Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

4-(2-Hydroxyethyl)-4*H*-1,2,4-triazole, an intermediate in the synthesis of iron–triazole spin-crossover compounds

Martin U. Schmidt,[a] Chunhua Hu,[a]* Jan W. Bats[b] and Jens Kühne[a]

[a]Institute of Inorganic and Analytical Chemistry, University of Frankfurt, Marie-Curie-Strasse 11, D-60439 Frankfurt am Main, Germany, and [b]Institute of Organic Chemistry, University of Frankfurt, Marie-Curie-Strasse 11, D-60439 Frankfurt am Main, Germany

Correspondence e-mail: chunhua.hu@chemie.uni-frankfurt.de

Key indicators

Single-crystal X-ray study
T = 150 K
Mean σ(C–C) = 0.002 Å
R factor = 0.041
wR factor = 0.100
Data-to-parameter ratio = 12.9

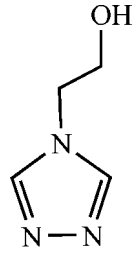
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 17 November 2005
Accepted 21 November 2005
Online 26 November 2005

The title 1,2,4-triazole derivative, $C_4H_7N_3O$, has been synthesized and characterized. Neighboring molecules are connected by intermolecular O—H···N hydrogen bonds, forming a linear chain arrangement along the crystallographic [101] direction.

Comment

The title compound, (hyetrz, I), has been used to react with divalent Fe or Cu complexes in order to investigate the interesting spin-crossover phenomena of Fe^{2+} compounds (Garcia, van Koningsbruggen, Bravic *et al.*, 1997; Garcia *et al.*, 2000, 2002) and to establish the structural model based on Cu^{2+} analogs (Garcia, van Koningsbruggen, Codjovi *et al.*, 1997; Garcia *et al.*, 2003). Although three metal complexes of the ligand have been structurally determined, the crystal structure of the free ligand itself is yet unknown. Here we report its structure.



(I)

The hydroxyethyl group represents the flexible part of the molecule (Fig. 1), and bends out of the plane of the triazole

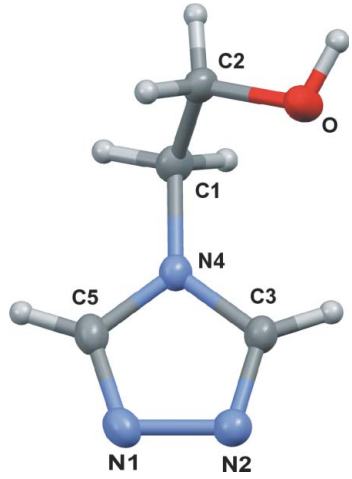


Figure 1
Displacement ellipsoid plot (50% probability level) for (I).

ring. The resulting torsion angle N4—C1—C2—O is 61.3 (2)°. This value is in the range of those observed in the metal coordination complexes: 48.2–64.8° in $[Cu(hyetrz)_3](ClO_4)_2\cdot 3H_2O$ (Garcia, van Koningsbruggen, Bravic *et al.*, 1997), 52.9–66.3° in $[Cu(hyetrz)_3](CF_3SO_3)_2\cdot H_2O$ (Garcia *et al.*, 2003), and 68.0 and 68.3° in $[Fe_3(hyetrz)_6(H_2O)_6](CF_3SO_3)_6$ (Garcia *et al.*, 2000). Obviously it is affected by the intermolecular interactions. The bond lengths and angles are almost identical to those in the above metal complexes.

In the crystal structure of (I), the molecules are connected by hydrogen bonds between N atoms of the triazole rings and H atoms of the hydroxy groups in neighboring molecules (Table 2), leading to a linear chain arrangement along the [101] direction (Fig. 2).

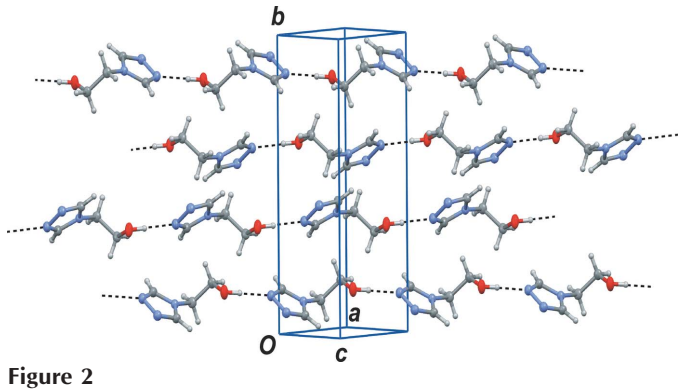


Figure 2
MERCURY (Bruno *et al.*, 2002) representation of the intermolecular hydrogen-bond (dashed lines) arrangement (C, grey; H, light gray; N, blue; O, red).

