Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

1,4-Bis(2-pyridyliminomethyl)benzene

Li-Hua Huo,[a] Shan Gao[a] and Seik Weng Ng[b]*

[a]College of Chemistry and Materials Science, Heilongjiang University, Harbin 150080, People's Republic of China, and [b]Department of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia
Correspondence e-mail: seikweng@um.edu.my

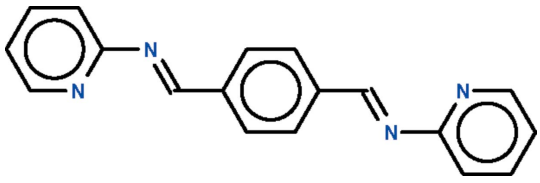
Received 28 September 2009; accepted 30 September 2009

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 $\bar{1}$ 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).

We thank the Natural Science Foundation of Heilongjiang Province (No. B200501), Heilongjiang University, China, and the University of Malaya for supporting this study.

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

References

Barbour, L. J. (2001). *J. Supramol. Chem.* **1**, 189–191.
D'Alelio, G. F., Crivello, J. V., Schönig, R. K. & Hümmer, T. F. (1967). *J. Macromol. Sci. Chem.* **1**, 1251–1258.
Higashi, T. (1995). *ABSCOR*. Rigaku Corporation, Tokyo, Japan.
Rigaku (1998). *RAPID-AUTO*. Rigaku Corporation, Tokyo, Japan.
Rigaku/MSC (2002). *CrystalClear*. Rigaku/MSC Inc., The Woodlands, Texas, USA.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Westrip, S. P. (2009). *publCIF*. In preparation.
Zhu, H.-L., Liu, Q.-X., Usman, A. & Fun, H.-K. (2003). *Z. Kristallogr. New Cryst. Struct.* **218**, 317–318.

supplementary materials

Acta Cryst. (2009). E**65**, o2659 [**doi:10.1107/S1600536809039853**]

1,4-Bis(2-pyridyliminomethyl)benzene

L.-H. Huo, S. Gao and S. W. Ng

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%.

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).

Figures

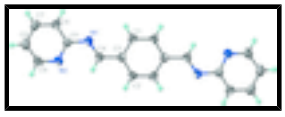


Fig. 1. Thermal ellipsoid plot (Barbour, 2001) of the title compound at the 50% probability level; hydrogen atoms are drawn as spheres of arbitrary radius.

1,4-Bis(2-pyridyliminomethyl)benzene

Crystal data

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

Data collection

Rigaku R-AXIS RAPID IP diffractometer	1657 independent reflections
Radiation source: fine-focus sealed tube	886 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.048

T = 293 K	θ_{max} = 27.5º
ω scans	θ_{min} = 3.5º
Absorption correction: Multi-scan (ABSCOR; Higashi, 1995)	h = −7→7
T_{min} = 0.976, T_{max} = 0.983	k = −24→24
7013 measured reflections	l = −8→8

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.048	H-atom parameters constrained
$wR(F^2)$ = 0.168	$w = 1/[\sigma^2(F_o^2) + (0.0811P)^2 + 0.0419P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.05	$(\Delta/\sigma)_{max}$ = 0.001
1657 reflections	$\Delta\rho_{max}$ = 0.15 e Å^{-3}
100 parameters	$\Delta\rho_{min}$ = −0.21 e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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

	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 (Å^2)

	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, °)

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 codes: (i) −*x*+1, −*y*+1, −*z*.

Fig. 1