# organic papers

# 3-(4-Fluorophenyl)-1,5-diphenyl-2-pyrazoline

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**Key indicators**

Single-crystal X-ray study
$T$ = 293 K
Mean $\sigma$(C–C) = 0.003 Å
$R$ factor = 0.050
$wR$ factor = 0.156
Data-to-parameter ratio = 16.5

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

The title compound, $C_{21}H_{17}FN_2$, crystallizes with two independent molecules in the asymmetric unit. The pyrazoline and 4-fluorophenyl rings are planar. The phenyl ring at the 5-position and the pyrazoline heterocycle are almost perpendicular.

## Comment

Five- and six-membered heterocyclic compounds are important constituents that often exist in biologically active natural products and synthetic compounds of medicinal interest (Gilchrist, 1998). Among them, 1,3,5-trisubstituted pyrazolines can be easily prepared from phenylhydrazine and chalcone derivatives (Nakamichi et al., 2002). Some 1,3,5-triaryl-substituted pyrazolines can also be used as probes in a biological environment (Fahrni et al., 2003). Here, we report the crystal structure of such a compound, (I).



(I)
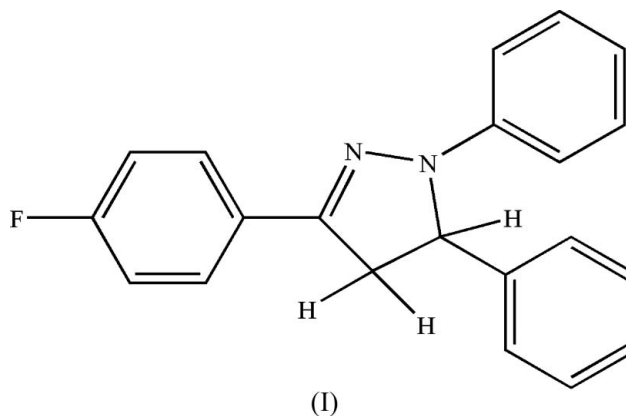
The structure of (I) (Fig. 1) contains two crystallographically independent molecules in the asymmetric unit, hereafter named $F1$ and $F2$. In both molecules, the C=N bond lengths are slightly longer than those found in similar structures [1.291 (2) Å (Rurack et al., 2000), 1.283 (2) Å for polymorph $\alpha$ (Kimura et al., 1977) and 1.293 (3)/1.291 (3) Å (Ge, 2006)]. In contrast, the N1—N2 and N3—N4 bond lengths are shorter than those found in the above-cited structures [1.394 (3), 1.390 (3) and 1.384 (2)/1.385 (2) Å, respectively]. The C—F bond lengths are slightly shorter than those found in similar structures [e.g. 1.370 (2) Å; Joshi et al., 1992].

All the bond lengths and angles for the phenyl and benzene rings in (I) are in normal ranges. In molecule $F1$, the pyrazoline ring and 4-fluorophenyl group define a plane ($P1$), the largest deviation being 0.068 (3) Å for atom N2. The dihedral angles between $P1$ and the phenyl rings at positions 1 and 5 of the pyrazoline are 12.64 (2) and 78.95 (3)°, respectively. The

dihedral angle between the phenyl rings is 88.51 (2)°. Similarly, in molecule *F*2, the pyrazoline and 4-fluorophenyl rings also define a plane (*P*2), the largest deviation being 0.072 (3) Å for atom C42. The dihedral angles between *P*2 and phenyl groups at positions 1 and 5 of the pyrazoline are 17.59 (2) and 75.29 (3)°, respectively. The dihedral angle between the two phenyl rings is 88.32 (3)°.

