Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

5-[(2-Benzylideneethylidene)amino]-1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-1*H*-pyrazole-3-carbonitrile

Shu-Yan Li, Ping Zhong,* Mao-Lin Hu, Yi Luo and Jin-Hai Li

Department of Chemistry, Wenzhou University, 325027 Wenzhou, People's Republic of China

Correspondence e-mail: zhongp0512@163.com

Received 18 April 2006
Accepted 9 May 2006

The title compound, $C_{20}H_{11}Cl_2F_3N_4$, is a tricyclic imine with an overall curved conformation. The pyrazole ring and the N-bound aromatic ring form a dihedral angle of 119.7 (2)°.

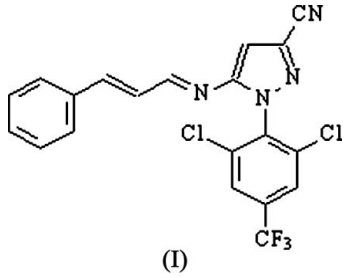
Key indicators

Single-crystal X-ray study
T = 273 K
Mean σ(C–C) = 0.004 Å
R factor = 0.052
wR factor = 0.129
Data-to-parameter ratio = 13.3

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

Comment

The title compound, (I) (Fig. 1 and Table 1), is an important starting material for the synthesis of various pyrazole derivatives, all of which are good insecticides (Hatton *et al.*, 1993).



(I)

As shown in Fig. 1, the molecule of (I) contains three planar groups forming an overall curved conformation, owing to substitution in the central pyrazole ring in adjacent positions. In the observed conformation, the pyrazole ring and the N-bound aromatic ring form a dihedral angle of 119.7 (2)°. The dihedral angle between the pyrazole and C2–C7 rings is 12.57 (1)°.

Experimental

According to the method of Hatton *et al.* (1993), reaction of 2,6-dichloro-4-(trifluoromethyl)aniline with a suspension of nitrosylsulfuric acid, followed by reaction with a solution of ethyl 2,3-dicyanopropionate in acetic acid, gave 5-amino-3-cyano-1-(2,6-dichloro-4-trifluoromethylphenyl)pyrazole, which was then reacted with cinnamaldehyde and hydrochloric acid in anhydrous ethanol to give the title compound, (I). This method is similar to that employed by others (Zhong, Yang & Shi, 2005; Zhong, Yang, Shi *et al.*, 2005; Chen *et al.*, 2005). Colourless single crystals of (I) suitable for X-ray analysis were obtained by slow evaporation of an anhydrous ethanol–acetone (3:1) solution (m.p. 433–433 K).

Crystal data

$C_{20}H_{11}Cl_2F_3N_4$
M_r = 435.23
Triclinic, $P\overline{1}$
a = 7.708 (5) Å
b = 9.503 (6) Å
c = 14.016 (9) Å
α = 86.064 (11)°
β = 84.310 (12)°
γ = 81.410 (12)°
V = 1008.6 (11) Å^3
Z = 2
D_x = 1.433 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.36 mm^{-1}
T = 273 (2) K
Block, colourless
0.31 × 0.23 × 0.17 mm

Data collection

Bruker APEX area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
T_{min} = 0.896, T_{max} = 0.941
5268 measured reflections
3490 independent reflections
2859 reflections with $I > 2\sigma(I)$
R_{int} = 0.013
θ_{max} = 25.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.052
$wR(F^2)$ = 0.129
S = 1.06
3490 reflections
262 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0593P)^2 + 0.2867P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.34 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

N1—N2	1.352 (3)	N4—C10	1.377 (3)
N1—C5	1.421 (3)	N4—C12	1.273 (3)
N1—C10	1.364 (3)	C8—C9	1.384 (4)
N2—C8	1.335 (3)	C8—C11	1.436 (4)
N3—C11	1.132 (4)	C9—C10	1.376 (4)
N2—N1—C5	119.7 (2)	N1—N2—C8	102.7 (2)
N2—N1—C10	113.93 (19)	C10—N4—C12	119.9 (2)
C5—N1—C10	126.2 (2)		

All H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H distances set at 0.93 Å and with $U_{iso}(H) = 1.2U_{eq}(C)$.

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*.

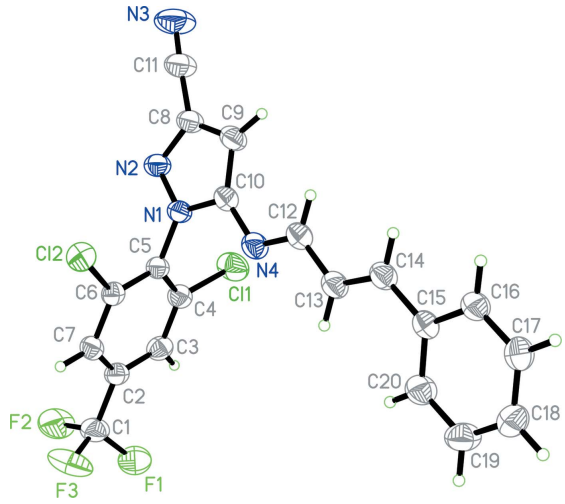


Figure 1
The molecular structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

This work was supported by the National Natural Science Foundation of China (grant No. 20572079) and the Natural Science Foundation of Zhejiang Province (grant No. Y205540).

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