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Crystal structure of 4-chloro-2-{(*E*)-[(3,4-dimethylphenyl)imino]methyl}phenol

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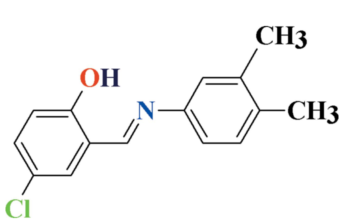
In the title compound, $C_{15}H_{14}ClNO$, which is isostructural with its bromo analogue [Tahir *et al.* (2012). *Acta Cryst.*, E**68**, o2730], the dihedral angle between the planes of the aromatic rings is 2.71 (7)° and an intramolecular O—H···N hydrogen bond closes an *S*(6) ring. In the crystal, extremely weak C—H···π interactions link the molecules into a three-dimensional network.

Keywords: crystal structure; phenol; intramolecular hydrogen bonding; C—H···π interactions.

CCDC reference: 1401503

1. Related literature

For related structures, see: Demircioğlu *et al.* (2014); Jin *et al.* (2012); Sun *et al.* (2013); Tahir *et al.* (2012).



2. Experimental

2.1. Crystal data

$C_{15}H_{14}ClNO$
M_r = 259.72
Monoclinic, $P2_1/n$
a = 12.1875 (10) Å
b = 7.4438 (5) Å
c = 14.3141 (12) Å
β = 101.549 (4)°
V = 1272.30 (17) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.29 mm^{-1}
T = 296 K
0.25 × 0.20 × 0.14 mm

2.2. Data collection

Bruker Kappa APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2007)
T_{min} = 0.933, T_{max} = 0.968
10293 measured reflections
2785 independent reflections
1871 reflections with $I > 2\sigma(I)$
R_{int} = 0.024

2.3. Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.116
S = 1.04
2785 reflections
166 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}

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

*Cg*1 and *Cg*2 are the centroids of the C1–C6 and C8–C13 benzene rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N1	0.82	1.87	2.5998 (19)	149
C3—H3···*Cg*1^{i}	0.93	2.98	3.732 (2)	139
C6—H6···*Cg*2^{ii}	0.93	2.93	3.576 (2)	128
C14—H14*B*···*Cg*2^{iii}	0.96	2.96	3.656 (2)	131

Symmetry codes: (i) $-x+\frac{1}{2}, y-\frac{1}{2}, -z+\frac{3}{2}$; (ii) $x+\frac{1}{2}, -y+\frac{3}{2}, z+\frac{1}{2}$; (iii) $-x+\frac{1}{2}, y+\frac{1}{2}, -z+\frac{1}{2}$.

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: *SHELXL2014* (Sheldrick, 2015); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012) and *PLATON* (Spek, 2009); software used to prepare material for publication: *WinGX* (Farrugia, 2012) and *PLATON*.

Acknowledgements

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.

Supporting information for this paper is available from the IUCr electronic archives (Reference: HB7424).

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supporting information

Acta Cryst. (2015). E**71**, o416 [doi:10.1107/S2056989015009354]

Crystal structure of 4-chloro-2-{(*E*)-[(3,4-dimethylphenyl)imino]methyl}phenol

Muhammad Salim, Muhammad Nawaz Tahir, Munawar Ali Munawar, Muhammad Shahid and Hazoor Ahmad Shad

S1. Comment

The title compound, (I, Fig. 1) has been synthesized in continuation of forming different derivatives of 3,4-dimethyl-aniline. (I) will also be utilized for synthesizing different metal complexes.

The crystal structures of 4-bromo-2-((*E*)-[(3,4-dimethylphenyl)imino]methyl)phenol (Tahir *et al.*, 2012), 2-((3,4-di-methylphenyl)carbonoimidoyl)-3-methoxyphenol (Demircioğlu *et al.*, 2014), *N*-[(*E*)-4-bromobenzylidene]-3,4-dimethyl-aniline (Sun *et al.*, 2013) and *N*-[(*E*)-4-fluorobenzylidene]-3,4-dimethylaniline (Jin *et al.*, 2012) have been published which are related to the title compound.

