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## Structure Reports

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## 2-(1*H*-Imidazo[4,5-*f*][1,10]phenanthroline-2-yl)phenol monohydrate

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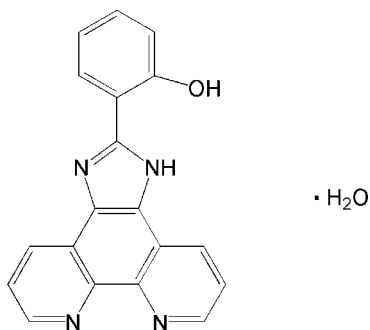
Received 18 June 2008; accepted 18 June 2008

 Key indicators: single-crystal X-ray study;  $T = 293$  K; mean  $\sigma(\text{C}-\text{C}) = 0.006$  Å;  $R$  factor = 0.094;  $wR$  factor = 0.206; data-to-parameter ratio = 14.4.

The asymmetric unit of the title compound,  $\text{C}_{19}\text{H}_{12}\text{N}_4\text{O}\cdot\text{H}_2\text{O}$ , contains one organic molecule and one solvent water molecule, which are connected by  $\text{N}-\text{H}\cdots\text{O}$  and  $\text{O}-\text{H}\cdots\text{N}$  hydrogen bonds. In addition, there is one intramolecular  $\text{O}-\text{H}\cdots\text{N}$  hydrogen bond. The organic molecule is essentially planar (r.m.s. deviation for all non-H atoms = 0.028 Å).

### Related literature

For related literature, see: Yin (2008). For a related structure, see: Sun *et al.* (2007).



### Experimental

#### Crystal data

 $\text{C}_{19}\text{H}_{12}\text{N}_4\text{O}\cdot\text{H}_2\text{O}$   
 $M_r = 330.34$ 

 Monoclinic,  $P2_1/c$   
 $a = 4.5272$  (9) Å

 $b = 19.822$  (4) Å  
 $c = 16.956$  (3) Å  
 $\beta = 94.15$  (3)°  
 $V = 1517.6$  (5) Å<sup>3</sup>  
 $Z = 4$ 

 Mo  $K\alpha$  radiation  
 $\mu = 0.10$  mm<sup>-1</sup>  
 $T = 293$  (2) K  
 $0.21 \times 0.17 \times 0.15$  mm

#### Data collection

 Rigaku R-Axis RAPID  
 diffractometer  
 Absorption correction: multi-scan  
 (ABSCOR; Higashi, 1995)  
 $T_{\min} = 0.975$ ,  $T_{\max} = 0.989$ 

 14107 measured reflections  
 3351 independent reflections  
 1342 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.177$ 

#### Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.094$   
 $wR(F^2) = 0.205$   
 $S = 1.02$   
 3351 reflections  
 232 parameters  
 3 restraints

 H atoms treated by a mixture of  
 independent and constrained  
 refinement  
 $\Delta\rho_{\max} = 0.20$  e Å<sup>-3</sup>  
 $\Delta\rho_{\min} = -0.21$  e Å<sup>-3</sup>
**Table 1**

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{O1}-\text{H1A}\cdots\text{N3}$	0.82	1.83	2.569 (5)	149
$\text{N4}-\text{H4}\cdots\text{O1W}$	0.86	1.90	2.744 (4)	169
$\text{O1W}-\text{HW12}\cdots\text{N2}^i$	0.863 (18)	1.91 (2)	2.715 (5)	155 (4)
$\text{O1W}-\text{HW12}\cdots\text{N1}^i$	0.863 (18)	2.62 (4)	3.255 (5)	131 (3)

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

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *PROCESS-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL-Plus* (Sheldrick, 2008); software used to prepare material for publication: *SHELXL97*.

This work was supported by the Program for Young Academic Backbone in Heilongjiang Provincial University (No. 1152 G053).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2727).

### References

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 Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.  
 Sun, M., Chen, G., Ling, B.-P. & Liu, Y.-X. (2007). *Acta Cryst.* **E63**, o1210–o1211.  
 Yin, G.-Q. (2008). *Acta Cryst.* **E64**, o1236.

