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(*S*)-2-Hydroxy-2-phenylacetic acid–(*R*)-2-aminobutanoic acid–water (1/1/0.5)

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Key indicators

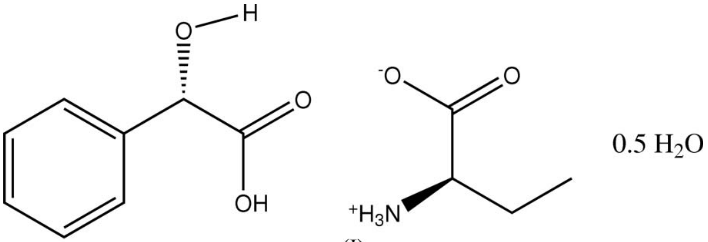
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.005 Å
R factor = 0.045
wR factor = 0.104
Data-to-parameter ratio = 7.8

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

The title complex, $C_8H_6O_3 \cdot C_4H_8NO_2 \cdot 0.5H_2O$, was obtained from an aqueous solution of racemic 2-aminobutyric acid and (*S*)-2-hydroxyphenylacetic acid. In the crystal structure, a two-dimensional network is formed *via* O—H···O [H···O = 1.63 (5)–2.52 (5) Å] and N—H···O [H···O = 1.91 (4)–2.30 (4) Å] hydrogen bonds.

Comment

The asymmetric unit of the title compound, (I), consists of two molecules of 2-aminobutyric acid, two molecules of 2-hydroxyphenylacetic acid and one molecule of water (Fig. 1 and Table 1). The absolute configuration of (*R*)-2-aminobutyric acid has been determined with reference to 2-hydroxyphenylacetic acid. The synthetic procedure is a useful method for separating the *R* isomer from a racemic mixture.



(I)

In the crystal structure, a two-dimensional network is formed *via* O—H···O and N—H···O hydrogen bonds (Table 2 and Fig. 2).

Experimental

DL-α-Aminobutyric acid (4.12 g) and D-mandelic acid (6.09 g) were mixed with water (6 ml) and heated to 349 K until the solid had dissolved. The solution was left to stand at room temperature for one week. The resulting single crystals were separated by filtration, washed with water (3 ml) and dried to obtain crystals of L-mandelic acid D-α-aminobutyric acid hemihydrate (Tashiro *et al.* 1980): $[\alpha]_D^{25}$ = −79.75° (*c* = 4.0, water).

Crystal data

$C_8H_8O_3 \cdot C_4H_9NO_2 \cdot 0.5H_2O$
$M_r = 264.28$
Monoclinic, $P2_1$
$a = 6.0017$ (7) Å
$b = 8.4357$ (9) Å
$c = 26.733$ (3) Å
$\beta = 94.614$ (2)°
$V = 1349.0$ (3) Å^3
$Z = 8$
$D_x = 1.301$ Mg m^{-3}
Mo *K*α radiation
$\mu = 0.10$ mm^{-1}
$T = 293$ (2) K
Prism, colorless
0.50 × 0.47 × 0.17 mm

doi:10.1107/S1600536806018605

Data collection

Bruker SMART CCD diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
$T_{\min} = 0.748$, $T_{\max} = 0.980$
8010 measured reflections
3134 independent reflections
2378 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.104$
$\theta_{\max} = 27.0°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.045$
$wR(F^2) = 0.104$
$S = 0.92$
3134 reflections
401 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0478P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.027$
$\Delta\rho_{\max} = 0.24$ e Å^{-3}
$\Delta\rho_{\min} = -0.19$ e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.021 (2)

Table 1
Selected bond lengths (Å).

O1—C1	1.233 (3)	O7—C13	1.259 (3)
O2—C1	1.247 (3)	O8—C17	1.227 (4)
O3—C5	1.210 (4)	O9—C17	1.294 (4)
O4—C5	1.313 (4)	O10—C18	1.420 (4)
O5—C6	1.424 (4)	N1—C2	1.479 (3)
O6—C13	1.221 (3)	N2—C14	1.482 (3)

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O10—H10*A*···O8	0.81 (5)	2.19 (5)	2.667 (3)	119 (4)
O10—H10*A*···O1	0.81 (5)	2.29 (4)	2.908 (3)	134 (4)
N2—H16···O11	1.02 (5)	2.03 (5)	2.959 (4)	150 (4)
O11—H11*A*···O1	0.91 (2)	2.10 (2)	2.962 (4)	159 (3)
N1—H14*A*···O5	0.82 (4)	2.30 (4)	2.962 (4)	139 (3)
O11—H11*B*···O3	0.86 (2)	2.52 (5)	3.194 (4)	136 (6)
O4—H4···O2$^{\rm i}$	0.92 (4)	1.65 (4)	2.561 (3)	168 (3)
O5—H5···O8$^{\rm ii}$	0.79 (5)	2.20 (5)	2.904 (3)	148 (5)
O9—H9*A*···O7$^{\rm iii}$	0.87 (5)	1.63 (5)	2.505 (3)	177 (3)
N1—H13···O2$^{\rm ii}$	0.88 (3)	1.91 (4)	2.786 (3)	172 (3)
N1—H15···O6$^{\rm iv}$	0.91 (5)	1.93 (5)	2.787 (3)	158 (4)
N2—H17···O7$^{\rm iii}$	0.90 (3)	1.95 (3)	2.820 (3)	161 (2)
N2—H18*A*···O10$^{\rm v}$	0.79 (3)	2.19 (3)	2.953 (4)	161 (3)

