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2-{[2-Chloro-5-(trifluoromethyl)phenyl]iminomethyl]phenol

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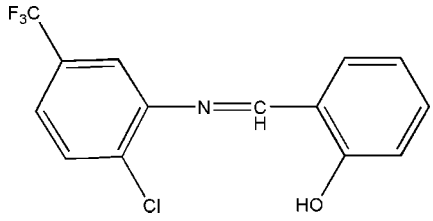
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.003 Å; disorder in main residue; R factor = 0.030; wR factor = 0.070; data-to-parameter ratio = 11.0.

In the title molecule, $C_{14}H_{19}ClF_3NO$, an intramolecular O—H···N hydrogen bond influences the molecular conformation; the two benzene rings make a dihedral angle of 47.7 (3)°. The crystal packing exhibits no classical intermolecular hydrogen bonds. One CF~3~ group is disordered over two positions; the site occupancy factors are 0.7 and 0.3.

Related literature

For related literature, see: Alemi & Shaabani (2000); Alizadeh *et al.* (1999); Johnson *et al.* (1996); Kim & Shin (1999); Wang & Zheng (2007).



Experimental

Crystal data

$C_{14}H_9ClF_3NO$
M_r = 299.67
Monoclinic, $P2_1/c$
a = 12.979 (6) Å
b = 7.418 (3) Å
c = 13.881 (6) Å
β = 101.064 (7)°
V = 1311.6 (10) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.32 mm^{-1}
T = 298 (2) K
0.28 × 0.22 × 0.15 mm

Data collection

Bruker APEX-II area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2004)
T_{min} = 0.916, T_{max} = 0.954
7694 measured reflections
2303 independent reflections
1411 reflections with $I > 2\sigma(I)$
R_{int} = 0.029

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.030
$wR(F^2)$ = 0.070
S = 0.96
2303 reflections
210 parameters
69 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.12 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N1	0.82	1.87	2.5975 (19)	147

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2004); 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: CV2348).

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supplementary materials

Acta Cryst. (2007). E**63**, o4677 [**doi:10.1107/S1600536807057017**]

2-{[2-Chloro-5-(trifluoromethyl)phenyl]iminomethyl]phenol

M.-H. Yang and Y.-F. Zheng

Comment

Schiff base ligands have significant importance in chemistry, especially in the development of Schiff base complexes (Johnson *et al.*, 1996; Alizadeh *et al.*, 1999; Wang & Zheng, 2007). Schiff bases that have solvent-dependent UV/vis spectra (solvatochromicity) can be suitable NLO (non-linear optically active) materials (Alemi & Shaabani, 2000). They are also useful in the asymmetric oxidation of methyl phenyl sulfide and are enantioselective (Kim & Shin, 1999). In this paper, we report the synthesis and crystal structure of the title compound, (I).

The molecular structure of the title compound is ramification of Schiff base (Fig. 1) The C7—N1 bond length is 1.283 (2) Å, indicative of a C═N double bond. The C—Cl, C—O and C—C distances are unremarkable. The dihedral angle between the two benzene rings is 47.7 (3) Å.

Experimental

Under nitrogen, a mixture of 2-chloro-5-(trifluoromethyl)aniline (1.95 g, 10 mmol), Na_2SO_4 (3.0 g) and 2-hydroxybenzaldehyde (1.22 g, 10 mmol) in absolute ethanol (20 ml) was refluxed for about 12 h to yield a yellow precipitate. The product was collected by vacuum filtration and washed with ethanol. The crude solid was redissolved in CH_2Cl_2 (100 ml) and washed with water (2 *x* 15 ml) and brine (8 ml). After drying over Na_2SO_4, the solvent was removed under vacuum, and a yellow solid was isolated in 90% yield (2.70 g). Colourless single crystals of the Schiff base, (I), suitable for X-ray analysis were grown from CH_2Cl_2 and absolute ethanol (4:1) by slow evaporation of the solvents at room temperature over a period of about three weeks.

