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5-(4-Fluorophenyl)-1-phenylpyrazole

Daniel E. Lynch[a]* and Ian McClenaghan[b]

[a]School of Science and the Environment, Coventry University, Coventry CV1 5FB, England, and [b]Key Organics Ltd, Highfield Industrial Estate, Camelford, Cornwall PL32 9QZ, England

Correspondence e-mail: apx106@coventry.ac.uk

Key indicators

Single-crystal X-ray study
T = 150 K
Mean σ(C–C) = 0.005 Å
R factor = 0.082
wR factor = 0.238
Data-to-parameter ratio = 16.3

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

The asymmetric unit of the title compound, $C_{15}H_{11}F_1N_2$, comprises two molecules with dihedral angles of 50.6 (1)/49.2 (1) and 51.5 (1)/53.3 (1)° between the pyrazole and, respectively, the phenyl and 4-fluorophenyl rings. One intermolecular C—H···F close contact is noted for each unique molecule.

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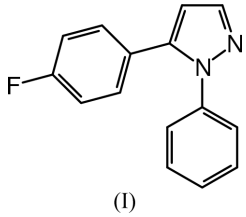
Comment

The title compound, (I), was prepared by the addition of phenylhydrazine to 1-(*N,N*-dimethylamino)-2-(4-fluorobenzoyl)ethene. However, in this reaction there are two possible products (Fig. 2). One is formed *via* the hydrazone intermediate which subsequently cyclizes to the 1,3-substituted pyrazole; the other is formed *via* the Michael intermediate, which cyclizes to the 1,5-substituted product, *i.e.* the title compound. The asymmetric unit of this compound comprises two molecules with dihedral angles of 50.6 (1)/49.2 (1) and 51.5 (1)/53.3 (1)° between the pyrazole and, respectively, the phenyl and 4-fluorophenyl rings. One intermolecular C—H···F close contact is noted for each unique molecule.



(I)

Experimental

The title compound was obtained from Key Organics Ltd and crystals were grown from an ethanol solution.

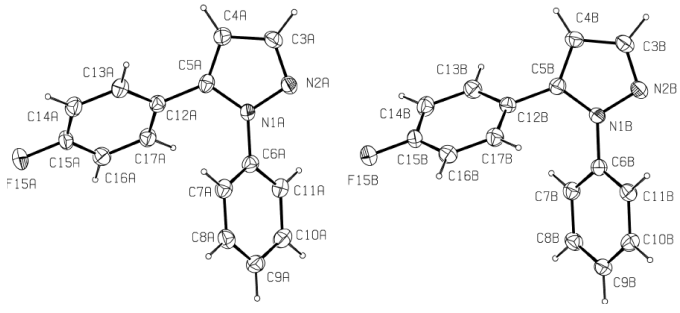


Figure 1
The molecular configuration and atom-numbering scheme for the title compound, showing 50% probability ellipsoids.

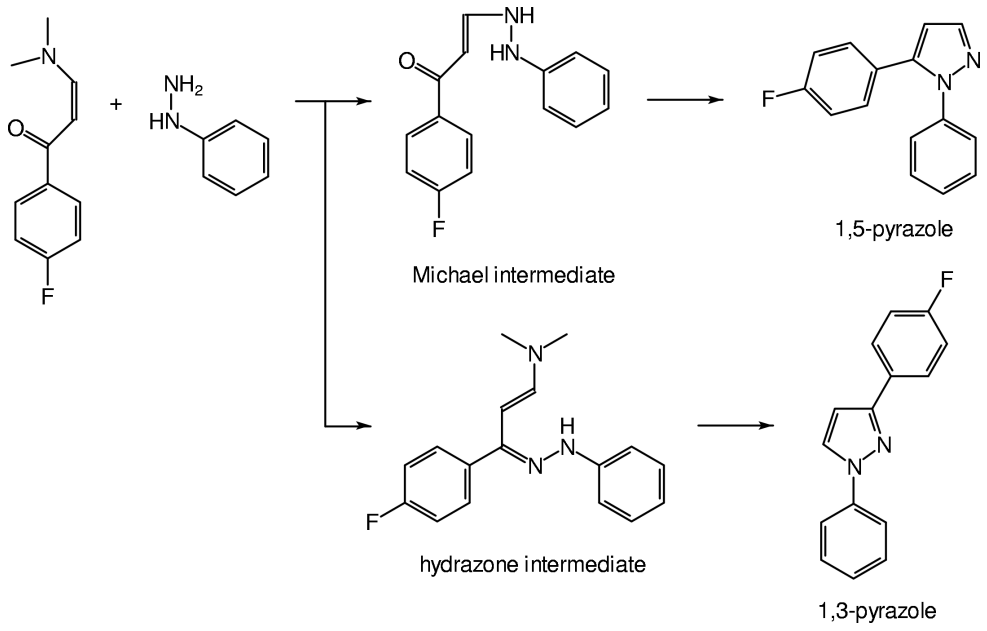


Figure 2
Reaction scheme showing two possible intermediates and subsequent products for the reaction of phenylhydrazine with 1-(*N*,*N*-dimethylamino)-2-(4-fluorobenzoyl)ethene.

Crystal data

$C_{15}H_{11}FN_2$
M_r = 238.26
Triclinic, $P\overline{1}$
a = 7.847 (2) Å
b = 7.904 (2) Å
c = 19.551 (4) Å
α = 90.20 (3)°
β = 100.92 (3)°
γ = 90.61 (3)°
V = 1190.5 (4) Å^3
Z = 4
D_x = 1.329 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 16018 reflections
θ = 2.9–27.5°
μ = 0.09 mm^{-1}
T = 150 (2) K
Block, yellow
0.20 × 0.18 × 0.10 mm

Data collection

Bruker–Nonius KappaCCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SORTAV*; Blessing, 1995)
T_{min} = 0.982, T_{max} = 0.991
17989 measured reflections
5311 independent reflections
3979 reflections with $I > 2\sigma(I)$
R_{int} = 0.065
θ_{max} = 27.5°
$h = -10 \rightarrow 10$
$k = -10 \rightarrow 10$
$l = -23 \rightarrow 25$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.082
$wR(F^2)$ = 0.238
S = 1.17
5311 reflections
326 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0756P)^2 + 2.8942P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.32 e Å^{-3}
$\Delta\rho_{min}$ = −0.33 e Å^{-3}
Extinction correction: *SHELXL*97
Extinction coefficient: 0.077 (9)

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

D—H···A	D—H	H···A	D···A	D—H···A
C3A—H3A···F15A^{i}	0.95	2.48	3.415 (4)	169
C4B—H4B···F15B^{ii}	0.95	2.44	3.385 (4)	171

Symmetry codes: (i) $-x, -y, 1-z$; (ii) $-x, 2-y, -z$.

All H atoms were included in the refinement, at calculated positions, as riding models, with C—H distances set to 0.95 Å. The R_{int} value of 0.065 was the result of weak high-angle data.

Data collection: *DENZO* (Otwinowski & Minor, 1997) and *COLLECT* (Hooft, 1998); cell refinement: *DENZO* and *COLLECT*; data reduction: *DENZO* and *COLLECT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *PLATON*97 (Spek, 1997); software used to prepare material for publication: *SHELXL*97.

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