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2,4-Dichloro-6-{[4-chloro-3-(trifluoromethyl)phenyl]iminomethyl}phenol

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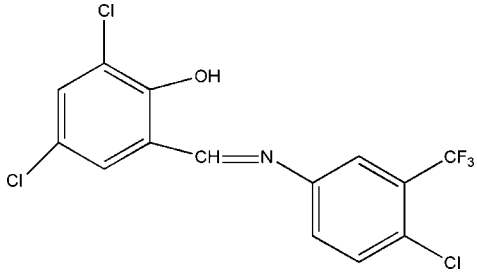
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.003 Å; R factor = 0.031; wR factor = 0.080; data-to-parameter ratio = 12.6.

In the title Schiff base, $C_{14}H_7Cl_3F_3NO$, one intramolecular hydrogen bond stabilizes the molecular structure. The dihedral angle between the two benzene rings in the molecule is 47.86 (4)°.

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

$C_{14}H_7Cl_3F_3NO$
M_r = 368.56
Monoclinic, $P2_1/c$
a = 8.6093 (6) Å
b = 22.9730 (16) Å
c = 7.9014 (5) Å
β = 111.204 (1)°
V = 1456.95 (17) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.66 mm^{-1}
T = 298 (2) K
0.19 × 0.16 × 0.15 mm

Data collection

Bruker APEX II area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.885, T_{max} = 0.907
8909 measured reflections
2523 independent reflections
1704 reflections with $I > 2\sigma(I)$
R_{int} = 0.037

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.080
S = 0.90
2523 reflections
200 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 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	1.88	2.5957 (19)	145

Data collection: *APEX2* (Bruker, 2004); cell refinement: *APEX2*; data reduction: *APEX2*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1998); 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: IS2185).

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supplementary materials

Acta Cryst. (2007). E**63**, o3401 [**doi:10.1107/S1600536807031972**]

2,4-Dichloro-6-{[4-chloro-3-(trifluoromethyl)phenyl]iminomethyl}phenol

C.-N. Zhang and M.-H. Yang

Comment

Schiff base ligands have significant importance in chemistry, especially, in the development of Schiff base complexes, because Schiff base ligands are potentially capable of forming stable complexes with metal ions (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 (nonlinear optical active) materials (Alemi & Shaabani, 2000). They are also useful in asymmetric oxidation of methyl phenyl sulfide and enantioselective (Kim & Shin, 1999). In this paper, we report here the synthesis and crystal structure of the title compound, (I).

The molecular structure of the title compound (Fig. 1) contains one intramolecular hydrogen bond (Table 1). The C8—N1 is 1.278 (2) Å, indicative of standard C=N double bond. The other C—N, C—Cl and C—C distances show no remarkable features. The dihedral angle between two benzene rings in the title molecule is 47.86 (4)°.

Experimental

Under nitrogen, a mixture of 4-chloro-3-(trifluoromethyl)benzenamine (1.92 g, 10 mmol), Na_2SO_4 (3.0 g) and 3,5-dichloro-2-hydroxybenzaldehyde (1.66 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 × 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 92% yield (3.1 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 one week.

Refinement

All H atoms were placed in calculated positions (C—H = 0.93 and O—H = 0.82 Å) and refined using a riding model, with U_{iso}(H) = 1.2U_{eq}(C) and 1.5U_{eq}(O).

Figures

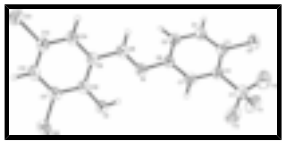


Fig. 1. The molecular structure of (I), showing the atomic numbering scheme. Non-H atoms are shown as 50% probability displacement ellipsoids.

