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L-Ornithine nitrate

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.037
wR factor = 0.090
Data-to-parameter ratio = 7.0

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

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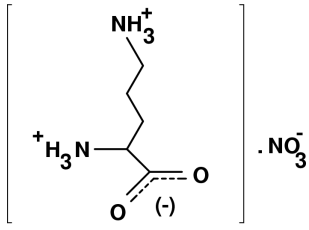
In the title compound, $C_5H_{13}N_2O_2^+\cdot NO_3^-$, both the α- and δ-amino N atoms form strong N—H···O hydrogen bonds with the carboxyl group and nitrate anions. The straight side-chain conformation shows an all *trans* form.

Comment

Ornithine is an important amino acid, which induces the release of growth hormones and thus encourages the mechanism of muscle building. The crystal structure of L-ornithine hydrochloride (Chiba *et al.*, 1967) has been solved. In the present study, the crystal stucture of L-ornithine nitrate, (I), has been determined.



(I)

The asymmetric part of the asymmetric unit contains one ornithine cation and one nitrate anion. The ornithine residue contains two planar groups, *viz*. the carboxyl group and the aliphatic side chain. The C—O bond distances [1.238 (3) and 1.258 (3) Å] and O—C—C angles [117.0 (2) and 116.1 (2)°] of the carboxyl group indicate the resonance form shown above. The backbone conformation angle ψ^1 [−39.2 (3)°] indicates a *cis* form. The α-amino N atom deviates from the carboxyl plane by 0.854 (4) Å. This tendency for the C—N bond to twist is found in various amino acids (Lakshiminarayanan *et al.*, 1967). The side-chain conformation angles χ^1, χ^2 and χ^3 [−173.5 (2), −169.4 (2) and 172.2 (2)°, respectively] correspond to *trans* forms having a fully extended configuration. The maximum deviation from the mean plane of the side-chain atoms is 0.151 (2) Å for C^γ. The side-chain plane forms a dihedral angle of 78° with the carboxyl plane.

The amino atom N1 of the ornithine forms strong N—H···O hydrogen bonds with the carboxyl and nitrate groups (Table 2). The ornithine residue is involved in both zigzag (*Z*2) and straight (*S*2) head-to-tail sequences. The δ-amino atom N2 forms strong N—H···O hydrogen bonds with nitrate atoms O2 and O3, and also with the carboxyl O1*a* atom (Fig. 2).

Experimental

The title compound was crystallized by slow evaporation from an aqueous solution of L-ornithine and nitric acid (1:1).

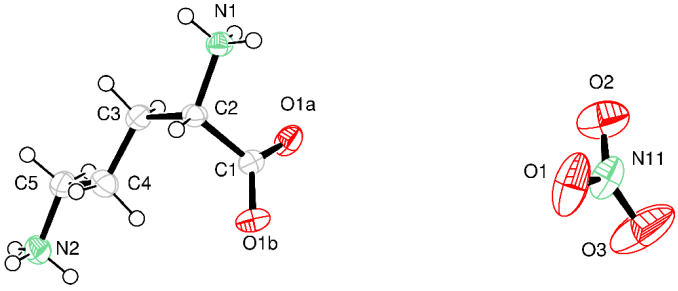


Figure 1
The molecular structure of the title compound, (I), showing the atomic numbering scheme and 50% probability displacement ellipsoids (Johnson, 1976).