Refinement

All H atoms were placed in calculated positions [Csp^2—H = 0.93 Å, O—H = 0.82 Å] and refined using a riding model, with U_{iso}(H) = 1.2U_{eq}(C, O). One trifluoromethyl group (at C13) was treated as disordered between two orientations with the refined occupancies of 0.70 (3) and 0.30 (3), respectively. A number of bond restraints has been applied for this group in the refinement.

Figures

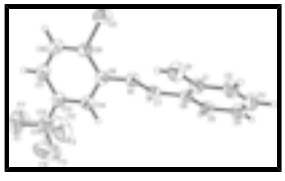


Fig. 1. The molecular structure of (I), showing the atomic numbering scheme, disordered CF_3 group and 30% probability displacement ellipsoids.

2-{[2-Chloro-5-(trifluoromethyl)phenyl]iminomethyl]phenol

Crystal data

$C_{14}H_9ClF_3NO$	F_{000} = 608
M_r = 299.67	D_x = 1.518 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 2303 reflections
a = 12.979 (6) Å	θ = 3.0–25.2º
b = 7.418 (3) Å	μ = 0.32 mm^{-1}
c = 13.881 (6) Å	T = 298 (2) K
β = 101.064 (7)º	Block, colourless
V = 1311.6 (10) Å^3	0.28 × 0.22 × 0.15 mm
Z = 4	

Data collection

Bruker APEX-II area-detector diffractometer	2303 independent reflections
Radiation source: fine-focus sealed tube	1411 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.029
T = 298(2) K	θ_{max} = 25.2º
φ and ω scan	θ_{min} = 3.0º
Absorption correction: multi-scan (SADABS; Sheldrick, 2004)	h = −15→14
T_{min} = 0.916, T_{max} = 0.954	k = −8→8
7694 measured reflections	l = −16→16

