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4-(3-Carboxyphenyl)pyridinium nitrate

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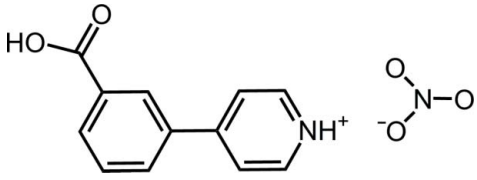
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.050; wR factor = 0.127; data-to-parameter ratio = 13.0.

In the title salt, $C_{12}H_{10}NO_2^+\cdot NO_3^-$, the dihedral angle between the pyridine ring and the benzene ring of the 4-(3-carboxyphenyl)pyridinium cation is 30.14 (2)°. Inversion-related pairs of cations are linked into dimers by pairs of O—H···O hydrogen bonds. Pairs of dimers are linked by N—H···O and C—H···O hydrogen bonds involving nitrate anions as acceptors, generating supramolecular chains along the diagonal of the *bc* plane.

Related literature

For structures of similar compounds, see: Jin *et al.* (2003); Bei *et al.* (2004); Rademeyer (2005); Wang (2006); Yu *et al.* (2006).



Experimental

Crystal data

$C_{12}H_{10}NO_2^+\cdot NO_3^-$
M_r = 262.22
Triclinic, $P\overline{1}$
a = 5.2545 (11) Å
b = 7.0617 (14) Å
c = 16.469 (3) Å
α = 97.39 (3)°
β = 92.96 (5)°
γ = 106.05 (3)°
V = 580.0 (2) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.12 mm^{-1}
T = 293 K
0.15 × 0.13 × 0.10 mm

Data collection

Bruker SMART diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.982, T_{max} = 0.988
4634 measured reflections
2255 independent reflections
1599 reflections with $I > 2\sigma(I)$
R_{int} = 0.042

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.127
S = 1.00
2255 reflections
174 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C10—H10···O4^{i}	0.93	2.42	3.225 (3)	145
C11—H11···O5^{ii}	0.93	2.49	3.122 (3)	125
O1—H1···O2^{iii}	0.82	1.82	2.624 (2)	167
N2—H2···O4^{ii}	0.86	1.89	2.748 (3)	174

Symmetry codes: (i) $x+1, y+1, z$; (ii) $-x+1, -y+1, -z$; (iii) $-x, -y+3, -z+1$.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PK2401).

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supplementary materials

Acta Cryst. (2012). E**68**, o1322 [doi:10.1107/S1600536812013918]

4-(3-Carboxyphenyl)pyridinium nitrate

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Comment

The title compound consists of a 3-(pyridin-4-yl)benzoic acid cation and a nitrate anion (Fig. 1). The nitric acid is deprotonated and the pyridine ring accepts the proton to produce the protonated organic cation, namely 3-(pyridin-4-yl)benzoic acid nitrate. The dihedral angle between pyridine ring and the benzene ring of the 3-(pyridin-4-yl)benzoic acid is 30.14 (2)°. The two components are linked by O—H···O [O1—H1···O2, 2.624 (2) Å] hydrogen bonds to form the cation dimers (Fig. 2), and further though N—H···O and C—H···O [N2—H2···O4, 2.748 (3) Å; C10—H10···O4, 3.225 (3) Å; C11—H11···O5, 3.122 (3)Å] hydrogen bonds. The cation dimers are thus connected by the nitrate anions into extended one-dimensional supramolecular chains (Fig. 2).

Experimental

The title compound was prepared by a hydrothermal method. An aqueous solution (20 mL) containing 3-(pyridin-4-yl)benzoic acid (0.10 mmol) and samarium nitrate hexahydrate (0.10 mmol) was placed in a Parr Teflon-lined stainless steel vessel (25 mL) under autogenous pressure, and then heated to 433 K for 72 h and subsequently cooled to room temperature at a rate of 5 K an hour. The targeted Sm^{3+} complex was not synthesized. Unintentionally, colorless single crystals of the title compound suitable for X-ray analysis were obtained from the reaction mixture.

Refinement

All H atoms were positioned geometrically (C-H = 0.93Å, O-H = 0.82 Å and N-H = 0.86 Å) and allowed to ride on their parent atoms, with U_{iso}(H) values equal to 1.2U_{eq}(C, N) or 1.5U_{eq}(O).

