Acta Crystallographica Section E
**Structure Reports Online**
ISSN 1600-5368

# *N*,*N*′-Bis(4-pyridylmethylene)octane-1,8-diamine

**Goutam Kumar Patra,[a] Anindita Mukherjee,[a] Partha Mitra[a] and Seik Weng Ng[b]***

[a]Department of Chemistry, Vijaygarh Jyotish Ray College, 8/2 Vijaygarh, Jadavpur, Kolkata 700 032, India, and [b]Department of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia
Correspondence e-mail: seikweng@um.edu.my

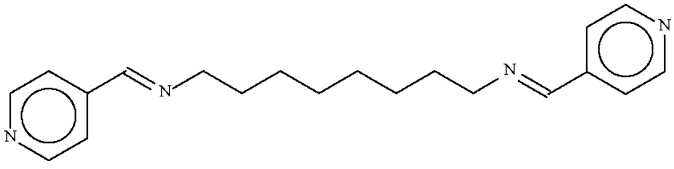
Received 24 June 2009; accepted 26 June 2009

Key indicators: single-crystal X-ray study; $T$ = 140 K; mean $\sigma$(C–C) = 0.002 Å; $R$ factor = 0.048; $wR$ factor = 0.138; data-to-parameter ratio = 18.9.

The complete molecule of the title compound, $C_{20}H_{26}N_4$, is generated by a crystallographic centre of inversion and the central eight-carbon chain adopts a fully extended conformation. In the crystal, the molecules pack in layers parallel to (010).

## Related literature

There are only few crystallographic reports of Schiff bases derived from 1,2-octanediamine; for details, see: Glidewell *et al.* (2005); Nathan *et al.* (2003); Viossat *et al.* (1997); Yamashita *et al.* (2003).



## Experimental

### *Crystal data*

$C_{20}H_{26}N_4$
$M_r$ = 322.45
Monoclinic, $P2_1/c$
$a$ = 11.6285 (4) Å
$b$ = 9.3821 (3) Å
$c$ = 8.8302 (3) Å
$\beta$ = 111.143 (2)°
$V$ = 898.52 (5) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 0.07 mm$^{-1}$
$T$ = 140 K
0.40 × 0.20 × 0.02 mm

### *Data collection*

Bruker SMART APEX area-detector diffractometer
Absorption correction: none
6110 measured reflections
2065 independent reflections
1588 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.023

### *Refinement*

$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.138
$S$ = 1.02
2065 reflections
109 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.31 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.23 e Å$^{-3}$

Data collection: *APEX2* (Bruker, 2008); cell refinement: *SAINT* (Bruker, 2008); data reduction: *SAINT*; 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).

The authors thank Vijaygarh Jyotish Ray College and the University of Malaya for supporting this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2836).

## References

Barbour, L. J. (2001). *J. Supramol. Chem.* **1**, 189–191.
Bruker (2008). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Glidewell, C., Low, J. N., Skakle, J. M. S. & Wardell, J. L. (2005). *Acta Cryst.* E**61**, o3551–o3553.
Nathan, L. C., Koehne, J. E., Gilmore, J. M., Hannibal, K. A., Dewhirst, W. E. & Mai, T. D. (2003). *Polyhedron*, **22**, 887–894.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Viossat, B., Dung, N. Y., Labouze, X., Morgant, G., Lancelot, J. C., Perrine, D. & Robba, M. (1997). *J. Inorg. Biochem.* **65**, 163–166.
Westrip, S. P. (2009). *publCIF*. In preparation.
Yamashita, S., Nihei, M. & Oshio, H. (2003). *Chem. Lett.* pp. 808–809.

