Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

4-(2-Chlorophenyl)-3-methyl-1-phenyl-6-(2-pyridyl)pyrazolo[3,4-*b*]pyridine

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Key indicators

Single-crystal X-ray study
T = 193 K
Mean σ(C–C) = 0.004 Å
R factor = 0.067
wR factor = 0.140
Data-to-parameter ratio = 16.7

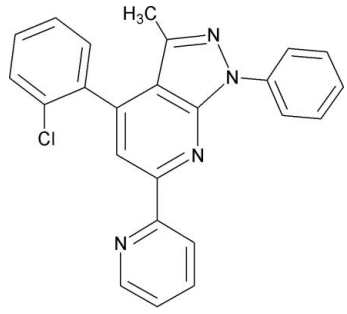
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 12 April 2005
Accepted 14 April 2005
Online 23 April 2005

The title compound, $C_{24}H_{17}N_4Cl$, was synthesized by the reaction of 5-amino-3-methyl-1-phenylpyrazole with 3-(2-chlorophenyl)-1-(2-pyridyl)prop-2-en-1-one in glycol under microwave irradition. X-ray crystal structure analysis reveals that the substituted pyridine ring is almost coplanar with the pyrazolo[3,4-*b*]pyridine moiety.

Comment

The pyrazolo[3,4-*b*]pyridine system has many interesting biological and pharmacological properties, such as active antitubercular action and action against Gram-positive and Gram-negative bacteria, and is used in the treatment of a wide variety of stress-related illnesses (Sekikawa *et al.*, 1973; Kuczynski *et al.*, 1979; El-Dean *et al.*, 1991; Chen, 1995). As part of our programme aimed at employing microwave irradiation for the preparation of heterocyclic compounds (Tu *et al.*, 2004), we have recently synthesized pyrazolo[3,4-*b*]-pyridine derivatives under microwave irradiation. We report here the crystal structure of the title compound, (I).



(I)

The dihedral angle between the pyrazole plane and N1/C1–C5 pyridine ring is 2.6 (1)°, indicating that they are almost coplanar (Fig. 1). The N4/C19–C23 pyridine ring and C13–C18 benzene ring form dihedral angles of 4.4 (1) and 63.0 (1)°, respectively, with the attached pyridine ring. The C7–C12 phenyl ring forms a dihedral angle of 24.2 (1)° with the pyrazole ring. In the crystal structure, the molecules pack as layers parallel to the *ac* plane.

Experimental

Compound (I) was prepared by the reaction of 5-amino-3-methyl-1-phenylpyrazole (2 mmol) with 3-(2-chlorophenyl)-1-(2-pyridyl)prop-2-en-1-one (2 mmol) in glycol (1 ml) under microwave irradiation (yield 77%, m.p. 437 K). Single crystals of (I) suitable for X-ray diffraction were obtained by slow evaporation of an ethanol solution (95%).

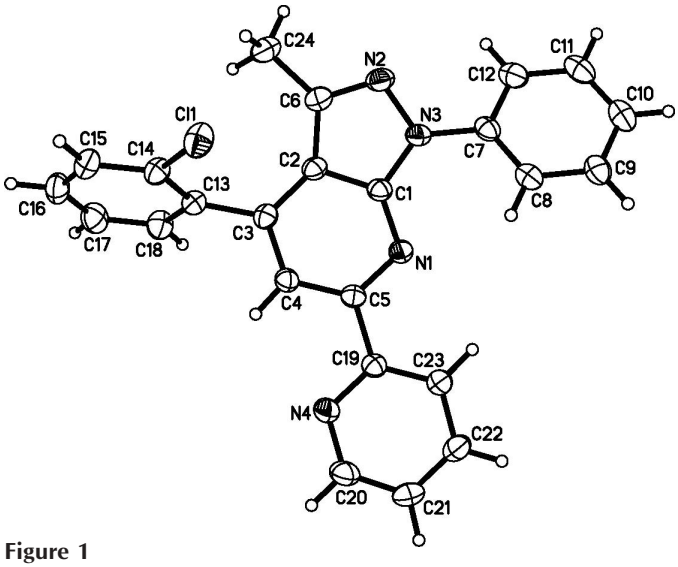


Figure 1
The molecular structure of (I), showing 40% probability displacement ellipsoids and the atom-numbering scheme.

