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Ammonium 2,6-dicarboxy-4-nitrophenolate

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Key indicators

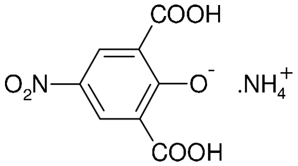
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.059
wR factor = 0.197
Data-to-parameter ratio = 11.3

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

The title compound, $NH_4^+\cdot C_8H_4NO_7^-$ consists of a 2,6-dicarboxy-4-nitrophenolate anion and an ammonium cation, both of which possess crystallographic twofold rotation symmetry. All the O atoms of the anion and the H atoms of the cation contribute to hydrogen bonds, forming a three-dimensional network.

Comment

Supramolecular chemistry, broadly the chemistry of multicomponent molecular assemblies in which the component structural units are typically held together by a variety of weaker non-covalent interactions, has developed rapidly over recent years (Lindoy & Atkinson, 2000). Non-covalent bonds, such as electrostatic interactions (Price & Stone, 1987), hydrogen bonding (Jeffrey, 2003), van der Waals interactions, halogen–halogen interactions (Bent, 1968), π–π stacking (Hunter & Sanders, 1990), anion–π interactions (Tarakeshwar & Dongwook, 2004), halogen–π stacking (Berg & Seddon, 2003), and CH_3–π facial hydrogen bonding (Desiraju, 1995), form the main toolbox in modern supramolecular chemistry. We can use this toolbox to describe the crystallization process as a self-assembly process. Each one of these forces has its importance in describing the complete theory of how building blocks take their final geometric positions to form a model of packing that is different from or similar to another with the same synthons.



(I)

As an extension of studies on weak non-covalent bonds in crystal systems, the crystal structure of the title compound, (I), is reported here.

The title compound, (I), consists of a dicarboxy-4-nitrophenolate anion and an ammonium cation, both of which possess C_2 symmetry (Fig. 1). All the bond lengths are within normal ranges (Allen *et al.*, 1987). In the anion, the dihedral angle between the two carboxy groups is 44.9 (2)°. The dihedral angle between the O1/C5/O2 plane of the carboxy group and the benzene ring is 25.8 (2)°.

In the crystal structure, molecules are linked together by intermolecular N—H···O and O—H···O hydrogen bonds, forming a three-dimensional network (Table 1 and Fig. 2).

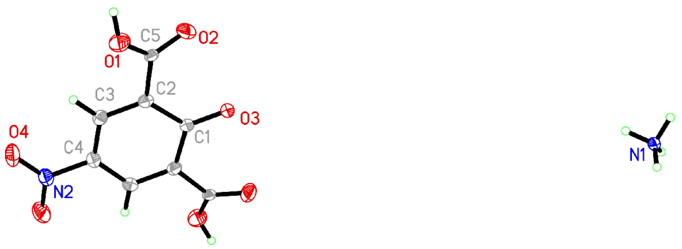


Figure 1
The structure of (I), showing the atom-numbering scheme and displacement ellipsoids drawn at the 30% probability level.

Experimental

2,4-Dicarboxy-4-nitrophenol (0.1 mmol, 22.6 mg) was dissolved in methanol (10 ml). To the methanol solution was added an ammonia solution (5 ml, 30%). The mixture was stirred at room temperature for 10 min to give a clear colourless solution. After allowing the solution to stand in air for 5 d, colourless block-shaped crystals were formed on slow evaporation of the solvent.

