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Crystal structure of 2-{[(2-chlorophenyl)-imino]methyl}phenol

Matheswaran Saranya,[a] Annamalai Subashini,[a]* Chidambaram Arunagiri[b] and Packianathan Thomas Muthiah[c]

[a]PG & Research Department of Chemistry, Seethalakshmi Ramaswami College, Tiruchirappalli 620 002, Tamil Nadu, India, [b]PG & Research Department of Physics, Government Arts College, Ariyalur 621 713, Tamil Nadu, India, and [c]School of Chemistry, Bharathidasan University, Tiruchirappalli 620 024, Tamil Nadu, India. *Correspondence e-mail: asubashini2k4@yahoo.co.in

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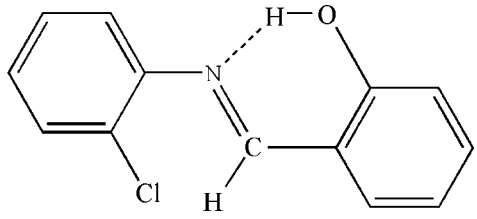
In the title compound, $C_{13}H_{10}ClNO$, the dihedral angle between the planes of the aromatic rings is 51.42 (9)° and an intramolecular O—H···N hydrogen bond closes an $S(6)$ ring. The Cl atom and the N atom are *syn*. No directional interactions beyond van der Waals contacts are observed in the crystal.

Keywords: crystal structure; 2-{[(2-chlorophenyl)imino]methyl}phenol; Schiff base; van der Waals contacts.

CCDC reference: 1038374

1. Related literature

For related structures recently reported by us and background to Schiff bases, see: Arunagiri *et al.* (2013*a*,*b*). For a related structure, see: Chumakov *et al.* (2005).



2. Experimental

2.1. Crystal data

$C_{13}H_{10}ClNO$
M_r = 231.67
Orthorhombic, $P2_12_12_1$
a = 6.8591 (2) Å
b = 12.1829 (4) Å
c = 13.5405 (5) Å
V = 1131.50 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.31 mm^{-1}
T = 293 K
0.30 × 0.25 × 0.20 mm

2.2. Data collection

Bruker Kappa APEXII CCD diffractometer
6509 measured reflections
2744 independent reflections
2315 reflections with $I > 2\sigma(I)$
R_{int} = 0.017

2.3. Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.097
S = 1.06
2744 reflections
146 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}
Absolute structure: Flack (1983)
Absolute structure parameter: 0.01 (7)

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N1	0.82	1.88	2.611 (2)	147

Data collection: *APEX2* (Bruker, 2008); cell refinement: *SAINT* (Bruker, 2008); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2009); software used to prepare material for publication: *PLATON*.

Acknowledgements

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Supporting information for this paper is available from the IUCr electronic archives (Reference: HB7335).

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supporting information

Acta Cryst. (2015). E**71**, o48 [https://doi.org/10.1107/S2056989014026978]

Crystal structure of 2-{[(2-chlorophenyl)imino]methyl}phenol

Matheswaran Saranya, Annamalai Subashini, Chidambaram Arunagiri and Packianathan Thomas Muthiah

S1. Comment

As part of our ongoing studies of Schiff bases (Arunagiri *et al.*, 2013a,b), we now describe the synthesis and structure of the title compound.

