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(E,E)-N^1,N^6-Bis[4-(dimethylamino)benzylidene]hexane-1,6-diamine

Zhi-Dong Lin,[a]* Zhi-Dong Lin,[b] Li-Ming Liu[c] and Ya-Min Huang[a]

[a]School of Materials Science and Technology, Wuhan Institute of Chemical Technology, Wuhan, 430073, People's Republic of China, [b]State Key Laboratory of New Nonferrous Metal Materials, Gansu University of Technology, Lanzhou 730050, People's Republic of China, and [c]Kunming Institute of Physics, Kunming 650223, People's Republic of China

Correspondence e-mail: zhidong.lin@126.com

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Key indicators

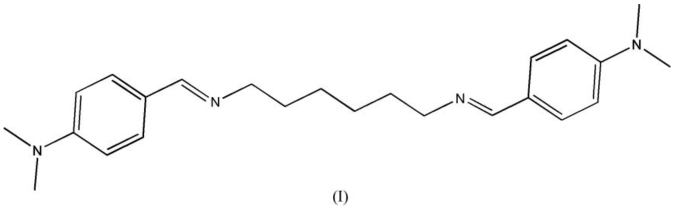
Single-crystal X-ray study
T = 292 K
Mean σ(C–C) = 0.004 Å
R factor = 0.062
wR factor = 0.167
Data-to-parameter ratio = 15.3

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

The title compound, $C_{24}H_{34}N_4$, is a Schiff base synthesized by the reaction of hexane-1,6-diamine with 4-(dimethylamino)benzaldehyde in ethanol. It crystallizes with one half-molecule in the asymmetric unit; there is a centre of symmetry at the mid-point of the central C—C bond. Since there are no strong hydrogen-bond-forming groups, the molecules interact through C—H···π hydrogen bonds, forming layers in the ac plane.

Comment

Much research has been devoted to the physicochemical characterization of substituted aromatic Schiff bases, because these compounds show remarkable photochromic properties. Photochromism arises from intramolecular H-atom transfer, together with a change in the π-electron configuration. The effect of intermolecular interactions, such as π–π charge transfer or hydrogen bonding, on H-atom transfer processes has been investigated in the solid state (Hadjoudis *et al.*, 1987; Puranik *et al.*, 1992). In the design of solid materials, one of the key steps is the understanding of how the constituent molecules are packed, what kinds of interactions play a role in crystal packing and how they interplay (Desiraju, 1989). In this paper, we report the crystal structure of the title Schiff base, (I) (Fig. 1).



(I)

In the crystal structure of (I) (Fig. 1) there is one half-molecule in the asymmetric unit; there is a centre of symmetry at the mid-point of the central C—C bond. The C═N unit has a *trans* configuration. All the bond lengths and angles are within expected ranges (You *et al.*, 2004, Munro & Camp, 2003). The planar benzylidene group is attached at C10.

There are no strong hydrogen-bond-forming groups, such as –COOH, –NH_2CO–, –OH or –NO_2, in the crystal structure, so weak interactions must play determining roles in the crystal packing (Fig. 2). The molecules interact through C—H···π hydrogen bonds, forming layers in the ac plane. The hydrogen bond length and C10—H10B···π(benzene ring)^{i} angle are 3.796 (3) Å and 156°, respectively [symmetry code: (i) x, $-y+1$, z]. In the third direction (b axis), there are only

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ordinary, weaker, van der Waals interactions, consistent with the formation of thin plates.

Experimental

Hexane-1,6-diamine (1.16 g, 10 mmol) was added slowly to an ethanol solution (100 ml) of 4-(dimethylamino)benzaldehyde (2.98 g, 20 mmol). The mixture was stirred for 15 min, refluxed for 6 h and the volume then reduced to 10 ml by vacuum evaporation. A yellow precipitate was obtained from the solution after allowing it to stand at room temperature for 12 h. The solid was filtered off and washed with cold ethanol. Yellow crystals of (I) were obtained by slow evaporation of an ethanol solution of the compound. The crystals were dried in a vacuum desiccator using anhydrous $CaCl_2$ (yield 64%). Analysis calculated for $C_{24}H_{34}N_4$: C 76.15, H 9.05, N 14.80%; found: C 76.41, H 9.21, N 14.56%.

