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2-(1*H*-Pyrrolo[2,3-*b*]pyridin-2-yl)-pyridine

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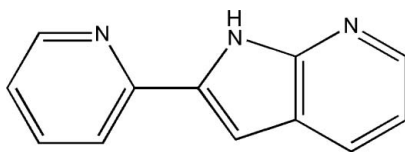
Received 1 May 2012; accepted 24 May 2012

 Key indicators: single-crystal X-ray study; $T = 200$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.064; wR factor = 0.145; data-to-parameter ratio = 15.8.

In the title compound, $\text{C}_{12}\text{H}_9\text{N}_3$, the dihedral angle between the pyridine and azaindole rings is $6.20(2)^\circ$. In the crystal, pairs of $\text{N}-\text{H}\cdots\text{N}$ hydrogen bonds link molecules into inversion dimers.

Related literature

For the production of luminescent organic/organometallic compounds, see: Liu *et al.* (2000). For related structures, see: Sakamoto *et al.* (1996); Huang *et al.* (2011).



Experimental

Crystal data

 $\text{C}_{12}\text{H}_9\text{N}_3$
 $M_r = 195.22$
 Monoclinic, $P2_1/c$
 $a = 10.1416(10)$ Å

 $b = 13.7428(14)$ Å
 $c = 6.7395(7)$ Å
 $\beta = 94.331(2)^\circ$
 $V = 936.63(16)$ Å³
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 0.09$ mm⁻¹
 $T = 200$ K
 $0.55 \times 0.15 \times 0.05$ mm

Data collection

 Bruker SMART APEX CCD diffractometer
 Absorption correction: multi-scan (SADABS; Bruker, 2001)
 $T_{\min} = 0.938$, $T_{\max} = 0.996$

 7069 measured reflections
 2154 independent reflections
 1792 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.056$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.064$
 $wR(F^2) = 0.145$
 $S = 1.19$
 2154 reflections

 136 parameters
 H-atom parameters constrained
 $\Delta\rho_{\max} = 0.25$ e Å⁻³
 $\Delta\rho_{\min} = -0.20$ e Å⁻³
Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{N2}-\text{H2}\cdots\text{N1}^i$	0.88	2.10	2.944 (2)	162

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

Data collection: SMART (Bruker, 2001); cell refinement: SAINT (Bruker, 2001); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: ORTEP-3 (Farrugia, 1997); software used to prepare material for publication: WinGX (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RK2358).

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supporting information

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2-(1*H*-Pyrrolo[2,3-*b*]pyridin-2-yl)pyridine**Ping-Hsin Huang, Yuh-Sheng Wen and Jiun-Yi Shen****S1. Comment**

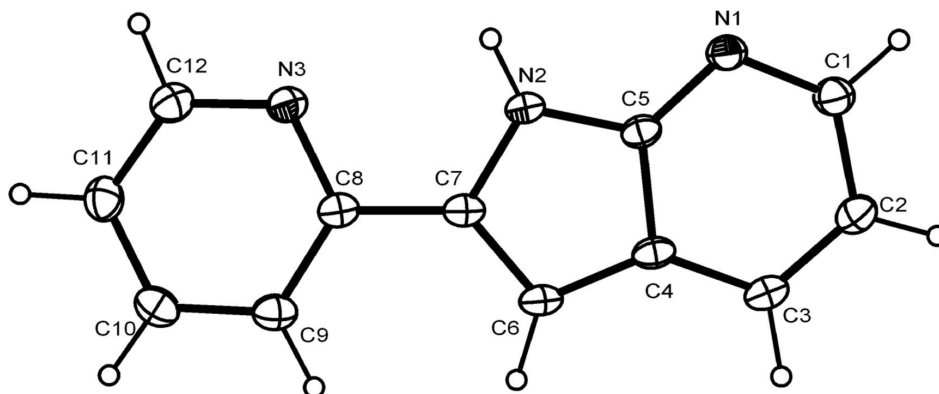
The title compound, has been shown to be an precursor for the production of luminescent organic/organometallic compound (Liu *et al.*, 2000). A one pot synthesis of a 7-azaindole substituted in the 2-position has been achieved by Pd complex catalyzed Cross-coupling reaction of 2-bromopyridine (Sakamoto *et al.*, 1996), in high yield (see Scheme). The molecular structure is shown in Fig. 1. The dihedral angle between the pyridine and azaindole rings is 6.20 (2)°, and that between the pyridine and pyrrole rings at 7-azaindole is 0.35 (2)° (Huang *et al.*, 2011). Weak intermolecular N2—H2···N1ⁱ (see Table 1) interactions help to stabilize the crystal structure - formation of centrosymmetrical dimers. Symmetry code: (i) -x+1, -y+2, -z.