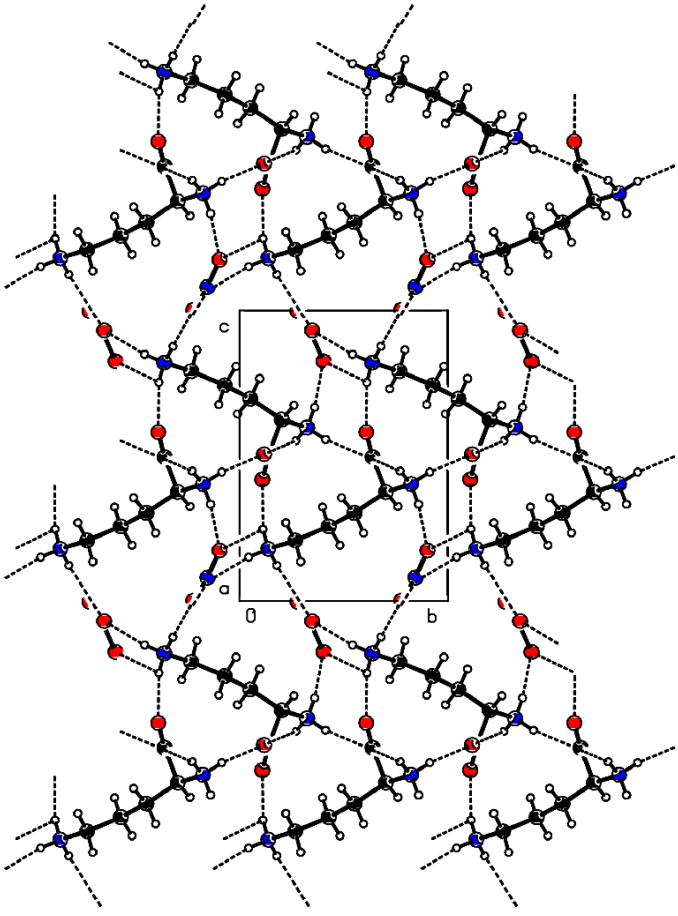


Figure 2
The packing of the title molecules, viewed down the *a* axis.

Crystal data

$C_5H_{13}N_2O_2^+\cdot NO_3^-$
M_r = 195.18
Monoclinic, $P2_1$
a = 5.1944 (6) Å
b = 7.803 (1) Å
c = 11.050 (1) Å
β = 98.75 (1)°
V = 442.66 (9) Å^3
Z = 2
D_x = 1.464 Mg m^{-3}
D_m = 1.438 Mg m^{-3}
D_m measured by flotation in a mixture of carbon tetrachloride and xylene
Mo $K\alpha$ radiation
Cell parameters from 24 reflections
θ = 9.8–14.4°
μ = 0.13 mm^{-1}
T = 293 (2) K
Needle, colorless
0.6 × 0.3 × 0.3 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
ω-2θ scans
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.887, T_{max} = 0.956
1295 measured reflections
963 independent reflections
919 reflections with $I > 2\sigma(I)$
R_{int} = 0.0316
θ_{max} = 25.0°
$h = -1 \rightarrow 6$
$k = -1 \rightarrow 9$
$l = -13 \rightarrow 13$
3 standard reflections
frequency: 60 min
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.090
S = 1.16
838 reflections
119 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.06P)^2 + 0.0457P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}
Extinction correction: *SHELXL*97
Extinction coefficient: 0.64 (5)

Table 1
Selected geometric parameters (Å, °).

O1*A*—C1	1.238 (3)	O1*B*—C1	1.258 (3)
O1*A*—C1—O1*B*	126.8 (2)	O1*B*—C1—C2	116.14 (19)
O1*A*—C1—C2	117.02 (18)		
O1*A*—C1—C2—N1	−39.2 (3)	C2—C3—C4—C5	−169.4 (2)
N1—C2—C3—C4	−173.54 (19)	C3—C4—C5—N2	172.15 (18)

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*A*···O1*B*^{i}	0.89	1.93	2.813 (3)	169
N1—H1*B*···O1^{ii}	0.89	1.93	2.818 (3)	172
N1—H1*C*···O1*B*^{iii}	0.89	2.06	2.911 (3)	161
N2—H2*A*···O2^{iv}	0.89	2.01	2.899 (4)	173
N2—H2*B*···O3^{v}	0.89	2.02	2.911 (4)	179
N2—H2*C*···O1*A*^{ii}	0.89	2.03	2.900 (3)	165

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

All 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_{eq} of the carrier atom. The Friedel pairs were merged during the final cycles of refinement.

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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