Acta Crystallographica Section E
Structure Reports
Online

ISSN 1600-5368

Sarcosine ammonium nitrate

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Received 13 December 2004
Accepted 18 April 2005
Online 14 May 2005

Key indicators

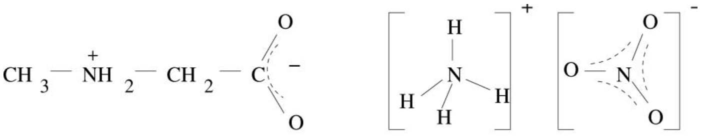
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.041
wR factor = 0.130
Data-to-parameter ratio = 11.8

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

In the title compound, $C_3H_7NO_2\cdot NH_4^+\cdot NO_3^-$, the sarcosine zwitterions have an almost perfectly planar N—C—COO main chain and assemble in chains *via* hydrogen bonds. The ammonium and nitrate ions are arranged in sheets that alternate with sheets of sarcosine chains. The whole structure is stabilized by an extensive three-dimensional network of hydrogen bonds.

Comment

Sarcosine (N-methylglycine, $CH_3NH_2^+\cdot CH_2COO^-$) is an α-amino acid found in many biological materials (Mostad & Natarajan, 1989). Several structural studies of sarcosine with inorganic acids and metallic ions have been published, spanning a variety of applications in which the sarcosine molecule plays a role. We report here the crystal structure of this amino acid cocrystallized with ammonium nitrate, *viz.* the title compound, (I), which could be particularly relevant given the importance of hydrogen-bonded interactions in chemistry and biology. This is the first reported crystal structure of an amino acid cocrystallized with ammonium nitrate.



(I)

The ionization state of the sarcosine molecule inferred from the C—O distances in the carboxyl group was found to be a zwitterionic form with a protonated amino group and a deprotonated carboxylate group. The sarcosine skeleton including atoms O1, O2, C1 and C2 is planar within 0.003 (2) Å. The N atom deviates 0.090 (3) Å from this plane. The title compound is slightly less distorted from planarity than pure sarcosine (Mostad & Natarajan, 1989), the corresponding values of the torsion angles O1—C1—C2—N1 and O2—C1—C2—N1 being 173.7 (2) and −6.8 (2)°. The methyl group breaks the almost perfect planarity of the whole main chain, and atom C3 is displaced by 1.435 (4) Å from the previously mentioned least-squares plane, in the same direction as the N atom. The nitrate anion, which is planar within 0.0016 (8) Å, deviates slightly from the usual (non-crystallographic) D_{3h} symmetry; one of the N—O bonds is 0.010 (3) Å shorter than the other two. In addition, two of the O—N—O angles deviate by about 2° from the ideal 120° value. The three-dimensional hydrogen-bonded network can be described as the stacking of linear chains of head-to-tail hydrogen-bonded sarcosine zwitterions, running along the *a*

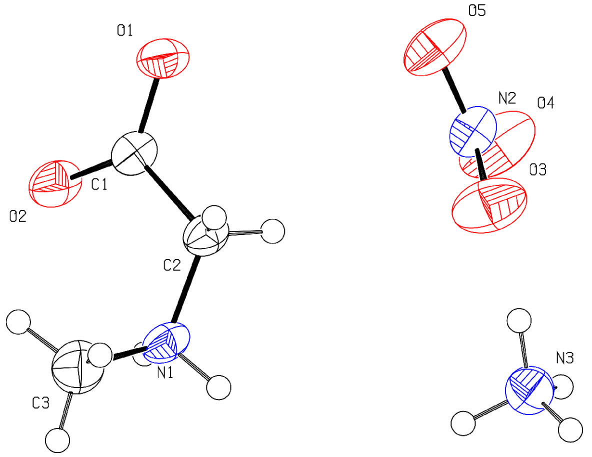


Figure 1
ORTEPII (Johnson, 1976) plot of the title compound. Displacement ellipsoids are drawn at the 50% probability level.

axis between sheets of nitrates and ammonium ions. Furthermore, each sarcosine molecule is hydrogen-bonded to another sarcosine in a neighbouring chain related by an inversion centre. The ammonium and nitrate ions are arranged in a two-dimensional network in which each nitrate is anchored to four ammonium cations *via* bifurcated hydrogen bonds and, conversely, each ammonium is anchored to four nitrate anions *via* the same bifurcated hydrogen bonds.

Experimental

Colourless block-shaped crystals were obtained by recrystallization of the solution resulting from pouring an excess of nitric acid directly over sarcosine crystals (0.5 g) as purchased from Aldrich (98%), followed by neutralization with ammonia solution (25%).