Crystal data

$NH_4^+ \cdot C_8H_4NO_7^-$
$M_r = 244.16$
Orthorhombic, *Ibca*
$a = 7.128$ (3) Å
$b = 13.460$ (3) Å
$c = 19.731$ (5) Å
$V = 1893.1$ (8) Å^3
$Z = 8$
$D_x = 1.713$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 872 reflections
$\theta = 2.3$–25.7°
$\mu = 0.15$ mm^{-1}
$T = 293$ (2) K
Block, colourless
0.35 × 0.28 × 0.25 mm

Data collection

Bruker SMART CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.948$, $T_{\max} = 0.963$
5300 measured reflections
1038 independent reflections
919 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.024$
$\theta_{\max} = 27.0°$
$h = -8 \rightarrow 9$
$k = -16 \rightarrow 17$
$l = -25 \rightarrow 20$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.059$
$wR(F^2) = 0.197$
$S = 1.12$
1038 reflections
92 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.117P)^2 + 2.7596P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.55$ e Å^{-3}
$\Delta\rho_{\min} = -0.52$ e Å^{-3}
Extinction correction: *SHELXL*
Extinction coefficient: 0.006 (2)

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
O1—H1$\cdots$O4$^{\rm i}$	0.846 (10)	2.48 (3)	3.172 (4)	139 (4)
N1—H1$B\cdots$O2$^{\rm ii}$	0.892 (10)	2.209 (15)	3.053 (3)	158 (3)
N1—H1$A\cdots$O2$^{\rm iii}$	0.892 (10)	2.46 (4)	2.948 (3)	115 (3)
N1—H1$A\cdots$O3$^{\rm iii}$	0.892 (10)	1.966 (16)	2.832 (2)	163 (4)

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

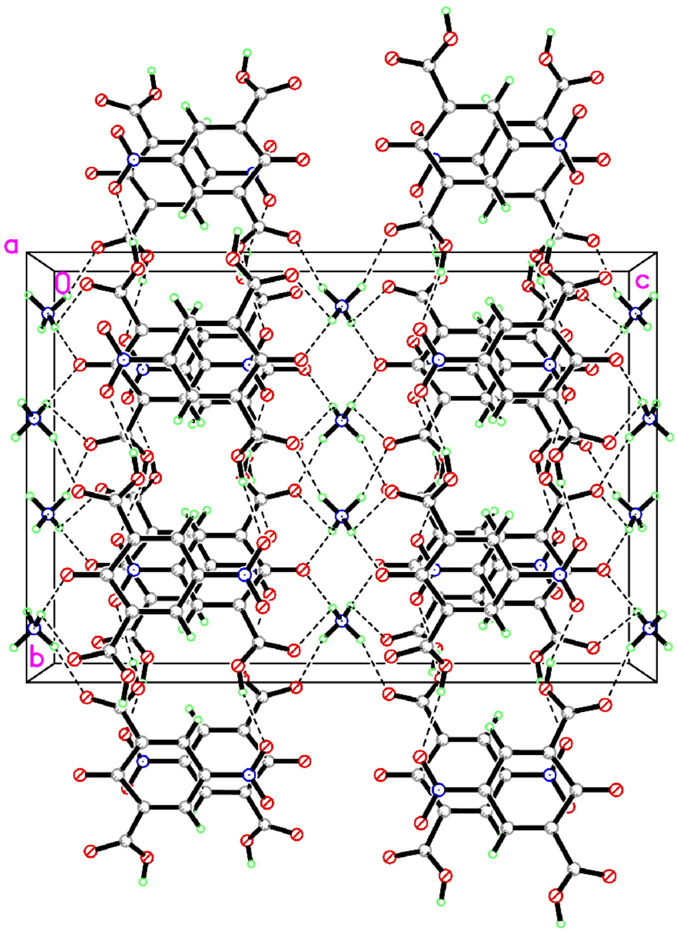


Figure 2
The crystal packing of (I), viewed along the *a* axis. Dashed lines indicate intermolecular hydrogen bonds.

Atoms H1*A* and H1*B* were located in a Fourier difference map and refined isotropically, with the N—H and H$\cdots$H distances restrained to 0.90 (1) and 1.43 (2) Å, respectively. Atom H1 was also located in a difference Fourier map and refined isotropically, and the $U_{\rm iso}$(H) value fixed at 0.08 Å^2. Atom H3 was placed in an idealized position and allowed to ride on its parent atom, with C—H = 0.96 Å, and $U_{\rm iso}$(H) fixed at 0.08 Å^2.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

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