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2-[(*E*)-(2,3-Dimethylphenyl)imino-methyl]phenol

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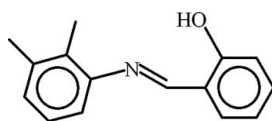
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Key indicators: single-crystal X-ray study; $T = 296$ K; mean $\sigma(\text{C}-\text{C}) = 0.009$ Å; R factor = 0.078; wR factor = 0.157; data-to-parameter ratio = 8.4.

In the title compound, $\text{C}_{15}\text{H}_{15}\text{NO}$, the almost planar 2,3-dimethylaniline unit and the salicylaldehyde group (r.m.s. deviations of 0.0156 and 0.0109 Å, respectively) are oriented at a dihedral angle of 43.69 (9)° with respect to each other. An $S(6)$ ring motif is formed due to intramolecular $\text{O}-\text{H}\cdots\text{N}$ hydrogen bonding. In the crystal, $\text{C}-\text{H}\cdots\pi$ interactions occur between the 2,3-dimethylaniline unit and the salicylaldehyde group, where the CH is from the *o*-methyl group.

Related literature

For background to Schiff bases synthesized from 2,3-dimethylaniline and for related structures, see: Tahir *et al.* (2010*a,b*); Tariq *et al.* (2010). For graph-set notation, see: Bernstein *et al.* (1995).



Experimental

Crystal data

$\text{C}_{15}\text{H}_{15}\text{NO}$	$V = 1244.0$ (2) Å ³
$M_r = 225.28$	$Z = 4$
Orthorhombic, $P2_12_12_1$	Mo $K\alpha$ radiation
$a = 7.5641$ (7) Å	$\mu = 0.08$ mm ⁻¹
$b = 12.5889$ (13) Å	$T = 296$ K
$c = 13.0643$ (14) Å	$0.32 \times 0.12 \times 0.10$ mm

Data collection

Bruker Kappa APEXII CCD diffractometer	9729 measured reflections
Absorption correction: multi-scan (SADABS; Bruker, 2005)	1316 independent reflections
$T_{\min} = 0.980$, $T_{\max} = 0.985$	687 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.085$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.078$	157 parameters
$wR(F^2) = 0.157$	H-atom parameters constrained
$S = 1.11$	$\Delta\rho_{\text{max}} = 0.11$ e Å ⁻³
1316 reflections	$\Delta\rho_{\text{min}} = -0.13$ e Å ⁻³

Table 1

Hydrogen-bond geometry (Å, °).

Cg1 is the centroid of the C1–C6 ring.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1–H1 \cdots N1	0.82	1.85	2.582 (6)	148
C7–H7A \cdots Cg1 ⁱ	0.96	2.92	3.782 (6)	150

 Symmetry code: (i) $-x + \frac{1}{2}, -y + 1, z - \frac{1}{2}$.

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, Vice Chancellor, University of Sargodha, Pakistan.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BQ2232).

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supporting information

Acta Cryst. (2010). E66, o2439 [https://doi.org/10.1107/S1600536810033398]

2-[(*E*)-(2,3-Dimethylphenyl)iminomethyl]phenol

M. Nawaz Tahir, Muhammad Ilyas Tariq, Shahbaz Ahmad, Muhammad Sarfraz and Riaz H. Tariq

S1. Comment

We have reported crystal structures of Schiff bases synthesized from 2,3-dimethylaniline (Tahir *et al.*, 2010*a*, 2010*b*), (Tariq *et al.*, 2010) and in continuation of this work, we report herein the structure and synthesis of the title compound (I, Fig. 1). The title compound has been synthesized for the preparation of different organometallic compounds.

In (I), the 2,3-dimethylaniline moiety A (C1–C8/N1) and the group B (C9–C15/O1) of salicylaldehyde are planar with r.m.s. deviations of 0.0156 and 0.0109 Å, respectively. The dihedral angle between A/B is 43.69 (9)°. The title molecule essentially consists of monomers. In the title molecule an S(6) ring motif (Bernstein *et al.*, 1995) is formed due to intramolecular H-bonding of O—H···N type (Table 1, Fig. 1). There exist C—H··· π interaction (Table 1) which plays important role in stabilizing the molecules.