An *ORTEP* view of the asymmetric unit is shown in Figure 1. The asymmetric unit contains a molecule of Schiff base. The compound crystallizes in the orthorhombic space group $P2_12_12_1$. The dihedral angle between the salicylidene moiety and amino phenyl plane is 51.42 (9)°. The two torsional angles τ1 (N—C—C—C) and τ2 (C—N—C—C) defining the confirmation of the molecule. In the present crystal structure, the torsion angles are 3.2 (3)° (N1—C7—C8—C9), -179.23 (2)° (N1—C7—C8—C13), 47.5 (2)° (C7—N1—C1—C6), -174.48 (2)° (C8—C7—N1—C1) and -135.60 (2)° (N1—C7—C1—C2). The N1—C7 distance of 1.275 (2) Å is normal double bond values and agree well with those observed in other azomethines. The C1—N1—C7 bond angle of 118.70 (2)° in the Schiff base ligand has a normal value. The C3—C2—C1 angle is 121.15 (2)° is larger than typical hexagonal of 120°. The C8—C9—C10 angle is 119.53 (2)° is smaller than typical hexagonal of 120°. This is due to effect of substitution on Cl & OH of the two aromatic rings. The two benzene rings (amino phenyl and salicylaldehyde) and the azomethine group are practically coplanar, as a result of intramolecular O—H···N (O1—H1···N1 with bond length of 2.611 (2) Å and bond angle of 147°) hydrogen bond involving the hydroxy O-atom and azomethine N-atom with graph-set notation S(6), as shown in Figure 2. Similar intramolecular hydrogen bonds are reported for the crystal structures of 2-(naphthalene-2-yliminomethyl) phenol and *N*-acetyl-4-[(2-hydroxybenzylidene)-amino]benzenesulfonamide monohydrate (Arunagiri *et al.*, 2013 (*a*); Chumakov *et al.*, 2005).

S2. Experimental

An ethanol solution (25 ml) of chlorophenyl amine (0.25 mole) was mixed with hydroxy benzaldehyde (0.25 mole) and the contents were refluxed for 3 h and kept aside for crystallization. After a few days a pale yellow colour precipitate was formed. Recrystallization was from $CHCl_3$/ethanol solution to form yellow needles. FT—IR (KBr pellet) in cm^{-1}: 3437(O—H), 1614 cm^{-1}(C=N stretching); ^{1}H—NMR (400 MHz, DMSO– d^6) in δ (p.p.m.) 13.17 (s,1*H*, aromatic O—H), 8.63 (s, 1H,*C*=N), 6.93 - 7.50 (m,8*H*, CH aromatic),^{13}C—NMR (400 MHz, DMSO-d^6) in δ (p.p.m.): 163.3 (C=N), 161.4 (phenolic OH), Electronic spectrum, λmax: 275 and 340 nm (due to intraligand π–π* and n–π* transitions); fluorescence spectra, 432 nm (attributed to the n–π* transition).

S3. Refinement

All H atoms were positioned geometrically and treated as riding. The C—H and O—H bond lengths are 0.93 Å and 0.82 Å respectively.

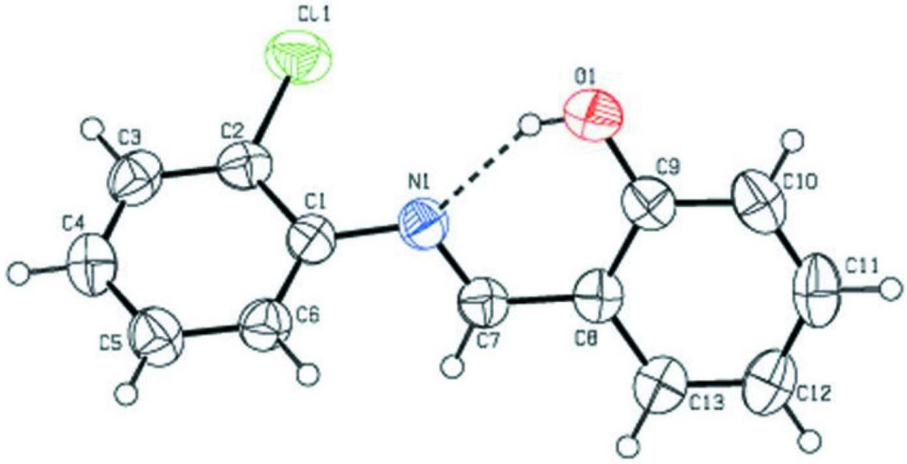

Figure 1

Molecular structure of the title compound with displacement ellipsoids drawn at 50% probability level. Dashed line indicates intramolecular hydrogen bond.

