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Key indicators

Single-crystal X-ray study
 $T = 294\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.004\text{ \AA}$
 R factor = 0.050
 wR factor = 0.124
Data-to-parameter ratio = 14.3For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.1,4-Bis[4-(di-*p*-tolylamino)benzyl]-2,3-diaza-1,3-butadieneIn the title compound, $\text{C}_{42}\text{H}_{38}\text{N}_4$, the two independent molecules are each located on an inversion centre. The central $\text{C}=\text{N}-\text{N}=\text{C}$ linkage is therefore planar.Received 19 October 2006
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Comment

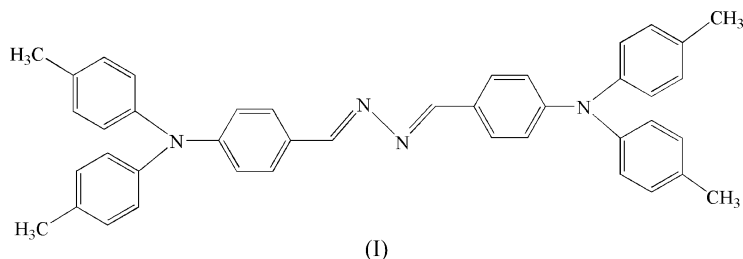
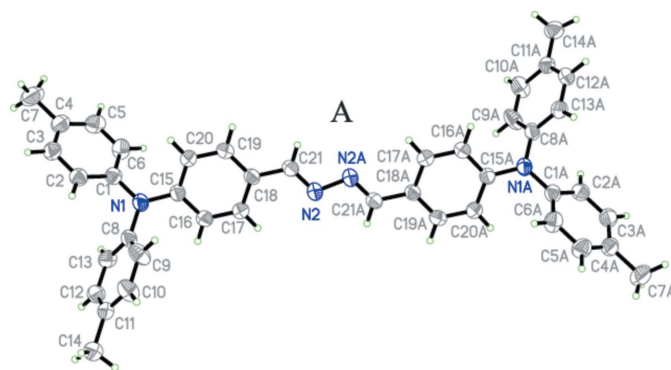
Recently, a number of azine derivatives containing both a diimine linkage and an $\text{N}-\text{N}$ bond have been investigated in terms of their crystallography and coordination chemistry (Kesslen *et al.*, 1999; Armstrong *et al.*, 1998; Xu *et al.*, 2005). We report here the crystal structure of the title compound, (I), in which two di-*p*-tolylaminobenzyl units are directly linked through imine N atoms. This molecule is structurally related to, for example, 1,4-bis(4-dimethylaminobenzyl)-2,3-diaza-1,3-butadiene (Wang *et al.*, 2005).The asymmetric unit cell of (I) contains two independent molecules. Each molecule (Fig. 1 for molecule *A* and Fig. 2 for molecule *B*) has an inversion centre at the mid-point of the central $\text{N}-\text{N}$ bond, making the $\text{C}=\text{N}-\text{N}=\text{C}$ linkage planar. This configuration agrees with that commonly found in a number of azine compounds (*e.g.* Zheng & Zhao, 2006; Duan *et al.*, 2005; Şengül *et al.*, 2004). In the two molecules, the

Figure 1

The structure of the first independent molecule (*A*) in the asymmetric unit of (I). Displacement ellipsoids are drawn at the 35% probability level. Atoms labelled with the suffix 'A' are generated by the symmetry operation $(-x, 1 - y, -z)$.

