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N-[(*E*)-3,4-Dimethoxybenzylidene]-2,3-dimethylaniline

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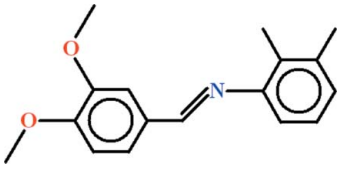
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.004 Å; R factor = 0.061; wR factor = 0.211; data-to-parameter ratio = 19.9.

In the title compound, $C_{17}H_{19}NO_2$, the aromatic rings are oriented at a dihedral angle of 59.27 (12)°. In the crystal, inversion dimers linked by pairs of weak C—H···O interactions generate $R_2^2(12)$ loops.

Related literature

For related structures, see: Sarfraz *et al.* (2010); Tahir *et al.* (2010*a*,*b*); Tariq *et al.* (2010).



Experimental

Crystal data

$C_{17}H_{19}NO_2$
M_r = 269.33
Triclinic, $P\overline{1}$
a = 7.0144 (4) Å
b = 7.4488 (4) Å
c = 15.6202 (8) Å
α = 81.987 (2)°
β = 81.009 (3)°
γ = 73.527 (2)°
V = 769.12 (7) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 296 K
0.34 × 0.25 × 0.22 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.972, T_{max} = 0.983
8993 measured reflections
3688 independent reflections
2028 reflections with $I > 2\sigma(I)$
R_{int} = 0.019

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.061
$wR(F^2)$ = 0.211
S = 1.08
3688 reflections
185 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C16—H16B···O2^{i}	0.96	2.51	3.454 (3)	167

Symmetry code: (i) $-x+1, -y+3, -z$.

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; 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) and *PLATON* (Spek, 2009); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *PLATON*.

The authors acknowledge the provision of funds for the purchase of the diffractometer and encouragement by Dr Muhammad Akram Chaudhary, former Vice Chancellor, University of Sargodha. Pakistan.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB6358).

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supporting information

Acta Cryst. (2011). E**67**, o2378 [doi:10.1107/S1600536811032892]

N-[(*E*)-3,4-Dimethoxybenzylidene]-2,3-dimethylaniline

M. Nawaz Tahir, Muhammad Ilyas Tariq and Riaz H. Tariq

S1. Comment

We have reported crystal structures of Schiff bases containining 2,3-dimethylaniline moiety *i.e.* (II) *N*-[(*E*)-4-chloro-benzylidene] -2,3-dimethylaniline (Tahir *et al.*, 2010*a*), (III) *i.e.*, 2-[(*E*)-(2,3-dimethylphenyl)iminomethyl]phenol (Tahir *et al.*, 2010*b*), (IV) *i.e.*, *N*-{(*E*)-[4-(dimethylamino)phenyl] methylidene}-2,3-dimethylaniline (Sarfraz *et al.*, 2010) and (V) *i.e.*, (2*Z*)-2-[(2,3-dimethylphenyl)imino]-1,2-diphenylethanone (Tariq *et al.*, 2010). The title compound (I), (Fig. 1) is in continuation to synthesize various compounds of 2,3-dimethylaniline.

In (I), the group A (C1—C8/N1) of 2,3-dimethylaniline and the group B (C9—C17/O1/O2) of 3,4-dimethoxy-benzaldehyde are close to planar with r.m.s. deviations of 0.010 and 0.041 Å, respectively. The dihedral angle between A/B is 60.57 (4)°. The molecules are linked in the form of dimers due to inter-molecular hydrogen bonds of C—H···O type with $R_2^2(12)$ ring motif (Table 1, Fig. 2). There does not exist any kind of significant π-interactions.

S2. Experimental

Equimolar quantities of 2,3-dimethylaniline and 3,4-dimethoxybenzaldehyde were refluxed in methanol for 30 min. The solution was kept at room temperature which affoarded colorless prisms after 48 h.

S3. Refinement

The H-atoms were positioned geometrically (C–H = 0.93–0.96 Å) and refined as riding with $U_{iso}(H) = xU_{eq}(C)$, where x = 1.5 for methyl and x = 1.2 for other H-atoms.