Computing details

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT* (Bruker, 1997); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

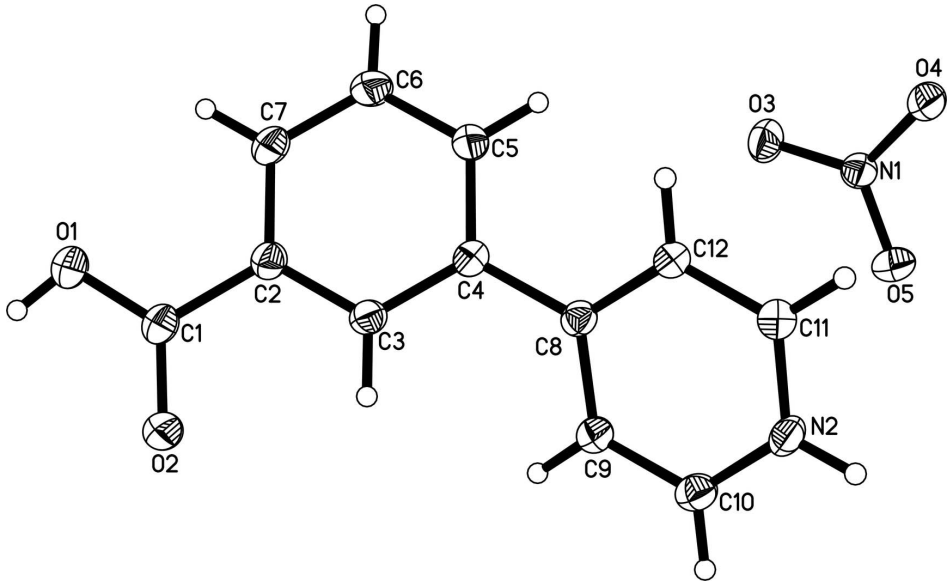

Figure 1

Thermal ellipsoid plot of the title compound (30% probability level), hydrogen atoms are drawn as spheres of arbitrary radius.

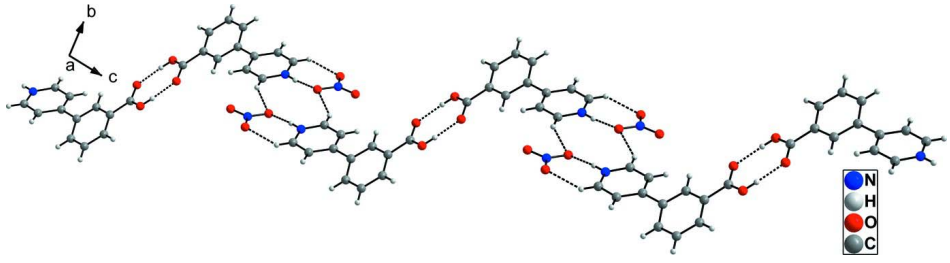

Figure 2

The one-dimensional hydrogen-bonded supramolecular chains in the crystal structure. Dashed lines denote hydrogen bonds.

4-(3-Carboxyphenyl)pyridinium nitrate

Crystal data

$C_{12}H_{10}NO_2^+ \cdot NO_3^-$
$M_r = 262.22$
Triclinic, $P\overline{1}$
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$a = 5.2545\ (11)$ Å
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$c = 16.469\ (3)$ Å
$\alpha = 97.39\ (3)°$
$\beta = 92.96\ (5)°$
$\gamma = 106.05\ (3)°$
$V = 580.0\ (2)$ Å^3
$Z = 2$
$F(000) = 272$
$D_x = 1.502$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2373 reflections
$\theta = 3.0–27.5°$
$\mu = 0.12$ mm^{-1}
$T = 293$ K
Block, colourless
0.15 × 0.13 × 0.10 mm

Data collection

Bruker SMART diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.982, T_{max} = 0.988
4634 measured reflections
2255 independent reflections
1599 reflections with $I > 2\sigma(I)$
R_{int} = 0.042
θ_{max} = 26.0°, θ_{min} = 3.0°
h = −4→6
k = −8→8
l = −20→17