S2. Experimental

Equimolar quantities of 2,3-dimethylaniline and salicylaldehyde were refluxed in methanol for 45 min. The resulting solution was kept at room temperature which afforded colorless needles of (I) after 72 h.

S3. Refinement

The H-atoms were positioned geometrically (O–H = 0.82, C–H = 0.93–0.96 Å) and refined as riding with $U_{\text{iso}}(\text{H}) = xU_{\text{eq}}(\text{C})$, where $x = 1.5$ for methyl and $x = 1.2$ for all other H-atoms. In the absence of significant anomalous scattering factor, Friedal pairs were merged.

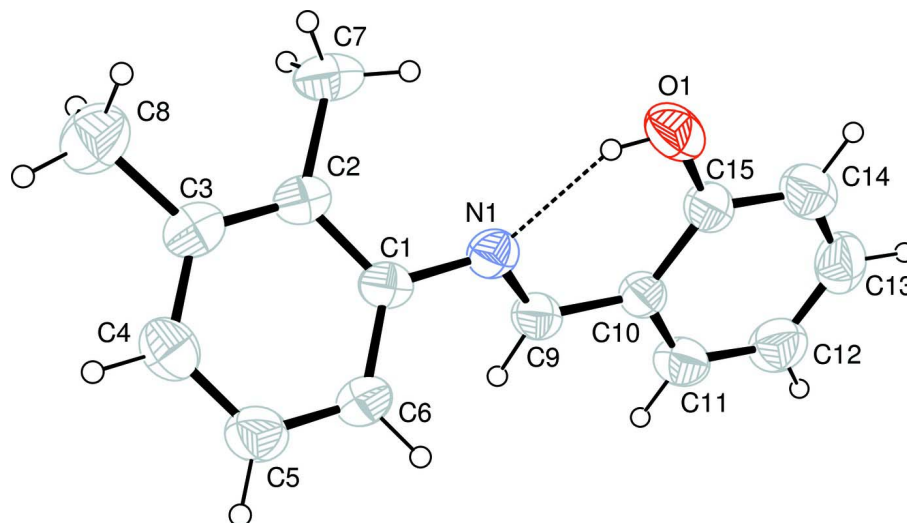


Figure 1

View of the title compound with the atom numbering scheme. The thermal ellipsoids are drawn at the 30% probability level. The dotted line represents the intramolecular H-bonding.

2-[(*E*)-(2,3-Dimethylphenyl)iminomethyl]phenol

Crystal data

$C_{15}H_{15}NO$

$M_r = 225.28$

Orthorhombic, $P2_12_12_1$

Hall symbol: P 2ac 2ab

$a = 7.5641$ (7) Å

$b = 12.5889$ (13) Å

$c = 13.0643$ (14) Å

$V = 1244.0$ (2) Å³

$Z = 4$

$F(000) = 480$

$D_x = 1.203$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 687 reflections

$\theta = 2.3$ – 25.2°

$\mu = 0.08$ mm⁻¹

$T = 296$ K

Needle, colorless

$0.32 \times 0.12 \times 0.10$ mm

Data collection

Bruker Kappa APEXII CCD

diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

Detector resolution: 8.1 pixels mm⁻¹

ω scans

Absorption correction: multi-scan

(*SADABS*; Bruker, 2005)

$T_{\min} = 0.980$, $T_{\max} = 0.985$

9729 measured reflections

1316 independent reflections

687 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.085$

$\theta_{\max} = 25.2^\circ$, $\theta_{\min} = 2.3^\circ$

$h = -9 \rightarrow 8$

$k = -15 \rightarrow 15$

$l = -15 \rightarrow 15$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.078$

$wR(F^2) = 0.157$

$S = 1.11$

1316 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

$$w = 1/[\sigma^2(F_o^2) + (0.0624P)^2]$$

where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$

$$\Delta\rho_{\max} = 0.11 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -0.13 \text{ e } \text{\AA}^{-3}$$

