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3,5-Dichloro-*N*-(4-fluorobenzylidene)aniline

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.002 Å
R factor = 0.037
wR factor = 0.106
Data-to-parameter ratio = 18.2

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

In the title compound, $C_{13}H_8Cl_2FN$, the central C=N bond length is 1.2699 (18) Å and the bond length between the C atom of the aromatic ring and the C atom of the imine group is 1.4644 (19) Å. This arrangement corresponds to a conjugated C=N moiety.

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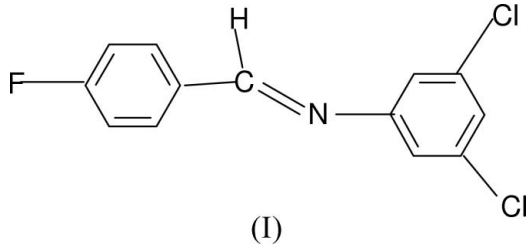
Comment

Schiff base compounds have been of great interest for many years. They play an important role in the development of coordination chemistry related to catalysis and enzymatic reactions, magnetism and molecular architectures. As an extension of work on the structural characterization of Schiff base compounds, the crystal structure of the title compound, (I), is reported here.



(I)

All the bond lengths in (I) (Fig. 1) are within normal ranges (Allen *et al.*, 1987). The C7=N1 bond length is 1.2699 (18) Å and the C1=C7 bond length is 1.4644 (19) Å. This arrangement corresponds to a conjugated C=N group. The dihedral angle between the benzene rings is 37.9 (5)°.

Experimental

3,5-Dichloroaniline (162 mg, 1 mmol) and 4-fluorobenzaldehyde (124 mg, 1 mmol) were stirred in ethanol (10 ml) for 1 h. After allowing the resulting solution to stand in air for 15 d, white crystals were formed on slow evaporation of the solvent. The crystals were isolated, washed with ethanol and dried. Elemental analysis found: C 58.36, H 2.97, N 5.20, F 7.13%; calculated for $C_{13}H_8Cl_2FN$: C 58.24, H 3.01, N 5.22, F 7.09%.

Crystal data

$C_{13}H_8Cl_2FN$
M_r = 268.10
Monoclinic, $P2_1/c$
a = 14.1311 (7) Å
b = 3.8481 (2) Å
c = 22.0365 (11) Å
β = 94.752 (1)°
V = 1194.18 (10) Å^3
Z = 4
D_x = 1.491 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1023 reflections
θ = 4.4–28.6°
μ = 0.53 mm^{-1}
T = 298 (2) K
Block, white
0.60 × 0.47 × 0.39 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.742, T_{max} = 0.820
13224 measured reflections
2863 independent reflections
2506 reflections with $I > 2\sigma(I)$
R_{int} = 0.017
θ_{max} = 28.0°
$h = -18 \rightarrow 18$
$k = -5 \rightarrow 5$
$l = -28 \rightarrow 29$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.106
S = 1.05
2863 reflections
157 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0573P)^2 + 0.3432P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.38 e Å^{-3}
$\Delta\rho_{min}$ = −0.51 e Å^{-3}

The H atom on C7 was located in a difference Fourier map and its positional parameters was refined with a fixed U_{iso}(H) value of 1.2 Å^2. The other H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C).

Data collection: *SMART* (Siemens, 1996); cell refinement: *SMART*; data reduction: *SAINT* (Siemens, 1996); 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*.

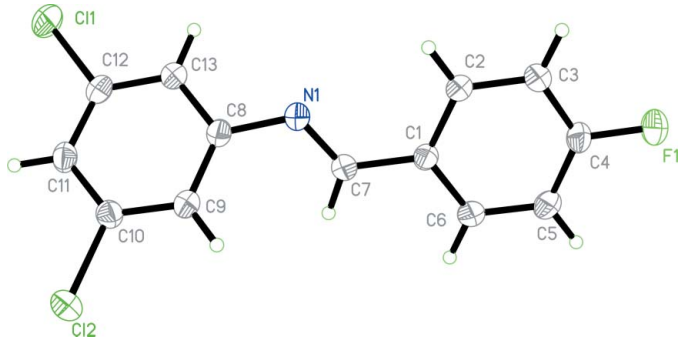


Figure 1
The molecular structure of (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme.

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