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(*E*)-4-Methyl-2-(*N*-phenylcarboximidoyl)phenol

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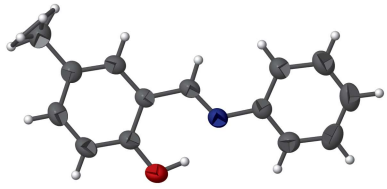
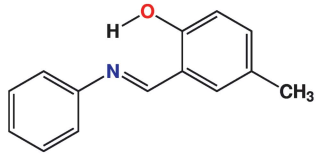
Structural data: full structural data are available from iucrdata.iucr.org

The title compound, $C_{14}H_{13}NO$, is not planar with the dihedral angle between the planes of the two aryl rings being 6.22 (11)°. The configuration about the imine bond is *E*. An intramolecular O—H···N hydrogen bond generates an *S*(6) loop. In the crystal, molecules assemble into columns parallel to the *a* axis. The methyl group is disordered over two positions rotated from each other by 60°.

3D view



Chemical scheme



Structure description

We report here, as part of our on-going research (Ida Malarselvi *et al.*, 2016; Swetha *et al.*, 2017), the synthesis and the X-ray crystal structure of the title methylated Schiff base compound, Fig.1, synthesized from the condensation reaction of equimolar amounts of 5-methylsalicylaldehyde and aniline in a mixture of DMSO and CCl_4.

The benzene and phenyl rings deviate from co-planarity with the dihedral angle between the two rings being 6.22 (11)°. The molecule has an *E* configuration about the C=N bond; the C2—C7=N1—C8 torsion angle is −177.73 (17)°. There is an intramolecular O1—H1···N1 hydrogen bond with an H···N distance of 1.73 (3) Å generating an *S*(6) loop, see Table 1 and Fig. 1. In the crystal, molecules assemble into columns parallel to the *a* axis, Fig. 2.

Swetha *et al.* (2017) have reported the crystal structure of (*E*)-4-fluoro-2-[(phenylimino)methyl]phenol, in which the molecule is essentially planar (r.m.s. deviation = 0.022 Å) and the dihedral angle between the planes of the two aryl rings is 0.69 (15)°.

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N1	0.96 (3)	1.73 (3)	2.603 (2)	148 (3)

Synthesis and crystallization

5-Methylsalicylaldehyde (0.64 g, 0.0047 mol) was dissolved in a mixture of DMSO (7.5 ml) and CCl_4 (7.5 ml). To this solution, aniline (0.42 g, 0.0045 mol) was added drop-wise with constant stirring for 1 h. During this time, the solution turned deep yellow. On standing for two weeks and with slow evaporation of the solvent, orange crystals of the title compound were deposited.

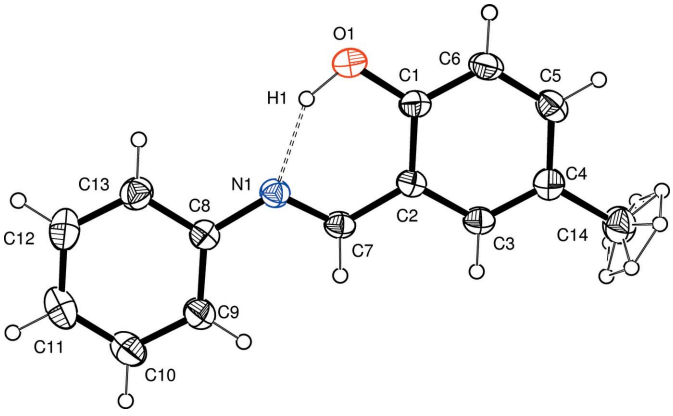


Figure 1
A view of the title compound with displacement ellipsoids drawn at the 30% probability level. The dashed lines indicate a hydrogen-bonding interaction. The methyl-H atoms are statistically disordered.

