Table 1. *Selected geometric parameters (Å, °)*

O1—C1	1.393 (8)	C5—C9	1.411 (9)
O2—C2	1.422 (8)	C6—C7	1.400 (10)
O2—C3	1.439 (8)	C7—C8	1.364 (10)
O3—C5	1.387 (8)	C8—C9^{i}	1.415 (8)
O3—C4	1.438 (9)	C9—C9^{i}	1.426 (12)
N1—C15	1.331 (9)	C11—C12	1.344 (10)
N1—C11	1.353 (8)	C12—C13	1.395 (9)
N1—C10	1.487 (9)	C13—C14	1.387 (9)
C1—C2	1.490 (10)	C13—C13^{ii}	1.472 (13)
C3—C4	1.428 (11)	C14—C15	1.352 (10)
C5—C6	1.350 (9)		
C2—O2—C3	111.7 (6)	C8—C7—C6	121.9 (7)
C5—O3—C4	120.3 (6)	C7—C8—C9^{i}	119.1 (7)
C15—N1—C11	119.5 (6)	C5—C9—C8^{i}	121.9 (6)
C15—N1—C10	121.3 (6)	C5—C9—C9^{i}	118.7 (7)
C11—N1—C10	119.2 (6)	C8^{i}—C9—C9^{i}	119.3 (7)
O1—C1—C2	108.9 (6)	C12—C11—N1	120.6 (6)
O2—C2—C1	109.9 (6)	C11—C12—C13	121.8 (6)
O2—C3—C4	110.6 (6)	C14—C13—C12	115.3 (6)
C3—C4—O3	113.1 (7)	C14—C13—C13^{ii}	122.5 (7)
C6—C5—O3	125.0 (7)	C12—C13—C13^{ii}	122.2 (7)
C6—C5—C9	120.9 (7)	C15—C14—C13	121.6 (7)
O3—C5—C9	114.1 (6)	N1—C15—C14	121.2 (7)
C5—C6—C7	120.1 (7)		

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

Data collection was stopped at 24.8° in θ because the last shell (>22° in θ) contained less than 20% observed reflections. The PF_6^- anion is severely disordered and the largest peaks on the residual electron-density map are located in the vicinity of the disordered F atoms. The anion was refined with constrained P—F bond lengths and equal populations of disordered F atoms. The difficulty in modelling the disorder is presumably the main cause of the rather high residual indices. All H-atoms were placed in calculated positions and refined in riding mode with $U(H) = 1.5U_{iso}(C)$.

Data collection: *CAD-4 EXPRESS* (Enraf–Nonius, 1995). Cell refinement: *CAD-4 EXPRESS*. Data reduction: *GX* (Mallinson & Muir, 1985). Program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1993). Program(s) used to refine structure: *SHELXL93* (Sheldrick, 1993). Software used to prepare material for publication: *SHELXL93*.

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: CF1184). Services for accessing these data are described at the back of the journal.

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L-Threonine at 12 K

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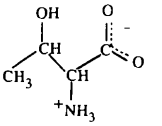
Abstract

The crystal structure of L-threonine, $C_4H_9NO_3$, was redetermined at 12 K. The present X-ray data allowed the determination of more accurate molecular geometry and of all the H-atom positions. The precision of the C—C, C—N and C—O distances is 0.002 Å or better, while that of the H-atom distances is 0.02 Å. The shape of the molecule relative to the C^{α}—C^{β} bond corresponds to the staggered (D_{3d}) conformation, with the H atoms at C^{α} and C^{β} *trans* to each other, yielding the least-crowded molecular conformation. All H atoms of the NH_3 and OH groups are involved in intermolecular hydrogen bonds, which interconnect the molecules to form a three-dimensional network.

