organic compounds

1,4-Bis(2-pyridylmethyleneamino-methyl)benzene

Chao Li, Fu-An Sun, Ming-Yang He, Huan Xu and Qun Chen*

Key Laboratory of Fine Petro-Chemical technology, Jiangsu Polytechnic University, Changzhou 213164, People's Republic of China

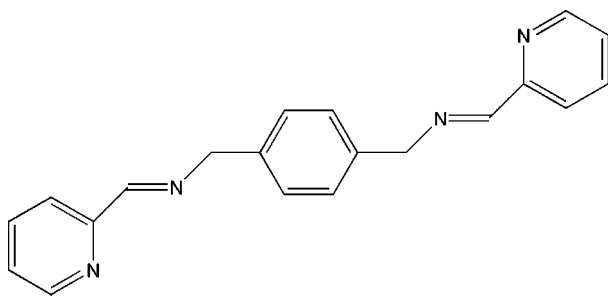Correspondence e-mail: chenqunjpu@yahoo.com

The asymmetric unit of the centrosymmetric title compound, $C_{20}H_{18}N_4$, contains one half-molecule. The pyridine and benzene rings are oriented at a dihedral angle of 77.21 (7)°.

Related literature

For general background, see: Barboiu *et al.* (2006); Keegan *et al.* (2002); Yue *et al.* (2004). For bond-length data, see: Allen *et al.* (1987).

Experimental

Crystal data

$C_{20}H_{18}N_4$	$\gamma = 82.242$ (8)°
$M_r = 314.38$	$V = 414.9$ (4) Å^3
Triclinic, $P\bar{1}$	$Z = 1$
$a = 4.527$ (3) Å	Mo $K\alpha$ radiation
$b = 10.117$ (6) Å	$\mu = 0.08$ mm^{-1}
$c = 10.456$ (6) Å	$T = 296$ (2) K
$\alpha = 61.086$ (7)°	$0.32 \times 0.30 \times 0.23$ mm
$\beta = 88.543$ (8)°	

Data collection

Bruker SMART CCD area-detector diffractometer	2909 measured reflections
	1449 independent reflections
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2000)	1250 reflections with $I > 2\sigma(I)$
$T_{min} = 0.976$, $T_{max} = 0.990$	$R_{int} = 0.021$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.036$	109 parameters
$wR(F^2) = 0.105$	H-atom parameters constrained
$S = 1.01$	$\Delta\rho_{max} = 0.14$ e Å^{-3}
1449 reflections	$\Delta\rho_{min} = -0.18$ e Å^{-3}

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

References

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supporting information

1,4-Bis(2-pyridylmethyleneaminomethyl)benzene

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S1. Comment

Bipyridyl-type bidentate Schiff base ligands have been utilized intensively to assemble various coordination polymers with interesting topologies and fascinating structural diversities (Barboiu *et al.*, 2006; Keegan *et al.*, 2002; Yue *et al.*, 2004). We report herein the crystal structure of the title compound.

The asymmetric unit of the title compound (Fig. 1) contains one-half of the centrosymmetric molecule, where the bond lengths (Allen *et al.*, 1987) and angles are within normal ranges. Rings A (N1/C1-C5) and B (C8-C10/C8A-C10A) are, of course, planar, and they are oriented at a dihedral angle of 77.21 (7)° [symmetry code: (A) 1 - x, 1 - y, 1 - z].

S2. Experimental

The title compound was prepared from the condensation reaction between pyridine-2-carboxaldehyde (100 mmol) and 1,4-benzenedimethanamine (50 mmol) in tetrahydrofuran (yield; 83%). Crystals suitable for X-ray analysis were obtained by slow evaporation of a methanol solution at room temperature.

S3. Refinement

H atoms were positioned geometrically, with C-H = 0.93 and 0.97 Å for aromatic and methylene H, respectively, and constrained to ride on their parent atoms, with $U_{iso}(H) = 1.2U_{eq}(C)$.
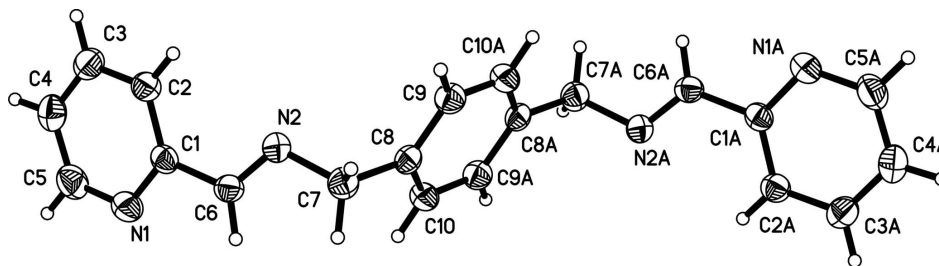
Figure 1

The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level [symmetry code: (A) 1 - x, 1 - y, 1 - z].