# supporting information

*Acta Cryst.* (2009). E**65**, o1728 [doi:10.1107/S1600536809024623]

## *N*,*N*′-Bis(4-pyridylmethylene)octane-1,8-diamine

**Goutam Kumar Patra, Anindita Mukherjee, Partha Mitra and Seik Weng Ng**

### S1. Experimental

1,8-Diaminooctane (0.145 g, 1 mmol) was dissolved in methanol (15 ml) and to this was added 4-pyridine-carboxaldehyde (0.215 g, 2 mmol). The mixture was heated for 4 h. The solid that formed was recrystallized from methanol in 70% yield; m.p. 393 K.

### S2. Refinement

H atoms were placed in calculated positions (C-H = 0.95-0.99 Å) and were included in the refinement in the riding model approximation, with $U_{iso}$(H) set to 1.2$U_{eq}$(C).

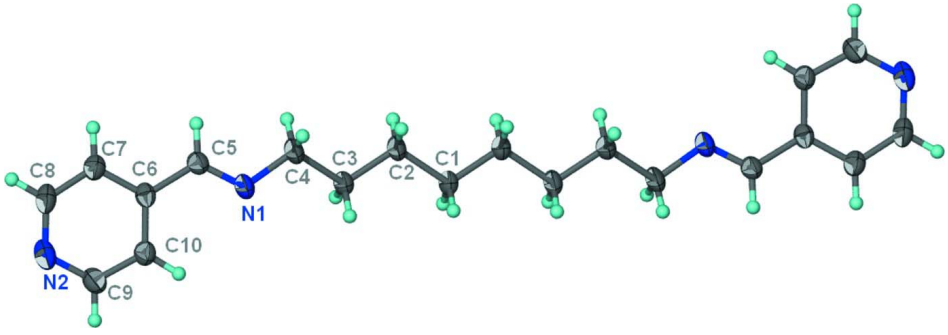



**Figure 1**

Displacement ellipsoid plot (Barbour, 2001) of $C_{20}H_{26}N_2$ at the 70% probability level; H atoms are drawn as spheres of arbitrary radius.

### *N*,*N*′-Bis(4-pyridylmethylene)octane-1,8-diamine

*Crystal data*

$C_{20}H_{26}N_4$
$M_r$ = 322.45
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a$ = 11.6285 (4) Å
$b$ = 9.3821 (3) Å
$c$ = 8.8302 (3) Å
$\beta$ = 111.143 (2)°
$V$ = 898.52 (5) Å$^3$
$Z$ = 2
$F$(000) = 348
$D_x$ = 1.192 Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å
Cell parameters from 1645 reflections
$\theta$ = 2.2–27.3°
$\mu$ = 0.07 mm$^{-1}$
$T$ = 140 K
Plate, light yellow
0.40 × 0.20 × 0.02 mm

*Data collection*

Bruker SMART APEX area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega$ scans
6110 measured reflections
2065 independent reflections
1588 reflections with $I > 2\sigma(I)$
$R_{int} = 0.023$
$\theta_{max} = 27.5°$, $\theta_{min} = 1.9°$
$h = -15 \rightarrow 15$
$k = -12 \rightarrow 11$
$l = -11 \rightarrow 11$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.048$
$wR(F^2) = 0.138$
$S = 1.02$
2065 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
$w = 1/[\sigma^2(F_o^2) + (0.0697P)^2 + 0.2588P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.31$ e Å$^{-3}$
$\Delta\rho_{min} = -0.23$ e Å$^{-3}$

