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## Structure Reports

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## 2,3-Dimethyl-*N*-[(*E*)-4-nitrobenzylidene]-aniline

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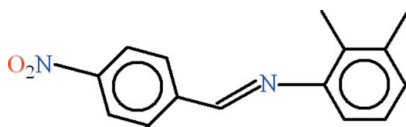
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 Key indicators: single-crystal X-ray study;  $T = 296$  K; mean  $\sigma(\text{C}-\text{C}) = 0.003$  Å;  $R$  factor = 0.047;  $wR$  factor = 0.111; data-to-parameter ratio = 11.0.

In the title compound,  $\text{C}_{15}\text{H}_{14}\text{N}_2\text{O}_2$ , the aromatic rings are oriented at a dihedral angle of  $24.52(5)^\circ$ . The dihedral angle between the nitro group and its parent benzene ring is  $9.22(16)^\circ$ . In the crystal, molecules interact through aromatic  $\pi-\pi$  stacking interactions [centroid-centroid separations =  $3.8158(14)$  and  $3.9139(14)$  Å].

### Related literature

 For structural systematics of related compounds, see: Harada *et al.* (2004).


### Experimental

#### Crystal data

 $\text{C}_{15}\text{H}_{14}\text{N}_2\text{O}_2$ 
 $M_r = 254.28$ 

 Orthorhombic,  $P2_12_12_1$ 
 $a = 7.1969(5)$  Å

 $b = 11.8023(7)$  Å

 $c = 15.3721(8)$  Å

 $V = 1305.71(14)$  Å<sup>3</sup>
 $Z = 4$ 

 Mo  $K\alpha$  radiation

 $\mu = 0.09$  mm<sup>-1</sup>
 $T = 296$  K

 $0.32 \times 0.14 \times 0.14$  mm

#### Data collection

Bruker Kappa APEXII CCD diffractometer

Absorption correction: multi-scan (SADABS; Bruker, 2005)

 $T_{\min} = 0.986$ ,  $T_{\max} = 0.987$ 

13172 measured reflections

1917 independent reflections

 1253 reflections with  $I > 2\sigma(I)$ 
 $R_{\text{int}} = 0.057$ 

#### Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.047$ 
 $wR(F^2) = 0.111$ 
 $S = 1.02$ 

1917 reflections

174 parameters

H-atom parameters constrained

 $\Delta\rho_{\text{max}} = 0.12$  e Å<sup>-3</sup>
 $\Delta\rho_{\text{min}} = -0.14$  e Å<sup>-3</sup>

Data collection: APEX2 (Bruker, 2007); cell refinement: SAINT (Bruker, 2007); 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 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: HB5464).

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## supporting information

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**2,3-Dimethyl-*N*-[(*E*)-4-nitrobenzylidene]aniline**

**Muhammad Ilyas Tariq, Shahbaz Ahmad, M. Nawaz Tahir, Muhammad Sarfaraz and Ishtiaq Hussain**

**S1. Comment**

Torsional, vibration and central bond length of *N*-benzylideneanilines (Harada *et al.*, 2004) has been studied for seven compounds at different temperatures. The title compound (I, Fig. 1) is another example due to change of substitutions at both phenyl rings for which the same study can be undertaken. The title compound has been prepared for derivatization.