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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	-0.1515 (5)	0.5069 (3)	0.2310 (3)	0.0897 (19)
N1	-0.0156 (5)	0.3687 (4)	0.1080 (3)	0.0627 (17)
C1	0.0128 (6)	0.3279 (4)	0.0080 (4)	0.056 (2)
C2	0.0758 (6)	0.3945 (5)	-0.0690 (5)	0.059 (2)
C3	0.0952 (6)	0.3556 (5)	-0.1668 (4)	0.065 (2)
C4	0.0551 (7)	0.2503 (6)	-0.1881 (5)	0.077 (3)
C5	-0.0066 (7)	0.1849 (5)	-0.1113 (5)	0.083 (3)
C6	-0.0298 (7)	0.2231 (5)	-0.0142 (5)	0.072 (2)
C7	0.1219 (8)	0.5080 (4)	-0.0424 (5)	0.088 (3)
C8	0.1642 (9)	0.4236 (5)	-0.2532 (4)	0.106 (3)
C9	0.0214 (6)	0.3121 (4)	0.1866 (4)	0.064 (2)
C10	-0.0210 (7)	0.3453 (4)	0.2888 (4)	0.061 (2)
C11	0.0197 (8)	0.2804 (5)	0.3715 (4)	0.081 (2)
C12	-0.0244 (10)	0.3084 (6)	0.4696 (5)	0.095 (3)
C13	-0.1103 (10)	0.4022 (7)	0.4868 (6)	0.097 (3)
C14	-0.1526 (7)	0.4687 (5)	0.4063 (6)	0.088 (3)
C15	-0.1088 (7)	0.4403 (5)	0.3083 (5)	0.068 (3)
H1	-0.11767	0.48168	0.17655	0.1075*
H4	0.06981	0.22390	-0.25406	0.0926*
H5	-0.03254	0.11425	-0.12564	0.0997*
H6	-0.07406	0.17895	0.03678	0.0859*
H7A	0.24802	0.51622	-0.04157	0.1311*
H7B	0.07492	0.52507	0.02387	0.1311*
H7C	0.07187	0.55492	-0.09262	0.1311*
H8A	0.08868	0.48428	-0.26179	0.1586*
H8B	0.16581	0.38290	-0.31528	0.1586*
H8C	0.28187	0.44699	-0.23737	0.1586*
H9	0.07767	0.24716	0.17715	0.0767*
H11	0.07817	0.21654	0.36011	0.0969*
H12	0.00398	0.26397	0.52398	0.1147*
H13	-0.14067	0.42136	0.55328	0.1166*
H14	-0.21052	0.53261	0.41862	0.1054*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.084 (3)	0.075 (3)	0.110 (4)	0.023 (3)	0.003 (3)	-0.009 (3)
N1	0.049 (3)	0.061 (3)	0.078 (3)	-0.008 (2)	0.003 (3)	-0.001 (3)
C1	0.038 (3)	0.050 (4)	0.081 (4)	-0.001 (3)	-0.005 (3)	-0.001 (3)
C2	0.045 (3)	0.057 (4)	0.075 (4)	-0.002 (3)	-0.009 (3)	0.010 (4)
C3	0.052 (3)	0.071 (5)	0.073 (4)	0.001 (3)	-0.015 (3)	0.018 (4)
C4	0.071 (4)	0.083 (5)	0.077 (4)	0.005 (3)	-0.009 (3)	-0.015 (4)
C5	0.078 (4)	0.071 (5)	0.101 (5)	-0.011 (4)	0.004 (4)	-0.010 (4)
C6	0.071 (4)	0.063 (4)	0.081 (4)	-0.012 (3)	0.009 (3)	0.005 (3)
C7	0.084 (4)	0.057 (4)	0.122 (5)	-0.011 (4)	-0.007 (4)	0.015 (4)
C8	0.118 (6)	0.113 (6)	0.086 (5)	-0.006 (5)	-0.005 (4)	0.019 (4)
C9	0.049 (3)	0.056 (4)	0.087 (4)	0.001 (3)	0.005 (3)	-0.003 (4)
C10	0.055 (3)	0.057 (4)	0.071 (4)	-0.003 (3)	0.004 (3)	-0.005 (3)
C11	0.090 (4)	0.066 (4)	0.086 (4)	-0.004 (4)	-0.002 (4)	-0.007 (4)
C12	0.114 (6)	0.089 (6)	0.083 (5)	-0.024 (5)	0.003 (4)	-0.003 (4)
C13	0.084 (5)	0.112 (7)	0.096 (5)	-0.030 (5)	0.019 (4)	-0.031 (5)
C14	0.067 (4)	0.078 (5)	0.118 (6)	-0.001 (3)	0.003 (4)	-0.018 (5)
C15	0.054 (3)	0.065 (5)	0.085 (5)	-0.003 (3)	0.005 (3)	-0.006 (4)

