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(E)-N-[2-(Pyridin-2-yl)isoindolin-1-ylidene]pyridin-2-amine

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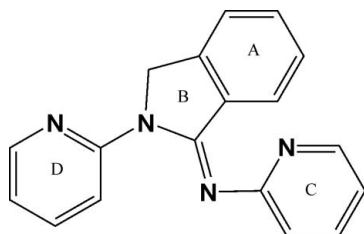
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Key indicators: single-crystal X-ray study; $T = 295$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å; R factor = 0.038; wR factor = 0.115; data-to-parameter ratio = 16.1.

A new bis(pyridyl) compound, $\text{C}_{18}\text{H}_{14}\text{N}_4$, was prepared by the reaction of phthalaldehyde and 2-aminopyridine in toluene. In the crystal structure, π - π stacking interactions exist between two adjacent molecules.

Related literature

Two corresponding complexes with 5-methyl-4,5-dihydroisoxazol-3-ylamine (Akkurt *et al.*, 2006) and aniline (Takahashi *et al.*, 2005) instead of 2-aminopyridine have similar structures.



Experimental

Crystal data

 $\text{C}_{18}\text{H}_{14}\text{N}_4$ $M_r = 286.33$ Triclinic, $P\bar{1}$ $a = 8.2571$ (17) Å $b = 8.2797$ (17) Å $c = 12.521$ (3) Å $\alpha = 105.97$ (3)° $\beta = 92.13$ (3)° $\gamma = 118.51$ (3)° $V = 708.7$ (4) Å³ $Z = 2$ Mo $K\alpha$ radiation $\mu = 0.08$ mm⁻¹ $T = 295$ (2) K $0.36 \times 0.25 \times 0.21$ mm

Data collection

Rigaku RAXIS-RAPID
diffractometer
Absorption correction: multi-scan
(*ABSCOR*; Higashi, 1995)
 $T_{\min} = 0.969$, $T_{\max} = 0.980$

6990 measured reflections
3208 independent reflections
2492 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.015$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.038$
 $wR(F^2) = 0.115$
 $S = 1.13$
3208 reflections

199 parameters
H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.18$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.21$ e Å⁻³

Table 1

 π - π contacts (Å, °) for the title compound. $\text{Cg}R$ is the centroid of ring R .

$\text{Cg}1$	$\text{Cg}2$	$\text{Cg}1 \cdots \text{Cg}2$ (Å)	Dihedral angle (°)	$\langle \text{Cg} \cdots \text{Perp} \rangle$ (Å)
$\text{Cg}A$	$\text{Cg}D^i$	3.8672 (13)	7.94 (1)	3.63 (7)
$\text{Cg}B$	$\text{Cg}B^i$	4.3836 (13)	0.00	3.48 (1)
$\text{Cg}B$	$\text{Cg}D^i$	4.0391 (13)	7.86 (1)	3.58 (12)
$\text{Cg}B$	$\text{Cg}D^{ii}$	4.2714 (14)	7.86 (1)	3.53 (13)
$\text{Cg}D$	$\text{Cg}D^{ii}$	3.9380 (12)	0.00	3.48 (1)

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

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MS, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BG2102).

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supplementary materials

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(*E*)-*N*-[2-(Pyridin-2-yl)isoindolin-1-ylidene]pyridin-2-amine

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Comment

In recent years, N-heterocyclic complexes have attracted much attention in the area of coordination and supramolecular chemistry. Infinite metal-organic frameworks are assembled through the metal coordination of pyridone- or pyridine-based bridging complexes. Accordingly, we have designed and synthesized a new bis(pyridyl) complex, *viz.* (*E*)-*N*-(2-(pyridin-2-yl)isoindolin-1-ylidene)pyridin-2-amine, (I). Two already reported complexes (Akkurt *et al.*, 2006; Takahashi *et al.*, 2005), respectively with 5-methyl-4,5-dihydroisoxazol-3-ylamine and aniline instead of 2-aminopyridine, have a similar structure. In comparison with the typical linear bis(pyridyl) disposition such as in 4,4-bipyridyl, the two pyridyl functions in (I) are more separated and form an acute angle, which may provide novel coordination modes in metal-organic structures.

