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1,4-Bis(2-pyridyliminomethyl)benzene

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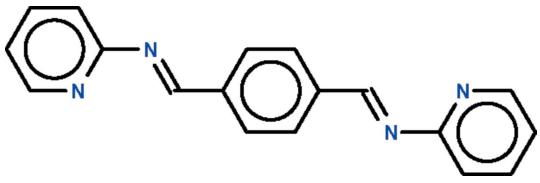
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.048; wR factor = 0.168; data-to-parameter ratio = 16.6.

In the crystal structure of the title compound, $C_{18}H_{14}N_4$, the molecule assumes $\overline{1}$ site symmetry with the centroid of the benzene ring located on the inversion center. The molecule is almost flat, with a dihedral angle of 2.70 (9)° between the pyridine and benzene rings.

Related literature

For the synthesis, see: D'Alelio *et al.* (1967). Terephthaldehyde condenses directly with 2-aminopyridine to form 4-(bis(2-pyridylamino)methyl)benzaldehyde; see: Zhu *et al.* (2003).



Experimental

Crystal data

$C_{18}H_{14}N_4$
M_r = 286.33
Monoclinic, $P2_1/n$
a = 6.1579 (8) Å
b = 18.911 (3) Å
c = 6.5956 (11) Å
β = 109.746 (5)°
V = 722.90 (18) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 293 K
0.30 × 0.26 × 0.21 mm

Data collection

Rigaku R-AXIS RAPID IP diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.976, T_{max} = 0.983
7013 measured reflections
1657 independent reflections
886 reflections with $I > 2\sigma(I)$
R_{int} = 0.048

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.168
S = 1.05
1657 reflections
100 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.15 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalClear* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU2625).

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supporting information

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S1. Experimental

To a solution of terephthaladehyde (1 mmol) in methanol was added a solution of 2-aminopyridine (2 mmol) and cobalt acetate trihydrate (1 mmol) in methanol. The mixture was heated to 333 K for one hour. The pale yellow solution was filtered. Colorless crystals were isolated from the filtrate after several days. CH&N elemental analysis. Calc. for $C_{18}H_{14}N_4$: C 75.51, H 4.93, N 19.57%; found: C 75.53, H 4.98, N 19.53%.

S2. Refinement

Carbon-bound H-atoms were placed in calculated positions (C—H 0.93 Å) and were included in the refinement in the riding model approximation, with U(H) set to 1.2U(C).

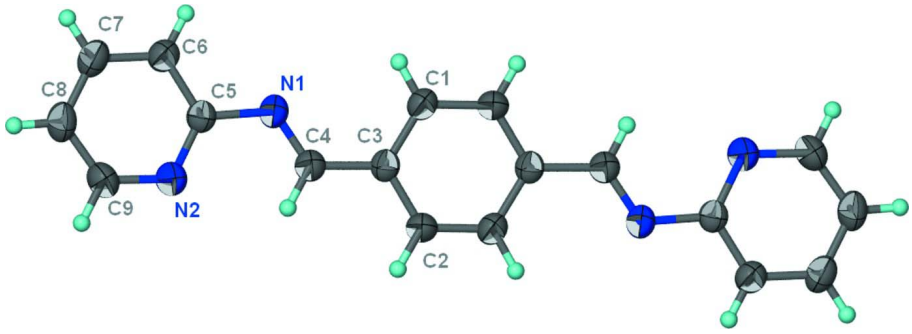

Figure 1

Thermal ellipsoid plot (Barbour, 2001) of the title compound at the 50% probability level; hydrogen atoms are drawn as spheres of arbitrary radius.

1,4-Bis(2-pyridyliminomethyl)benzene

Crystal data

$C_{18}H_{14}N_4$
M_r = 286.33
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
a = 6.1579 (8) Å
b = 18.911 (3) Å
c = 6.5956 (11) Å
β = 109.746 (5)°
V = 722.90 (18) Å^3
Z = 2
F(000) = 300
D_x = 1.315 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 3577 reflections
θ = 3.5–27.5°
μ = 0.08 mm^{-1}
T = 293 K
Prism, colorless
0.30 × 0.26 × 0.21 mm

