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

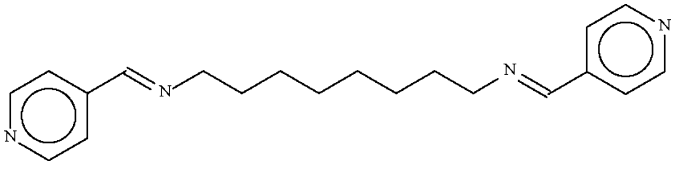
Received 24 June 2009; accepted 26 June 2009

Key indicators: single-crystal X-ray study; T = 140 K; mean σ(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
β = 111.143 (2)°
V = 898.52 (5) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 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.

supplementary materials

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

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

G. K. Patra, A. Mukherjee, P. Mitra and S. W. Ng

Experimental

1,8-Diaminooctane (0.145 g, 1 mmol) was dissolved in methanol (15 ml) and to this was added 4-pyridinecarboxaldehyde (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.

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 1.2U_{eq}(C).

Figures

Fig. 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

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

Data collection

Bruker SMART APEX area-detector diffractometer	1588 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	R_{int} = 0.023
Monochromator: graphite	θ_{max} = 27.5º
T = 140 K	θ_{min} = 1.9º

ω scans	$h = -15 \rightarrow 15$
Absorption correction: None	$k = -12 \rightarrow 11$
6110 measured reflections	$l = -11 \rightarrow 11$
2065 independent reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.048$	H-atom parameters constrained
$wR(F^2) = 0.138$	$w = 1/[\sigma^2(F_o^2) + (0.0697P)^2 + 0.2588P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.02$	$(\Delta/\sigma)_{max} = 0.001$
2065 reflections	$\Delta\rho_{max} = 0.31$ e Å^{-3}
109 parameters	$\Delta\rho_{min} = -0.23$ 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	0.28339 (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 (Å^2)

	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, °)

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 codes: (i) −*x*+1, −*y*+1, −*z*+1.

Fig. 1