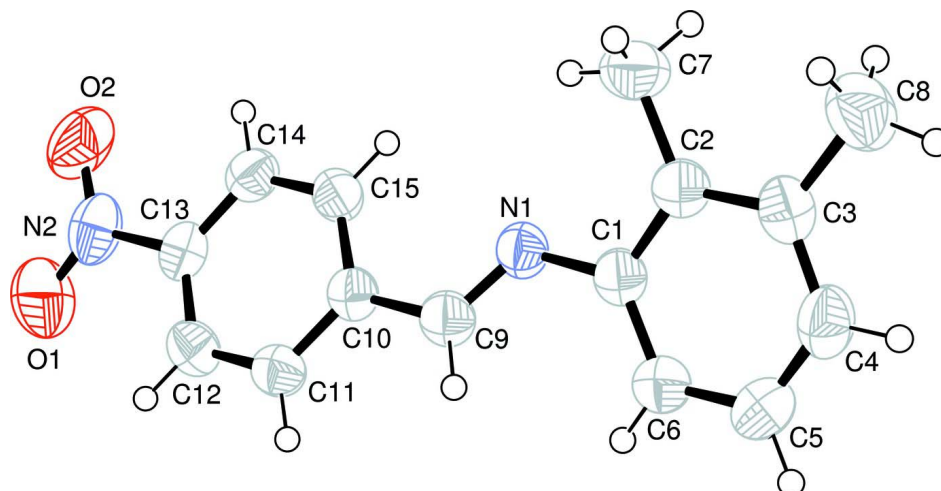
The molecules of (I) are essentially monomeric having no intra or inter-molecular H-bondings. The phenyl rings A (C1—C6) and B (C10—C15) are planar with r. m. s. deviation of 0.0065 and 0.0022 Å respectively. The dihedral angle between A/B is 24.52 (5)°. The nitro group C (O1/N2/O2) is oriented at 9.22 (16)° with the parent phenyl ring. It is to be noted that the nitro substituted phenyl ring B has smaller bond lengths [1.365 (3)–1.387 (3) Å], whereas the 2,3-dimethyl substituted ring has longer bond lengths 1.373 (3)–1.401 (3) Å. The value of C=N bond length at room temperature for (I) is 1.262 (3) Å which is in compatible with the studies of Harada *et al.*, 2004. The molecules are stabilized due to  $\pi$ – $\pi$  interactions between the centroids of phenyl rings with separation of 3.8158 (14) and 3.9139 (14) Å.

**S2. Experimental**

Equimolar quantities of 2,3-dimethylaniline and 4-nitro benzaldehyde were refluxed in methanol for 15 minutes resulting in yellow color precipitates. The contents of the flask were dried at room temperature and washed with methanol and ethanol, respectively. The washed crude material afforded yellow needles of (I) in the solution of diethyl ether at room temperature by slow evaporation after 24 h.

**S3. Refinement**

In the absence of anomalous scattering, all Friedal pairs were merged. Although all H-atoms were appeared in Fourier difference map but positioned geometrically (C–H = 0.93–0.96 Å) and refined as riding with  $U_{\text{iso}}(\text{H}) = xU_{\text{eq}}(\text{C})$ , where  $x = 1.2$  for aryl C–H and  $x = 1.5$  methyl H-atoms.

**Figure 1**

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

### 2,3-Dimethyl-*N*-[(*E*)-4-nitrobenzylidene]aniline

#### Crystal data

$C_{15}H_{14}N_2O_2$   
 $M_r = 254.28$   
 Orthorhombic,  $P2_12_12_1$   
 Hall symbol:  $P\ 2ac\ 2ab$   
 $a = 7.1969\ (5)\ \text{\AA}$   
 $b = 11.8023\ (7)\ \text{\AA}$   
 $c = 15.3721\ (8)\ \text{\AA}$   
 $V = 1305.71\ (14)\ \text{\AA}^3$   
 $Z = 4$

$F(000) = 536$   
 $D_x = 1.294\ \text{Mg m}^{-3}$   
 Mo  $K\alpha$  radiation,  $\lambda = 0.71073\ \text{\AA}$   
 Cell parameters from 1334 reflections  
 $\theta = 2.1\text{--}25.4^\circ$   
 $\mu = 0.09\ \text{mm}^{-1}$   
 $T = 296\ \text{K}$   
 Needle, yellow  
 $0.32 \times 0.14 \times 0.14\ \text{mm}$

