Acta Crystallographica Section C
Crystal Structure Communications
ISSN 0108-2701

4-(4-Hydroxybenzylideneamino)-4*H*-1,2,4-triazole hemihydrate

Dun-Ru Zhu, Yan Xu, Yong-Jiang Liu, You Song, Yong Zhang* and Xiao-Zeng You

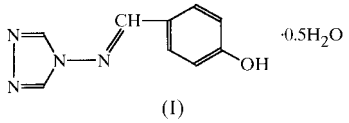
Coordination Chemistry Institute, State Key Laboratory of Coordination Chemistry, Nanjing University, Nanjing 210093, People's Republic of China
Correspondence e-mail: xyz@nju.edu.cn

Received 18 October 1999
Accepted 9 November 1999

In the title compound, 4-(4*H*-1,2,4-triazol-4-yliminomethyl)-phenol hemihydrate, $C_9H_8N_4O{\cdot}0.5H_2O$ or (I)$\cdot 0.5H_2O$, molecules of (I) are arranged as layers running along the *b* axis through intermolecular O—H···N and C—H···O hydrogen bonds. These layers are stabilized by hydrogen-bonded water molecules to form three-dimensional networks.

Comment

The aroyl Schiff bases of 4-amino-1,2,4-triazole have received considerable attention over the past few decades (Kitaev *et al.*, 1971; Mazza *et al.*, 1976; Kargin *et al.*, 1988). It is of interest that some of them are anti-inflammatory agents (Gupta & Bhargava, 1978) and new coccidiostatic drugs (Colautti *et al.*, 1971). As a continuation of our study on the structure of Schiff-base-containing substituted 1,2,4-triazole (Shanmuga Sundara Raj *et al.*, 1999), we report here the title structure, (I).



(I)

An *ORTEP*II (Johnson, 1976) diagram of (I) with numbering scheme is shown in Fig. 1. Compared to 9-(4*H*-1,2,4-triazol-4-ylimino)-4,5-diazafluorene (Shanmuga Sundara Raj *et al.*, 1999), molecules of (I) are essentially planar [the maximum displacement from the least-squares mean plane through the whole molecule is 0.073 (2) Å for C9]. The bond lengths and angles observed in the structure are in the normal ranges. In contrast with 2-(2-hydroxybenzylidene)-1-(2-picoloyl)hydrazine hemihydrate (Wang *et al.*, 1998), molecules of (I) are arranged as layers running along the *b* axis through strong intermolecular O1—H11···N4($-\frac{1}{2}+x$, $-\frac{1}{2}-y$, $\frac{1}{2}+z$) hydrogen bonds and weak C9—H9···O1($\frac{1}{2}-x$, $-\frac{1}{2}+y$, $-\frac{1}{2}-z$) ones. These layers are stabilized by water molecules to form three-dimensional networks through strong O1*W*—H1*W*···N3 hydrogen bonds and weak C7—H7···O1*W*(x, $-y$, $\frac{1}{2}+z$) ones. The geometry of these interactions are listed in Table 2. In the packing of molecules of the title compound, the water molecules (O1*W*) lie on crystallographic twofold axes.

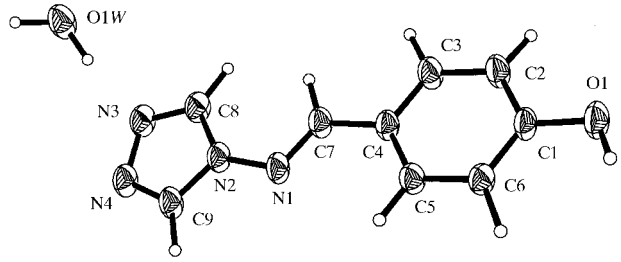


Figure 1
The structure of (I) showing 50% probability displacement ellipsoids with the numbering scheme.

Experimental

The title compound was prepared by condensation of equivalent amounts of *p*-hydroxybenzaldehyde and 4-amino-1,2,4-triazole in ethanol for 5 h (Kitaev *et al.*, 1971). Diffraction-quality crystals were obtained by recrystallization from ethanol.

