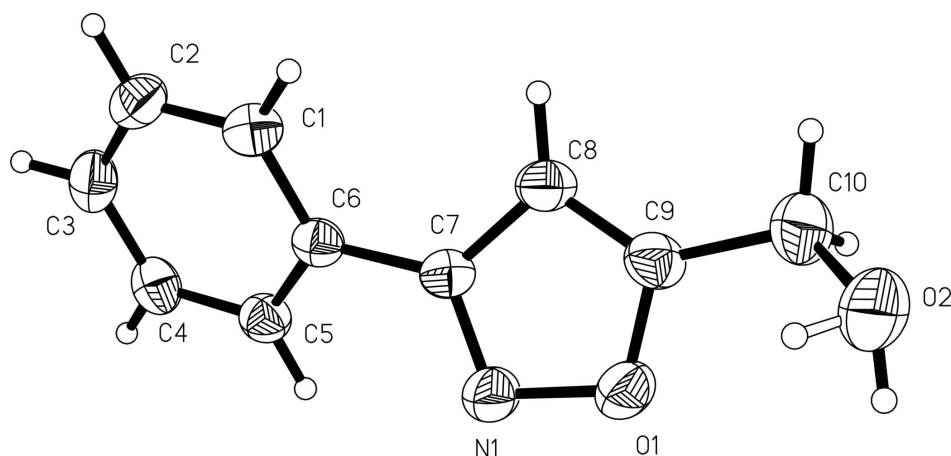
In (I) (Fig. 1), the bond lengths and angles of the isoxazole ring are normal and comparable to those reported for related structures (Tian & Li, 2006; Tang *et al.*, 2006). The mean planes of the benzene (C1—C6) and isoxazole (C7—C9/N1/O1) rings make a dihedral angle of 25.82 (3)°. Intermolecular O—H···O hydrogen bonds (Table 1) link the molecules into ribbons extended along the *c* axis. The crystal packing is further stabilized by weak C—H···O and C—H···N interactions (Table 1).

**S2. Experimental**

A round-bottomed flask was charged with benzaldoxime (5.0 g, 41.3 mmol) in 20 ml *N,N*-dimethyl formamide, and then *N*-chlorosuccinimide (1.20 g, 9.1 mmol) was added to the solution. Heating until *N*-chlorosuccinimide was solved, and the mixture was stirred at room temperature for 20 min, into the above solution was added *N*-chlorosuccinimide (4.80 g, 36.4 mmol) in batches under 308 K. After 3 h, propargyl alcohol (2.78 g, 49.6 mmol) was added, then the saturated solution of CuSO<sub>4</sub>·5H<sub>2</sub>O (0.62 g, 2.48 mmol) and L-ascorbic acid (1.75 g, 9.92 mmol) were added also. The solution of K<sub>2</sub>CO<sub>3</sub> (3.14 g, 45.5 mmol) was added to the mixture and was stirred for 1 h. The reaction mixture was diluted with the saturated solution of ethylenediaminetetraacetic acid, and then was extracted with dichloromethane (3 times per 50 ml), and the extracts were dried over anhydrous Na<sub>2</sub>SO<sub>4</sub>. The solution was evaporated to afford a residue, which was purified by a silica-gel column chromatography (petroleum ether / ethyl acetate, 3:1 by volume) to afford a pale yellow solid (yield: 61.7%, m.p. 325–326 K). The crystals of (I) were obtained from petroleum ether / ethyl acetate / dichloromethane (3:1:1, V/V/V) by slow evaporation at room temperature.

**S3. Refinement**

All H atoms were placed in calculated positions, with C—H = 0.93 or 0.97 Å, O—H = 0.86, 0.88 Å, and included in the final cycles of refinement using a riding model, with  $U_{\text{iso}}(\text{H}) = 1.2-1.5U_{\text{eq}}(\text{C}, \text{O})$ . The hydroxyl H atom was treated as disordered over two positions with equal occupancies fixed to 0.5.

**Figure 1**

The molecular structure of (I), with atom labels and 40% probability displacement ellipsoids for non-H atoms.

