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Glycine–D-tartaric acid (1/1)

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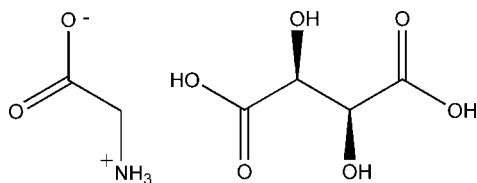
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Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.001$ Å; R factor = 0.037; wR factor = 0.112; data-to-parameter ratio = 19.9.

In the title co-crystal, $\text{C}_2\text{H}_5\text{NO}_2 \cdot \text{C}_4\text{H}_6\text{O}_6$, the glycine molecule is present in the zwitterion form. In the tartaric acid molecule there is a short intramolecular $\text{O}-\text{H} \cdots \text{O}$ contact. In the crystal, the tartaric acid molecules are linked *via* pairs of $\text{O}-\text{H} \cdots \text{O}$ hydrogen bonds, forming inversion dimers. These dimers are linked *via* a number of $\text{O}-\text{H} \cdots \text{O}$ and $\text{N}-\text{H} \cdots \text{O}$ hydrogen bonds involving the two components, forming a three-dimensional network.

Related literature

For related structures, see: Kvick *et al.* (1980). For a description of the Cambridge Structural Database, see: Allen (2002).



Experimental

Crystal data

$\text{C}_2\text{H}_5\text{NO}_2 \cdot \text{C}_4\text{H}_6\text{O}_6$
 $M_r = 225.16$
 Monoclinic, $P2_1/n$
 $a = 4.8387$ (2) Å
 $b = 9.2913$ (4) Å
 $c = 20.0273$ (8) Å
 $\beta = 90.171$ (1)°

$V = 900.38$ (6) Å³
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 0.16$ mm⁻¹
 $T = 293$ K
 $0.30 \times 0.20 \times 0.20$ mm

Data collection

Bruker Kappa APEXII diffractometer
 Absorption correction: multi-scan (SADABS; Bruker, 2003)
 $T_{\min} = 0.954$, $T_{\max} = 0.969$

12500 measured reflections
 3282 independent reflections
 2685 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.033$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.037$
 $wR(F^2) = 0.112$
 $S = 1.07$
 3282 reflections
 165 parameters

H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\text{max}} = 0.49$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.22$ e Å⁻³

Table 1
 Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
$\text{N1}-\text{H1A} \cdots \text{O1}^i$	0.953 (19)	2.20 (2)	2.9509 (11)	135.2 (16)
$\text{N1}-\text{H1A} \cdots \text{O3}^i$	0.953 (19)	2.21 (2)	2.9386 (11)	132.2 (15)
$\text{N1}-\text{H1B} \cdots \text{O6}^{ii}$	0.909 (16)	2.041 (16)	2.9188 (10)	162.0 (14)
$\text{N1}-\text{H1C} \cdots \text{O7}^{ii}$	0.914 (18)	2.172 (17)	2.9492 (13)	142.4 (14)
$\text{O2}-\text{H2A} \cdots \text{O8}^{iii}$	0.93 (2)	1.64 (2)	2.5473 (8)	167 (2)
$\text{O3}-\text{H3A} \cdots \text{O4}^{iv}$	0.870 (18)	1.849 (18)	2.7122 (8)	171.0 (16)
$\text{O4}-\text{H4A} \cdots \text{O3}^v$	0.81 (2)	2.09 (2)	2.7654 (10)	141.1 (18)
$\text{O4}-\text{H4A} \cdots \text{O6}$	0.81 (2)	2.251 (18)	2.6743 (9)	112.9 (16)
$\text{O5}-\text{H5} \cdots \text{O7}$	0.944 (19)	1.612 (19)	2.5459 (9)	169.2 (18)

Symmetry codes: (i) $x + \frac{1}{2}, -y + \frac{1}{2}, z - \frac{1}{2}$; (ii) $-x + \frac{5}{2}, y - \frac{1}{2}, -z + \frac{1}{2}$; (iii) $-x + 1, -y, -z + 1$; (iv) $x + 1, y, z$; (v) $-x + 1, -y + 1, -z + 1$.

Data collection: APEX2 (Bruker, 2004); cell refinement: APEX2 and SAINT-NT (Bruker, 2004); data reduction: SAINT-NT and XPREP (Bruker, 2003); program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: ORTEP-32 (Farrugia, 2012); software used to prepare material for publication: PLATON (Spek, 2009).