The title compound is isostructural to 4-bromo-2-((*E*)-[(3,4-dimethyl phenyl)imino]methyl)phenol (Tahir *et al.*, 2012) and is almost planar with r. m. s. deviation of 0.0325 Å, with maximum deviation of 0.0803 (9) Å for Cl1 atom from the mean square plane. There exist intramolecular H-bonding of O—H···N type (Table 1, Fig. 1) with *S*(6) ring motif. There exist C—H···π interactions (Table 1).

S2. Experimental

Equimolar quantities of 5-chlorosalicylaldehyde and 3,4-dimethylaniline were refluxed in methanol for 3 h. The solution was kept at room temperature for crystallization which affoarded light yellow plates after 72 h.

S3. Refinement

The H atoms were positioned geometrically (C–H = 0.93–0.96 Å, O—H= 0.82 Å) and refined as riding with U_{iso}(H) = xU_{eq}(C, O), where x = 1.5 for methyl & hydroxy and x = 1.2 for other H-atoms.

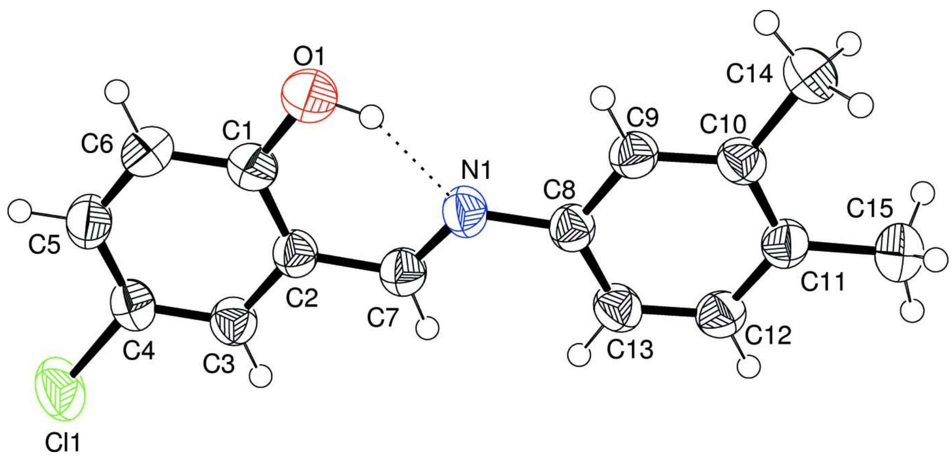

Figure 1

View of the title compound with displacement ellipsoids drawn at the 50% probability level. The dotted line shows intramolecular H-bonding.

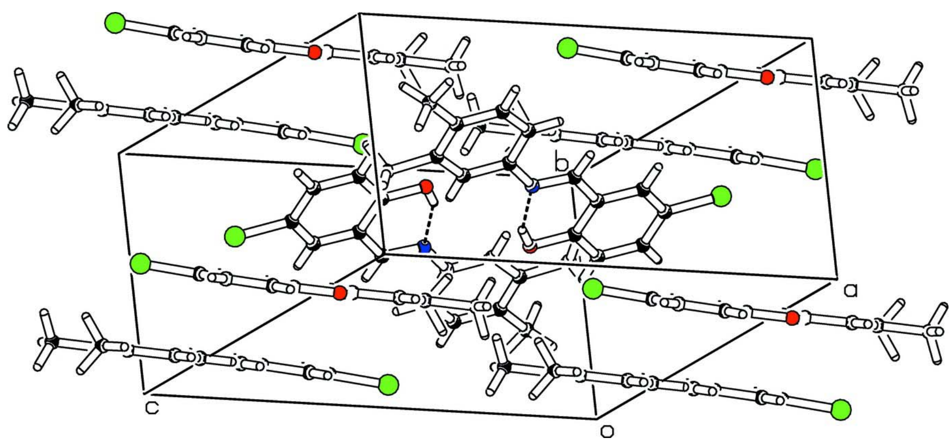

Figure 2

Packing diagram for the title compound.