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.030	H-atom parameters constrained
$wR(F^2)$ = 0.070	$w = 1/[\sigma^2(F_o^2) + (0.0314P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 0.96	$(\Delta/\sigma)_{max} < 0.001$
2303 reflections	$\Delta\rho_{max}$ = 0.12 e Å^{-3}
210 parameters	$\Delta\rho_{min}$ = −0.16 e Å^{-3}
69 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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}	Occ. (<1)
Cl1	0.63136 (4)	0.08790 (6)	0.59424 (3)	0.0854 (2)	
O1	0.40859 (9)	0.40057 (17)	0.42934 (8)	0.0778 (3)	
H1	0.4706	0.3721	0.4451	0.117*	
N1	0.58895 (10)	0.27658 (15)	0.40482 (9)	0.0545 (3)	
C8	0.69623 (12)	0.24343 (18)	0.44034 (10)	0.0519 (4)	
C7	0.54804 (12)	0.24459 (18)	0.31476 (11)	0.0528 (4)	
H7	0.5896	0.1956	0.2738	0.063*	
C6	0.43864 (12)	0.28297 (19)	0.27537 (10)	0.0512 (4)	
C5	0.39664 (14)	0.2422 (2)	0.17731 (11)	0.0652 (4)	
H5	0.4397	0.1934	0.1376	0.078*	
C1	0.37309 (13)	0.3581 (2)	0.33403 (12)	0.0592 (4)	
C14	0.77401 (13)	0.29778 (19)	0.39131 (11)	0.0565 (4)	
H14	0.7558	0.3553	0.3309	0.068*	
C9	0.72630 (14)	0.15890 (19)	0.53128 (11)	0.0604 (4)	
C12	0.87901 (13)	0.2676 (2)	0.43115 (12)	0.0614 (4)	
C11	0.90654 (15)	0.1808 (2)	0.52090 (13)	0.0745 (5)	
H11	0.9768	0.1594	0.5476	0.089*	
C4	0.29257 (17)	0.2735 (2)	0.13898 (14)	0.0813 (5)	
H4	0.2649	0.2448	0.0739	0.098*	
C2	0.26852 (15)	0.3908 (2)	0.29453 (15)	0.0773 (5)	
H2	0.2248	0.4415	0.3330	0.093*	
C3	0.22978 (16)	0.3476 (2)	0.19782 (17)	0.0866 (6)	
H3	0.1594	0.3691	0.1717	0.104*	
C10	0.82995 (16)	0.1266 (2)	0.57015 (12)	0.0741 (5)	
H10	0.8483	0.0678	0.6302	0.089*	
C13	0.96069 (17)	0.3228 (3)	0.37635 (16)	0.0797 (5)	0.70 (3)
F3	0.9374 (6)	0.4774 (8)	0.3282 (6)	0.1087 (17)	0.70 (3)
F1	1.0542 (5)	0.3515 (13)	0.4326 (4)	0.1155 (19)	0.70 (3)
F2	0.9751 (7)	0.2058 (7)	0.3093 (5)	0.1148 (16)	0.70 (3)
C13'	0.96069 (17)	0.3228 (3)	0.37635 (16)	0.0797 (5)	0.30 (3)
F1'	1.0556 (10)	0.290 (4)	0.4232 (15)	0.146 (6)	0.30 (3)
F2'	0.951 (2)	0.231 (3)	0.2911 (15)	0.170 (7)	0.30 (3)
F3'	0.957 (2)	0.4929 (17)	0.350 (2)	0.131 (6)	0.30 (3)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0968 (4)	0.0917 (4)	0.0741 (3)	0.0008 (3)	0.0328 (3)	0.0167 (2)
O1	0.0701 (8)	0.0978 (9)	0.0688 (7)	0.0127 (7)	0.0216 (6)	−0.0104 (6)
N1	0.0546 (9)	0.0567 (8)	0.0526 (8)	0.0022 (6)	0.0110 (6)	−0.0008 (6)
C8	0.0556 (11)	0.0490 (9)	0.0510 (9)	0.0032 (8)	0.0102 (8)	−0.0045 (7)
C7	0.0571 (11)	0.0469 (9)	0.0583 (10)	−0.0016 (8)	0.0209 (8)	−0.0001 (7)
C6	0.0509 (10)	0.0478 (9)	0.0552 (9)	−0.0044 (7)	0.0108 (8)	0.0043 (7)
C5	0.0714 (13)	0.0601 (11)	0.0624 (11)	−0.0095 (9)	0.0083 (9)	0.0014 (8)
C1	0.0545 (12)	0.0570 (10)	0.0674 (11)	0.0005 (8)	0.0147 (9)	0.0049 (8)
C14	0.0583 (12)	0.0579 (10)	0.0536 (9)	0.0036 (8)	0.0115 (8)	−0.0011 (7)
C9	0.0685 (12)	0.0595 (10)	0.0547 (10)	0.0027 (8)	0.0157 (8)	−0.0002 (8)
C12	0.0548 (11)	0.0659 (11)	0.0630 (10)	0.0009 (9)	0.0096 (8)	−0.0062 (8)
C11	0.0610 (12)	0.0867 (13)	0.0705 (11)	0.0109 (10)	−0.0006 (10)	−0.0023 (10)
C4	0.0799 (15)	0.0759 (13)	0.0779 (12)	−0.0108 (11)	−0.0101 (11)	0.0056 (10)
C2	0.0593 (13)	0.0732 (13)	0.1010 (15)	0.0071 (10)	0.0194 (10)	0.0066 (11)
C3	0.0573 (13)	0.0765 (13)	0.1162 (17)	−0.0031 (10)	−0.0077 (13)	0.0165 (12)
C10	0.0781 (14)	0.0836 (13)	0.0571 (10)	0.0129 (11)	0.0042 (10)	0.0082 (9)
C13	0.0599 (15)	0.0961 (18)	0.0825 (15)	−0.0006 (14)	0.0125 (12)	−0.0028 (14)
F3	0.079 (2)	0.129 (4)	0.126 (3)	−0.006 (2)	0.0405 (17)	0.032 (2)
F1	0.063 (3)	0.174 (4)	0.107 (3)	−0.030 (3)	0.0110 (19)	−0.017 (4)
F2	0.107 (3)	0.125 (4)	0.128 (3)	−0.0154 (18)	0.064 (2)	−0.0488 (19)
C13'	0.0599 (15)	0.0961 (18)	0.0825 (15)	−0.0006 (14)	0.0125 (12)	−0.0028 (14)
F1'	0.045 (6)	0.182 (12)	0.210 (14)	0.024 (7)	0.020 (7)	0.094 (9)
F2'	0.133 (10)	0.278 (18)	0.116 (7)	−0.051 (9)	0.070 (6)	−0.053 (7)
F3'	0.116 (10)	0.084 (7)	0.206 (13)	−0.007 (5)	0.061 (8)	0.036 (6)

