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N-[4-(Dimethylamino)benzylidene]-4-ethoxyaniline

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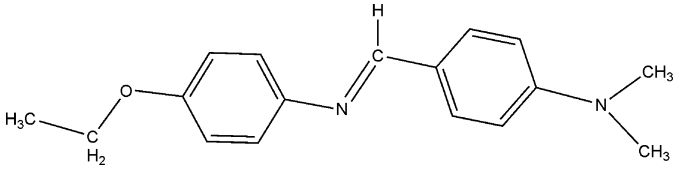
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.005 Å; R factor = 0.051; wR factor = 0.164; data-to-parameter ratio = 14.1.

In the title compound, $C_{17}H_{20}N_2O$, the molecular core is planar, with a central C—N═C—C torsion angle of −179.3 (3)°. However, the overall geometry is not planar, with a dihedral angle of 61.96 (1)° between the two benzene rings, which adopt a *trans* configuration with respect to the C═N bond [1.269 (4) Å]. The bond lengths and angles are within normal ranges

Related literature

For biological activities, see: Yang *et al.* (2000). For related synthesis, see: Mondal *et al.* (2001); Tarafder *et al.* (2002).



Experimental

Crystal data

$C_{17}H_{20}N_2O$
M_r = 268.35
Monoclinic, $P2_1/c$
a = 9.586 (3) Å
b = 16.678 (7) Å
c = 9.722 (3) Å
β = 109.319 (4)°
V = 1466.7 (9) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 298 (2) K
0.34 × 0.27 × 0.19 mm

Data collection

Siemens SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.97, T_{max} = 0.99
7422 measured reflections
2589 independent reflections
1323 reflections with $I > 2\sigma(I)$
R_{int} = 0.036

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.051
$wR(F^2)$ = 0.164
S = 1.02
2589 reflections
184 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.14 e Å^{-3}

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BG2150).

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supplementary materials

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N-[4-(Dimethylamino)benzylidene]-4-ethoxyaniline

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Comment

Schiff bases have been intensively investigated recently owing to their strong coordination capability and diverse biological activities, such as antibacterial, antitumor activities *etc*. (Yang *et al.*, 2000; Mondal *et al.*, 2001; Tarafder *et al.*, 2002). We report here the synthesis and crystal structure of the title new Schiff base $C_{17}H_{20}N_2O$, (I).

The molecular structure of (I) is shown in Fig. 1. The molecular core is planar, with a central C—N═C—C torsion angle of −179.3 (3)°. The overall geometry instead, is not, with a dihedral angle of 61.96 (1)° between the two benzene rings, which adopt a *trans* configuration with respect to the C═N bond [1.269 (4) Å]. The bond lengths and angles are within normal ranges.

Experimental

P-dimethylamino benzaldehyde (5 mmol, 746.0 mg) in absolute ethanol (15 ml) was added dropwise to a absolute ethanol solution (5 ml) of *p*-ethoxyaniline (5 mmol, 685.9 mg). The mixture was heated under reflux with stirring for 3 h and then filtered. The resulting clear solution was kept at room temperature for 10 days, after which large pale-yellow block-shaped crystals of the title compound suitable for X-ray diffraction analysis were obtained.

Refinement

All H-atoms were positioned geometrically and refined using a riding model, with C—H = 0.96 Å (methyl), 0.97(methylene), 0.93 Å (methenyl), 0.93 Å (aromatic), and U_{iso}(H) = 1.2U_{eq}(C,*N*).

Figures

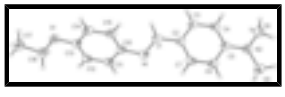

Fig. 1. A molecular view of (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme.