4-Chloro-2-{(*E*)-[(3,4-dimethylphenyl)imino]methyl}phenol

Crystal data

$C_{15}H_{14}ClNO$
$M_r = 259.72$
Monoclinic, $P2_1/n$
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$b = 7.4438$ (5) Å
$c = 14.3141$ (12) Å
$\beta = 101.549$ (4)°
$V = 1272.30$ (17) Å^3
$Z = 4$
$F(000) = 544$
$D_x = 1.356$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1871 reflections
$\theta = 2.0$–27.0°
$\mu = 0.29$ mm^{-1}
$T = 296$ K
Plate, light yellow
0.25 × 0.20 × 0.14 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 7.80 pixels mm^{-1}
ω scans

Absorption correction: multi-scan (*SADABS*; Bruker, 2007)
T_{min} = 0.933, T_{max} = 0.968
10293 measured reflections
2785 independent reflections
1871 reflections with $I > 2\sigma(I)$
R_{int} = 0.024
θ_{max} = 27.0°, θ_{min} = 2.0°
$h = -15 \rightarrow 12$
$k = -8 \rightarrow 9$
$l = -18 \rightarrow 15$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.116
S = 1.04
2785 reflections
166 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
$w = 1/[\sigma^2(F_o^2) + (0.0519P)^2 + 0.2053P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}

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 $F^2 > \sigma(F^2)$ 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}
Cl1	0.31558 (4)	0.47763 (8)	0.94032 (3)	0.0702 (2)
O1	0.45252 (11)	0.6419 (2)	0.58212 (9)	0.0684 (4)
H1	0.4036	0.6151	0.5361	0.103*
N1	0.26240 (12)	0.51118 (17)	0.49303 (10)	0.0442 (4)
C1	0.41674 (14)	0.6064 (2)	0.66249 (12)	0.0462 (4)
C2	0.31233 (14)	0.5273 (2)	0.66205 (11)	0.0400 (4)
C3	0.28167 (14)	0.4894 (2)	0.74847 (12)	0.0434 (4)
H3	0.2128	0.4363	0.7492	0.052*
C4	0.35292 (14)	0.5305 (2)	0.83271 (12)	0.0447 (4)
C5	0.45476 (15)	0.6104 (2)	0.83316 (12)	0.0499 (4)
H5	0.5022	0.6383	0.8907	0.060*
C6	0.48620 (15)	0.6486 (2)	0.74880 (13)	0.0524 (5)
H6	0.5549	0.7035	0.7493	0.063*
C7	0.23682 (15)	0.4821 (2)	0.57324 (12)	0.0432 (4)
H7	0.1679	0.4304	0.5753	0.052*
C8	0.18970 (13)	0.4694 (2)	0.40504 (11)	0.0394 (4)
C9	0.23021 (14)	0.5050 (2)	0.32363 (12)	0.0414 (4)
H9	0.3016	0.5534	0.3296	0.050*
C10	0.16807 (14)	0.4712 (2)	0.23319 (12)	0.0407 (4)