S2. Experimental

The compound was synthesized by the following procedure (Liu *et al.*, 2000); (Sakamoto *et al.*, 1996). A solution of 1-(benzenesulfonyl)-2-(2-pyridyl)-7-azaindole (2.00 g, 5.97 mmol), ethanol (340 ml), and 10% aqueous NaOH (34 ml) was heated at reflux overnight. The resulting mixture was concentrated, and the residue was dissolved in CH₂Cl₂. The organic solution was washed with water and aqueous Na₂CO₃, dried, and concentrated. The residue was purified by column chromatography using CH₂Cl₂/CH₃OH (20:1) as eluent, followed by recrystallization from CH₂Cl₂ and hexane to yield 0.82 g (70%) of title compound as a white solid. Crystals suitable for X-ray diffraction were grown from a CH₂Cl₂ solution layered with hexane at room temperature. ¹H NMR (CDCl₃): 10.90 (br s, 1H), 8.69 (ddd, 1H, J = 4.8, 1.6, 1.0 Hz), 8.46 (dd, 1H, J = 4.8, 1.6 Hz), 7.98 (dd, 1H, J = 7.8, 1.3 Hz), 7.85 (m, 1H), 7.76 (td, 1H, J = 7.8, 1.7 Hz), 7.24 (ddd, 1H, J = 7.8, 4.8, 1.2 Hz), 7.12 (dd, 1H, J = 4.8, 1.8 Hz), 6.99 (d, 1H, J = 1.8 Hz). Anal. Calcd for C₁₂H₉N₃: C, 73.83; H, 4.65; N, 21.52. Found: C, 73.26; H, 4.48; N, 21.58.

S3. Refinement

H atoms were located geometrically and treated as riding atoms, with C—H = 0.93 Å, and with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

**Figure 1**

Molecular structure of title compound with the atom numbering scheme. Displacement ellipsoids are drawn at 30% probability level. H atoms are shown as small spheres of the arbitrary radii.

2-(1*H*-Pyrrolo[2,3-*b*]pyridin-2-yl)pyridine

Crystal data

$C_{12}H_9N_3$

$M_r = 195.22$

Monoclinic, $P2_1/c$

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

$a = 10.1416$ (10) Å

$b = 13.7428$ (14) Å

$c = 6.7395$ (7) Å

$\beta = 94.331$ (2)°

$V = 936.63$ (16) Å³

$Z = 4$

$F(000) = 408$

$D_x = 1.384$ Mg m⁻³

$D_m = 1.384$ Mg m⁻³

D_m measured by not measured

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 1871 reflections

$\theta = 2.5$ – 26.3 °

$\mu = 0.09$ mm⁻¹

$T = 200$ K

Needle, colourless

$0.55 \times 0.15 \times 0.05$ mm

Data collection

Bruker SMART APEX CCD
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

ω scans

Absorption correction: multi-scan

(*SADABS*; Bruker, 2001)

$T_{\min} = 0.938$, $T_{\max} = 0.996$

7069 measured reflections

2154 independent reflections

1792 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.056$

$\theta_{\max} = 27.5$ °, $\theta_{\min} = 2.0$ °

$h = -13 \rightarrow 13$

$k = -17 \rightarrow 17$

$l = -8 \rightarrow 8$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.064$

$wR(F^2) = 0.145$

$S = 1.19$

2154 reflections

136 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

$w = 1/[\sigma^2(F_o^2) + (0.0366P)^2 + 0.2976P]$

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

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

$\Delta\rho_{\max} = 0.25$ e Å⁻³

$\Delta\rho_{\min} = -0.20$ e Å⁻³

Special details

Geometry. All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'s 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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
N1	0.66995 (16)	0.94501 (12)	0.0034 (2)	0.0382 (4)
N2	0.50593 (15)	0.92225 (11)	0.2357 (2)	0.0324 (4)
H2	0.4394	0.9513	0.1684	0.039*
N3	0.27130 (16)	0.91454 (12)	0.4136 (2)	0.0371 (4)
C1	0.7961 (2)	0.92562 (16)	-0.0253 (3)	0.0418 (5)
H1	0.8296	0.9475	-0.1454	0.050*
C2	0.8818 (2)	0.87517 (16)	0.1101 (3)	0.0412 (5)
H2A	0.9707	0.8639	0.0808	0.049*
C3	0.8377 (2)	0.84179 (14)	0.2859 (3)	0.0391 (5)
H3	0.8948	0.8070	0.3790	0.047*
C4	0.70684 (19)	0.86035 (13)	0.3238 (3)	0.0333 (4)
C5	0.62979 (18)	0.91210 (13)	0.1741 (3)	0.0316 (4)
C6	0.62305 (19)	0.84091 (13)	0.4777 (3)	0.0351 (5)
H6	0.6466	0.8073	0.5984	0.042*
C7	0.50115 (19)	0.87982 (13)	0.4198 (3)	0.0323 (4)
C8	0.37880 (18)	0.87873 (13)	0.5192 (3)	0.0327 (4)
C9	0.3725 (2)	0.84151 (14)	0.7108 (3)	0.0411 (5)
H9	0.4501	0.8179	0.7828	0.049*
C10	0.2536 (2)	0.83931 (15)	0.7945 (3)	0.0465 (6)
H10	0.2474	0.8138	0.9244	0.056*
C11	0.1429 (2)	0.87497 (16)	0.6860 (3)	0.0460 (5)
H11	0.0586	0.8738	0.7388	0.055*
C12	0.1579 (2)	0.91213 (16)	0.5003 (3)	0.0440 (5)
H12	0.0817	0.9380	0.4283	0.053*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0389 (9)	0.0415 (9)	0.0336 (9)	0.0069 (7)	-0.0001 (7)	0.0021 (7)
N2	0.0326 (8)	0.0329 (8)	0.0306 (8)	0.0031 (6)	-0.0059 (6)	0.0030 (7)
N3	0.0347 (9)	0.0376 (9)	0.0382 (9)	-0.0009 (7)	-0.0026 (7)	0.0040 (7)
C1	0.0422 (11)	0.0459 (12)	0.0373 (11)	0.0069 (9)	0.0026 (9)	0.0005 (9)
C2	0.0352 (11)	0.0435 (12)	0.0444 (12)	0.0067 (9)	-0.0013 (9)	-0.0031 (10)
C3	0.0366 (11)	0.0361 (11)	0.0426 (12)	0.0037 (8)	-0.0104 (9)	0.0006 (9)
C4	0.0379 (10)	0.0259 (9)	0.0341 (10)	-0.0004 (8)	-0.0101 (8)	-0.0009 (8)
C5	0.0336 (10)	0.0281 (9)	0.0319 (10)	0.0027 (8)	-0.0050 (8)	-0.0030 (8)

