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m-Carboxyphenylammonium nitrate

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.002 Å
R factor = 0.040
wR factor = 0.057
Data-to-parameter ratio = 10.4

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

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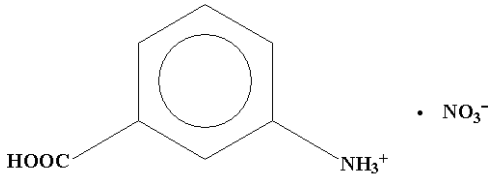
The crystal structure of the title compound, $C_7H_8NO_2^+\cdot NO_3^-$, consists of anionic and cationic layers linked by a complex three-dimensional hydrogen-bond network. Each cationic layer contains organic groups $(NH_3C_6H_4COOH)^+$, and each anionic layer contains inorganic $(NO_3)^-$. The structure is stabilized by two types of hydrogen-bonding interaction: anion–cation and cation–cation contacts.

Comment

Organic–inorganic hybrid materials have received increasing attention during the past few decades (Mazeaud *et al.*, 2000; Soghomonian *et al.*, 1995; Mayer *et al.*, 1999). They are of intense interest (Sigel *et al.*, 1998; Baker *et al.*, 1992) in the field of new materials chemistry as they can exhibit synergic properties, such as electrical, magnetic and optical properties (Kagan *et al.*, 1999; Hill, 1998).



(I)

Systematic investigation of organic–inorganic hybrid materials, including amino acids and various inorganic acids, led us to investigate crystals of *m*-carboxyphenylammonium nitrate, (I), which is described in this paper. The structure of (I) is composed of cationic $(NH_3C_6H_4COOH)^+$ and anionic $[(NO_3)^-]$ layers alternating along the *a* axis.

Each nitrate ion is an acceptor of three hydrogen bonds from three neighbouring ammonium groups. The keto O atom of the carboxylic acid group is also an acceptor of one H atom, donated by the neighbouring carboxylic acid group.

Two types of hydrogen bonding, N1—H···N2 and O1—H···O2, ensure the cohesion of the structure (Table 1). Nitrate anions link ammonium groups in a three-dimensional array, and cation–cation interactions between carboxylic acid groups link them in a one-dimensional quasi-linear array.

Experimental

Brown single crystals of the title salt were obtained by slow evaporation at room temperature of an equimolar solution of gc=^st_head3_bgcolour]>*m*-aminobenzoic and nitric acids.

Crystal data

$C_7H_8NO_2^+\cdot NO_3^-$
M_r = 200.15
Monoclinic, $C2/c$
a = 31.838 (2) Å
b = 5.208 (1) Å
c = 11.117 (3) Å
β = 108.06 (4)°
V = 1752.4 (7) Å^3
Z = 8
D_x = 1.517 Mg m^{-3}
Mo Kα radiation
Cell parameters from 25 reflections
θ = 10–14°
μ = 0.13 mm^{-1}
T = 298 K
Prism, brown
0.60 × 0.40 × 0.30 mm

Data collection

Enraf–Nonius MACH3 diffractometer
$\theta/2\theta$ scans
2923 measured reflections
2551 independent reflections
1654 reflections with $I > 3\sigma(I)$
R_{int} = 0.018
θ_{max} = 30.0°
$h = 0 \rightarrow 44$
$k = 0 \rightarrow 7$
$l = -15 \rightarrow 14$
2 standard reflections
every 60 reflections
intensity decay: 4.2%

Refinement

Refinement on F
R = 0.040
wR = 0.057
S = 1.13
1654 reflections
159 parameters
All H-atom parameters refined
$w = 4F_o^2/[\sigma^2(F_o^2) + 0.0016F_o^4]$
$(\Delta/\sigma)_{max}$ = 0.006
$\Delta\rho_{max}$ = 0.14 e Å^{-3}
$\Delta\rho_{min}$ = −0.07 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H···O2^{i}	0.90 (2)	1.78 (2)	2.676 (1)	177 (2)
N1—H1n···O4^{ii}	0.90 (2)	2.03 (2)	2.883 (2)	159 (2)
N1—H3n···O3	0.91 (2)	1.98 (2)	2.842 (2)	158 (2)
N1—H2n···O3^{iii}	0.92 (2)	1.97 (2)	2.849 (2)	161 (2)

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

Data collection: *CAD*-4 *Operations Manual* (Enraf–Nonius, 1989); cell refinement: *CAD*-4 *Operations Manual*; data reduction: *BEGIN SDP* (Frenz, 1985); program(s) used to solve structure: *MULTAN* (Main *et al.*, 1980); program(s) used to refine structure: *LSFM* in *SDP*; molecular graphics: *ORTEP*II (Johnson, 1976); software used to prepare material for publication: *CIF VAX* in *MolEN* (Fair, 1990).

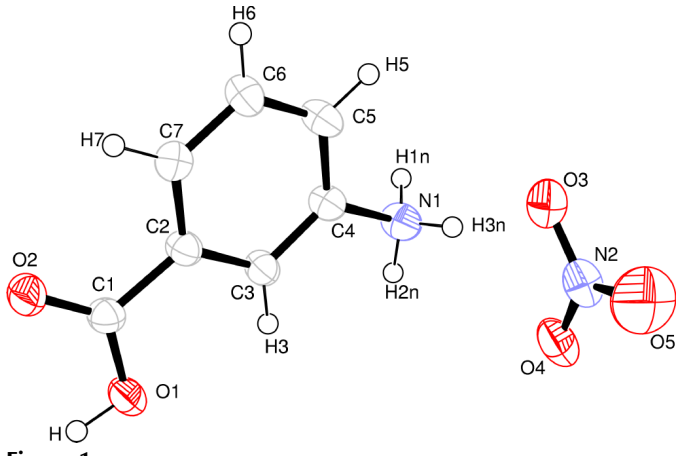


Figure 1
An *ORTEP*II (Johnson, 1976) view of the title compound with the atomic labelling scheme. Displacement ellipsoids are drawn at the 50% probability level.

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