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2-(5-Amino-2H-tetrazol-2-yl)acetic acid

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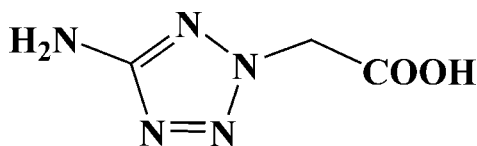
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Key indicators: single-crystal X-ray study; $T = 296$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.044; wR factor = 0.124; data-to-parameter ratio = 13.0.

In the title molecule, $\text{C}_3\text{H}_5\text{N}_5\text{O}_2$, the tetrazole ring and carboxyl group form a dihedral angle of $82.25(14)^\circ$. In the crystal, adjacent molecules are linked through $\text{O}-\text{H}\cdots\text{N}$, $\text{N}-\text{H}\cdots\text{O}$ and $\text{N}-\text{H}\cdots\text{N}$ hydrogen bonds into layers parallel to the bc plane.

Related literature

For background to tetrazole compounds, see: Zhao *et al.* (2008). For the use of 5-aminotetrazole-1-acetic acid in coordination chemistry, see: Li *et al.* (2010); Shen *et al.* (2011); Yang *et al.* (2008). For the crystal structures of similar compounds, see: Bryden (1956); Klapötke *et al.* (2009). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$\text{C}_3\text{H}_5\text{N}_5\text{O}_2$
 $M_r = 143.12$
 Monoclinic, $C2/c$
 $a = 18.381(4)$ Å
 $b = 4.4429(9)$ Å
 $c = 14.846(3)$ Å
 $\beta = 90.850(3)^\circ$

$V = 1212.2(4)$ Å³
 $Z = 8$
 Mo $K\alpha$ radiation
 $\mu = 0.13$ mm⁻¹
 $T = 296$ K
 $0.28 \times 0.19 \times 0.15$ mm

Data collection

Bruker APEXII CCD diffractometer
 Absorption correction: multi-scan (SADABS; Bruker, 2008)
 $T_{\min} = 0.970$, $T_{\max} = 0.980$

3040 measured reflections
 1193 independent reflections
 890 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.024$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.044$
 $wR(F^2) = 0.124$
 $S = 1.03$
 1193 reflections

92 parameters
 H-atom parameters constrained
 $\Delta\rho_{\max} = 0.21$ e Å⁻³
 $\Delta\rho_{\min} = -0.19$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{N5}-\text{H5B}\cdots\text{O1}^{\text{i}}$	0.86	2.36	3.080 (3)	141
$\text{N5}-\text{H5A}\cdots\text{N4}^{\text{ii}}$	0.86	2.23	3.064 (3)	163
$\text{O2}-\text{H2}\cdots\text{N1}^{\text{iii}}$	0.82	1.85	2.665 (2)	172

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

Data collection: APEX2 (Bruker, 2008); cell refinement: SAINT (Bruker, 2008); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: ORTEP-3 (Farrugia, 1997); software used to prepare material for publication: SHELXL97.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV5277).

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supporting information

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2-(5-Amino-2*H*-tetrazol-2-yl)acetic acid

Guo-Chun Zhang, Cheng-Fang Qiao, Chun-Sheng Zhou and Zheng-Qiang Xia

S1. Comment

In recent years, numerous tetrazole ligands were used to construct coordination compounds, which have been the subject of an intense research effort owing to their unique structures and potential applications in advanced materials (Zhao *et al.*, 2008). However, the study of coordination compounds with disubstituted tetrazole ligands is comparatively scarce.

Recently, Li *et al.* (2010) reported a series of lanthanide-based compounds with 5-aminotetrazole-1-acetic acid, which possesses intriguing topological structures and predominant optics performance. Inspired by this interesting work, we report here the crystal structure of a 2,5-disubstituted tetrazole compound, (5-Amino-2*H*-tetrazole-2-yl)acetic acid, (**I**).