1,4-Bis(2-pyridylmethyleneaminomethyl)benzene

Crystal data

$C_{20}H_{18}N_4$	$c = 10.456$ (6) Å
$M_r = 314.38$	$\alpha = 61.086$ (7)°
Triclinic, $P\bar{1}$	$\beta = 88.543$ (8)°
Hall symbol: -P 1	$\gamma = 82.242$ (8)°
$a = 4.527$ (3) Å	$V = 414.9$ (4) Å³
$b = 10.117$ (6) Å	$Z = 1$

$F(000) = 166$

$D_x = 1.258$ Mg m^{-3}

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

Cell parameters from 1582 reflections

$\theta = 2.2$–$27.0°$

$\mu = 0.08$ mm^{-1}

$T = 296$ K

Block, colorless

$0.32 \times 0.30 \times 0.23$ mm

Data collection

Bruker SMART CCD area-detector
 diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

φ and ω scans

Absorption correction: multi-scan
 (*SADABS*; Sheldrick, 2000)

$T_{min} = 0.976$, $T_{max} = 0.990$

2909 measured reflections

1449 independent reflections

1250 reflections with $I > 2\sigma(I)$

$R_{int} = 0.021$

$\theta_{max} = 25.0°$, $\theta_{min} = 2.2°$

$h = -5\rightarrow5$

$k = -12\rightarrow12$

$l = -12\rightarrow11$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.036$

$wR(F^2) = 0.105$

$S = 1.01$

1449 reflections

109 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

$w = 1/[\sigma^2(F_o^2) + (0.0582P)^2 + 0.0501P]$
 where $P = (F_o^2 + 2F_c^2)/3$

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

$\Delta\rho_{max} = 0.14$ e Å^{-3}

$\Delta\rho_{min} = -0.18$ e Å^{-3}

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'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 (Å²)

	x	y	z	$U_{iso}*/U_{eq}$
N1	0.8015 (3)	0.26368 (14)	1.18773 (13)	0.0628 (3)
N2	0.4321 (2)	0.26607 (12)	0.89307 (11)	0.0516 (3)
C1	0.7265 (3)	0.20335 (14)	1.10637 (13)	0.0477 (3)
C2	0.8567 (3)	0.06149 (15)	1.12895 (14)	0.0536 (3)
H2	0.7948	0.0215	1.0722	0.064*
C3	1.0786 (3)	−0.01952 (17)	1.23630 (16)	0.0622 (4)
H3	1.1727	−0.1140	1.2519	0.075*
C4	1.1584 (4)	0.04142 (19)	1.31980 (16)	0.0673 (4)
H4	1.3071	−0.0110	1.3937	0.081*
C5	1.0143 (4)	0.18146 (19)	1.29230 (17)	0.0714 (5)
H5	1.0687	0.2215	1.3503	0.086*
C6	0.4970 (3)	0.29926 (14)	0.98916 (14)	0.0497 (3)