The authors thank Sona Engineering College, Salem, for providing the sample to carry out the X-ray study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BV2215).

References

- Allen, F. H. (2002). *Acta Cryst.* **B58**, 380–388.
 Bruker (2003). SADABS, SAINT-NT and XPREP. Bruker AXS Inc., Madison, Wisconsin, USA.
 Bruker (2004). APEX2. Bruker AXS Inc., Madison, Wisconsin, USA.
 Farrugia, L. J. (2012). *J. Appl. Cryst.* **45**, 849–854.
 Kvick, Å., Canning, W. M., Koetzle, T. F. & Williams, G. J. B. (1980). *Acta Cryst.* **B36**, 115–120.
 Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
 Spek, A. L. (2009). *Acta Cryst.* **D65**, 148–155.

supporting information

Acta Cryst. (2013). E69, o236 [doi:10.1107/S1600536813000822]

Glycine–D-tartaric acid (1/1)

T. Mohandas, C. Ranjith Dev Inbaseelan, S. Saravanan and P. Sakthivel

S1. Comment

Glycine is the simplest amino acid that is not optically active. It is essential for biosynthesis of nucleic acids as well as the biosynthesis of bile acids, creatine phosphate and other amino acids. Its geometric features of non covalent interactions at atomic resolution are important in the structural assembly and functions of proteins.

In the title compound(I), glycine is in the zwitterionic form. The tartaric acid molecule is in the un-ionized state. The angle between the planes of the half molecules O1/O2/C1/C2/O3 and O5/O6/C4/C3/O4 is 62.74 (3)°, which is closer to the value of 54.6° found in the structure of tartaric acid.

Atoms C5,C6,O7,N1 are planar with the N1 atom is slightly displaced out of this plane by -0.518 (1)°.

The relevant torsion angles are O7—C5—C6—N1 of -158.33 (3)° and O8—C5—C6—N1 of 23.08 (3)°. These can be compared with the corresponding values in pure Γ glycine 167.1 (1)° and -15.4 (1)°, respectively (Kvick *et al.*, (1980), which is more distorted from planarity.

The molecular structure of (I) is shown in the (Fig.1) and selected geometric parameters listed in Table 1. The bond lengths for C=N, C=O, C—C are within normal ranges (Allen 2002). The dihedral angle between planes of D-tartaric acid and glycine is 51.14 (9)°. The molecules related by the 2_1 screw along *b* axis are linked by intermolecular O—H...O hydrogen bond generating a supramolecular chain.

The carbon skeleton of tartaric molecule is non-planar with a C1—C2—C3—C4 torsion angle of 177.8 (1)°. Fig.2 shows the packing diagram in which there are a large number of N—H...O and O—H...O hydrogen bonds.

S2. Experimental

Colourless single crystals were grown as transparent needles by slow evaporation method from a saturated aqueous solution containing glycine and D-tartaric acid in a 1:1 stoichiometric ratio.

S3. Refinement

All the hydrogen atoms were geometrically fixed and allowed to ride on their parent atoms with C—H = 0.97 and 0.98 Å, and $U_{iso} = 1.2_{eq}(C)$. Hydrogen atoms attached to O and N were refined isotropically.