### (3-Phenylisoxazol-5-yl)methanol

#### Crystal data

$C_{10}H_9NO_2$

$M_r = 175.18$

Monoclinic,  $C2/c$

Hall symbol:  $-C 2yc$

$a = 41.03 (4) \text{ \AA}$

$b = 5.694 (5) \text{ \AA}$

$c = 7.348 (7) \text{ \AA}$

$\beta = 98.51 (2)^\circ$

$V = 1698 (3) \text{ \AA}^3$

$Z = 8$

$F(000) = 736$

$D_x = 1.371 \text{ Mg m}^{-3}$

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

Cell parameters from 1357 reflections

$\theta = 3.0\text{--}28.1^\circ$

$\mu = 0.10 \text{ mm}^{-1}$

$T = 298 \text{ K}$

Plate, colourless

$0.55 \times 0.45 \times 0.02 \text{ mm}$

#### Data collection

Bruker SMART APEX  
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

phi and  $\omega$  scans

3328 measured reflections

1500 independent reflections

1182 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.059$

$\theta_{\text{max}} = 25.1^\circ$ ,  $\theta_{\text{min}} = 2.0^\circ$

$h = -48 \rightarrow 43$

$k = -6 \rightarrow 5$

$l = -8 \rightarrow 8$

#### Refinement

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.054$

$wR(F^2) = 0.119$

$S = 1.05$

1500 reflections

118 parameters

0 restraints

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

$w = 1/[\sigma^2(F_o^2) + (0.0354P)^2 + 0.7771P]$

where  $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\text{max}} < 0.001$

$\Delta\rho_{\text{max}} = 0.16 \text{ e \AA}^{-3}$

$\Delta\rho_{\text{min}} = -0.23 \text{ e \AA}^{-3}$

*Special details*

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

**Refinement.** Refinement of  $F^2$  against ALL reflections. The weighted  $R$ -factor  $wR$  and goodness of fit  $S$  are based on  $F^2$ , conventional  $R$ -factors  $R$  are based on  $F$ , with  $F$  set to zero for negative  $F^2$ . The threshold expression of  $F^2 > \sigma(F^2)$  is used only for calculating  $R$ -factors(gt) etc. and is not relevant to the choice of reflections for refinement.  $R$ -factors based on  $F^2$  are statistically about twice as large as those based on  $F$ , and  $R$ -factors based on ALL data will be even larger.

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )*

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
C1	0.15963 (5)	0.9135 (4)	0.2841 (2)	0.0424 (5)	
H1	0.1439	1.0293	0.2497	0.051*	
C2	0.19149 (5)	0.9476 (4)	0.2556 (3)	0.0470 (6)	
H2	0.1973	1.0855	0.2009	0.056*	
C3	0.21488 (5)	0.7785 (4)	0.3078 (3)	0.0484 (6)	
H3	0.2366	0.8022	0.2889	0.058*	
C4	0.20619 (5)	0.5744 (4)	0.3878 (3)	0.0457 (6)	
H4	0.2221	0.4604	0.4237	0.055*	
C5	0.17421 (5)	0.5374 (4)	0.4152 (2)	0.0403 (5)	
H5	0.1685	0.3980	0.4682	0.048*	
C6	0.15054 (5)	0.7074 (3)	0.3639 (2)	0.0352 (5)	
C7	0.11668 (5)	0.6746 (4)	0.4006 (2)	0.0370 (5)	
C8	0.09363 (5)	0.8478 (4)	0.4305 (3)	0.0438 (5)	
H8	0.0961	1.0098	0.4236	0.053*	
C9	0.06769 (5)	0.7318 (4)	0.4705 (3)	0.0460 (6)	
C10	0.03668 (5)	0.8061 (5)	0.5327 (3)	0.0629 (7)	
H10A	0.0377	0.7646	0.6615	0.076*	
H10B	0.0350	0.9757	0.5237	0.076*	
N1	0.10486 (4)	0.4641 (3)	0.4183 (2)	0.0501 (5)	
O1	0.07313 (3)	0.4982 (3)	0.4643 (2)	0.0543 (4)	
O2	0.00792 (4)	0.7069 (3)	0.4334 (3)	0.0808 (6)	
H2B	0.0046	0.5589	0.4396	0.121*	0.50
H2A	0.0167	0.6698	0.3350	0.121*	0.50

*Atomic displacement parameters ( $\text{\AA}^2$ )*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
C1	0.0450 (13)	0.0391 (13)	0.0412 (10)	-0.0012 (10)	-0.0003 (9)	0.0019 (10)
C2	0.0546 (14)	0.0453 (14)	0.0412 (11)	-0.0104 (12)	0.0076 (9)	0.0033 (10)
C3	0.0405 (12)	0.0642 (17)	0.0415 (11)	-0.0082 (12)	0.0098 (9)	-0.0076 (11)
C4	0.0425 (13)	0.0513 (16)	0.0438 (11)	0.0086 (11)	0.0081 (9)	-0.0007 (11)
C5	0.0471 (12)	0.0362 (13)	0.0377 (10)	0.0027 (10)	0.0066 (8)	0.0018 (9)
C6	0.0393 (11)	0.0346 (12)	0.0308 (9)	-0.0001 (10)	0.0018 (7)	-0.0019 (8)
C7	0.0381 (11)	0.0332 (12)	0.0384 (10)	-0.0013 (10)	0.0015 (8)	-0.0001 (9)
C8	0.0378 (12)	0.0346 (13)	0.0571 (12)	0.0000 (11)	0.0006 (9)	-0.0002 (10)