H6	0.3968	0.3873	0.9862	0.060*
C7	0.2103 (3)	0.37330 (16)	0.77804 (14)	0.0560 (4)
H7A	0.1281	0.4543	0.7986	0.067*
H7B	0.0484	0.3210	0.7748	0.067*
C8	0.3559 (3)	0.43975 (14)	0.63283 (13)	0.0470 (3)
C9	0.3629 (3)	0.37288 (15)	0.54431 (14)	0.0541 (3)
H9	0.2705	0.2866	0.5733	0.065*
C10	0.4953 (3)	0.56793 (15)	0.58621 (14)	0.0544 (4)
H10	0.4935	0.6150	0.6438	0.065*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0703 (8)	0.0659 (7)	0.0620 (7)	−0.0068 (6)	−0.0016 (6)	−0.0391 (6)
N2	0.0562 (7)	0.0502 (6)	0.0452 (6)	−0.0045 (5)	0.0029 (5)	−0.0215 (5)
C1	0.0499 (7)	0.0519 (7)	0.0441 (7)	−0.0121 (6)	0.0107 (5)	−0.0246 (6)
C2	0.0571 (8)	0.0527 (7)	0.0524 (7)	−0.0080 (6)	0.0060 (6)	−0.0268 (6)
C3	0.0614 (9)	0.0552 (8)	0.0598 (8)	−0.0025 (6)	0.0032 (7)	−0.0214 (7)
C4	0.0614 (9)	0.0776 (10)	0.0520 (8)	−0.0078 (8)	−0.0027 (7)	−0.0231 (8)
C5	0.0784 (11)	0.0846 (11)	0.0626 (9)	−0.0120 (9)	−0.0046 (8)	−0.0441 (9)
C6	0.0521 (7)	0.0461 (7)	0.0512 (7)	−0.0057 (5)	0.0079 (6)	−0.0245 (6)
C7	0.0507 (8)	0.0607 (8)	0.0542 (8)	−0.0029 (6)	0.0009 (6)	−0.0271 (7)
C8	0.0393 (6)	0.0488 (7)	0.0470 (7)	0.0033 (5)	−0.0071 (5)	−0.0206 (6)
C9	0.0563 (8)	0.0498 (7)	0.0571 (8)	−0.0099 (6)	−0.0004 (6)	−0.0258 (6)
C10	0.0593 (8)	0.0566 (8)	0.0539 (8)	−0.0048 (6)	−0.0020 (6)	−0.0326 (6)

Geometric parameters (Å, º)

N1—C1	1.3358 (17)	C6—C1	1.472 (2)
N1—C5	1.332 (2)	C6—H6	0.9300
N2—C6	1.2555 (17)	C7—H7A	0.9700
N2—C7	1.4620 (18)	C7—H7B	0.9700
C1—C2	1.383 (2)	C8—C7	1.5078 (19)
C2—C3	1.373 (2)	C8—C9	1.3832 (19)
C2—H2	0.9300	C8—C10	1.383 (2)
C3—C4	1.367 (2)	C9—C10^i	1.379 (2)
C3—H3	0.9300	C9—H9	0.9300
C4—C5	1.372 (2)	C10—C9^i	1.379 (2)
C4—H4	0.9300	C10—H10	0.9300
C5—H5	0.9300		
C5—N1—C1	116.79 (13)	N2—C6—H6	118.9
C6—N2—C7	117.39 (12)	C1—C6—H6	118.9
N1—C1—C2	122.69 (13)	N2—C7—C8	109.34 (11)
N1—C1—C6	115.30 (12)	N2—C7—H7A	109.8
C2—C1—C6	122.01 (12)	C8—C7—H7A	109.8
C3—C2—C1	119.09 (13)	N2—C7—H7B	109.8
C3—C2—H2	120.5	C8—C7—H7B	109.8

C1—C2—H2	120.5	H7A—C7—H7B	108.3
C4—C3—C2	118.73 (14)	C9—C8—C7	121.61 (12)
C4—C3—H3	120.6	C10—C8—C7	120.48 (11)
C2—C3—H3	120.6	C10^i—C9—C8	121.07 (13)
C3—C4—C5	118.57 (14)	C10—C8—C9	117.88 (12)
C3—C4—H4	120.7	C10^i—C9—H9	119.5
C5—C4—H4	120.7	C8—C9—H9	119.5
N1—C5—C4	124.10 (14)	C9^i—C10—C8	121.05 (12)
N1—C5—H5	117.9	C9^i—C10—H10	119.5
C4—C5—H5	117.9	C8—C10—H10	119.5
N2—C6—C1	122.13 (12)		
C5—N1—C1—C2	1.0 (2)	C3—C4—C5—N1	−0.7 (2)
C5—N1—C1—C6	−178.28 (12)	N2—C6—C1—N1	170.79 (11)
C1—N1—C5—C4	0.3 (2)	N2—C6—C1—C2	−8.52 (19)
C7—N2—C6—C1	−177.26 (11)	C9—C8—C7—N2	90.82 (14)
C6—N2—C7—C8	115.21 (13)	C10—C8—C7—N2	−87.19 (15)
N1—C1—C2—C3	−2.0 (2)	C7—C8—C9—C10^i	−178.00 (12)
C6—C1—C2—C3	177.27 (11)	C10—C8—C9—C10^i	0.1 (2)
C1—C2—C3—C4	1.6 (2)	C7—C8—C10—C9^i	178.03 (12)
C2—C3—C4—C5	−0.3 (2)	C9—C8—C10—C9^i	−0.1 (2)

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