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2-{(1*E*)-1-[(4-Chlorophenyl)imino]ethyl}-4-methylphenol

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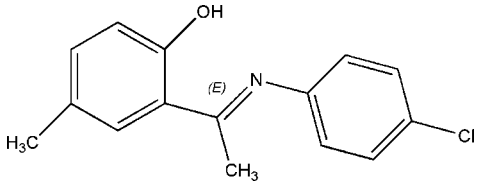
Key indicators: single-crystal X-ray study; T = 273 K; mean σ(C–C) = 0.004 Å; R factor = 0.048; wR factor = 0.155; data-to-parameter ratio = 14.0.

The title compound, $C_{15}H_{14}ClNO$, displays a *trans* configuration with respect to the C=N double bond [C—C=N—C = 175.3 (2)°], with a twist by 58.67 (8)° of the two benzene rings about the cental C=N bond. The crystal structure is stabilized by intramolecular O—H···N and intermolecular C—H···O hydrogen bonds.

Related literature

Chemistry and biological activity: Carcelli *et al.* (1995); Salem (1998).



Experimental

Crystal data

$C_{15}H_{14}ClNO$
M_r = 259.72
Monoclinic, $P2_1/c$
a = 13.254 (6) Å
b = 8.285 (3) Å
c = 12.078 (6) Å
β = 95.640 (9)°
V = 1320.0 (10) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.28 mm^{-1}
T = 273 (2) K
0.14 × 0.10 × 0.09 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
T_{min} = 0.962, T_{max} = 0.978
6701 measured reflections
2330 independent reflections
1376 reflections with $I > 2\sigma(I)$
R_{int} = 0.042

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.155
S = 1.00
2330 reflections
167 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.13 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C9—H9*C*···O1^{i}	0.96	2.50	3.358 (3)	149
O1—H1···N1	0.82	1.80	2.529 (3)	147

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

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FL2169).

References

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Salem, A. A. (1998). *Microchem. J.* **60**, 51–66.
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supplementary materials

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2-{(1*E*)-1-[(4-Chlorophenyl)imino]ethyl}-4-methylphenol

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Comment

Schiff bases have been extensively used as ligands in the field of coordination chemistry due to their ability to coordinate to metal ions (Salem, 1998) and their biological activity (Carcelli *et al.*, 1995). As an extension of our work on the structural characterization of Schiff bases, the title compound, (I),was synthesized and its crystal structure is reported here.

The title compound,(I), displays a *trans* conformation with respect to the C=N double bond (C2—C8=N1—C10 torsion = 175.3 (2)°, Fig. 1.)·The crystal structure is stabilized by an intramolecular O—H···N and intermolecular C—H···O hydrogen bonds(Table 1. and Fig 2.). The dihedral angle between the two benzene rings is 58.67 (8)°.

Experimental

4-chloroaniline(0.01 mol,1.27 g) was dissolved in anhydrous ethanol (20 ml), and 1-(2-hydroxy-5-methylphenyl)ethanone (0.01 mol, 1.50 g) was added. The reaction mixture was refluxed for 4 h with stirring, then the resulting precipitate was collected by filtration, washed several times with ethanol and dried *in vacuo* (yield 83%). The compound (1.0 mmol,0.26 g) was dissolved in dimethylformamide (15 ml) and kept at room temperature for 30 d to obtain yellow single crystals suitable for X-ray diffraction.

Refinement

All H atoms were positioned geometrically and treated as riding on their parent atoms,with *C*—*H*(methyl) = 0.96 Å, C—H(aromatic) = 0.93 Å,*O*—H = 0.82 Å and with U_{iso}(H) =1.5U_{eq}(C_{methyl},*O*) and 1.2U_{eq}($C_{aromatic}$).

Figures

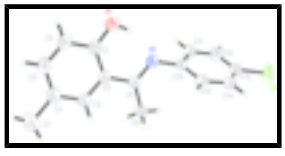

Fig. 1. The molecular structure of compound (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

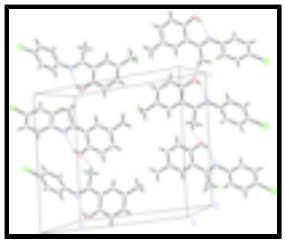

Fig. 2. The crystal packing of (I), viewed along the *b* axis. Dashed lines show intra-and intermolecular hydrogen bonds.

