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Key indicators

Single-crystal X-ray study
T = 293 K
Mean $\sigma(\text{C}-\text{C}) = 0.003 \text{ \AA}$
R factor = 0.036
wR factor = 0.087
Data-to-parameter ratio = 8.3

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

7-(4-Methylphenyl)pyrazolo[1,5-a]pyrimidine-3-carbonitrile

The title compound [systematic name: 7-(4-methylphenyl)pyrazolo[2,3-a]pyrimidine-3-carbonitrile], $\text{C}_{14}\text{H}_{10}\text{N}_4$, crystallizes in space group $P2_12_12_1$. The pyrazolopyrimidine ring system is essentially planar and makes a dihedral angle of $42.3 (2)^\circ$ with the benzene ring.

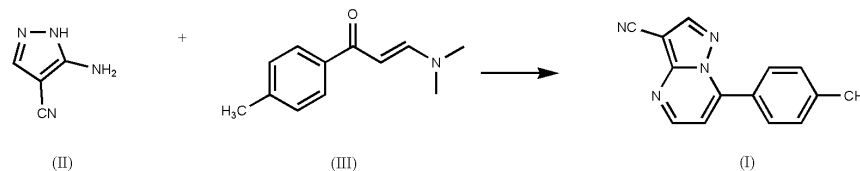
Received 10 June 2004

Accepted 28 June 2004

Online 9 July 2004

Comment

Many pyrazolo[1,5-a]pyrimidine derivatives have been reported, showing various biological activities, *e.g.* antibacterial (Zoni & Vicini, 1998), insulin-releasing (Maren, 1976), anti-inflammatory (Li *et al.*, 1995) and antitumor (Yoshino *et al.*, 1992). It has been documented that enamines are important and versatile synthons for the synthesis of a number of novel heterocycles (Olivera *et al.*, 2000; Hernandez *et al.*, 2003), especially for the synthesis of pyrazolo[1,5-a]pyrimidines (Al-Enezi *et al.*, 1997; Dawood *et al.*, 1999). In this paper, we report the synthesis and crystal structure of the title compound, (I).



All ring atoms in the pyrazolopyrimidine moiety are almost coplanar, the largest deviation from the mean plane being $0.032 (2) \text{ \AA}$ for atom N2. The dihedral angle between the five-membered ring and the fused six-membered ring is $3.2 (2)^\circ$, whereas the dihedral angle between the mean plane of the pyrazolopyrimidine moiety and the benzene ring is $42.3 (2)^\circ$. The geometry of the pyrazolopyrimidine system is very similar to that reported in the related compounds 2,7-dimethyl-5-acetylaminopyrazolo[1,5-a]pyrimidine (Ballard *et al.*, 1975), 6-(2-hydroxybenzoyl)-2-(4-nitrophenyl)pyrazolo[1,5-a]pyrimidine (Cannon *et al.*, 2001), 6-(2-hydroxybenzoyl)-2-phenylpyrazolo[1,5-a]pyrimidine (Quesada *et al.*, 2001) and 2-hydroxyphenyl-2-methylpyrazolo[1,5-a]pyrimidin-6-yl ketone (Quiroga *et al.*, 2000).

Experimental

Compound (I) was prepared by reaction of (II) (2 mmol, 0.40 g) and (III) (2 mmol, 0.35 g) in glacial acetic acid (15 ml), with stirring for 15 h at room temperature. The mixture was then evaporated on a rotary evaporator to remove acetic acid, and (I) was crystallized from a mixture of EtOH-DMF.

Crystal data

$C_{14}H_{10}N_4$
 $M_r = 234.26$
 Orthorhombic, $P2_12_12_1$
 $a = 7.404$ (3) Å
 $b = 10.276$ (4) Å
 $c = 14.963$ (5) Å
 $V = 1138.4$ (7) Å³
 $Z = 4$
 $D_x = 1.367$ Mg m⁻³

Mo $K\alpha$ radiation
 Cell parameters from 696
 reflections
 $\theta = 3.4$ – 23.1°
 $\mu = 0.09$ mm⁻¹
 $T = 293$ (2) K
 Prism, yellow
 $0.26 \times 0.22 \times 0.18$ mm

Data collection

Bruker SMART 1K CCD area-
 detector diffractometer
 φ and ω scans
 Absorption correction: none
 6603 measured reflections
 1364 independent reflections

1097 reflections with $I > 2\sigma(I)$
 $R_{int} = 0.038$
 $\theta_{max} = 26.4^\circ$
 $h = -9 \rightarrow 4$
 $k = -12 \rightarrow 12$
 $l = -16 \rightarrow 18$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.036$
 $wR(F^2) = 0.087$
 $S = 1.06$
 1364 reflections
 165 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0427P)^2 + 0.1275P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{max} = 0.001$
 $\Delta\rho_{max} = 0.14$ e Å⁻³
 $\Delta\rho_{min} = -0.12$ e Å⁻³
 Extinction correction: *SHELXL97*
 Extinction coefficient: 0.035 (4)

Table 1

Selected geometric parameters (Å, °).

N1—C1	1.323 (3)	N4—C3	1.133 (3)
N1—N2	1.371 (2)	C1—C2	1.400 (3)
N2—C7	1.372 (3)	C2—C4	1.385 (3)
N2—C4	1.385 (3)	C2—C3	1.426 (3)
N3—C5	1.314 (3)	C5—C6	1.396 (3)
N3—C4	1.341 (3)	C5—H5	0.9300
C1—N1—N2	103.7 (2)	N1—C1—C2	113.3 (2)
N1—N2—C4	112.5 (2)	C4—C2—C1	105.3 (2)
C5—N3—C4	115.1 (2)	N2—C4—C2	105.3 (2)
C1—N1—N2—C7	177.5 (2)	C1—C2—C3—N4	166 (11)
C1—N1—N2—C4	0.0 (3)	C5—N3—C4—N2	-2.4 (3)
N2—N1—C1—C2	0.2 (3)	C5—N3—C4—C2	175.6 (3)
N1—C1—C2—C4	-0.4 (3)	N1—N2—C4—N3	178.1 (2)
N1—C1—C2—C3	-176.3 (3)	C7—N2—C4—N3	0.5 (3)
C4—C2—C3—N4	-0.9 (1)		

All H atoms were placed in calculated positions, with C—H = 0.93 or 0.96 Å, and included in the final cycles of refinement using a riding model, with $U_{iso}(H) = 1.2U_{eq}(C)$. In the absence of significant anomalous dispersion effects, Friedel pairs were averaged.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 1999); program(s) used to solve

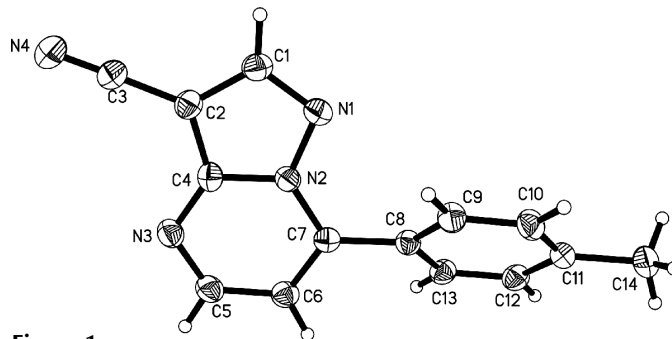


Figure 1

View of (I), with displacement ellipsoids drawn at the 40% probability level.

structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1999); software used to prepare material for publication: *SHELXTL*.

This project was supported by the Natural Science Foundation of Shandong Province (grant No. Y2003B01).

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