Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

4-Allyl-3-(pyrazin-2-yl)-Δ^2-1*H*-1,2,4-triazole-5(4*H*)-thione

Irena Wawrzycka-Gorczyca,[a]* Agata Siwek[b] and Maria Dobosz[b]

[a]Faculty of Chemistry, Maria Curie-Sklodowska University, 20031 Lublin, Poland, and [b]Department of Organic Chemistry, Faculty of Pharmacy, Medical University, 20081 Lublin, Poland

Correspondence e-mail: iwawrz@hermes.umcs.lublin.pl

Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.043
wR factor = 0.131
Data-to-parameter ratio = 13.0

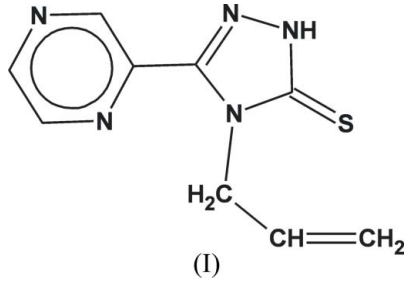
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 30 November 2005
Accepted 5 December 2005
Online 10 December 2005

The molecule of the title compound, $C_9H_9N_5S$, has a non-planar conformation. In the crystal structure, molecules are connected by N—H···N hydrogen bonds along the *b* axis. Weak C—H···S interactions complete the crystal packing.

Comment

Organic compounds containing aromatic heterocyclic rings have received considerable attention among medicinal chemists because many of them play a role in various biochemical processes. 1,2,4-Triazole and pyrazine derivatives belong to an aromatic heterocyclic group exhibiting a wide range of biological activities, such as antifungal (Demirayak *et al.*, 2000; Doležal *et al.*, 2000; Doležal *et al.*, 2003), antibacterial (Pandeya *et al.*, 2000), anticancer (Invidiata *et al.*, 1991), antiviral (Todoulou *et al.*, 1994), anti-inflammatory (Sahin *et al.*, 2001), antitubercular (Doležal *et al.*, 1996). Chemical modifications leading to the combination of two or more heterocyclic and non-heterocyclic systems produce compounds of significantly enhanced biological profile compared to the parent nuclei. We have therefore combined the 1,2,4-triazole group with the pyrazin-2-yl nucleus, since both of these systems possess well documented biological activities. We present here the crystal structure of 4-allyl-3-(pyrazin-2-yl)-Δ^2-1,2,4-triazoline-5-thione, (I) (Fig. 1).



(I)

The triazole plane forms dihedral angles of 76.8 (2)° and 6.1 (1)° with the propene and pyrazine planes, respectively. In the crystal structure, molecules are linked by intermolecular N—H···N (triazole···pyrazine) hydrogen bonds and C—H···S (pyrazine···triazole) weak interactions (Fig. 2 and Table 2) along the [010] direction.

Experimental

Yellow crystals of (I) (Dobosz *et al.*, 2006) were obtained by slow evaporation of an ethanol solution at room temperature.

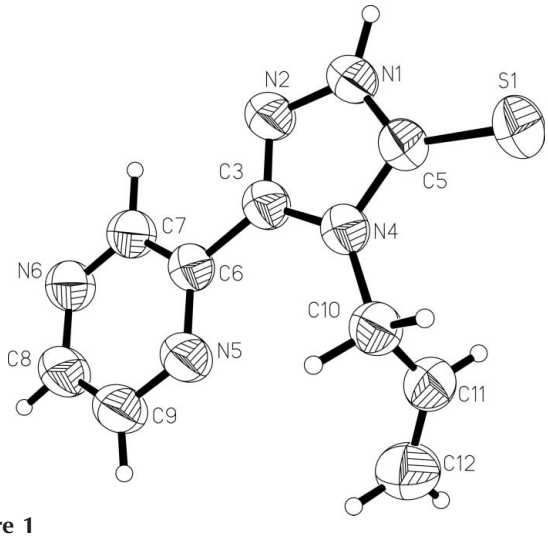


Figure 1
The molecular structure of (I), with the atom numbering. Displacement ellipsoids are drawn at the 50% probability level.

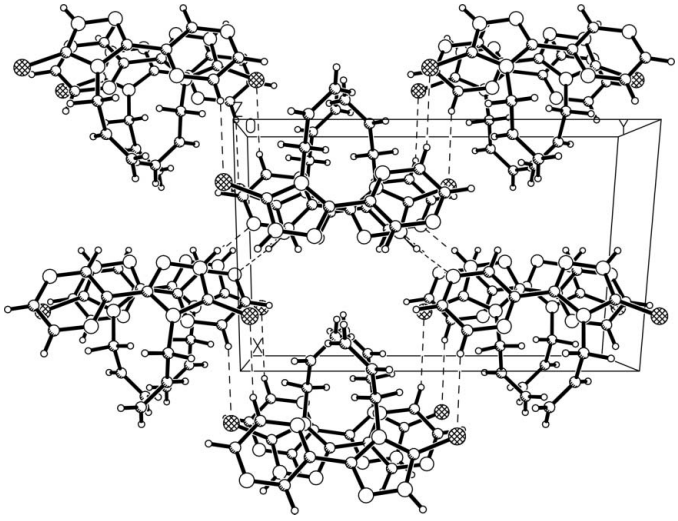


Figure 2
The crystal packing of (I). Dashed lines indicate hydrogen bonds.