Comment

L-Threonine (*threo*-α-amino-β-hydroxy-*n*-butyric acid) is an especially important amino acid. It is a significant constituent of many common proteins, such as egg albumin, human γ-globulin, β-lactoglobulin, gelatin, human serum albumin, insulin, silk fibroin and hemoglobin. L-Threonine plays a crucial role in many biological processes (Craig & Dekker, 1986; White, Berget & Nall, 1987; Krause, Volz & Lipscomb, 1987; Gouax, Krause & Lipscomb, 1987; Fierke & Benkovic, 1989; Raag *et al.*, 1991; Waldrop *et al.*, 1992; Chen *et al.*, 1993). From the X-ray analysis of L-lacate dehydrogenase, the threonine was identified as an active site residue that plays a major role in the control of catalysis and specificity (Bur *et al.*, 1989; Wigley *et al.*, 1992; Sakowicz *et al.*, 1992, 1993). This specificity is closely related to the conformation of L-threonine and its ability to form hydrogen bonds (Wigley *et al.*, 1992; Sakowicz *et al.*, 1993). We decided to redetermine the crystal structure of L-threonine, (I), at a low temperature (12 K) because



(I)

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the previous report of the room-temperature structure (Shoemaker *et al.*, 1950) did not provide information about the location of the H atoms and the geometry of the hydrogen bonds.

The shape of the molecule of L-threonine (Fig. 1) relative to the C2—C3 (C^{α}—C^{β}) bond corresponds to the staggered conformation. Of the three positions available for groups attached to the C3 (C^{γ}) atom, the most crowded is the position between C1 and N1, which is occupied by the H atom. Thus, the H atoms at C^{α} and C^{β} are *trans* to each other; this is the most stable configuration for threonine. In contrast, in L-allothreonine, this position is occupied by atom C4 (Swaminathan & Srinivasan, 1975*a*,*b*). The side-chain conformation is described by the torsion angles χ^{11}, χ^{12} and χ^{13} around C^{α}—C^{β}, determining the positions of the γ atoms with respect to the N atom (Edsall *et al.*, 1966; Lakshminarayanan, Sasisekharan & Ramachandran, 1967). These angles are −174.82 (9), −54.6 (1) and 65 (1)° for C4, O3 and H5, respectively. For comparison, χ^{11} and χ^{12} at room temperature, as determined by Shoemaker *et al.* (1950), are −174 and −55°, respectively. The torsion angles Ψ_1 (N1—C2—C1—O1) and Ψ_2 (N1—C2—C1—O2), describing the torsions of the two C—O bonds around C1—C2, are −25.3 (2) and 155.5 (1)°, respectively, at 12 K, which are comparable to the angles determined at room temperature (−26 and 157°, respectively; Shoemaker *et al.*, 1950).

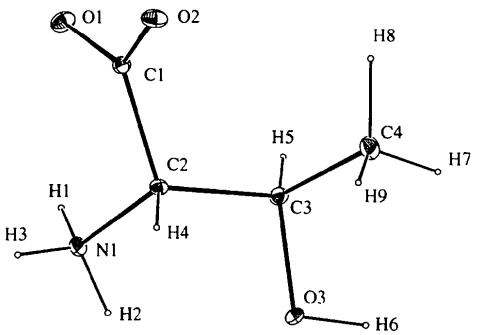

Fig. 1. *ORTEP* (Johnson, 1971) drawing showing the molecular structure of the title compound and the crystallographic numbering scheme (50% probability displacement ellipsoids).

