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(*S*)-1-Hydroxypropan-2-aminium (2*R*,3*R*)-3-carboxy-2,3-dihydroxypropanoate monohydrate

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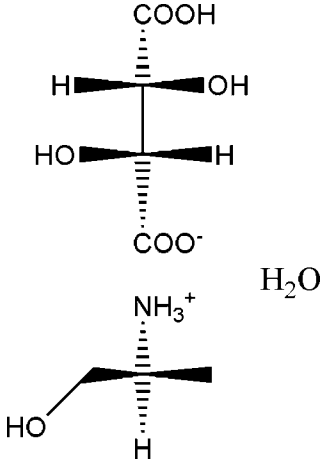
Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.002 Å; R factor = 0.029; wR factor = 0.075; data-to-parameter ratio = 7.8.

The chiral title compound, $C_4H_{10}NO^+\cdot C_4H_5O_6^-\cdot H_2O$, is a hydrated molecular salt in which the tartaric acid has transferred one proton to the (*S*)-2-aminopropan-1-ol molecule. The crystal structure is stabilized by a three-dimensional network of N—H···O and O—H···O hydrogen bonds. The absolute configuration was assigned on the basis of the starting materials.

Related literature

For the synthesis, see: Bai *et al.* (2004); For background, see: Humljan *et al.* (2006).



Experimental

Crystal data

$C_4H_{10}NO^+\cdot C_4H_5O_6^-\cdot H_2O$
M_r = 243.22
Orthorhombic, $P2_12_12_1$
a = 7.533 (2) Å
b = 7.701 (2) Å
c = 19.288 (5) Å
V = 1118.9 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.13 mm^{-1}
T = 294 (2) K
0.24 × 0.22 × 0.18 mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
T_{min} = 0.969, T_{max} = 0.977
6331 measured reflections
1359 independent reflections
1280 reflections with $I > 2\sigma(I)$
R_{int} = 0.024

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.028
$wR(F^2)$ = 0.074
S = 1.06
1359 reflections
174 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···O8^{i}	0.89 (3)	1.78 (3)	2.677 (2)	176 (3)
O4—H4···O3^{ii}	0.89 (2)	2.01 (3)	2.885 (2)	169 (2)
O5—H5···O2^{iii}	0.82 (3)	1.87 (3)	2.676 (2)	167 (3)
O6—H6···O2^{iv}	0.85 (3)	1.77 (3)	2.6091 (19)	173 (3)
N1—H1*D*···O1^{v}	0.93 (3)	2.05 (3)	2.945 (2)	159 (2)
N1—H1*E*···O5^{iii}	0.95 (3)	1.91 (3)	2.852 (2)	168 (2)
N1—H1*F*···O6^{i}	0.95 (3)	2.26 (3)	3.121 (2)	150 (2)
O8—H8*A*···O3	0.85 (3)	1.95 (3)	2.784 (2)	169 (3)
O8—H8*B*···O4^{vi}	0.81 (3)	2.06 (3)	2.865 (2)	173 (3)

Symmetry codes: (i) $x, y+1, z$; (ii) $x-\frac{1}{2}, -y+\frac{1}{2}, -z+2$; (iii) $x+\frac{1}{2}, -y+\frac{1}{2}, -z+2$; (iv) $x, y-1, z$; (v) $-x+1, y-\frac{1}{2}, -z+\frac{3}{2}$; (vi) $x+1, y, z$.

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

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2687).

References

Bai, G. Y., Chen, L. G., Xing, P., Li, Y. & Yan, X. L. (2004). *Fine Chem.* **21**, 943–945.
Bruker (1997). *SADABS*, *SMART*, *SAINT* and *SHELXTL*. Bruker AXS Inc., Madison, Wisconsin, USA.
Humljan, J., Kotnik, M., Boniface, A., Solmajer, T., Urleb, U., Blanot, D. & Gobec, S. (2006). *Tetrahedron*, **62**, 10980–10988.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

supporting information

Acta Cryst. (2008). E**64**, o422 [doi:10.1107/S1600536808000391]

(*S*)-1-Hydroxypropan-2-aminium (2*R*,3*R*)-3-carboxy-2,3-dihydroxypropanoate monohydrate

Xin-Yu Tang, Xi-Long Yan, Ping Zhang, Ling Qin and Yueguang Yin

S1. Comment

The title compound, (I), (Fig. 1), is a hydrated (2*R*,3*R*)-tartrate salt of (*S*)-2-aminopropan-1-ol. (*S*)-2-aminopropan-1-ol is a key intermediate for the synthesis of potential inhibitors of the bacterial peptidoglycan biosynthesis enzymes MurD and MurE (Humljan *et al.*, 2006).

