Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

(*m*-Carboxyphenyl)ammonium perchlorate at 223 K

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Key indicators

Single-crystal X-ray study
T = 223 K
Mean σ(C–C) = 0.003 Å
R factor = 0.036
wR factor = 0.140
Data-to-parameter ratio = 11.8

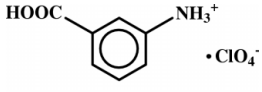
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 27 February 2003
Accepted 20 March 2003
Online 31 March 2003

The title compound, $C_7H_8N^+\cdot ClO_4^-$, is built up from (*m*-carboxyphenyl)ammonium cations and perchlorate anions. Crystal cohesion is ensured by strong cation–anion and cation–cation hydrogen bonds, between the carboxylic acid groups of the organic cations and the O atoms of the anions, and also between amine groups and carboxylic acid groups.

Comment

During the past few decades, organic–inorganic hybrid materials have been receiving increasing attention (Mazeaud *et al.*, 2000; Soghomonian *et al.*, 1995; Mayer *et al.*, 1999) owing to their electrical, magnetic and optical properties (Kagan *et al.*, 1999; Hill, 1998). This study is a part of systematic investigation of organic–inorganic hybrid materials, including amino acids with nitric [(*m*-carboxyphenyl)ammonium nitrate (Benali-Cherif, Cherouana *et al.*, (2002) and L-histidinium dinitrate (Benali-Cherif, Benguedouar *et al.*, 2002)], phosphoric [(*m*-carboxyphenyl)ammonium phosphate (Benali-Cherif, Bendheif *et al.*, 2002) and (*p*-carboxyphenyl)-ammonium dihydrogenmonophosphate monohydrate (Benali-Cherif, Abouimrane *et al.*, 2002)], and hydrochloric (3-aminobenzoic acid hydrochloride;Arora *et al.*, 1973) acids. The (*m*-carboxyphenyl)ammonium perchlorate structure, (I), is composed of cationic ($HCOO–C_6H_4–NH_3^+$) and anionic (ClO_4^-) layers alternating along the *c* axis. All bond lengths and angles of the organic cation are within normal ranges and are in good agreement with those observed in (*m*-carboxyphenyl)ammonium nitrate, (*m*-carboxyphenyl)ammonium phosphate and 3-aminobenzoic acid hydrochloride. In the title compound, the perchlorate anion is not disordered at 223 K, and it is stabilized by strong interactions with its environment. The average Cl—O bond distances and O—Cl—O bond angles are 1.4384 (15) Å and 109.47 (10)°, respectively, confirming a tetrahedral configuration (Table 1), similar to other perchlorates studied at low temperature. Perchlorate anions (ClO_4^-), surrounded by four (*m*-carboxyphenyl)-ammonium residues *via* hydrogen bonds (Table 2), play an important role in stabilizing the crystal structure.



(I)

Two types of hydrogen bonds are observed in this structure, *viz*. cation–cation and anion–cation interactions.

For the cation–cation interactions, each (*m*-carboxyphenyl)ammonium cation is connected to its neighbour,

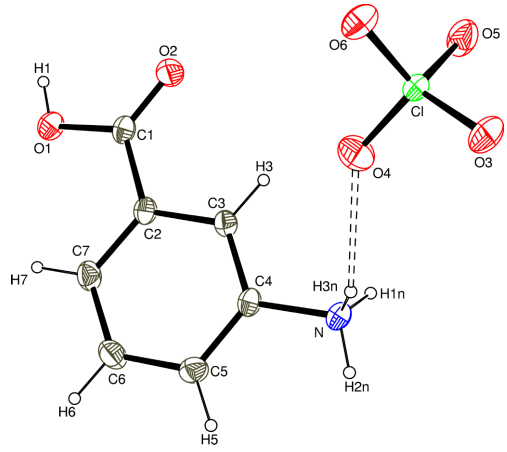


Figure 1
ORTEP-3 (Farrugia, 1997) view of the structure of (I), with the atom-numbering scheme and 50% probability displacement ellipsoids. The open dashed bond indicates one of the hydrogen bonds.