#### Data collection

Bruker Kappa APEXII CCD  
 diffractometer  
 Radiation source: fine-focus sealed tube  
 Graphite monochromator  
 Detector resolution:  $7.40\ \text{pixels mm}^{-1}$   
 $\omega$  scans  
 Absorption correction: multi-scan  
 (*SADABS*; Bruker, 2005)  
 $T_{\min} = 0.986$ ,  $T_{\max} = 0.987$

13172 measured reflections  
 1917 independent reflections  
 1253 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.057$   
 $\theta_{\max} = 28.6^\circ$ ,  $\theta_{\min} = 2.2^\circ$   
 $h = -8 \rightarrow 9$   
 $k = -15 \rightarrow 15$   
 $l = -20 \rightarrow 20$

#### Refinement

Refinement on  $F^2$   
 Least-squares matrix: full  
 $R[F^2 > 2\sigma(F^2)] = 0.047$   
 $wR(F^2) = 0.111$   
 $S = 1.02$   
 1917 reflections  
 174 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  
 $w = 1/[\sigma^2(F_o^2) + (0.0482P)^2 + 0.0883P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} < 0.001$   
 $\Delta\rho_{\max} = 0.12\ \text{e \AA}^{-3}$   
 $\Delta\rho_{\min} = -0.14\ \text{e \AA}^{-3}$

*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 ( $\text{\AA}^2$ )*

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	0.1409 (4)	−0.19301 (18)	0.70198 (14)	0.0997 (9)
O2	0.1083 (4)	−0.06237 (19)	0.79842 (12)	0.0941 (9)
N1	0.1128 (3)	0.34130 (16)	0.47092 (11)	0.0485 (7)
N2	0.1253 (3)	−0.0943 (2)	0.72311 (16)	0.0684 (9)
C1	0.1231 (3)	0.42218 (18)	0.40278 (13)	0.0457 (7)
C2	0.1509 (3)	0.5351 (2)	0.42653 (14)	0.0488 (8)
C3	0.1581 (4)	0.61833 (19)	0.36160 (15)	0.0549 (8)
C4	0.1353 (4)	0.5864 (2)	0.27595 (17)	0.0624 (10)
C5	0.1052 (4)	0.4755 (2)	0.25272 (16)	0.0650 (10)
C6	0.0972 (4)	0.3935 (2)	0.31593 (14)	0.0550 (8)
C7	0.1768 (4)	0.5654 (2)	0.52133 (14)	0.0679 (10)
C8	0.1878 (5)	0.7409 (2)	0.38401 (19)	0.0820 (13)
C9	0.1573 (4)	0.23940 (19)	0.45751 (14)	0.0495 (8)
C10	0.1434 (3)	0.15342 (18)	0.52625 (14)	0.0448 (7)
C11	0.1832 (3)	0.04156 (19)	0.50760 (15)	0.0525 (8)
C12	0.1753 (4)	−0.0397 (2)	0.57139 (15)	0.0551 (9)
C13	0.1287 (3)	−0.0075 (2)	0.65402 (14)	0.0500 (8)
C14	0.0878 (3)	0.1021 (2)	0.67504 (15)	0.0523 (8)
C15	0.0953 (3)	0.18289 (19)	0.61064 (14)	0.0496 (8)
H4	0.14039	0.64145	0.23274	0.0748*
H5	0.09027	0.45617	0.19450	0.0779*
H6	0.07448	0.31854	0.30059	0.0659*
H7A	0.09112	0.62429	0.53696	0.1016*
H7B	0.30167	0.59128	0.53059	0.1016*
H7C	0.15399	0.49972	0.55663	0.1016*
H8A	0.18433	0.78558	0.33184	0.1229*
H8B	0.30655	0.74981	0.41166	0.1229*
H8C	0.09161	0.76571	0.42285	0.1229*
H9	0.20007	0.21822	0.40278	0.0594*
H11	0.21572	0.02105	0.45120	0.0630*
H12	0.20116	−0.11509	0.55867	0.0661*
H14	0.05543	0.12165	0.73165	0.0627*
H15	0.06802	0.25797	0.62382	0.0596*