N-[4-(Dimethylamino)benzylidene]-4-ethoxyaniline

Crystal data

$C_{17}H_{20}N_2O$	F_{000} = 576
M_r = 268.35	D_x = 1.215 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 1506 reflections
a = 9.586 (3) Å	θ = 2.3–23.3°

b = 16.678 (7) Å	μ = 0.08 mm^{-1}
c = 9.722 (3) Å	T = 298 (2) K
β = 109.319 (4)º	Block, light yellow
V = 1466.7 (9) Å^3	0.34 × 0.27 × 0.19 mm
Z = 4	

Data collection

Siemens SMART CCD area-detector diffractometer	2589 independent reflections
Radiation source: fine-focus sealed tube	1323 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.036
T = 298(2) K	θ_{max} = 25.0º
φ and ω scans	θ_{min} = 2.3º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −11→11
T_{min} = 0.97, T_{max} = 0.99	k = −19→15
7422 measured reflections	l = −11→11

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.051	H-atom parameters constrained
$wR(F^2)$ = 0.164	$w = 1/[\sigma^2(F_o^2) + (0.0571P)^2 + 0.7834P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.02	$(\Delta/\sigma)_{max} < 0.001$
2589 reflections	$\Delta\rho_{max}$ = 0.18 e Å^{-3}
184 parameters	$\Delta\rho_{min}$ = −0.14 e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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 $F^2 > 2\text{sigma}(F^2)$ 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	0.5988 (3)	0.11288 (15)	0.4352 (3)	0.0543 (7)
N2	0.2098 (3)	0.13050 (17)	−0.2456 (3)	0.0614 (8)
O1	0.8309 (2)	0.13646 (13)	1.0402 (2)	0.0614 (6)
C1	0.4827 (3)	0.15105 (18)	0.3643 (4)	0.0521 (8)
H1	0.4384	0.1832	0.4163	0.063*
C2	0.4153 (3)	0.14752 (18)	0.2077 (3)	0.0479 (8)
C3	0.2738 (3)	0.17601 (19)	0.1395 (4)	0.0567 (9)
H3	0.2237	0.1999	0.1960	0.068*
C4	0.2044 (3)	0.17042 (19)	−0.0081 (4)	0.0566 (9)
H4	0.1082	0.1893	−0.0488	0.068*
C5	0.2761 (3)	0.13677 (18)	−0.0982 (4)	0.0493 (8)
C6	0.4203 (3)	0.10872 (19)	−0.0297 (4)	0.0547 (8)
H6	0.4723	0.0863	−0.0858	0.066*
C7	0.4858 (3)	0.11380 (19)	0.1179 (4)	0.0559 (9)
H7	0.5811	0.0939	0.1598	0.067*
C8	0.0542 (4)	0.1494 (2)	−0.3144 (4)	0.0716 (11)
H8A	−0.0036	0.1185	−0.2696	0.107*
H8B	0.0248	0.1368	−0.4163	0.107*
H8C	0.0386	0.2055	−0.3026	0.107*
C9	0.2890 (4)	0.1011 (2)	−0.3392 (4)	0.0782 (11)
H9A	0.3837	0.1269	−0.3137	0.117*
H9B	0.2332	0.1127	−0.4390	0.117*
H9C	0.3026	0.0442	−0.3268	0.117*
C10	0.6552 (3)	0.11975 (18)	0.5892 (3)	0.0475 (8)
C11	0.6938 (3)	0.05080 (19)	0.6712 (4)	0.0509 (8)
H11	0.6818	0.0013	0.6245	0.061*
C12	0.7501 (3)	0.05387 (19)	0.8218 (4)	0.0515 (8)
H12	0.7724	0.0066	0.8755	0.062*
C13	0.7731 (3)	0.12667 (18)	0.8921 (3)	0.0485 (8)
C14	0.7365 (3)	0.19622 (19)	0.8103 (4)	0.0542 (8)
H14	0.7519	0.2457	0.8570	0.065*
C15	0.6778 (3)	0.19303 (19)	0.6611 (4)	0.0554 (9)
H15	0.6531	0.2403	0.6077	0.066*
C16	0.8842 (4)	0.0675 (2)	1.1264 (3)	0.0629 (9)
H16A	0.9620	0.0425	1.0981	0.075*
H16B	0.8049	0.0290	1.1124	0.075*
C17	0.9428 (4)	0.0927 (2)	1.2824 (4)	0.0781 (11)
H17A	1.0181	0.1325	1.2944	0.117*
H17B	0.9841	0.0470	1.3421	0.117*
H17C	0.8639	0.1146	1.3109	0.117*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0525 (16)	0.0502 (17)	0.0639 (18)	0.0000 (14)	0.0244 (14)	−0.0015 (14)
N2	0.0514 (16)	0.075 (2)	0.0631 (18)	0.0029 (14)	0.0266 (14)	−0.0008 (16)
O1	0.0751 (15)	0.0487 (14)	0.0638 (15)	0.0040 (11)	0.0275 (12)	−0.0021 (12)
C1	0.0502 (19)	0.0427 (19)	0.070 (2)	−0.0031 (15)	0.0294 (17)	−0.0041 (16)

