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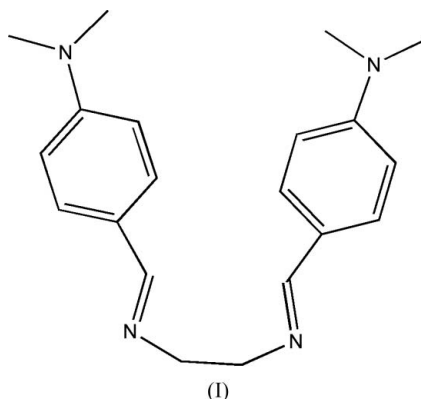
Key indicators

Single-crystal X-ray study
 $T = 298\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.004\text{ \AA}$
 R factor = 0.079
 wR factor = 0.230
Data-to-parameter ratio = 15.8For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.*N,N'*-Bis[4-(dimethylamino)benzylidene]-ethane-1,2-diamine

The title compound, $\text{C}_{20}\text{H}_{26}\text{N}_4$, shows a distinctly V-shaped structure. In the crystal structure, parallel rings and short intermolecular contacts indicate the presence of aromatic stacking interactions. A twofold rotation axis passes through the mid-point of the central C—C bond.

Comment

The crystal structure of *N,N'*-bis(4-(dimethylamino)benzylidene)-1,2-diaminocyclohexane has been reported previously (Jones *et al.*, 1998); we report here the crystal structure of *N,N'*-bis[4-(dimethylamino)benzylidene]-1,2-diaminoethane, (I). The molecular structure of (I) is illustrated in Fig. 1, with selected bond lengths and bond angles listed in Table 1.



The molecular structure of (I) exhibits a distinct V shape. A twofold rotation axis passes through the mid-point of the C10—C10ⁱ bond (symmetry code as in Table 1). The C9—N2 bond length of 1.251 (4) Å is consistent with double-bond character. Other bond lengths and angles in (I) lie within the expected ranges. In the molecular packing, the distance between parallel rings is 3.597 Å, which indicates the presence of aromatic stacking interactions.

Experimental

A mixture of 1,2-diaminoethane (1 mmol) and 4-dimethylamino-benzaldehyde (2 mol) in ethanol (40 ml) was refluxed for 3 h and then cooled to room temperature with stirring. The solution was filtered and concentrated to dryness. The resulting residue was washed with ethanol and dried in a vacuum. The yellow product was dissolved in dichloromethane and the solution was evaporated slowly in a dark place at room temperature. After two weeks, red block crystals were obtained. The overall yield was 75%. CHN elemental analysis on the red platelets: found (calculated) for $\text{C}_{20}\text{H}_{26}\text{N}_4$ (%): C 74.35 (74.50), H 8.10 (8.13), N 17.55 (17.38). IR (KBr): 3423, 3030, 1645, 1630, 1450, 1380, 1280, 1115, 850, 803, 771, 680, 637 cm^{-1} .

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Crystal data

$C_{20}H_{26}N_4$
 $M_r = 322.45$
 Monoclinic, $C2/c$
 $a = 24.151$ (10) Å
 $b = 6.503$ (3) Å
 $c = 12.390$ (5) Å
 $\beta = 114.869$ (8)°
 $V = 1765.5$ (12) Å³
 $Z = 4$

$D_x = 1.213$ Mg m⁻³
 Mo $K\alpha$ radiation
 Cell parameters from 1200 reflections
 $\theta = 3.2$ – 25°
 $\mu = 0.07$ mm⁻¹
 $T = 298$ (2) K
 Plate, red
 $0.31 \times 0.30 \times 0.11$ mm

Data collection

Bruker APEX diffractometer
 φ and ω scans
 Absorption correction: multi-scan
 (SADABS; Sheldrick, 1996)
 $T_{\min} = 0.978$, $T_{\max} = 0.992$
 4624 measured reflections
 1721 independent reflections

1347 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.028$
 $\theta_{\text{max}} = 26.0^\circ$
 $h = -20 \rightarrow 29$
 $k = -8 \rightarrow 7$
 $l = -15 \rightarrow 8$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.079$
 $wR(F^2) = 0.230$
 $S = 1.08$
 1721 reflections
 109 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.1093P)^2 + 2.2949P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} < 0.001$
 $\Delta\rho_{\text{max}} = 0.32$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.27$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

C9–N2	1.251 (4)	C1–N1	1.432 (4)
C10–N2	1.440 (3)	C2–N1	1.428 (4)
C10–C10 ⁱ	1.506 (6)		
N2–C10–C10 ⁱ	111.5 (2)	C3–N1–C1	120.9 (3)
C9–N2–C10	116.6 (2)	C2–N1–C1	117.3 (3)
C3–N1–C2	121.2 (2)		
C7–C6–C9–N2	177.8 (3)	C4–C3–N1–C1	–178.3 (3)
C5–C6–C9–N2	–2.7 (4)	C10–C10 ⁱ –N2–C9	–130.5 (3)
C4–C3–N1–C2	–7.6 (4)		

Symmetry code: (i) $-x + 1, y, -z + \frac{3}{2}$.

The aromatic and aliphatic H atoms were placed at calculated positions and refined using the riding-model approximation, with C–H = 0.93 – 0.97 Å and $U_{\text{iso}} = 1.2U_{\text{eq}}(\text{C})$.

Data collection: SMART (Bruker, 2001); cell refinement: SAINT (Bruker, 2001); data reduction: SAINT; program(s) used to solve

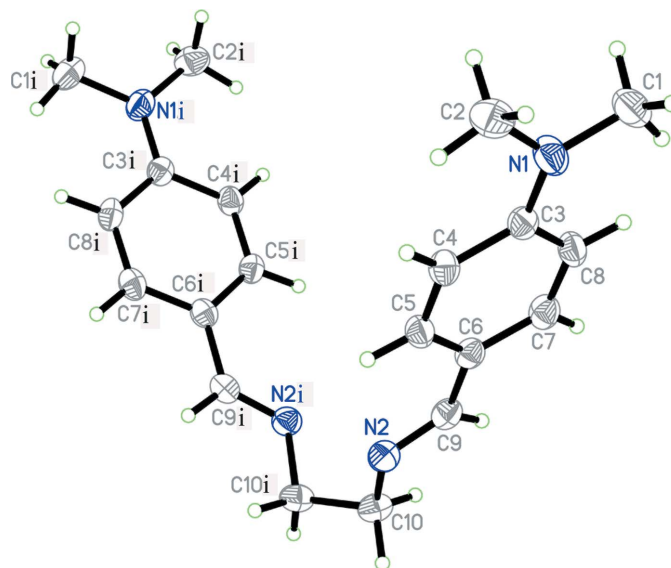


Figure 1

ORTEPII (Johnson, 1976) plot of (I). Displacement ellipsoids are drawn at the 30% probability level. [Symmetry code: (i) $-x + 1, y, -z + \frac{3}{2}$.]

structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: ORTEPII (Johnson, 1976); software used to prepare material for publication: SHELXL97.

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References

- Bruker (2001). *SADABS*, *SAINT* and *SMART*. Bruker AXS Inc., Madison, Wisconsin, USA.
 Johnson, C. K. (1976). *ORTEPII*. Report ORNL-5138. Oak Ridge National Laboratory, Tennessee, USA.
 Jones, V. A., Sripang, S., Thornton-Pett, M. & Kee, T. P. (1998). *J. Organomet. Chem.* pp. 199–218.
 Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
 Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.