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Ammonium 4-(4-carboxyphenoxy)-benzoate

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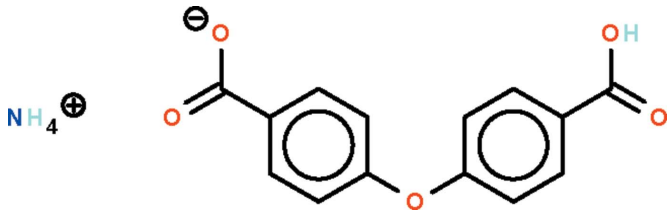
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.002 Å; R factor = 0.049; wR factor = 0.146; data-to-parameter ratio = 14.1.

The anions of the title salt, $NH_4^+\cdot HO_2CC_6H_4$–O–$C_6H_4CO_2^-$, are linked by intermolecular –$CO_2H\cdots O_2C$– hydrogen bonds, forming a polyanionic chain in the crystal; adjacent chains are connected through the ammonium cation into a layer structure, with the ammonium cation serving as hydrogen-bond donor to four carboxylate O atoms. The cation and anion both lie on special positions of 2 site symmetry. In the anion, the rings make a dihedral angle of 65.3 (1)°. The acid H atom is disordered about the special position.

Related literature

For the crystal structures of two modifications of oxy-4,4′-bis(benzoic acid), see: Dey & Desiraju (2005); Potts *et al.* (2007).



Experimental

Crystal data

$NH_4^+\cdot C_{14}H_9O_5^-$
M_r = 275.25
Orthorhombic, *Pnna*
a = 6.1916 (1) Å
b = 28.5483 (6) Å
c = 7.1123 (1) Å
V = 1257.17 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.11 mm^{-1}
T = 293 K
0.50 × 0.40 × 0.30 mm

Data collection

Bruker SMART APEX diffractometer
3444 measured reflections
1434 independent reflections
1279 reflections with $I > 2\sigma(I)$
R_{int} = 0.014

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.146
S = 1.04
1434 reflections
102 parameters
6 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.30 e Å^{-3}
$\Delta\rho_{min}$ = −0.42 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···O1^{i}	0.84 (1)	1.70 (3)	2.490 (2)	156 (6)
N1—H11···O1^{i}	0.88 (1)	2.14 (1)	2.962 (2)	155 (1)
N1—H12···O2	0.88 (1)	2.10 (2)	2.827 (1)	139 (2)

Symmetry code: (i) $-x+\frac{3}{2}, -y+1, z$.

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2010).

We thank Dr Yun-Xia Yang of Northeast Normal University for the diffraction measurements, and the University of Malaya for supporting this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HG2754).

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Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.

supporting information

Acta Cryst. (2010). E**66**, o3345 [https://doi.org/10.1107/S1600536810048841]

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S1. Comment

We have been studying the co-crystals of carboxylic acids and amines. In the present study, the reaction of 4,4′-oxybis(benzoic acid) and tri-*n*-propylamine is expected to yield either the neutral co-crystal or the ammonium carboxylate. However, the amine has probably decomposed after being left in solution for several weeks. The product is ammonium hydrogen 4,4′-oxybis(benzoate) (Scheme I, Fig. 1). The non-hydrogen atoms of the benzoate portion of the anion nearly flat (r.m.s. deviation 0.10 Å); the two planes are aligned 65.3 (1) °. The anions are linked by an intermolecular –CO_2H···O_2C– hydrogen bond to form a polyanionic chain; adjacent chains are connected through the ammonium cation into a layer structure. The ammonium cation is hydrogen-bond donor to four carboxylate O atoms (Fig. 2). The cation and anion both lie on special positions of *2* site symmetry. The parent carboxylic acid itself crystallizes in two modifications (Dey & Desiraju, 2005; Potts *et al.*, 2007).