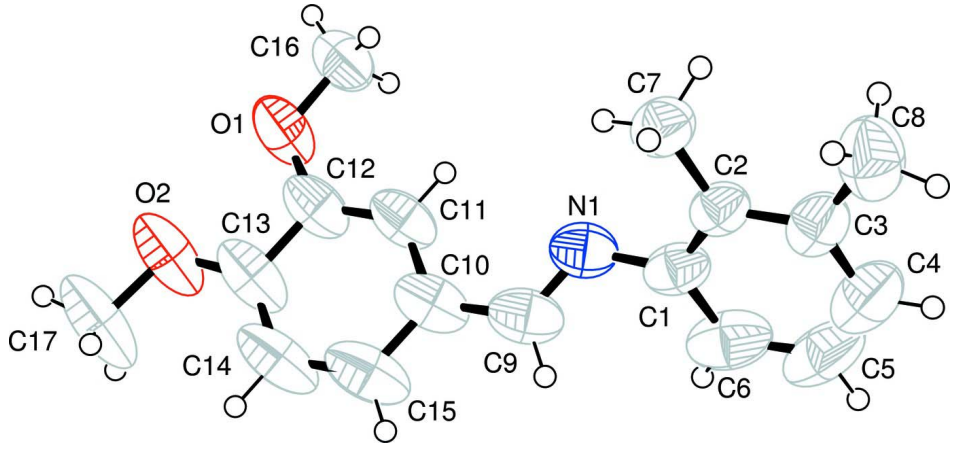

Figure 1

View of (I) with displacement ellipsoids drawn at the 50% probability level.

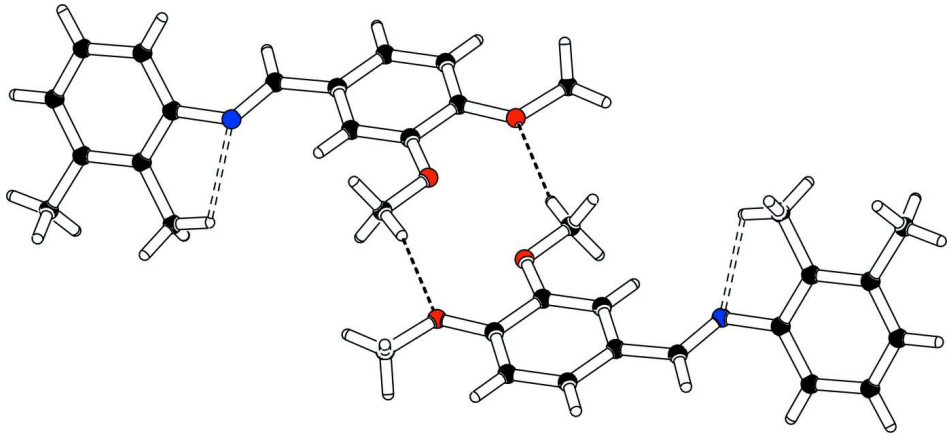

Figure 2

The partial packing of (I) showing that molecules form inversion dimers. The dotted lines represent the H-bondings.

N-[(*E*)-3,4-Dimethoxybenzylidene]-2,3-dimethylaniline

Crystal data

$C_{17}H_{19}NO_2$
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Hall symbol: -P 1
$a = 7.0144$ (4) Å
$b = 7.4488$ (4) Å
$c = 15.6202$ (8) Å
$\alpha = 81.987$ (2)°
$\beta = 81.009$ (3)°
$\gamma = 73.527$ (2)°
$V = 769.12$ (7) Å^3
$Z = 2$
$F(000) = 288$
$D_x = 1.163$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2028 reflections
$\theta = 2.7$–$28.4°$
$\mu = 0.08$ mm^{-1}
$T = 296$ K
Prism, colorless
0.34 × 0.25 × 0.22 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 7.50 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
$T_{min} = 0.972$, $T_{max} = 0.983$
8993 measured reflections
3688 independent reflections
2028 reflections with $I > 2\sigma(I)$
$R_{int} = 0.019$
$\theta_{max} = 28.4°$, $\theta_{min} = 2.7°$
$h = -9 \rightarrow 8$
$k = -9 \rightarrow 9$
$l = -20 \rightarrow 20$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.061$
$wR(F^2) = 0.211$
$S = 1.08$
3688 reflections
185 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
$w = 1/[\sigma^2(F_o^2) + (0.0973P)^2 + 0.0736P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.19$ e Å^{-3}
$\Delta\rho_{min} = -0.18$ e Å^{-3}