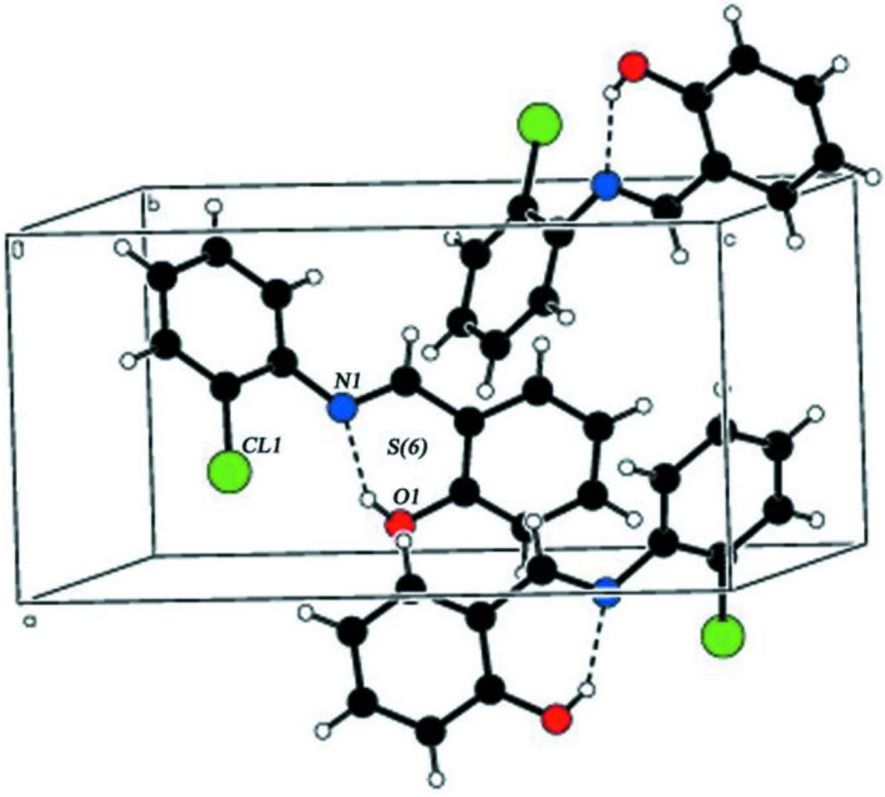

Figure 2

Hydrogen bonding interaction of title compound.

2-{[(2-Chlorophenyl)imino]methyl}phenol

Crystal data

$C_{13}H_{10}ClNO$
$M_r = 231.67$
Orthorhombic, $P2_12_12_1$
Hall symbol: P 2ac 2ab
$a = 6.8591$ (2) Å
$b = 12.1829$ (4) Å
$c = 13.5405$ (5) Å
$V = 1131.50$ (6) Å^3
$Z = 4$
$F(000) = 480$
$D_x = 1.360$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 45 reflections
$\theta = 3.0$–$28.3°$
$\mu = 0.31$ mm^{-1}
$T = 293$ K
Cut needle, yellow
0.30 × 0.25 × 0.20 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
6509 measured reflections
2744 independent reflections
2315 reflections with $I > 2\sigma(I)$
$R_{int} = 0.017$
$\theta_{max} = 28.3°$, $\theta_{min} = 3.0°$
$h = -9 \rightarrow 7$
$k = -13 \rightarrow 16$
$l = -18 \rightarrow 10$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.034$
$wR(F^2) = 0.097$
$S = 1.06$
2744 reflections
146 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
$w = 1/[\sigma^2(F_o^2) + (0.0488P)^2 + 0.0823P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.17$ e Å^{-3}
$\Delta\rho_{min} = -0.17$ e Å^{-3}
Absolute structure: Flack (1983)
Absolute structure parameter: 0.01 (7)

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 on F^2 for ALL reflections except those flagged by the user for potential systematic errors. Weighted *R*-factors *wR* and all goodnesses 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 observed criterion of $F^2 > \sigma(F^2)$ is used only for calculating -*R*-factor-obs *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	0.22873 (7)	0.87326 (5)	0.81891 (4)	0.0781 (2)
O1	0.41345 (19)	0.60666 (15)	0.63294 (11)	0.0742 (5)
N1	0.0830 (2)	0.68972 (13)	0.69278 (10)	0.0531 (4)
C1	−0.0473 (2)	0.72426 (14)	0.76845 (12)	0.0486 (5)