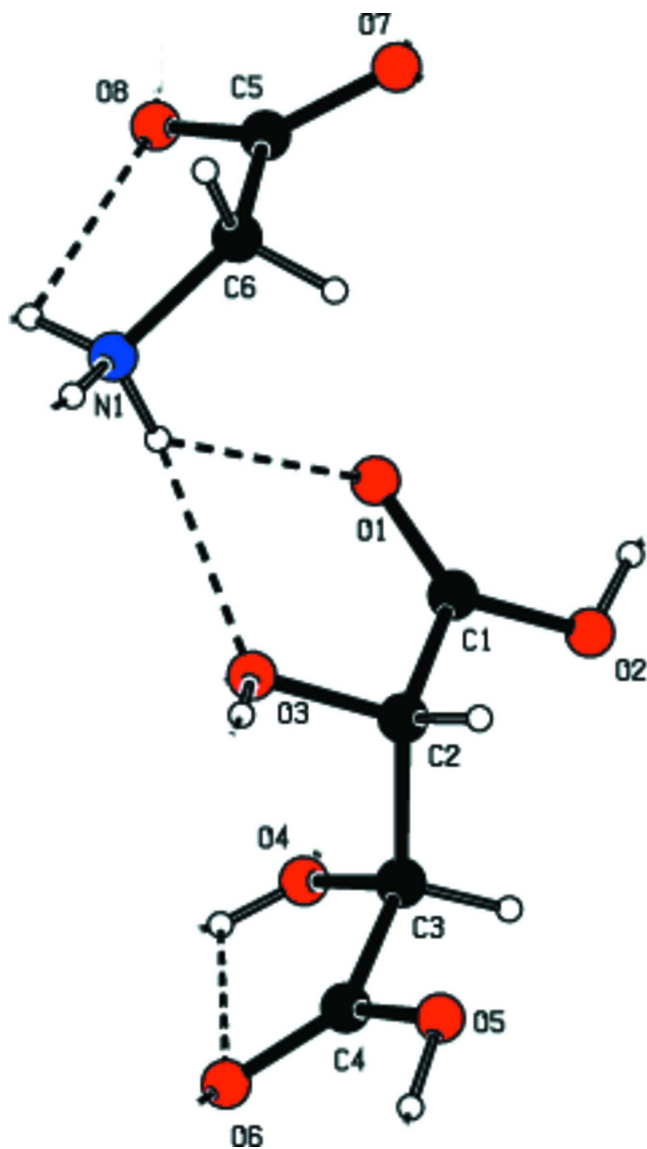
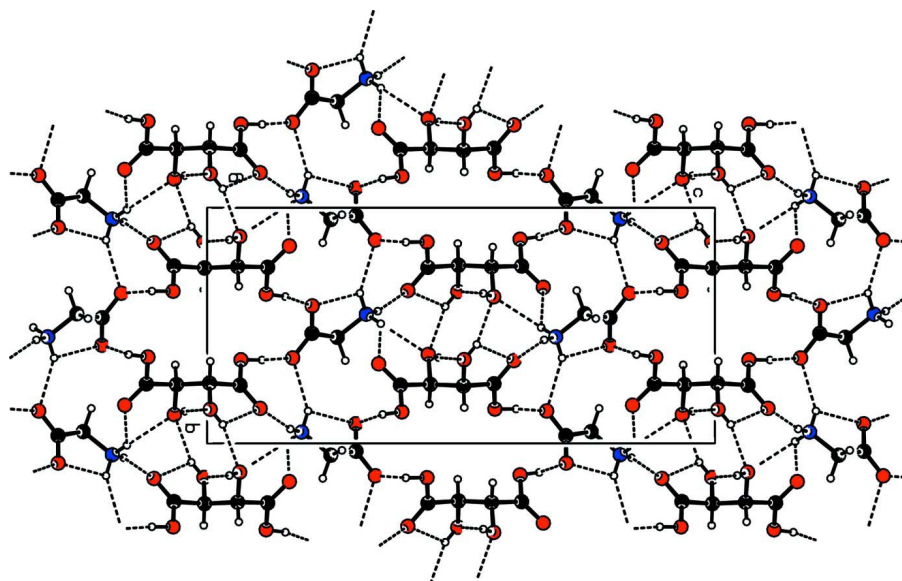


Figure 1

The molecular structure and labelling scheme for (I) with displacement ellipsoid of non-H atoms are drawn at the 30% probability level.

**Figure 2**

A packing diagram for (I) is shown. Dashed line indicates intra and inter molecular N—H...O and O—H...O hydrogen bonding interactions

Glycine–D-tartaric acid (1/1)

Crystal data

$C_2H_5NO_2 \cdot C_4H_6O_6$

$M_r = 225.16$

Monoclinic, $P2_1/n$

Hall symbol: $-P 2_1n$

$a = 4.8387$ (2) Å

$b = 9.2913$ (4) Å

$c = 20.0273$ (8) Å

$\beta = 90.171$ (1)°

$V = 900.38$ (6) Å³

$Z = 4$

$F(000) = 472$

$D_x = 1.661$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 1585 reflections

$\theta = 2.0$ – 25.0 °

$\mu = 0.16$ mm⁻¹

$T = 293$ K

Prism, colorless

$0.30 \times 0.20 \times 0.20$ mm

Data collection

Bruker Kappa APEXII
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

ω and φ scan

Absorption correction: multi-scan

(*SADABS*; Bruker, 2003)