## supporting information

*Acta Cryst.* (2008). E64, o1331 [doi:10.1107/S1600536808018527]

**2-(1*H*-Imidazo[4,5-*f*][1,10]phenanthrolin-2-yl)phenol monohydrate**

Wen-Zhi Zhang, Li Li and Ying-Hui Xiao

**S1. Comment**

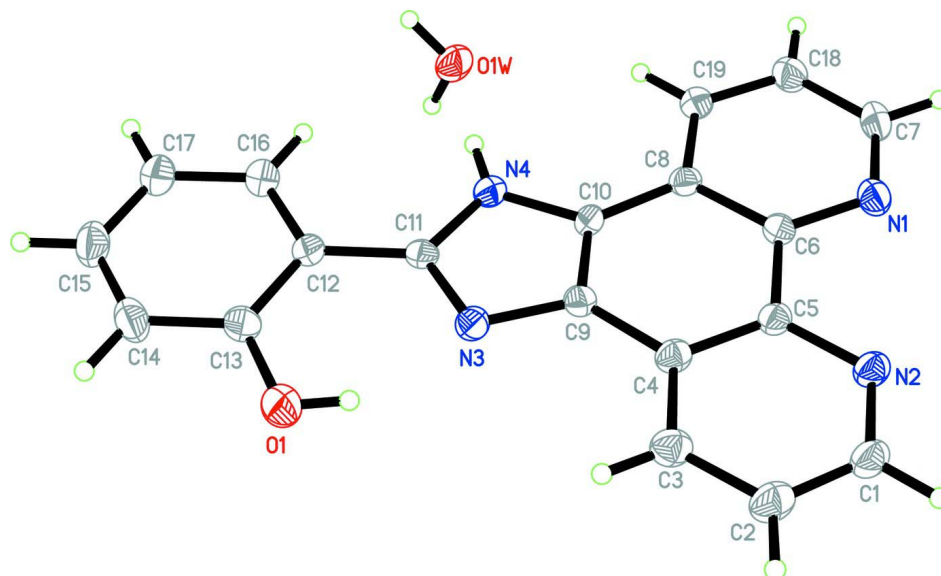
1,10-Phenanthroline and its derivatives are commonly used as ligands in metal-organic coordination polymers (Sun *et al.*, 2007; Yin, 2008). The title compound was synthesized from [4,5-*f*]1,10-phenanthroline. All bond lengths are within normal ranges. The H<sub>2</sub>O molecules links the 2-(1*H*-imidazo[4,5-*f*][1,10]phenanthrolin-2-yl)phenol molecules by hydrogen bonds to the nitrogen atoms of the imidazo-phenanthroline ring systems.

**S2. Experimental**

1,10-Phenanthroline-5,6-dione (1.5 mmol) and 2-hydroxybenzaldehyde (1.5 mmol) were dissolved in CH<sub>3</sub>COOH/CH<sub>3</sub>COONH<sub>4</sub> (1:1) solution (30 ml). The mixture was refluxed for 1.5 h under argon, after cooling, this mixture was diluted with water and neutralized with concentrated aqueous ammonia, immediately resulting a yellow precipitate, which was washed with water, acetone and diethyl ether respectively. Crystals of the title compound were obtained by recrystallization from dichloromethane.

**S3. Refinement**

C- and N-bound H atoms were positioned geometrically (N-H = 0.86 Å and C-H = 0.93-0.96 Å) and refined as riding, with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{carrier})$ . The water H-atoms were located in a difference Fourier map, and were refined with distance restraints of O-H = 0.85±0.01 Å and HW11···HW12 = 1.35±0.01 Å and with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{O})$ .



**Figure 1**

A perspective view of the title compound, showing the atomic numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

## 2-(1H-Imidazo[4,5-f][1,10]phenanthrolin-2-yl)phenol monohydrate

### Crystal data

$C_{19}H_{12}N_4O \cdot H_2O$

$M_r = 330.34$

Monoclinic,  $P2_1/c$

Hall symbol:  $-P\ 2_1/c$

$a = 4.5272\ (9)\ \text{\AA}$

$b = 19.822\ (4)\ \text{\AA}$

$c = 16.956\ (3)\ \text{\AA}$

$\beta = 94.15\ (3)^\circ$

$V = 1517.6\ (5)\ \text{\AA}^3$

$Z = 4$

$F(000) = 688$

$D_x = 1.446\ \text{Mg m}^{-3}$

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

Cell parameters from 6908 reflections

$\theta = 3.0\text{--}27.5^\circ$

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

$T = 293\ \text{K}$

Block, pale yellow

$0.21 \times 0.17 \times 0.15\ \text{mm}$

### Data collection

Rigaku R-Axis RAPID  
diffractometer

Radiation source: rotating anode

Graphite monochromator

Detector resolution:  $10.0\ \text{pixels mm}^{-1}$

$\omega$  scans

Absorption correction: multi-scan

(*ABSCOR*; Higashi, 1995)

