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N,*N*′-Bis(4-dimethylaminobenzylidene)-ethane-1,2-diamine

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Key indicators

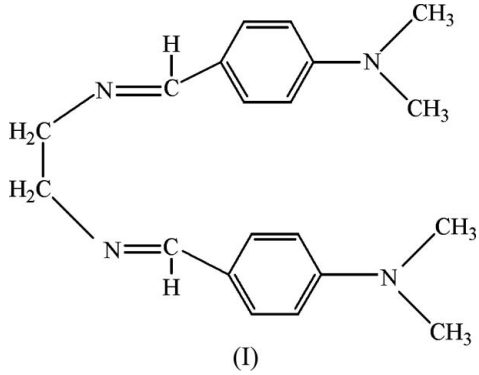
Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.003 Å
R factor = 0.041
wR factor = 0.122
Data-to-parameter ratio = 9.8

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

The title compound, $C_{20}H_{26}N_4$, was prepared by a condensation reaction between *p*-dimethylaminobenzaldehyde and ethylenediamine. The molecule contains a crystallographically imposed twofold axis of symmetry.

Comment

Schiff bases are used extensively as ligands in the field of coordination chemistry (Yamada, 1999). The molecular structure of the title compound, (I), is shown in Fig. 1.



(I)

The two arms of the Schiff base are each essentially planar and are related by a crystallographically imposed twofold axis of symmetry. The bond parameters within the imine groups are comparable with those reported in the literature (Huang & Xu, 1989; Mirkhani *et al.*, 2004).

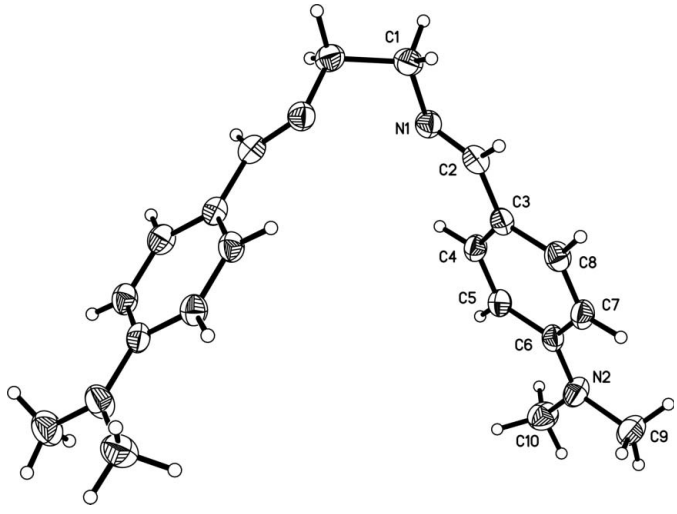


Figure 1
The structure of the title compound, showing 30% probability displacement ellipsoids and the atom-numbering scheme for the asymmetric unit. Unlabelled atoms are related to labelled atoms by $-x, y, -\frac{1}{2} - z$.

Experimental

The title compound was prepared by the reaction of *p*-dimethylaminobenzaldehyde and ethylenediamine (molar ratio 2:1) in absolute ethanol. The mixture was heated under reflux with stirring for 10 h, and the solvent was evaporated in a rotary vacuum evaporator. The resulting solution was filtered and the filtrate allowed to stand in air for about three weeks, after which large yellow block-shaped crystals suitable for X-ray analysis were formed. Elemental analysis found: C 74.54, H 8.17, N 17.29%; calculated for $C_{20}H_{26}N_4$: C 74.50, H 8.13, N 17.37%.

Crystal data

$C_{20}H_{26}N_4$
M_r = 322.44
Monoclinic, $C2/c$
a = 24.218 (16) Å
b = 6.534 (4) Å
c = 12.433 (8) Å
β = 114.872 (10)°
V = 1785 (2) Å^3
Z = 4
D_x = 1.200 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1166 reflections
θ = 3.3–25.6°
μ = 0.07 mm^{-1}
T = 298 (2) K
Block, yellow
0.37 × 0.13 × 0.08 mm

Data collection

Siemens SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.974, T_{max} = 0.994
4438 measured reflections
1577 independent reflections
990 reflections with $I > 2\sigma(I)$
R_{int} = 0.030
θ_{max} = 25.0°
$h = -20 \rightarrow 28$
$k = -7 \rightarrow 7$
$l = -14 \rightarrow 14$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.122
S = 1.02
1577 reflections
161 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0566P)^2 + 0.44P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.16 e Å^{-3}
$\Delta\rho_{min}$ = −0.12 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

N1—C2	1.258 (2)	N2—C10	1.426 (3)
N1—C1	1.454 (3)	N2—C9	1.438 (3)
N2—C6	1.375 (3)		
C2—N1—C1	116.41 (18)	C10—N2—C9	117.6 (2)
C6—N2—C10	121.17 (18)	N1—C2—C3	125.7 (2)
C6—N2—C9	120.6 (2)	N1—C2—H3	120.1 (11)

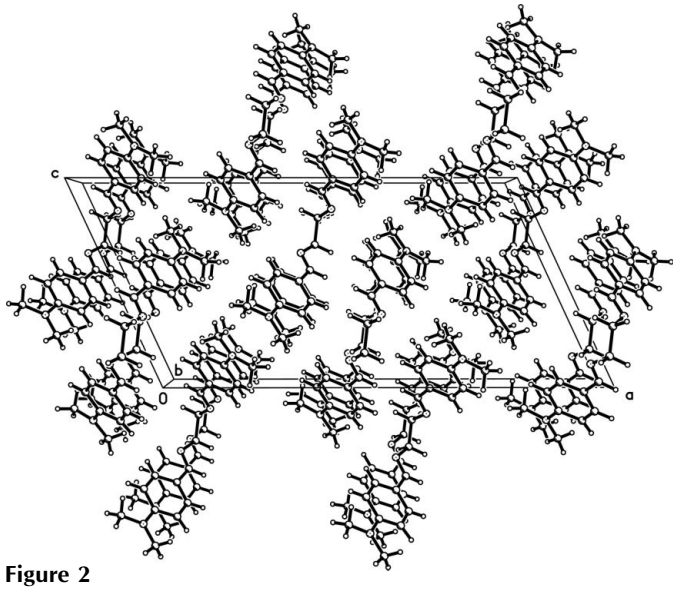


Figure 2
The crystal packing of the title compound.

All H atoms were located in a difference Fourier synthesis and refined isotropically.

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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