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L-Ornithinium sulfate monohydrate

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.008 Å
R factor = 0.059
wR factor = 0.171
Data-to-parameter ratio = 8.6

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

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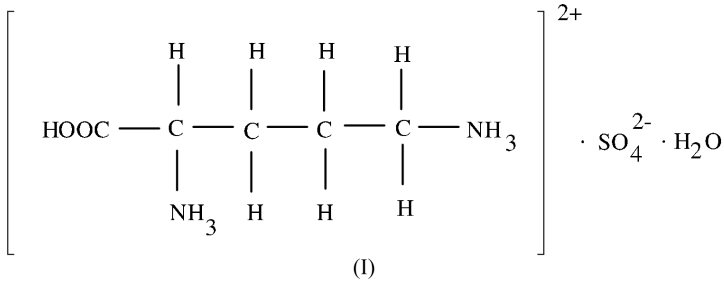
In the title compound, $C_5H_{14}N_2O_2^{2+}\cdot SO_4^{2-}\cdot H_2O$, the ornithinium cation forms a strong O—H···O hydrogen bond with the sulfate anion. One backbone conformation angle is in an eclipsed conformation, while the other two are in a *trans–trans* staggered conformation. All the amino and carboxylate groups and the sulfate anions are involved in hydrogen bonding. The amino groups are also involved in a three-centred hydrogen bond with the O atoms of the sulfate anion.

Comment

L-Ornithine helps to elevate levels of human growth hormone, assists in repairing muscles and tissues, stimulates the pancreas to release insulin and helps regenerate the liver, in addition to being necessary for the proper functioning of the immune system (Bucchi *et al.*, 1990). The crystal structures of L-ornithine hydrochloride (Chiba *et al.*, 1967), L-ornithine nitrate (Ramaswamy *et al.*, 2002) and bis(L-ornithinium) chloride nitrate sulfate (Ramaswamy *et al.*, 2004) have been solved. In the present study, the crystal structure of L-ornithinium sulfate monohydrate, (I) (Fig. 1), obtained by the recrystallization of L-ornithine from sulfuric acid, is reported.



(I)

The average S—O bond distance and O—S—O bond angle in (I) conform to tetrahedral symmetry. The unsymmetrical C—O bond distances [1.1957 (6) and 1.3162 (7) Å] and O—C—C bond angles [123.0 (5) and 111.5 (5)°] clearly confirm the protonation of the carboxyl group. Both amino groups are also protonated.

The backbone conformation angle ψ^1 (O1*A*—C1—C2—N1) indicates a *cis* conformation [−9.3 (8) Å]. The deviation of this amino N atom from the carbonyl plane is very small [0.208 (9) Å]. An eclipsed conformation is observed about C2—C3, with torsion angles N1—C2—C3—C4 = −130.3 (5)° and C1—C2—C3—C4 = 110.4 (6)°. The other angles, χ^2 (C2—C3—C4—C5) and χ^3 (C3—C4—C5—N2), have fully extended *trans–trans* conformations [178.2 (5) and −170.8 (5)°, respectively]. The maximum deviation of the side-chain atoms from their mean plane is 0.41 (1) Å for C3.

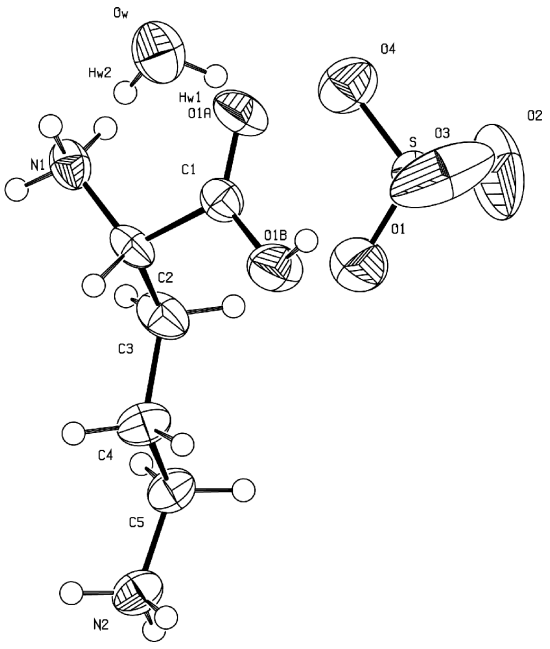


Figure 1
The molecular structure of (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

