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A 1:1 proton transfer compound of 2-aminobenzoic acid with nitric acid

S. Asath Bahadur,[a] R. Sayee Kannan[b] and B. Sridhar[c]*

[a]Department of Basic Sciences, Kalasalingam University, Krishnan kovil 626 190, India, [b]Department of Chemistry, Thiagarajar College, Madurai 625 009, India, and [c]Laboratory of X-ray Crystallography, Indian Institute of Chemical Technology, Hyderabad 500 007, India
Correspondence e-mail: sshiya@yahoo.com

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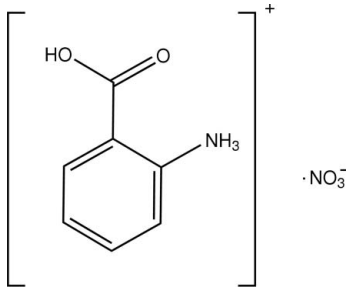
Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.003 Å; R factor = 0.049; wR factor = 0.146; data-to-parameter ratio = 10.4.

The asymmetric unit of the title compound, 2-carboxyanilinium nitrate, $C_7H_8NO_2^+\cdot NO_3^-$, consists of a 2-carboxyanilinium cation protonated at the amino group and a nitrate anion. The carboxyl group of 2-carboxyanilinium lies in the benzene-ring plane and a characteristic $S(6)$-type motif forms *via* an intramolecular N—H···O hydrogen bond between the carbonyl O atom and the amino group. The structure exhibits strong classical O—H···O and three-centered N—H···O interactions. Aggregation of cations and anions through hydrogen bonds form infinite one-dimensional hydrogen-bonded ribbons extending along [10$\bar{1}$].

Related literature

In all essential details, the molecular geometry of the title compound is in good agreement with those of similar structures (Brown & Ehrenberg, 1985; Takazawa *et al.*, 1986). For information on the uses of the title compound, see: He *et al.* (2003). For details of hydrogen-bonding motifs, see: Bernstein *et al.* (1995) and Jeffrey & Saenger (1991).



Experimental

Crystal data

$C_7H_8NO_2^+\cdot NO_3^-$
M_r = 200.15
Monoclinic, $P2_1/n$
a = 12.2368 (7) Å
b = 5.0082 (3) Å
c = 14.8395 (9) Å
β = 108.270 (1)°
V = 863.58 (9) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.13 mm^{-1}
T = 294 (2) K
0.20 × 0.15 × 0.09 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Absorption correction: none
6687 measured reflections
1498 independent reflections
1415 reflections with $I > 2\sigma(I)$
R_{int} = 0.042

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.146
S = 1.06
1498 reflections
144 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.44 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1O···O3	0.75 (3)	1.93 (3)	2.667 (2)	170 (3)
N1—H1N···O2	0.85 (4)	2.00 (4)	2.678 (3)	136 (3)
N1—H1N···O3^{i}	0.85 (4)	2.42 (3)	3.056 (3)	132 (3)
N1—H2N···O4^{ii}	0.91 (4)	1.99 (4)	2.891 (3)	173 (3)
N1—H2N···O5^{ii}	0.91 (4)	2.48 (4)	3.154 (3)	131 (3)
N1—H2N···N2^{ii}	0.91 (4)	2.58 (4)	3.443 (3)	159 (3)
N1—H3N···O4^{iii}	0.79 (4)	2.49 (3)	2.950 (2)	119 (3)
N1—H3N···O2^{i}	0.79 (4)	2.53 (4)	2.980 (2)	117 (3)
C4—H4···O5^{iv}	0.93	2.34	3.237 (3)	163
C6—H6···O5^{v}	0.93	2.59	3.378 (3)	143

Symmetry codes: (i) $-x+\frac{3}{2}, y-\frac{1}{2}, -z+\frac{3}{2}$; (ii) $x-\frac{1}{2}, -y+\frac{5}{2}, z-\frac{1}{2}$; (iii) $-x+\frac{3}{2}, y-\frac{3}{2}, -z+\frac{3}{2}$; (iv) $x-\frac{1}{2}, -y+\frac{3}{2}, z-\frac{1}{2}$; (v) $-x+1, -y+2, -z+2$.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *DIAMOND* (Brandenburg & Putz, 2005) and *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SJ2301).

