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5-(2-Chlorophenyl)-3-(4-chlorophenyl)-1-phenyl-2-pyrazoline

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.041
wR factor = 0.112
Data-to-parameter ratio = 17.0

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

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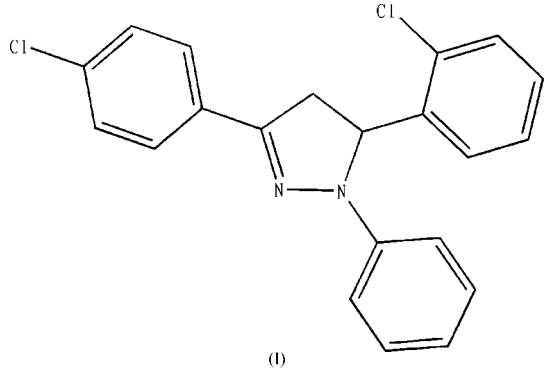
In the title structure, $C_{21}H_{16}Cl_2N_2$, the pyrazoline ring makes dihedral angles of 6.76 (9), 7.52 (10) and 81.88 (10)°, respectively, with the 4-chlorophenyl ring, the phenyl ring and the 2-chlorophenyl ring. The 5-phenyl ring is almost perpendicular to the pyrazoline ring.

Comment

Pyrazoline-based fluorophores have attracted much interest because of their simple structure and favorable photophysical properties, such as large extinction coefficient and quantum yield (Rivett *et al.*, 1983). The published data identify pyrazoline fluorophores as a platform for the development of PET-based cation fluorescent sensors (Fahrni *et al.*, 2003). Among them, 1,3,5-trisubstituted pyrazolines can be easily prepared from phenylhydrazine and chalcone derivatives (Nakamichi *et al.*, 2002). We report the crystal structure of the title compound, (I).



(I)

In (I) (Fig. 1), the C═N bond length [1.297 (2) Å] is longer and the N1—N2 bond length [1.380 (2) Å] is shorter than those in the similar structures reported by Rurack *et al.* (2000), Kimura *et al.* (1977) and Ge (2006) [C═N = 1.291 (2), 1.283 (2) and 1.293 (3) Å, respectively, and N—N = 1.394 (3), 1.390 (3) and 1.384 (2) Å, respectively]. The C—Cl bond lengths [1.750 (2) and 1.751 (2) Å] are slightly longer than that in a similar structure (1.745 Å; Kimura *et al.*, 1977). All the bond lengths and angles fall in the normal ranges. The pyrazoline ring makes dihedral angles of 6.76 (9), 7.52 (10) and 81.88 (10)°, respectively, with the *p*-chlorophenyl, phenyl and 2-chlorophenyl rings.

Experimental

Compound (I) was synthesized by reaction of phenylhydrazine (0.02 mol) and 1-(4-chlorophenyl)-3-(2-chlorophenyl)-2-propenyl-1-

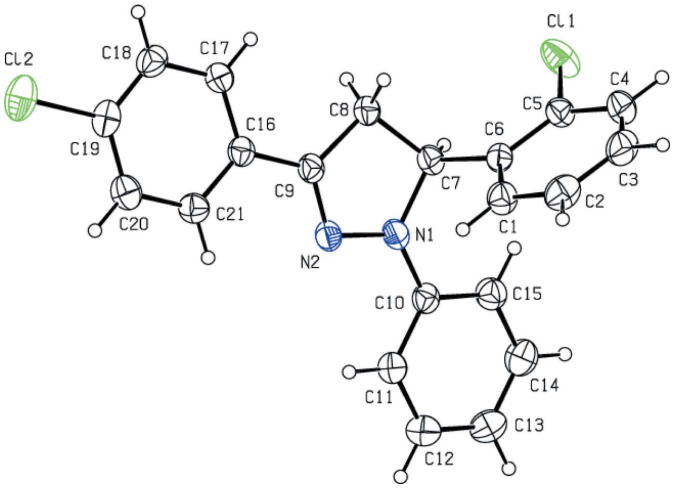


Figure 1
The molecular structure of (I), showing the atom-labeling scheme, with displacement ellipsoids drawn at the 30% probability level.

ketone (0.02 mol) in acetic acid solution (40 ml). Single crystals of (I) suitable for X-ray measurements were obtained by recrystallization from EtOH at room temperature.

Crystal data

$C_{21}H_{16}Cl_2N_2$
M_r = 367.26
Triclinic, $P\overline{1}$
a = 8.3520 (17) Å
b = 9.5020 (19) Å
c = 11.751 (2) Å
α = 89.57 (3)°
β = 80.43 (3)°
γ = 81.83 (3)°
V = 910.1 (3) Å^3
Z = 2
D_x = 1.340 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.36 mm^{-1}
T = 293 (2) K
Block, yellow
0.45 × 0.44 × 0.44 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
ω scans
Absorption correction: none
4139 measured reflections
3865 independent reflections
3098 reflections with $I > 2\sigma(I)$
R_{int} = 0.013
θ_{max} = 27.0°
3 standard reflections
every 100 reflections
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.112
S = 1.06
3865 reflections
227 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0478P)^2 + 0.3091P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.28 e Å^{-3}
$\Delta\rho_{min}$ = −0.48 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.238 (8)

H atoms were positioned geometrically and allowed to ride on their parent atoms, with C—H distances in the range 0.93–0.97 Å and U_{iso}(H) = 1.2U_{eq}(C).

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *NRCVAX* (Gabe *et al.*, 1989); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL/PC* (Sheldrick, 1990); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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