C2	0.0066 (2)	0.80739 (14)	0.83346 (13)	0.0513 (5)
C3	−0.1161 (3)	0.84060 (16)	0.90860 (14)	0.0606 (6)
C4	−0.2937 (3)	0.78949 (18)	0.92067 (14)	0.0672 (7)
C5	−0.3476 (3)	0.70587 (18)	0.85879 (16)	0.0668 (7)
C6	−0.2258 (3)	0.67361 (15)	0.78292 (13)	0.0563 (5)
C7	0.0161 (2)	0.67467 (14)	0.60596 (13)	0.0506 (5)
C8	0.1350 (2)	0.63031 (15)	0.52664 (12)	0.0501 (5)
C9	0.3282 (3)	0.59651 (15)	0.54312 (14)	0.0556 (5)
C10	0.4336 (3)	0.54992 (17)	0.46648 (17)	0.0676 (7)
C11	0.3501 (3)	0.53771 (17)	0.37489 (16)	0.0716 (8)
C12	0.1616 (3)	0.57133 (18)	0.35676 (15)	0.0701 (7)
C13	0.0551 (3)	0.61655 (16)	0.43201 (13)	0.0597 (6)
H1	0.33750	0.63660	0.67120	0.1110*
H3	−0.07910	0.89710	0.95080	0.0730*
H4	−0.37710	0.81180	0.97090	0.0810*
H5	−0.46660	0.67070	0.86790	0.0800*
H6	−0.26410	0.61710	0.74100	0.0680*
H7	−0.11310	0.69270	0.59300	0.0610*
H10	0.56110	0.52680	0.47710	0.0810*
H11	0.42230	0.50620	0.32410	0.0860*
H12	0.10740	0.56340	0.29420	0.0840*
H13	−0.07260	0.63860	0.42020	0.0720*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0627 (3)	0.0739 (3)	0.0977 (4)	−0.0117 (2)	−0.0077 (2)	−0.0088 (3)
O1	0.0569 (7)	0.0894 (11)	0.0762 (9)	0.0072 (8)	−0.0098 (6)	−0.0086 (8)
N1	0.0541 (7)	0.0507 (8)	0.0545 (7)	0.0050 (6)	−0.0011 (6)	−0.0023 (6)
C1	0.0520 (9)	0.0442 (9)	0.0496 (8)	0.0093 (7)	−0.0039 (7)	0.0014 (7)
C2	0.0536 (8)	0.0423 (8)	0.0579 (9)	0.0038 (7)	−0.0103 (7)	0.0030 (7)
C3	0.0738 (12)	0.0493 (10)	0.0588 (10)	0.0110 (8)	−0.0099 (8)	−0.0079 (8)
C4	0.0715 (12)	0.0656 (12)	0.0644 (11)	0.0088 (10)	0.0122 (9)	−0.0050 (10)
C5	0.0633 (10)	0.0610 (12)	0.0761 (12)	−0.0017 (9)	0.0086 (9)	−0.0019 (10)
C6	0.0597 (9)	0.0477 (9)	0.0614 (9)	0.0011 (8)	−0.0033 (8)	−0.0063 (8)
C7	0.0516 (8)	0.0436 (8)	0.0566 (9)	0.0050 (7)	−0.0025 (7)	0.0009 (7)
C8	0.0578 (8)	0.0392 (8)	0.0533 (9)	−0.0004 (7)	0.0033 (7)	0.0024 (7)
C9	0.0547 (8)	0.0453 (9)	0.0667 (10)	−0.0036 (7)	0.0040 (8)	0.0034 (8)
C10	0.0609 (10)	0.0551 (11)	0.0869 (14)	0.0012 (9)	0.0190 (10)	0.0028 (10)
C11	0.0956 (15)	0.0490 (11)	0.0703 (13)	0.0000 (11)	0.0317 (11)	−0.0017 (9)
C12	0.0957 (14)	0.0612 (12)	0.0533 (10)	−0.0001 (12)	0.0053 (10)	−0.0001 (9)
C13	0.0702 (10)	0.0531 (10)	0.0559 (9)	0.0019 (9)	0.0001 (8)	0.0025 (8)