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  doi:10.1107/S160053680701999X

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supplementary materials

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A 1:1 proton transfer compound of 2-aminobenzoic acid with nitric acid

S. A. Bahadur, R. S. Kannan and B. Sridhar

Comment

2-aminobenzoic acid (anthralinic acid) is a useful derivatizing agent for carbohydrate analyses (He *et al.*, 2003). Depending upon on the pH of a buffer, the 2-amionbenzoic acid can be either positively or negatively charged or neutral, since it has both a carboxyl group and an amino group. In the present study, 2-aminobenzoic acid was reacted with nitric acid and the structure of the product, (I), is reported.

The asymmetric unit of (I) consists of a 2-aminobenzoic acid cation protonated at the carboxylate group, and a nitrate anion. A strong O—H···O hydrogen bond links the 2-aminobenzoic acid cation to nitrate anion (Fig. 1). N—O bond lengths for the nitrate anion range from 1.233 (2) to 1.238 (2)°, and O—N—O bond angles ranges from 118.93 (18) to 120.89 (18)°.

The torsion angle C3—C2—C1—O1, -173.1 (2)°, clearly shows the coplanarity of the carboxyl group and the benzene ring and forms an intramolecular N—H···O hydrogen bond between the amino N atom and the carboxyl O atom thereby forming a characteristic S(6)-type motif (Bernstein *et al.*, 1995).

N—H···O and O—H···O hydrogen bonds stabilize the crystal structure. All the oxygen atoms are participating in the hydrogen bonding network. The three 2-amino H atoms are involved in hydrogen bonding network with three-centre associations (Jeffrey & Saenger, 1991) with the acceptor atoms. The three H atoms of the amino group are involved in extensive N^{+}—H···O^{-} hydrogen bonding interactions with O-atom acceptors of three different nitrate anions (Table 2). In addition, a glide-related cation-cation interaction is also observed through an N—H···O hydrogen bond. The structure can be considered as consisting of an infinite one-dimensional hydrogen-bonded ribbons extended diagonally as illustrated in Fig.2. Each ribbon consists of pairs of cations and anions, with the aromatic groups of the cations being parallel. Weak C—H···O interactions are also noticed in the crystal structure. A short interatomic contact is obseved between nitrate anions [O4···O4 = 2.381 Å] which is a consequence of the dense packing of the components by the hydrogen bonding.

Experimental

2-aminobenzoic acid and nitric acid were mixed in a 1:1 stoichiometric ratio and dissolved in water. Crystal were obtained by slow evaporation.

Refinement

All N-bound and O-bound H atoms were located in difference Fourier map and their positions and isotropic displacement parameters were refined. All other H atoms were positioned geometrically and treated as riding on their parent C atoms, with C—H distance = 0.93 Å, and with U_{iso}(H) = 1.2U_{eq}(C).

Figures

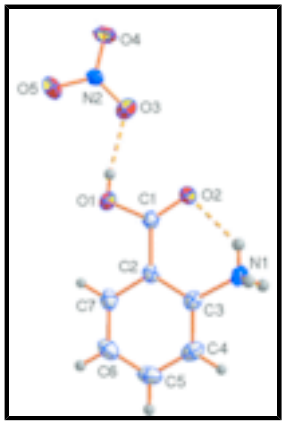

Fig. 1. A view of the (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as small spheres of arbitrary radii. Dashed lines indicate hydrogen bonds.

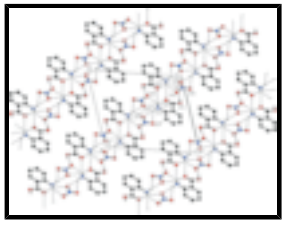

Fig. 2. A view of the packing, showing the infinite one-dimensional hydrogen-bonded ribbons. Dashed lines indicate O—H···O and N—H···O hydrogen bonds. H atoms not involved in hydrogen bonding have been removed for clarity. Only atoms involved in hydrogen bonding are labelled. [symmetry code: (i) -*x* + 3/2, *y* - 1/2, -*z* + 3/2; (ii) *x* - 1/2, -*y* + 5/2, *z* - 1/; (iii) -*x* + 3/2, *y* - 3/2, -*z* + 3/2.].