2,4-Dichloro-6-{[4-chloro-3-(trifluoromethyl)phenyl]iminomethyl}phenol

Crystal data

$C_{14}H_7Cl_3F_3NO$	F_{000} = 736
M_r = 368.56	D_x = 1.680 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 2502 reflections
a = 8.6093 (6) Å	θ = 1.7–28.0º
b = 22.9730 (16) Å	μ = 0.66 mm^{-1}
c = 7.9014 (5) Å	T = 298 (2) K
β = 111.204 (1)º	Block, colourless
V = 1456.95 (17) Å^3	0.19 × 0.16 × 0.15 mm
Z = 4	

Data collection

Bruker APEX II area-detector diffractometer	2523 independent reflections
Radiation source: fine-focus sealed tube	1704 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.037
T = 298(2) K	θ_{max} = 25.2º
φ and ω scans	θ_{min} = 1.8º
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	h = −10→10
T_{min} = 0.885, T_{max} = 0.907	k = −27→26
8909 measured reflections	l = −8→9

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.031	H-atom parameters constrained
$wR(F^2)$ = 0.080	$w = 1/[\sigma^2(F_o^2) + (0.0476P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 0.90	$(\Delta/\sigma)_{max} < 0.001$
2523 reflections	$\Delta\rho_{max}$ = 0.25 e Å^{-3}
200 parameters	$\Delta\rho_{min}$ = −0.25 e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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	0.15918 (7)	0.52233 (2)	0.33997 (8)	0.0804 (2)
Cl2	0.79951 (8)	0.09612 (2)	0.71667 (8)	0.0815 (2)
Cl3	1.25114 (7)	0.22761 (3)	1.22425 (8)	0.0825 (2)
O1	0.62110 (17)	0.20466 (5)	0.60598 (19)	0.0613 (4)
H1	0.5829	0.2367	0.5663	0.092*
N1	0.59189 (19)	0.31700 (7)	0.6135 (2)	0.0522 (4)
C9	0.8203 (2)	0.26618 (8)	0.8258 (2)	0.0479 (5)
C3	0.2901 (2)	0.46309 (8)	0.4173 (3)	0.0535 (5)
C10	0.7643 (2)	0.21157 (8)	0.7483 (3)	0.0498 (5)
C14	0.9707 (2)	0.27044 (8)	0.9732 (3)	0.0546 (5)
H14	1.0077	0.3066	1.0253	0.066*
C7	0.4266 (2)	0.37778 (8)	0.3681 (3)	0.0532 (5)
H7	0.4491	0.3518	0.2896	0.064*
C8	0.7238 (2)	0.31842 (8)	0.7560 (3)	0.0518 (5)
H8	0.7584	0.3536	0.8161	0.062*
C6	0.4947 (2)	0.36810 (8)	0.5533 (3)	0.0482 (5)
C11	0.8632 (2)	0.16297 (8)	0.8196 (3)	0.0565 (5)
C12	1.0111 (2)	0.16771 (9)	0.9657 (3)	0.0616 (5)
H12	1.0749	0.1348	1.0127	0.074*
