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Key indicators

Single-crystal X-ray study

$T = 293$ K

Mean $\sigma(\text{C}-\text{C}) = 0.004$ Å

R factor = 0.061

wR factor = 0.173

Data-to-parameter ratio = 12.2

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

L-Aspartic acid monohydrate

In the title compound, $\text{C}_4\text{H}_7\text{NO}_4 \cdot \text{H}_2\text{O}$, the screw-related aspartic acid molecules are linked along the a axis by $\text{N}-\text{H} \cdots \text{O}$ hydrogen bonds to form helical structures. The adjacent helices are inter-linked through $\text{O}-\text{H} \cdots \text{O}$ hydrogen bonds and also by the water molecules through $\text{N}-\text{H} \cdots \text{O}(\text{W})$ and $\text{O}(\text{W})-\text{H} \cdots \text{O}$ hydrogen bonds, to form a three-dimensional network.

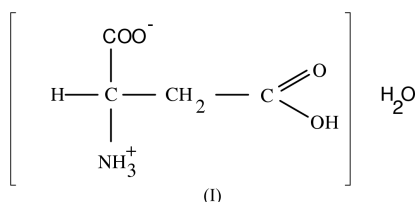
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Comment

Aspartic acid is a non-essential amino acid, widely distributed in proteins, which plays a major role in the energy cycle of the human body. The crystal structures of L-aspartic acid (Derissen *et al.*, 1968), DL-aspartic acid (Rao, 1973; Sequeira *et al.*, 1989), DL-aspartic acid nitrate monohydrate (Asath Bahadur & Rajaram, 1995), bis(DL-aspartic acid) sulfate (Srinivasan *et al.*, 2001) and L-aspartic acid nitrate-L-aspartic acid (1/1) (Sridhar *et al.*, 2002) have been reported. In the present paper, the crystal structure of L-aspartic acid monohydrate, (I), is reported.



The asymmetric unit of (I) contains one aspartic acid molecule and one water molecule (Fig. 1). The equality of C—O bond distances [1.240 (4) and 1.259 (4) Å] and O—C—C bond angles [118.3 (3) and 115.3 (3)°] (Table 1) characterize the deprotonated carboxylate group. The backbone conformation angle ψ^1 of -10.8 (4)° indicates the *cis* form. The side chain shows a *gauche* II conformation [$\chi^1 = -71.8$ (3)°]. The branched chain conformation angles χ^{11} and χ^{21} correspond to the *cis* and *trans* forms. The C' atom is in the *gauche* I [52.7 (3)°] conformation with respect to the C' atom. The molecular structure is stabilized by a weak intramolecular $\text{N1}-\text{H1B} \cdots \text{O3}$ hydrogen bond.

The screw-related aspartic acid molecules are linked along the a axis by $\text{N1}-\text{H1A} \cdots \text{O1}^i$ hydrogen bonds to form a helical structure (Table 2 and Fig. 2). This helical structure is further stabilized by $\text{N1}-\text{H1C} \cdots \text{O3}^{ii}$ hydrogen bonds, which link the molecules translated by one unit along the a axis. The adjacent helices are interlinked through $\text{O4}-\text{H4} \cdots \text{O2}^{iii}$ hydrogen bonds and also by the water molecules through $\text{N1}-\text{H1B} \cdots \text{O11}^{iv}$, $\text{O11}-\text{H11} \cdots \text{O2}^v$ and $\text{O11}-\text{H12} \cdots \text{O2}^j$

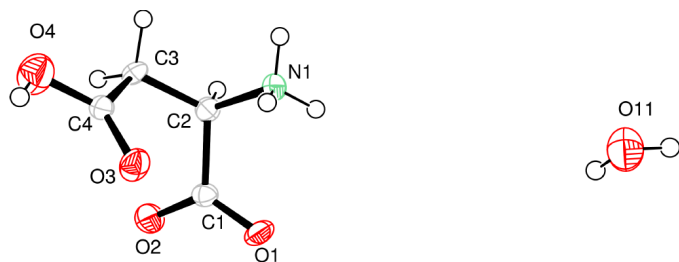


Figure 1
The asymmetric unit of the title compound, showing 50% probability displacement ellipsoids (Johnson, 1976) and the atom-numbering scheme.

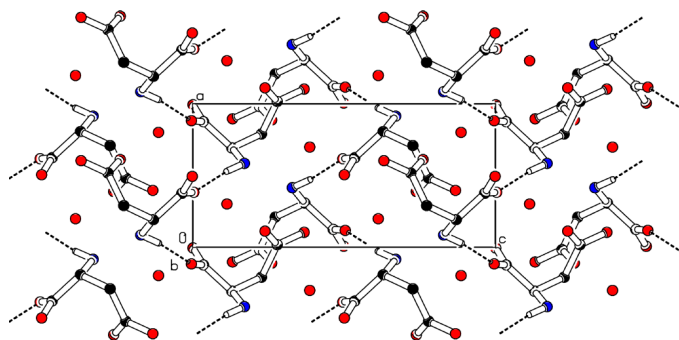


Figure 2
A view of the helical structures formed along the *a* axis. For clarity, all H atoms except H1A have been omitted.