If the 12 K atomic displacement parameters are compared with the room-temperature values [obtained by us and similar to those obtained by Shoemaker *et al.* (1950)], a decrease by a factor of about four is found between the averaged U_{eq} values: 0.0059 (13) at 12 K and 0.023 (7) Å^2 at 295 K. This seems to be a rather small ratio; among the few investigated examples of ultra-low-temperature and room-temperature structures of organic molecules, ratios of about five, for a lysergic acid derivative (Luger & Zobel, 1993), or even ten, for a crown ether complex (Luger *et al.*, 1992), have been seen. The distribution of U_{eq} values *versus* atomic distances from the molecular mass centre at 12 K is a linear function of the atomic distance from the molecular mass centre (differing by about 3σ from a constant), while in the room-temperature structure the vibrations of the 'outer' atoms are more pronounced. For C—C, C—O and C—N bond lengths, the e.s.d.'s at 12 K are 0.002 Å or smaller, while for H-atom distances, this quantity is 0.02 Å. The approximately 6σ difference between the two C—O distances in the carboxy group is a consequence of the hydrogen bonds, O2 being involved in two and O1 in only one hydrogen bond (Table 3). The differences among the C—N—H and H—N—H bond angles can also be attributed to the existence of hydrogen bonds. This effect has been noted previously in a low-temperature study of L-alanine (Destro, Marsh & Bianchi, 1988). The angle C3—C4—H8 is larger than both C3—C4—H7 and C3—C4—H9, which can be explained by weak interaction of the H7 and H9 atoms with the hydroxy group.

The contraction of the cell volume from room temperature to 12 K amounts to 2.1%. The lattice parameters at room temperature are: a = 13.608 (3), b = 7.736 (2) and c = 5.146 (2) Å. In contrast to the decrease of the lattice constants b and c, there is an increase of the lattice constant a with decreasing temperature. This axis is nearly along the direction of the strongest hydrogen bond, O3—H6···O1.

In the crystal of L-threonine, there are four non-linear intermolecular hydrogen bonds (see Table 3 and Fig. 2). Two H atoms (H1 and H3) of the NH_3 group form

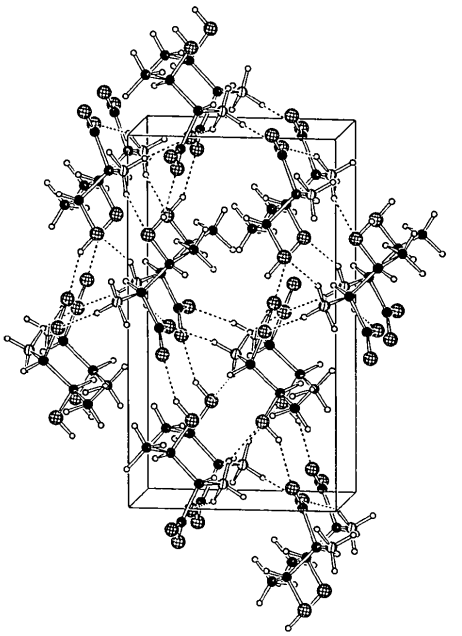

Fig. 2. Crystal structure as viewed along the c axis; b axis across the page, c axis down (*SCHAKAL92*; Keller, 1992).

shorter hydrogen bonds [N···O distances of 2.869 (1) and 2.786 (2) Å, respectively] than the third H atom (H2) [N···O 3.050 (1) Å]. One of the O atoms (O2) of the carboxy group is an acceptor of two hydrogen bonds; the other O atom (O1) forms only one hydrogen bond, but this is a shorter hydrogen bond, involving the H atom of the hydroxy group with an O···O distance of 2.651 (1) Å. Each molecule of L-threonine interconnects four neighbouring molecules by hydrogen bonds, forming a three-dimensional network (Fig. 2). The short N···O contacts are comparable with the N···O distances of the N—H···O hydrogen bonds in related amino acids, such as glycine (Iitaka, 1960; Power, Turner & Moore, 1976; Kvick *et al.*, 1980; Shimon, Lahar & Leiserowitz, 1986) and alanine (Dunitz & Ryan, 1966; Lehmann, Koetzle & Hamilton, 1972). The methyl groups pack around one of the twofold screw axes with a C···C separation of 3.79 Å. This distance is longer in the structure of alanine, in which the methyl groups, also packed around a twofold screw axis, are separated by 3.68 Å (Dunitz, & Ryan, 1966; Lehmann, Koetzle & Hamilton, 1972).

Experimental

L-Threonine was obtained from the Aldrich Chemical Co. The crystal used for the measurements was obtained by recrystallization from water.