Geometric parameters (Å, °)

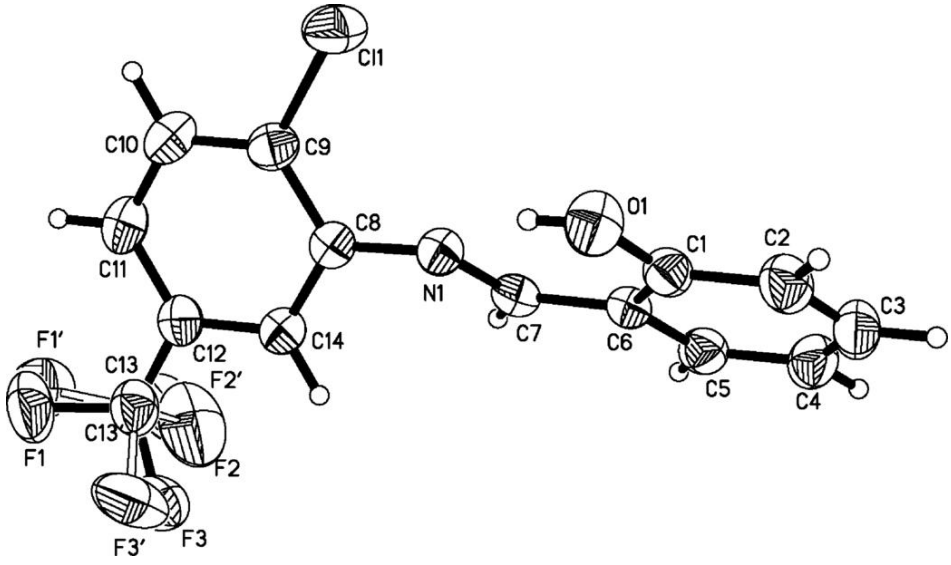
Cl1—C9	1.7242 (17)	C14—H14	0.9300
O1—C1	1.3520 (18)	C9—C10	1.371 (2)
O1—H1	0.8200	C12—C11	1.387 (2)
N1—C7	1.2831 (18)	C12—C13	1.477 (2)
N1—C8	1.4068 (19)	C11—C10	1.370 (2)
C8—C14	1.382 (2)	C11—H11	0.9300
C8—C9	1.396 (2)	C4—C3	1.374 (3)
C7—C6	1.449 (2)	C4—H4	0.9300
C7—H7	0.9300	C2—C3	1.378 (2)
C6—C5	1.399 (2)	C2—H2	0.9300
C6—C1	1.401 (2)	C3—H3	0.9300
C5—C4	1.373 (2)	C10—H10	0.9300
C5—H5	0.9300	C13—F2	1.312 (5)
C1—C2	1.384 (2)	C13—F1	1.329 (5)
C14—C12	1.387 (2)	C13—F3	1.333 (5)
C7—N1—C8	120.38 (13)	C11—C12—C13	120.32 (18)
C14—C8—C9	118.20 (15)	C14—C12—C13	119.83 (17)