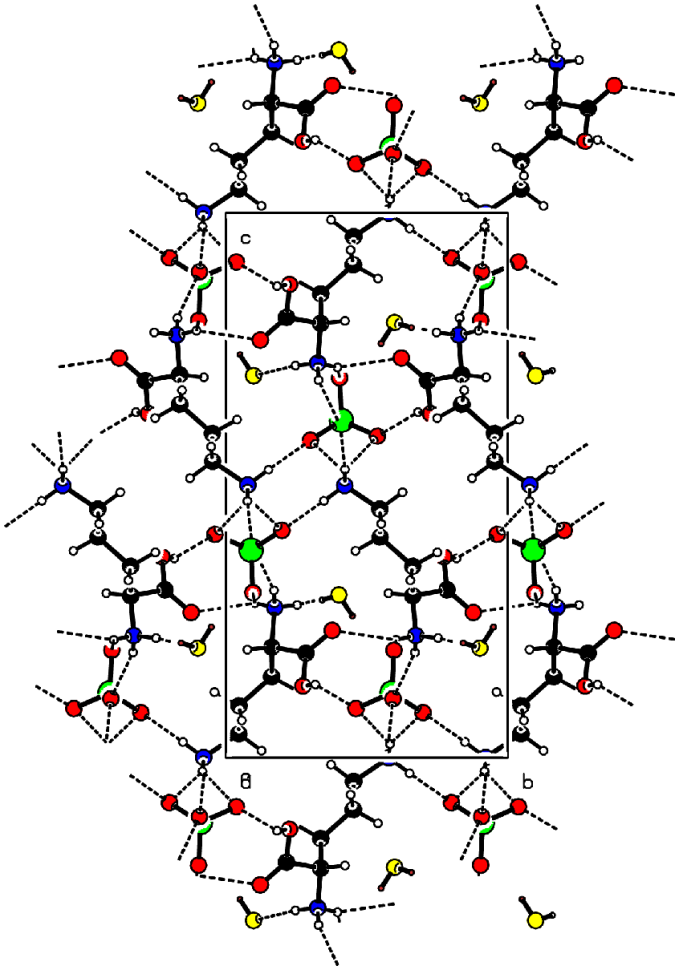


Figure 2
A packing diagram for (I), viewed down the *a* axis. Dashed lines indicate the hydrogen bonds.

The hydroxyl group of the ornithinium cation forms a strong O—H···O hydrogen bond with one O atom of the sulfate anion (Fig. 2, Table 2). Atoms N1 and N2 form one two-centred and two three-centred hydrogen bonds, leading to class III behaviour (Jeffrey & Saenger, 1991). Both N atoms in the ornithinium cation connect O atoms of two different sulfate anions, thus forming a chain running along the *a* axis (N1—H1*A*···O4^{iii} and N1—H1*C*···O3^{ii}; Table 2) and a similar zigzag head-to-tail sequence along the *a* axis (N2—H2*A*···O3^{iv} and N2—H2*C*···O2^{vi}; Table 2). The water molecule connects two ornithinium cations to form an infinite chain, also along the *a* axis (N1—H1*B*···O*W*—H*W*2···O1*A*^{vii}; Table 2). Through the three-centred bond, this water molecule connects two 2_1 screw-related sulfate anions along the *b* axis.

Experimental

The title compound was formed by mixing a 1 *M* solution of L-ornithine with a 1 *M* solution of sulfuric acid, followed by crystallization by slow evaporation under ambient conditions.

Crystal data

$C_5H_{14}N_2O_2^{2+}\cdot SO_4^{2-}\cdot H_2O$
M_r = 248.26
Orthorhombic, $P2_12_12_1$
a = 6.1589 (2) Å
b = 9.682 (6) Å
c = 18.714 (6) Å
V = 1115.9 (8) Å^3
Z = 4
D_x = 1.478 Mg m^{-3}
D_m = 1.475 (5) Mg m^{-3}
D_m measured by flotation, using a mixture of CCl_4 and xylene
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
θ = 11.3–14.2°
μ = 0.31 mm^{-1}
T = 293 (2) K
Block, colourless
0.3 × 0.3 × 0.2 mm

