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5*H*-Imidazo[4,5-*f*][1,10]phenanthroline

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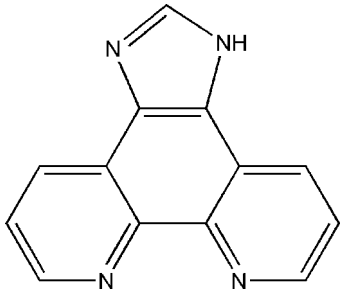
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.003 Å; R factor = 0.042; wR factor = 0.123; data-to-parameter ratio = 9.4.

The title molecule, $C_{13}H_8N_4$, is is essentially planar [r.m.s. deviation for all non-H atoms = 0.025 (3) Å]. In the crystal, molecules are connected through one weak bifurcated N—H···(N,N) hydrogen bond and three π–π stacking interactions between pyridine and imidazole rings [centroid–centroid distance = 3.631 (8) Å] and between pyridine and benzene rings [centroid–centroid distances = 3.675 (5) and 3.666 (2) Å].

Related literature

For our previous work based on 1,10-phenanthroline as anauxiliary ligand, see: Song *et al.* (2009); Hao *et al.* (2008). For background to 1,10-phenanthroline complexes, see: Chesnut *et al.* (1999).



Experimental

Crystal data

$C_{13}H_8N_4$ M_r = 220.23
Orthorhombic, *Pbca*
a = 14.569 (2) Å
b = 7.8623 (12) Å
c = 17.042 (3) Å
V = 1952.1 (5) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 296 K
0.26 × 0.18 × 0.16 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2007)
T_{min} = 0.980, T_{max} = 0.985
5772 measured reflections
1756 independent reflections
1025 reflections with $I > 2\sigma(I)$
R_{int} = 0.053

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.123
S = 1.00
1756 reflections
186 parameters
All H-atom parameters refined
$\Delta\rho_{max}$ = 0.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.15 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N3—H8···N1^{i}	0.92 (3)	2.47 (3)	3.104 (3)	126 (2)
N3—H8···N2^{i}	0.92 (3)	2.18 (3)	3.017 (3)	150 (2)

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

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BX2404).

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Chesnut, D.-J., Haushalter, R.-C. & Zubieta, J. (1999). *Inorg. Chim. Acta*, **292**, 41–51.
Hao, X.-M., Gu, C.-S., Song, W.-D. & Liu, J.-W. (2008). *Acta Cryst.* E**64**, m1052.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Song, W.-D., Wang, H., Hu, S.-W., Qin, P.-W. & Li, S.-J. (2009). *Acta Cryst.* E**65**, m701.

supplementary materials

Acta Cryst. (2012). E**68**, o1448 [doi:10.1107/S1600536812016595]

5*H*-Imidazo[4,5-*f*][1,10]phenanthroline

Shao-Wei Tong, Wen-Dong Song, Dong-Liang Miao and Jing-Bo An

Comment

(1,10)phenanthroline is widely used to synthetize metal-complex as a auxiliary ligand. In our laboratory earlier studies, we have successfully obtained some metal-complex with (1,10)phenanthroline.We report here the crystal structure of the title compound, Fig. 1. The title compound, is essentially planar (r.m.s. deviation for all non-H atoms = 0.025 (3)Å). In the crystal the molecules are connected through one weak bifurcated N—H···N hydrogen bonds, Fig. 2, Table 1 and π-π stacking interactions between pyridine and imidazole rings [distance centroid – centroid 3.631 (8) Å] and between pyridine and benzene rings [distance centroid–centroid 3.675 (5); 3.666 (2) Å] respectively.

Experimental

Imidazo(4,5-f)(1,10)phenanthroline was purchased from Jinan Henghua science and technology limited company and recristallized of an alkaline solution.

Refinement

All H-atoms in this structure were located from differences Fourier syntheses and were refined isotropically.