Geometric parameters (\AA , $^\circ$)

O1—C15	1.352 (7)	C13—C14	1.382 (11)
O1—H1	0.8200	C14—C15	1.370 (10)
N1—C1	1.420 (7)	C4—H4	0.9300
N1—C9	1.281 (7)	C5—H5	0.9300
C1—C6	1.389 (8)	C6—H6	0.9300
C1—C2	1.394 (8)	C7—H7A	0.9600
C2—C7	1.511 (8)	C7—H7B	0.9600
C2—C3	1.376 (8)	C7—H7C	0.9600
C3—C4	1.388 (10)	C8—H8A	0.9600
C3—C8	1.510 (8)	C8—H8B	0.9600
C4—C5	1.379 (9)	C8—H8C	0.9600
C5—C6	1.368 (9)	C9—H9	0.9300
C9—C10	1.435 (7)	C11—H11	0.9300
C10—C15	1.392 (8)	C12—H12	0.9300
C10—C11	1.389 (8)	C13—H13	0.9300
C11—C12	1.370 (9)	C14—H14	0.9300
C12—C13	1.366 (11)		
O1 \cdots N1	2.582 (6)	H1 \cdots H7B	2.5300
O1 \cdots H8C ⁱ	2.8900	H4 \cdots H8B	2.2700
N1 \cdots O1	2.582 (6)	H5 \cdots C8 ^v	3.0400
N1 \cdots H1	1.8500	H5 \cdots H8A ^v	2.2400
N1 \cdots H7B	2.3600	H6 \cdots C9	2.6800
C1 \cdots C6 ⁱⁱ	3.520 (7)	H6 \cdots H9	2.3300
C2 \cdots C6 ⁱⁱ	3.503 (8)	H6 \cdots C2 ⁱⁱⁱ	2.8400

C6...C2 ⁱⁱⁱ	3.503 (8)	H6...C3 ⁱⁱⁱ	3.0600
C6...C1 ⁱⁱⁱ	3.520 (7)	H7A...C8	3.0700
C1...H1	3.0900	H7A...C12 ^{vii}	3.0400
C2...H6 ⁱⁱ	2.8400	H7A...C13 ^{vii}	2.9500
C2...H14 ^{iv}	2.9200	H7B...N1	2.3600
C3...H6 ⁱⁱ	3.0600	H7B...H1	2.5300
C5...H8A ^v	3.0800	H7C...C8	2.7600
C6...H9	2.6500	H7C...H8A	2.3900
C7...H8A	2.8900	H8A...C7	2.8900
C7...H8C	2.9200	H8A...H7C	2.3900
C8...H7A	3.0700	H8A...C5 ^{vi}	3.0800
C8...H7C	2.7600	H8A...H5 ^{vi}	2.2400
C8...H5 ^{vi}	3.0400	H8B...H4	2.2700
C9...H1	2.3800	H8C...C7	2.9200
C9...H6	2.6800	H8C...O1 ^{vii}	2.8900
C12...H7A ⁱ	3.0400	H8C...C15 ^{vii}	2.9100
C13...H7A ⁱ	2.9500	H9...C6	2.6500
C15...H8C ⁱ	2.9100	H9...H6	2.3300
H1...N1	1.8500	H9...H11	2.4200
H1...C1	3.0900	H11...H9	2.4200
H1...C9	2.3800	H14...C2 ^{viii}	2.9200
C15—O1—H1	109.00	C4—C5—H5	120.00
C1—N1—C9	120.2 (5)	C6—C5—H5	120.00
N1—C1—C2	119.9 (5)	C1—C6—H6	120.00
C2—C1—C6	120.0 (5)	C5—C6—H6	120.00
N1—C1—C6	120.0 (5)	C2—C7—H7A	110.00
C1—C2—C3	119.5 (6)	C2—C7—H7B	109.00
C1—C2—C7	118.8 (5)	C2—C7—H7C	109.00
C3—C2—C7	121.7 (6)	H7A—C7—H7B	109.00
C2—C3—C4	120.2 (5)	H7A—C7—H7C	109.00
C2—C3—C8	122.0 (5)	H7B—C7—H7C	109.00
C4—C3—C8	117.9 (5)	C3—C8—H8A	109.00
C3—C4—C5	119.9 (6)	C3—C8—H8B	109.00
C4—C5—C6	120.5 (6)	C3—C8—H8C	109.00
C1—C6—C5	119.9 (6)	H8A—C8—H8B	109.00
N1—C9—C10	122.3 (5)	H8A—C8—H8C	109.00
C9—C10—C15	121.8 (5)	H8B—C8—H8C	110.00
C11—C10—C15	118.0 (5)	N1—C9—H9	119.00
C9—C10—C11	120.2 (5)	C10—C9—H9	119.00
C10—C11—C12	121.5 (6)	C10—C11—H11	119.00
C11—C12—C13	119.5 (7)	C12—C11—H11	119.00
C12—C13—C14	120.6 (7)	C11—C12—H12	120.00
C13—C14—C15	119.8 (6)	C13—C12—H12	120.00
O1—C15—C14	118.6 (5)	C12—C13—H13	120.00
C10—C15—C14	120.7 (6)	C14—C13—H13	120.00
O1—C15—C10	120.7 (5)	C13—C14—H14	120.00
C3—C4—H4	120.00	C15—C14—H14	120.00