Crystal data

$C_4H_9NO_3$
M_r = 119.12
Orthorhombic
$P2_12_12_1$
a = 13.628 (2) Å
b = 7.618 (1) Å
c = 5.110 (1) Å
V = 530.5 (1) Å^3
Z = 4
D_x = 1.491 Mg m^{-3}
D_m = 1.45 Mg m^{-3}
D_m measured by floation in C_6H_6/CCl_4 at room temperature
Ag $K\alpha$ radiation (X-ray tube)
λ = 0.5609 Å
Cell parameters from 30 reflections
θ = 15–30°
μ = 0.077 mm^{-1}
T = 12 K
Prism
0.58 × 0.36 × 0.33 mm
Colourless

Data collection

Huber four-circle diffractometer
ω–2θ scans
Absorption correction: none
2141 measured reflections
1132 independent reflections
1066 reflections with $F > 2\sigma(F)$
R_{int} = 0.021
θ_{max} = 25.0°
$h = -20 \rightarrow 0$
$k = -11 \rightarrow 11$
$l = 0 \rightarrow 7$
3 standard reflections
frequency: 90 min
intensity decay: 0.9%

Refinement

Refinement on F
R = 0.026
wR = 0.030
S = 2.866
1066 reflections
109 parameters
H atoms refined isotropically
Weighting scheme based on measured e.s.d.'s
$(\Delta/\sigma)_{max}$ = 0.00276
$\Delta\rho_{max}$ = 0.406 e Å^{-3}
$\Delta\rho_{min}$ = −0.336 e Å^{-3}
Extinction correction: none
Scattering factors from *International Tables for X-ray Crystallography* (Vol. IV)
Absolute configuration: Flack (1983)
Flack parameter = 0.0 (1)

Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters (Å^2)*

$U_{eq} = (1/3)\sum_i\sum_j U^{ij} a_i^* a_j^* \mathbf{a}_i.\mathbf{a}_j.$

	x	y	z	U_{eq}
C1	0.49723 (7)	0.1780 (2)	0.3011 (2)	0.0047 (4)
C2	0.39881 (7)	0.1014 (2)	0.3943 (2)	0.0041 (4)
C3	0.31954 (6)	0.2421 (2)	0.4281 (2)	0.0051 (4)
C4	0.29324 (7)	0.3347 (2)	0.1741 (2)	0.0078 (4)
N1	0.41238 (6)	0.0079 (2)	0.6482 (2)	0.0051 (4)
O1	0.55951 (5)	0.2099 (2)	0.4745 (2)	0.0070 (3)
O2	0.50549 (5)	0.2032 (1)	0.0591 (1)	0.0069 (3)
O3	0.23687 (5)	0.1472 (1)	0.5280 (2)	0.0064 (3)

Table 2. *Selected geometric parameters (Å, °)*

C1—C2	1.538 (1)	C3—H5	0.93 (3)
C1—O1	1.251 (1)	C4—H7	0.91 (2)
C1—O2	1.257 (1)	C4—H8	1.07 (2)
C2—C3	1.532 (2)	C4—H9	1.00 (2)
C2—N1	1.491 (2)	N1—H1	0.85 (2)
C2—H4	0.95 (2)	N1—H2	0.90 (2)
C3—C4	1.520 (2)	N1—H3	0.84 (2)
C3—O3	1.433 (1)	O3—H6	0.89 (2)
C2—C1—O1	116.51 (9)	O3—C3—H5	112 (1)
C2—C1—O2	116.15 (9)	C3—C4—H7	108 (1)
O1—C1—O2	127.3 (1)	C3—C4—H8	113 (1)
C1—C2—C3	112.6 (1)	C3—C4—H9	107 (1)
C1—C2—N1	110.01 (8)	H7—C4—H8	109 (2)
C1—C2—H4	110 (1)	H7—C4—H9	107 (2)
C3—C2—N1	108.88 (8)	H8—C4—H9	113 (2)
C3—C2—H4	108 (1)	C2—N1—H1	113 (2)
N1—C2—H4	106 (1)	C2—N1—H2	110 (1)
C2—C3—C4	113.24 (9)	C2—N1—H3	106 (1)
C2—C3—O3	104.0 (1)	H1—N1—H2	107 (2)
C2—C3—H5	110 (1)	H1—N1—H3	107 (2)
C4—C3—O3	110.68 (8)	H2- N1—H3	114 (2)
C4—C3—H5	107 (2)	C3—O3—H6	107 (2)
O1—C1—C2—C3	96.3 (1)	C1—C2—C3—C4	62.9 (1)
O1—C1—C2—N1	−25.3 (2)	C1—C2—C3—O3	−176.91 (8)
O2—C1—C2—C3	−82.9 (1)	N1—C2—C3—C4	−174.82 (9)
O2—C1—C2—N1	155.5 (1)	N1—C2—C3—O3	−54.6 (1)