Crystal data

$C_9H_9N_5S$
M_r = 219.27
Monoclinic, $P2_1/c$
a = 9.736 (2) Å
b = 14.750 (2) Å
c = 7.913 (2) Å
β = 112.57 (3)°
V = 1049.3 (4) Å^3
Z = 4
D_x = 1.388 Mg m^{-3}
Cu $K\alpha$ radiation
Cell parameters from 97 reflections
θ = 6–20.5°
μ = 2.54 mm^{-1}
T = 293 (2) K
Prism, yellow
0.6 × 0.25 × 0.1 mm

Data collection

Kuma KM-4 four-circle diffractometer
ω–2θ scans
Absorption correction: spherical (Dwiggins, 1975) with modifications.
T_{min} = 0.129, T_{max} = 0.236
2367 measured reflections
2242 independent reflections
1213 reflections with $I > 2\sigma(I)$
R_{int} = 0.055
θ_{max} = 80.3°
$h = 0 \rightarrow 11$
$k = -18 \rightarrow 0$
$l = -9 \rightarrow 9$
3 standard reflections
every 100 reflections
intensity decay: 1.4%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.131
S = 1.03
2242 reflections
173 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0796P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.31 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0130 (12)

Table 1
Selected geometric parameters (Å, °).

S1—C5	1.671 (2)	N4—C3	1.380 (3)
N1—C5	1.335 (3)	N4—C10	1.475 (3)
N1—N2	1.367 (3)	C10—C11	1.479 (4)
N2—C3	1.303 (3)	C11—C12	1.304 (4)
N4—C5	1.378 (3)		
C10—N4—C3—C6	2.3 (4)	C3—N4—C10—C11	83.9 (3)
N4—C3—C6—N5	5.8 (4)	N4—C10—C11—C12	−128.6 (3)

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1*N*···N6^{i}	0.95 (3)	1.91 (3)	2.844 (3)	168 (3)
C9—H9···S1^{ii}	0.92 (3)	2.92 (3)	3.780 (3)	156 (3)

Symmetry codes: (i) $-x, y+\frac{1}{2}, -z+\frac{1}{2}$; (ii) $-x+1, y-\frac{1}{2}, -z+\frac{3}{2}$.

All H atoms were found in a difference Fourier map and were refined isotropically.

Data collection: *KM-4 Software* (Kuma, 1991); cell refinement: *KM-4 Software*; data reduction: *KM-4 Software*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL/PC* (Sheldrick, 1990); software used to prepare material for publication: *SHELXL97*.

References

Demirayak, S., Benkli, K. & Güven, K. (2000). *Eur. J. Med. Chem.* **35**, 1037–1040.
Dobosz, M., Siwek, A. & Wawrzycka-Gorczyca, I. (2006). In preparation.
Doležal, M., Hartl, J., Lyčka, A., Buchta, V. & Odlerová, Ž. (1996). *Collect. Czech. Chem. Commun.* **61**, 1102–1108.
Doležal, M., Jampílek, J., Osicka, Z., Kuneš, J., Buchta, V. & Víchová, P. (2003). *Farmaco*, **58**, 1105–1111.
Doležal, M., Vicik, R., Miletin, M. & Král'ová, K. (2000). *Chem. Pap.* **54**, 245–248.
Dwiggins, C. W. Jr (1975). *Acta Cryst.* A**31**, 146–148.
Invidiata, F. P., Grimaudo, S., Giammanco, P. & Giammanco, L. (1991). *Farmaco*, **46**, 1489–1495.
Kuma Diffraction (1991). *KM4 Software*. Kuma Diffraction, Wrocław, Poland.
Pandeya, S. N., Sriram, D., Nath, G. & De Clercq, E. (2000). *Arzneim.-Forsch. Drug Res.* **50**, 55–59.
Sahin, G., Palaska, E., Kelicen, P., Demirdamar, R. & Altmok, G. (2001). *Arzneim.-Forsch.* **51**, 478–484.
Sheldrick, G. M. (1990). *SHELXTL/PC*. User's Manual. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Todoulou, O. G., Papadaki-Valiraki, A., Filippatos, E. C., Ikeda, S. & De Clercq, E. (1994). *Eur. J. Med. Chem.* **29**, 127–131.