C9	0.0384 (12)	0.0413 (14)	0.0562 (12)	0.0046 (11)	0.0001 (9)	-0.0029 (11)
C10	0.0400 (13)	0.0669 (19)	0.0812 (16)	0.0018 (13)	0.0068 (11)	-0.0049 (14)
N1	0.0402 (11)	0.0408 (12)	0.0702 (11)	0.0002 (9)	0.0112 (8)	0.0017 (9)
O1	0.0395 (9)	0.0458 (11)	0.0781 (10)	-0.0054 (8)	0.0105 (7)	0.0018 (8)
O2	0.0340 (9)	0.0818 (15)	0.1241 (15)	-0.0034 (9)	0.0039 (9)	-0.0057 (12)

*Geometric parameters (Å, °)*

C1—C2	1.368 (3)	C7—N1	1.306 (3)
C1—C6	1.387 (3)	C7—C8	1.406 (3)
C1—H1	0.9300	C8—C9	1.322 (3)
C2—C3	1.373 (3)	C8—H8	0.9300
C2—H2	0.9300	C9—O1	1.351 (3)
C3—C4	1.373 (3)	C9—C10	1.476 (3)
C3—H3	0.9300	C10—O2	1.410 (3)
C4—C5	1.373 (3)	C10—H10A	0.9700
C4—H4	0.9300	C10—H10B	0.9700
C5—C6	1.383 (3)	N1—O1	1.406 (2)
C5—H5	0.9300	O2—H2B	0.8561
C6—C7	1.466 (3)	O2—H2A	0.8798
C2—C1—C6	120.5 (2)	N1—C7—C6	120.73 (18)
C2—C1—H1	119.7	C8—C7—C6	128.09 (19)
C6—C1—H1	119.7	C9—C8—C7	105.4 (2)
C1—C2—C3	120.1 (2)	C9—C8—H8	127.3
C1—C2—H2	119.9	C7—C8—H8	127.3
C3—C2—H2	119.9	C8—C9—O1	110.0 (2)
C2—C3—C4	119.9 (2)	C8—C9—C10	133.2 (2)
C2—C3—H3	120.1	O1—C9—C10	116.5 (2)
C4—C3—H3	120.1	O2—C10—C9	114.7 (2)
C5—C4—C3	120.4 (2)	O2—C10—H10A	108.6
C5—C4—H4	119.8	C9—C10—H10A	108.6
C3—C4—H4	119.8	O2—C10—H10B	108.6
C4—C5—C6	120.1 (2)	C9—C10—H10B	108.6
C4—C5—H5	120.0	H10A—C10—H10B	107.6
C6—C5—H5	120.0	C7—N1—O1	105.53 (16)
C5—C6—C1	119.00 (19)	C9—O1—N1	107.91 (15)
C5—C6—C7	120.49 (19)	C10—O2—H2B	119.6
C1—C6—C7	120.46 (18)	C10—O2—H2A	96.2
N1—C7—C8	111.11 (19)	H2B—O2—H2A	84.0
C6—C1—C2—C3	-0.7 (3)	N1—C7—C8—C9	1.2 (2)
C1—C2—C3—C4	0.3 (3)	C6—C7—C8—C9	-175.60 (17)
C2—C3—C4—C5	0.4 (3)	C7—C8—C9—O1	-0.9 (2)
C3—C4—C5—C6	-0.7 (3)	C7—C8—C9—C10	173.2 (2)
C4—C5—C6—C1	0.4 (3)	C8—C9—C10—O2	131.4 (3)
C4—C5—C6—C7	-177.04 (16)	O1—C9—C10—O2	-54.8 (3)
C2—C1—C6—C5	0.3 (3)	C8—C7—N1—O1	-1.0 (2)

C2—C1—C6—C7	177.73 (16)	C6—C7—N1—O1	176.11 (15)
C5—C6—C7—N1	-24.9 (3)	C8—C9—O1—N1	0.4 (2)
C1—C6—C7—N1	157.73 (18)	C10—C9—O1—N1	-174.81 (17)
C5—C6—C7—C8	151.63 (19)	C7—N1—O1—C9	0.4 (2)
C1—C6—C7—C8	-25.7 (3)		

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>
O2—H2 <i>B</i> ...O2 <sup>i</sup>	0.86	1.89	2.669 (4)	151
O2—H2 <i>A</i> ...O2 <sup>ii</sup>	0.88	2.09	2.677 (5)	124
C8—H8...N1 <sup>iii</sup>	0.93	2.61	3.542 (4)	177
C10—H10 <i>B</i> ...O2 <sup>iv</sup>	0.97	2.58	3.352 (4)	137

Symmetry codes: (i)  $-x, -y+1, -z+1$ ; (ii)  $-x, y, -z+1/2$ ; (iii)  $x, y+1, z$ ; (iv)  $-x, -y+2, -z+1$ .