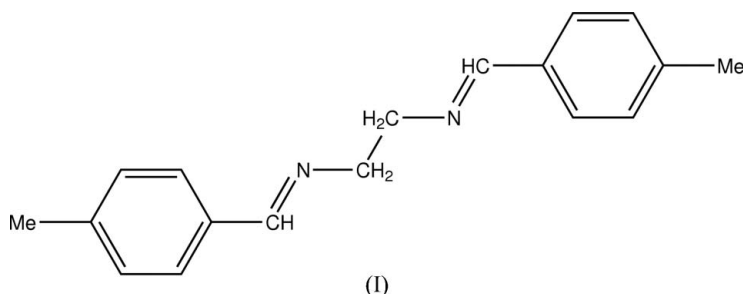
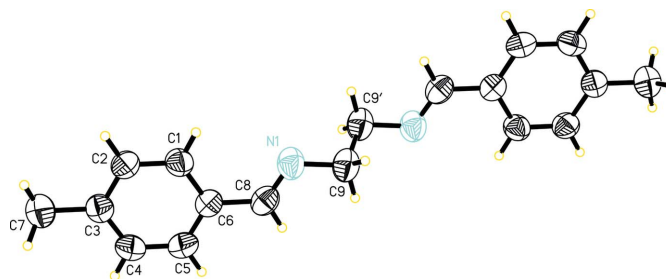


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bohari@pkrisc.cc.ukm.my**Key indicators**Single-crystal X-ray study
 $T = 298\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.003\text{ \AA}$
 R factor = 0.056
 wR factor = 0.165
Data-to-parameter ratio = 16.1For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.**(*E,E*)-*N,N'*-Bis(4-tolylmethylidene)ethylenediamine**The non-planar molecule of the title compound, $\text{C}_{18}\text{H}_{20}\text{N}_2$, is centrosymmetric about the central point of the ethylene bond and poses *E* configuration across each azomethine $\text{C}=\text{N}$ bond.

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CommentThe continuing interest in the Schiff bases of ethylenediamine derivatives is driven by the development of supramolecular assemblies (Thalladi *et al.*, 1995), complexations with metals, and their biological activities (Patel *et al.*, 2005). The title compound, (I), is similar to (*E,E*)-*N,N'*-bis(1-phenylethylidene)ethylenediamine, (II) (Benson *et al.*, 2006), except that the methyl group is attached at the 4-position of the benzene ring instead of the azomethine group.In the molecule of the title compound, (I) (Fig. 1), the bond lengths and angles are within normal ranges (Allen *et al.*, 1987). Like in (II), the molecule maintains its centrosymmetry about the ethylene bridge and the *E* configuration about the azomethine $\text{C}=\text{N}$ bonds. It also adopts a staggered conformation about the $\text{C}_9-\text{C}_9'$ bond, required by the centrosymmetry. The C_1-C_8 tolylmethylidene fragment is nearly planar, having a total puckering amplitude, Q_T , of $0.074(3)\text{ \AA}$ (Cremer & Pople, 1975). In contrast to compound (II), the**Figure 1**

The molecular structure with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

entire molecule is not planar because the dihedral angle between the planar bridging N1/C9/C9ⁱ/N1ⁱ and C1–C8 tolylmethyldene fragments is 61.65 (17)°.

In the crystal structure, although there are no significant π – π interactions, there are C–H·· π interactions, the closest H··centroid distance being 2.80 Å, occurring between C2/H2 and the ring centroid of (C1–C6)ⁱⁱ with an angle at H of 138° [symmetry code: (ii) $-\frac{1}{2} - x, -\frac{1}{2} + y, \frac{3}{2} - z$]. These interactions lead to the formation of columns along the *a* axis.

Experimental

A mixture of ethylenediamine (0.45 g, 0.015 mol) and 4-methylbenzaldehyde (4.0 g, 0.030 mol) in absolute ethanol (100 ml) was heated in a water bath at 323 K for 3 h. The mixture was then cooled to 273 K in an ice bath. The resulting white precipitate was filtered off, washed with cold ethanol and then dried under vacuum. Crystals suitable for X-ray investigation were obtained by recrystallization from a mixture of chloroform and ethanol (1:1) (yield 3.23 g, 81.5%; m.p. 415.2–416.5 K).

Crystal data

C₁₈H₂₀N₂
M_r = 264.36
 Monoclinic, *P*2₁/*n*
a = 6.842 (2) Å
b = 7.531 (2) Å
c = 14.933 (5) Å
 β = 100.801 (7)°
V = 755.8 (4) Å³

Z = 2
D_x = 1.162 Mg m⁻³
 Mo *K*α radiation
 μ = 0.07 mm⁻¹
T = 298 (2) K
 Block, colorless
 0.42 × 0.28 × 0.16 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
 ω scans
 Absorption correction: multi-scan (SADABS; Bruker, 2000)
T_{min} = 0.971, *T_{max}* = 0.989

4098 measured reflections
 1484 independent reflections
 935 reflections with *I* > 2σ(*I*)
R_{int} = 0.025
 θ_{\max} = 26.0°

Refinement

Refinement on *F*²
R [*F*² > 2σ(*F*²)] = 0.056
wR (*F*²) = 0.165
S = 1.05
 1484 reflections
 92 parameters
 H-atom parameters constrained

$$w = 1/[\sigma^2(F_o^2) + (0.0854P)^2 + 0.0506P]$$

where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.18 \text{ e } \text{Å}^{-3}$
 $\Delta\rho_{\min} = -0.12 \text{ e } \text{Å}^{-3}$

H atoms were positioned geometrically with C–H = 0.93, 0.96 and 0.97 Å for aromatic, methyl and methylene H atoms, respectively, and constrained to ride on their parent atoms, with *U_{iso}*(H) = *xU_{eq}*(C,N) where *x* = 1.5 for methyl H and *x* = 1.2 for all other H atoms.

Data collection: SMART (Bruker, 2000); cell refinement: SAINT; data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997a); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997a); molecular graphics: SHELXTL (Sheldrick, 1997b); software used to prepare material for publication: SHELXTL, PARST (Nardelli, 1995) and PLATON (Spek, 2003).

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References

- Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
- Benson, R. E., Roy, T. G., Dey, B. K., Barua, K. K. & Tiekink, E. R. T. (2006). *Acta Cryst.* **E62**, o1971–o1972.
- Bruker (2000). SADABS (Version 2.01), SMART (Version 5.630) and SAINT (Version 6.36a). Bruker AXS Inc., Madison, Wisconsin, USA.
- Cremer, D. & Pople, J. A. (1975). *J. Am. Chem. Soc.* **97**, 1354–1358.
- Nardelli, M. (1995). *J. Appl. Cryst.* **28**, 659.
- Patel, N., Parekh, H. & Patel, M. (2005). *Transition Met. Chem.* **30**, 13–17.
- Sheldrick, G. M. (1997a). SHELXS97 and SHELXL97. University of Göttingen, Germany.
- Sheldrick, G. M. (1997b). SHELXTL. Version 5.1. Bruker AXS Inc., Madison, Wisconsin, USA.
- Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.
- Thalladi, V. R., Panneerselvam, K., Carrell, C. J., Carrell, H. L. & Desiraju, G. R. (1995). *J. Chem. Soc. Chem. Commun.* pp. 341–342.