Data collection

Rigaku R-AXIS RAPID IP diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.976, T_{max} = 0.983
7013 measured reflections
1657 independent reflections
886 reflections with $I > 2\sigma(I)$
R_{int} = 0.048
θ_{max} = 27.5°, θ_{min} = 3.5°
$h = -7 \rightarrow 7$
$k = -24 \rightarrow 24$
$l = -8 \rightarrow 8$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.168
S = 1.05
1657 reflections
100 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
$w = 1/[\sigma^2(F_o^2) + (0.0811P)^2 + 0.0419P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.15 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
N1	0.2738 (3)	0.57623 (8)	0.4070 (3)	0.0484 (5)
N2	0.4005 (3)	0.67692 (8)	0.6348 (3)	0.0547 (5)
C1	0.3212 (3)	0.48484 (9)	0.0748 (3)	0.0490 (5)
H1	0.2001	0.4745	0.1242	0.059*
C2	0.6436 (3)	0.55629 (10)	0.0822 (3)	0.0501 (6)
H2	0.7408	0.5945	0.1371	0.060*
C3	0.4653 (3)	0.54201 (9)	0.1610 (3)	0.0422 (5)
C4	0.4303 (3)	0.58674 (9)	0.3268 (3)	0.0470 (5)
H4	0.5285	0.6251	0.3762	0.056*
C5	0.2518 (3)	0.62320 (9)	0.5657 (3)	0.0427 (5)
C6	0.0719 (4)	0.61176 (10)	0.6427 (3)	0.0505 (6)
H6	−0.0267	0.5735	0.5940	0.061*
C7	0.0405 (4)	0.65755 (10)	0.7920 (3)	0.0566 (6)
H7	−0.0817	0.6513	0.8431	0.068*
C8	0.1919 (4)	0.71275 (11)	0.8649 (4)	0.0585 (6)
H8	0.1762	0.7443	0.9673	0.070*
C9	0.3676 (4)	0.71989 (10)	0.7815 (4)	0.0598 (6)
H9	0.4701	0.7572	0.8310	0.072*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0544 (10)	0.0491 (9)	0.0460 (11)	−0.0014 (8)	0.0225 (9)	−0.0062 (7)
N2	0.0572 (11)	0.0523 (10)	0.0595 (12)	−0.0048 (8)	0.0260 (9)	−0.0111 (8)
C1	0.0530 (12)	0.0510 (11)	0.0503 (13)	−0.0033 (9)	0.0268 (10)	−0.0034 (9)

C2	0.0523 (12)	0.0492 (11)	0.0540 (13)	−0.0120 (9)	0.0250 (11)	−0.0078 (9)
C3	0.0472 (11)	0.0413 (10)	0.0389 (11)	0.0030 (8)	0.0158 (9)	0.0011 (8)
C4	0.0505 (12)	0.0453 (11)	0.0478 (13)	−0.0031 (9)	0.0202 (10)	−0.0036 (9)
C5	0.0452 (11)	0.0419 (10)	0.0415 (11)	0.0036 (8)	0.0156 (9)	0.0002 (8)
C6	0.0544 (13)	0.0496 (11)	0.0531 (14)	−0.0030 (9)	0.0256 (11)	−0.0022 (9)
C7	0.0674 (14)	0.0548 (12)	0.0588 (14)	0.0064 (10)	0.0361 (12)	0.0009 (10)
C8	0.0741 (14)	0.0513 (12)	0.0564 (14)	0.0079 (11)	0.0305 (12)	−0.0071 (10)
C9	0.0673 (14)	0.0500 (11)	0.0639 (15)	−0.0090 (10)	0.0247 (12)	−0.0159 (10)

Geometric parameters (Å, º)

N1—C4	1.262 (2)	C3—C4	1.455 (3)
N1—C5	1.414 (2)	C4—H4	0.9300
N2—C9	1.330 (2)	C5—C6	1.383 (3)
N2—C5	1.340 (2)	C6—C7	1.373 (3)
C1—C2^{i}	1.369 (3)	C6—H6	0.9300
C1—C3	1.392 (3)	C7—C8	1.374 (3)
C1—H1	0.9300	C7—H7	0.9300
C2—C1^{i}	1.369 (3)	C8—C9	1.376 (3)
C2—C3	1.391 (3)	C8—H8	0.9300
C2—H2	0.9300	C9—H9	0.9300
C4—N1—C5	119.30 (17)	N2—C5—N1	120.16 (16)
C9—N2—C5	117.11 (17)	C6—C5—N1	117.58 (17)
C2^{i}—C1—C3	120.54 (17)	C7—C6—C5	119.28 (19)
C2^{i}—C1—H1	119.7	C7—C6—H6	120.4
C3—C1—H1	119.7	C5—C6—H6	120.4
C1^{i}—C2—C3	121.24 (17)	C6—C7—C8	119.14 (19)
C1^{i}—C2—H2	119.4	C6—C7—H7	120.4
C3—C2—H2	119.4	C8—C7—H7	120.4
C2—C3—C1	118.21 (17)	C7—C8—C9	117.83 (19)
C2—C3—C4	120.26 (17)	C7—C8—H8	121.1
C1—C3—C4	121.52 (16)	C9—C8—H8	121.1
N1—C4—C3	123.46 (18)	N2—C9—C8	124.36 (19)
N1—C4—H4	118.3	N2—C9—H9	117.8
C3—C4—H4	118.3	C8—C9—H9	117.8
N2—C5—C6	122.26 (17)		
C1^{i}—C2—C3—C1	−0.5 (3)	C4—N1—C5—N2	−2.1 (3)
C1^{i}—C2—C3—C4	−179.58 (18)	C4—N1—C5—C6	177.18 (19)
C2^{i}—C1—C3—C2	0.5 (3)	N2—C5—C6—C7	1.3 (3)
C2^{i}—C1—C3—C4	179.57 (18)	N1—C5—C6—C7	−177.98 (17)
C5—N1—C4—C3	−179.24 (17)	C5—C6—C7—C8	−1.5 (3)
C2—C3—C4—N1	−179.11 (19)	C6—C7—C8—C9	0.8 (3)
C1—C3—C4—N1	1.9 (3)	C5—N2—C9—C8	−0.2 (3)

C9—N2—C5—C6	−0.5 (3)	C7—C8—C9—N2	0.1 (4)
C9—N2—C5—N1	178.83 (18)		

Symmetry code: (i) −*x*+1, −*y*+1, −*z*.