2-carboxyanilinium nitrate

Crystal data

$C_7H_8NO_2^+ \cdot NO_3^-$	F_{000} = 416
M_r = 200.15	D_x = 1.539 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 5597 reflections
a = 12.2368 (7) Å	θ = 2.6–27.9º
b = 5.0082 (3) Å	μ = 0.13 mm^{-1}
c = 14.8395 (9) Å	*T* = 294 (2) K
β = 108.270 (1)º	Block, colorless
V = 863.58 (9) Å^3	0.20 × 0.15 × 0.09 mm
Z = 4	

Data collection

Bruker SMART APEX CCD area-detector diffractometer	1415 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	R_{int} = 0.042
Monochromator: graphite	θ_{max} = 25.0º
T = 294(2) K	θ_{min} = 2.9º
ω scans	*h* = −14→14
Absorption correction: none	*k* = −5→5
6687 measured reflections	*l* = −17→17

1498 independent reflections

Refinement

Refinement on F^2	H atoms treated by a mixture of independent and constrained refinement
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.0638P)^2 + 0.3928P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.050$	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2) = 0.146$	$\Delta\rho_{max} = 0.44$ e Å^{-3}
$S = 1.06$	$\Delta\rho_{min} = -0.21$ e Å^{-3}
1498 reflections	Extinction correction: SHELXL97, $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
144 parameters	Extinction coefficient: 0.209 (18)
Primary atom site location: structure-invariant direct methods	
Secondary atom site location: difference Fourier map	
Hydrogen site location: inferred from neighbouring sites	

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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.63021 (16)	0.9765 (4)	0.84294 (13)	0.0392 (5)
C2	0.54112 (15)	0.7649 (3)	0.82574 (12)	0.0365 (5)
C3	0.51308 (15)	0.6048 (4)	0.74515 (12)	0.0374 (5)
C4	0.42748 (19)	0.4147 (4)	0.72904 (16)	0.0507 (6)
H4	0.4093	0.3094	0.6747	0.061*
C5	0.36898 (19)	0.3818 (5)	0.79429 (18)	0.0586 (6)
H5	0.3114	0.2535	0.7838	0.070*
C6	0.3953 (2)	0.5372 (5)	0.87449 (17)	0.0576 (6)
H6	0.3557	0.5141	0.9182	0.069*
C7	0.48004 (19)	0.7262 (4)	0.88997 (15)	0.0484 (6)
H7	0.4973	0.8309	0.9444	0.058*
N1	0.57349 (17)	0.6312 (5)	0.67506 (13)	0.0469 (5)
H1N	0.620 (3)	0.762 (8)	0.685 (2)	0.089 (11)*
H2N	0.523 (3)	0.667 (7)	0.617 (3)	0.087 (9)*
H3N	0.609 (3)	0.500 (7)	0.673 (2)	0.087 (11)*
O1	0.65438 (15)	1.0888 (3)	0.92666 (10)	0.0544 (5)
H1O	0.696 (3)	1.202 (6)	0.931 (2)	0.071 (9)*
O2	0.67464 (13)	1.0449 (3)	0.78371 (10)	0.0533 (5)