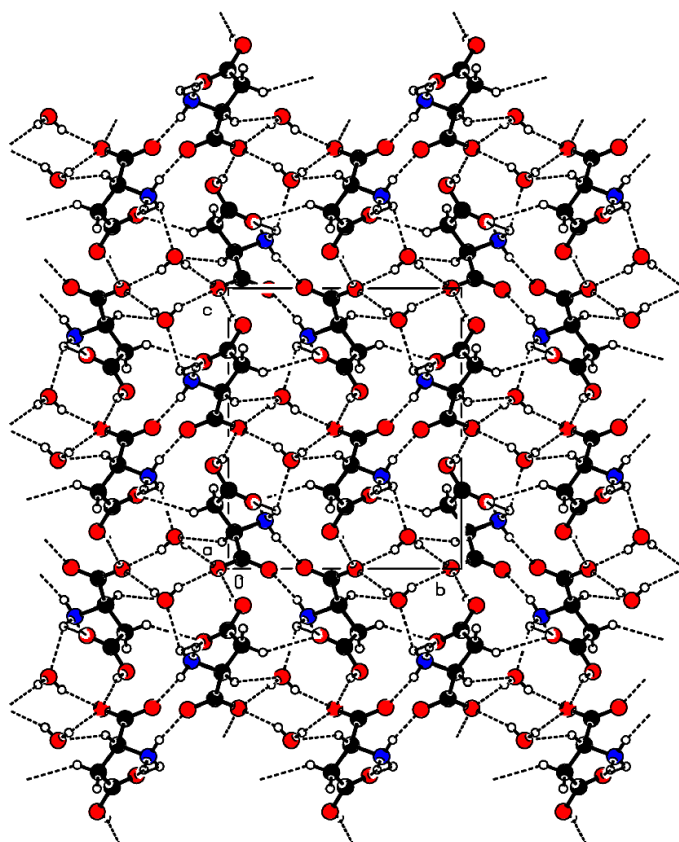


Figure 3
Hydrogen-bonding network, viewed down the *a* axis.

hydrogen bonds, to form a three-dimensional network. Within the network, the $O4-H4 \cdots O2^{iii}$ hydrogen bonds link the screw-related molecules, to form zigzag chains along the *c* axis. A class II hydrogen-bonding pattern is observed in the present structure, having two two-centered hydrogen bonds and one three-centered hydrogen bond (Jeffrey & Saenger, 1991). In the present study, the water molecule shows a planar $1B-1/D$ orientation (Jeffrey & Saenger, 1991). All the symmetry codes are as in Table 2. A view of the molecular packing down the *a* axis is shown in Fig. 3.

Experimental

The title compound was crystallized from an aqueous solution when attempts were made to grow single crystals of a complex of L-aspartic acid with sulfuric acid.

Crystal data

$C_4H_7NO_4 \cdot H_2O$
 $M_r = 151.12$
Orthorhombic, $P2_12_12_1$
 $a = 5.587$ (4) Å
 $b = 9.822$ (5) Å
 $c = 11.813$ (9) Å
 $V = 648.2$ (8) Å³
 $Z = 4$
 $D_x = 1.548$ Mg m⁻³
 $D_m = 1.54$ Mg m⁻³

D_m measured by flotation in a mixture of carbon tetrachloride and xylene
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
 $\theta = 8.0$ – 13.8°
 $\mu = 0.14$ mm⁻¹
 $T = 293$ (2) K
Block, colorless
 $0.3 \times 0.3 \times 0.3$ mm

Data collection

Enraf–Nonius CAD-4 diffractometer
 ω - 2θ scans
Absorption correction: ψ scan (North *et al.*, 1968)
 $T_{\min} = 0.958$, $T_{\max} = 0.958$
1318 measured reflections
1132 independent reflections
1091 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.085$
 $\theta_{\text{max}} = 24.6^\circ$
 $h = 0 \rightarrow 6$
 $k = 0 \rightarrow 11$
 $l = -14 \rightarrow 14$
3 standard reflections
frequency: 60 min
intensity decay: none

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.061$
 $wR(F^2) = 0.173$
 $S = 1.06$
1132 reflections
93 parameters
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.136P)^2 + 0.3381P]$
where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} < 0.001$
 $\Delta\rho_{\text{max}} = 0.33$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.54$ e Å⁻³

Table 1
Selected geometric parameters (Å, °).

O1—C1	1.240 (4)	C4—O3	1.244 (4)
O2—C1	1.259 (4)	C4—O4	1.322 (4)
O1—C1—O2	126.2 (3)	O2—C1—C2	115.3 (3)
O1—C1—C2	118.3 (3)		
O1—C1—C2—N1	−10.8 (4)	N1—C2—C3—C4	−71.9 (3)
O2—C1—C2—N1	173.9 (3)	C1—C2—C3—C4	52.8 (3)
O1—C1—C2—C3	−136.2 (3)	C2—C3—C4—O3	−2.9 (4)
O2—C1—C2—C3	48.5 (3)	C2—C3—C4—O4	177.0 (3)

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

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
N1—H1A \cdots O1 ⁱ	0.89	1.93	2.813 (4)	171
N1—H1C \cdots O3 ⁱⁱ	0.89	2.02	2.809 (4)	147
O4—H4 \cdots O2 ⁱⁱⁱ	0.82	2.15	2.933 (4)	161
N1—H1B \cdots O11 ^{iv}	0.89	2.22	2.854 (4)	128
O11—H11 \cdots O2 ^v	0.78	2.06	2.837 (4)	170
O11—H12 \cdots O2 ⁱ	0.80	2.05	2.817 (4)	160
N1—H1B \cdots O3	0.89	2.55	3.093 (4)	120

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

The H atoms of the water molecule were located from a difference Fourier map and their isotropic displacement parameters were refined [$U_{\text{iso}}(\text{H}) = 0.04$ (1) and 0.07 (2) Å²]. All other H atoms were placed in geometrically calculated positions and included in the refinement in the riding-model approximation, with U_{iso} equal to $1.2U_{\text{eq}}$ of the carrier atom. The data set includes 442 Friedel pairs; however, the lack of any significant anomalous effects precludes the confirmation of the absolute configuration from the diffraction data, and it has been assumed.

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *CAD-4 Software*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 1999); software used to prepare material for publication: *SHELXL97*.

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