The molecule structure of (I) is shown in Fig. 1. Each of the individual rings is essentially planar. The benzene ring A (C7—C12) and five-membered B (N3/C6/C7/C12/C13) lie almost on the same plane, subtending a dihedral angle of 2.1 (2)°. The pyridyl rings C (N1/C1—C5) and D (N4/C14—C18) make a dihedral angle of 102.1 (2)° with each other. The dihedral angles between rings A/C and B/C are 102.2 (2) and 100.1 (2)°, respectively. The dihedral angles between rings A/D and B/D are both 7.9 (2)°. In the crystal structure, π - π stacking interactions exist between adjacent molecules (Table 1) defining a three-dimensional structure.

Experimental

To a solution of phthalaldehyde in toluene was added a solution of 2-aminopyridine in toluene. The mixture was refluxed for 10 h, and a yellow precipitate was obtained. Colorless crystals were obtained by recrystallization of the material from methanol with a yield of 60%. Analysis calculated for C₁₈H₁₄N₄: C 75.51, H 4.93, N 19.57%. Found: C 75.56, H 4.90, N 19.55%.

Refinement

C-bound H atoms were placed at calculated positions, with phenyl C—H = 0.95 Å and methylene C—H = 0.97 Å and $U_{iso}(H) = 1.2U_{eq}(C)$, and included in the refinement in the riding-model approximation.

Figures

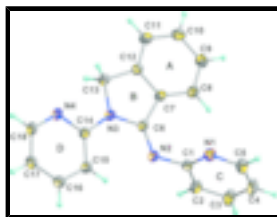


Fig. 1. ORTEP plot (Johnson, 1976) of title complex, with displacement ellipsoids drawn at 30% probability level.

supplementary materials

(E)—N-[2-(Pyridin-2-yl)isoindolin-1-ylidene]pyridin-2-amine

Crystal data

$C_{18}H_{14}N_4$	$Z = 2$
$M_r = 286.33$	$F_{000} = 300$
Triclinic, $P\bar{1}$	$D_x = 1.342 \text{ Mg m}^{-3}$
Hall symbol: -P 1	Mo $K\alpha$ radiation
$a = 8.2571 (17) \text{ \AA}$	$\lambda = 0.71073 \text{ \AA}$
$b = 8.2797 (17) \text{ \AA}$	Cell parameters from 5618 reflections
$c = 12.521 (3) \text{ \AA}$	$\theta = 3.0\text{--}27.4^\circ$
$\alpha = 105.97 (3)^\circ$	$\mu = 0.08 \text{ mm}^{-1}$
$\beta = 92.13 (3)^\circ$	$T = 295 (2) \text{ K}$
$\gamma = 118.51 (3)^\circ$	Prism, colorless
$V = 708.7 (4) \text{ \AA}^3$	$0.36 \times 0.25 \times 0.21 \text{ mm}$

Data collection

Rigaku RAXIS-RAPID diffractometer	3208 independent reflections
Radiation source: fine-focus sealed tube	2492 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\text{int}} = 0.015$
Detector resolution: $10.000 \text{ pixels mm}^{-1}$	$\theta_{\text{max}} = 27.5^\circ$
$T = 295(2) \text{ K}$	$\theta_{\text{min}} = 3.0^\circ$
ω scans	$h = -10 \rightarrow 10$
Absorption correction: multi-scan ABCOR (Higashi, 1995)	$k = -10 \rightarrow 10$
$T_{\text{min}} = 0.969$, $T_{\text{max}} = 0.980$	$l = -14 \rightarrow 16$
6990 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
$R[F^2 > 2\sigma(F^2)] = 0.038$	H-atom parameters constrained
$wR(F^2) = 0.115$	$w = 1/[\sigma^2(F_o^2) + (0.054P)^2 + 0.0939P]$
$S = 1.13$	where $P = (F_o^2 + 2F_c^2)/3$
3208 reflections	$(\Delta/\sigma)_{\text{max}} < 0.001$
199 parameters	$\Delta\rho_{\text{max}} = 0.18 \text{ e \AA}^{-3}$
Primary atom site location: structure-invariant direct methods	$\Delta\rho_{\text{min}} = -0.21 \text{ e \AA}^{-3}$
	Extinction correction: none

