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

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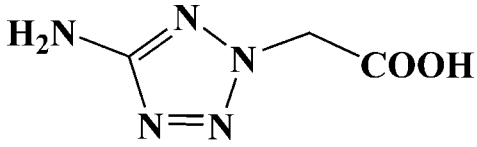
Key indicators: single-crystal X-ray study; $T$ = 296 K; mean $\sigma$(C–C) = 0.003 Å; $R$ factor = 0.044; $wR$ factor = 0.124; data-to-parameter ratio = 13.0.

In the title molecule, $C_3H_5N_5O_2$, the tetrazole ring and carboxyl group form a dihedral angle of 82.25 (14)°. In the crystal, adjacent molecules are linked through O—H···N, N—H···O and N—H···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

$C_3H_5N_5O_2$
$M_r$ = 143.12
Monoclinic, $C2/c$
$a$ = 18.381 (4) Å
$b$ = 4.4429 (9) Å
$c$ = 14.846 (3) Å
$\beta$ = 90.850 (3)°
$V$ = 1212.2 (4) Å$^3$
$Z$ = 8
Mo $K\alpha$ radiation
$\mu$ = 0.13 mm$^{-1}$
$T$ = 296 K
0.28 × 0.19 × 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 $I > 2\sigma(I)$
$R_{int}$ = 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, °).

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N5—H5$B$···O1$^{i}$ | 0.86 | 2.36 | 3.080 (3) | 141 |
| N5—H5$A$···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) $x, -y+1, z-\frac{1}{2}$; (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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# supplementary materials

*Acta Cryst.* (2012). E**68**, o1330 [doi:10.1107/S1600536812014389]

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

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

### 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.

### 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.

### 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 $U_{iso}$(H) = 1.2$U_{eq}$(C,*N*) or 1.5$U_{eq}$(O).

### Computing details

Data collection: *APEX2* (Bruker, 2008); cell refinement: *SAINT* (Bruker, 2008); data reduction: *SAINT* (Bruker, 2008); 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* (Sheldrick, 2008).

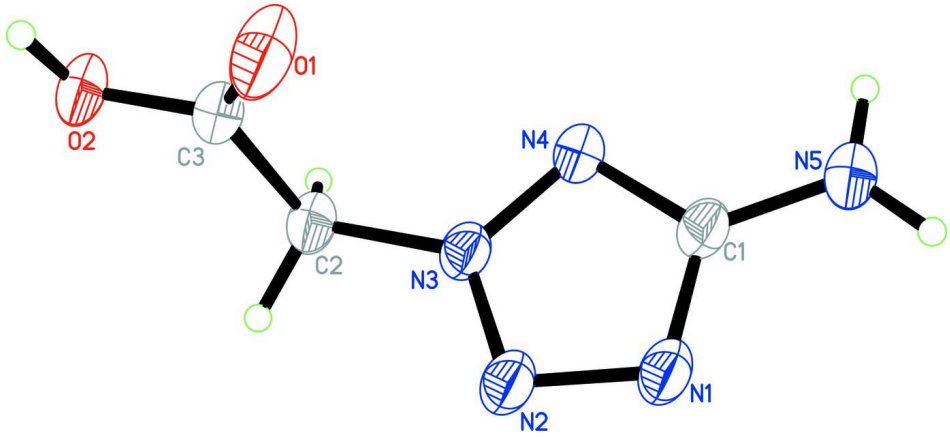


**Figure 1**

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

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

*Crystal data*

$C_3H_5N_5O_2$
$M_r$ = 143.12
Monoclinic, *C*2/*c*
Hall symbol: -C 2yc
*a* = 18.381 (4) Å
*b* = 4.4429 (9) Å
*c* = 14.846 (3) Å
*β* = 90.850 (3)°
*V* = 1212.2 (4) Å$^3$
*Z* = 8
*F*(000) = 592
$D_x$ = 1.568 Mg m$^{-3}$
$D_m$ = 1.568 Mg m$^{-3}$
$D_m$ measured by not measured
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 734 reflections
*θ* = 3.5–22.2°
*μ* = 0.13 mm$^{-1}$
*T* = 296 K
Block, colourless
0.28 × 0.19 × 0.15 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 $I > 2\sigma(I)$
$R_{int}$ = 0.024
$\theta_{max}$ = 26.0°, $\theta_{min}$ = 2.2°
*h* = −22→22
*k* = −5→4
*l* = −13→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 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.19 e Å$^{-3}$

*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 (Å²)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| 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 (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| 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 (Å, º)*

| | | | |
|---|---|---|---|
| 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, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N5—H5*B*···O1$^{i}$ | 0.86 | 2.36 | 3.080 (3) | 141 |
| N5—H5*A*···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.