In the crystal, the (*S*)-2-aminopropan-1-ol molecule is in a cationic form, and has a positively charged amino group. The tartaric acid molecule is a semi-tartrate ion, with a neutral carboxylic acid group at one end and a negatively charged carboxylate group at the other (Fig. 1). The bond distances and angles in the cation and the anion are normal. The chiralities of the carbon atoms (C2 S, C5 *R*, C6 *R*) were assigned according to the known absolute structures of the starting materials.

In the crystal structure of (I), an extensive hydrogen-bond network is built up (Table 1).

S2. Experimental

The title compound was prepared by the procedure of Bai *et al.* (2004). Colourless single crystals of (I) were grown by slow evaporation of a solution of methanol and water.

S3. Refinement

Anomalous dispersion was negligible and Friedel pairs were merged before refinement.

The N– and O-bound H atoms were located in difference maps and their positions were freely refined with U_{iso}(H) = 1.5U_{eq}(carrier).

The C-bound H atoms were positioned geometrically (C—H = 0.96–0.98 Å) and refined as riding with U_{iso}(H) = 1.2U_{eq}(C).

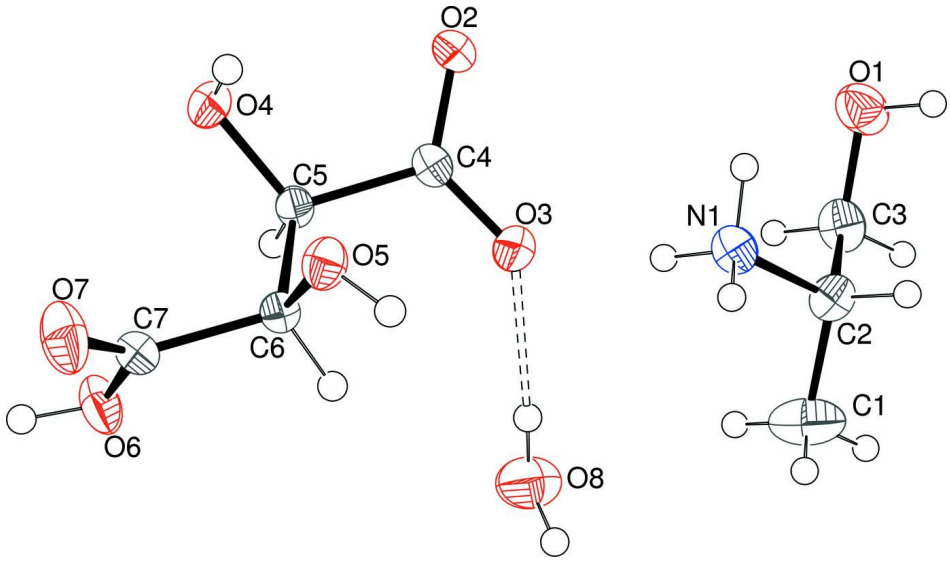


Figure 1

A view of the molecular structure of (I). Displacement ellopsoids are drawn at the 50% probability level and H atoms are shown as spheres of arbitrary radius. The hydrogen bond is indicated by a double dashed line.

(*S*)-1-hydroxypropan-2-aminium (2*R*,3*R*)-3-carboxy -2,3-dihydroxypropanoate monohydrate

Crystal data

$C_3H_{10}NO^+·C_4H_5O_6^-·H_2O$
M_r = 243.22
Orthorhombic, $P2_12_12_1$
Hall symbol: P 2ac 2ab
a = 7.533 (2) Å
b = 7.701 (2) Å
c = 19.288 (5) Å
V = 1118.9 (5) Å^3
Z = 4
$F(000)$ = 520
D_x = 1.444 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 3930 reflections
θ = 2.9–26.4°
μ = 0.13 mm^{-1}
T = 294 K
Block, colourless
0.24 × 0.22 × 0.18 mm

Data collection

Bruker SMART CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
T_{min} = 0.969, T_{max} = 0.977
6331 measured reflections
1359 independent reflections
1280 reflections with $I > 2\sigma(I)$
R_{int} = 0.024
θ_{max} = 26.4°, θ_{min} = 2.1°
h = −9→6
k = −9→9
l = −17→24

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.028
$wR(F^2)$ = 0.074
S = 1.06
1359 reflections
174 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: difmap (N-H and O-H) and geom (C-H)
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0475P)^2 + 0.1468P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.25$ e Å^{-3}
$\Delta\rho_{min} = -0.17$ e Å^{-3}
Extinction correction: *SHELXL*,
$Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.067 (5)