C5—C4—H4	120.00		
C9—N1—C1—C2	-141.7 (5)	C3—C4—C5—C6	0.4 (8)
C9—N1—C1—C6	41.3 (7)	C4—C5—C6—C1	-1.5 (8)
C1—N1—C9—C10	-173.7 (4)	N1—C9—C10—C11	179.1 (5)
N1—C1—C2—C7	3.3 (7)	N1—C9—C10—C15	1.5 (8)
C6—C1—C2—C3	0.0 (7)	C9—C10—C11—C12	-177.8 (6)
C6—C1—C2—C7	-179.7 (5)	C15—C10—C11—C12	-0.1 (9)
N1—C1—C6—C5	178.3 (5)	C9—C10—C15—O1	-2.5 (8)
C2—C1—C6—C5	1.2 (8)	C9—C10—C15—C14	178.0 (5)
N1—C1—C2—C3	-177.0 (4)	C11—C10—C15—O1	179.8 (5)
C1—C2—C3—C4	-1.1 (7)	C11—C10—C15—C14	0.3 (8)
C7—C2—C3—C4	178.7 (5)	C10—C11—C12—C13	0.0 (10)
C7—C2—C3—C8	0.2 (8)	C11—C12—C13—C14	-0.1 (11)
C1—C2—C3—C8	-179.5 (5)	C12—C13—C14—C15	0.3 (10)
C2—C3—C4—C5	0.9 (8)	C13—C14—C15—O1	-179.9 (6)
C8—C3—C4—C5	179.3 (5)	C13—C14—C15—C10	-0.4 (9)

Symmetry codes: (i) $-x+1/2, -y+1, z+1/2$; (ii) $x+1/2, -y+1/2, -z$; (iii) $x-1/2, -y+1/2, -z$; (iv) $-x-1/2, -y+1, z-1/2$; (v) $-x, y-1/2, -z-1/2$; (vi) $-x, y+1/2, -z-1/2$; (vii) $-x+1/2, -y+1, z-1/2$; (viii) $-x-1/2, -y+1, z+1/2$.

Hydrogen-bond geometry ($\text{\AA}, ^\circ$)

Cg1 is the centroid of the C1—C6 ring.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1—H1 \cdots N1	0.82	1.85	2.582 (6)	148
C7—H7A \cdots Cg1 ^{vii}	0.96	2.92	3.782 (6)	150

Symmetry code: (vii) $-x+1/2, -y+1, z-1/2$.