*Atomic displacement parameters (Å<sup>2</sup>)*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
O1	0.131 (2)	0.0586 (12)	0.1094 (16)	0.0005 (15)	0.0004 (17)	0.0307 (12)
O2	0.1205 (19)	0.1055 (16)	0.0563 (11)	-0.0025 (15)	-0.0044 (13)	0.0275 (12)
N1	0.0509 (12)	0.0484 (11)	0.0463 (11)	0.0052 (10)	0.0029 (10)	0.0042 (9)
N2	0.0614 (15)	0.0707 (16)	0.0731 (16)	-0.0068 (14)	-0.0072 (13)	0.0266 (13)
C1	0.0431 (14)	0.0477 (12)	0.0463 (12)	0.0035 (11)	0.0067 (11)	0.0043 (10)
C2	0.0454 (15)	0.0529 (13)	0.0482 (12)	0.0020 (12)	0.0069 (11)	0.0015 (11)
C3	0.0515 (16)	0.0504 (13)	0.0628 (15)	0.0051 (12)	0.0070 (12)	0.0082 (11)
C4	0.0660 (19)	0.0615 (16)	0.0596 (16)	0.0045 (15)	0.0068 (14)	0.0193 (13)
C5	0.079 (2)	0.0708 (17)	0.0453 (12)	0.0029 (16)	0.0008 (14)	0.0040 (12)
C6	0.0614 (16)	0.0526 (14)	0.0509 (14)	0.0027 (13)	0.0009 (13)	-0.0010 (12)
C7	0.081 (2)	0.0651 (16)	0.0577 (14)	-0.0020 (16)	0.0041 (14)	-0.0097 (13)
C8	0.105 (3)	0.0539 (15)	0.087 (2)	-0.0044 (18)	0.009 (2)	0.0079 (15)
C9	0.0467 (15)	0.0539 (13)	0.0479 (12)	0.0039 (12)	0.0081 (12)	0.0010 (11)
C10	0.0406 (13)	0.0467 (12)	0.0471 (13)	0.0009 (11)	0.0030 (11)	0.0026 (10)
C11	0.0578 (16)	0.0514 (13)	0.0483 (12)	0.0057 (12)	0.0043 (11)	-0.0031 (11)
C12	0.0608 (17)	0.0424 (12)	0.0621 (15)	0.0015 (12)	0.0011 (13)	0.0007 (11)
C13	0.0436 (14)	0.0550 (14)	0.0515 (12)	-0.0029 (12)	-0.0050 (12)	0.0116 (11)
C14	0.0521 (15)	0.0601 (16)	0.0447 (12)	0.0018 (13)	-0.0007 (11)	0.0014 (12)
C15	0.0521 (15)	0.0456 (12)	0.0512 (13)	0.0046 (12)	0.0015 (12)	0.0005 (11)

*Geometric parameters (Å, °)*

O1—N2	1.215 (3)	C12—C13	1.368 (3)
O2—N2	1.224 (3)	C13—C14	1.365 (3)
N1—C1	1.419 (3)	C14—C15	1.376 (3)
N1—C9	1.262 (3)	C4—H4	0.9300
N2—C13	1.476 (3)	C5—H5	0.9300
C1—C2	1.396 (3)	C6—H6	0.9300
C1—C6	1.390 (3)	C7—H7A	0.9600
C2—C3	1.401 (3)	C7—H7B	0.9600
C2—C7	1.512 (3)	C7—H7C	0.9600
C3—C4	1.379 (3)	C8—H8A	0.9600
C3—C8	1.502 (3)	C8—H8B	0.9600
C4—C5	1.374 (3)	C8—H8C	0.9600
C5—C6	1.373 (3)	C9—H9	0.9300
C9—C10	1.468 (3)	C11—H11	0.9300
C10—C11	1.381 (3)	C12—H12	0.9300
C10—C15	1.387 (3)	C14—H14	0.9300
C11—C12	1.373 (3)	C15—H15	0.9300
C1—N1—C9	120.49 (18)	C5—C4—H4	119.00
O1—N2—O2	123.9 (2)	C4—C5—H5	120.00
O1—N2—C13	118.2 (2)	C6—C5—H5	120.00
O2—N2—C13	118.0 (2)	C1—C6—H6	120.00
N1—C1—C2	117.16 (18)	C5—C6—H6	120.00