C13	1.0638 (2)	0.22165 (9)	1.0415 (3)	0.0569 (5)
C4	0.3564 (2)	0.45298 (9)	0.6018 (3)	0.0587 (5)
H4	0.3321	0.4782	0.6808	0.070*
C2	0.3256 (2)	0.42545 (8)	0.2980 (3)	0.0513 (5)
C5	0.4583 (2)	0.40582 (8)	0.6696 (3)	0.0547 (5)
H5	0.5027	0.3993	0.7942	0.066*
C1	0.2572 (3)	0.43443 (11)	0.0974 (3)	0.0731 (6)
F1	0.09308 (19)	0.43127 (7)	0.02775 (19)	0.1100 (5)
F2	0.3073 (2)	0.39374 (7)	0.00968 (18)	0.1127 (5)
F3	0.2992 (2)	0.48465 (7)	0.0468 (2)	0.1208 (6)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0838 (4)	0.0581 (3)	0.0883 (4)	0.0195 (3)	0.0179 (3)	0.0103 (3)
Cl2	0.1047 (5)	0.0476 (3)	0.0908 (5)	0.0039 (3)	0.0337 (4)	0.0002 (3)
Cl3	0.0610 (3)	0.1032 (5)	0.0728 (4)	0.0193 (3)	0.0113 (3)	−0.0040 (3)
O1	0.0639 (9)	0.0526 (8)	0.0627 (9)	0.0000 (6)	0.0172 (7)	0.0020 (7)
N1	0.0568 (10)	0.0503 (9)	0.0517 (10)	0.0042 (7)	0.0226 (9)	0.0066 (7)
C9	0.0518 (11)	0.0493 (11)	0.0488 (12)	0.0044 (9)	0.0255 (10)	0.0052 (9)
C3	0.0551 (12)	0.0422 (11)	0.0609 (14)	0.0016 (9)	0.0181 (10)	0.0050 (9)
C10	0.0539 (11)	0.0532 (12)	0.0489 (12)	0.0025 (9)	0.0264 (10)	0.0063 (9)
C14	0.0550 (12)	0.0570 (12)	0.0570 (13)	0.0049 (10)	0.0266 (10)	−0.0020 (10)
C7	0.0585 (11)	0.0509 (11)	0.0523 (13)	−0.0019 (9)	0.0225 (10)	−0.0017 (9)
C8	0.0565 (12)	0.0486 (11)	0.0553 (13)	0.0008 (9)	0.0262 (11)	0.0018 (9)
C6	0.0515 (11)	0.0450 (10)	0.0480 (12)	0.0001 (8)	0.0180 (9)	0.0048 (9)
C11	0.0689 (13)	0.0473 (11)	0.0617 (14)	0.0062 (10)	0.0335 (11)	0.0049 (9)
C12	0.0653 (13)	0.0604 (13)	0.0636 (14)	0.0192 (11)	0.0289 (12)	0.0128 (11)
C13	0.0522 (11)	0.0709 (14)	0.0518 (12)	0.0122 (10)	0.0238 (10)	0.0040 (10)
C4	0.0655 (13)	0.0529 (12)	0.0577 (14)	0.0047 (10)	0.0225 (11)	−0.0061 (10)
C2	0.0541 (11)	0.0501 (11)	0.0464 (12)	−0.0030 (9)	0.0142 (9)	0.0065 (9)
C5	0.0591 (12)	0.0554 (12)	0.0478 (12)	0.0046 (9)	0.0172 (10)	0.0022 (9)
C1	0.0815 (17)	0.0714 (16)	0.0591 (15)	0.0084 (13)	0.0167 (13)	0.0058 (12)
F1	0.0860 (10)	0.1488 (15)	0.0682 (10)	0.0080 (9)	−0.0045 (8)	0.0074 (8)
F2	0.1564 (14)	0.1246 (13)	0.0533 (9)	0.0440 (11)	0.0332 (9)	0.0051 (8)
F3	0.1825 (17)	0.0976 (12)	0.0735 (10)	−0.0228 (10)	0.0358 (10)	0.0324 (8)