$T_{\min} = 0.975$ ,  $T_{\max} = 0.989$

14107 measured reflections

3351 independent reflections

1342 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.177$

$\theta_{\max} = 27.5^\circ$ ,  $\theta_{\min} = 3.2^\circ$

$h = -5 \rightarrow 5$

$k = -25 \rightarrow 25$

$l = -21 \rightarrow 21$

### Refinement

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.094$

$wR(F^2) = 0.205$

$S = 1.03$

3351 reflections

232 parameters

3 restraints

Primary atom site location: structure-invariant  
direct methods

Secondary atom site location: difference Fourier map  
 Hydrogen site location: inferred from neighbouring sites  
 H atoms treated by a mixture of independent and constrained refinement

$$w = 1/[\sigma^2(F_o^2) + (0.0767P)^2]$$

where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} = 0.006$   
 $\Delta\rho_{\max} = 0.20 \text{ e } \text{\AA}^{-3}$   
 $\Delta\rho_{\min} = -0.21 \text{ e } \text{\AA}^{-3}$

*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  $F^2 > 2\sigma(F^2)$  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	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.8402 (11)	0.1329 (2)	1.0945 (2)	0.0583 (13)
H1	0.9502	0.1313	1.1429	0.070*
C2	0.6283 (11)	0.0844 (3)	1.0794 (2)	0.0632 (14)
H2	0.5933	0.0519	1.1172	0.076*
C3	0.4704 (10)	0.0846 (2)	1.0080 (2)	0.0568 (12)
H3	0.3234	0.0526	0.9964	0.068*
C4	0.5324 (9)	0.1337 (2)	0.9525 (2)	0.0454 (11)
C5	0.7451 (9)	0.1833 (2)	0.9742 (2)	0.0436 (10)
C6	0.8102 (9)	0.2370 (2)	0.9201 (2)	0.0434 (10)
C7	1.0598 (11)	0.3337 (2)	0.8980 (3)	0.0622 (13)
H7	1.1926	0.3669	0.9163	0.075*
C8	0.6649 (9)	0.2387 (2)	0.8427 (2)	0.0414 (10)
C9	0.3919 (9)	0.1377 (2)	0.8750 (2)	0.0419 (10)
C10	0.4603 (9)	0.1867 (2)	0.8232 (2)	0.0413 (10)
C11	0.1276 (9)	0.1180 (2)	0.7673 (2)	0.0421 (10)
C12	-0.0845 (9)	0.0871 (2)	0.7108 (2)	0.0467 (11)
C13	-0.2259 (10)	0.0279 (2)	0.7296 (3)	0.0544 (12)
C14	-0.4299 (11)	-0.0019 (3)	0.6760 (3)	0.0685 (14)
H14	-0.5268	-0.0411	0.6895	0.082*
C15	-0.4894 (11)	0.0265 (3)	0.6030 (3)	0.0740 (16)
H15	-0.6268	0.0062	0.5671	0.089*
C16	-0.1476 (10)	0.1140 (2)	0.6352 (2)	0.0610 (13)
H16	-0.0506	0.1529	0.6205	0.073*
C17	-0.3502 (11)	0.0840 (3)	0.5825 (3)	0.0717 (15)
H17	-0.3924	0.1028	0.5327	0.086*
C18	0.9353 (10)	0.3391 (2)	0.8210 (2)	0.0587 (13)
H18	0.9871	0.3745	0.7887	0.070*
C19	0.7362 (10)	0.2917 (2)	0.7935 (2)	0.0486 (11)
H19	0.6485	0.2946	0.7423	0.058*