## Experimental

The title compound was prepared by reaction of phenylhydrazine (0.02 mol) and 1-(4-fluorophenyl)-3-phenyl-2-propenyl-1-ketone (0.02 mol) dissolved in acetic acid (40 ml). Single crystals suitable for X-ray measurements were obtained by recrystallization from EtOH at 298 K.
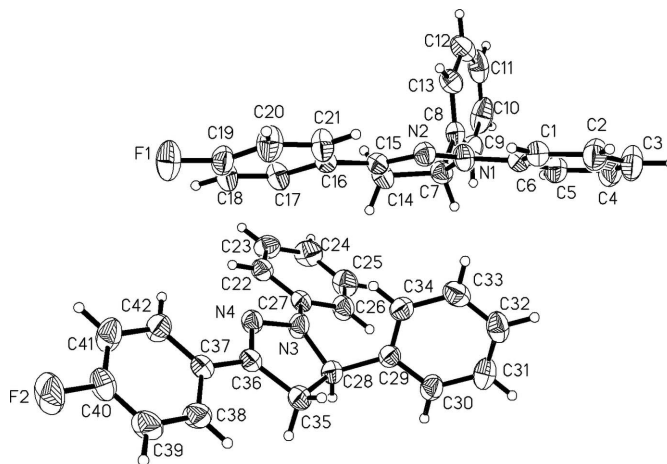


**Figure 1**
The asymmetric unit of (I), showing the atom-labelling scheme, with displacement ellipsoids drawn at the 30% probability level.

### Crystal data

| | |
|---|---|
| $C_{21}H_{17}FN_2$ | $V = 1678.2$ (6) Å$^3$ |
| $M_r = 316.37$ | $Z = 4$ |
| Triclinic, $P\bar{1}$ | $D_x = 1.252$ Mg m$^{-3}$ |
| $a = 11.491$ (2) Å | Mo $K\alpha$ radiation |
| $b = 11.728$ (2) Å | $\mu = 0.08$ mm$^{-1}$ |
| $c = 13.601$ (3) Å | $T = 293$ (2) K |
| $\alpha = 89.44$ (3)° | Block, colourless |
| $\beta = 71.07$ (3)° | $0.23 \times 0.22 \times 0.19$ mm |
| $\gamma = 76.07$ (3)° | |

### Data collection

| | |
|---|---|
| Enraf–Nonius CAD-4 diffractometer | 3538 reflections with $I > 2\sigma(I)$ |
| $\omega$ scans | $R_{int} = 0.030$ |
| Absorption correction: none | $\theta_{max} = 27.2°$ |
| 7526 measured reflections | 3 standard reflections |
| 7160 independent reflections | every 100 reflections |
| | intensity decay: <1% |

### Refinement

| | |
|---|---|
| Refinement on $F^2$ | $w = 1/[\sigma^2(F_o^2) + (0.0765P)^2$ |
| $R[F^2 > 2\sigma(F^2)] = 0.050$ | $+ 0.0731P]$ |
| $wR(F^2) = 0.156$ | where $P = (F_o^2 + 2F_c^2)/3$ |
| $S = 1.01$ | $(\Delta/\sigma)_{max} < 0.001$ |
| 7160 reflections | $\Delta\rho_{max} = 0.18$ e Å$^{-3}$ |
| 434 parameters | $\Delta\rho_{min} = -0.16$ e Å$^{-3}$ |
| H-atom parameters constrained | Extinction correction: *SHELXL97* |
| | Extinction coefficient: 0.023 (2) |

All H atoms were positioned geometrically and refined using a riding model, with C—H = 0.93 (aromatic CH), 0.97 (methylene CH$_2$) or 0.98 Å (methine CH). Isotropic displacement parameters for H atoms were fixed at $U_{iso}$(H) = 1.2$U_{eq}$(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*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL/PC* (Sheldrick, 1997*b*); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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

| | | | |
|---|---|---|---|
| F1—C19 | 1.366 (2) | F2—C40 | 1.357 (2) |
| N1—N2 | 1.374 (2) | N3—N4 | 1.378 (2) |
| N1—C6 | 1.396 (3) | N3—C27 | 1.396 (2) |
| N1—C7 | 1.469 (3) | N3—C28 | 1.477 (3) |
| N2—C15 | 1.298 (2) | N4—C36 | 1.295 (2) |
| C1—C2 | 1.379 (3) | C22—C23 | 1.376 (3) |
| C3—C4 | 1.368 (4) | C25—C26 | 1.386 (3) |
| C7—C8 | 1.531 (3) | C29—C30 | 1.374 (3) |
| C8—C9 | 1.368 (3) | C37—C38 | 1.399 (3) |
| C16—C21 | 1.372 (3) | | |
| N1—C7—C8 | 112.05 (17) | N3—C28—C29 | 112.28 (17) |