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
N1	-0.09225 (17)	0.76516 (17)	0.87717 (10)	0.0466 (3)
N2	-0.11473 (15)	0.63183 (17)	0.68229 (9)	0.0435 (3)
N3	0.08028 (14)	0.75228 (15)	0.55829 (8)	0.0379 (3)
N4	0.03406 (16)	0.81571 (18)	0.39661 (9)	0.0465 (3)
C1	-0.13993 (17)	0.60736 (19)	0.78836 (11)	0.0388 (3)
C2	-0.2270 (2)	0.4209 (2)	0.79558 (12)	0.0492 (3)
H2	-0.2595	0.3133	0.7320	0.059*
C3	-0.2642 (3)	0.3984 (2)	0.89801 (13)	0.0597 (4)
H3	-0.3208	0.2751	0.9050	0.072*
C4	-0.2171 (3)	0.5599 (2)	0.99041 (13)	0.0598 (4)
H4	-0.2428	0.5480	1.0604	0.072*
C5	-0.1313 (2)	0.7384 (2)	0.97623 (12)	0.0528 (4)
H5	-0.0981	0.8476	1.0388	0.063*
C6	0.04936 (17)	0.71127 (17)	0.65899 (10)	0.0356 (3)
C7	0.23566 (17)	0.76891 (17)	0.72090 (11)	0.0371 (3)
C8	0.2882 (2)	0.7566 (2)	0.82419 (12)	0.0469 (3)
H8	0.2006	0.7114	0.8690	0.056*
C9	0.4738 (2)	0.8131 (2)	0.85819 (13)	0.0531 (4)
H9	0.5114	0.8066	0.9271	0.064*
C10	0.6052 (2)	0.8793 (2)	0.79186 (13)	0.0506 (3)
H10	0.7292	0.9157	0.8164	0.061*
C11	0.55360 (19)	0.8919 (2)	0.68939 (12)	0.0447 (3)
H11	0.6415	0.9367	0.6447	0.054*
C12	0.36805 (18)	0.83610 (18)	0.65505 (11)	0.0377 (3)
C13	0.27804 (17)	0.83251 (19)	0.54836 (11)	0.0399 (3)
H13	0.3312	0.9626	0.5438	0.048*
H14	0.2921	0.7496	0.4822	0.048*
C14	-0.04689 (17)	0.73947 (17)	0.47444 (10)	0.0358 (3)
C15	-0.24000 (19)	0.6558 (2)	0.47075 (12)	0.0456 (3)
H15	-0.2938	0.6035	0.5259	0.055*
C16	-0.3486 (2)	0.6527 (2)	0.38339 (12)	0.0495 (3)
H16	-0.4780	0.5959	0.3784	0.059*
C17	-0.2669 (2)	0.7331 (2)	0.30345 (12)	0.0511 (4)
H17	-0.3383	0.7337	0.2445	0.061*
C18	-0.0762 (2)	0.8124 (2)	0.31402 (12)	0.0543 (4)
H18	-0.0198	0.8674	0.2603	0.065*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0504 (7)	0.0451 (6)	0.0436 (6)	0.0217 (5)	0.0095 (5)	0.0187 (5)
N2	0.0378 (6)	0.0553 (7)	0.0393 (6)	0.0200 (5)	0.0125 (5)	0.0248 (5)
N3	0.0355 (5)	0.0429 (6)	0.0355 (6)	0.0172 (5)	0.0113 (4)	0.0179 (5)
N4	0.0425 (6)	0.0589 (7)	0.0364 (6)	0.0209 (5)	0.0124 (5)	0.0220 (5)