Special details

Geometry. Bond distances, angles *etc*. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

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 $F^2 > \sigma(F^2)$ 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.4243 (2)	1.3278 (2)	0.06049 (11)	0.1032 (6)
O2	0.0678 (3)	1.5334 (3)	0.09093 (12)	0.1237 (7)
N1	0.4479 (2)	0.7156 (3)	0.26807 (10)	0.0781 (6)
C1	0.4907 (3)	0.5385 (3)	0.31797 (12)	0.0724 (7)
C2	0.6399 (3)	0.4985 (2)	0.37272 (11)	0.0653 (6)
C3	0.6892 (3)	0.3227 (3)	0.42177 (13)	0.0801 (7)
C4	0.5942 (5)	0.1908 (3)	0.41376 (19)	0.1067 (10)
C5	0.4515 (5)	0.2251 (4)	0.3599 (2)	0.1191 (11)
C6	0.3959 (4)	0.4001 (4)	0.31104 (18)	0.1058 (10)
C7	0.7449 (3)	0.6439 (3)	0.38007 (15)	0.0814 (7)
C8	0.8467 (4)	0.2768 (3)	0.48259 (17)	0.1107 (10)
C9	0.2673 (3)	0.8109 (4)	0.26475 (13)	0.0873 (8)
C10	0.2098 (3)	0.9939 (4)	0.21549 (13)	0.0872 (8)
C11	0.3509 (3)	1.0665 (3)	0.15843 (12)	0.0804 (7)
C12	0.2991 (3)	1.2443 (3)	0.11668 (13)	0.0845 (7)
C13	0.1014 (3)	1.3574 (4)	0.13272 (14)	0.0982 (9)
C14	−0.0383 (3)	1.2866 (5)	0.18777 (16)	0.1098 (12)
C15	0.0153 (3)	1.1059 (5)	0.22878 (16)	0.1091 (12)
C16	0.6230 (3)	1.2208 (3)	0.03706 (18)	0.1017 (9)
C17	−0.1297 (4)	1.6586 (5)	0.1040 (2)	0.1511 (14)
H4	0.62832	0.07416	0.44610	0.1282*
H5	0.38993	0.13205	0.35542	0.1429*
H6	0.29718	0.42404	0.27438	0.1267*
H7A	0.71156	0.74586	0.33535	0.1221*
H7B	0.88706	0.58857	0.37339	0.1221*
H7C	0.70333	0.69060	0.43618	0.1221*
H8A	0.84583	0.15970	0.51705	0.1659*
H8B	0.81876	0.37504	0.52020	0.1659*
H8C	0.97589	0.26637	0.44934	0.1659*
H9	0.16648	0.76071	0.29555	0.1047*
H11	0.48208	0.99265	0.14874	0.0964*
H14	−0.16955	1.36030	0.19753	0.1317*
H15	−0.08069	1.05903	0.26580	0.1308*
H16A	0.69124	1.18297	0.08799	0.1523*
H16B	0.69194	1.29576	−0.00456	0.1523*
H16C	0.62060	1.11121	0.01184	0.1523*

