Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2-Chloro-4-(3,5-dimethyl-1*H*-pyrazol-1-yl)-pyrimidine

Wei-Min Liu, You-Quan Zhu, Yi-Feng Wang, Gong-Chun Li and Hua-Zheng Yang*

State Key Laboratory and Institute of Elemento-Organic Chemistry, Nankai University, Tianjin 300071, People's Republic of China

Correspondence e-mail: youquan_zhu@mail.nankai.edu.cn

Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
Disorder in main residue
R factor = 0.036
wR factor = 0.106
Data-to-parameter ratio = 10.7

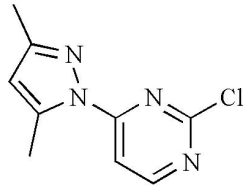
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 10 May 2005
Accepted 13 May 2005
Online 21 May 2005

In the crystal structure of the title compound, $C_9H_9ClN_4$, there are non-classical intramolecular C—H···N hydrogen bonds and intermolecular C—H···π interactions.

Comment

Pyrimidines are very important molecules in biology and have many applications in the areas of pesticides and pharmaceuticals (Condon *et al.*, 1993). For example, Imazosulfuron, Ethirmol and Mepanipyrim have been commercialized as agrochemicals (Maeno *et al.*, 1990). Pyrimidine derivatives have also been developed as antiviral agents, such as AZT, which is the most widely used anti-AIDS drug (Gilchrist, 1997). In order to discover more biologically active pyrimidine compounds, the title compound, (I), was synthesized and its crystal structure determined (Fig. 1).



(I)

The pyrimidine and pyrazole rings are located on a mirror plane and thus are crystallographically required to be coplanar, consistent with the extensive conjugation observed for this compound. The only atoms, in fact, that are not located on the mirror plane are the methyl H atoms, which are present

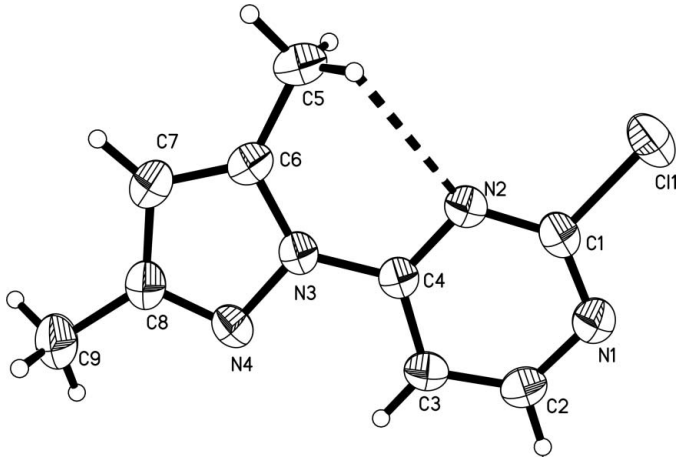


Figure 1
View of the title compound, (I), with displacement ellipsoids for non-H atoms drawn at the 50% probability level. The dashed line indicates a hydrogen bond.

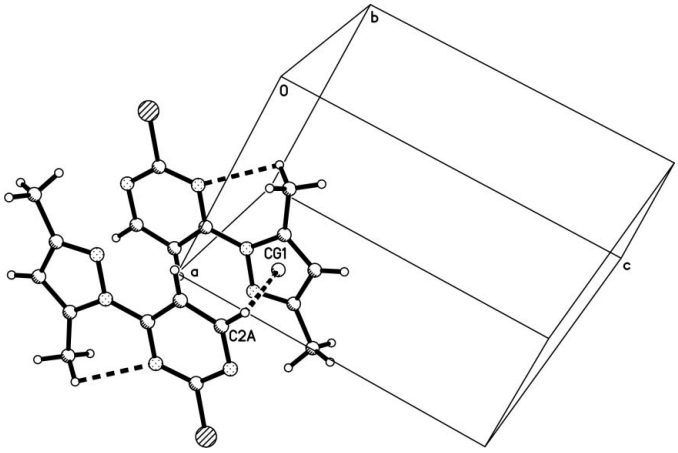


Figure 2
Part of the packing of (I), showing intermolecular C—H···π interactions as dashed lines [symmetry code: (A) $2-x, -y, -z$].

in 50% occupancy and are disordered about the plane. The structure of (I) also involves C—H···N interactions (Fig. 1 and Table 2). The crystal packing is further stabilized by intermolecular C—H···π interactions involving the C6/C7/C8/N3/N4 pyrazole rings (centroid *Cg*1) with a C2···*Cg*1 distance of 3.323 (2) Å (Fig. 2).