2-{(1E)-1-[(4-Chlorophenyl)imino]ethyl}-4-methylphenol

Crystal data

$C_{15}H_{14}ClNO$	F_{000} = 544
M_r = 259.72	D_x = 1.307 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 1014 reflections
a = 13.254 (6) Å	θ = 2.9–19.5º
b = 8.285 (3) Å	μ = 0.28 mm^{-1}
c = 12.078 (6) Å	T = 273 (2) K
β = 95.640 (9)º	Block, yellow
V = 1320.0 (10) Å^3	0.14 × 0.10 × 0.09 mm
Z = 4	

Data collection

Bruker APEXII CCD area-detector diffractometer	2330 independent reflections
Radiation source: fine-focus sealed tube	1376 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.042
T = 273(2) K	θ_{max} = 25.0º
φ and ω scans	θ_{min} = 1.5º
Absorption correction: multi-scan (SADABS; Sheldrick, 2003)	h = −15→15
T_{min} = 0.962, T_{max} = 0.978	k = −8→9
6701 measured reflections	l = −14→14

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.048	$w = 1/[\sigma^2(F_o^2) + (0.082P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.155	$(\Delta/\sigma)_{max}$ = 0.001
S = 1.00	$\Delta\rho_{max}$ = 0.13 e Å^{-3}
2330 reflections	$\Delta\rho_{min}$ = −0.17 e Å^{-3}
167 parameters	Extinction correction: SHELXL97 (Sheldrick, 1997a), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.009 (2)
Secondary atom site location: difference Fourier map	

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 $F^2 > 2\text{sigma}(F^2)$ 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	1.38320 (6)	0.11834 (12)	0.47045 (8)	0.1083 (4)
O1	0.88869 (14)	0.1765 (3)	0.02565 (14)	0.0819 (6)
H1	0.9377	0.1657	0.0720	0.123*
N1	0.98204 (16)	0.1218 (2)	0.21468 (16)	0.0593 (6)
C1	0.8031 (2)	0.1469 (3)	0.0733 (2)	0.0636 (7)
C2	0.80493 (19)	0.0957 (3)	0.18390 (19)	0.0544 (6)
C3	0.71244 (19)	0.0670 (3)	0.2254 (2)	0.0650 (7)
H3	0.7124	0.0326	0.2987	0.078*
C4	0.6208 (2)	0.0874 (4)	0.1628 (3)	0.0779 (8)
C5	0.6225 (2)	0.1373 (4)	0.0542 (3)	0.0822 (9)
H5	0.5617	0.1515	0.0100	0.099*
C6	0.7118 (2)	0.1662 (4)	0.0102 (2)	0.0783 (9)
H6	0.7108	0.1994	−0.0635	0.094*
C7	0.5225 (2)	0.0569 (5)	0.2120 (3)	0.1153 (13)
H7A	0.5257	0.1035	0.2850	0.173*
H7B	0.5114	−0.0573	0.2169	0.173*
H7C	0.4677	0.1049	0.1655	0.173*
C8	0.90082 (19)	0.0743 (3)	0.25395 (19)	0.0527 (6)
C9	0.89928 (18)	−0.0049 (3)	0.36422 (18)	0.0611 (7)
H9A	0.9671	−0.0344	0.3922	0.092*
H9B	0.8577	−0.1000	0.3565	0.092*
H9C	0.8720	0.0684	0.4151	0.092*
C10	1.07746 (19)	0.1175 (3)	0.2786 (2)	0.0569 (7)
C11	1.1540 (2)	0.0262 (4)	0.2436 (2)	0.0687 (8)
H11	1.1423	−0.0358	0.1794	0.082*
C12	1.2482 (2)	0.0251 (4)	0.3027 (2)	0.0778 (8)
H12	1.2994	−0.0402	0.2802	0.093*
C13	1.2658 (2)	0.1204 (4)	0.3943 (2)	0.0680 (8)
C14	1.1917 (2)	0.2165 (3)	0.4280 (2)	0.0686 (8)
H14	1.2049	0.2831	0.4897	0.082*
C15	1.0969 (2)	0.2150 (3)	0.3705 (2)	0.0633 (7)
H15	1.0458	0.2799	0.3938	0.076*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0686 (6)	0.1324 (9)	0.1179 (8)	−0.0129 (5)	−0.0205 (5)	0.0054 (6)
O1	0.0709 (12)	0.1126 (17)	0.0618 (11)	0.0009 (12)	0.0052 (9)	0.0263 (11)
N1	0.0600 (13)	0.0624 (14)	0.0553 (12)	0.0004 (11)	0.0037 (10)	0.0098 (10)
C1	0.0665 (17)	0.0623 (17)	0.0611 (16)	0.0021 (14)	0.0011 (13)	0.0058 (13)
C2	0.0596 (15)	0.0487 (15)	0.0544 (14)	0.0028 (12)	0.0033 (12)	0.0014 (11)
C3	0.0643 (17)	0.0696 (18)	0.0612 (15)	−0.0003 (14)	0.0071 (13)	−0.0047 (13)
C4	0.0638 (18)	0.086 (2)	0.083 (2)	−0.0003 (16)	0.0042 (15)	−0.0106 (17)
C5	0.0651 (19)	0.090 (2)	0.087 (2)	0.0096 (17)	−0.0120 (16)	−0.0007 (17)
C6	0.082 (2)	0.085 (2)	0.0654 (17)	0.0067 (17)	−0.0089 (16)	0.0097 (14)
C7	0.070 (2)	0.154 (4)	0.123 (3)	−0.007 (2)	0.014 (2)	−0.001 (2)
C8	0.0603 (15)	0.0455 (15)	0.0519 (13)	0.0011 (12)	0.0039 (12)	0.0008 (11)
C9	0.0686 (16)	0.0626 (16)	0.0517 (14)	−0.0031 (14)	0.0048 (12)	0.0038 (12)
C10	0.0579 (15)	0.0578 (16)	0.0549 (15)	−0.0032 (13)	0.0047 (12)	0.0117 (12)
C11	0.0622 (16)	0.074 (2)	0.0697 (16)	−0.0018 (15)	0.0052 (14)	−0.0093 (14)
C12	0.0628 (17)	0.081 (2)	0.090 (2)	0.0011 (16)	0.0088 (16)	−0.0023 (17)
C13	0.0571 (16)	0.0700 (19)	0.0761 (19)	−0.0085 (15)	0.0030 (14)	0.0143 (15)
C14	0.0824 (19)	0.0631 (18)	0.0587 (15)	−0.0165 (17)	−0.0019 (14)	0.0085 (14)
C15	0.0692 (17)	0.0607 (17)	0.0608 (15)	0.0024 (14)	0.0106 (13)	0.0065 (14)