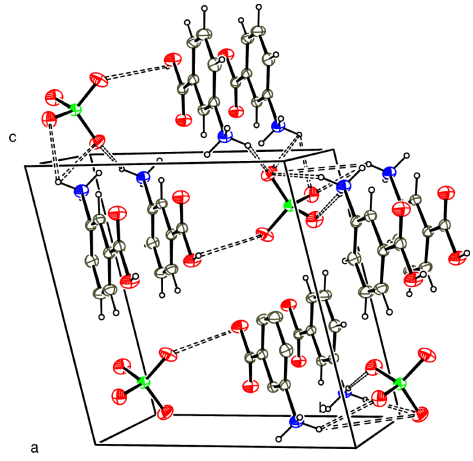


Figure 2
View of the ionic stacking, showing the three-dimensional network of hydrogen bonds, as open dashed bonds.

parallel to the *bc* diagonal, by a strong hydrogen bond [N—H1N···O2^{i} = 2.822 (2) Å)].

For the anion–cation interactions, two H atoms of the ammonium group are linked through hydrogen bonds to O3, O4 and O6 atoms of perchlorate, while the third is linked to atom O2 of the carboxylic acid group. The carboxylic acid group is not deprotonated and its H atom is involved in the strongest interaction with the perchlorate anion *via* O1—H1···O5^{iv} = 2.748 (2) Å.

Experimental

The title compound was crystallized from a 1:1 aqueous solution of 3-aminobenzoic acid and perchlorate acid. Brown crystals grew after a few days.

Crystal data

$C_7H_8N^+\cdot ClO_4^-$
M_r = 237.59
Triclinic, $P\overline{1}$
a = 5.0886 (2) Å
b = 9.3338 (7) Å
c = 10.1159 (7) Å
α = 103.904 (3)°
β = 95.153 (5)°
γ = 98.779 (5)°
V = 456.90 (5) Å^3
Z = 2
D_x = 1.727 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1629 reflections
θ = 2.1–26.4°
μ = 0.43 mm^{-1}
T = 223 (2) K
Prism, brown
0.4 × 0.3 × 0.3 mm

Data collection

Nonius KappaCCD diffractometer
φ scans
Absorption correction: none
3143 measured reflections
1629 independent reflections
1532 reflections with $I > 2\sigma(I)$
R_{int} = 0.034
θ_{max} = 26.4°
$h = -5 \rightarrow 5$
$k = -11 \rightarrow 10$
$l = -12 \rightarrow 12$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.140
S = 1.27
1629 reflections
138 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0849P)^2 + 0.1634P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.46 e Å^{-3}
$\Delta\rho_{min}$ = −0.62 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

C1—O2	1.220 (2)	O4—Cl	1.4364 (15)
C1—O1	1.326 (2)	O5—Cl	1.4442 (15)
O3—Cl	1.4330 (15)	O6—Cl	1.4399 (16)
O2—C1—O1	123.4 (2)	O4—Cl—O6	108.97 (10)
O2—C1—C2	123.00 (18)	O3—Cl—O5	109.10 (10)
O1—C1—C2	113.63 (17)	O4—Cl—O5	109.21 (10)
O3—Cl—O4	110.46 (11)	O6—Cl—O5	109.15 (9)
O3—Cl—O6	109.93 (10)		

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

D—H···A	D—H	H···A	D···A	D—H···A
N—H1N···O2^{i}	0.89	2.00	2.822 (2)	153
N—H2N···O3^{ii}	0.89	2.09	2.931 (3)	158
N—H3N···O4	0.89	2.20	2.912 (3)	137
N—H3N···O6^{iii}	0.89	2.36	2.943 (2)	124
O1—H1···O5^{iv}	0.82	1.94	2.748 (2)	170

Symmetry codes: (i) $1-x, 1-y, -z$; (ii) $2-x, 2-y, -z$; (iii) $1-x, 2-y, -z$; (iv) $-x, 1-y, -z$.

Data collection: *KappaCCD Reference Manual* (Nonius, 1998); cell refinement: *DENZO* and *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO* and *SCALEPACK*; program(s) used to solve structure: *SIR*2002 (Burla *et al.*, 2003); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*-3 (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *PARST* (Nardelli, 1995).

This work was supported by Mentouri-Constantine University, Algeria. We thank Dr M. Pierrot and Dr M. Giorgi from LBS–UMR 6517, Faculté des Sciences et Techniques de Saint Jérôme, Marseille, France, for data collection.

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