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

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| N1 | 0.28339 (13) | 0.52618 (14) | 0.97725 (16) | 0.0353 (3) |
| N2 | 0.09040 (12) | 0.40434 (14) | 1.39134 (15) | 0.0326 (3) |
| C1 | 0.48329 (13) | 0.46639 (14) | 0.56773 (16) | 0.0248 (3) |
| H1A | 0.5601 | 0.4388 | 0.6573 | 0.030* |
| H1B | 0.4353 | 0.3784 | 0.5261 | 0.030* |
| C2 | 0.40867 (13) | 0.56437 (15) | 0.63471 (17) | 0.0264 (3) |
| H2A | 0.4584 | 0.6500 | 0.6818 | 0.032* |
| H2B | 0.3340 | 0.5961 | 0.5442 | 0.032* |
| C3 | 0.36981 (13) | 0.49380 (15) | 0.76402 (17) | 0.0265 (3) |
| H3A | 0.3086 | 0.4184 | 0.7125 | 0.032* |
| H3B | 0.4426 | 0.4476 | 0.8451 | 0.032* |
| C4 | 0.31509 (18) | 0.59651 (17) | 0.8495 (2) | 0.0413 (4) |
| H4A | 0.3748 | 0.6740 | 0.8979 | 0.050* |
| H4B | 0.2400 | 0.6397 | 0.7697 | 0.050* |
| C5 | 0.20006 (13) | 0.58108 (14) | 1.01734 (16) | 0.0250 (3) |
| H5 | 0.1598 | 0.6647 | 0.9631 | 0.030* |
| C6 | 0.16301 (12) | 0.51912 (15) | 1.14647 (15) | 0.0225 (3) |
| C7 | 0.07925 (13) | 0.58973 (15) | 1.19920 (17) | 0.0265 (3) |
| H7 | 0.0446 | 0.6782 | 1.1522 | 0.032* |
| C8 | 0.04704 (13) | 0.52910 (16) | 1.32146 (18) | 0.0303 (4) |
| H8 | −0.0092 | 0.5793 | 1.3576 | 0.036* |
| C9 | 0.17031 (14) | 0.33682 (16) | 1.33808 (18) | 0.0304 (3) |
| H9 | 0.2018 | 0.2473 | 1.3852 | 0.036* |
| C10 | 0.20944 (13) | 0.38956 (15) | 1.21893 (17) | 0.0263 (3) |
| H10 | 0.2673 | 0.3380 | 1.1869 | 0.032* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| N1 | 0.0532 (8) | 0.0291 (7) | 0.0383 (7) | 0.0066 (6) | 0.0343 (7) | 0.0070 (6) |
| N2 | 0.0390 (7) | 0.0354 (7) | 0.0306 (7) | −0.0071 (5) | 0.0212 (6) | −0.0029 (5) |
| C1 | 0.0282 (7) | 0.0273 (7) | 0.0236 (7) | 0.0019 (5) | 0.0148 (6) | 0.0008 (5) |
| C2 | 0.0339 (7) | 0.0257 (7) | 0.0274 (7) | −0.0007 (6) | 0.0203 (6) | 0.0006 (6) |
| C3 | 0.0338 (7) | 0.0256 (7) | 0.0260 (7) | 0.0022 (6) | 0.0181 (6) | 0.0023 (6) |
| C4 | 0.0682 (11) | 0.0283 (8) | 0.0490 (10) | 0.0084 (7) | 0.0473 (9) | 0.0090 (7) |
| C5 | 0.0318 (7) | 0.0225 (7) | 0.0238 (7) | 0.0000 (5) | 0.0139 (6) | 0.0003 (5) |
| C6 | 0.0244 (7) | 0.0245 (7) | 0.0202 (6) | −0.0037 (5) | 0.0101 (5) | −0.0032 (5) |
| C7 | 0.0270 (7) | 0.0277 (7) | 0.0274 (7) | 0.0002 (5) | 0.0130 (6) | −0.0023 (6) |
| C8 | 0.0304 (7) | 0.0348 (8) | 0.0323 (8) | −0.0035 (6) | 0.0191 (6) | −0.0066 (6) |
| C9 | 0.0387 (8) | 0.0270 (7) | 0.0297 (7) | −0.0027 (6) | 0.0174 (6) | 0.0010 (6) |
| C10 | 0.0308 (7) | 0.0252 (7) | 0.0267 (7) | 0.0001 (5) | 0.0151 (6) | −0.0017 (5) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| N1—C5 | 1.2558 (18) | C3—H3B | 0.99 |
| N1—C4 | 1.4643 (18) | C4—H4A | 0.99 |
| N2—C8 | 1.334 (2) | C4—H4B | 0.99 |
| N2—C9 | 1.3421 (18) | C5—C6 | 1.4758 (18) |
| C1—C1$^{i}$ | 1.522 (2) | C5—H5 | 0.95 |
| C1—C2 | 1.5225 (18) | C6—C10 | 1.3889 (19) |
| C1—H1A | 0.99 | C6—C7 | 1.3898 (18) |
| C1—H1B | 0.99 | C7—C8 | 1.3860 (19) |
| C2—C3 | 1.5227 (18) | C7—H7 | 0.95 |
| C2—H2A | 0.99 | C8—H8 | 0.95 |
| C2—H2B | 0.99 | C9—C10 | 1.3800 (19) |
| C3—C4 | 1.4998 (19) | C9—H9 | 0.95 |
| C3—H3A | 0.99 | C10—H10 | 0.95 |
| | | | |
| C5—N1—C4 | 117.82 (13) | C3—C4—H4A | 109.3 |
| C8—N2—C9 | 116.48 (12) | N1—C4—H4B | 109.3 |
| C1$^{i}$—C1—C2 | 113.46 (14) | C3—C4—H4B | 109.3 |
| C1$^{i}$—C1—H1A | 108.9 | H4A—C4—H4B | 108.0 |
| C2—C1—H1A | 108.9 | N1—C5—C6 | 121.75 (13) |
| C1$^{i}$—C1—H1B | 108.9 | N1—C5—H5 | 119.1 |
| C2—C1—H1B | 108.9 | C6—C5—H5 | 119.1 |
| H1A—C1—H1B | 107.7 | C10—C6—C7 | 117.76 (12) |
| C3—C2—C1 | 113.18 (11) | C10—C6—C5 | 121.82 (12) |
| C3—C2—H2A | 108.9 | C7—C6—C5 | 120.42 (12) |
| C1—C2—H2A | 108.9 | C8—C7—C6 | 118.97 (13) |
| C3—C2—H2B | 108.9 | C8—C7—H7 | 120.5 |
| C1—C2—H2B | 108.9 | C6—C7—H7 | 120.5 |
| H2A—C2—H2B | 107.8 | N2—C8—C7 | 123.85 (13) |
| C4—C3—C2 | 113.11 (12) | N2—C8—H8 | 118.1 |
| C4—C3—H3A | 109.0 | C7—C8—H8 | 118.1 |