Geometric parameters (Å, °)

Cl1—C13	1.728 (3)	C7—H7B	0.9600
O1—C1	1.344 (3)	C7—H7C	0.9600
O1—H1	0.8200	C8—C9	1.487 (3)
N1—C8	1.280 (3)	C9—H9A	0.9600
N1—C10	1.416 (3)	C9—H9B	0.9600
C1—C6	1.374 (4)	C9—H9C	0.9600
C1—C2	1.400 (4)	C10—C11	1.365 (4)
C2—C3	1.390 (3)	C10—C15	1.376 (3)
C2—C8	1.467 (3)	C11—C12	1.376 (3)
C3—C4	1.377 (4)	C11—H11	0.9300
C3—H3	0.9300	C12—C13	1.361 (4)
C4—C5	1.377 (4)	C12—H12	0.9300
C4—C7	1.505 (4)	C13—C14	1.357 (4)
C5—C6	1.365 (4)	C14—C15	1.374 (3)
C5—H5	0.9300	C14—H14	0.9300
C6—H6	0.9300	C15—H15	0.9300
C7—H7A	0.9600		
C1—O1—H1	109.5	N1—C8—C9	123.6 (2)
C8—N1—C10	121.9 (2)	C2—C8—C9	118.8 (2)
O1—C1—C6	118.4 (2)	C8—C9—H9A	109.5
O1—C1—C2	121.9 (2)	C8—C9—H9B	109.5
C6—C1—C2	119.7 (3)	H9A—C9—H9B	109.5
C3—C2—C1	117.6 (2)	C8—C9—H9C	109.5