S2. Experimental

4,4′-Oxybis(benzoic acid) (0.25 mmol, 0.065 g) was dissolved in a water-ethanol (50 ml/100 ml *v*/*v*) mixture. Tri-*n*-propylamine (33% aqueous solution) was added until the solution registered a neutral pH. The mixture was then set aside for a several weeks; colorless crystals were isolated.

S3. Refinement

Carbon-bound H-atoms were placed in calculated positions (C–H 0.93 Å) and were included in the refinement in the riding model approximation, with U_{iso}(H) set to 1.2U_{eq}(C).

The acid and ammonium H-atoms were located in a difference Fourier map, and were refined with distance restraints of O–H 0.84±0.01 and N–H 0.88±0.01 Å. The temperature factor of the acid H atom was refined whereas that of the ammonium H atoms were tied by a factor of 1.2 times. For the ammonium H-atoms, because the N atom lies on a special position, the H···H distance was restrained to 1.43±0.01 Å.

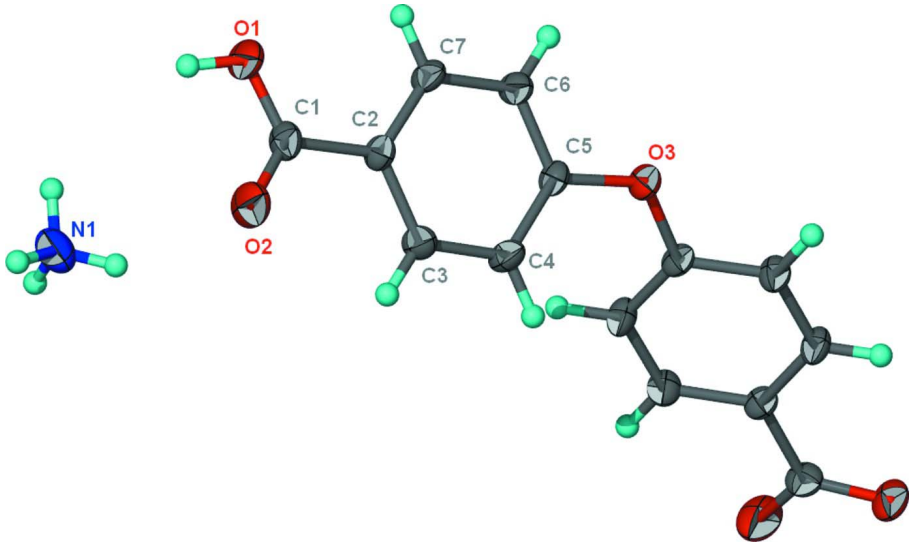

Figure 1

Thermal ellipsoid plot (Barbour, 2001) of $[NH_4]^+$ $[HO_2CC_6H_4–O–C_6H_4CO_2]^-$ at the 50% probability level. Hydrogen atoms are drawn as spheres of arbitrary radius.