Experimental

The compound was prepared from monoformyl hydrazine, triethyl orthoformate and 2-ethanolamine according to the general method described by Bayer *et al.* (1974). m.p.: 357 K by DTA. ^{1}H NMR (250 MHz) (DMSO): 3.66 (*t*, 2H, CH_2), 4.09 (*t*, 2H, CH_2), 5.10 (*s*, 1H, OH), 8.48 (*s*, 2H, CH). Recrystallization from methanol results in single crystals suitable for X-ray measurement.

Crystal data

$C_4H_7N_3O$	D_x = 1.400 Mg m^{-3}
M_r = 113.13	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 39 reflections
a = 5.5894 (18) Å	θ = 2.8–28.0°
b = 14.444 (5) Å	μ = 0.11 mm^{-1}
c = 7.013 (4) Å	T = 150 (2) K
β = 108.56 (3)°	Block, colourless
V = 536.7 (4) Å^3	0.23 × 0.18 × 0.18 mm
Z = 4	

Data collection

Siemens SMART 1K CCD area-detector diffractometer	976 reflections with $I > 2\sigma(I)$
	R_{int} = 0.095
ω scans	θ_{max} = 28.0°
Absorption correction: none	$h = -7 \rightarrow 7$
8131 measured reflections	$k = -19 \rightarrow 18$
1301 independent reflections	$l = -9 \rightarrow 9$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0324P)^2 + 0.1227P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.041	
$wR(F^2)$ = 0.100	
S = 1.08	$(\Delta/\sigma)_{max} < 0.001$
1301 reflections	$\Delta\rho_{max}$ = 0.20 e Å^{-3}
101 parameters	$\Delta\rho_{min}$ = −0.25 e Å^{-3}
All H-atom parameters refined	

Table 1
Selected bond length.

N1—N2	1.3923 (17)	N1—C5	1.3031 (19)
N2—C3	1.308 (2)	N4—C1	1.466 (2)
C3—N4	1.3505 (19)	C1—C2	1.509 (2)
N4—C5	1.3594 (17)	C2—O	1.4197 (17)

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

D—H···A	D—H	H···A	D···A	D—H···A
O—H1···N2^{i}	0.90 (2)	1.85 (2)	2.754 (2)	178 (2)

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

All H atoms were located in difference Fourier syntheses and were refined freely with isotropic displacement parameters.

Data collection: *SMART* (Siemens, 1995); cell refinement: *SMART*; data reduction: *SAINT* (Siemens, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *MERCURY* (Bruno *et al.*, 2002); software used to prepare material for publication: *SHELXL97*.

This work was supported by the Deutsche Forschungsgemeinschaft under the auspices of the Forschergruppe 412 on 'Spin- and Charge-Correlations in Low-Dimensional Metal-organic Solids'.

References

Bayer, H. O., Cook, R. S. & von Meyer, W. C. (1974). US Patent No. 3 821 376.
Bruno, I. J., Cole, J. C., Edgington, P. R., Kessler, M. K., Macrae, C. F., McCabe, P., Pearson, J. & Taylor, R. (2002). *Acta Cryst.* B**58**, 389–397.
Garcia, Y., Guionneau, P., Bravic, G., Chasseau, D., Howard, J. A. K., Kahn, O., Ksenofontov, V., Reiman, S. & Gütlich, P. (2000). *Eur. J. Inorg. Chem.* pp. 1531–1538.
Garcia, Y., Ksenofontov, V. & Gütlich, P. (2002). *Hyperfine Interact.* **139/140**, 543–551.
Garcia, Y., van Koningsbruggen, P. J., Bravic, G., Chasseau, D. & Kahn, O. (2003). *Eur. J. Inorg. Chem.* pp. 356–362.
Garcia, Y., van Koningsbruggen, P. J., Bravic, G., Guionneau, P., Chasseau, D., Cascarano, G. L., Moscovici, J., Lambert, K., Michalowicz, A. & Kahn, O. (1997). *Inorg. Chem.* **36**, 6357–6365.
Garcia, Y., van Koningsbruggen, P. J., Codjovi, E., Lapouyade, R., Kahn, O. & Rabardel, L. (1997). *J. Mater. Chem.* **7**, 857–858.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Siemens (1995). *SMART* and *SAINT*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.