Geometric parameters (Å, º)

Cl1—C2	1.7333 (15)	C9—C10	1.386 (3)
O1—C9	1.355 (2)	C10—C11	1.374 (3)
O1—H1	0.8200	C11—C12	1.378 (3)

N1—C7	1.275 (2)	C12—C13	1.369 (3)
N1—C1	1.423 (2)	C3—H3	0.9300
C1—C6	1.385 (2)	C4—H4	0.9300
C1—C2	1.392 (2)	C5—H5	0.9300
C2—C3	1.381 (3)	C6—H6	0.9300
C3—C4	1.378 (3)	C7—H7	0.9300
C4—C5	1.370 (3)	C10—H10	0.9300
C5—C6	1.381 (3)	C11—H11	0.9300
C7—C8	1.453 (2)	C12—H12	0.9300
C8—C13	1.404 (2)	C13—H13	0.9300
C8—C9	1.406 (2)		

C9—O1—H1	109.00	C11—C12—C13	119.17 (19)
C1—N1—C7	118.70 (13)	C8—C13—C12	121.26 (18)
N1—C1—C6	121.68 (15)	C2—C3—H3	120.00
C2—C1—C6	118.00 (15)	C4—C3—H3	120.00
N1—C1—C2	120.24 (13)	C3—C4—H4	120.00
Cl1—C2—C3	118.93 (14)	C5—C4—H4	120.00
C1—C2—C3	121.15 (15)	C4—C5—H5	120.00
Cl1—C2—C1	119.90 (12)	C6—C5—H5	120.00
C2—C3—C4	119.59 (17)	C1—C6—H6	120.00
C3—C4—C5	120.14 (19)	C5—C6—H6	120.00
C4—C5—C6	120.22 (19)	N1—C7—H7	119.00
C1—C6—C5	120.87 (17)	C8—C7—H7	119.00
N1—C7—C8	122.21 (13)	C9—C10—H10	120.00
C7—C8—C13	120.01 (14)	C11—C10—H10	120.00
C9—C8—C13	118.56 (16)	C10—C11—H11	119.00
C7—C8—C9	121.39 (15)	C12—C11—H11	119.00
O1—C9—C10	118.96 (18)	C11—C12—H12	120.00
C8—C9—C10	119.53 (18)	C13—C12—H12	120.00
O1—C9—C8	121.51 (17)	C8—C13—H13	119.00
C9—C10—C11	120.17 (19)	C12—C13—H13	119.00
C10—C11—C12	121.3 (2)		

C7—N1—C1—C2	−135.60 (17)	N1—C7—C8—C9	3.2 (3)
C7—N1—C1—C6	47.5 (2)	N1—C7—C8—C13	−179.23 (17)
C1—N1—C7—C8	−174.48 (16)	C7—C8—C9—O1	−1.9 (3)
N1—C1—C2—Cl1	2.9 (2)	C7—C8—C9—C10	177.01 (17)
C6—C1—C2—Cl1	179.83 (13)	C13—C8—C9—O1	−179.45 (18)
C6—C1—C2—C3	−1.7 (3)	C13—C8—C9—C10	−0.6 (3)
N1—C1—C2—C3	−178.70 (16)	C7—C8—C13—C12	−177.66 (18)
C2—C1—C6—C5	0.9 (3)	C9—C8—C13—C12	0.0 (3)
N1—C1—C6—C5	177.85 (17)	O1—C9—C10—C11	179.40 (19)
Cl1—C2—C3—C4	179.58 (15)	C8—C9—C10—C11	0.5 (3)
C1—C2—C3—C4	1.1 (3)	C9—C10—C11—C12	0.2 (3)
C2—C3—C4—C5	0.3 (3)	C10—C11—C12—C13	−0.8 (3)
C3—C4—C5—C6	−1.1 (3)	C11—C12—C13—C8	0.7 (3)
C4—C5—C6—C1	0.5 (3)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N1	0.82	1.88	2.611 (2)	147