N1—C1—C6	122.56 (19)	C2—C7—H7A	109.00
C2—C1—C6	120.2 (2)	C2—C7—H7B	109.00
C1—C2—C3	119.2 (2)	C2—C7—H7C	109.00
C1—C2—C7	119.7 (2)	H7A—C7—H7B	110.00
C3—C2—C7	121.1 (2)	H7A—C7—H7C	109.00
C2—C3—C4	118.9 (2)	H7B—C7—H7C	109.00
C2—C3—C8	121.1 (2)	C3—C8—H8A	109.00
C4—C3—C8	119.9 (2)	C3—C8—H8B	109.00
C3—C4—C5	121.8 (2)	C3—C8—H8C	109.00
C4—C5—C6	119.6 (2)	H8A—C8—H8B	109.00
C1—C6—C5	120.2 (2)	H8A—C8—H8C	109.00
N1—C9—C10	121.6 (2)	H8B—C8—H8C	109.00
C9—C10—C11	119.8 (2)	N1—C9—H9	119.00
C9—C10—C15	121.1 (2)	C10—C9—H9	119.00
C11—C10—C15	119.1 (2)	C10—C11—H11	120.00
C10—C11—C12	120.7 (2)	C12—C11—H11	120.00
C11—C12—C13	118.7 (2)	C11—C12—H12	121.00
N2—C13—C12	118.7 (2)	C13—C12—H12	121.00
N2—C13—C14	118.9 (2)	C13—C14—H14	121.00
C12—C13—C14	122.4 (2)	C15—C14—H14	121.00
C13—C14—C15	118.6 (2)	C10—C15—H15	120.00
C10—C15—C14	120.6 (2)	C14—C15—H15	120.00
C3—C4—H4	119.00		
C9—N1—C1—C2	-153.3 (2)	C2—C3—C4—C5	0.2 (4)
C9—N1—C1—C6	30.1 (4)	C8—C3—C4—C5	-179.1 (3)
C1—N1—C9—C10	-178.4 (2)	C3—C4—C5—C6	0.1 (4)
O1—N2—C13—C12	-9.2 (3)	C4—C5—C6—C1	-1.3 (4)
O1—N2—C13—C14	171.7 (2)	N1—C9—C10—C11	176.3 (2)
O2—N2—C13—C12	170.3 (3)	N1—C9—C10—C15	-5.4 (4)
O2—N2—C13—C14	-8.8 (3)	C9—C10—C11—C12	178.5 (2)
N1—C1—C2—C3	-178.7 (2)	C15—C10—C11—C12	0.1 (3)
N1—C1—C2—C7	2.6 (3)	C9—C10—C15—C14	-178.2 (2)
C6—C1—C2—C3	-2.0 (3)	C11—C10—C15—C14	0.2 (3)
C6—C1—C2—C7	179.3 (2)	C10—C11—C12—C13	-0.5 (4)
N1—C1—C6—C5	178.8 (2)	C11—C12—C13—N2	-178.3 (2)
C2—C1—C6—C5	2.3 (4)	C11—C12—C13—C14	0.8 (4)
C1—C2—C3—C4	0.8 (4)	N2—C13—C14—C15	178.6 (2)
C1—C2—C3—C8	-180.0 (3)	C12—C13—C14—C15	-0.5 (3)
C7—C2—C3—C4	179.4 (2)	C13—C14—C15—C10	0.0 (3)
C7—C2—C3—C8	-1.3 (4)		