2-(4-Chlorophenyl)-5-methyl-1*H*-pyrazol-3(2*H*)-one

Xue-Min Duan,[a]* Mei-Lian Fan,[b] Peng-Wu Zheng,[a] Jiang-Sheng Li[c] and Peng-Mian Huang[c]

[a]School of Pharmacy, Jiangxi Science and Technology Normal University, Nanchang 330013, People's Republic of China, [b]College of Chemistry and Chemical Engineering, Hunan University, Changsha 410082, People's Republic of China, and [c]College of Pharmaceuticals and Biotechnology, Tianjin University, Tianjin 300072, People's Republic of China

Correspondence e-mail:
dxmlhp@yahoo.com.cn

Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.003 Å
R factor = 0.038
wR factor = 0.111
Data-to-parameter ratio = 12.6

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

In the title compound, $C_{10}H_9ClN_2O$, the benzene ring is twisted with respect to the pyrazole plane, with a dihedral angle of 15.81 (11)°. The centroid-to-centroid separation of 3.721 (4) Å indicates π–π stacking between parallel benzene rings.

Comment

The tautomerism of pyrazolin-5-ones is well known. The crystal structure of the title compound, (I), exhibits the NH tautomer in the crystal state.

(I)
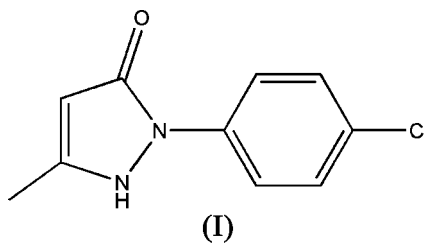
The molecular structure of (I) is illustrated in Fig. 1. The pyrazole ring is essentially planar, with a mean deviation of 0.0155 Å, but atom H2*A* is not coplanar with the ring plane, showing an sp^3 hybrid nature for atom N2. The dihedral angle between the pyrazole and benzene ring planes is 15.81 (11)°. The bond lengths and angles are normal (Table 1).

N—H···O intermolecular hydrogen bonding occurs in the crystal structure of (I) (Table 2) and π–π stacking is also observed between parallel benzene rings (Fig. 2), the centroid-to-centroid and face-to-face separations being 3.721 (4) and 3.466 (6) Å, respectively.

Experimental

2-(4-Chlorophenyl)-5-methyl-1*H*-pyrazol-3(2*H*)-one was prepared according to the literature method of Liu & Li (2004). Single crystals of (I) suitable for X-ray analysis were obtained by evaporation of an ethanol solution.

Crystal data

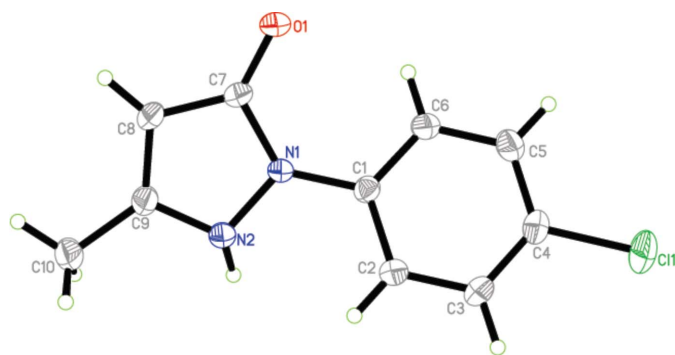|	
$C_{10}H_9ClN_2O$	V = 481.4 (7) Å^3
M_r = 208.64	Z = 2
Triclinic, $P\bar{1}$	D_x = 1.439 Mg m^{-3}
a = 5.885 (5) Å	Mo $K\alpha$ radiation
b = 7.704 (7) Å	μ = 0.36 mm^{-1}
c = 11.38 (1) Å	T = 294 (2) K
α = 105.980 (13)°	Block, colourless
β = 94.719 (14)°	0.30 × 0.26 × 0.22 mm
γ = 101.250 (13)°	

Figure 1
The molecular structure of (I), with 30% probability displacement ellipsoids (arbitrary spheres for H atoms).

Data collection

Bruker SMART CCD area-detector diffractometer	2397 measured reflections
φ and ω scans	1669 independent reflections
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	1421 reflections with $I > 2\sigma(I)$
$T_{min} = 0.899$, $T_{max} = 0.925$	$R_{int} = 0.025$
	$\theta_{max} = 25.0°$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.054P)^2$
$R[F^2 > 2\sigma(F^2)] = 0.038$	$+ 0.1893P]$
$wR(F^2) = 0.111$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.07$	$(\Delta/\sigma)_{max} = 0.003$
1669 reflections	$\Delta\rho_{max} = 0.21$ e Å^{-3}
132 parameters	$\Delta\rho_{min} = -0.26$ e Å^{-3}
H atoms treated by a mixture of independent and constrained refinement	

Table 1
Selected bond lengths (Å).

Cl1—C4	1.753 (2)	N1—C1	1.417 (2)
O1—C7	1.256 (2)	N1—C7	1.392 (2)
N1—N2	1.400 (2)	N2—C9	1.355 (3)

Table 2
Hydrogen-bond geometry (Å, °).

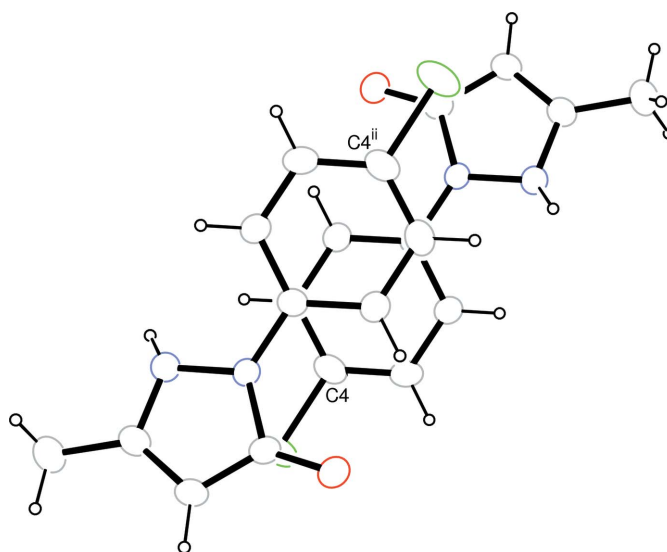| D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
N2—H2A$\cdots$O1^i	0.84 (3)	1.90 (3)	2.737 (3)	179 (2)

Symmetry code: (i) $x + 1, y, z$.

Figure 2
The π–π stacking between parallel benzene rings of (I). [Symmetry code: (ii) $1 - x, -y, 1 - z$.]

Methyl H atoms were placed in calculated psitions, with C—H = 0.96 Å, and the torsion angles were refined to fit the electron density. They were treated as riding, with $U_{iso}(H) = 1.5 \ U_{eq}(C)$. Aromatic H atoms were positioned geometrically, with C—H = 0.93 Å, and they were refined in riding mode, with $U_{iso}(H) = 1.2 \ U_{eq}(C)$. Atom H2A was located in a difference Fourier map and refined isotropically.

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*.

References

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Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.