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C1	0.0331 (6)	0.0476 (7)	0.0390 (7)	0.0198 (5)	0.0102 (5)	0.0200 (6)
C2	0.0617 (9)	0.0436 (8)	0.0409 (7)	0.0244 (7)	0.0166 (6)	0.0157 (6)
C3	0.0843 (11)	0.0460 (8)	0.0501 (9)	0.0282 (8)	0.0240 (8)	0.0259 (7)
C4	0.0844 (12)	0.0613 (10)	0.0399 (8)	0.0360 (9)	0.0236 (7)	0.0260 (7)
C5	0.0688 (10)	0.0514 (8)	0.0391 (7)	0.0315 (8)	0.0112 (7)	0.0144 (6)
C6	0.0385 (6)	0.0340 (6)	0.0350 (6)	0.0174 (5)	0.0109 (5)	0.0142 (5)
C7	0.0376 (7)	0.0349 (6)	0.0402 (7)	0.0175 (5)	0.0102 (5)	0.0159 (5)
C8	0.0445 (7)	0.0557 (8)	0.0479 (8)	0.0250 (6)	0.0138 (6)	0.0280 (7)
C9	0.0488 (8)	0.0617 (9)	0.0538 (9)	0.0262 (7)	0.0057 (6)	0.0302 (7)
C10	0.0381 (7)	0.0512 (8)	0.0626 (9)	0.0202 (6)	0.0061 (6)	0.0247 (7)
C11	0.0370 (7)	0.0435 (7)	0.0531 (8)	0.0181 (6)	0.0127 (6)	0.0193 (6)
C12	0.0384 (6)	0.0343 (6)	0.0400 (7)	0.0173 (5)	0.0108 (5)	0.0135 (5)
C13	0.0358 (6)	0.0455 (7)	0.0389 (7)	0.0187 (5)	0.0137 (5)	0.0175 (6)
C14	0.0401 (7)	0.0334 (6)	0.0322 (6)	0.0174 (5)	0.0093 (5)	0.0107 (5)
C15	0.0409 (7)	0.0533 (8)	0.0451 (7)	0.0206 (6)	0.0144 (6)	0.0251 (6)
C16	0.0398 (7)	0.0583 (9)	0.0497 (8)	0.0224 (6)	0.0098 (6)	0.0217 (7)
C17	0.0506 (8)	0.0644 (9)	0.0399 (7)	0.0295 (7)	0.0063 (6)	0.0196 (7)
C18	0.0530 (8)	0.0729 (10)	0.0383 (7)	0.0273 (8)	0.0137 (6)	0.0287 (7)

Geometric parameters (Å, °)

N1—C1	1.3325 (19)	C8—C9	1.380 (2)
N1—C5	1.3432 (18)	C8—H8	0.9300
N2—C6	1.2797 (17)	C9—C10	1.385 (2)
N2—C1	1.4060 (16)	C9—H9	0.9300
N3—C6	1.3953 (15)	C10—C11	1.383 (2)
N3—C14	1.4024 (16)	C10—H10	0.9300
N3—C13	1.4656 (16)	C11—C12	1.3827 (19)
N4—C14	1.3338 (16)	C11—H11	0.9300
N4—C18	1.3378 (18)	C12—C13	1.4903 (18)
C1—C2	1.3892 (19)	C13—H13	0.9700
C2—C3	1.371 (2)	C13—H14	0.9700
C2—H2	0.9300	C14—C15	1.3953 (18)
C3—C4	1.377 (2)	C15—C16	1.375 (2)
C3—H3	0.9300	C15—H15	0.9300
C4—C5	1.368 (2)	C16—C17	1.374 (2)
C4—H4	0.9300	C16—H16	0.9300
C5—H5	0.9300	C17—C18	1.370 (2)
C6—C7	1.4839 (18)	C17—H17	0.9300
C7—C12	1.3867 (18)	C18—H18	0.9300
C7—C8	1.3947 (18)		
C1—N1—C5	117.37 (12)	C10—C9—H9	119.3
C6—N2—C1	121.20 (12)	C11—C10—C9	120.57 (14)
C6—N3—C14	128.75 (11)	C11—C10—H10	119.7
C6—N3—C13	112.22 (10)	C9—C10—H10	119.7
C14—N4—C18	118.85 (10)	C12—C11—C10	118.32 (13)
C14—N4—C18	117.72 (12)	C12—C11—H11	120.8
N1—C1—C2	122.43 (12)	C10—C11—H11	120.8
N1—C1—N2	117.73 (12)	C11—C12—C7	121.37 (12)