Crystal data

$C_{24}H_{34}N_4$
$M_r = 378.55$
Monoclinic, $P2_1/n$
$a = 6.1695$ (15) Å
$b = 6.6209$ (16) Å
$c = 27.417$ (6) Å
$\beta = 93.212$ (5)°
$V = 1118.2$ (5) Å^3
$Z = 2$

$D_x = 1.124$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2600 reflections
$\theta = 2.3$–26.6°
$\mu = 0.07$ mm^{-1}
$T = 292$ (2) K
Block, yellow
0.20 × 0.10 × 0.06 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.992$, $T_{\max} = 0.996$
7590 measured reflections

1976 independent reflections
949 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.070$
$\theta_{\max} = 25.0°$
$h = -7 \rightarrow 6$
$k = -7 \rightarrow 7$
$l = -32 \rightarrow 32$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.062$
$wR(F^2) = 0.167$
$S = 0.99$
1976 reflections
129 parameters

H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.079P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.003$
$\Delta\rho_{\max} = 0.17$ e Å^{-3}
$\Delta\rho_{\min} = -0.12$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

C1—N1	1.443 (3)	C8—C9	1.441 (3)
C2—N1	1.436 (3)	C9—N2	1.261 (3)
C3—N1	1.371 (3)	C10—N2	1.456 (3)
N1—C3—C4	121.7 (3)	N2—C9—C8	125.3 (3)
N1—C3—C5	121.5 (2)	C3—N1—C2	120.8 (2)
C4—C3—C5	116.7 (2)	C3—N1—C1	121.2 (2)
C7—C8—C6	116.0 (2)	C2—N1—C1	117.3 (2)
C7—C8—C9	123.4 (3)	C9—N2—C10	118.0 (3)
C6—C8—C9	120.5 (3)		
C7—C8—C9—N2	2.1 (4)	C5—C3—N1—C1	174.9 (2)
C6—C8—C9—N2	−176.6 (3)	C8—C9—N2—C10	177.7 (2)
N2—C10—C11—C12	172.5 (2)	C11—C10—N2—C9	141.8 (3)
C4—C3—N1—C1	−5.3 (4)		

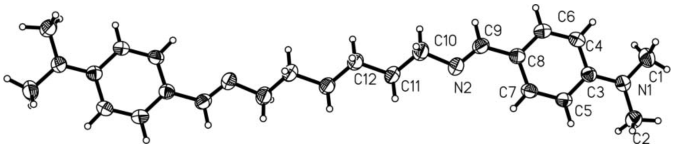

Figure 1
The molecular structure of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level. Unlabelled atoms are related to labelled atoms by the symmetry operator $(2 - x, -y, -z)$.

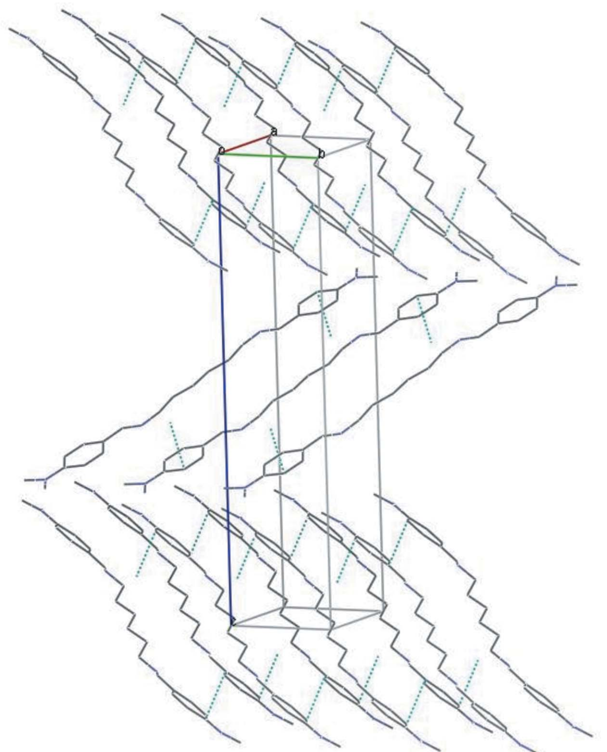

Figure 2
The crystal packing of (I). Dashed lines indicate C—H$\cdots\pi$ interactions.

All H atoms were positioned geometrically and refined using a riding model, with C—H distances in the range 0.93–0.97 Å. The isotropic displacement parameters were set equal to $1.5U_{\rm eq}$(parent atom) for methyl H atoms and $1.2U_{\rm eq}$(parent atom) for the remaining H atoms.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

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