Experimental

2-Chloro-4-hydrazinopyrimidine (0.3 g, 2 mmol) and pentane-2,4-dione (0.25 g, 2.5 mmol) were mixed in methanol (15 ml). The mixture was refluxed for 8 h. The solvent was then evaporated under vacuum. The resulting light-yellow precipitate was recrystallized from methanol and crystals of (I) suitable for X-ray diffraction studies were obtained (m.p. 414–415 K). Analysis found (calculated): C 51.64 (51.81), H 4.35 (4.35), N 26.61% (26.85%). ^{1}H NMR (300 MHz, $CDCl_3$): δ 2.291, 2.725 (2*s*, 6H, $2CH_3$), 6.060 (*s*, 1H, CH of pyrazole ring), 7.831,7.849 (*d*, 1H, CH of the the pyrimidine ring), 8.524, 8.540 (*d*, 1H, CH of the pyrimidine ring).

Crystal data

$C_9H_9ClN_4$	D_x = 1.425 Mg m^{-3}
M_r = 208.65	Mo $K\alpha$ radiation
Monoclinic, $P2_1/m$	Cell parameters from 571 reflections
a = 7.336 (4) Å	θ = 3.1–26.2°
b = 6.607 (4) Å	μ = 0.36 mm^{-1}
c = 10.092 (6) Å	T = 293 (2) K
β = 96.387 (9)°	Block, yellow
V = 486.1 (5) Å^3	0.32 × 0.26 × 0.18 mm
Z = 2	

Data collection

Bruker SMART CCD area-detector diffractometer	934 independent reflections
φ and ω scans	713 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	R_{int} = 0.024
T_{min} = 0.895, T_{max} = 0.938	θ_{max} = 25.0°
2461 measured reflections	$h = -7 \rightarrow 8$
	$k = -7 \rightarrow 7$
	$l = -10 \rightarrow 12$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0615P)^2 + 0.096P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.036	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2)$ = 0.106	$\Delta\rho_{max}$ = 0.17 e Å^{-3}
S = 1.03	$\Delta\rho_{min}$ = −0.19 e Å^{-3}
934 reflections	
87 parameters	
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

N1—C1	1.311 (4)	N3—C6	1.387 (3)
N1—C2	1.337 (3)	N3—C4	1.398 (3)
N2—C1	1.322 (4)	N4—C8	1.310 (3)
N2—C4	1.335 (3)	C2—C3	1.364 (4)
N3—N4	1.384 (3)		
C1—N2—C4	114.7 (2)	C6—N3—C4	131.6 (2)
N4—N3—C6	111.4 (2)	C8—N4—N3	104.8 (2)
N4—N3—C4	117.0 (2)	C2—C3—C4	116.0 (2)

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C5—H5*B*···N2	0.96	2.52	2.921 (4)	105

H atoms attached to C atoms were placed in calculated positions and treated as riding atoms [C—H = 0.93 and 0.96 Å, and U_{iso} = $1.2U_{eq}$(C) or U_{iso} = $1.5U_{eq}$(C methyl)]. The disordered methyl H atoms were intially located in a difference map and then refined with constrained C—H distances of 0.96 Å and occupy factors of 0.5.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 1999); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1999); software used to prepare material for publication: *SHELXTL*.

This work was supported by the National Key Project for Basic Research (No. 2003CB114400), the National Natural Science Foundation of China (No. 20372040) and the Research Fund for the Doctoral Programme of Higher Education.

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