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Bis(β-alanine) hydrogen nitrate

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.002 Å
R factor = 0.033
wR factor = 0.092
Data-to-parameter ratio = 8.8

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

In the title compound, $2C_3H_7NO_2.H^+\cdot NO_3^-$, both the alanine residues, related by a center of symmetry, are linked by a strong symmetric O—H···O hydrogen bond with an O···O distance of 2.467 (2) Å. The N atom and one of the O atoms of the nitrate anion lie on the twofold axis.

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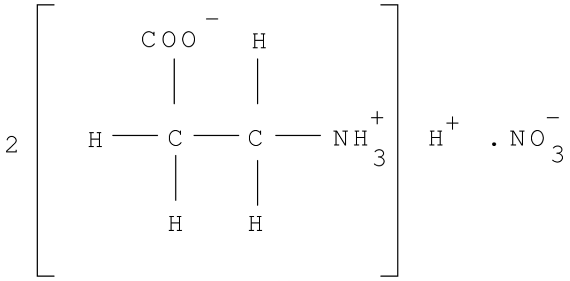
Comment

In amino acid–inorganic acid complexes, when the number of H atoms liberated from the inorganic acid is less than the number of amino acids, the H atom is shared by two amino acids, resulting in short symmetric O—H···O hydrogen bonds, as evidenced in triglycine sulfate (Kay, 1977), leading to phase transitions. In order to look for similar compounds, a systematic study of the behavior of hydrogen bonding in amino acid–inorganic acid complexes was undertaken. In this context, the crystal structure of L-phenylalanine L-phenylalaninium perchlorate (Srinivasan & Rajaram, 1997), hydrogen bis[L-lysinium (2+)] dichloride perchlorate (Srinivasan *et al.*, 2001*a*), L-lysine L-lysinium dichloride nitrate (Srinivasan *et al.*, 2001*b*), L-phenylalanine-nitric acid (2/1) (Srinivasan *et al.*, 2001*c*) and bis(L-proline) hydrogen perchlorate (Pandiarajan *et al.*, 2001) have been reported. A similar stucture, L-phenylalanine L-phenylalaninium formate, has been reported by Görbitz & Etter (1992). As part of this program, the crystal structure of β-alanine reacted with nitric acid was undertaken to study the nature of the hydrogen bonding in the presence of an inorganic acid.



(I)

The asymmetric unit contains one β-alanine residue and a nitrate anion which lies on the twofold axis. The backbone conformation angles ψ^1 and ψ^2 are −5.2 (2) and 174.9 (1)°, respectively, for the alanine residue. The straight-chain conformation angle χ^1 is in *gauche* I form [63.6 (2)°]. This tendency of twisting of the C—N bond is found in various amino acids (Lakshminarayanan *et al.*, 1967).

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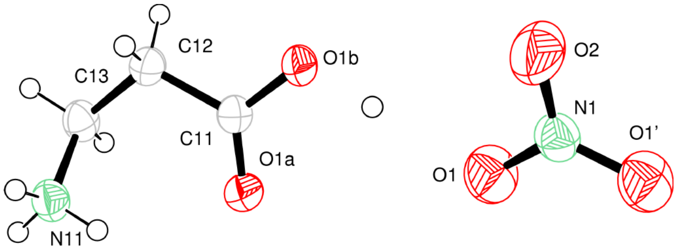

Figure 1
The molecular structure of (I), with the atom-numbering scheme and 50% probability displacement ellipsoids (Johnson, 1976).

The nitrate anion plays a vital role in forming hydrogen bonds with the alanine residue and stabilizing the structure. The H1*B* atom, which lies on a center of symmetry, links the two alanine residues through a strong symmetric O—H⋯O hydrogen bond [O1*B*⋯O1*B*($1/2-x, 1/2-y, 1-z$) 2.467 (2) Å]. The large U_{iso} value of H1*B* suggests that this atom may have positional or flip-flop disorder, leading to the switching of roles of the cation and zwitterion in a time-averaged equilibrium (Jeffrey & Saenger, 1991). A similar feature of short hydrogen bonding has been observed in L-phenylalanine L-phenylalaninium formate, L-phenylalanine L-phenylalaninium perchlorate, hydrogen bis[L-lysinium (2+)] dichloride perchlorate, L-lysine L-lysinium dichloride nitrate, L-phenylalanine-nitric acid (2/1) and bis(L-proline) hydrogen perchlorate. In these compounds, the hydrogen bond can be termed a possible symmetric hydrogen bond. At low temperature, the crystal of (I) may change to the non-centrosymmetric space group *Cc*, triggering a structural phase transition leading to interesting physical properties.

The O1 and O2 atoms of the nitrate anion, as acceptors, link the amino N atom in a three-centered hydrogen bond involving the alanine residue. This O2 atom of the nitrate anion, sitting on the twofold axis, links two symmetry-related β-alanine residues. A three-centered hydrogen bond is observed involving the alanine residue (amino N atom) and the carboxyl O1*A* (intramolecular hydrogen bond) and O1*B* (*Z*2 head-to-tail sequence) atoms. A glide-related head-to-tail sequence is observed, since N11—H2*B*⋯O1B($x, -y, z-1/2$) connects two glide-related amino acids (Vijayan, 1988).

