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Hydrogen bonding in 1-carboxypropanaminium nitrate

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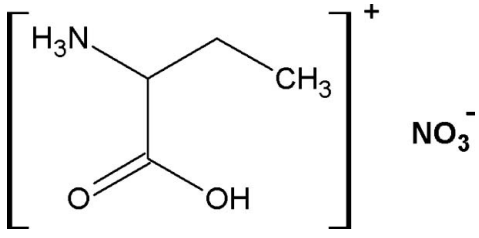
Key indicators: single-crystal X-ray study; T = 150 K; mean σ(C–C) = 0.002 Å; R factor = 0.039; wR factor = 0.109; data-to-parameter ratio = 13.2.

There are two crystallographically independent cations and two anions in the asymmetric unit of the title compound, $C_4H_5NO_2^+\cdot NO_3^-$. In the crystal, the 1-carboxypropanaminium cations and nitrate anions are linked to each other through strong N—H···O and O—H···O hydrogen bonds, forming a three-dimensional complex network. C—H···O interactions also occur.

Related literature

For background to inorganic–organic hybrid materials, see: Benali-Cherif, Allouche *et al.* (2007); Benali-Cherif, Kateb *et al.* (2007); Messai *et al.* (2009); Cherouana *et al.* (2003). Changes in illuminated volume were kept to a minimum, and were taken into account (Görbitz, 1999) by multi-scan inter-frame scaling.



Experimental

Crystal data

$C_4H_{10}NO_2^+\cdot NO_3^-$
M_r = 166.14
Monoclinic, $P2_1/c$
a = 18.274 (2) Å
b = 5.6052 (4) Å
c = 16.536 (2) Å
β = 116.224 (16)°
V = 1519.4 (3) Å^3
Z = 8
Cu $K\alpha$ radiation
μ = 1.18 mm^{-1}
T = 150 K
0.1 × 0.02 × 0.01 mm

Data collection

Oxford Xcalibur Atlas Gemini ultra diffractometer
Absorption correction: analytical (*CrysAlis PRO*; Oxford Diffraction, 2010)
T_{min} = 0.987, T_{max} = 0.999
14871 measured reflections
2683 independent reflections
2441 reflections with $I > 2\sigma(I)$
R_{int} = 0.054

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.109
S = 1.08
2683 reflections
203 parameters
H-atom parameters not refined
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.31 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N1A—H1A···O1A^{i}	0.89	2.11	2.8590 (18)	141
N1A—H1A···O5B^{ii}	0.89	2.48	2.9464 (18)	113
N1A—H1B···O3B^{iii}	0.89	2.01	2.8877 (17)	169
N1A—H1B···O4B^{iii}	0.89	2.44	3.0033 (16)	121
N1A—H1C···O4B	0.89	1.93	2.8162 (16)	173
O2A—H2O···O3B^{iv}	0.82	1.84	2.6295 (17)	160
N1B—H3C···O1B^{v}	0.89	2.08	2.8470 (16)	143
N1B—H3C···O5A^{v}	0.89	2.50	2.946 (2)	111
N1B—H3D···O3A^{vi}	0.89	2.47	2.9917 (16)	118
N1B—H3D···O4A^{vi}	0.89	2.02	2.9025 (16)	169
N1B—H3E···O3A^{vii}	0.89	1.94	2.8126 (16)	168
O2B—H4···O4A	0.82	1.84	2.6206 (16)	159
C4A—H4B···O3B^{iii}	0.96	2.58	3.382 (2)	141
C2B—H6···O3A^{vi}	0.98	2.57	3.189 (2)	121

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

Data collection: *Gemini User Manual* (Oxford Diffraction, 2006); cell refinement: *CrysAlis PRO* (Oxford Diffraction, 2010); data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SIR2004* (Burla *et al.*, 2005); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *PLATON* (Spek, 2009); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RU2030).

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