Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

5-Amino-1-(1,5-dimethyl-1*H*-pyrazol-4-ylcarbonyl)-3-methylsulfanyl-1*H*-1,2,4-triazole

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.043
wR factor = 0.138
Data-to-parameter ratio = 12.8

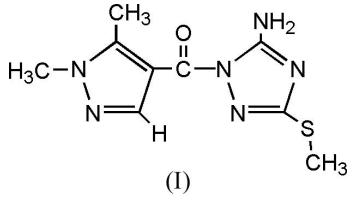
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 1 March 2005
Accepted 30 March 2005
Online 9 April 2005

In the title compound, $C_9H_{12}N_6OS$, the pyrazole and triazole rings are nearly coplanar, forming a dihedral angle of 6.50 (9)°. There are N—H···N intermolecular hydrogen-bond interactions in the crystal structure, providing stabilization.

Comment

Many pyrazole and triazole derivatives have been reported to show various biological activities, such as antifungal (Chen & Li, 2000), herbicidal (Ren *et al.*, 2000), insecticidal (Huang *et al.*, 1996) and other activities (Kopp *et al.*, 2001). Thus, we paid special attention to the possibility of obtaining a pyrazole ring connected to a triazole ring *via* a carbonyl group. In order to develop new biological activities, we synthesized the title compound, (I), the structure of which is reported here.



(I)

Bond distances and angles (Table 1) are as expected for this type of compound. The pyrazole and triazole rings are nearly coplanar, the dihedral angle between them being 6.50 (9)°. A weak intramolecular N—H···O hydrogen-bond interaction is observed (Table 2). In the crystal structure, centrosymmetrically related molecules are linked in dimers through the formation of intermolecular N—H···N hydrogen-bond interactions (Table 2).

Experimental

A mixture of 1,5-dimethylpyrazol-4-ylcarbonyl hydrazide (3 mmol) and CIDT (*N*-cyanoimido-*S*,*S*-dimethylthiocarbonate) (2 mmol) in acetonitrile (15 ml) was refluxed for 8 h (monitored by thin-layer chromatography) until a solid product formed; the solution was cooled and the product filtered off. The pure product was isolated by recrystallization from dimethylformamide (m.p. 514 K).

Crystal data

$C_9H_{12}N_6OS$
M_r = 252.31
Monoclinic, $P2_1/n$
a = 7.642 (5) Å
b = 10.100 (7) Å
c = 15.250 (10) Å
β = 101.275 (8)°
V = 1154.3 (13) Å^3
Z = 4
D_x = 1.458 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2811 reflections
θ = 2.4–27.8°
μ = 0.28 mm^{-1}
T = 293 (2) K
Prism, colourless
0.59 × 0.38 × 0.20 mm

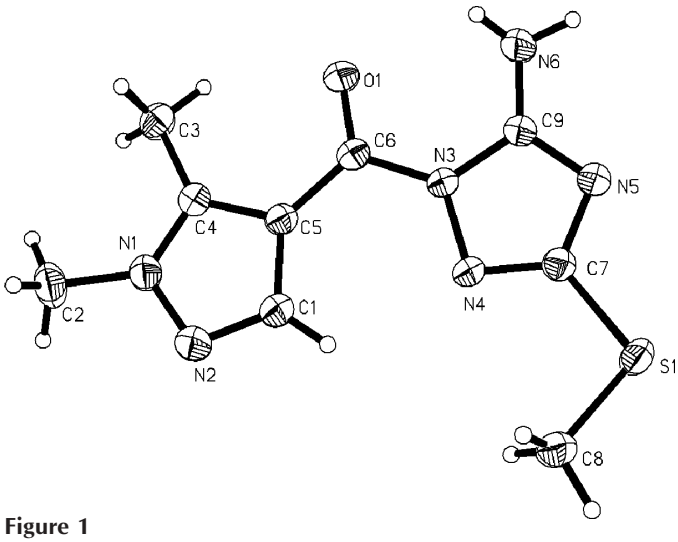


Figure 1
View of the title compound, with 35% probability ellipsoids.