N2	0.85489 (14)	1.6057 (3)	0.98956 (11)	0.0415 (5)
O3	0.79176 (15)	1.4943 (3)	0.91758 (11)	0.0636 (5)
O4	0.92357 (15)	1.7801 (4)	0.98375 (13)	0.0725 (6)
O5	0.84897 (18)	1.5455 (4)	1.06845 (12)	0.0719 (6)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0382 (10)	0.0427 (10)	0.0382 (10)	−0.0009 (8)	0.0140 (8)	−0.0070 (7)
C2	0.0353 (9)	0.0376 (10)	0.0371 (9)	0.0022 (7)	0.0119 (7)	−0.0006 (7)
C3	0.0333 (9)	0.0388 (10)	0.0378 (9)	0.0057 (7)	0.0080 (7)	−0.0016 (7)
C4	0.0470 (12)	0.0432 (11)	0.0532 (12)	−0.0026 (9)	0.0031 (9)	−0.0067 (9)
C5	0.0439 (12)	0.0529 (13)	0.0743 (15)	−0.0114 (10)	0.0119 (11)	0.0099 (11)
C6	0.0495 (12)	0.0646 (14)	0.0643 (14)	−0.0043 (10)	0.0259 (11)	0.0121 (11)
C7	0.0525 (12)	0.0538 (12)	0.0444 (11)	−0.0006 (9)	0.0231 (9)	−0.0013 (9)
N1	0.0460 (11)	0.0555 (12)	0.0405 (10)	0.0033 (9)	0.0156 (8)	−0.0127 (8)
O1	0.0615 (10)	0.0615 (10)	0.0441 (8)	−0.0206 (8)	0.0223 (7)	−0.0189 (7)
O2	0.0551 (9)	0.0644 (10)	0.0486 (8)	−0.0201 (7)	0.0282 (7)	−0.0137 (7)
N2	0.0404 (9)	0.0412 (9)	0.0440 (9)	−0.0065 (7)	0.0147 (7)	0.0037 (7)
O3	0.0621 (10)	0.0713 (11)	0.0534 (10)	−0.0141 (8)	0.0122 (8)	−0.0146 (8)
O4	0.0667 (11)	0.0738 (12)	0.0704 (11)	−0.0337 (9)	0.0122 (9)	0.0206 (9)
O5	0.0864 (14)	0.0809 (12)	0.0531 (10)	−0.0183 (10)	0.0287 (9)	0.0121 (8)

Geometric parameters (Å, °)

C1—O2	1.219 (2)	C6—C7	1.369 (3)
C1—O1	1.310 (2)	C6—H6	0.9300
C1—C2	1.484 (3)	C7—H7	0.9300
C2—C3	1.391 (3)	N1—H1N	0.85 (4)
C2—C7	1.397 (3)	N1—H2N	0.91 (4)
C3—C4	1.380 (3)	N1—H3N	0.79 (4)
C3—N1	1.459 (3)	O1—H1O	0.75 (3)
C4—C5	1.383 (3)	N2—O5	1.233 (2)
C4—H4	0.9300	N2—O4	1.234 (2)
C5—C6	1.373 (4)	N2—O3	1.238 (2)
C5—H5	0.9300		
O2—C1—O1	122.96 (19)	C7—C6—H6	120.1
O2—C1—C2	123.13 (17)	C5—C6—H6	120.1
O1—C1—C2	113.88 (17)	C6—C7—C2	121.4 (2)
C3—C2—C7	117.79 (18)	C6—C7—H7	119.3
C3—C2—C1	121.98 (16)	C2—C7—H7	119.3
C7—C2—C1	120.21 (17)	C3—N1—H1N	114 (2)
C4—C3—C2	121.07 (18)	C3—N1—H2N	110 (2)
C4—C3—N1	117.77 (18)	H1N—N1—H2N	103 (3)
C2—C3—N1	121.16 (17)	C3—N1—H3N	111 (2)
C3—C4—C5	119.5 (2)	H1N—N1—H3N	107 (3)
C3—C4—H4	120.2	H2N—N1—H3N	110 (3)
C5—C4—H4	120.2	C1—O1—H1O	110 (2)

C6—C5—C4	120.5 (2)	O5—N2—O4	118.93 (18)
C6—C5—H5	119.8	O5—N2—O3	120.18 (17)
C4—C5—H5	119.8	O4—N2—O3	120.89 (18)
C7—C6—C5	119.8 (2)		
O2—C1—C2—C3	8.8 (3)	C2—C3—C4—C5	−0.3 (3)
O1—C1—C2—C3	−173.12 (17)	N1—C3—C4—C5	179.4 (2)
O2—C1—C2—C7	−169.4 (2)	C3—C4—C5—C6	0.2 (3)
O1—C1—C2—C7	8.7 (3)	C4—C5—C6—C7	0.0 (4)
C7—C2—C3—C4	0.2 (3)	C5—C6—C7—C2	−0.1 (3)
C1—C2—C3—C4	−177.97 (17)	C3—C2—C7—C6	0.0 (3)
C7—C2—C3—N1	−179.47 (18)	C1—C2—C7—C6	178.24 (19)
C1—C2—C3—N1	2.3 (3)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1O···O3	0.75 (3)	1.93 (3)	2.667 (2)	170 (3)
N1—H1N···O2	0.85 (4)	2.00 (4)	2.678 (3)	136 (3)
N1—H1N···O3^{i}	0.85 (4)	2.42 (3)	3.056 (3)	132 (3)
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Fig. 1

