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D-Serinium D-serine nitrate

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.026
wR factor = 0.074
Data-to-parameter ratio = 6.2

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

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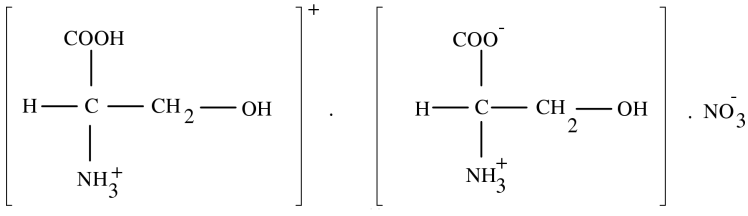
In the title compound, $C_3H_8O_3N^+\cdot NO_3^-\cdot C_3H_7O_3N$, the serinium and the serine as zwitterion are held together by a strong O—H···O hydrogen bond. The serinium cation has a *gauche* I conformation and the serine molecule has a *gauche* II conformation for the hydroxyl O atom. The nitrate anion links the amino N atom of molecule 1 extending in a chain running along the *a* axis.

Comment

The crystal structures of L-serine (Benedetti *et al.*, 1972), DL-serine (Shoemaker *et al.*, 1953; Frey *et al.*, 1973; Kistenmacher *et al.*, 1974) and L-serine monohydrate (Frey *et al.*, 1973) have been reported previously. In the present study, the structure determination of the product of D-serine reacted with nitric acid was undertaken.

The geometry of the two crystallographically independent serine and serinium constituents are similar and agree well with earlier X-ray studies of DL-serine (Shoemaker *et al.*, 1953) and L-serine (Benedetti *et al.*, 1972). The conformation angle ψ_1 is −1.5 (3) and −3.9 (3)° for serinium and serine, respectively. This tendency of the C—N bond to twist is found in various amino acids (Lakshiminarayanan *et al.*, 1967). The straight side-chain conformation angle χ_1 for the serinium cation is in a *gauche* I conformation [63.8 (3)°] and for the serine molecule is in a *gauche* II conformation [−66.4 (3)°].



(I)

The nitrate anion plays a vital role in the hydrogen bonding with both ions and in stabilizing the structure. Serine and serinium are connected by a strong O—H···O hydrogen bond O1*B*—H1*B*···O2*A*^{iv}. The nitrate anion, as acceptor, hydrogen bonds with the amino N and hydroxyl O atom of both molecules in a three-dimensional network. The nitrate anion links the amino N atom of the serinium cation resulting in a chain running along the *a* axis. The hydroxyl O atom of serinium, as acceptor, links the amino N atom of serinium.

The serine molecule is engaged in a straight (S1) head-to-tail sequence, since the N21—H21*C*···O2*B*^{iv} hydrogen bond connects two amino acids separated by a period along the *a*

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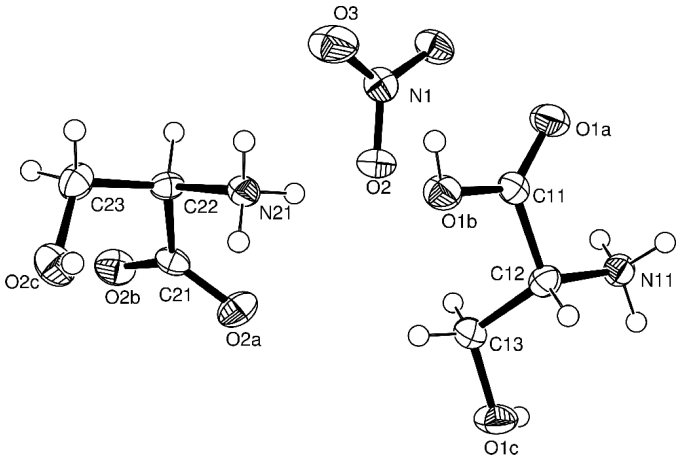

Figure 1
The structure of the asymmetric unit showing the atomic numbering scheme and 50% probability displacement ellipsoids (Johnson, 1976).