C2	0.0479 (18)	0.0387 (18)	0.061 (2)	−0.0032 (14)	0.0239 (16)	−0.0009 (15)
C3	0.052 (2)	0.054 (2)	0.071 (2)	0.0082 (16)	0.0306 (18)	−0.0053 (17)
C4	0.0463 (18)	0.055 (2)	0.073 (2)	0.0083 (16)	0.0253 (17)	0.0002 (18)
C5	0.0455 (18)	0.0440 (19)	0.066 (2)	−0.0046 (14)	0.0281 (16)	0.0000 (16)
C6	0.0495 (19)	0.055 (2)	0.069 (2)	−0.0002 (15)	0.0317 (17)	−0.0051 (17)
C7	0.0392 (17)	0.053 (2)	0.079 (3)	0.0021 (15)	0.0237 (17)	−0.0010 (18)
C8	0.056 (2)	0.087 (3)	0.072 (2)	−0.0053 (19)	0.0212 (18)	0.000 (2)
C9	0.075 (2)	0.097 (3)	0.074 (2)	0.009 (2)	0.039 (2)	0.001 (2)
C10	0.0418 (17)	0.047 (2)	0.060 (2)	−0.0020 (14)	0.0245 (15)	−0.0031 (17)
C11	0.0505 (19)	0.0389 (19)	0.066 (2)	−0.0018 (14)	0.0235 (16)	−0.0057 (16)
C12	0.0498 (19)	0.0391 (19)	0.069 (2)	0.0011 (14)	0.0250 (17)	0.0032 (17)
C13	0.0462 (18)	0.045 (2)	0.061 (2)	0.0013 (15)	0.0273 (15)	−0.0017 (17)
C14	0.063 (2)	0.0372 (19)	0.071 (2)	−0.0010 (15)	0.0330 (18)	−0.0045 (17)
C15	0.062 (2)	0.042 (2)	0.071 (2)	0.0049 (15)	0.0325 (18)	0.0033 (17)
C16	0.066 (2)	0.061 (2)	0.063 (2)	0.0080 (18)	0.0234 (18)	0.0030 (19)
C17	0.085 (3)	0.082 (3)	0.063 (2)	0.004 (2)	0.018 (2)	0.000 (2)

Geometric parameters (Å, °)

N1—C1	1.269 (4)	C8—H8C	0.9600
N1—C10	1.418 (4)	C9—H9A	0.9600
N2—C5	1.366 (4)	C9—H9B	0.9600
N2—C9	1.450 (4)	C9—H9C	0.9600
N2—C8	1.453 (4)	C10—C11	1.378 (4)
O1—C13	1.370 (4)	C10—C15	1.389 (4)
O1—C16	1.415 (4)	C11—C12	1.384 (4)
C1—C2	1.445 (4)	C11—H11	0.9300
C1—H1	0.9300	C12—C13	1.375 (4)
C2—C3	1.383 (4)	C12—H12	0.9300
C2—C7	1.387 (4)	C13—C14	1.385 (4)
C3—C4	1.370 (4)	C14—C15	1.372 (4)
C3—H3	0.9300	C14—H14	0.9300
C4—C5	1.398 (4)	C15—H15	0.9300
C4—H4	0.9300	C16—C17	1.492 (4)
C5—C6	1.402 (4)	C16—H16A	0.9700
C6—C7	1.366 (4)	C16—H16B	0.9700
C6—H6	0.9300	C17—H17A	0.9600
C7—H7	0.9300	C17—H17B	0.9600
C8—H8A	0.9600	C17—H17C	0.9600
C8—H8B	0.9600		
C1—N1—C10	119.5 (3)	H9A—C9—H9B	109.5
C5—N2—C9	121.7 (3)	N2—C9—H9C	109.5
C5—N2—C8	121.1 (3)	H9A—C9—H9C	109.5
C9—N2—C8	117.1 (3)	H9B—C9—H9C	109.5
C13—O1—C16	117.8 (2)	C11—C10—C15	118.4 (3)
N1—C1—C2	123.9 (3)	C11—C10—N1	118.6 (3)
N1—C1—H1	118.0	C15—C10—N1	122.9 (3)
C2—C1—H1	118.0	C10—C11—C12	121.2 (3)
C3—C2—C7	116.2 (3)	C10—C11—H11	119.4