O1	-0.1730 (7)	-0.00281 (16)	0.80052 (18)	0.0763 (11)
H1A	-0.0499	0.0189	0.8278	0.114*
N1	1.0015 (8)	0.28440 (19)	0.94675 (19)	0.0546 (10)
N2	0.9002 (8)	0.18203 (19)	1.04526 (18)	0.0504 (10)
N3	0.1823 (7)	0.09440 (17)	0.84045 (18)	0.0449 (9)
N4	0.2873 (7)	0.17430 (17)	0.75510 (17)	0.0458 (9)
H4	0.2814	0.1979	0.7125	0.055*
O1W	0.3484 (8)	0.24505 (18)	0.61814 (17)	0.0688 (10)
HW12	0.195 (7)	0.257 (2)	0.588 (2)	0.083*
HW11	0.444 (9)	0.219 (2)	0.590 (2)	0.083*

*Atomic displacement parameters (Å<sup>2</sup>)*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
C1	0.074 (4)	0.061 (3)	0.039 (2)	0.011 (3)	-0.006 (2)	0.001 (2)
C2	0.075 (4)	0.071 (4)	0.044 (3)	0.008 (3)	0.004 (2)	0.013 (2)
C3	0.064 (3)	0.055 (3)	0.052 (3)	0.001 (3)	0.007 (2)	0.008 (2)
C4	0.049 (3)	0.048 (3)	0.039 (2)	0.007 (2)	0.0045 (19)	0.002 (2)
C5	0.046 (3)	0.044 (3)	0.041 (2)	0.008 (2)	-0.0006 (19)	-0.003 (2)
C6	0.045 (3)	0.039 (3)	0.046 (2)	0.005 (2)	0.002 (2)	-0.005 (2)
C7	0.069 (4)	0.053 (3)	0.063 (3)	-0.012 (3)	-0.009 (2)	-0.009 (3)
C8	0.043 (3)	0.040 (3)	0.041 (2)	0.007 (2)	0.0010 (19)	0.0004 (19)
C9	0.040 (3)	0.039 (3)	0.047 (2)	0.001 (2)	0.0010 (19)	0.000 (2)
C10	0.039 (3)	0.042 (3)	0.041 (2)	0.004 (2)	-0.0061 (19)	-0.001 (2)
C11	0.043 (3)	0.035 (2)	0.047 (2)	0.009 (2)	0.0010 (19)	-0.003 (2)
C12	0.044 (3)	0.042 (3)	0.053 (3)	0.004 (2)	-0.004 (2)	-0.002 (2)
C13	0.055 (3)	0.046 (3)	0.062 (3)	0.006 (2)	0.002 (2)	-0.006 (2)
C14	0.060 (4)	0.056 (3)	0.088 (4)	-0.010 (3)	0.001 (3)	-0.022 (3)
C15	0.066 (4)	0.078 (4)	0.075 (4)	-0.003 (3)	-0.016 (3)	-0.022 (3)
C16	0.058 (3)	0.057 (3)	0.066 (3)	-0.001 (3)	-0.009 (2)	-0.003 (3)
C17	0.072 (4)	0.071 (4)	0.069 (3)	-0.001 (3)	-0.019 (3)	-0.007 (3)
C18	0.069 (4)	0.049 (3)	0.057 (3)	-0.007 (2)	0.001 (2)	0.004 (2)
C19	0.054 (3)	0.046 (3)	0.046 (2)	0.001 (2)	0.000 (2)	0.002 (2)
O1	0.077 (2)	0.066 (2)	0.083 (2)	-0.0178 (19)	-0.0115 (18)	0.0141 (19)
N1	0.063 (3)	0.047 (2)	0.053 (2)	-0.011 (2)	-0.0019 (18)	-0.0013 (19)
N2	0.059 (2)	0.052 (2)	0.0394 (19)	0.0082 (19)	0.0000 (17)	0.0002 (18)
N3	0.043 (2)	0.046 (2)	0.0449 (19)	0.0014 (18)	0.0012 (16)	0.0004 (17)
N4	0.046 (2)	0.044 (2)	0.0463 (19)	0.0008 (18)	-0.0033 (16)	0.0060 (17)
O1W	0.077 (3)	0.071 (3)	0.0559 (19)	0.000 (2)	-0.0092 (16)	0.0158 (17)

*Geometric parameters (Å, °)*

C1—N2	1.323 (5)	C11—N3	1.332 (5)
C1—C2	1.370 (6)	C11—N4	1.353 (5)
C1—H1	0.9300	C11—C12	1.443 (5)
C2—C3	1.360 (5)	C12—C13	1.384 (6)
C2—H2	0.9300	C12—C16	1.400 (5)
C3—C4	1.397 (5)	C13—O1	1.353 (5)