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.127
S = 1.00
2255 reflections
174 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.063P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.039 (7)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
N2	0.5337 (3)	0.8423 (2)	0.07114 (11)	0.0357 (4)
H2	0.6254	0.8387	0.0295	0.043*
O2	0.1639 (3)	1.3909 (2)	0.43108 (10)	0.0541 (5)
O1	−0.2183 (3)	1.2586 (2)	0.48279 (11)	0.0555 (5)
H1	−0.1765	1.3685	0.5113	0.083*
C4	0.0785 (4)	0.8582 (3)	0.27490 (12)	0.0316 (5)
C8	0.2414 (4)	0.8503 (3)	0.20449 (13)	0.0306 (5)
C12	0.1417 (4)	0.7172 (3)	0.13261 (13)	0.0352 (5)
H12	−0.0275	0.6284	0.1292	0.042*
C10	0.6380 (4)	0.9746 (3)	0.13859 (13)	0.0370 (5)
H10	0.8073	1.0623	0.1400	0.044*
C9	0.4953 (4)	0.9804 (3)	0.20526 (13)	0.0341 (5)
H9	0.5685	1.0726	0.2519	0.041*
C3	0.1074 (4)	1.0373 (3)	0.32576 (12)	0.0332 (5)
H3	0.2408	1.1501	0.3185	0.040*

C1	−0.0351 (4)	1.2460 (3)	0.43713 (14)	0.0394 (5)
C5	−0.1169 (4)	0.6893 (3)	0.28921 (14)	0.0384 (5)
H5	−0.1356	0.5674	0.2568	0.046*
C11	0.2897 (4)	0.7157 (3)	0.06729 (14)	0.0384 (5)
H11	0.2208	0.6260	0.0196	0.046*
C7	−0.2581 (4)	0.8815 (3)	0.39976 (14)	0.0410 (5)
H7	−0.3726	0.8898	0.4404	0.049*
C2	−0.0603 (4)	1.0497 (3)	0.38714 (13)	0.0349 (5)
C6	−0.2820 (5)	0.7011 (3)	0.35072 (14)	0.0454 (6)
H6	−0.4108	0.5872	0.3595	0.054*
O3	0.2280 (3)	0.3289 (2)	0.18749 (10)	0.0466 (4)
O5	0.5525 (3)	0.3893 (2)	0.10947 (10)	0.0513 (5)
N1	0.3185 (4)	0.3064 (2)	0.12032 (11)	0.0355 (4)
O4	0.1696 (3)	0.1940 (2)	0.05948 (10)	0.0479 (5)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N2	0.0348 (10)	0.0396 (9)	0.0369 (11)	0.0138 (7)	0.0154 (8)	0.0091 (8)
O2	0.0551 (11)	0.0408 (9)	0.0583 (11)	0.0013 (7)	0.0264 (9)	−0.0027 (7)
O1	0.0538 (11)	0.0479 (10)	0.0593 (12)	0.0076 (8)	0.0287 (9)	−0.0062 (8)
C4	0.0293 (11)	0.0351 (11)	0.0310 (12)	0.0097 (8)	0.0049 (9)	0.0057 (8)
C8	0.0289 (11)	0.0306 (10)	0.0345 (12)	0.0104 (8)	0.0059 (9)	0.0075 (8)
C12	0.0317 (11)	0.0327 (10)	0.0390 (13)	0.0057 (8)	0.0102 (10)	0.0017 (9)
C10	0.0311 (12)	0.0372 (11)	0.0440 (14)	0.0093 (9)	0.0066 (10)	0.0102 (10)
C9	0.0304 (11)	0.0353 (10)	0.0354 (12)	0.0077 (8)	0.0055 (9)	0.0038 (9)
C3	0.0312 (11)	0.0341 (10)	0.0318 (12)	0.0051 (8)	0.0053 (9)	0.0047 (9)
C1	0.0409 (13)	0.0431 (12)	0.0346 (12)	0.0113 (10)	0.0125 (10)	0.0052 (9)
C5	0.0415 (13)	0.0315 (11)	0.0394 (13)	0.0054 (9)	0.0124 (10)	0.0032 (9)
C11	0.0383 (13)	0.0349 (11)	0.0398 (13)	0.0077 (9)	0.0090 (10)	0.0015 (9)
C7	0.0411 (13)	0.0458 (12)	0.0350 (13)	0.0081 (10)	0.0160 (10)	0.0068 (10)
C2	0.0353 (12)	0.0375 (11)	0.0316 (12)	0.0097 (9)	0.0064 (10)	0.0041 (9)
C6	0.0453 (14)	0.0393 (12)	0.0457 (14)	−0.0001 (10)	0.0159 (11)	0.0071 (10)
O3	0.0551 (11)	0.0481 (9)	0.0378 (10)	0.0147 (7)	0.0171 (8)	0.0054 (7)
O5	0.0345 (10)	0.0517 (9)	0.0570 (11)	−0.0034 (7)	0.0119 (8)	0.0011 (8)
N1	0.0376 (11)	0.0296 (9)	0.0397 (11)	0.0085 (7)	0.0093 (9)	0.0061 (8)
O4	0.0348 (9)	0.0587 (10)	0.0393 (9)	0.0008 (7)	0.0076 (7)	−0.0064 (7)