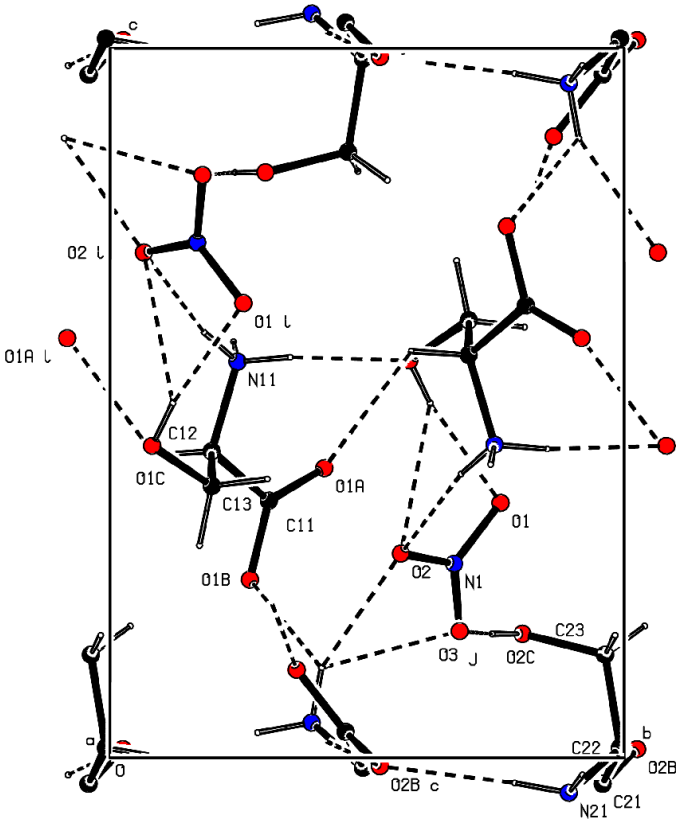

Figure 2
The packing viewed down the *a* axis.

axis, and a zigzag (Z2) head-to-tail sequence, since N21—H21*B*···O2*B*^{v} connects two 2_1-related amino acids (Vijayan, 1988).

Experimental

The title compound was crystallized in aqueous solution from a 2:1 stoichiometric ratio of D-serine and nitric acid. Colorless needle-shaped crystals were obtained.

Crystal data

$C_3H_8NO_3^+\cdot NO_3^-\cdot C_3H_7NO_3$
M_r = 273.21
Monoclinic, $P2_1$
a = 5.929 (1) Å
b = 8.195 (7) Å
c = 11.503 (2) Å
β = 100.06 (1)°
V = 550.3 (5) Å^3
Z = 2
D_x = 1.649 Mg m^{-3}
D_m = 1.63 Mg m^{-3}
D_m measured by flotation in bromoform and xylene
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
θ = 10.0–13.9°
μ = 0.16 mm^{-1}
T = 293 (2) K
Needle, colorless
0.50 × 0.20 × 0.07 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
ω–2θ scans
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.962, T_{max} = 0.988
1533 measured reflections
1030 independent reflections
908 reflections with $I > 2\sigma(I)$
R_{int} = 0.019
θ_{max} = 25.0°
$h = -1 \rightarrow 7$
$k = -1 \rightarrow 9$
$l = -13 \rightarrow 13$
25 standard reflections
every 3 reflections
frequency: 60 min
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.026
$wR(F^2)$ = 0.074
S = 0.95
1030 reflections
166 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0554P)^2 + 0.0361P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.16 e Å^{-3}
$\Delta\rho_{min}$ = −0.15 e Å^{-3}
Extinction correction: *SHELXL*97

Table 1
Selected geometric parameters (Å, °).

O1*A*—C11	1.210 (3)	O2*B*—C21	1.240 (4)
O1*B*—C11	1.297 (3)	O2*A*—C21	1.259 (4)
O1*A*—C11—C12—N11	−1.5 (3)	O2*A*—C21—C22—N21	−3.9 (3)
N11—C12—C13—O1*C*	63.8 (3)	N21—C22—C23—O2*C*	−66.4 (3)

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N11—H11*A*···O2^{i}	0.89	2.09	2.972 (3)	170
N11—H11*B*···O1^{ii}	0.89	2.08	2.963 (3)	171
N11—H11*C*···O1C^{iii}	0.89	1.97	2.853 (4)	173
O1C—H1*C*···O1^{i}	0.82	2.02	2.833 (3)	168
O1C—H1*C*···O2^{i}	0.82	2.55	3.112 (3)	127
O1B—H1*B*···O2*A*^{iv}	0.82	1.66	2.462 (3)	164
N21—H21*A*···O2	0.89	2.25	3.084 (3)	155
N21—H21*A*···O1*B*	0.89	2.48	2.979 (3)	116
N21—H21*A*···O3	0.89	2.53	2.965 (4)	111
N21—H21*B*···O2*B*^{v}	0.89	2.16	3.048 (4)	172
N21—H21*C*···O2*B*^{iv}	0.89	1.99	2.863 (3)	167
O2C—H2*C*···O3^{vi}	0.82	2.01	2.792 (3)	159

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

The reflection/parameter ratio is 6.20 in spite of the fact that data for 1030 of the possible 1038 reflections have been collected which has resulted in a reasonable final R factor of 0.026. All H atoms were fixed by geometric restraints using *HFIX* and allowed to ride on the parent atom.

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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