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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.5541 (2)	0.9115 (2)	0.77366 (8)	0.0413 (4)
H1	0.611 (4)	0.989 (4)	0.7999 (16)	0.062*
O2	0.14604 (17)	0.39481 (16)	0.92596 (8)	0.0324 (3)
O3	0.42454 (16)	0.30294 (16)	0.92082 (7)	0.0285 (3)
O4	0.01406 (16)	0.07039 (17)	0.94283 (7)	0.0279 (3)
H4	0.002 (3)	0.110 (3)	0.9859 (13)	0.042*
O5	0.30427 (18)	0.05497 (16)	1.04183 (6)	0.0244 (3)
H5	0.406 (3)	0.086 (3)	1.0507 (12)	0.037*
O6	0.2651 (2)	−0.28770 (17)	0.91791 (7)	0.0324 (3)
H6	0.218 (4)	−0.387 (4)	0.9212 (13)	0.049*
O7	0.1836 (2)	−0.27117 (18)	1.02899 (7)	0.0380 (4)
N1	0.6127 (2)	0.5901 (2)	0.84455 (8)	0.0280 (4)
H1D	0.561 (3)	0.510 (3)	0.8145 (13)	0.042*
H1E	0.665 (3)	0.529 (3)	0.8822 (13)	0.042*
H1F	0.521 (3)	0.666 (3)	0.8599 (12)	0.042*
C1	0.8957 (3)	0.5543 (4)	0.78287 (12)	0.0517 (6)
H1A	0.8387	0.4739	0.7520	0.078*
H1B	0.9459	0.4921	0.8213	0.078*
H1C	0.9882	0.6146	0.7585	0.078*
C2	0.7608 (3)	0.6838 (2)	0.80928 (9)	0.0288 (4)
H2	0.8185	0.7610	0.8428	0.035*
C3	0.6849 (3)	0.7920 (3)	0.75103 (10)	0.0333 (4)
H3A	0.7805	0.8555	0.7289	0.040*
H3B	0.6330	0.7154	0.7167	0.040*
C4	0.2611 (2)	0.2769 (2)	0.92464 (8)	0.0198 (3)
C5	0.1966 (2)	0.0871 (2)	0.92587 (8)	0.0204 (3)
H5A	0.2126	0.0400	0.8791	0.025*
C6	0.3130 (2)	−0.0200 (2)	0.97483 (8)	0.0202 (3)
H6A	0.4360	−0.0185	0.9583	0.024*
C7	0.2464 (2)	−0.2062 (2)	0.97795 (9)	0.0236 (4)
O8	0.7125 (2)	0.1422 (2)	0.85702 (9)	0.0460 (4)

H8A	0.633 (4)	0.190 (4)	0.8814 (15)	0.055*
H8B	0.802 (4)	0.119 (4)	0.8783 (15)	0.055*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0473 (9)	0.0330 (7)	0.0436 (8)	0.0065 (7)	−0.0122 (7)	−0.0017 (7)
O2	0.0262 (6)	0.0181 (6)	0.0529 (8)	0.0018 (5)	0.0047 (6)	−0.0008 (6)
O3	0.0223 (6)	0.0244 (6)	0.0388 (7)	−0.0023 (5)	0.0013 (5)	0.0022 (6)
O4	0.0199 (6)	0.0271 (6)	0.0368 (7)	−0.0029 (6)	−0.0025 (5)	0.0002 (6)
O5	0.0243 (6)	0.0266 (6)	0.0224 (6)	−0.0045 (5)	−0.0013 (5)	−0.0019 (5)
O6	0.0449 (8)	0.0189 (6)	0.0333 (7)	−0.0063 (6)	0.0090 (6)	−0.0044 (5)
O7	0.0538 (9)	0.0273 (6)	0.0329 (7)	−0.0120 (7)	0.0100 (7)	0.0029 (6)
N1	0.0337 (9)	0.0260 (7)	0.0244 (7)	−0.0005 (8)	0.0006 (6)	0.0017 (6)
C1	0.0465 (13)	0.0641 (15)	0.0445 (12)	0.0226 (13)	0.0113 (10)	0.0148 (11)
C2	0.0276 (9)	0.0329 (9)	0.0259 (8)	−0.0018 (9)	−0.0010 (7)	0.0022 (7)
C3	0.0421 (11)	0.0314 (9)	0.0265 (8)	−0.0037 (9)	−0.0002 (8)	0.0062 (7)
C4	0.0244 (8)	0.0181 (7)	0.0169 (7)	−0.0002 (7)	−0.0004 (7)	0.0006 (6)
C5	0.0211 (7)	0.0177 (7)	0.0225 (7)	−0.0016 (6)	0.0008 (7)	−0.0008 (7)
C6	0.0195 (7)	0.0184 (7)	0.0228 (7)	−0.0003 (7)	0.0012 (6)	0.0000 (6)
C7	0.0230 (8)	0.0187 (8)	0.0291 (8)	0.0013 (7)	0.0000 (7)	0.0004 (7)
O8	0.0416 (9)	0.0528 (10)	0.0435 (9)	0.0115 (8)	−0.0096 (7)	−0.0171 (7)