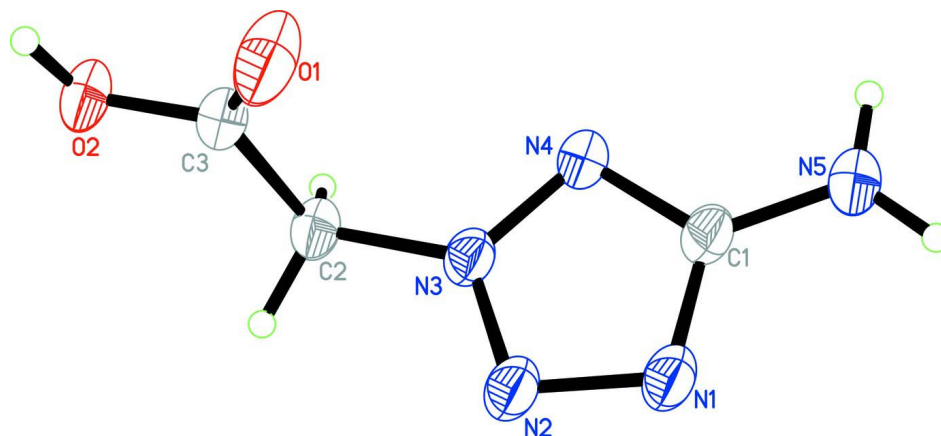
As shown in Fig. 1, the tetrazole ring (C1/N1—N4) is essentially planar with an r.m.s. deviation of 0.008 °. The carboxyl group (O1/C3/O2) and tetrazole ring are inclined at a dihedral angle of 82.25 (14) °. All bond lengths and angles are in the normal ranges (Allen *et al.*, 1987). The torsion angles N4—N3—C2—C3 = -80.6 (2) °, N2—N3—C2—C3 = 101.8 (2) °, O1—C3—C2—N3 = -3.6 (3) °, O2—C3—C2—N3 = 178.80 (17) °. In the crystal structure, intermolecular O—H···N, N—H···O and N—H···N hydrogen bonds (Table 1) link the molecules into a two-dimensional framework parallel to the *bc* plane.

S2. Experimental

The compound was obtained commercially (Aldrich). Colourless crystals suitable for the X-ray diffraction study were obtained by slow evaporation of an ethanol/water (2:1 *v/v*) solution of the compound (**I**) at room temperature.

S3. Refinement

All H atoms were placed in geometrically idealized positions, with C—H = 0.97 Å, N—H = 0.86 Å and O—H = 0.82 Å, and were thereafter treated as riding with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C}, \text{N})$ or $1.5U_{\text{eq}}(\text{O})$.

**Figure 1**

The molecular structure of (I) showing the atom numbering scheme and 30% probability displacement ellipsoids.

2-(5-Amino-2H-tetrazol-2-yl)acetic acid

Crystal data

$C_3H_5N_5O_2$
 $M_r = 143.12$
 Monoclinic, $C2/c$
 Hall symbol: $-C 2yc$
 $a = 18.381(4) \text{ \AA}$
 $b = 4.4429(9) \text{ \AA}$
 $c = 14.846(3) \text{ \AA}$
 $\beta = 90.850(3)^\circ$
 $V = 1212.2(4) \text{ \AA}^3$
 $Z = 8$
 $F(000) = 592$

$D_x = 1.568 \text{ Mg m}^{-3}$
 $D_m = 1.568 \text{ Mg m}^{-3}$
 D_m measured by not measured
 Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
 Cell parameters from 734 reflections
 $\theta = 3.5\text{--}22.2^\circ$
 $\mu = 0.13 \text{ mm}^{-1}$
 $T = 296 \text{ K}$
 Block, colourless
 $0.28 \times 0.19 \times 0.15 \text{ mm}$

Data collection

Bruker APEXII CCD
 diffractometer
 Radiation source: fine-focus sealed tube
 Graphite monochromator
 φ and ω scans
 Absorption correction: multi-scan
 (SADABS; Bruker, 2008)
 $T_{\min} = 0.970$, $T_{\max} = 0.980$

3040 measured reflections
 1193 independent reflections
 890 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.024$
 $\theta_{\max} = 26.0^\circ$, $\theta_{\min} = 2.2^\circ$
 $h = -22 \rightarrow 22$
 $k = -5 \rightarrow 4$
 $l = -13 \rightarrow 18$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.044$
 $wR(F^2) = 0.124$
 $S = 1.03$
 1193 reflections
 92 parameters
 0 restraints
 Primary atom site location: structure-invariant
 direct methods

Secondary atom site location: difference Fourier
 map
 Hydrogen site location: inferred from
 neighbouring sites
 H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.0657P)^2 + 0.3572P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.002$
 $\Delta\rho_{\max} = 0.21 \text{ e \AA}^{-3}$
 $\Delta\rho_{\min} = -0.19 \text{ e \AA}^{-3}$

