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N,*N*-Dimethyl-4-[(*E*)-phenyliminomethyl]aniline

Lei Zheng, Xiu-juan Yin, Cong-ling Yang, Ying Li and Shu-fan Yin*

College of Chemistry, Sichuan University, Chengdu 610064, People's Republic of China
Correspondence e-mail: chuandayouji217@163.com

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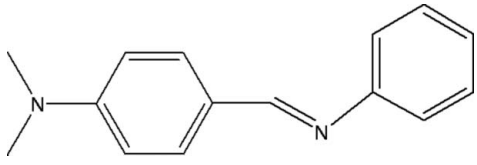
Key indicators: single-crystal X-ray study; T = 292 K; mean σ(C–C) = 0.003 Å; R factor = 0.047; wR factor = 0.150; data-to-parameter ratio = 14.8.

The title compound, $C_{15}H_{16}N_2$, contains two aromatic rings linked through an imino group. The molecule exhibits an *E* configuration with respect to the C=N bond. The dihedral angle between the aromatic rings is 61.96 (1)°.

Related literature

For the physical properties and physiological activity of Schiff bases, see: Hodnett & Dunn (1970); Nyarku & Mavuso (1998); Tang & Vanslyke (1987); Yu *et al.* (2001). For related structures, see: Ahmet *et al.* (1994); Nakai *et al.* (1976); Wang & Wang (2007, 2008).



Experimental

Crystal data

$C_{15}H_{16}N_2$ M_r = 224.30
Monoclinic, $P2_1/c$
a = 9.441 (4) Å
b = 8.356 (3) Å
c = 17.245 (5) Å
β = 110.97 (2)°
V = 1270.4 (8) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.07 mm^{-1}
T = 292 (2) K
0.52 × 0.48 × 0.46 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: none
3023 measured reflections
2328 independent reflections
1336 reflections with $I > 2\sigma(I)$
R_{int} = 0.012
3 standard reflections
every 200 reflections
intensity decay: 1.8%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.150
S = 1.02
2328 reflections
157 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.13 e Å^{-3}
$\Delta\rho_{min}$ = −0.14 e Å^{-3}

Data collection: *DIFRAC* (Gabe *et al.*, 1993); cell refinement: *NRCVAX* (Gabe *et al.*, 1989); data reduction: *NRCVAX*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia,1997); software used to prepare material for publication: *SHELXL97*.

The authors thank Mr Zhi-Hua Mao, Sichuan University, for the X-ray data collection.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PV2134).

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supporting information

Acta Cryst. (2009). E**65**, o506 [doi:10.1107/S1600536809003791]

N,*N*-Dimethyl-4-[(*E*)-phenyliminomethyl]aniline

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S1. Comment

Schiff base, because of its unique light, electric, magnetic and other physical material properties (Tang & Vanslyke, 1987; Yu *et al.*, 2001), good coordination chemistry performance, unique anti-bacterial, anti-cancer and other physiological activities (Nyarku & Mavuso, 1998; Hodnett & Dunn, 1970), has aroused broad, systematic and in-depth theoretical and applied research. Several crystal sturctures of schiff bases, which are closely related to the title compound, have been reported (eg., Ahmet *et al.*, 1994; Nakai *et al.*, 1976; Wang & Wang, 2008; Wang & Wang, 2007). We report herein the crystal sturcture of the title schiff base, N,N-dimethyl-4-[(E)-(phenylimino)methyl]benzenamine, (I).

The molecule of the title compound (Fig. 1) adopts an E configuration probably owing to the steric effect. The C(10)–N(2)–C(9)–C(6) and C(7)–C(6)–C(9)–N(2) torsion angles are -176.70 (15) and 9.2 (3)°, respectively. There are no intermolecular hydrogen-bonding interactions in the crystal structure. The packing is essentially stabilized *via* van der Waals forces.

S2. Experimental

To a solution of *N*,*N*-dimethyl-4-aminobenzaldehyde (0.75 g, 5 mmol) in ethanol (10 ml) and aniline (0.91 ml, 10 mmol) were added three drops of acetic acid as a catalyst. The mixture was heated to reflux and the reaction monitored by TLC. After completion of the reaction, on cooling to room temperature, crystals were obtained. Colourless crystals suitable for X-ray analysis were obtained by slow evaporation of an ethyl acetate solution at room temperature.