Geometric parameters (Å, º)

O1—C3	1.417 (3)	C1—C2	1.512 (3)
O1—H1	0.89 (3)	C1—H1A	0.9600
O2—C4	1.256 (2)	C1—H1B	0.9600
O3—C4	1.249 (2)	C1—H1C	0.9600
O4—C5	1.419 (2)	C2—C3	1.511 (3)
O4—H4	0.89 (2)	C2—H2	0.9800
O5—C6	1.4166 (19)	C3—H3A	0.9700
O5—H5	0.82 (3)	C3—H3B	0.9700
O6—C7	1.325 (2)	C4—C5	1.540 (2)
O6—H6	0.85 (3)	C5—C6	1.530 (2)
O7—C7	1.202 (2)	C5—H5A	0.9800
N1—C2	1.492 (2)	C6—C7	1.520 (2)
N1—H1D	0.93 (3)	C6—H6A	0.9800
N1—H1E	0.95 (3)	O8—H8A	0.85 (3)
N1—H1F	0.95 (3)	O8—H8B	0.81 (3)
C3—O1—H1	106 (2)	C2—C3—H3A	109.0
C5—O4—H4	106.3 (16)	O1—C3—H3B	109.0
C6—O5—H5	105.4 (17)	C2—C3—H3B	109.0
C7—O6—H6	108.7 (17)	H3A—C3—H3B	107.8
C2—N1—H1D	110.4 (16)	O3—C4—O2	124.44 (16)
C2—N1—H1E	106.4 (15)	O3—C4—C5	117.66 (15)
H1D—N1—H1E	108 (2)	O2—C4—C5	117.89 (14)

C2—N1—H1F	112.7 (15)	O4—C5—C6	111.34 (13)
H1D—N1—H1F	107 (2)	O4—C5—C4	113.31 (14)
H1E—N1—H1F	112 (2)	C6—C5—C4	109.88 (13)
C2—C1—H1A	109.5	O4—C5—H5A	107.3
C2—C1—H1B	109.5	C6—C5—H5A	107.3
H1A—C1—H1B	109.5	C4—C5—H5A	107.3
C2—C1—H1C	109.5	O5—C6—C7	109.44 (13)
H1A—C1—H1C	109.5	O5—C6—C5	108.48 (13)
H1B—C1—H1C	109.5	C7—C6—C5	110.12 (13)
N1—C2—C3	108.85 (16)	O5—C6—H6A	109.6
N1—C2—C1	109.68 (17)	C7—C6—H6A	109.6
C3—C2—C1	111.56 (16)	C5—C6—H6A	109.6
N1—C2—H2	108.9	O7—C7—O6	124.11 (15)
C3—C2—H2	108.9	O7—C7—C6	123.73 (15)
C1—C2—H2	108.9	O6—C7—C6	112.17 (14)
O1—C3—C2	113.08 (15)	H8A—O8—H8B	114 (3)
O1—C3—H3A	109.0		

N1—C2—C3—O1	57.1 (2)	C4—C5—C6—O5	58.54 (17)
C1—C2—C3—O1	178.27 (18)	O4—C5—C6—C7	51.92 (18)
O3—C4—C5—O4	169.20 (14)	C4—C5—C6—C7	178.28 (13)
O2—C4—C5—O4	−12.4 (2)	O5—C6—C7—O7	5.5 (2)
O3—C4—C5—C6	44.0 (2)	C5—C6—C7—O7	−113.67 (19)
O2—C4—C5—C6	−137.61 (15)	O5—C6—C7—O6	−174.79 (15)
O4—C5—C6—O5	−67.82 (17)	C5—C6—C7—O6	66.06 (18)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···O8^{i}	0.89 (3)	1.78 (3)	2.677 (2)	176 (3)
O4—H4···O3^{ii}	0.89 (2)	2.01 (3)	2.885 (2)	169 (2)
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