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# 4-Chloro-1-[2,6-dichloro-4-(trifluoromethyl)-phenyl]-5-(4-methylbenzylideneamino)-1*H*-pyrazole-3-carbonitrile

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The molecular structure of the title tricyclic imine, $C_{19}H_{10}Cl_3F_3N_4$, has an overall Y-shape, with each of the three rings being essentially planar. The dihedral angles between the pyrazole ring and the two benzene rings are 72.28 (14) and 25.6 (2)°.

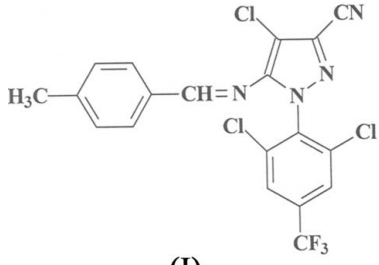
**Key indicators**

Single-crystal X-ray study
*T* = 298 K
Mean σ(C–C) = 0.007 Å
*R* factor = 0.073
*wR* factor = 0.209
Data-to-parameter ratio = 13.4

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

## Comment

The title compound, (I), is similar to the very effective imine-containing insecticides which are used for treating animals such as cows and sheep (Philippe, 1997, 2000).




(I)

The molecular structure of (I) is shown in Fig. 1. The molecule contains three essentially planar rings, forming an overall Y-shape. The dihedral angles between the pyrazole ring and the C1–C6 and C12–C17 benzene rings are 72.28 (14) and 25.6 (2)°, respectively.

## Experimental

According to the method of Zhong *et al.*, (2005), using 5-amino-3-cyano-1-(2,6-dichloro-4-trifluoromethylphenyl)-pyrazole, we obtained 1-(2,6-dichloro-4-trifluoromethylphenyl)-3-cyano-5-[(4-methylbenzylidene)amino]-1*H*-pyrazole, which was then reacted with sulfinyl dichloride (0.36 ml) in ethyl acetate (8 ml) under ice cooling and a stream of nitrogen (Okui, 2005). After stirring for 1 h, the vessel was left at room temperature and stirred further. The reaction was monitored at intervals by thin-layer chromatography until completion. Saturated aqueous sodium hydrogen carbonate solution (2 ml) was added and the organic layer was washed with saturated aqueous sodium hydrogen carbonate solution (15 ml) and water (15 ml) several times. The organic layer was purified by silica-gel column chromatography. Removal of the solvent gave the title compound (92% yield). Colourless single crystals suitable for X-ray analysis were obtained by slow evaporation of an anhydrous ethanol–acetone (3:1) solution of (I) (m.p. 451–453 K).

*Crystal data*

$C_{19}H_{10}Cl_3F_3N_4$
$M_r$ = 457.66
Monoclinic, $P2_1/c$
$a$ = 17.678 (4) Å
$b$ = 10.262 (2) Å
$c$ = 11.477 (3) Å
$\beta$ = 106.935 (4)°
$V$ = 1991.8 (8) Å$^3$
$Z$ = 4
$D_x$ = 1.526 Mg m$^{-3}$
Mo $K\alpha$ radiation
$\mu$ = 0.50 mm$^{-1}$
$T$ = 298 (2) K
Block, colourless
0.23 × 0.18 × 0.13 mm

*Data collection*

Bruker APEX area-detector diffractometer
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
$T_{min}$ = 0.894, $T_{max}$ = 0.938
10217 measured reflections
3517 independent reflections
2685 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.032
$\theta_{max}$ = 25.0°

*Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)]$ = 0.074
$wR(F^2)$ = 0.209
$S$ = 1.07
3517 reflections
263 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1002P)^2 + 2.0911P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.71 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.34 e Å$^{-3}$

**Table 1**
Selected geometric parameters (Å, °).

| | | | |
|---|---|---|---|
| Cl3—C9 | 1.745 (4) | N4—C12 | 1.279 (5) |
| F3—C1 | 1.305 (6) | N4—C10 | 1.374 (5) |
| N1—N2 | 1.346 (5) | C8—C9 | 1.396 (6) |
| N1—C10 | 1.374 (5) | C8—C11 | 1.427 (6) |
| N1—C5 | 1.422 (5) | C9—C10 | 1.360 (6) |
| N2—C8 | 1.329 (6) | C12—C13 | 1.454 (6) |
| N3—C11 | 1.131 (6) | | |
| N2—N1—C10 | 113.2 (3) | C9—C8—C11 | 128.3 (4) |
| N2—N1—C5 | 120.0 (3) | C10—C9—C8 | 106.2 (4) |
| C10—N1—C5 | 126.7 (3) | C10—C9—Cl3 | 130.0 (3) |
| C8—N2—N1 | 103.8 (3) | C8—C9—Cl3 | 123.8 (3) |
| C12—N4—C10 | 121.1 (4) | C9—C10—N1 | 105.0 (4) |
| F3—C1—F1 | 103.7 (5) | C9—C10—N4 | 137.6 (4) |
| N2—C8—C9 | 111.9 (4) | N1—C10—N4 | 117.1 (3) |
| N2—C8—C11 | 119.7 (4) | N4—C12—C13 | 122.6 (4) |

All H atoms were initially located in a difference Fourier map but were eventually placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H distances in the range 0.93–0.96 Å and with $U_{iso}$(H) = 1.2$U_{eq}$(C), or 1.5$U_{eq}$(C) for methyl C atoms. The large displacement parameters of atoms F1, F2 and F3 may indicate rotational disorder of the trifluoromethyl group. However, attempts to refine the $CF_3$ group using a disordered model were unsuccessful.

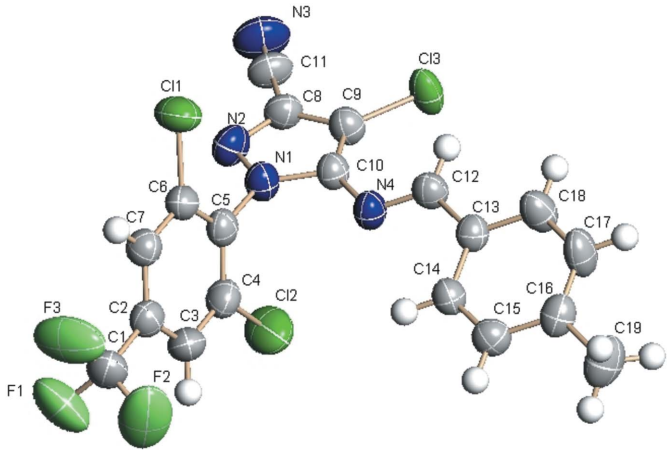



**Figure 1**
The molecular structure of (I), showing displacement ellipsoids at the 50% probability level and H atoms as small spheres of arbitrary radii.

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); 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, 2002); software used to prepare material for publication: *SHELXL97*.

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