Geometric parameters (Å, °)

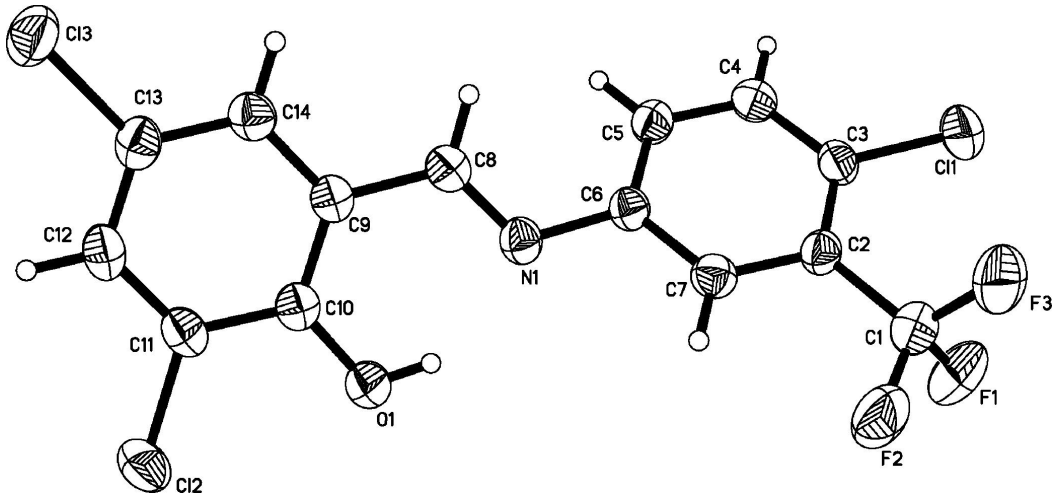
Cl1—C3	1.7314 (19)	C7—C6	1.383 (2)
Cl2—C11	1.731 (2)	C7—C2	1.384 (2)
Cl3—C13	1.738 (2)	C7—H7	0.9300
O1—C10	1.344 (2)	C8—H8	0.9300
O1—H1	0.8200	C6—C5	1.379 (3)
N1—C8	1.278 (2)	C11—C12	1.380 (3)
N1—C6	1.420 (2)	C12—C13	1.380 (3)
C9—C14	1.397 (3)	C12—H12	0.9300
C9—C10	1.403 (2)	C4—C5	1.375 (3)
C9—C8	1.450 (2)	C4—H4	0.9300
C3—C4	1.379 (3)	C2—C1	1.492 (3)
C3—C2	1.392 (3)	C5—H5	0.9300
C10—C11	1.393 (2)	C1—F3	1.314 (3)
C14—C13	1.370 (2)	C1—F1	1.320 (3)
C14—H14	0.9300	C1—F2	1.325 (3)
C10—O1—H1	109.5	C12—C11—Cl2	120.17 (15)
C8—N1—C6	120.14 (16)	C10—C11—Cl2	118.53 (16)
C14—C9—C10	119.68 (17)	C11—C12—C13	119.55 (18)
C14—C9—C8	119.35 (17)	C11—C12—H12	120.2

C10—C9—C8	120.97 (17)	C13—C12—H12	120.2
C4—C3—C2	120.18 (17)	C14—C13—C12	120.67 (19)
C4—C3—Cl1	118.25 (16)	C14—C13—Cl3	119.87 (16)
C2—C3—Cl1	121.56 (15)	C12—C13—Cl3	119.47 (15)
O1—C10—C11	119.00 (17)	C5—C4—C3	120.43 (19)
O1—C10—C9	122.50 (16)	C5—C4—H4	119.8
C11—C10—C9	118.49 (18)	C3—C4—H4	119.8
C13—C14—C9	120.34 (18)	C7—C2—C3	118.71 (17)
C13—C14—H14	119.8	C7—C2—C1	118.97 (19)
C9—C14—H14	119.8	C3—C2—C1	122.32 (18)
C6—C7—C2	121.02 (18)	C4—C5—C6	120.13 (19)
C6—C7—H7	119.5	C4—C5—H5	119.9
C2—C7—H7	119.5	C6—C5—H5	119.9
N1—C8—C9	121.22 (18)	F3—C1—F1	107.0 (2)
N1—C8—H8	119.4	F3—C1—F2	106.4 (2)
C9—C8—H8	119.4	F1—C1—F2	104.2 (2)
C5—C6—C7	119.50 (17)	F3—C1—C2	113.49 (19)
C5—C6—N1	122.99 (17)	F1—C1—C2	112.8 (2)
C7—C6—N1	117.39 (17)	F2—C1—C2	112.34 (19)
C12—C11—C10	121.27 (18)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N1	0.82	1.88	2.5957 (19)	145

Fig. 1


Cl3
C13
C14
C8
C9
C12
C10
C11
O1
Cl2
N1
C6
C5
C4
C3
Cl1
C2
C7
C1
F3
F1
F2