Geometric parameters (Å, º)

N2—C11	1.338 (3)	C9—H9	0.9300
N2—C10	1.339 (3)	C3—C2	1.385 (3)
N2—H2	0.8600	C3—H3	0.9300
O2—C1	1.263 (3)	C1—C2	1.487 (3)
O1—C1	1.267 (3)	C5—C6	1.377 (3)
O1—H1	0.8200	C5—H5	0.9300
C4—C3	1.391 (3)	C11—H11	0.9300
C4—C5	1.398 (3)	C7—C6	1.388 (3)
C4—C8	1.481 (3)	C7—C2	1.393 (3)
C8—C12	1.392 (3)	C7—H7	0.9300

C8—C9	1.393 (3)	C6—H6	0.9300
C12—C11	1.360 (3)	O3—N1	1.235 (2)
C12—H12	0.9300	O5—N1	1.240 (2)
C10—C9	1.364 (3)	N1—O4	1.272 (2)
C10—H10	0.9300		

C11—N2—C10	121.3 (2)	O2—C1—O1	123.68 (19)
C11—N2—H2	119.4	O2—C1—C2	118.7 (2)
C10—N2—H2	119.4	O1—C1—C2	117.61 (19)
C1—O1—H1	109.5	C6—C5—C4	120.80 (19)
C3—C4—C5	118.4 (2)	C6—C5—H5	119.6
C3—C4—C8	120.40 (18)	C4—C5—H5	119.6
C5—C4—C8	121.07 (17)	N2—C11—C12	120.49 (19)
C12—C8—C9	116.8 (2)	N2—C11—H11	119.8
C12—C8—C4	121.07 (18)	C12—C11—H11	119.8
C9—C8—C4	122.08 (18)	C6—C7—C2	119.0 (2)
C11—C12—C8	120.60 (19)	C6—C7—H7	120.5
C11—C12—H12	119.7	C2—C7—H7	120.5
C8—C12—H12	119.7	C3—C2—C7	120.33 (18)
N2—C10—C9	119.82 (19)	C3—C2—C1	119.46 (18)
N2—C10—H10	120.1	C7—C2—C1	120.2 (2)
C9—C10—H10	120.1	C5—C6—C7	120.6 (2)
C10—C9—C8	121.00 (19)	C5—C6—H6	119.7
C10—C9—H9	119.5	C7—C6—H6	119.7
C8—C9—H9	119.5	O3—N1—O5	122.40 (18)
C2—C3—C4	120.76 (18)	O3—N1—O4	119.71 (18)
C2—C3—H3	119.6	O5—N1—O4	117.89 (19)
C4—C3—H3	119.6		

C3—C4—C8—C12	−147.6 (2)	C8—C4—C5—C6	−174.7 (2)
C5—C4—C8—C12	28.9 (3)	C10—N2—C11—C12	−0.6 (3)
C3—C4—C8—C9	29.6 (3)	C8—C12—C11—N2	0.0 (3)
C5—C4—C8—C9	−154.0 (2)	C4—C3—C2—C7	1.1 (3)
C9—C8—C12—C11	0.5 (3)	C4—C3—C2—C1	−176.26 (19)
C4—C8—C12—C11	177.82 (19)	C6—C7—C2—C3	0.9 (3)
C11—N2—C10—C9	0.6 (3)	C6—C7—C2—C1	178.2 (2)
N2—C10—C9—C8	0.0 (3)	O2—C1—C2—C3	−10.7 (3)
C12—C8—C9—C10	−0.6 (3)	O1—C1—C2—C3	168.3 (2)
C4—C8—C9—C10	−177.83 (18)	O2—C1—C2—C7	172.0 (2)
C5—C4—C3—C2	−2.4 (3)	O1—C1—C2—C7	−9.0 (3)
C8—C4—C3—C2	174.15 (18)	C4—C5—C6—C7	0.1 (4)
C3—C4—C5—C6	1.8 (3)	C2—C7—C6—C5	−1.5 (4)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C10—H10···O4^{i}	0.93	2.42	3.225 (3)	145
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