C3—C2—C1	121.1 (3)	C12—C11—H11	119.4
C7—C2—C1	122.6 (3)	C13—C12—C11	120.1 (3)
C4—C3—C2	122.6 (3)	C13—C12—H12	120.0
C4—C3—H3	118.7	C11—C12—H12	120.0
C2—C3—H3	118.7	O1—C13—C12	124.8 (3)
C3—C4—C5	121.0 (3)	O1—C13—C14	116.2 (3)
C3—C4—H4	119.5	C12—C13—C14	119.0 (3)
C5—C4—H4	119.5	C15—C14—C13	120.8 (3)
N2—C5—C4	122.3 (3)	C15—C14—H14	119.6
N2—C5—C6	121.1 (3)	C13—C14—H14	119.6
C4—C5—C6	116.7 (3)	C14—C15—C10	120.5 (3)
C7—C6—C5	121.1 (3)	C14—C15—H15	119.8
C7—C6—H6	119.4	C10—C15—H15	119.8
C5—C6—H6	119.4	O1—C16—C17	108.3 (3)
C6—C7—C2	122.4 (3)	O1—C16—H16A	110.0
C6—C7—H7	118.8	C17—C16—H16A	110.0
C2—C7—H7	118.8	O1—C16—H16B	110.0
N2—C8—H8A	109.5	C17—C16—H16B	110.0
N2—C8—H8B	109.5	H16A—C16—H16B	108.4
H8A—C8—H8B	109.5	C16—C17—H17A	109.5
N2—C8—H8C	109.5	C16—C17—H17B	109.5
H8A—C8—H8C	109.5	H17A—C17—H17B	109.5
H8B—C8—H8C	109.5	C16—C17—H17C	109.5
N2—C9—H9A	109.5	H17A—C17—H17C	109.5
N2—C9—H9B	109.5	H17B—C17—H17C	109.5
C10—N1—C1—C2	−179.3 (3)	C1—C2—C7—C6	178.3 (3)
N1—C1—C2—C3	166.0 (3)	C1—N1—C10—C11	132.5 (3)
N1—C1—C2—C7	−12.1 (5)	C1—N1—C10—C15	−49.7 (4)
C7—C2—C3—C4	1.2 (5)	C15—C10—C11—C12	1.7 (4)
C1—C2—C3—C4	−177.1 (3)	N1—C10—C11—C12	179.7 (3)
C2—C3—C4—C5	−1.5 (5)	C10—C11—C12—C13	−2.2 (4)
C9—N2—C5—C4	175.3 (3)	C16—O1—C13—C12	6.5 (4)
C8—N2—C5—C4	−7.8 (5)	C16—O1—C13—C14	−173.4 (3)
C9—N2—C5—C6	−5.3 (5)	C11—C12—C13—O1	−178.6 (3)
C8—N2—C5—C6	171.6 (3)	C11—C12—C13—C14	1.2 (4)
C3—C4—C5—N2	−179.9 (3)	O1—C13—C14—C15	180.0 (3)
C3—C4—C5—C6	0.7 (5)	C12—C13—C14—C15	0.1 (4)
N2—C5—C6—C7	−178.9 (3)	C13—C14—C15—C10	−0.6 (4)
C4—C5—C6—C7	0.5 (5)	C11—C10—C15—C14	−0.4 (4)
C5—C6—C7—C2	−0.9 (5)	N1—C10—C15—C14	−178.2 (3)
C3—C2—C7—C6	0.0 (5)	C13—O1—C16—C17	179.4 (3)

Fig. 1