C11	0.06064 (14)	0.3993 (2)	0.22426 (12)	0.0429 (4)
C12	0.02122 (14)	0.3625 (2)	0.30650 (12)	0.0455 (4)
H12	−0.0499	0.3133	0.3010	0.055*
C13	0.08330 (14)	0.3962 (2)	0.39585 (12)	0.0456 (4)
H13	0.0544	0.3701	0.4497	0.055*
C14	0.21523 (18)	0.5150 (3)	0.14640 (13)	0.0576 (5)
H14A	0.2165	0.4083	0.1089	0.086*
H14B	0.2901	0.5603	0.1659	0.086*
H14C	0.1693	0.6042	0.1090	0.086*
C15	−0.01190 (16)	0.3653 (3)	0.12815 (13)	0.0599 (5)
H15A	0.0236	0.2788	0.0943	0.090*
H15B	−0.0225	0.4756	0.0927	0.090*
H15C	−0.0832	0.3200	0.1360	0.090*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0742 (4)	0.1002 (4)	0.0366 (3)	−0.0049 (3)	0.0120 (2)	0.0047 (2)
O1	0.0658 (9)	0.0930 (10)	0.0483 (8)	−0.0276 (8)	0.0159 (7)	0.0033 (7)
N1	0.0472 (8)	0.0498 (8)	0.0349 (8)	−0.0009 (6)	0.0069 (6)	−0.0023 (6)
C1	0.0493 (10)	0.0475 (10)	0.0428 (10)	−0.0042 (8)	0.0116 (8)	0.0025 (7)
C2	0.0427 (9)	0.0390 (9)	0.0376 (9)	0.0015 (7)	0.0061 (7)	−0.0012 (7)
C3	0.0430 (10)	0.0469 (10)	0.0407 (9)	0.0001 (7)	0.0093 (8)	−0.0005 (7)
C4	0.0493 (11)	0.0476 (10)	0.0364 (9)	0.0048 (8)	0.0065 (8)	0.0002 (7)
C5	0.0519 (11)	0.0500 (10)	0.0432 (10)	−0.0005 (8)	−0.0013 (8)	−0.0027 (8)
C6	0.0476 (11)	0.0523 (11)	0.0550 (12)	−0.0103 (8)	0.0048 (9)	−0.0008 (9)
C7	0.0440 (10)	0.0450 (9)	0.0404 (10)	−0.0016 (7)	0.0080 (8)	−0.0015 (7)
C8	0.0421 (10)	0.0383 (9)	0.0376 (9)	0.0011 (7)	0.0073 (7)	−0.0016 (7)
C9	0.0404 (9)	0.0421 (9)	0.0423 (10)	−0.0036 (7)	0.0102 (7)	−0.0015 (7)
C10	0.0480 (10)	0.0368 (9)	0.0389 (9)	0.0015 (7)	0.0125 (7)	0.0007 (7)
C11	0.0482 (10)	0.0368 (9)	0.0417 (10)	0.0013 (7)	0.0040 (7)	−0.0007 (7)
C12	0.0410 (9)	0.0474 (10)	0.0482 (10)	−0.0044 (8)	0.0091 (8)	0.0017 (8)
C13	0.0467 (10)	0.0520 (10)	0.0400 (10)	−0.0016 (8)	0.0132 (8)	0.0029 (8)
C14	0.0672 (13)	0.0661 (12)	0.0422 (10)	−0.0091 (9)	0.0171 (9)	0.0008 (8)
C15	0.0621 (12)	0.0674 (13)	0.0461 (11)	−0.0079 (10)	0.0008 (9)	−0.0017 (9)

Geometric parameters (Å, º)

Cl1—C4	1.7365 (17)	C8—C13	1.389 (2)
O1—C1	1.336 (2)	C9—C10	1.386 (2)
O1—H1	0.8200	C9—H9	0.9300
N1—C7	1.267 (2)	C10—C11	1.396 (2)
N1—C8	1.422 (2)	C10—C14	1.505 (2)
C1—C6	1.387 (2)	C11—C12	1.385 (2)
C1—C2	1.401 (2)	C11—C15	1.500 (2)
C2—C3	1.391 (2)	C12—C13	1.372 (2)
C2—C7	1.452 (2)	C12—H12	0.9300
C3—C4	1.372 (2)	C13—H13	0.9300

C3—H3	0.9300	C14—H14A	0.9600
C4—C5	1.375 (2)	C14—H14B	0.9600
C5—C6	1.368 (2)	C14—H14C	0.9600
C5—H5	0.9300	C15—H15A	0.9600
C6—H6	0.9300	C15—H15B	0.9600
C7—H7	0.9300	C15—H15C	0.9600
C8—C9	1.379 (2)		