Computing details

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT* (Bruker, 2007); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

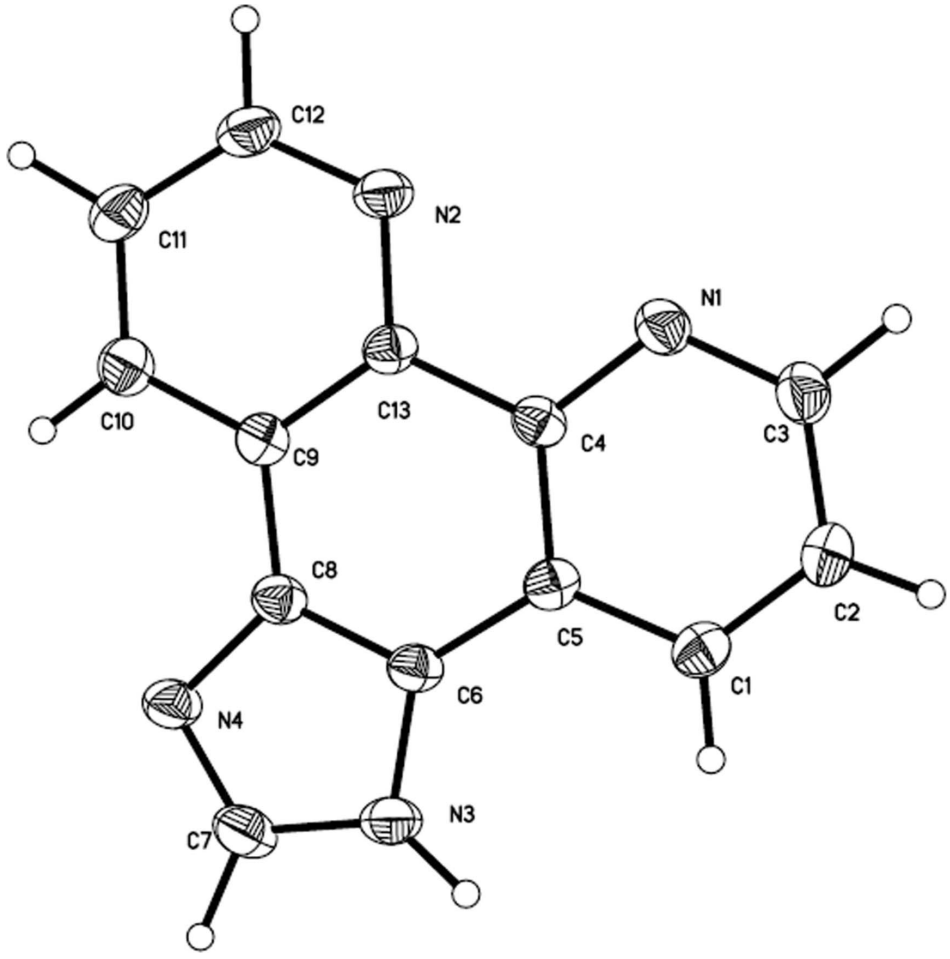

Figure 1

Molecular configuration and atom numbering scheme for the title complex showing 30% probability ellipsoids.

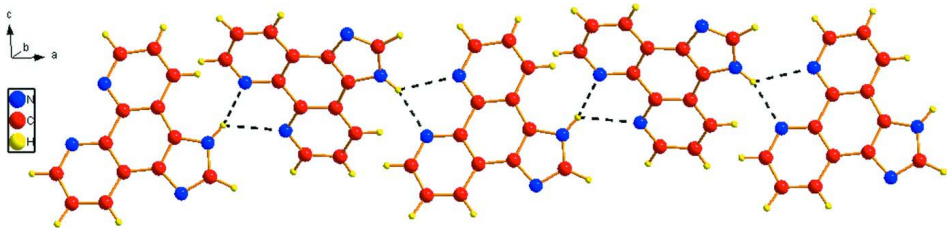

Figure 2

Part of the crystal structure showing one dimensional chain along (100).

5*H*-Imidazo[4,5-*f*][1,10]phenanthroline

Crystal data

$C_{13}H_8N_4$
M_r = 220.23
Orthorhombic, *Pbca*
Hall symbol: -P 2ac 2ab
a = 14.569 (2) Å
b = 7.8623 (12) Å
c = 17.042 (3) Å
V = 1952.1 (5) Å^3
Z = 8
F(000) = 912
D_x = 1.499 Mg m^{-3}
Mo *Kα* radiation, *λ* = 0.71073 Å