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R -factor wR and goodness of fit S are based on F^2 , conventional R -factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R -factors(gt) *etc.* and is not relevant to the choice of reflections for refinement. R -factors based on F^2 are statistically about twice as large as those based on F , and R -factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
O2	0.17856 (8)	0.1746 (3)	0.30324 (8)	0.0527 (4)
H2	0.1626	0.2644	0.3470	0.079*
N2	0.18104 (10)	0.4658 (4)	0.01590 (11)	0.0493 (5)
N3	0.15090 (8)	0.2586 (4)	0.06465 (10)	0.0414 (4)
C3	0.14844 (11)	0.2824 (5)	0.22938 (12)	0.0426 (5)
N4	0.08911 (9)	0.1468 (4)	0.03036 (11)	0.0485 (5)
N1	0.13778 (10)	0.4994 (4)	-0.05556 (11)	0.0500 (5)
C2	0.18346 (11)	0.1507 (5)	0.14771 (12)	0.0449 (5)
H2A	0.2348	0.2010	0.1487	0.054*
H2B	0.1793	-0.0668	0.1499	0.054*
O1	0.10122 (10)	0.4680 (4)	0.22631 (10)	0.0752 (6)
C1	0.08229 (11)	0.3035 (5)	-0.04569 (13)	0.0479 (5)
N5	0.02757 (11)	0.2722 (6)	-0.10567 (13)	0.0787 (8)
H5A	-0.0064	0.1434	-0.0962	0.094*
H5B	0.0264	0.3809	-0.1536	0.094*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O2	0.0661 (10)	0.0609 (10)	0.0308 (8)	0.0097 (8)	-0.0064 (6)	-0.0009 (6)
N2	0.0611 (10)	0.0547 (11)	0.0320 (9)	-0.0062 (9)	-0.0015 (7)	0.0015 (7)
N3	0.0464 (9)	0.0479 (10)	0.0300 (8)	0.0011 (7)	0.0009 (7)	-0.0019 (7)
C3	0.0479 (11)	0.0467 (12)	0.0329 (10)	0.0005 (10)	-0.0036 (8)	-0.0002 (8)
N4	0.0490 (9)	0.0622 (11)	0.0341 (9)	-0.0039 (8)	-0.0029 (7)	0.0042 (8)
N1	0.0604 (11)	0.0588 (12)	0.0309 (9)	-0.0029 (9)	-0.0027 (7)	0.0027 (7)
C2	0.0506 (11)	0.0502 (12)	0.0337 (10)	0.0068 (10)	-0.0047 (8)	0.0013 (8)
O1	0.0878 (12)	0.0979 (14)	0.0398 (9)	0.0459 (11)	-0.0038 (8)	-0.0048 (8)
C1	0.0483 (11)	0.0651 (14)	0.0303 (10)	0.0030 (10)	0.0015 (8)	0.0015 (9)
N5	0.0607 (12)	0.125 (2)	0.0503 (12)	-0.0216 (12)	-0.0165 (9)	0.0320 (12)

Geometric parameters (\AA , $^\circ$)

O2—C3	1.312 (2)	N4—C1	1.331 (3)
O2—H2	0.8200	N1—C1	1.351 (3)
N2—N3	1.300 (2)	C2—H2A	0.9700
N2—N1	1.325 (2)	C2—H2B	0.9700

N3—N4	1.334 (2)	C1—N5	1.341 (2)
N3—C2	1.444 (2)	N5—H5A	0.8600
C3—O1	1.198 (2)	N5—H5B	0.8600
C3—C2	1.500 (3)		
C3—O2—H2	109.5	N3—C2—H2A	109.1
N3—N2—N1	105.66 (16)	C3—C2—H2A	109.1
N2—N3—N4	114.75 (16)	N3—C2—H2B	109.1
N2—N3—C2	122.39 (16)	C3—C2—H2B	109.1
N4—N3—C2	122.81 (17)	H2A—C2—H2B	107.8
O1—C3—O2	125.45 (18)	N4—C1—N5	124.7 (2)
O1—C3—C2	123.87 (18)	N4—C1—N1	111.56 (17)
O2—C3—C2	110.64 (17)	N5—C1—N1	123.72 (19)
C1—N4—N3	101.42 (17)	C1—N5—H5A	120.0
N2—N1—C1	106.60 (16)	C1—N5—H5B	120.0
N3—C2—C3	112.53 (16)	H5A—N5—H5B	120.0
N1—N2—N3—N4	0.2 (2)	O1—C3—C2—N3	-3.6 (3)
N1—N2—N3—C2	177.93 (17)	O2—C3—C2—N3	178.80 (17)
N2—N3—N4—C1	-0.1 (2)	N3—N4—C1—N5	179.7 (2)
C2—N3—N4—C1	-177.82 (17)	N3—N4—C1—N1	0.0 (2)
N3—N2—N1—C1	-0.2 (2)	N2—N1—C1—N4	0.2 (2)
N2—N3—C2—C3	101.8 (2)	N2—N1—C1—N5	-179.6 (2)
N4—N3—C2—C3	-80.6 (2)		

Hydrogen-bond geometry (Å, °)

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
N5—H5B...O1 ⁱ	0.86	2.36	3.080 (3)	141
N5—H5A...N4 ⁱⁱ	0.86	2.23	3.064 (3)	163
O2—H2...N1 ⁱⁱⁱ	0.82	1.85	2.665 (2)	172

Symmetry codes: (i) $x, -y+1, z-1/2$; (ii) $-x, -y, -z$; (iii) $x, -y+1, z+1/2$.