C6	0.0390 (11)	0.0298 (10)	0.0344 (10)	-0.0013 (8)	-0.0106 (8)	0.0053 (8)
C7	0.0382 (10)	0.0253 (9)	0.0321 (10)	-0.0037 (8)	-0.0065 (8)	0.0015 (8)
C8	0.0357 (10)	0.0253 (9)	0.0358 (10)	-0.0038 (7)	-0.0054 (8)	-0.0002 (8)
C9	0.0453 (12)	0.0367 (11)	0.0401 (11)	-0.0023 (9)	-0.0050 (9)	0.0062 (9)
C10	0.0566 (14)	0.0433 (12)	0.0397 (12)	-0.0035 (10)	0.0054 (10)	0.0083 (10)
C11	0.0410 (12)	0.0458 (12)	0.0521 (13)	-0.0032 (10)	0.0094 (10)	0.0023 (10)
C12	0.0393 (11)	0.0444 (12)	0.0473 (12)	0.0000 (9)	-0.0027 (9)	0.0011 (10)

Geometric parameters (Å, °)

N1—C5	1.328 (2)	C4—C6	1.415 (3)
N1—C1	1.335 (3)	C4—C5	1.420 (3)
N2—C5	1.360 (2)	C6—C7	1.376 (3)
N2—C7	1.376 (2)	C6—H6	0.9500
N2—H2	0.8800	C7—C8	1.454 (3)
N3—C12	1.329 (3)	C8—C9	1.395 (3)
N3—C8	1.349 (2)	C9—C10	1.369 (3)
C1—C2	1.396 (3)	C9—H9	0.9500
C1—H1	0.9500	C10—C11	1.383 (3)
C2—C3	1.377 (3)	C10—H10	0.9500
C2—H2A	0.9500	C11—C12	1.371 (3)
C3—C4	1.393 (3)	C11—H11	0.9500
C3—H3	0.9500	C12—H12	0.9500
C5—N1—C1	114.66 (18)	C7—C6—H6	126.4
C5—N2—C7	109.17 (15)	C4—C6—H6	126.4
C5—N2—H2	125.4	N2—C7—C6	109.17 (17)
C7—N2—H2	125.4	N2—C7—C8	120.62 (16)
C12—N3—C8	116.82 (17)	C6—C7—C8	130.19 (18)
N1—C1—C2	124.1 (2)	N3—C8—C9	122.01 (18)
N1—C1—H1	117.9	N3—C8—C7	115.95 (17)
C2—C1—H1	117.9	C9—C8—C7	122.04 (18)
C3—C2—C1	120.04 (19)	C10—C9—C8	119.5 (2)
C3—C2—H2A	120.0	C10—C9—H9	120.2
C1—C2—H2A	120.0	C8—C9—H9	120.2
C2—C3—C4	118.22 (19)	C9—C10—C11	118.7 (2)
C2—C3—H3	120.9	C9—C10—H10	120.7
C4—C3—H3	120.9	C11—C10—H10	120.7
C3—C4—C6	137.09 (19)	C12—C11—C10	118.2 (2)
C3—C4—C5	116.24 (18)	C12—C11—H11	120.9
C6—C4—C5	106.67 (17)	C10—C11—H11	120.9
N1—C5—N2	125.47 (17)	N3—C12—C11	124.7 (2)
N1—C5—C4	126.71 (18)	N3—C12—H12	117.6
N2—C5—C4	107.81 (17)	C11—C12—H12	117.6
C7—C6—C4	107.17 (17)		

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>
N2—H2 \cdots N1 ⁱ	0.88	2.10	2.944 (2)	162

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