Cell parameters from 799 reflections
θ = 2.2–27.5°
μ = 0.10 mm^{-1}
T = 296 K
Block, yellow
0.26 × 0.18 × 0.16 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2007)
T_{min} = 0.980, T_{max} = 0.985
5772 measured reflections
1756 independent reflections
1025 reflections with $I > 2\sigma(I)$
R_{int} = 0.053
θ_{max} = 25.2°, θ_{min} = 2.4°
h = −17→10
k = −9→9
l = −20→20

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.123
S = 1.00
1756 reflections
186 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
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0606P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.15 e Å^{-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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
N2	0.08583 (13)	0.0741 (3)	0.18218 (11)	0.0428 (6)
C13	0.17857 (16)	0.0868 (3)	0.18200 (12)	0.0349 (6)
C4	0.22247 (15)	0.1620 (3)	0.25102 (12)	0.0347 (6)
N1	0.16716 (13)	0.2161 (3)	0.30974 (10)	0.0423 (6)
C5	0.31923 (15)	0.1740 (3)	0.25518 (12)	0.0355 (6)
N3	0.46339 (14)	0.1051 (3)	0.17574 (13)	0.0471 (6)
N4	0.39502 (14)	−0.0018 (3)	0.06803 (11)	0.0449 (6)
C11	0.09449 (19)	−0.0623 (4)	0.05615 (15)	0.0487 (7)
C12	0.04717 (19)	−0.0004 (3)	0.12071 (16)	0.0494 (7)
C3	0.20665 (19)	0.2840 (3)	0.37251 (14)	0.0460 (7)
C2	0.30087 (18)	0.3045 (3)	0.38092 (14)	0.0439 (7)
C1	0.35746 (19)	0.2504 (3)	0.32252 (13)	0.0416 (6)
C6	0.37040 (15)	0.1101 (3)	0.18996 (12)	0.0365 (6)
C7	0.4727 (2)	0.0392 (3)	0.10225 (15)	0.0514 (7)

C8	0.32970 (16)	0.0437 (3)	0.12418 (12)	0.0373 (6)
C9	0.23250 (15)	0.0280 (3)	0.11878 (12)	0.0356 (6)
C10	0.18762 (19)	−0.0478 (3)	0.05489 (14)	0.0445 (7)
H7	0.5396 (16)	0.027 (3)	0.0759 (12)	0.042 (6)*
H6	0.2264 (16)	−0.088 (3)	0.0121 (15)	0.056 (8)*
H4	−0.0192 (17)	−0.012 (3)	0.1232 (13)	0.045 (7)*
H1	0.4230 (16)	0.270 (3)	0.3229 (13)	0.051 (8)*
H5	0.0590 (16)	−0.125 (3)	0.0140 (15)	0.063 (8)*
H3	0.1640 (15)	0.322 (3)	0.4153 (13)	0.046 (7)*
H2	0.3235 (16)	0.353 (3)	0.4266 (14)	0.053 (7)*
H8	0.5057 (19)	0.136 (4)	0.2135 (18)	0.074 (9)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N2	0.0304 (12)	0.0574 (14)	0.0407 (12)	−0.0012 (10)	−0.0020 (9)	0.0005 (10)
C13	0.0326 (13)	0.0403 (15)	0.0318 (12)	−0.0009 (11)	−0.0029 (11)	0.0052 (10)
C4	0.0343 (13)	0.0379 (14)	0.0319 (11)	0.0024 (12)	0.0035 (11)	0.0054 (10)
N1	0.0396 (12)	0.0519 (14)	0.0355 (11)	0.0021 (10)	0.0037 (10)	0.0001 (9)
C5	0.0350 (14)	0.0389 (14)	0.0326 (12)	−0.0016 (11)	−0.0027 (11)	0.0075 (10)
N3	0.0308 (12)	0.0644 (15)	0.0462 (13)	0.0046 (11)	−0.0024 (11)	0.0001 (11)
N4	0.0334 (12)	0.0646 (15)	0.0368 (11)	0.0021 (11)	0.0034 (10)	0.0000 (10)
C11	0.0435 (17)	0.0584 (18)	0.0441 (15)	−0.0023 (14)	−0.0125 (13)	−0.0028 (13)
C12	0.0326 (15)	0.0651 (19)	0.0505 (15)	−0.0029 (14)	−0.0084 (13)	−0.0022 (13)
C3	0.0488 (17)	0.0546 (18)	0.0346 (14)	0.0041 (13)	0.0018 (12)	−0.0029 (11)
C2	0.0511 (17)	0.0462 (16)	0.0344 (13)	−0.0027 (13)	−0.0045 (12)	−0.0036 (11)
C1	0.0403 (15)	0.0443 (15)	0.0403 (14)	−0.0014 (13)	−0.0053 (13)	0.0029 (11)
C6	0.0305 (13)	0.0445 (15)	0.0344 (12)	0.0013 (11)	0.0015 (10)	0.0047 (11)
C7	0.0401 (17)	0.0647 (19)	0.0495 (15)	0.0122 (15)	0.0068 (14)	0.0010 (13)
C8	0.0335 (14)	0.0447 (16)	0.0338 (12)	0.0021 (12)	0.0013 (11)	0.0039 (10)
C9	0.0375 (14)	0.0372 (14)	0.0321 (12)	0.0020 (11)	−0.0006 (10)	0.0048 (10)
C10	0.0471 (17)	0.0518 (17)	0.0346 (13)	0.0026 (14)	−0.0025 (12)	0.0009 (11)