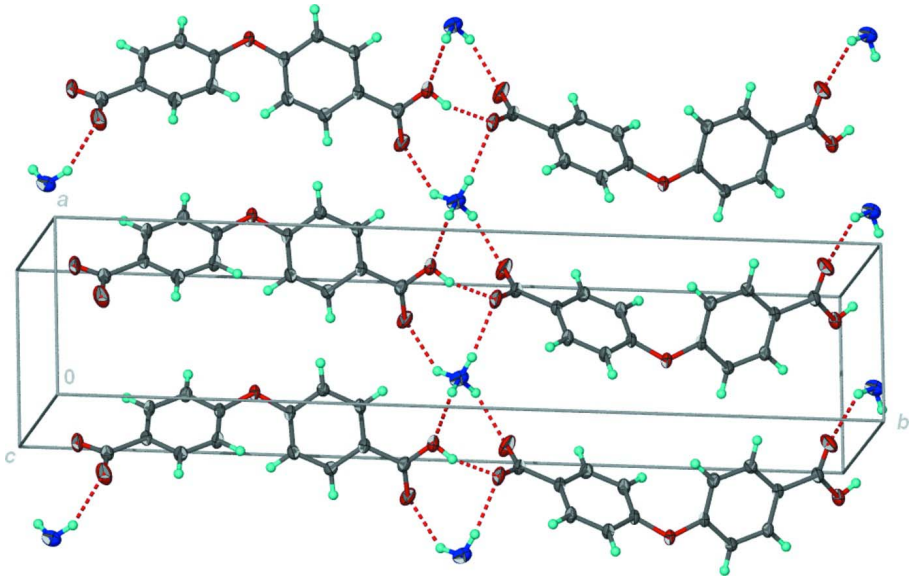

Figure 2

Layer structure projected onto the unit cell.

Ammonium 4-(4-carboxyphenoxy)benzoate

Crystal data

$NH_4^+ \cdot C_{14}H_9O_5^-$
$M_r = 275.25$
Orthorhombic, *Pnna*
Hall symbol: -P 2a 2bc
$a = 6.1916$ (1) Å
$b = 28.5483$ (6) Å
$c = 7.1123$ (1) Å
$V = 1257.17$ (4) Å^3
$Z = 4$
$F(000) = 576$
$D_x = 1.454$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2311 reflections
$\theta = 2.9$–27.6°

μ = 0.11 mm^{-1}
T = 293 K

Block, colorless
0.50 × 0.40 × 0.30 mm

Data collection

Bruker SMART APEX diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
3444 measured reflections
1434 independent reflections

1279 reflections with $I > 2\sigma(I)$
R_{int} = 0.014
θ_{max} = 27.5°, θ_{min} = 2.9°
h = −6→8
k = −36→29
l = −9→5

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.146
S = 1.04
1434 reflections
102 parameters
6 restraints
Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0922P)^2 + 0.4317P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.30 e Å^{-3}
$\Delta\rho_{min}$ = −0.42 e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	y	z	U_{iso}*/U_{eq}	Occ. (<1)
O1	0.83559 (19)	0.46053 (3)	0.15346 (17)	0.0429 (4)	
H1	0.748 (8)	0.4828 (15)	0.140 (6)	0.10 (2)*	0.50
O2	0.5981 (2)	0.43933 (4)	0.37136 (18)	0.0536 (4)	
O3	1.1215 (2)	0.2500	0.2500	0.0325 (4)	
C1	0.7477 (2)	0.43024 (5)	0.26451 (19)	0.0320 (3)	
C2	0.8424 (2)	0.38203 (4)	0.25651 (17)	0.0266 (3)	
C3	0.7341 (2)	0.34508 (5)	0.34202 (18)	0.0302 (3)	
H3	0.6034	0.3506	0.4026	0.036*	
C4	0.8184 (2)	0.30004 (5)	0.33813 (18)	0.0304 (3)	
H4	0.7450	0.2754	0.3950	0.036*	
C5	1.0136 (2)	0.29244 (4)	0.24811 (16)	0.0254 (3)	
C6	1.1244 (2)	0.32879 (5)	0.16242 (18)	0.0292 (3)	
H6	1.2555	0.3232	0.1027	0.035*	
C7	1.0374 (2)	0.37357 (4)	0.16673 (18)	0.0298 (3)	
H7	1.1105	0.3981	0.1089	0.036*	
N1	0.2500	0.5000	0.2884 (4)	0.0503 (5)	
H11	0.3506 (16)	0.5123 (6)	0.2161 (16)	0.060*	
H12	0.308 (3)	0.4771 (5)	0.355 (2)	0.060*	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0450 (7)	0.0203 (5)	0.0633 (8)	0.0051 (4)	0.0098 (5)	0.0037 (4)