S3. Refinement

H atoms were positioned geometrically (C—H = 0.93–0.96 Å) and included in the refinement using a riding model, with U_{iso}(H) = 1.2U_{eq} (methylene C, aromatic C), U_{iso}(H) = 1.5U_{eq} (methyl C).

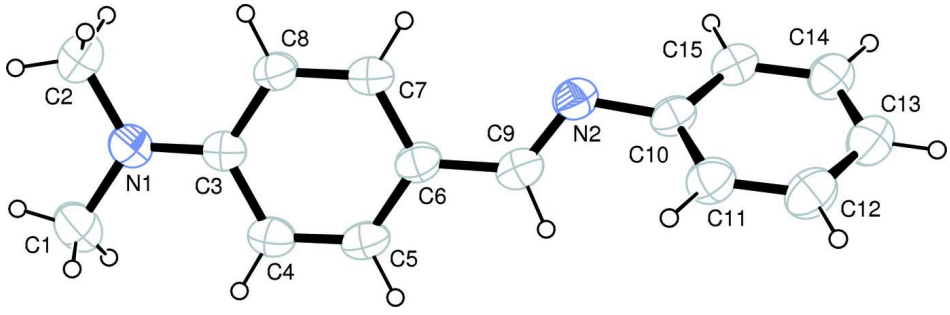

Figure 1

The molecular structure of (I), with displacement ellipsoids drawn at the 30% probability level.

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Crystal data

$C_{15}H_{16}N_2$
$M_r = 224.30$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 9.441$ (4) Å
$b = 8.356$ (3) Å
$c = 17.245$ (5) Å
$\beta = 110.97$ (2)°
$V = 1270.4$ (8) Å^3
$Z = 4$
$F(000) = 480$
$D_x = 1.173$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 20 reflections
$\theta = 4.4$–$7.1°$
$\mu = 0.07$ mm^{-1}
$T = 292$ K
Block, colourless
0.52 × 0.48 × 0.46 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega/2\theta$ scans
3023 measured reflections
2328 independent reflections
1336 reflections with $I > 2\sigma(I)$
$R_{int} = 0.012$
$\theta_{max} = 25.5°$, $\theta_{min} = 2.3°$
$h = -11 \rightarrow 11$
$k = -10 \rightarrow 0$
$l = -20 \rightarrow 10$
3 standard reflections every 200 reflections
intensity decay: 1.8%

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.047$
$wR(F^2) = 0.150$
$S = 1.02$
2328 reflections
157 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0913P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.13$ e Å^{-3}
$\Delta\rho_{min} = -0.14$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008)
Extinction coefficient: 0.032 (10)

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
N1	0.30901 (17)	1.50607 (18)	−0.07311 (10)	0.0722 (5)
N2	0.28787 (18)	0.86291 (19)	0.13032 (9)	0.0668 (5)
C1	0.3837 (2)	1.4806 (2)	−0.13194 (12)	0.0815 (6)