C3—H3	0.9300	C13—C14	1.380 (6)
C4—C5	1.407 (6)	C14—C15	1.368 (6)
C4—C9	1.420 (5)	C14—H14	0.9300
C5—N2	1.351 (4)	C15—C17	1.360 (7)
C5—C6	1.449 (5)	C15—H15	0.9300
C6—N1	1.334 (5)	C16—C17	1.370 (6)
C6—C8	1.424 (5)	C16—H16	0.9300
C7—N1	1.318 (5)	C17—H17	0.9300
C7—C18	1.389 (5)	C18—C19	1.361 (6)
C7—H7	0.9300	C18—H18	0.9300
C8—C19	1.393 (5)	C19—H19	0.9300
C8—C10	1.410 (5)	O1—H1A	0.8200
C9—C10	1.360 (5)	N4—H4	0.8600
C9—N3	1.378 (5)	O1W—HW12	0.863 (18)
C10—N4	1.370 (4)	O1W—HW11	0.841 (18)
N2—C1—C2	124.9 (4)	C13—C12—C16	117.8 (4)
N2—C1—H1	117.5	C13—C12—C11	120.3 (4)
C2—C1—H1	117.5	C16—C12—C11	121.8 (4)
C3—C2—C1	118.7 (4)	O1—C13—C14	117.4 (4)
C3—C2—H2	120.7	O1—C13—C12	122.0 (4)
C1—C2—H2	120.7	C14—C13—C12	120.6 (4)
C2—C3—C4	118.9 (4)	C15—C14—C13	119.9 (5)
C2—C3—H3	120.5	C15—C14—H14	120.1
C4—C3—H3	120.5	C13—C14—H14	120.1
C3—C4—C5	118.6 (4)	C17—C15—C14	120.8 (5)
C3—C4—C9	124.4 (4)	C17—C15—H15	119.6
C5—C4—C9	117.1 (4)	C14—C15—H15	119.6
N2—C5—C4	121.4 (4)	C17—C16—C12	121.0 (5)
N2—C5—C6	117.6 (4)	C17—C16—H16	119.5
C4—C5—C6	121.0 (3)	C12—C16—H16	119.5
N1—C6—C8	122.8 (4)	C15—C17—C16	119.8 (5)
N1—C6—C5	117.3 (3)	C15—C17—H17	120.1
C8—C6—C5	119.9 (4)	C16—C17—H17	120.1
N1—C7—C18	124.1 (4)	C19—C18—C7	118.8 (4)
N1—C7—H7	117.9	C19—C18—H18	120.6
C18—C7—H7	117.9	C7—C18—H18	120.6
C19—C8—C10	126.0 (3)	C18—C19—C8	119.5 (4)
C19—C8—C6	117.2 (4)	C18—C19—H19	120.3
C10—C8—C6	116.8 (4)	C8—C19—H19	120.3
C10—C9—N3	110.6 (3)	C13—O1—H1A	109.5
C10—C9—C4	122.0 (4)	C7—N1—C6	117.6 (4)
N3—C9—C4	127.4 (4)	C1—N2—C5	117.4 (4)
C9—C10—N4	105.8 (3)	C11—N3—C9	104.6 (3)
C9—C10—C8	123.2 (3)	C11—N4—C10	107.3 (3)
N4—C10—C8	130.9 (4)	C11—N4—H4	126.3
N3—C11—N4	111.5 (3)	C10—N4—H4	126.3
N3—C11—C12	122.5 (4)	HW12—O1W—HW11	105 (3)

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N4—C11—C12                      125.9 (4)

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*Hydrogen-bond geometry (Å, °)*

<i>D—H...A</i>	<i>D—H</i>	<i>H...A</i>	<i>D...A</i>	<i>D—H...A</i>
O1—H1A...N3	0.82	1.83	2.569 (5)	149
N4—H4...O1W	0.86	1.90	2.744 (4)	169
O1W—HW12...N2 <sup>i</sup>	0.86 (2)	1.91 (2)	2.715 (5)	155 (4)
O1W—HW12...N1 <sup>i</sup>	0.86 (2)	2.62 (4)	3.255 (5)	131 (3)

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