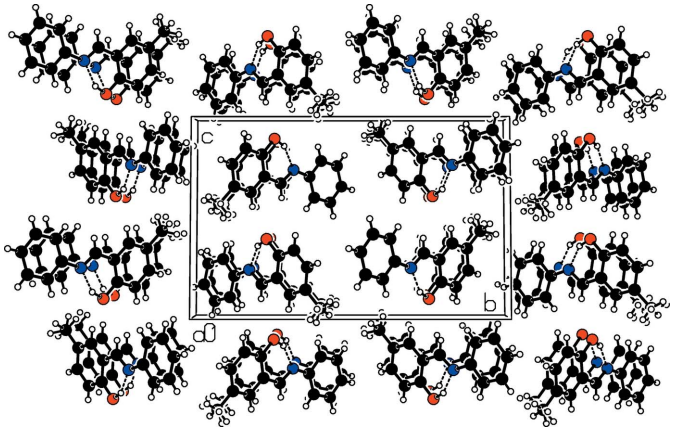


Figure 2
A perspective view of the molecular packing of the title compound, viewed down the *a* axis. The hydrogen bonds are shown as dashed lines (see Table 1).

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{14}H_{13}NO$
M_r	211.25
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	296
a, b, c (Å)	4.6976 (4), 19.3656 (18), 12.3116 (12)
β (°)	95.831 (3)
V (Å^3)	1114.21 (18)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.08
Crystal size (mm)	0.15 × 0.10 × 0.10
Data collection	
Diffractometer	Bruker Kappa APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2004)
T_{min}, T_{max}	0.699, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	20153, 2825, 1527
R_{int}	0.043
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.673
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.054, 0.169, 1.05
No. of reflections	2825
No. of parameters	149
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.21, −0.18

Computer programs: *APEX2*, *SAINT* and *XPREP* (Bruker, 2004), *SHELXT2014/5* (Sheldrick, 2015*a*), *ORTEP-3 for Windows* (Farrugia, 2012), *SHELXL2018/1* (Sheldrick, 2015*b*), *PLATON* (Spek, 2009) and *publCIF* (Westrip, 2010).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The methyl group was found to be disordered over two positions rotated from each other by 60°, and was refined as an idealized disordered methyl group.

Acknowledgements

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full crystallographic data

IUCrData (2018). **3**, x180464 [https://doi.org/10.1107/S2414314618004649]

(*E*)-4-Methyl-2-(*N*-phenylcarboximidoyl)phenol

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(I)

