Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

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

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

College of Chemistry and Chemical Engineering, Qiqihar University, Qiqihar 161006, Heilongjiang Province, People's Republic of China
Correspondence e-mail: zhangwenzhi1968@yahoo.com.cn

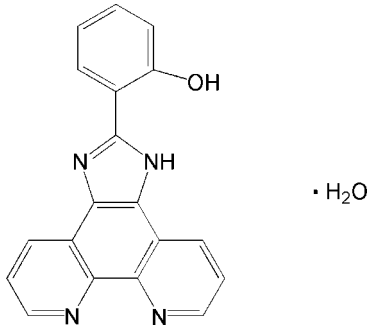
Received 18 June 2008; accepted 18 June 2008

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–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, $C_{19}H_{12}N_4O\cdot H_2O$, contains one organic molecule and one solvent water molecule, which are connected by N—H···O and O—H···N hydrogen bonds. In addition, there is one intramolecular O—H···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

$C_{19}H_{12}N_4O\cdot H_2O$
M_r = 330.34
Monoclinic, $P2_1/c$
a = 4.5272 (9) Å
b = 19.822 (4) Å
c = 16.956 (3) Å
β = 94.15 (3)°
V = 1517.6 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 293 (2) K
0.21 × 0.17 × 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_{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^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
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^{i}	0.863 (18)	1.91 (2)	2.715 (5)	155 (4)
O1W—HW12···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

Higashi, T. (1995). *ABSCOR*. Rigaku Corporation, Tokyo, Japan.
Rigaku (1998). *PROCESS-AUTO*. Rigaku Corporation, Tokyo, Japan.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Sun, M., Chen, G., Ling, B.-P. & Liu, Y.-X. (2007). *Acta Cryst.* E**63**, o1210–o1211.
Yin, G.-Q. (2008). *Acta Cryst.* E**64**, o1236.

supplementary materials

Acta Cryst. (2008). E**64**, o1331 [**doi:10.1107/S1600536808018527**]

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

W.-Z. Zhang, L. Li and Y.-H. Xiao

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_2O molecules links the 2-(1H-imidazo[4,5-f][1,10]phenanthrolin-2-yl)phenol molecules by hydrogen bonds to the nitrogen atoms of the imidazo-phenantholine ring systems.

Experimental

1,10-Phenanthroline-5,6-dione (1.5 mmol) and 2-hydroxybenzaldehyde (1.5 mmol) were dissolved in $CH_3COOHCH_3COONH_4$ (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 re-crystallization from dichloromethane.

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 $U_{iso}(H) = 1.2U_{eq}$(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 $U_{iso}(H) = 1.2U_{eq}(O)$.

Figures

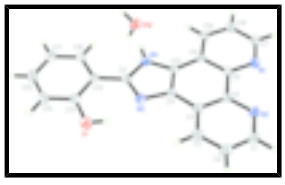


Fig. 1. A perspective view of the title compound, showing the atomic numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

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

Crystal data

$C_{19}H_{12}N_4O·H_2O$	F_{000} = 688
M_r = 330.34	D_x = 1.446 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 6908 reflections

a = 4.5272 (9) Å	θ = 3.0–27.5º
b = 19.822 (4) Å	μ = 0.10 mm^{-1}
c = 16.956 (3) Å	T = 293 (2) K
β = 94.15 (3)º	Block, pale yellow
V = 1517.6 (5) Å^3	0.21 × 0.17 × 0.15 mm
Z = 4	

Data collection

Rigaku R-AXIS RAPID diffractometer	3351 independent reflections
Radiation source: rotating anode	1342 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.177
Detector resolution: 10.0 pixels mm^{-1}	θ_{max} = 27.5º
T = 293(2) K	θ_{min} = 3.2º
ω scans	h = −5→5
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	k = −25→25
T_{min} = 0.975, T_{max} = 0.989	l = −21→21
14107 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.094	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.205	$w = 1/[\sigma^2(F_o^2) + (0.0767P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.03	$(\Delta/\sigma)_{max}$ = 0.006
3351 reflections	$\Delta\rho_{max}$ = 0.20 e Å^{-3}
232 parameters	$\Delta\rho_{min}$ = −0.21 e Å^{-3}
3 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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 $F^2 > 2\text{sigma}(F^2)$ 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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{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^2)

	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)

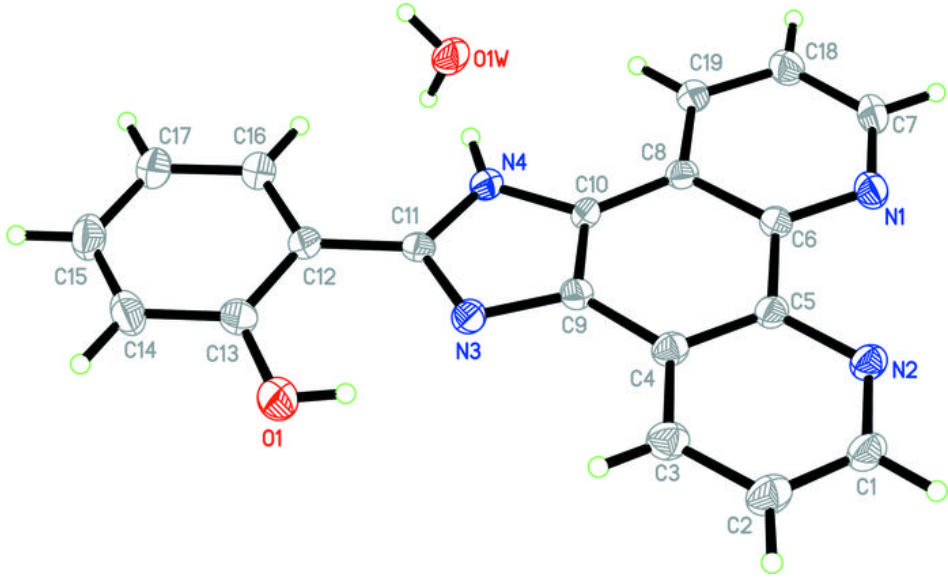
N2—C1—H1	117.5	C13—C12—C11	120.3 (4)
C2—C1—H1	117.5	C16—C12—C11	121.8 (4)
C3—C2—C1	118.7 (4)	O1—C13—C14	117.4 (4)
C3—C2—H2	120.7	O1—C13—C12	122.0 (4)
C1—C2—H2	120.7	C14—C13—C12	120.6 (4)
C2—C3—C4	118.9 (4)	C15—C14—C13	119.9 (5)
C2—C3—H3	120.5	C15—C14—H14	120.1
C4—C3—H3	120.5	C13—C14—H14	120.1
C3—C4—C5	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)
N4—C11—C12	125.9 (4)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
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^{i}	0.863 (18)	1.91 (2)	2.715 (5)	155 (4)
O1W—HW12···N1^{i}	0.863 (18)	2.62 (4)	3.255 (5)	131 (3)

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

Fig. 1


O1W
C19
C18
C7
C17
C16
N4
C8
C10
N1
C11
C6
C15
C12
C5
N3
C9
C14
C13
N2
C4
O1
C3
C1
C2