H17A	−0.22229	1.60982	0.08122	0.2265*
H17B	−0.12956	1.78039	0.07430	0.2265*
H17C	−0.16937	1.66912	0.16514	0.2265*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0793 (9)	0.1041 (11)	0.0950 (11)	0.0173 (8)	−0.0053 (8)	0.0011 (8)
O2	0.0955 (11)	0.1343 (14)	0.0975 (12)	0.0434 (10)	−0.0131 (9)	−0.0186 (10)
N1	0.0689 (10)	0.1016 (12)	0.0657 (10)	−0.0269 (9)	−0.0016 (7)	−0.0135 (8)
C1	0.0726 (11)	0.0870 (13)	0.0648 (10)	−0.0362 (10)	0.0107 (9)	−0.0220 (9)
C2	0.0683 (10)	0.0677 (11)	0.0609 (10)	−0.0251 (8)	0.0103 (8)	−0.0157 (8)
C3	0.0919 (13)	0.0699 (12)	0.0725 (12)	−0.0256 (10)	0.0236 (10)	−0.0164 (9)
C4	0.133 (2)	0.0838 (15)	0.1044 (19)	−0.0482 (15)	0.0309 (16)	−0.0238 (13)
C5	0.144 (2)	0.1027 (19)	0.133 (2)	−0.0808 (18)	0.034 (2)	−0.0442 (18)
C6	0.1058 (17)	0.139 (2)	0.0977 (17)	−0.0668 (16)	0.0115 (13)	−0.0523 (16)
C7	0.0819 (12)	0.0803 (12)	0.0893 (14)	−0.0328 (10)	−0.0139 (10)	−0.0060 (10)
C8	0.124 (2)	0.0967 (16)	0.0917 (17)	−0.0090 (15)	−0.0065 (15)	0.0061 (13)
C9	0.0686 (12)	0.1318 (18)	0.0640 (12)	−0.0304 (12)	−0.0026 (9)	−0.0174 (12)
C10	0.0633 (11)	0.1337 (19)	0.0587 (11)	−0.0106 (11)	−0.0090 (9)	−0.0217 (12)
C11	0.0590 (10)	0.1120 (16)	0.0585 (10)	0.0010 (10)	−0.0108 (8)	−0.0156 (10)
C12	0.0670 (11)	0.1122 (16)	0.0570 (11)	0.0084 (11)	−0.0100 (9)	−0.0159 (10)
C13	0.0765 (13)	0.130 (2)	0.0626 (12)	0.0260 (13)	−0.0180 (10)	−0.0259 (12)
C14	0.0621 (12)	0.167 (3)	0.0755 (14)	0.0215 (14)	−0.0105 (11)	−0.0365 (15)
C15	0.0625 (12)	0.178 (3)	0.0730 (14)	−0.0054 (15)	−0.0046 (10)	−0.0264 (16)
C16	0.0696 (12)	0.0984 (16)	0.122 (2)	−0.0017 (11)	−0.0060 (12)	−0.0103 (14)
C17	0.114 (2)	0.163 (3)	0.118 (2)	0.0679 (19)	−0.0177 (17)	−0.035 (2)

Geometric parameters (Å, º)

O1—C12	1.358 (3)	C14—C15	1.383 (5)
O1—C16	1.416 (3)	C4—H4	0.9300
O2—C13	1.355 (3)	C5—H5	0.9300
O2—C17	1.436 (4)	C6—H6	0.9300
N1—C1	1.414 (3)	C7—H7A	0.9600
N1—C9	1.270 (3)	C7—H7B	0.9600
C1—C2	1.396 (3)	C7—H7C	0.9600
C1—C6	1.400 (4)	C8—H8A	0.9600
C2—C3	1.403 (3)	C8—H8B	0.9600
C2—C7	1.497 (3)	C8—H8C	0.9600
C3—C4	1.363 (4)	C9—H9	0.9300
C3—C8	1.504 (4)	C11—H11	0.9300
C4—C5	1.354 (5)	C14—H14	0.9300
C5—C6	1.400 (4)	C15—H15	0.9300
C9—C10	1.451 (4)	C16—H16A	0.9600
C10—C11	1.400 (3)	C16—H16B	0.9600
C10—C15	1.384 (4)	C16—H16C	0.9600
C11—C12	1.368 (3)	C17—H17A	0.9600

