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6,7,8,9-Tetrahydro-2*H*-1,2,4-triazolo[4,3-*a*]-azepin-3(5*H*)-one

Gui-Sheng Yu, Hai-Zhen Xu* and Xin Zhang

College of Chemistry and Life Science, Tianjin Normal University, Weijin Road No. 241, Tianjin, People's Republic of China

Correspondence e-mail: tj_xhz@126.com

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Key indicators

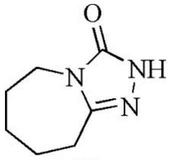
Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.004 Å
R factor = 0.058
wR factor = 0.154
Data-to-parameter ratio = 14.1

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

In the title compound, $C_7H_{11}N_3O$, the seven-membered hetero-ring adopts a chair conformation. The five-membered ring is essentially coplanar with the fused back of the chair. The compound is stabilized by a strong intermolecular N—H···O hydrogen bond, forming a chain.

Comment

Recently, bicyclic 1,2,4-triazol-3(2*H*)-ones have been designed and synthesized as potential 5-HT2 antagonists (Yoshifumi *et al.*, 1992). It was noticed that many hetero-ring compounds possess high herbicidal activities; however, the use of their derivatives as herbicides has rarely been reported. This provides us with a chance to obtain the herbicidal lead compound with bicyclic 1,2,4-triazol-3(2*H*)-ones. In this paper, we describe the crystal structure of the title compound, (I).



(I)

In (I), the seven-membered heterocyclic ring adopts a chair conformation. The five-membered ring is essentially coplanar with the fused back of the chair, *viz.* atoms C1, N1, C6 and C5 (Fig. 1). The dihedral angles formed by the plane C1/C2/C4/C5 with C1/C5/C6/C7/N1/N2/N3 and C2/C3/C4 are 51.9 (1) and 56.1 (2)°, respectively. The packing form of the molecule is a sandwich, and the compound is stabilized by an intermolecular

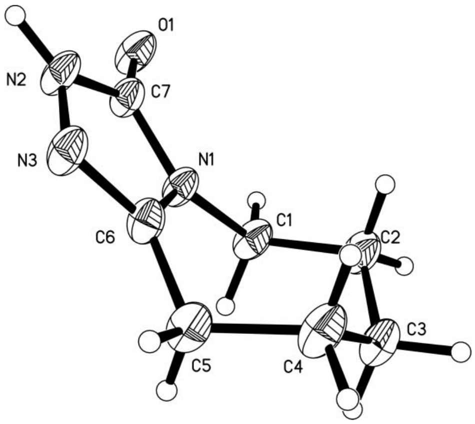


Figure 1
View of the title compound, with displacement ellipsoids drawn at the 30% probability level.

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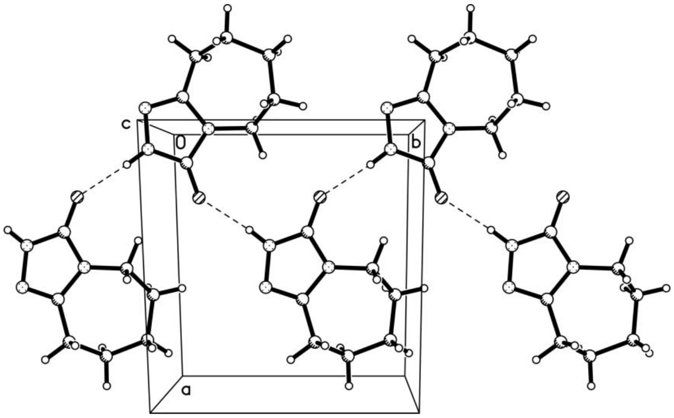

Figure 2
The packing of (I), viewed along the *c* axis. Dashed lines indicate hydrogen bonds.

N—H···O hydrogen bond, forming a chain along the *b* axis (Fig. 2 and Table 2).

Experimental

The title compound, (I), was synthesized by the procedure of Petersen & Tietze (1957). The product was recrystallized from ethanol, affording colorless crystals suitable for X-ray analysis.

Crystal data

$C_7H_{11}N_3O$
$M_r = 153.19$
Monoclinic, $P2_1/n$
$a = 9.069$ (9) Å
$b = 7.884$ (8) Å
$c = 10.780$ (11) Å
$\beta = 111.279$ (17)°
$V = 718.2$ (12) Å^3
$Z = 4$

$D_x = 1.417$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1141 reflections
$\theta = 3.3$–25.3°
$\mu = 0.10$ mm^{-1}
$T = 294$ (2) K
Prism, colorless
0.28 × 0.24 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.973$, $T_{\max} = 0.980$
3655 measured reflections

1426 independent reflections
898 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.049$
$\theta_{\max} = 26.1°$
$h = -11 \rightarrow 8$
$k = -9 \rightarrow 9$
$l = -13 \rightarrow 12$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.058$
$wR(F^2) = 0.155$
$S = 1.07$
1426 reflections
101 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.08P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.004$
$\Delta\rho_{\max} = 0.26$ e Å^{-3}
$\Delta\rho_{\min} = -0.25$ e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.032 (8)

Table 1
Selected torsion angles (°).

C7—N1—C1—C2	122.9 (2)	C3—C4—C5—C6	−74.0 (3)
N1—C1—C2—C3	75.2 (3)	C4—C5—C6—N3	−122.6 (3)

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···O1$^{\rm i}$	0.86	1.95	2.776 (3)	160

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

The H atom bonded to N2 was located in a difference map but then placed in a calculated position. All other H atoms were positioned geometrically. The H atoms were refined using a riding model, with N—H = 0.86 Å and C—H = 0.97 Å, and with $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}({\rm C,N})$.

Data collection: *SMART* (Bruker, 1999); 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*.

References

Bruker (1999). *SMART*, *SAINT* and *SHELXTL*. Bruker AXS Inc., Madison, Wisconsin, USA.
Petersen, S. & Tietze, E. (1957). *Chem. Ber.* **90**, 909–921.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Yoshifumi, W., Hiroyuki, U., Shozo, K., Hirotaka, Y., Toshiro, S., Tsuyoshi, T., Yoshiyuki, M., Megumi, Y. & Munefumi, K. (1992). *J. Med. Chem.* **35**, 189–194.