C1—O1—H1	109.5	C8—C9—H9	118.9
C7—N1—C8	122.85 (15)	C10—C9—H9	118.9
O1—C1—C6	118.44 (15)	C9—C10—C11	118.83 (15)
O1—C1—C2	122.14 (15)	C9—C10—C14	120.27 (16)
C6—C1—C2	119.42 (15)	C11—C10—C14	120.89 (15)
C3—C2—C1	119.12 (15)	C12—C11—C10	118.45 (15)
C3—C2—C7	119.72 (15)	C12—C11—C15	120.34 (16)
C1—C2—C7	121.15 (15)	C10—C11—C15	121.20 (16)
C4—C3—C2	120.07 (16)	C13—C12—C11	122.41 (16)
C4—C3—H3	120.0	C13—C12—H12	118.8
C2—C3—H3	120.0	C11—C12—H12	118.8
C3—C4—C5	120.82 (16)	C12—C13—C8	119.34 (15)
C3—C4—Cl1	119.80 (14)	C12—C13—H13	120.3
C5—C4—Cl1	119.37 (13)	C8—C13—H13	120.3
C6—C5—C4	119.86 (16)	C10—C14—H14A	109.5
C6—C5—H5	120.1	C10—C14—H14B	109.5
C4—C5—H5	120.1	H14A—C14—H14B	109.5
C5—C6—C1	120.69 (16)	C10—C14—H14C	109.5
C5—C6—H6	119.7	H14A—C14—H14C	109.5
C1—C6—H6	119.7	H14B—C14—H14C	109.5
N1—C7—C2	121.73 (16)	C11—C15—H15A	109.5
N1—C7—H7	119.1	C11—C15—H15B	109.5
C2—C7—H7	119.1	H15A—C15—H15B	109.5
C9—C8—C13	118.75 (15)	C11—C15—H15C	109.5
C9—C8—N1	116.19 (14)	H15A—C15—H15C	109.5
C13—C8—N1	125.06 (14)	H15B—C15—H15C	109.5
C8—C9—C10	122.23 (15)		

O1—C1—C2—C3	178.21 (15)	C7—N1—C8—C9	−178.57 (14)
C6—C1—C2—C3	−1.3 (2)	C7—N1—C8—C13	1.2 (3)
O1—C1—C2—C7	−0.9 (3)	C13—C8—C9—C10	0.4 (2)
C6—C1—C2—C7	179.60 (15)	N1—C8—C9—C10	−179.85 (13)
C1—C2—C3—C4	0.4 (2)	C8—C9—C10—C11	0.3 (2)
C7—C2—C3—C4	179.50 (14)	C8—C9—C10—C14	179.07 (14)
C2—C3—C4—C5	0.5 (3)	C9—C10—C11—C12	−0.8 (2)
C2—C3—C4—Cl1	−178.37 (12)	C14—C10—C11—C12	−179.62 (15)
C3—C4—C5—C6	−0.4 (3)	C9—C10—C11—C15	178.03 (15)
Cl1—C4—C5—C6	178.42 (13)	C14—C10—C11—C15	−0.7 (2)
C4—C5—C6—C1	−0.5 (3)	C10—C11—C12—C13	0.8 (3)
O1—C1—C6—C5	−178.16 (16)	C15—C11—C12—C13	−178.10 (15)

C2—C1—C6—C5	1.4 (3)	C11—C12—C13—C8	−0.1 (3)
C8—N1—C7—C2	−179.54 (13)	C9—C8—C13—C12	−0.5 (2)
C3—C2—C7—N1	−178.66 (14)	N1—C8—C13—C12	179.79 (15)
C1—C2—C7—N1	0.4 (3)		

Hydrogen-bond geometry (Å, º)

Cg1 and Cg2 are the centroids of the C1–C6 and C8–C13 benzene rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N1	0.82	1.87	2.5998 (19)	149
C3—H3···*Cg*1^{i}	0.93	2.98	3.732 (2)	139
C6—H6···*Cg*2^{ii}	0.93	2.93	3.576 (2)	128
C14—H14*B*···*Cg*2^{iii}	0.96	2.96	3.656 (2)	131

Symmetry codes: (i) −*x*+1/2, *y*−1/2, −*z*+3/2; (ii) *x*+1/2, −*y*+3/2, *z*+1/2; (iii) −*x*+1/2, *y*+1/2, −*z*+1/2.