H1A	0.4831	1.4372	−0.1037	0.122*
H1B	0.3924	1.5807	−0.1572	0.122*
H1C	0.3254	1.4071	−0.1740	0.122*
C2	0.2456 (3)	1.6630 (2)	−0.07117 (15)	0.0907 (7)
H2A	0.1369	1.6571	−0.0944	0.136*
H2B	0.2810	1.7363	−0.1031	0.136*
H2C	0.2768	1.6997	−0.0148	0.136*
C3	0.28724 (19)	1.3833 (2)	−0.02654 (11)	0.0587 (5)
C4	0.2055 (2)	1.4036 (2)	0.02656 (12)	0.0687 (5)
H4	0.1636	1.5029	0.0300	0.082*
C5	0.1867 (2)	1.2792 (2)	0.07319 (12)	0.0686 (5)
H5	0.1329	1.2965	0.1082	0.082*
C6	0.2449 (2)	1.1275 (2)	0.07036 (11)	0.0616 (5)
C7	0.3258 (2)	1.1071 (2)	0.01746 (10)	0.0636 (5)
H7	0.3669	1.0073	0.0142	0.076*
C8	0.3462 (2)	1.2297 (2)	−0.02946 (11)	0.0625 (5)
H8	0.4004	1.2115	−0.0643	0.075*
C9	0.2222 (2)	0.9985 (2)	0.12090 (11)	0.0681 (5)
H9	0.1550	1.0160	0.1484	0.082*
C10	0.2496 (2)	0.7447 (2)	0.17785 (11)	0.0619 (5)
C11	0.1006 (2)	0.7114 (2)	0.16925 (12)	0.0715 (6)
H11	0.0217	0.7702	0.1321	0.086*
C12	0.0694 (2)	0.5918 (3)	0.21553 (13)	0.0795 (6)
H12	−0.0307	0.5700	0.2093	0.095*
C13	0.1848 (3)	0.5041 (2)	0.27093 (13)	0.0796 (6)
H13	0.1629	0.4243	0.3025	0.096*
C14	0.3326 (2)	0.5352 (2)	0.27936 (12)	0.0744 (6)
H14	0.4110	0.4757	0.3165	0.089*
C15	0.3645 (2)	0.6536 (2)	0.23315 (11)	0.0682 (5)
H15	0.4648	0.6733	0.2389	0.082*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0775 (11)	0.0677 (10)	0.0723 (11)	0.0087 (8)	0.0278 (9)	0.0044 (8)
N2	0.0681 (10)	0.0769 (11)	0.0590 (9)	0.0019 (8)	0.0270 (8)	−0.0015 (8)
C1	0.0882 (14)	0.0911 (14)	0.0695 (12)	−0.0005 (11)	0.0338 (11)	0.0092 (11)
C2	0.0945 (16)	0.0719 (13)	0.1018 (16)	0.0086 (11)	0.0305 (14)	0.0059 (12)
C3	0.0538 (10)	0.0656 (11)	0.0530 (10)	−0.0001 (8)	0.0146 (8)	−0.0077 (9)
C4	0.0696 (12)	0.0667 (11)	0.0716 (12)	0.0094 (9)	0.0276 (10)	−0.0083 (10)
C5	0.0684 (12)	0.0816 (14)	0.0637 (11)	0.0060 (10)	0.0333 (10)	−0.0109 (10)
C6	0.0620 (11)	0.0713 (12)	0.0535 (10)	0.0026 (9)	0.0231 (9)	−0.0057 (9)
C7	0.0682 (12)	0.0637 (11)	0.0630 (11)	0.0070 (9)	0.0285 (10)	−0.0066 (9)
C8	0.0669 (12)	0.0682 (12)	0.0580 (11)	0.0063 (9)	0.0290 (9)	−0.0048 (9)
C9	0.0657 (12)	0.0836 (14)	0.0594 (11)	0.0019 (10)	0.0278 (9)	−0.0064 (10)
C10	0.0642 (12)	0.0724 (11)	0.0528 (10)	−0.0030 (10)	0.0255 (9)	−0.0095 (9)
C11	0.0607 (12)	0.0852 (14)	0.0656 (12)	−0.0022 (10)	0.0191 (10)	−0.0030 (11)
C12	0.0657 (12)	0.0961 (15)	0.0779 (13)	−0.0151 (11)	0.0271 (11)	−0.0076 (12)

C13	0.0881 (15)	0.0816 (14)	0.0746 (13)	−0.0110 (12)	0.0358 (12)	−0.0003 (11)
C14	0.0770 (13)	0.0800 (13)	0.0680 (12)	0.0054 (11)	0.0281 (10)	0.0050 (11)
C15	0.0619 (12)	0.0796 (12)	0.0680 (12)	0.0011 (10)	0.0291 (10)	−0.0036 (11)

Geometric parameters (Å, º)