Data collection

Bruker APEX II CCD area-detector diffractometer	2024 independent reflections
φ and ω scans	1763 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	$R_{int} = 0.020$
$T_{min} = 0.882$, $T_{max} = 0.946$	$\theta_{max} = 25.0^\circ$
5982 measured reflections	$h = -9 \rightarrow 8$
	$k = -12 \rightarrow 10$
	$l = -18 \rightarrow 18$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.088P)^2 + 0.3815P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.043$	$(\Delta/\sigma)_{max} = 0.001$
$wR(F^2) = 0.138$	$\Delta\rho_{max} = 0.29$ e Å^{-3}
$S = 1.08$	$\Delta\rho_{min} = -0.50$ e Å^{-3}
2024 reflections	
158 parameters	
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

O1—C6	1.221 (3)	N5—C9	1.313 (3)
N1—C4	1.336 (3)	N5—C7	1.376 (3)
N2—C1	1.320 (3)	N6—C9	1.333 (3)
N3—C9	1.388 (3)	C1—C5	1.412 (3)
N4—C7	1.307 (3)	C4—C5	1.395 (3)
C4—N1—N2	113.28 (17)	N2—C1—C5	111.94 (19)
C1—N2—N1	104.29 (17)	N1—C4—C5	106.22 (18)
C9—N3—N4	108.46 (15)	C4—C5—C1	104.27 (19)
C7—N4—N3	101.66 (16)	N4—C7—N5	116.75 (19)
C9—N5—C7	103.03 (18)	N5—C9—N3	110.08 (17)

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

D—H···A	D—H	H···A	D···A	D—H···A
N6—H6B···O1	0.89	2.23	2.695 (3)	112
N6—H6A···N5^{i}	0.89	2.09	2.961 (3)	163

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

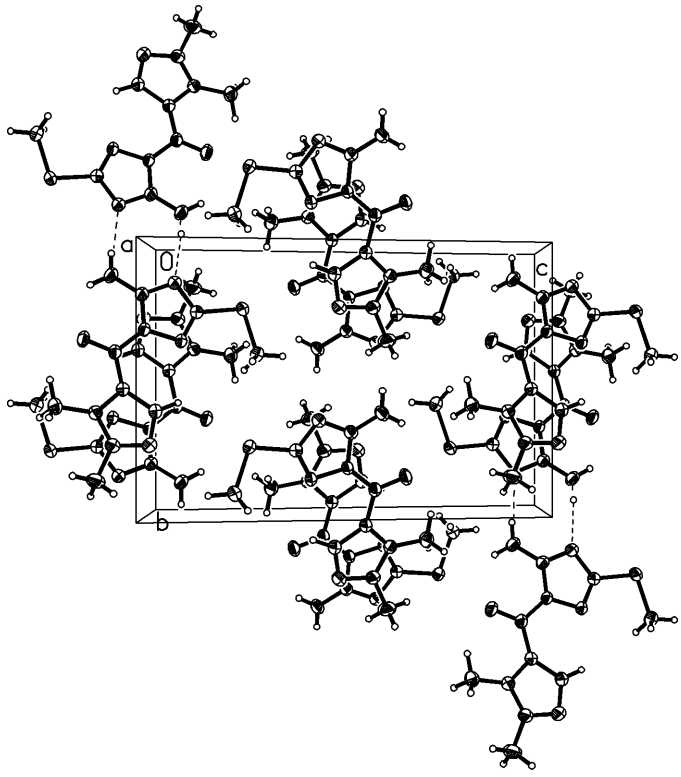


Figure 2
The molecular packing of the title compound, viewed along the *a* axis. Hydrogen bonds are shown as dashed lines.

All H atoms were placed in calculated positions, with C—H = 0.93 or 0.96 Å and N—H = 0.89 Å, and included in the final cycles of refinement using a riding model, with U_{iso}(H) set at $1.2U_{eq}$(C) for CH_2, and $1.5U_{eq}$(C,N) for NH, CH and CH_3 H atoms.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1999); 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, 1999); software used to prepare material for publication: *SHELXTL*.

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

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