$T_{\min} = 0.954$, $T_{\max} = 0.969$

12500 measured reflections

3282 independent reflections

2685 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.033$

$\theta_{\max} = 35.0$ °, $\theta_{\min} = 2.0$ °

$h = -7 \rightarrow 7$

$k = -14 \rightarrow 12$

$l = -27 \rightarrow 29$

2 standard reflections every 100 reflections

intensity decay: none

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.037$

$wR(F^2) = 0.112$

$S = 1.07$

3282 reflections

165 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 atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0603P)^2 + 0.1264P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$
 $\Delta\rho_{\max} = 0.49 \text{ e } \text{Å}^{-3}$
 $\Delta\rho_{\min} = -0.22 \text{ e } \text{Å}^{-3}$
 Extinction correction: *SHELXL97* (Sheldrick, 2008), $F_c^* = kFc[1 + 0.001x Fc^2 \lambda^3 / \sin(2\theta)]^{-1/4}$
 Extinction coefficient: 0.074 (5)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 $F^2 > 2\sigma(F^2)$ 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 (Å^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.44851 (16)	0.24734 (9)	0.61943 (4)	0.02360 (17)
C2	0.64567 (15)	0.25044 (9)	0.56018 (4)	0.02271 (17)
H2	0.7688	0.1668	0.5624	0.027*
C3	0.47689 (16)	0.24434 (9)	0.49514 (4)	0.02364 (17)
H3	0.3788	0.1521	0.4936	0.028*
C4	0.66706 (17)	0.25298 (9)	0.43493 (4)	0.02490 (18)
C5	1.19172 (16)	0.03299 (10)	0.29340 (4)	0.02399 (18)
C6	1.42473 (16)	0.05011 (10)	0.24364 (4)	0.02740 (19)
H6A	1.4296	0.1487	0.2278	0.033*
H6B	1.5996	0.0297	0.2655	0.033*
N1	1.38776 (19)	-0.04805 (10)	0.18645 (4)	0.03233 (19)
O1	0.44118 (15)	0.33804 (9)	0.66214 (4)	0.03694 (19)
O2	0.29078 (17)	0.13348 (8)	0.61631 (4)	0.0395 (2)
O3	0.80456 (13)	0.37788 (7)	0.56436 (3)	0.02782 (16)
O4	0.28015 (13)	0.35571 (8)	0.49377 (4)	0.03210 (17)
O5	0.83917 (16)	0.14540 (8)	0.43321 (4)	0.03596 (18)
O6	0.65303 (16)	0.35172 (9)	0.39549 (4)	0.03701 (19)
O7	1.15307 (17)	0.13761 (9)	0.33148 (4)	0.0417 (2)
O8	1.06398 (15)	-0.08344 (8)	0.29288 (4)	0.03465 (18)
H1A	1.257 (4)	-0.008 (2)	0.1562 (10)	0.074 (5)*
H1B	1.548 (3)	-0.0609 (17)	0.1637 (8)	0.054 (4)*
H1C	1.320 (3)	-0.1370 (19)	0.1966 (8)	0.054 (4)*
H2A	0.179 (4)	0.122 (2)	0.6533 (10)	0.084 (6)*
H3A	0.962 (4)	0.3630 (18)	0.5444 (8)	0.060 (5)*
H4A	0.323 (4)	0.419 (2)	0.4681 (9)	0.070 (5)*
H5	0.938 (4)	0.148 (2)	0.3926 (10)	0.072 (5)*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0228 (3)	0.0263 (4)	0.0218 (4)	-0.0020 (3)	0.0057 (3)	0.0023 (3)
C2	0.0223 (3)	0.0226 (4)	0.0233 (4)	-0.0009 (3)	0.0083 (3)	0.0002 (3)
C3	0.0237 (3)	0.0245 (4)	0.0228 (4)	-0.0023 (3)	0.0076 (3)	-0.0001 (3)
C4	0.0267 (3)	0.0266 (4)	0.0214 (4)	-0.0040 (3)	0.0066 (3)	-0.0039 (3)
C5	0.0221 (3)	0.0284 (4)	0.0215 (4)	0.0024 (3)	0.0093 (3)	0.0027 (3)
C6	0.0225 (3)	0.0333 (4)	0.0265 (4)	0.0000 (3)	0.0109 (3)	0.0026 (3)
N1	0.0387 (4)	0.0315 (4)	0.0269 (4)	0.0084 (3)	0.0162 (3)	0.0021 (3)
O1	0.0369 (3)	0.0426 (4)	0.0314 (4)	-0.0110 (3)	0.0154 (3)	-0.0113 (3)
O2	0.0484 (4)	0.0366 (4)	0.0335 (4)	-0.0202 (3)	0.0196 (3)	-0.0046 (3)
O3	0.0226 (3)	0.0297 (3)	0.0313 (3)	-0.0064 (2)	0.0107 (2)	-0.0030 (2)
O4	0.0259 (3)	0.0358 (4)	0.0347 (4)	0.0050 (2)	0.0120 (3)	0.0079 (3)
O5	0.0447 (4)	0.0324 (4)	0.0309 (4)	0.0075 (3)	0.0155 (3)	-0.0028 (3)
O6	0.0398 (4)	0.0399 (4)	0.0314 (4)	0.0031 (3)	0.0145 (3)	0.0089 (3)
O7	0.0490 (4)	0.0382 (4)	0.0380 (4)	-0.0039 (3)	0.0231 (3)	-0.0107 (3)
O8	0.0368 (3)	0.0314 (4)	0.0358 (4)	-0.0059 (3)	0.0189 (3)	0.0019 (3)