O2	0.0553 (8)	0.0374 (6)	0.0681 (8)	0.0191 (5)	0.0230 (6)	0.0050 (5)
O3	0.0327 (7)	0.0164 (6)	0.0485 (8)	0.000	0.000	−0.0001 (5)
C1	0.0339 (7)	0.0233 (6)	0.0387 (7)	0.0044 (5)	−0.0013 (5)	−0.0041 (5)
C2	0.0321 (7)	0.0194 (6)	0.0284 (6)	0.0019 (5)	−0.0005 (5)	−0.0016 (4)
C3	0.0309 (7)	0.0269 (7)	0.0329 (7)	0.0015 (5)	0.0058 (5)	−0.0014 (5)
C4	0.0366 (7)	0.0223 (6)	0.0323 (7)	−0.0030 (5)	0.0062 (5)	0.0024 (5)
C5	0.0328 (7)	0.0167 (6)	0.0266 (6)	0.0011 (4)	−0.0016 (5)	−0.0020 (4)
C6	0.0308 (7)	0.0219 (6)	0.0350 (7)	0.0006 (5)	0.0070 (5)	−0.0013 (5)
C7	0.0360 (8)	0.0183 (6)	0.0352 (7)	−0.0012 (5)	0.0062 (5)	0.0019 (4)
N1	0.0342 (10)	0.0516 (12)	0.0651 (13)	0.0082 (9)	0.000	0.000

Geometric parameters (Å, º)

O1—C1	1.2914 (18)	C3—H3	0.9300
O1—H1	0.841 (10)	C4—C5	1.385 (2)
O2—C1	1.2260 (18)	C4—H4	0.9300
O3—C5^{i}	1.3833 (13)	C5—C6	1.3852 (18)
O3—C5	1.3833 (13)	C6—C7	1.3876 (17)
C1—C2	1.4973 (17)	C6—H6	0.9300
C2—C7	1.3867 (19)	C7—H7	0.9300
C2—C3	1.3902 (18)	N1—H11	0.881 (7)
C3—C4	1.3880 (18)	N1—H12	0.882 (8)
C1—O1—H1	108 (4)	C5—C4—H4	120.6
C5^{i}—O3—C5	122.29 (15)	C3—C4—H4	120.6
O2—C1—O1	123.76 (13)	O3—C5—C4	123.65 (11)
O2—C1—C2	120.94 (13)	O3—C5—C6	114.94 (12)
O1—C1—C2	115.30 (12)	C4—C5—C6	121.19 (11)
C7—C2—C3	119.32 (11)	C5—C6—C7	119.25 (12)
C7—C2—C1	121.23 (12)	C5—C6—H6	120.4
C3—C2—C1	119.45 (12)	C7—C6—H6	120.4
C4—C3—C2	120.83 (12)	C2—C7—C6	120.55 (12)
C4—C3—H3	119.6	C2—C7—H7	119.7
C2—C3—H3	119.6	C6—C7—H7	119.7
C5—C4—C3	118.86 (12)	H11—N1—H12	108.6 (10)
O2—C1—C2—C7	−166.60 (14)	C5^{i}—O3—C5—C6	−151.57 (12)
O1—C1—C2—C7	12.97 (19)	C3—C4—C5—O3	174.06 (11)
O2—C1—C2—C3	12.8 (2)	C3—C4—C5—C6	−0.17 (19)
O1—C1—C2—C3	−167.60 (13)	O3—C5—C6—C7	−174.86 (10)
C7—C2—C3—C4	−0.1 (2)	C4—C5—C6—C7	−0.15 (19)
C1—C2—C3—C4	−179.57 (12)	C3—C2—C7—C6	−0.20 (19)
C2—C3—C4—C5	0.3 (2)	C1—C2—C7—C6	179.23 (12)
C5^{i}—O3—C5—C4	33.86 (10)	C5—C6—C7—C2	0.3 (2)

Symmetry code: (i) *x*, −*y*+1/2, −*z*+1/2.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···O1^{ii}	0.84 (1)	1.70 (3)	2.490 (2)	156 (6)
N1—H11···O1^{ii}	0.88 (1)	2.14 (1)	2.962 (2)	155 (1)
N1—H12···O2	0.88 (1)	2.10 (2)	2.827 (1)	139 (2)

Symmetry code: (ii) −*x*+3/2, −*y*+1, *z*.