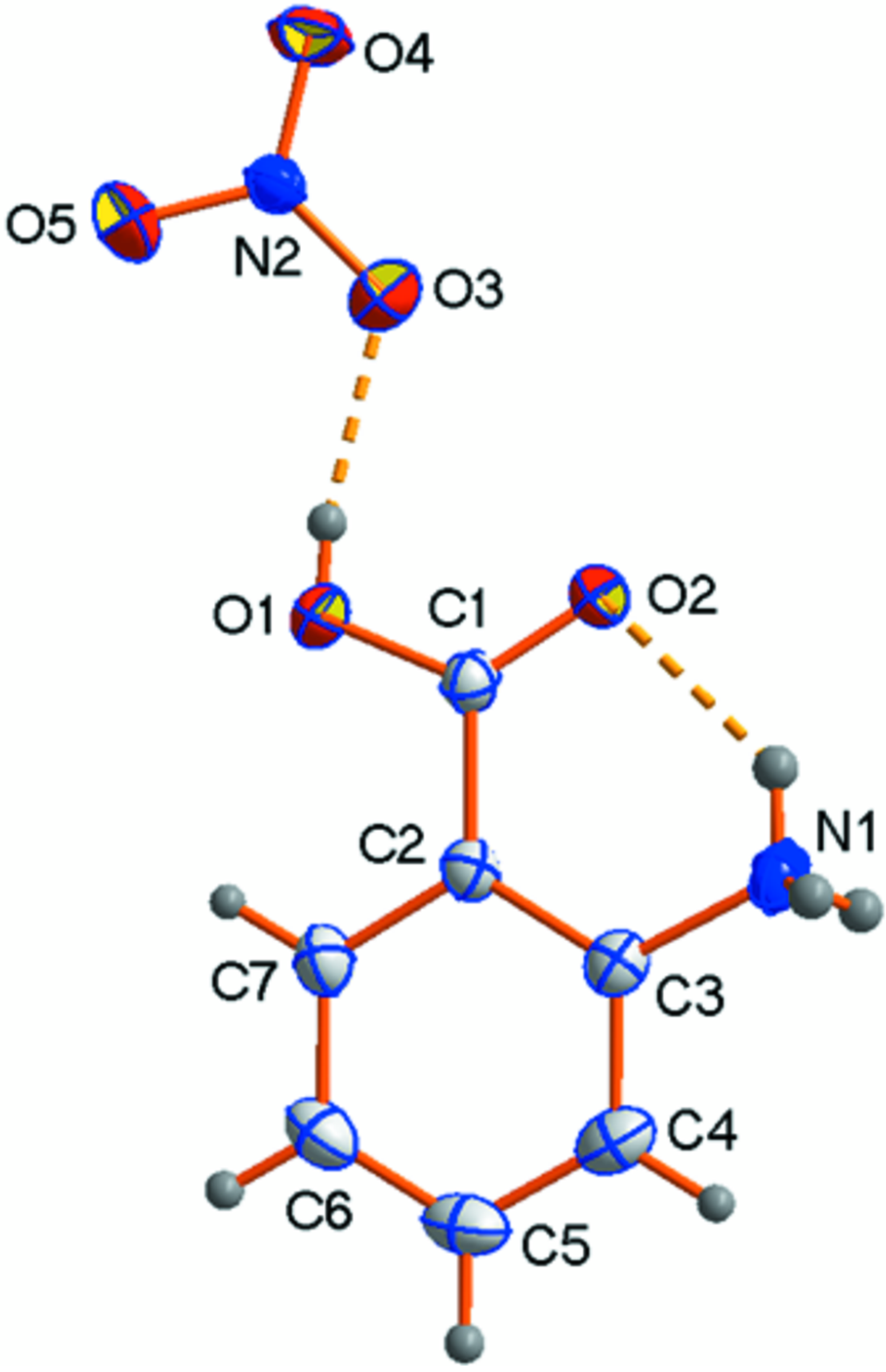

Fig. 2