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5-Chloro-1-(4-chlorophenyl)-4-(2-methoxybenzoylhydrazonomethyl)-3-methyl-1*H*-pyrazole

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Key indicators

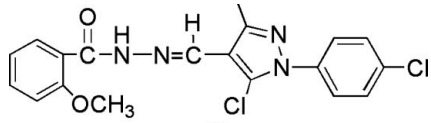
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.035
wR factor = 0.091
Data-to-parameter ratio = 13.6

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

In the title molecule, $C_{19}H_{16}C_{l2}N_4O_2$, all bond lengths and angles show normal values. The two benzene rings make a dihedral angle of 12.55 (2)°. The crystal packing is stabilized by weak intermolecular C—H···N hydrogen bonds and van der Waals forces.

Comment

Arylpyrazoles have a widespread occurrence as substructures in a large variety of compounds with important biological activities and pharmacological properties (Nizar & James, 2002). In the course of our systematic studies aimed at the synthesis of new bioactive compounds, we have synthesized the title compound, (I) (Fig. 1).



(I)

The bond lengths and angles (Table 1) in (I) are as expected for this type of compound. The pyrazole ring is planar, the largest deviation from planarity being 0.003 (4) Å for atom C8, and forms a dihedral angle of 50.45 (4)° with the C1–C6 benzene ring. The two benzene rings, C1–C6 and C13–C18, make a dihedral angle of 12.55 (2)°.

The crystal packing (Fig. 2) is stabilized by weak intermolecular C—H···N hydrogen bonds (Table 2) and van der Waals forces.

Experimental

To anhydrous ethanol (15 ml), a mixture of 2-methyloxybenzoylhydrazide (3 mmol, 0.500 g) and 5-chloro-1-(4-chlorophenyl)-3-methyl-1*H*-4-pyrazolaldehyde (3 mmol, 0.765 g), synthesized according to Li *et al.* (2004), was added and refluxed for 5 h. The solvent was removed under reduced pressure and the residue was recrystallized from ethanol (m.p. 458 K).

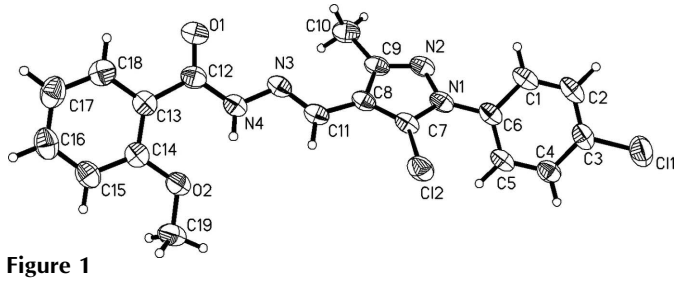


Figure 1
View of (I), shown with 35% probability displacement ellipsoids.

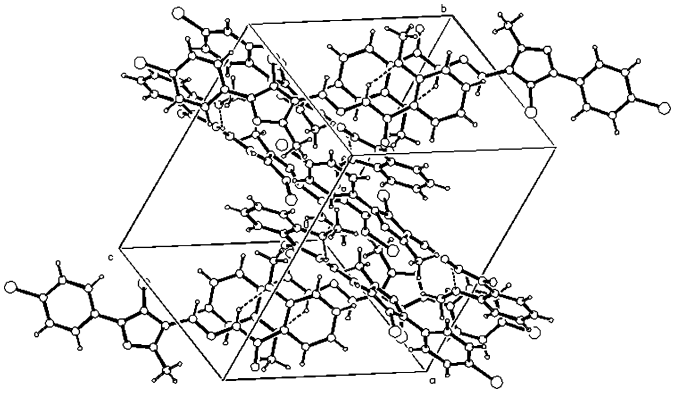


Figure 2
The packing of the title compound. Hydrogen bonds are shown as dashed lines.

Crystal data

$C_{19}H_{16}Cl_2N_4O_2$
M_r = 403.26
Monoclinic, $P2_1/n$
a = 9.3332 (10) Å
b = 16.7115 (19) Å
c = 12.3865 (14) Å
β = 101.839 (2)°
V = 1890.8 (4) Å^3
Z = 4
D_x = 1.417 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.37 mm^{-1}
T = 293 (2) K
Block, colourless
0.28 × 0.22 × 0.20 mm

Data collection

Bruker APEX-II CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.885, T_{max} = 0.998
(expected range = 0.824–0.929)
10116 measured reflections
3338 independent reflections
2462 reflections with $I > 2\sigma(I)$
R_{int} = 0.020
θ_{max} = 25.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.091
S = 1.04
3338 reflections
246 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0403P)^2 + 0.4272P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

O1—C12	1.222 (2)	N2—C9	1.316 (3)
O2—C14	1.365 (2)	N3—C11	1.278 (2)
N1—C7	1.354 (2)	C7—C8	1.367 (3)
N1—N2	1.374 (2)	C8—C9	1.418 (3)
C7—N1—N2	109.78 (17)	C7—C8—C9	103.59 (18)
C9—N2—N1	105.69 (15)	N2—C9—C8	111.88 (18)
N1—C7—C8	109.05 (17)		

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N4—H4A···O2	0.86	1.98	2.617 (2)	130
C2—H2···N3^{i}	0.93	2.54	3.421 (2)	158

Symmetry code: (i) $x+\frac{1}{2}, -y+\frac{1}{2}, z-\frac{1}{2}$.

All H atoms were placed in calculated positions, with C—H = 0.93 or 0.96 Å and N—H = 0.86 Å, and included in the final cycles of refinement using a riding model, with U_{iso}(H) set to 1.2U_{eq}(C,N) for CH and NH groups and 1.5U_{eq}(C) for methyl groups.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1999); 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, 1999); software used to prepare material for publication: *SHELXTL*.

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