C14—C8—N1	122.96 (13)	C10—C11—C12	119.86 (17)
C9—C8—N1	118.78 (14)	C10—C11—H11	120.1
N1—C7—C6	121.59 (14)	C12—C11—H11	120.1
N1—C7—H7	119.2	C5—C4—C3	119.25 (18)
C6—C7—H7	119.2	C5—C4—H4	120.4
C5—C6—C1	119.00 (15)	C3—C4—H4	120.4
C5—C6—C7	119.71 (15)	C3—C2—C1	119.47 (18)
C1—C6—C7	121.28 (14)	C3—C2—H2	120.3
C4—C5—C6	120.75 (18)	C1—C2—H2	120.3
C4—C5—H5	119.6	C4—C3—C2	121.66 (18)
C6—C5—H5	119.6	C4—C3—H3	119.2
O1—C1—C2	118.10 (15)	C2—C3—H3	119.2
O1—C1—C6	122.03 (15)	C11—C10—C9	120.22 (16)
C2—C1—C6	119.86 (16)	C11—C10—H10	119.9
C8—C14—C12	120.75 (15)	C9—C10—H10	119.9
C8—C14—H14	119.6	F2—C13—F1	106.5 (4)
C12—C14—H14	119.6	F2—C13—F3	105.3 (4)
C10—C9—C8	121.14 (15)	F1—C13—F3	104.5 (4)
C10—C9—Cl1	119.33 (13)	F2—C13—C12	113.4 (3)
C8—C9—Cl1	119.50 (13)	F1—C13—C12	114.0 (3)
C11—C12—C14	119.81 (16)	F3—C13—C12	112.4 (4)
C7—N1—C8—C14	46.70 (19)	C8—C14—C12—C13	178.50 (16)
C7—N1—C8—C9	−136.21 (14)	C14—C12—C11—C10	−0.5 (2)
C8—N1—C7—C6	−177.93 (12)	C13—C12—C11—C10	−178.58 (17)
N1—C7—C6—C5	−178.56 (13)	C6—C5—C4—C3	0.7 (3)
N1—C7—C6—C1	0.5 (2)	O1—C1—C2—C3	−179.45 (15)
C1—C6—C5—C4	−0.6 (2)	C6—C1—C2—C3	0.5 (2)
C7—C6—C5—C4	178.46 (14)	C5—C4—C3—C2	−0.2 (3)
C5—C6—C1—O1	179.94 (13)	C1—C2—C3—C4	−0.4 (3)
C7—C6—C1—O1	0.9 (2)	C12—C11—C10—C9	−0.4 (3)
C5—C6—C1—C2	0.0 (2)	C8—C9—C10—C11	1.4 (2)
C7—C6—C1—C2	−179.07 (13)	Cl1—C9—C10—C11	179.52 (13)
C9—C8—C14—C12	0.5 (2)	C11—C12—C13—F2	96.0 (5)
N1—C8—C14—C12	177.65 (13)	C14—C12—C13—F2	−82.1 (5)
C14—C8—C9—C10	−1.5 (2)	C11—C12—C13—F1	−26.1 (5)
N1—C8—C9—C10	−178.71 (13)	C14—C12—C13—F1	155.8 (5)
C14—C8—C9—Cl1	−179.58 (11)	C11—C12—C13—F3	−144.8 (4)
N1—C8—C9—Cl1	3.19 (18)	C14—C12—C13—F3	37.1 (5)
C8—C14—C12—C11	0.5 (2)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N1	0.82	1.87	2.5975 (19)	147

Fig. 1


Cl1
C10
C9
O1
C8
C1
C2
C11
N1
C3
F1′
C13
C12
C14
C7
C6
F2′
C5
C4
C13′
F1
F2
F3′
F3