Crystal data

$C_{14}H_{13}NO$
$M_r = 211.25$
Monoclinic, $P2_1/n$
$a = 4.6976$ (4) Å
$b = 19.3656$ (18) Å
$c = 12.3116$ (12) Å
$\beta = 95.831$ (3)°
$V = 1114.21$ (18) Å^3
$Z = 4$
$F(000) = 448$
$D_x = 1.259$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4170 reflections
$\theta = 2.7$–25.3°
$\mu = 0.08$ mm^{-1}
$T = 296$ K
Needle, orange
0.15 × 0.10 × 0.10 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω and φ scan
Absorption correction: multi-scan (SADABS; Bruker, 2004)
$T_{min} = 0.699$, $T_{max} = 0.746$
20153 measured reflections
2825 independent reflections
1527 reflections with $I > 2\sigma(I)$
$R_{int} = 0.043$
$\theta_{max} = 28.6°$, $\theta_{min} = 2.1°$
$h = -5\rightarrow6$
$k = -25\rightarrow26$
$l = -16\rightarrow16$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.054$
$wR(F^2) = 0.169$
$S = 1.05$
2825 reflections
149 parameters
0 restraints
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0565P)^2 + 0.5019P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.21$ e Å^{-3}
$\Delta\rho_{min} = -0.18$ e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. The carbon-bound H-atoms were placed in calculated positions (C—H = 0.93–0.96 Å) and were included in the refinement in the riding model approximation, with U_{iso}(H) set to 1.2–1.5U_{equiv}(C)·The OH H atom was located in a difference Fourier map and refined freely.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
C1	0.1821 (4)	0.78020 (11)	0.18545 (16)	0.0421 (5)	
C2	0.2951 (4)	0.77295 (10)	0.29511 (15)	0.0373 (4)	
C3	0.1864 (4)	0.81482 (11)	0.37342 (16)	0.0430 (5)	
H3	0.259387	0.809976	0.446105	0.052*	
C4	−0.0255 (4)	0.86316 (11)	0.34711 (18)	0.0464 (5)	
C5	−0.1323 (5)	0.86888 (11)	0.23773 (18)	0.0502 (6)	
H5	−0.274657	0.901142	0.217726	0.060*	
C6	−0.0319 (5)	0.82791 (12)	0.15850 (17)	0.0505 (6)	
H6	−0.109020	0.832407	0.086232	0.061*	
C7	0.5179 (4)	0.72355 (10)	0.32756 (16)	0.0405 (5)	
H7	0.589870	0.721013	0.400660	0.049*	
C8	0.8311 (4)	0.63294 (10)	0.29122 (16)	0.0401 (5)	
C9	0.9307 (5)	0.61802 (12)	0.39877 (19)	0.0533 (6)	
H9	0.861945	0.642702	0.455421	0.064*	
C10	1.1313 (5)	0.56665 (13)	0.4217 (2)	0.0625 (7)	
H10	1.196216	0.556890	0.493922	0.075*	
C11	1.2361 (5)	0.52984 (12)	0.3395 (2)	0.0653 (7)	
H11	1.370708	0.495170	0.355807	0.078*	
C12	1.1409 (5)	0.54455 (13)	0.2330 (2)	0.0663 (7)	
H12	1.211556	0.519957	0.176631	0.080*	
C13	0.9401 (5)	0.59586 (12)	0.20938 (19)	0.0531 (6)	
H13	0.877201	0.605578	0.136922	0.064*	
C14	−0.1393 (6)	0.90787 (13)	0.4329 (2)	0.0651 (7)	
H14A	−0.284475	0.938039	0.399146	0.098*	0.5
H14B	−0.219813	0.879186	0.485566	0.098*	0.5
H14C	0.013807	0.934903	0.468760	0.098*	0.5
H14D	−0.042513	0.896713	0.503169	0.098*	0.5
H14E	−0.107174	0.955566	0.416749	0.098*	0.5
H14F	−0.340794	0.899849	0.433555	0.098*	0.5
N1	0.6195 (3)	0.68309 (9)	0.25867 (13)	0.0416 (4)	
O1	0.2776 (4)	0.74103 (9)	0.10554 (12)	0.0595 (5)	
H1	0.427 (7)	0.7120 (16)	0.140 (2)	0.097 (10)*	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0427 (11)	0.0475 (12)	0.0359 (10)	−0.0030 (9)	0.0028 (8)	0.0041 (9)
C2	0.0344 (10)	0.0393 (10)	0.0378 (10)	−0.0050 (8)	0.0014 (8)	0.0039 (8)
C3	0.0439 (11)	0.0464 (12)	0.0380 (10)	−0.0040 (9)	0.0001 (9)	0.0013 (9)
C4	0.0466 (12)	0.0415 (11)	0.0514 (12)	−0.0039 (9)	0.0068 (10)	0.0010 (10)
C5	0.0463 (12)	0.0465 (12)	0.0571 (14)	0.0035 (10)	0.0021 (10)	0.0115 (10)
C6	0.0524 (13)	0.0573 (14)	0.0404 (11)	0.0031 (11)	−0.0018 (10)	0.0109 (10)
C7	0.0382 (11)	0.0460 (11)	0.0363 (10)	−0.0038 (9)	−0.0014 (8)	0.0024 (9)
C8	0.0343 (10)	0.0413 (11)	0.0444 (11)	−0.0045 (8)	0.0024 (8)	0.0006 (9)
C9	0.0559 (14)	0.0532 (13)	0.0497 (13)	0.0078 (11)	−0.0004 (10)	0.0013 (11)

C10	0.0654 (16)	0.0539 (14)	0.0649 (16)	0.0053 (12)	−0.0097 (12)	0.0062 (12)
C11	0.0550 (15)	0.0471 (14)	0.091 (2)	0.0068 (11)	−0.0067 (14)	−0.0006 (13)
C12	0.0588 (16)	0.0605 (16)	0.0800 (19)	0.0094 (12)	0.0097 (13)	−0.0170 (14)
C13	0.0510 (13)	0.0597 (14)	0.0481 (12)	0.0016 (11)	0.0029 (10)	−0.0057 (11)
C14	0.0708 (17)	0.0554 (15)	0.0692 (17)	0.0098 (12)	0.0074 (13)	−0.0064 (12)
N1	0.0392 (9)	0.0450 (10)	0.0400 (9)	−0.0004 (8)	0.0014 (7)	0.0012 (8)
O1	0.0679 (11)	0.0728 (11)	0.0370 (8)	0.0156 (9)	0.0008 (7)	−0.0007 (8)

Geometric parameters (Å, º)