Crystal data

$C_3H_7NO_2 \cdot NH_4^+ \cdot NO_3^-$
$M_r = 169.15$
Monoclinic, $P2_1/c$
$a = 5.7208$ (9) Å
$b = 7.9144$ (8) Å
$c = 17.447$ (2) Å
$\beta = 101.682$ (13)°
$V = 773.58$ (17) Å^3
$Z = 4$
$D_x = 1.452$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
$\theta = 6.6$–17.3°
$\mu = 0.14$ mm^{-1}
$T = 293$ (2) K
Block, colourless
0.43 × 0.40 × 0.39 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
ω–2θ scans
Absorption correction: none
2819 measured reflections
1423 independent reflections
901 reflections with $I > 2\sigma(I)$
$R_{\text{int}} = 0.037$
$\theta_{\max} = 25.5°$
$h = -6 \rightarrow 6$
$k = -9 \rightarrow 9$
$l = -21 \rightarrow 6$
3 standard reflections
frequency: 7200 min
intensity decay: 0.3%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.041$
$wR(F^2) = 0.130$
$S = 0.98$
1423 reflections
121 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0885P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.19$ e Å^{-3}
$\Delta\rho_{\min} = -0.26$ e Å^{-3}

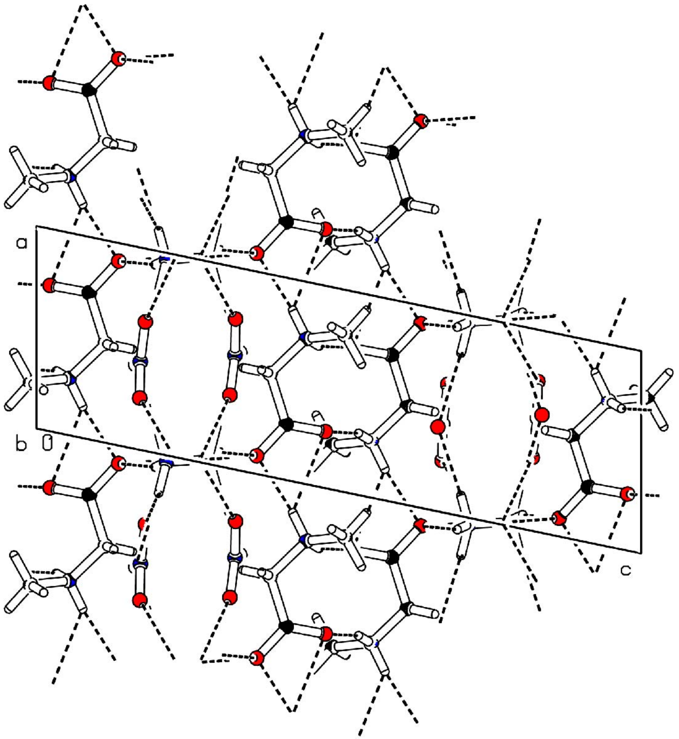


Figure 2
The packing, showing the layers of sarcosine chains alternating with the ammonium nitrate layers. Dashed lines represent the extensive hydrogen-bond network that stabilizes the structure

Table 1
Selected geometric parameters (Å, °).

O1—C1	1.261 (3)	O4—N2	1.243 (3)
O2—C1	1.234 (3)	O5—N2	1.231 (2)
O3—N2	1.241 (3)		
C3—N1—C2—C1	−75.5 (2)	O1—C1—C2—N1	176.4 (2)
O2—C1—C2—N1	−4.4 (3)		

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···O1$^{\text{i}}$	0.89	1.97	2.822 (2)	158
N1—H1A···O2$^{\text{i}}$	0.89	2.49	3.160 (2)	132
N1—H1B···O2$^{\text{ii}}$	0.89	1.95	2.826 (2)	167
N3—H4···O1$^{\text{iii}}$	0.94 (2)	1.92 (2)	2.839 (2)	164 (2)
N3—H5···O1$^{\text{i}}$	0.95 (2)	2.20 (2)	2.942 (2)	135 (2)
N3—H5···O5$^{\text{iii}}$	0.95 (2)	2.45 (3)	2.961 (3)	114 (2)
N3—H5···O3$^{\text{iv}}$	0.95 (2)	2.59 (3)	3.072 (3)	112 (2)
N3—H6···O4$^{\text{i}}$	0.92 (2)	2.05 (2)	2.946 (3)	164 (3)
N3—H6···O5$^{\text{i}}$	0.92 (2)	2.42 (3)	3.171 (3)	139 (3)
N3—H6···N2$^{\text{i}}$	0.92 (2)	2.55 (2)	3.443 (3)	164 (3)
N3—H7···O3	0.94 (2)	2.11 (2)	2.977 (3)	153 (3)
N3—H7···O4	0.94 (2)	2.31 (2)	3.151 (3)	149 (3)
N3—H7···N2	0.94 (2)	2.56 (2)	3.494 (3)	175 (3)

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

The ammonium H atoms were located in a difference Fourier map and refined isotropically subject to appropriate restraints to ensure an average tetrahedral geometry; all N—H distances were restrained to be equal within 0.02 Å, with a corresponding restraint on all H···H distances. All other H atoms were positioned geometrically and

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subsequently refined as riding, with the bond length also allowed to refine (N—H = 0.90 Å and C—H = 0.94–0.97 Å). $U_{iso}(H) = 1.2U_{eq}(N)$ for NH_2, $U_{iso}(H) = 1.2U_{eq}(C)$ for CH_2 and $1.5U_{eq}(C)$ for CH_3. Examination of the crystal structure with *PLATON* (Spek, 2003) showed that there are no solvent-accessible voids.

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *PLATON* (Spek, 2003); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

This work was supported by Fundação para a Ciência e a Tecnologia (FCT).

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