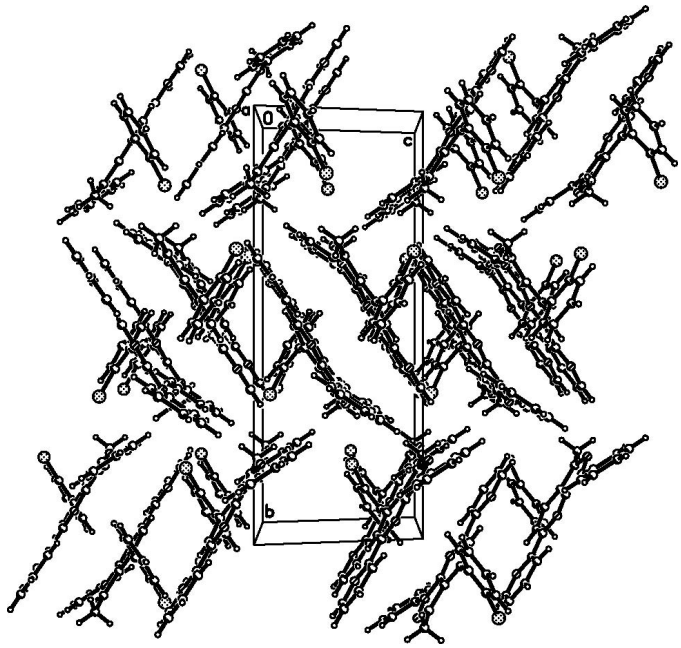


Figure 2
The molecular packing of (I), viewed along the *a* axis.

Crystal data

$C_{24}H_{17}ClN_4$	D_x = 1.367 Mg m^{-3}
M_r = 396.87	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 6741 reflections
a = 11.545 (2) Å	θ = 3.2–27.5°
b = 20.694 (3) Å	μ = 0.22 mm^{-1}
c = 8.5970 (15) Å	T = 193 (2) K
β = 110.147 (4)°	Plate, light yellow
V = 1928.3 (6) Å^3	0.38 × 0.30 × 0.10 mm
Z = 4	

Data collection

Rigaku Mercury CCD area-detector diffractometer	4401 independent reflections
	3457 reflections with $I > 2\sigma(I)$
ω scans	R_{int} = 0.048
Absorption correction: multi-scan (Jacobson, 1998)	θ_{max} = 27.5°
	$h = -14 \rightarrow 14$
T_{min} = 0.922, T_{max} = 0.979	$k = -21 \rightarrow 26$
21 550 measured reflections	$l = -11 \rightarrow 10$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0443P)^2 + 1.016P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.067	
$wR(F^2)$ = 0.140	
S = 1.16	$(\Delta/\sigma)_{max}$ = 0.001
4401 reflections	$\Delta\rho_{max}$ = 0.22 e Å^{-3}
263 parameters	$\Delta\rho_{min}$ = −0.34 e Å^{-3}
H-atom parameters constrained	

H atoms were placed in idealized positions and allowed to ride on their parent atoms, with C—H distances in the range 0.95–0.98 Å, and with U_{iso}(H) = 1.5U_{eq}(C) for methyl H atoms and 1.2 U_{eq}(C) for other H atoms.

Data collection: *CrystalClear* (Rigaku, 1999); cell refinement: *CrystalClear*; data reduction: *CrystalStructure* (Rigaku/MSC, 2003); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

The authors thank the Natural Science Foundation of China (grant No. 20372057) and the Key Laboratory of Biotechnology for Medicinal Plants of Jiangsu Province (grant No. 01AXL14) for financial support.

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