C3—C2—C8	121.1 (2)	H9A—C9—H9C	109.5
C1—C2—C8	121.3 (2)	H9B—C9—H9C	109.5
C4—C3—C2	122.9 (3)	C11—C10—C15	119.3 (2)
C4—C3—H3	118.5	C11—C10—N1	119.7 (2)
C2—C3—H3	118.5	C15—C10—N1	120.8 (2)
C3—C4—C5	117.6 (3)	C10—C11—C12	120.4 (3)
C3—C4—C7	120.9 (3)	C10—C11—H11	119.8
C5—C4—C7	121.5 (3)	C12—C11—H11	119.8
C6—C5—C4	121.3 (3)	C13—C12—C11	119.5 (3)
C6—C5—H5	119.3	C13—C12—H12	120.3
C4—C5—H5	119.3	C11—C12—H12	120.3
C5—C6—C1	120.9 (3)	C14—C13—C12	120.8 (3)
C5—C6—H6	119.6	C14—C13—Cl1	119.1 (2)
C1—C6—H6	119.6	C12—C13—Cl1	120.0 (2)
C4—C7—H7A	109.5	C13—C14—C15	119.7 (3)
C4—C7—H7B	109.5	C13—C14—H14	120.1
H7A—C7—H7B	109.5	C15—C14—H14	120.1
C4—C7—H7C	109.5	C14—C15—C10	120.1 (3)
H7A—C7—H7C	109.5	C14—C15—H15	119.9
H7B—C7—H7C	109.5	C10—C15—H15	119.9
N1—C8—C2	117.5 (2)		

O1—C1—C2—C3	−179.6 (2)	C1—C2—C8—N1	7.9 (3)
C6—C1—C2—C3	−0.3 (4)	C3—C2—C8—C9	10.3 (3)
O1—C1—C2—C8	1.0 (4)	C1—C2—C8—C9	−170.3 (2)
C6—C1—C2—C8	−179.7 (2)	C8—N1—C10—C11	119.2 (3)
C1—C2—C3—C4	−0.2 (4)	C8—N1—C10—C15	−66.4 (3)
C8—C2—C3—C4	179.2 (2)	C15—C10—C11—C12	3.2 (4)
C2—C3—C4—C5	0.5 (4)	N1—C10—C11—C12	177.7 (2)
C2—C3—C4—C7	−179.2 (3)	C10—C11—C12—C13	−2.3 (4)
C3—C4—C5—C6	−0.3 (5)	C11—C12—C13—C14	−0.1 (4)
C7—C4—C5—C6	179.4 (3)	C11—C12—C13—Cl1	179.1 (2)
C4—C5—C6—C1	−0.2 (5)	C12—C13—C14—C15	1.5 (4)
O1—C1—C6—C5	179.8 (3)	Cl1—C13—C14—C15	−177.68 (19)
C2—C1—C6—C5	0.5 (4)	C13—C14—C15—C10	−0.6 (4)
C10—N1—C8—C2	175.3 (2)	C11—C10—C15—C14	−1.8 (4)
C10—N1—C8—C9	−6.6 (4)	N1—C10—C15—C14	−176.2 (2)
C3—C2—C8—N1	−171.6 (2)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C9—H9C···O1^{i}	0.96	2.50	3.358 (3)	149
O1—H1···N1	0.82	1.80	2.529 (3)	147

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

Fig. 1

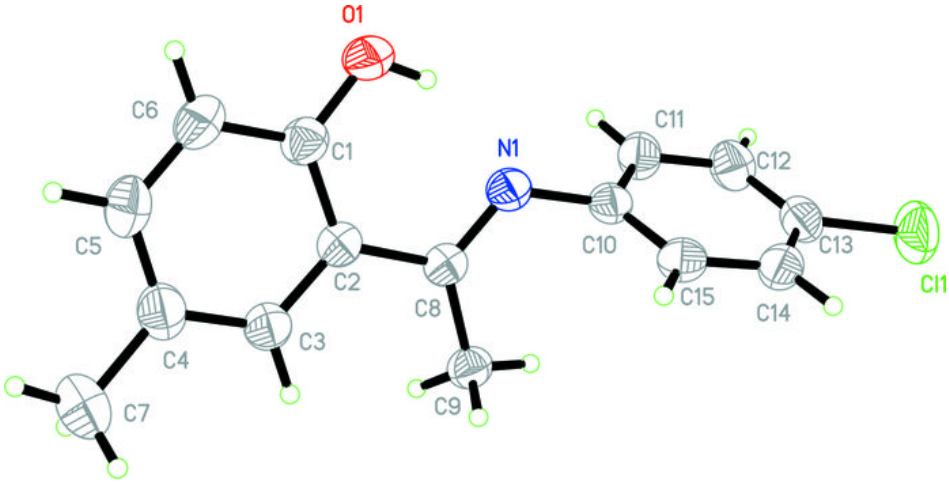

Fig. 2