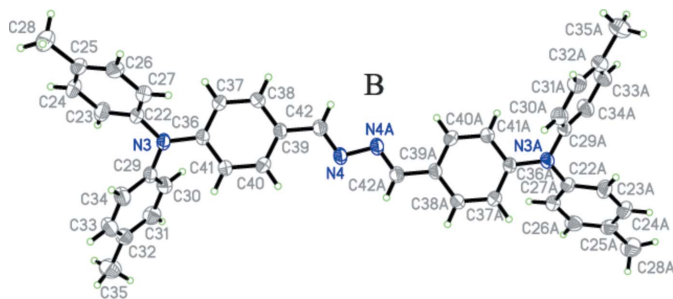


Figure 2

The structure of the other independent molecule, (B), in the asymmetric unit of (I). Displacement ellipsoids are drawn at the 35% probability level. Atoms labelled with the suffix 'A' are generated by the symmetry operation $(1 - x, 1 - y, -z)$.

$C=N-N$ angles [112.1 (3) and 112.4 (2) $^\circ$] deviate significantly from the ideal value of 120 $^\circ$ expected for an sp^2 -N atom as a consequence of the repulsion between the N lone pairs and the adjacent $C=N$ bonds. The two independent molecules adopt different conformations for the peripheral groups, *viz.* the terminal tolyl functionalities, as reflected in the significantly different values of the dihedral angles between the two terminal benzene rings [74.0 (2) and 63.4 (2) $^\circ$]. The C atoms of the methyl groups attached to the benzene rings do not deviate substantially from the planes of these rings: the deviations for atoms C7, C14, C28 and C35 are 0.0020 (2), 0.0011 (2), 0.0893 (2) and 0.0352 (2) Å, respectively.

Experimental

The title compound was synthesized by the reaction of 4-(di-*p*-tolylamino)benzaldehyde with hydrazine hydrate in refluxing ethanol (Liu *et al.*, 2004). Single crystals suitable for X-ray analysis were obtained by slow evaporation of a tetrahydrofuran solution at 298 K.

Crystal data

$C_{42}H_{38}N_4$	$V = 1712.1 (10) \text{ \AA}^3$
$M_r = 598.76$	$Z = 2$
Triclinic, $P\bar{1}$	$D_x = 1.161 \text{ Mg m}^{-3}$
$a = 11.142 (4) \text{ \AA}$	Mo $K\alpha$ radiation
$b = 12.562 (5) \text{ \AA}$	$\mu = 0.07 \text{ mm}^{-1}$
$c = 13.848 (5) \text{ \AA}$	$T = 294 (2) \text{ K}$
$\alpha = 72.191 (6)^\circ$	Block, colourless
$\beta = 84.891 (7)^\circ$	$0.32 \times 0.20 \times 0.12 \text{ mm}$
$\gamma = 68.143 (7)^\circ$	

Data collection

Bruker SMART CCD area-detector diffractometer	8794 measured reflections
φ and ω scans	6005 independent reflections
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	3032 reflections with $I > 2\sigma(I)$
$T_{\min} = 0.979$, $T_{\max} = 0.992$	$R_{\text{int}} = 0.027$
	$\theta_{\text{max}} = 25.0^\circ$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.050$
 $wR(F^2) = 0.124$
 $S = 1.03$
 6005 reflections
 419 parameters

H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.0442P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.002$
 $\Delta\rho_{\text{max}} = 0.15 \text{ e \AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.16 \text{ e \AA}^{-3}$

Table 1

Selected geometric parameters (Å, $^\circ$).

N2—C21	1.266 (3)	N4—C42	1.281 (3)
N2—N2 ⁱ	1.410 (3)	N4—N4 ⁱⁱ	1.415 (3)
C21—N2—N2 ⁱ	112.1 (3)	C42—N4—N4 ⁱⁱ	112.4 (2)
C19—C18—C21—N2	179.6 (2)	C40—C39—C42—N4	9.4 (3)

Symmetry codes: (i) $-x, -y + 1, -z$; (ii) $-x + 1, -y + 1, -z$.

All H atoms were positioned geometrically and refined as riding on their carrier atoms, with C—H bond lengths constrained to 0.93 (aromatic CH) or 0.96 Å (methyl CH₃). Isotropic displacement parameters for H atoms were fixed at $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$ for methyl groups and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ otherwise.

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

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