C2—C1—N2	119.60 (13)	C11—C12—C13	128.40 (12)
C3—C2—C1	118.84 (14)	C7—C12—C13	110.22 (11)
C3—C2—H2	120.6	N3—C13—C12	102.90 (10)
C1—C2—H2	120.6	N3—C13—H13	111.2
C2—C3—C4	119.44 (14)	C12—C13—H13	111.2
C2—C3—H3	120.3	N3—C13—H14	111.2
C4—C3—H3	120.3	C12—C13—H14	111.2
C5—C4—C3	118.07 (14)	H13—C13—H14	109.1
C5—C4—H4	121.0	N4—C14—C15	122.18 (12)
C3—C4—H4	121.0	N4—C14—N3	113.52 (11)
N1—C5—C4	123.85 (14)	C15—C14—N3	124.30 (11)
N1—C5—H5	118.1	C16—C15—C14	118.21 (12)
C4—C5—H5	118.1	C16—C15—H15	120.9
N2—C6—N3	122.49 (12)	C14—C15—H15	120.9
N2—C6—C7	131.41 (11)	C17—C16—C15	120.30 (13)
N3—C6—C7	106.04 (10)	C17—C16—H16	119.9
C12—C7—C8	120.14 (12)	C15—C16—H16	119.9
C12—C7—C6	108.58 (11)	C18—C17—C16	117.41 (13)
C8—C7—C6	131.20 (12)	C18—C17—H17	121.3
C9—C8—C7	118.22 (13)	C16—C17—H17	121.3
C9—C8—H8	120.9	N4—C18—C17	124.18 (13)
C7—C8—H8	120.9	N4—C18—H18	117.9
C8—C9—C10	121.37 (14)	C17—C18—H18	117.9
C8—C9—H9	119.3		
C5—N1—C1—C2	0.1 (2)	C9—C10—C11—C12	-0.2 (2)
C5—N1—C1—N2	174.56 (12)	C10—C11—C12—C7	0.0 (2)
C6—N2—C1—N1	73.68 (17)	C10—C11—C12—C13	-178.68 (13)
C6—N2—C1—C2	-111.73 (16)	C8—C7—C12—C11	0.08 (19)
N1—C1—C2—C3	-0.4 (2)	C6—C7—C12—C11	-177.06 (11)
N2—C1—C2—C3	-174.77 (14)	C8—C7—C12—C13	178.94 (12)
C1—C2—C3—C4	0.9 (3)	C6—C7—C12—C13	1.80 (14)
C2—C3—C4—C5	-1.1 (3)	C6—N3—C13—C12	0.29 (13)
C1—N1—C5—C4	-0.3 (2)	C14—N3—C13—C12	175.88 (10)
C3—C4—C5—N1	0.8 (3)	C11—C12—C13—N3	177.45 (12)
C1—N2—C6—N3	-174.52 (11)	C7—C12—C13—N3	-1.30 (14)
C1—N2—C6—C7	8.8 (2)	C18—N4—C14—C15	0.9 (2)
C14—N3—C6—N2	8.3 (2)	C18—N4—C14—N3	-179.11 (12)
C13—N3—C6—N2	-176.67 (12)	C6—N3—C14—N4	170.91 (11)
C14—N3—C6—C7	-174.30 (11)	C13—N3—C14—N4	-3.85 (16)
C13—N3—C6—C7	0.74 (13)	C6—N3—C14—C15	-9.1 (2)
N2—C6—C7—C12	175.52 (13)	C13—N3—C14—C15	176.12 (12)
N3—C6—C7—C12	-1.57 (13)	N4—C14—C15—C16	0.1 (2)
N2—C6—C7—C8	-1.2 (2)	N3—C14—C15—C16	-179.90 (12)
N3—C6—C7—C8	-178.27 (13)	C14—C15—C16—C17	-1.0 (2)
C12—C7—C8—C9	0.2 (2)	C15—C16—C17—C18	0.9 (2)
C6—C7—C8—C9	176.54 (13)	C14—N4—C18—C17	-1.0 (2)
C7—C8—C9—C10	-0.4 (2)	C16—C17—C18—N4	0.1 (2)
C8—C9—C10—C11	0.5 (2)		

supplementary materials

π - π contacts (\AA , $^\circ$) for the title compound

Cg1	Cg2	Cg1...Cg2 (\AA)	Dihedral angle ($^\circ$)	<Cg...Perp> (\AA)
CgA	CgD ⁱ	3.8672 (13)	7.94 (1)	3.63 (7)
CgB	CgB ⁱ	4.3836 (13)	0.00	3.48 (1)
CgB	CgD ⁱ	4.0391 (13)	7.86 (1)	3.58 (12)
CgB	CgD ⁱⁱ	4.2714 (14)	7.86 (1)	3.53 (13)
CgD	CgD ⁱⁱ	3.9380 (12)	0.00	3.48 (1)

Symmetry codes: i = $-x, 1 - y, 1 - z$; ii = $-x, 2 - y, 1 - z$

Ring code: as in Fig. 1

Fig. 1