Geometric parameters (Å, º)

N2—C12	1.326 (3)	C11—C10	1.362 (4)
N2—C13	1.355 (3)	C11—C12	1.387 (4)
C13—C9	1.411 (3)	C11—H5	1.01 (3)
C13—C4	1.464 (3)	C12—H4	0.97 (2)
C4—N1	1.353 (3)	C3—C2	1.390 (4)
C4—C5	1.415 (3)	C3—H3	1.00 (2)
N1—C3	1.327 (3)	C2—C1	1.360 (3)
C5—C1	1.410 (3)	C2—H2	0.93 (2)
C5—C6	1.429 (3)	C1—H1	0.97 (2)
N3—C7	1.362 (3)	C6—C8	1.372 (3)
N3—C6	1.377 (3)	C7—H7	1.08 (2)
N3—H8	0.92 (3)	C8—C9	1.424 (3)
N4—C7	1.314 (3)	C9—C10	1.403 (3)
N4—C8	1.396 (3)	C10—H6	0.98 (3)

C12—N2—C13	117.0 (2)	C2—C3—H3	120.2 (13)
N2—C13—C9	122.2 (2)	C1—C2—C3	119.2 (2)
N2—C13—C4	117.63 (19)	C1—C2—H2	121.8 (15)
C9—C13—C4	120.2 (2)	C3—C2—H2	119.0 (15)
N1—C4—C5	122.4 (2)	C2—C1—C5	119.3 (2)
N1—C4—C13	117.4 (2)	C2—C1—H1	123.0 (14)
C5—C4—C13	120.16 (19)	C5—C1—H1	117.5 (14)
C3—N1—C4	117.7 (2)	C8—C6—N3	105.7 (2)
C1—C5—C4	117.6 (2)	C8—C6—C5	122.9 (2)
C1—C5—C6	125.2 (2)	N3—C6—C5	131.3 (2)
C4—C5—C6	117.2 (2)	N4—C7—N3	114.5 (2)
C7—N3—C6	105.7 (2)	N4—C7—H7	124.9 (11)
C7—N3—H8	132.4 (17)	N3—C7—H7	120.5 (11)
C6—N3—H8	121.7 (17)	C6—C8—N4	111.3 (2)
C7—N4—C8	102.7 (2)	C6—C8—C9	121.0 (2)
C10—C11—C12	118.6 (2)	N4—C8—C9	127.7 (2)
C10—C11—H5	122.6 (13)	C10—C9—C13	118.2 (2)
C12—C11—H5	118.7 (13)	C10—C9—C8	123.4 (2)
N2—C12—C11	124.8 (2)	C13—C9—C8	118.4 (2)
N2—C12—H4	115.4 (14)	C11—C10—C9	119.2 (2)
C11—C12—H4	119.7 (14)	C11—C10—H6	124.2 (14)
N1—C3—C2	123.9 (2)	C9—C10—H6	116.6 (14)
N1—C3—H3	115.9 (13)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H8···N1^{i}	0.92 (3)	2.47 (3)	3.104 (3)	126 (2)
N3—H8···N2^{i}	0.92 (3)	2.18 (3)	3.017 (3)	150 (2)

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