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1-Acetyl-5-(4-chlorophenyl)-3-(4-fluorophenyl)-2-pyrazoline

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In the title compound, $C_{17}H_{14}ClFN_2O$, all bond lengths and angles show normal values. The two benzene rings make a dihehral angle of 82.17 (2)°. Weak intermolecular C—H···O hydrogen bonds stabilize the crystal packing.

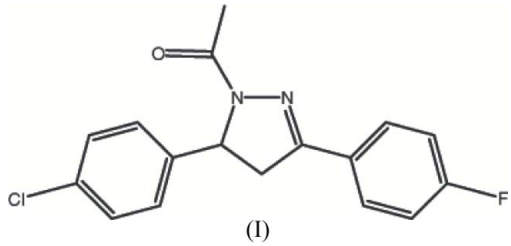
Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.003 Å
R factor = 0.041
wR factor = 0.118
Data-to-parameter ratio = 15.5

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

Comment

Pyrazoline and its derivatives are important and useful five-membered heterocyclic compounds, which are found to possess antiviral (Rawal *et al.*, 1963), antifungal (Dhal *et al.*, 1975) and immunosuppressive activities (Lombardino & Ottemes, 1981). 1-Acetyl-3,5-diaryl-2-pyrazolines have been found to inhibit monoamine oxidases (Manna *et al.*, 2002). As part of our ongoing investigation of pyrazolines and their metal complexes, we report here the crystal structure of the title compound, (I).



(I)

In the structure of (I) (Fig. 1), all bond lengths and angles are comparable with those in related structures (Guo *et al.*, 2006; Fahrni *et al.*, 2003; Kimura *et al.*, 1977). The mean plane of the N1/N2/C7–C9 pyrazoline ring makes dihedral angles of 4.36 (4) and 86.47 (1)° with the benzene rings C1–C6 and C10–C15, respectively. The dihedral angle between the two benzene rings is 82.17 (2)°.

The crystal packing of (I) is stabilized by weak intermolecular C—H···O hydrogen bonds (Table 1).

Experimental

1-(*p*-Fluorophenyl)-3-(*p*-chlorophenyl)-2-propenyl-1-ketone (0.02 mol) and hydrazine (0.02 mol) were mixed in acetic acid (40 ml) and stirred under reflux for 6 h; the mixture was then poured into ice–water to afford colourless solids. The solids were filtered off and washed with water until the pH of the solution was about 7.0. Finally, the crystals were dried at room temperature. Single crystals of compound (I) suitable for X-ray measurements were obtained by recrystallization from EtOH at room temperature.

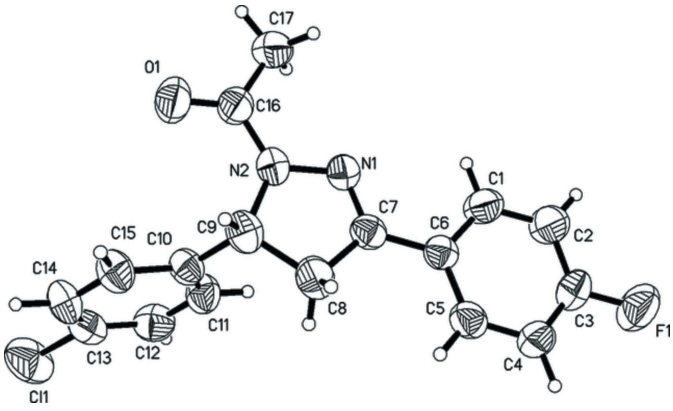


Figure 1
The molecular structure of (I), with the atom labelling scheme. Displacement ellipsoids are drawn at the 50% probability level.

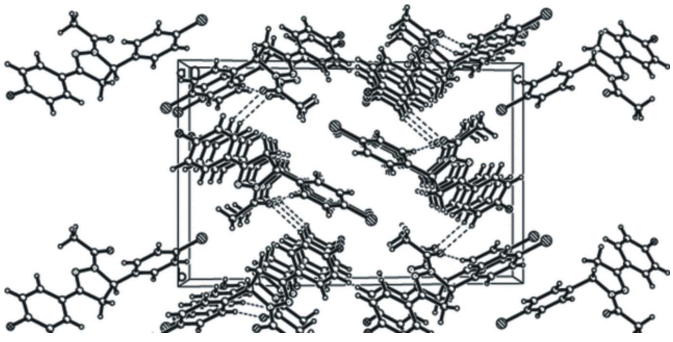


Figure 2
The packing of (I), viewed down the *c* axis, showing one layer of molecules connected by C—H···O hydrogen bonds (dashed lines). H atoms not involved in hydrogen bonding have been omitted.

Crystal data

$C_{17}H_{14}ClFN_2O$
M_r = 316.75
Monoclinic, $P2_1/c$
a = 6.119 (2) Å
b = 12.696 (5) Å
c = 19.812 (7) Å
β = 97.549 (7)°
V = 1525.8 (10) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.26 mm^{-1}
T = 294 (2) K
0.30 × 0.20 × 0.18 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
T_{min} = 0.925, T_{max} = 0.954
8612 measured reflections
3118 independent reflections
1772 reflections with $I > 2\sigma(I)$
R_{int} = 0.039

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.118
S = 1.01
3118 reflections
201 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C4—H4···O1^{i}	0.93	2.48	3.306 (3)	148
C11—H11···O1^{ii}	0.93	2.55	3.459 (3)	167

Symmetry codes: (i) $-x+1, y+\frac{1}{2}, -z+\frac{3}{2}$; (ii) $x+1, y, z$.

H atoms were positioned geometrically and allowed to ride on their parent atoms, with C—H distances of 0.93–0.98 Å and U_{iso}(H) = 1.2–1.5U_{eq}(C).

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); 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, 1997); software used to prepare material for publication: *SHELXTL*.

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References

Bruker (1997). *SADABS*, *SMART*, *SAINT* and *SHELXTL*. Bruker AXS Inc., Madison, Wisconsin, USA.
Dhal, P. N., Acharya, T. E. & Nayak, A. (1975). *J. Indian Chem. Soc.* **52**, 1196–1200.
Fahrni, C. J., Yang, L. C. & VanDerveer, D. G. (2003). *J. Am. Chem. Soc.* **125**, 3799–3812.
Guo, H.-M., Jian, F.-F., Zhou, L.-Y., Zhao, P.-S. & Zheng, J. (2006). *Acta Cryst.* E**62**, o4337–o4338.
Kimura, T., Kai, Y., Yasuoka, N. & Kasai, N. (1977). *Acta Cryst.* B**33**, 1786–1792.
Lombardino, G. & Ottemes, I. G. (1981). *J. Med. Chem.* **24**, 830–834.
Manna, F., Chimenti, F., Bolasco, A., Secci, D., Bizzarri, B., Befani, O., Turini, P., Mondovi, B., Alcaro, S. & Tafi, A. (2002). *Bioorg. Med. Chem. Lett.* **12**, 3629–3635.
Rawal, A. A., Thakor, V. M. & Shah, N. M. (1963). *J. Indian Chem. Soc.* **40**, 323–326.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.