| | | | |
|---|---|---|---|
| C2—C3—H3A | 109.0 | N2—C9—C10 | 123.94 (14) |
| C4—C3—H3B | 109.0 | N2—C9—H9 | 118.0 |
| C2—C3—H3B | 109.0 | C10—C9—H9 | 118.0 |
| H3A—C3—H3B | 107.8 | C9—C10—C6 | 119.00 (13) |
| N1—C4—C3 | 111.63 (12) | C9—C10—H10 | 120.5 |
| N1—C4—H4A | 109.3 | C6—C10—H10 | 120.5 |
| | | | |
| C1$^{i}$—C1—C2—C3 | 176.99 (14) | C5—C6—C7—C8 | −179.57 (13) |
| C1—C2—C3—C4 | 170.37 (14) | C9—N2—C8—C7 | 0.5 (2) |
| C5—N1—C4—C3 | −154.80 (15) | C6—C7—C8—N2 | −1.1 (2) |
| C2—C3—C4—N1 | −177.71 (14) | C8—N2—C9—C10 | 0.6 (2) |
| C4—N1—C5—C6 | −179.09 (14) | N2—C9—C10—C6 | −1.0 (2) |
| N1—C5—C6—C10 | −6.5 (2) | C7—C6—C10—C9 | 0.4 (2) |
| N1—C5—C6—C7 | 173.65 (13) | C5—C6—C10—C9 | −179.46 (13) |
| C10—C6—C7—C8 | 0.6 (2) | | |

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