Data collection

Nonius MACH 3 diffractometer
$\omega/2\theta$ scans
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.911, T_{max} = 0.940
1399 measured reflections
1172 independent reflections
1043 reflections with $I > 2\sigma(I)$
R_{int} = 0.029
θ_{max} = 25°
$h = 0 \rightarrow 7$
$k = -1 \rightarrow 11$
$l = -1 \rightarrow 22$
3 standard reflections
frequency: 60 min
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.059
$wR(F^2)$ = 0.171
S = 1.06
1172 reflections
137 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.112P)^2 + 1.3829P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.005
$\Delta\rho_{max}$ = 0.73 e Å^{-3}
$\Delta\rho_{min}$ = −0.37 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

O1*B*—C1	1.319 (7)	O1*A*—C1	1.197 (7)
O1*A*—C1—O1*B*	125.3 (6)	O1*B*—C1—C2	111.6 (5)
O1*A*—C1—C2	123.1 (5)		
O1*A*—C1—C2—N1	−9.3 (8)	C1—C2—C3—C4	110.4 (6)
O1*B*—C1—C2—N1	171.8 (5)	C2—C3—C4—C5	178.2 (5)
N1—C2—C3—C4	−130.3 (5)	C3—C4—C5—N2	−170.8 (5)

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

D—H···A	D—H	H···A	D···A	D—H···A
O1B—H1···O1^{i}	0.82	1.87	2.546 (7)	139
N1—H1A···O1A^{ii}	0.89	2.21	2.903 (6)	134
N1—H1A···O4^{iii}	0.89	2.34	3.003 (7)	132
N1—H1B···OW	0.89	1.91	2.790 (7)	169
N1—H1C···O3^{ii}	0.89	1.99	2.810 (7)	153
N2—H2A···O3^{iv}	0.89	1.86	2.729 (7)	165
N2—H2B···O2^{v}	0.89	1.94	2.781 (8)	158
N2—H2C···O2^{vi}	0.89	2.14	2.945 (10)	150
N2—H2C···O1^{vi}	0.89	2.35	3.136 (8)	148
OW—HW1···O4	0.88	1.88	2.726 (7)	162
OW—HW2···O4^{iii}	0.87	2.46	3.195 (7)	143
OW—HW2···O1A^{vii}	0.87	2.57	3.191 (7)	130

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

For the water molecule, the H atoms were located in a difference Fourier map and in these positions. All remaining H atoms were positioned geometrically and refined in the riding-model approximation, with C—H = 0.97–0.98, N—H = 0.89 and O—H = 0.82 Å, and with U_{iso}(H) = 1.2U_{eq} of the carrier atom (1.5U_{eq} for methyl and NH_3 H atoms).

Data collection: *CAD*-4 *EXPRESS* (Enraf–Nonius, 1994); cell refinement: *CAD*-4 *EXPRESS*; data reduction: *XCAD*4 (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*3 (Farrugia, 1997) and *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL*97.

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References

Bucchi, L., Hickson, J. F., Pivarnik, J. M., Wolinsky, I., McMahon, J. C. & Turner, S. D. (1990). *Nutr. Res.* **10**, 239–245.
Chiba, A., Ueki, T., Ashida, T., Sasada, Y. & Kakudo, M.(1967). *Acta Cryst.* **22**, 863–870.
Enraf–Nonius (1994). *CAD*-4 *EXPRESS*. Version 5.1/1.2. Enraf–Nonius, Delft, The Netherlands.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Harms, K. & Wocadlo, S. (1995). *XCAD*4. University of Marburg, Germany.
Jeffrey, G. A. & Saenger, W. (1991). *Hydrogen Bonding in Biological Structures*. Berlin: Springer Verlag.
North, A. C. T., Phillips, D. C. & Mathews, F. S. (1968). *Acta Cryst.* A**24**, 351–359.
Ramaswamy, S., Sridhar, B., Ramakrishnan, V. & Rajaram, R. K., (2002). *Acta Cryst.* E**58**, o646–o648.
Ramaswamy, S., Sridhar, B., Ramakrishnan, V. & Rajaram, R. K., (2004). *Acta Cryst.* E**60**, o768–o770.
Sheldrick, G. M. (1997). *SHELXS*97 and *SHELXL*97. University of Göttingen, Germany.
Spek, A. L. (2003). *J. Appl.Cryst.* **36**, 7–13.