Crystal data

$C_9H_8N_4O{\cdot}0.5H_2O$
M_r = 197.20
Monoclinic, C_2/c
a = 14.134 (2) Å
b = 12.491 (2) Å
c = 12.063 (2) Å
β = 119.483 (10)°
V = 1854.0 (5) Å^3
Z = 8
D_x = 1.413 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 36 reflections
θ = 5.22–9.01°
μ = 0.102 mm^{-1}
T = 293 (2) K
Block, colourless
0.30 × 0.26 × 0.20 mm

Data collection

Siemens *P*4 diffractometer
$2\theta/\omega$ scans
Absorption correction: empirical (North *et al.*, 1968)
T_{min} = 0.954, T_{max} = 0.968
2043 measured reflections
1642 independent reflections
1100 reflections with $I > 2\sigma(I)$
R_{int} = 0.021
θ_{max} = 25°
$h = -1 \rightarrow 16$
$k = -1 \rightarrow 14$
$l = -14 \rightarrow 12$
3 standard reflections every 97 reflections
intensity decay: 5.84%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.057
$wR(F^2)$ = 0.155
S = 1.166
1637 reflections
133 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0851P)^2 + 1.2289P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = -0.006$
$\Delta\rho_{max}$ = 0.28 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}
Extinction correction: *SHELXTL* (Siemens, 1995)
Extinction coefficient: 0.0022 (6)

Table 1
Selected geometric parameters (Å, °).

N1—C7	1.267 (2)	N3—N4	1.383 (2)
N1—N2	1.409 (2)	N4—C9	1.302 (2)
N2—C9	1.357 (2)	C1—O1	1.350 (2)
N2—C8	1.362 (2)	C4—C7	1.456 (3)
N3—C8	1.304 (3)		
C7—N1—N2	115.4 (2)	C8—N2—N1	132.3 (2)
C9—N2—C8	105.7 (2)	O1—C1—C6	123.0 (2)
C9—N2—N1	122.0 (2)	N1—C7—C4	122.5 (2)

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H11···N4^{i}	1.01	1.74	2.717 (2)	161
C9—H9···O1^{ii}	1.18	2.15	3.293 (3)	164
O1W—H1W···N3	1.02	1.89	2.898 (2)	169
C7—H7···O1W^{iii}	1.10	2.47	3.214 (2)	123

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

Data collection: *XSCANS* (Siemens, 1994); cell refinement: *XSCANS*; data reduction: *SHELXTL* (Siemens, 1995); program(s) used to solve structure: *SHELXTL*; program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

This work was funded by a state key project of the Fundamental Research and the National Nature Science Foundation of China and Nanjing University Talent Development Foundation.

Supplementary data for this paper are available from the IUCr electronic archives (Reference: NA1438). Services for accessing these data are described at the back of the journal.

References

Colautti, A., Ferlauto, R. J., Maurich, V., De Nardo, M., Nisi, C., Rubessa, F. & Runti, C. (1971). *Chim. Ther.* **6**, 367–379.
Gupta, A. K. & Bhargava, K. P. (1978). *Pharmazie*, **33**, 430–431.
Johnson, C. K. (1976). *ORTEP*II. Report ORNL-5138. Oak Ridge National Laboratory, Tennessee, USA.
Kargin, Yu. M., Kitaeva, M. Yu., Latypova, V. Z., Vafina, A. A., Zaripova, R. M. & Il'yasov, A. V. (1988). *Izv. Akad. Nauk SSSR Ser. Khim.* **3**, 607–611.
Kitaev, Yu. P., Savin, V. I., Zverev, V. V. & Popova, G. V. (1971). *Khim. Geterotsikl. Soedin.* **7**, 559–564.
Mazza, M., Montanari, L. & Pavanetto, F. (1976). *Farmaco Ed. Sci.* **31**, 334–344.
North, A. C. T., Phillips, D. C. & Mathews, F. S. (1968). *Acta Cryst.* A**24**, 351–359.
Shanmuga Sundara Raj, S., Fun, H.-K., Zhu, D.-R., Jian, F.-F., Zhang, K.-L. & You, X.-Z. (1999). *Acta Cryst.* C**55**, 1526–1528.
Siemens (1994). *XSCANS*. Version 2.1. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Siemens (1995). *SHELXTL*. Version 5.0. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Wang, Z.-X., Jian, F.-F., Duan, C.-Y., Bai, Z.-P. & You, X.-Z. (1998). *Acta Cryst.* C**54**, 1927–1929.