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

C1—O1	1.2014 (11)	C5—O7	1.2499 (11)
C1—O2	1.3058 (10)	C5—C6	1.5153 (10)
C1—C2	1.5250 (10)	C6—N1	1.4746 (13)
C2—O3	1.4141 (10)	C6—H6A	0.9700
C2—C3	1.5364 (13)	C6—H6B	0.9700
C2—H2	0.9800	N1—H1A	0.953 (19)
C3—O4	1.4063 (11)	N1—H1B	0.909 (16)
C3—C4	1.5212 (10)	N1—H1C	0.914 (18)
C3—H3	0.9800	O2—H2A	0.93 (2)
C4—O6	1.2124 (11)	O3—H3A	0.870 (18)
C4—O5	1.3015 (11)	O4—H4A	0.81 (2)
C5—O8	1.2460 (11)	O5—H5	0.944 (19)
O1—C1—O2	125.71 (7)	O8—C5—C6	117.12 (7)
O1—C1—C2	124.10 (7)	O7—C5—C6	115.63 (8)
O2—C1—C2	110.19 (7)	N1—C6—C5	110.92 (7)
O3—C2—C1	108.12 (7)	N1—C6—H6A	109.5
O3—C2—C3	111.63 (7)	C5—C6—H6A	109.5
C1—C2—C3	109.07 (6)	N1—C6—H6B	109.5
O3—C2—H2	109.3	C5—C6—H6B	109.5
C1—C2—H2	109.3	H6A—C6—H6B	108.0
C3—C2—H2	109.3	C6—N1—H1A	109.2 (12)
O4—C3—C4	110.90 (7)	C6—N1—H1B	111.6 (10)
O4—C3—C2	110.33 (7)	H1A—N1—H1B	107.6 (15)
C4—C3—C2	110.42 (6)	C6—N1—H1C	115.4 (10)
O4—C3—H3	108.4	H1A—N1—H1C	105.0 (16)
C4—C3—H3	108.4	H1B—N1—H1C	107.6 (14)

C2—C3—H3	108.4	C1—O2—H2A	113.3 (13)
O6—C4—O5	126.76 (7)	C2—O3—H3A	108.3 (11)
O6—C4—C3	121.57 (8)	C3—O4—H4A	111.9 (14)
O5—C4—C3	111.66 (7)	C4—O5—H5	109.4 (11)
O8—C5—O7	127.24 (7)		
O1—C1—C2—O3	-1.72 (12)	C1—C2—C3—C4	177.86 (7)
O2—C1—C2—O3	177.86 (8)	O4—C3—C4—O6	4.99 (12)
O1—C1—C2—C3	-123.29 (10)	C2—C3—C4—O6	-117.63 (9)
O2—C1—C2—C3	56.29 (9)	O4—C3—C4—O5	-175.95 (8)
O3—C2—C3—O4	-64.51 (8)	C2—C3—C4—O5	61.43 (9)
C1—C2—C3—O4	54.91 (8)	O8—C5—C6—N1	23.03 (11)
O3—C2—C3—C4	58.45 (8)	O7—C5—C6—N1	-158.29 (9)

Hydrogen-bond geometry (Å, °)

<i>D—H...A</i>	<i>D—H</i>	<i>H...A</i>	<i>D...A</i>	<i>D—H...A</i>
N1—H1A...O1 ⁱ	0.953 (19)	2.20 (2)	2.9509 (11)	135.2 (16)
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Symmetry codes: (i) $x+1/2, -y+1/2, z-1/2$; (ii) $-x+5/2, y-1/2, -z+1/2$; (iii) $-x+1, -y, -z+1$; (iv) $x+1, y, z$; (v) $-x+1, -y+1, -z+1$.