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

H atoms bonded to O and N atoms were located in difference Fourier maps and were refined isotropically, as were H2, H6, H14, and H18 [C—H = 0.93 (3)–0.97 (3) Å]. The remaining H atoms were placed in calculated positions, with C—H distances in the range 0.93–0.97 Å, and were refined using the riding-model approximation, with $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}({\rm C})$, or $1.5U_{\rm eq}({\rm C})$ for methyl H atoms. In the absence of significant anomalous dispersion effects, Friedel pairs were merged.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2000); software used to prepare material for publication: *SHELXTL*.

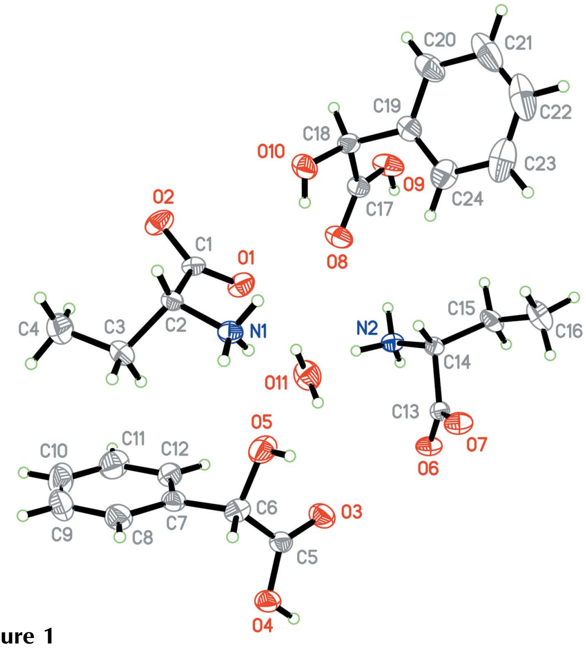


Figure 1
View of the asymmetric unit of (I), with displacement ellipsoids drawn at the 40% probability level. H atoms are represented by circles of arbitrary size.

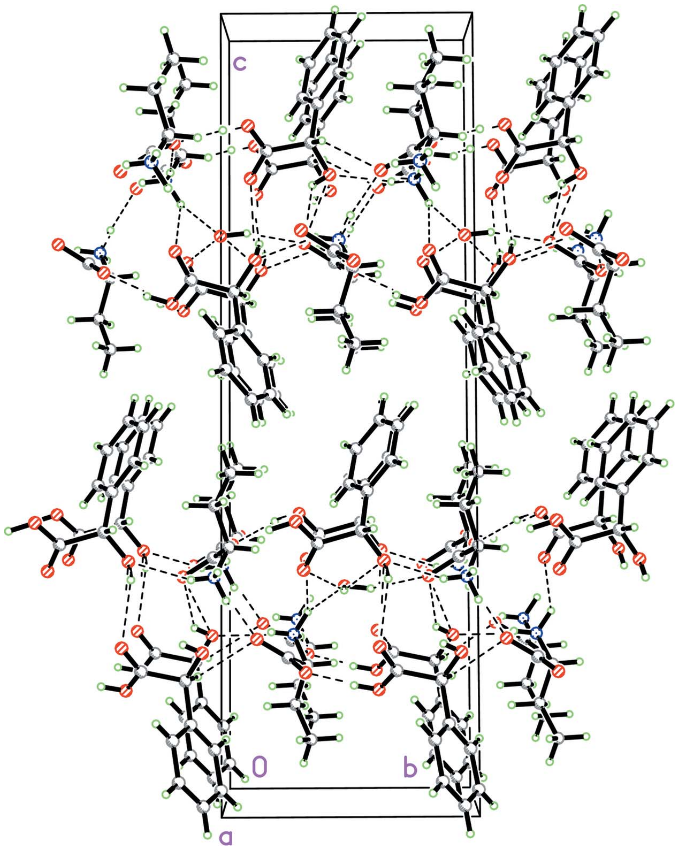


Figure 2
Packing plot, showing hydrogen bonds as dashed lines.

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