C1—O1	1.355 (2)	C9—C10	1.380 (3)
C1—C6	1.381 (3)	C9—H9	0.9300
C1—C2	1.407 (3)	C10—C11	1.369 (3)
C2—C3	1.396 (3)	C10—H10	0.9300
C2—C7	1.444 (3)	C11—C12	1.372 (4)
C3—C4	1.381 (3)	C11—H11	0.9300
C3—H3	0.9300	C12—C13	1.380 (3)
C4—C5	1.393 (3)	C12—H12	0.9300
C4—C14	1.505 (3)	C13—H13	0.9300
C5—C6	1.377 (3)	C14—H14A	0.9600
C5—H5	0.9300	C14—H14B	0.9600
C6—H6	0.9300	C14—H14C	0.9600
C7—N1	1.282 (2)	C14—H14D	0.9600
C7—H7	0.9300	C14—H14E	0.9600
C8—C13	1.377 (3)	C14—H14F	0.9600
C8—C9	1.389 (3)	O1—H1	0.96 (3)
C8—N1	1.418 (2)		
O1—C1—C6	119.16 (18)	C10—C9—H9	119.9
O1—C1—C2	121.36 (18)	C8—C9—H9	119.9
C6—C1—C2	119.48 (19)	C11—C10—C9	120.9 (2)
C3—C2—C1	118.42 (18)	C11—C10—H10	119.5
C3—C2—C7	119.98 (17)	C9—C10—H10	119.5
C1—C2—C7	121.61 (18)	C10—C11—C12	119.4 (2)
C4—C3—C2	122.52 (19)	C10—C11—H11	120.3
C4—C3—H3	118.7	C12—C11—H11	120.3
C2—C3—H3	118.7	C11—C12—C13	120.0 (2)
C3—C4—C5	117.4 (2)	C11—C12—H12	120.0
C3—C4—C14	121.6 (2)	C13—C12—H12	120.0
C5—C4—C14	120.9 (2)	C8—C13—C12	121.2 (2)
C6—C5—C4	121.6 (2)	C8—C13—H13	119.4
C6—C5—H5	119.2	C12—C13—H13	119.4
C4—C5—H5	119.2	C4—C14—H14A	109.5
C5—C6—C1	120.6 (2)	C4—C14—H14B	109.5
C5—C6—H6	119.7	H14A—C14—H14B	109.5
C1—C6—H6	119.7	C4—C14—H14C	109.5
N1—C7—C2	122.01 (18)	H14A—C14—H14C	109.5
N1—C7—H7	119.0	H14B—C14—H14C	109.5

C2—C7—H7	119.0	H14D—C14—H14E	109.5
C13—C8—C9	118.3 (2)	H14D—C14—H14F	109.5
C13—C8—N1	116.88 (18)	H14E—C14—H14F	109.5
C9—C8—N1	124.77 (19)	C7—N1—C8	121.95 (17)
C10—C9—C8	120.1 (2)	C1—O1—H1	106.9 (18)
O1—C1—C2—C3	−179.81 (18)	C3—C2—C7—N1	178.48 (18)
C6—C1—C2—C3	−0.2 (3)	C1—C2—C7—N1	−1.4 (3)
O1—C1—C2—C7	0.0 (3)	C13—C8—C9—C10	−0.7 (3)
C6—C1—C2—C7	179.64 (19)	N1—C8—C9—C10	178.0 (2)
C1—C2—C3—C4	−0.5 (3)	C8—C9—C10—C11	0.2 (4)
C7—C2—C3—C4	179.67 (18)	C9—C10—C11—C12	0.3 (4)
C2—C3—C4—C5	0.5 (3)	C10—C11—C12—C13	−0.3 (4)
C2—C3—C4—C14	−179.9 (2)	C9—C8—C13—C12	0.7 (3)
C3—C4—C5—C6	0.2 (3)	N1—C8—C13—C12	−178.1 (2)
C14—C4—C5—C6	−179.4 (2)	C11—C12—C13—C8	−0.2 (4)
C4—C5—C6—C1	−0.9 (3)	C2—C7—N1—C8	−177.73 (17)
O1—C1—C6—C5	−179.5 (2)	C13—C8—N1—C7	−175.27 (19)
C2—C1—C6—C5	0.9 (3)	C9—C8—N1—C7	6.0 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N1	0.96 (3)	1.73 (3)	2.603 (2)	148 (3)