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1-Acetyl-5-(4-methylphenyl)-3-(4-nitrophenyl)-2-pyrazoline

Huan-Mei Guo,[a] Fang-Fang Jian,[b]* Pu-Su Zhao,[b] Xiao-Zheng Sun[a] and Cui-Hua Lin[a]

[a]Department of Chemistry, Weifang College, Weifang 261061, People's Republic of China, and [b]New Materials and Function Coordination Chemistry Laboratory, Qingdao University of Science and Technology, Qingdao 266042, People's Republic of China

Correspondence e-mail: ffj2003@163169.net

Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.052
wR factor = 0.156
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.

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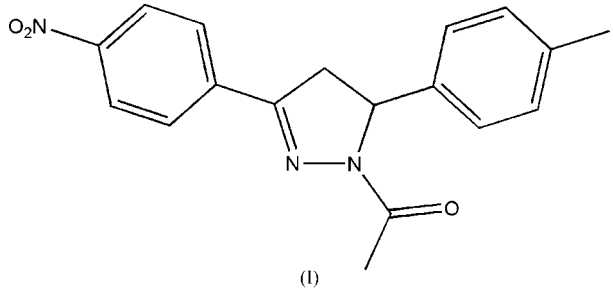
In the title molecule, $C_{18}H_{17}N_3O_3$, all bond lengths and angles show normal values. The two benzene rings make a dihedral angle of 87.27 (2)°. Weak intermolecular C—H···O hydrogen bonds stabilize the crystal packing.

Comment

Pyrazoline and some of its derivatives demonstrate antiviral (Rawal *et al.*, 1963), antifungal (Dhal *et al.*, 1975), and immunosuppressive (Lombardino & Ottemes, 1981) activities. 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 (I) (Fig. 1), all bond lengths and angles are normal (Fahrni *et al.*, 2003; Kimura *et al.*, 1977). The mean plane of pyrazoline ring N2/N3/C7–C8 makes dihedral angles of 9.36 (1) and 78.49 (2)° with benzene rings C1–C6 and C13–C17, respectively. The dihedral angle between the two benzene rings is 87.27 (2)°.

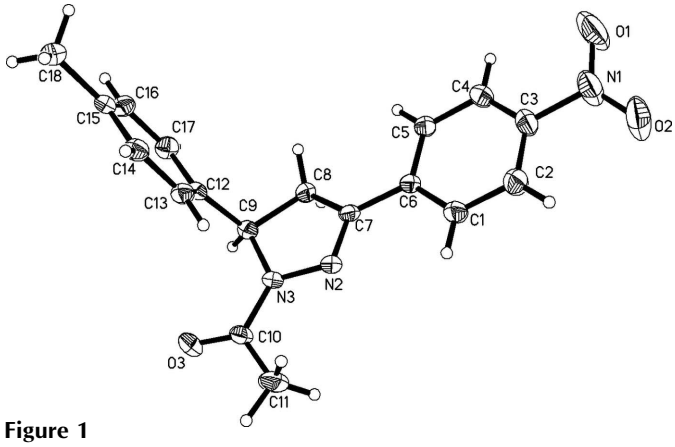


Figure 1
The molecular structure of (I), showing the atomic labelling and displacement ellipsoids drawn at the 30% probability level.

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

Experimental

3-(4-Methylphenyl)-1-(4-nitrophenyl)-2-propen-1-one (0.02 mol) and phenylhydrazine (0.02 mol) were mixed in acetic acid (40 ml), stirred and refluxed for 6 h. The mixture was then poured into ice–water, affording red solids. The solids were filtered and washed with water until the pH of the solution was about 7.0. The crystals were dried at room temperature. Single crystals of (I) suitable for X-ray measurements were obtained by recrystallization from EtOH at room temperature.

Crystal data

$C_{18}H_{17}N_3O_3$
M_r = 323.35
Monoclinic, $C2/c$
a = 24.072 (5) Å
b = 11.905 (2) Å
c = 11.759 (2) Å
β = 104.65 (3)°
V = 3260.3 (11) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 293 (2) K
0.4 × 0.4 × 0.2 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: none
7239 measured reflections
3545 independent reflections
2473 reflections with $I > 2\sigma(I)$
R_{int} = 0.073
3 standard reflections
every 100 reflections
intensity decay: none

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.052
$wR(F^2)$ = 0.156
S = 1.05
3545 reflections
218 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.32 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C1—H1A···O3^{i}	0.93	2.54	3.419 (5)	159
C8—H8A···O3^{ii}	0.97	2.57	3.357 (3)	138

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

H atoms were positioned geometrically and allowed to ride on their parent atoms, with C—H distances of 0.93–0.97 Å and with U_{iso}(H) = 1.2 or 1.5 times U_{eq} of the parent atom.

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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