

(*E,E*)-*N,N'*-Bis(1-phenylethylidene)ethylenediamine

Ronald E. Benson,^a Tapashi G. Roy,^b Benu K. Dey,^b Kanak K. Barua^b and Edward R. T. Tiekink^{c*}

^aRigaku Americas Corporation, 9009 New Trails Drive, The Woodlands, Texas 77381, USA,

^bDepartment of Chemistry, University of Chittagong, Chittagong 4331, Bangladesh, and

^cDepartment of Chemistry, The University of Texas at San Antonio, One UTSA Circle, San Antonio, Texas 78249-0698, USA

Correspondence e-mail:
edward.tiekink@utsa.edu

Key indicators

Single-crystal X-ray study

T = 113 K

Mean $\sigma(\text{C}-\text{C})$ = 0.002 Å

R factor = 0.043

wR factor = 0.117

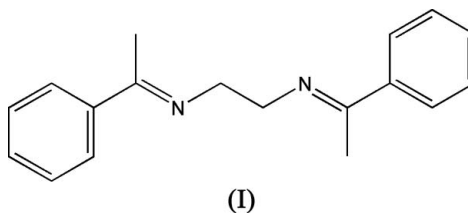
Data-to-parameter ratio = 18.1

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

The essentially planar title compound, C₁₈H₂₀N₂, is disposed about a center of inversion located at the mid-point of the ethylene bond and features an *E* configuration about each C=N bond.

Comment

The title compound, (I), was isolated in an attempt to prepare a macrocyclic ligand in connection with our ongoing interest in macrocyclic complexes of transition metals (*e.g.* Roy *et al.*, 2006); see *Experimental* for details. This molecule was first reported by Ferguson & Goodwin (1949) and now attracts interest as a ligand for transition metals with biological activity, *e.g.* antibacterial (Patel *et al.*, 2005). Compound (I) (Fig. 1 and Table 1) is centrosymmetric about the ethylene bridge and the configuration about the C=N bond is *E*. The entire molecule is essentially planar as evidenced in the values of the N1–C1–C4–C5, C3–N1–C1–C4 and N1–C3–C3ⁱ–N1ⁱ torsion angles of 6.15 (14), 178.62 (9) and 179.98 (11)°, respectively [symmetry code: (i) 1 – *x*, 1 – *y*, –*z*]. The observed configuration found for (I) contrasts with that observed in the only known crystal structure containing (I), in which it functions as a chelating ligand to an Mo(CO)₄ unit (Paz-Sandoval *et al.*, 1995). While there are no significant π – π interactions in the crystal structure of (I), there are C–H... π interactions with the closest being 2.70 Å, occurring between C2/H2B and the ring centroid of (C4–C9)ⁱⁱ with an angle at H of 141° [symmetry code: (ii) 1 – *x*, 1 – *y*, 1 – *z*]. These interactions lead to the formation of columns comprising off-set molecules.

**Experimental**

Compound (I) was isolated during reactions designed to form a new macrocyclic ligand following literature precedents (*e.g.* Bembi *et al.*, 1989; Roy *et al.*, 2001; Gasperov *et al.*, 2004). Thus, the reaction between acetophenone (excess), diaminoethane and HClO₄ in ethanol solution yielded an intractable product, but in the absence of acid yielded (I). Presumably, it is the bulky size of the phenyl substituents that preclude cyclization, as observed in the methyl analogs. Crystals for the X-ray analysis were grown by slow evaporation of a chloroform–xylene solution (1:5) of (I).

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Crystal data

C₁₈H₂₀N₂
 M_r = 264.36
 Monoclinic, P2₁/n
 a = 5.4713 (7) Å
 b = 14.1328 (17) Å
 c = 9.7392 (13) Å
 β = 105.7130 (5)°
 V = 724.94 (16) Å³

Z = 2
 D_x = 1.211 Mg m⁻³
 Mo Kα radiation
 μ = 0.07 mm⁻¹
 T = 113 (2) K
 Prism, colorless
 0.51 × 0.40 × 0.22 mm

Data collection

Rigaku R-Axis SPIDER
 diffractometer
 ω scans
 Absorption correction: numerical
 (Katayama, 1986; Paturle &
 Coppens, 1988)
 T_{min} = 0.978, T_{max} = 0.992

9051 measured reflections
 1666 independent reflections
 1617 reflections with I > 2σ(I)
 R_{int} = 0.034
 θ_{max} = 27.5°

Refinement

Refinement on F²
 R[F² > 2σ(F²)] = 0.043
 wR(F²) = 0.117
 S = 1.07
 1666 reflections
 92 parameters
 H-atom parameters constrained

w = 1/[σ²(F_o²) + (0.0589P)²
 + 0.2225P]
 where P = (F_o² + 2F_c²)/3
 (Δ/σ)_{max} < 0.001
 Δρ_{max} = 0.32 e Å⁻³
 Δρ_{min} = -0.15 e Å⁻³

Table 1

Selected geometric parameters (Å, °).

N1—C1	1.2772 (13)	C1—C2	1.5120 (14)
N1—C3	1.4668 (13)	C1—C4	1.4999 (14)
C1—N1—C3	119.82 (9)	C2—C1—C4	117.18 (8)
N1—C1—C2	125.77 (9)	N1—C3—C3 ⁱ	108.95 (11)

Symmetry code: (i) -x + 1, -y + 1, -z.

All H atoms were allowed to ride on their parent atoms at distances of 0.95 (aromatic H), 0.98 (methyl H) and 0.99 Å (methylene H), and with U_{iso}(H) values of 1.2U_{eq}(parent atom) for aromatic and methylene H atoms, and 1.5U_{eq}(parent atom) for methyl H atoms.

Data collection: *CrystalClear* (Rigaku/MS, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1994); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics:

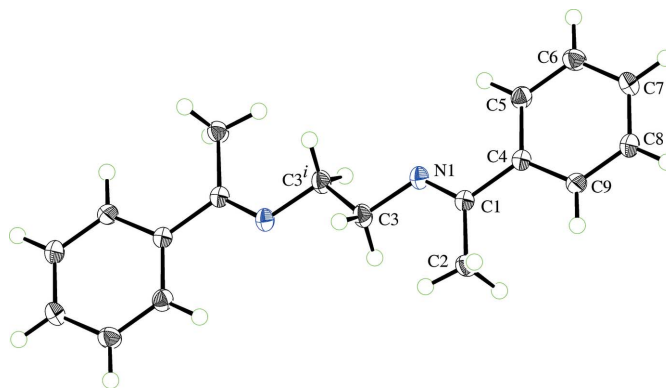


Figure 1

The molecular structure of (I), showing the crystallographic numbering scheme. Displacement ellipsoids are shown at the 50% probability level. [Symmetry code: (i) 1 - x, 1 - y, -z.]

ORTEP (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

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