N1—C3	1.363 (2)	C6—C7	1.394 (2)
N1—C1	1.444 (2)	C6—C9	1.449 (3)
N1—C2	1.447 (2)	C7—C8	1.361 (2)
N2—C9	1.274 (2)	C7—H7	0.9300
N2—C10	1.411 (2)	C8—H8	0.9300
C1—H1A	0.9600	C9—H9	0.9300
C1—H1B	0.9600	C10—C15	1.388 (3)
C1—H1C	0.9600	C10—C11	1.388 (3)
C2—H2A	0.9600	C11—C12	1.375 (3)
C2—H2B	0.9600	C11—H11	0.9300
C2—H2C	0.9600	C12—C13	1.375 (3)
C3—C4	1.403 (2)	C12—H12	0.9300
C3—C8	1.407 (2)	C13—C14	1.375 (3)
C4—C5	1.364 (2)	C13—H13	0.9300
C4—H4	0.9300	C14—C15	1.370 (3)
C5—C6	1.389 (2)	C14—H14	0.9300
C5—H5	0.9300	C15—H15	0.9300
C3—N1—C1	121.18 (15)	C8—C7—C6	121.63 (16)
C3—N1—C2	121.17 (16)	C8—C7—H7	119.2
C1—N1—C2	117.39 (17)	C6—C7—H7	119.2
C9—N2—C10	118.88 (16)	C7—C8—C3	121.55 (16)
N1—C1—H1A	109.5	C7—C8—H8	119.2
N1—C1—H1B	109.5	C3—C8—H8	119.2
H1A—C1—H1B	109.5	N2—C9—C6	124.65 (17)
N1—C1—H1C	109.5	N2—C9—H9	117.7
H1A—C1—H1C	109.5	C6—C9—H9	117.7
H1B—C1—H1C	109.5	C15—C10—C11	118.49 (18)
N1—C2—H2A	109.5	C15—C10—N2	118.89 (16)
N1—C2—H2B	109.5	C11—C10—N2	122.57 (18)
H2A—C2—H2B	109.5	C12—C11—C10	120.17 (19)
N1—C2—H2C	109.5	C12—C11—H11	119.9
H2A—C2—H2C	109.5	C10—C11—H11	119.9
H2B—C2—H2C	109.5	C13—C12—C11	120.63 (19)
N1—C3—C4	121.86 (16)	C13—C12—H12	119.7
N1—C3—C8	121.37 (16)	C11—C12—H12	119.7
C4—C3—C8	116.77 (17)	C12—C13—C14	119.64 (19)
C5—C4—C3	120.70 (16)	C12—C13—H13	120.2
C5—C4—H4	119.7	C14—C13—H13	120.2
C3—C4—H4	119.7	C15—C14—C13	120.05 (19)
C4—C5—C6	122.56 (16)	C15—C14—H14	120.0
C4—C5—H5	118.7	C13—C14—H14	120.0

C6—C5—H5	118.7	C14—C15—C10	121.00 (18)
C5—C6—C7	116.79 (17)	C14—C15—H15	119.5
C5—C6—C9	120.79 (17)	C10—C15—H15	119.5
C7—C6—C9	122.42 (17)		
C1—N1—C3—C4	−175.41 (16)	C10—N2—C9—C6	−176.70 (15)
C2—N1—C3—C4	−1.3 (3)	C5—C6—C9—N2	−170.32 (18)
C1—N1—C3—C8	4.7 (3)	C7—C6—C9—N2	9.2 (3)
C2—N1—C3—C8	178.74 (17)	C9—N2—C10—C15	−137.72 (18)
N1—C3—C4—C5	−179.28 (17)	C9—N2—C10—C11	44.8 (2)
C8—C3—C4—C5	0.6 (3)	C15—C10—C11—C12	0.7 (3)
C3—C4—C5—C6	−0.7 (3)	N2—C10—C11—C12	178.17 (16)
C4—C5—C6—C7	0.5 (3)	C10—C11—C12—C13	0.2 (3)
C4—C5—C6—C9	−179.94 (17)	C11—C12—C13—C14	−0.8 (3)
C5—C6—C7—C8	−0.3 (3)	C12—C13—C14—C15	0.4 (3)
C9—C6—C7—C8	−179.89 (17)	C13—C14—C15—C10	0.5 (3)
C6—C7—C8—C3	0.4 (3)	C11—C10—C15—C14	−1.0 (3)
N1—C3—C8—C7	179.43 (16)	N2—C10—C15—C14	−178.61 (16)
C4—C3—C8—C7	−0.5 (3)		