C12—C13	1.408 (3)	C17—H17B	0.9600
C13—C14	1.372 (3)	C17—H17C	0.9600
C12—O1—C16	118.63 (17)	C5—C6—H6	120.00
C13—O2—C17	118.4 (2)	C2—C7—H7A	109.00
C1—N1—C9	119.83 (19)	C2—C7—H7B	109.00
N1—C1—C2	118.28 (18)	C2—C7—H7C	109.00
N1—C1—C6	122.3 (2)	H7A—C7—H7B	109.00
C2—C1—C6	119.3 (2)	H7A—C7—H7C	109.00
C1—C2—C3	119.81 (18)	H7B—C7—H7C	109.00
C1—C2—C7	120.07 (16)	C3—C8—H8A	109.00
C3—C2—C7	120.11 (18)	C3—C8—H8B	109.00
C2—C3—C4	119.6 (2)	C3—C8—H8C	109.00
C2—C3—C8	121.02 (19)	H8A—C8—H8B	109.00
C4—C3—C8	119.4 (2)	H8A—C8—H8C	109.00
C3—C4—C5	121.7 (2)	H8B—C8—H8C	109.00
C4—C5—C6	120.3 (3)	N1—C9—H9	118.00
C1—C6—C5	119.3 (3)	C10—C9—H9	118.00
N1—C9—C10	123.5 (2)	C10—C11—H11	119.00
C9—C10—C11	121.3 (2)	C12—C11—H11	119.00
C9—C10—C15	120.1 (2)	C13—C14—H14	120.00
C11—C10—C15	118.5 (2)	C15—C14—H14	120.00
C10—C11—C12	121.1 (2)	C10—C15—H15	120.00
O1—C12—C11	125.7 (2)	C14—C15—H15	120.00
O1—C12—C13	114.90 (19)	O1—C16—H16A	109.00
C11—C12—C13	119.4 (2)	O1—C16—H16B	109.00
O2—C13—C12	114.7 (2)	O1—C16—H16C	109.00
O2—C13—C14	125.5 (3)	H16A—C16—H16B	109.00
C12—C13—C14	119.8 (3)	H16A—C16—H16C	109.00
C13—C14—C15	120.2 (3)	H16B—C16—H16C	109.00
C10—C15—C14	120.9 (2)	O2—C17—H17A	109.00
C3—C4—H4	119.00	O2—C17—H17B	109.00
C5—C4—H4	119.00	O2—C17—H17C	109.00
C4—C5—H5	120.00	H17A—C17—H17B	109.00
C6—C5—H5	120.00	H17A—C17—H17C	109.00
C1—C6—H6	120.00	H17B—C17—H17C	110.00
C16—O1—C12—C11	4.7 (3)	C8—C3—C4—C5	−180.0 (3)
C16—O1—C12—C13	−176.7 (2)	C3—C4—C5—C6	−0.6 (5)
C17—O2—C13—C12	−179.7 (2)	C4—C5—C6—C1	0.5 (4)
C17—O2—C13—C14	−0.3 (4)	N1—C9—C10—C11	8.8 (4)
C9—N1—C1—C2	−133.8 (2)	N1—C9—C10—C15	−166.8 (2)
C9—N1—C1—C6	49.3 (3)	C9—C10—C11—C12	−175.4 (2)
C1—N1—C9—C10	179.8 (2)	C15—C10—C11—C12	0.2 (3)
N1—C1—C2—C3	−178.66 (18)	C9—C10—C15—C14	174.7 (2)
N1—C1—C2—C7	2.3 (3)	C11—C10—C15—C14	−1.0 (4)
C6—C1—C2—C3	−1.7 (3)	C10—C11—C12—O1	179.8 (2)
C6—C1—C2—C7	179.2 (2)	C10—C11—C12—C13	1.2 (3)

N1—C1—C6—C5	177.5 (2)	O1—C12—C13—O2	−1.3 (3)
C2—C1—C6—C5	0.6 (4)	O1—C12—C13—C14	179.3 (2)
C1—C2—C3—C4	1.7 (3)	C11—C12—C13—O2	177.4 (2)
C1—C2—C3—C8	−178.9 (2)	C11—C12—C13—C14	−2.0 (3)
C7—C2—C3—C4	−179.3 (2)	O2—C13—C14—C15	−178.1 (2)
C7—C2—C3—C8	0.2 (3)	C12—C13—C14—C15	1.2 (4)
C2—C3—C4—C5	−0.5 (4)	C13—C14—C15—C10	0.3 (4)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C16—H16*B*···O2^{i}	0.96	2.51	3.454 (3)	167

Symmetry code: (i) −*x*+1, −*y*+3, −*z*.