Table 3. *Hydrogen-bonding geometry (Å, °)*

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O2^i	0.85 (2)	2.03 (2)	2.869 (1)	170 (2)
N1—H2···O3^{ii}	0.90 (2)	2.23 (2)	3.050 (1)	150 (2)
N1—H3···O2^{iii}	0.84 (2)	1.97 (2)	2.786 (2)	163 (2)
O3—H6···O1^{iv}	0.89 (2)	1.82 (2)	2.651 (1)	154 (3)

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

The clear colourless crystal was mounted on a beryllium needle with its c axis along the φ axis of the diffractometer and sealed in a capillary (0.01 mm wall thickness) to prevent sublimation of the crystal in the vacuum. The measurement was performed on a large four-circle Eulerian cradle (Huber, type 512) equipped with a double-stage closed-cycle He refrigerator (Air Products) and a Be vacuum chamber around the cold head. The vacuum was achieved using a turbomolecular pump to reduce the pressure to less than 1×10^{-4} mbar (1 bar = 10^5 Pa) and was stable during the entire measurement. The

crystal was cooled to 12 K with a cooling rate of 1 K min^{-1}. During the cooling procedure, several reflections were monitored by φ scan to monitor the crystal quality. The alignment of the crystal was controlled by the *C*8 routine (King & Finger, 1979), based on centring of one reflection in eight equivalent positions. During the cooling of the crystal from room temperature to 12 K, no phase transition was observed.

Data collection: *DIF*4 (Stoe & Cie, 1991*a*). Cell refinement: *DIF*4. Data reduction: *REDU*4 (Stoe & Cie, 1991*b*). Program(s) used to solve structure: *Xtal*3.2 (Hall, Flack & Stewart, 1992). Program(s) used to refine structure: *Xtal*3.2 *CRYLSQ*. Molecular graphics: *ORTEP*II (Johnson, 1971) and *SCHAKAL*92 (Keller, 1992). Software used to prepare material for publication: *Xtal*3.2 *BONDLA CIFIO*.

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Pyridinium Trifluoroacetate: Spoked Columns of Hydrogen-Bonded Cyclic Dimers

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Abstract

The crystal structure of $C_5H_6N^+.C_2F_3O_2^-$ consists of three unique ion pairs. Each unique ion pair packs along a threefold screw axis to generate a distinct spoked column. The three distinct spoked columns are pseudosymmetrically related through a threefold screw axis. Each column comprises an ionic core and non-polar spokes. Columns pack in a manner that maximizes the non-polar interactions between them.

Comment

Evaporation of water from a mixture of pyridine and trifluoroacetic acid results in the crystallization of $C_5H_6N^+.C_2F_3O_2^-$, (I), as clear colourless block-shaped crystals (m.p. = 355 K). Structural characterization of the title compound reveals three rectangular-shaped ion pairs of $C_5H_6N^+.C_2F_3O_2^-$ (identified as N1, N2, N3) within the asymmetric unit cell (Fig. 1). Proton transfer