Experimental

Crystals of (I) were grown from an aqueous solution of a 2:1 stoichiometric ratio of β-alanine and nitric acid by slow evaporation.

Crystal data

$2C_3H_7NO_2\cdot H^+\cdot NO_3^-$
$M_r = 241.21$
Monoclinic, $C2/c$
$a = 19.791$ (1) Å
$b = 5.3220$ (3) Å
$c = 10.974$ (1) Å
$\beta = 113.923$ (6)°
$V = 1056.57$ (13) Å^3
$Z = 4$
$D_x = 1.516$ Mg m^{-3}
$D_m = 1.502$ Mg m^{-3}
D_m measured by flotation using a mixture of carbon tetrachloride and xylene
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
$\theta = 11.3$–14.0°
$\mu = 0.14$ mm^{-1}
$T = 293$ (2) K
Needle, colorless
0.6 × 0.4 × 0.2 mm

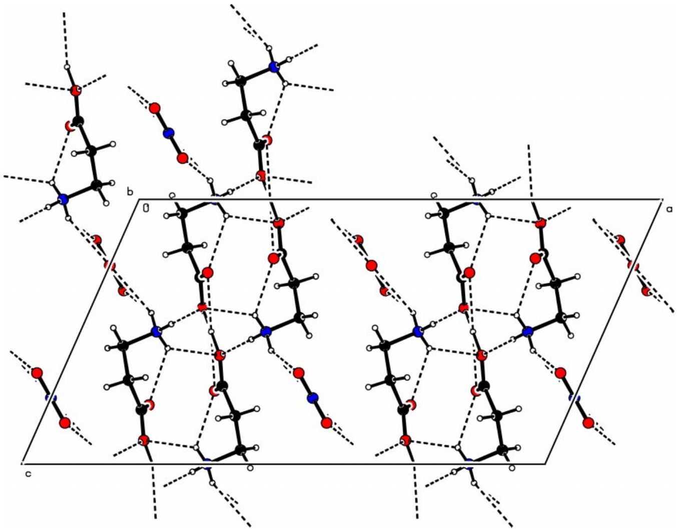

Figure 2
Packing diagram of (I) viewed down the *b* axis.

Data collection

Enraf–Nonius CAD-4 diffractometer
ω–2θ scans
Absorption correction: ψ scan (North *et al.*, 1968)
  $T_{min} = 0.863$, $T_{max} = 0.970$
941 measured reflections
914 independent reflections
798 reflections with $I > 2\sigma(I)$
$R_{int} = 0.014$
$\theta_{max} = 25.0°$
$h = 0 \rightarrow 23$
$k = 0 \rightarrow 6$
$l = -13 \rightarrow 11$
3 standard reflections
  frequency: 60 min
  intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.033$
$wR(F^2) = 0.092$
$S = 1.09$
914 reflections
104 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0459P)^2 + 0.6820P]$
  where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.31$ e Å^{-3}
$\Delta\rho_{min} = -0.18$ e Å^{-3}
Extinction correction: *SHELXL*97
Extinction coefficient: 0.103 (7)

Table 1
Selected geometric parameters (Å, °).

O1*A*—C11	1.2204 (19)	N1—O2	1.235 (3)
O1*B*—C11	1.3030 (17)	N1—O1	1.2419 (15)
O1*A*—C11—C12—C13	−5.2 (2)	C11—C12—C13—N11	63.60 (19)
O1*B*—C11—C12—C13	174.93 (13)		

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

D—H⋯*A*	*D*—H	H⋯*A*	*D*⋯*A*	*D*—H⋯*A*
O1*B*—H1*B*⋯O1*B*^{i}	1.2333 (10)	1.2333 (10)	2.467 (2)	180
N11—H1*A*⋯O1*A*	0.87 (2)	2.29 (2)	2.8971 (18)	126.5 (17)
N11—H1*A*⋯O1*B*^{ii}	0.87 (2)	2.34 (2)	3.0517 (18)	139.1 (17)
N11—H2*B*⋯O1*B*^{iii}	0.87 (2)	2.01 (3)	2.877 (2)	175 (2)
N11—H3*C*⋯O1^{ii}	0.89 (2)	2.10 (3)	2.908 (2)	150 (2)
N11—H3*C*⋯O2^{iv}	0.89 (2)	2.40 (2)	3.0779 (15)	133.2 (18)

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

All the H atoms were located and refined isotropically. The C—H and N—H bond lengths are 0.94 (2)–0.97 (2) and 0.87 (2)–0.89 (2) Å, respectively.

Data collection: *CAD*-4 *Software* (Enraf–Nonius, 1989); cell refinement: *CAD*-4 *Software*; data reduction: *CAD*-4 *Software*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 1999); software used to prepare material for publication: *SHELXL*97.

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