Sodium pyridine-3-carboxylate

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The title compound, also known as sodium nicotinate, $Na^+ \cdot C_6H_4NO_2^-$, consists of two unique Na atoms coordinated to two unique pyridine-3-carboxylate ligands through the N atoms and carboxylate groups. One Na atom and one pyridine-3-carboxylate ligand lie on a twofold axis. Extensive Na coordination results in a three-dimensional array comprising infinite NaO_2CR chains linked by intrachain Na—N bonds.

Comment

The title compound, (I), is used as a precursor in therapeutic formulations, because its progenitor nicotinic acid, commonly known as the B-vitamin niacin, is a necessary component of human nutrition (Prinzo & Benoist, 2002; O'Neil, 2006). In addition, the achievement and elucidation of pyridine-carboxylate coordination complexes has been the focus of supramolecular and coordination complex research (Huang et al., 2005; Batten & Harris, 2001). Pyridinecarboxylate ligands display versatile coordinating modes owing to the presence of two carboxylate O atoms as well as the pyridine N-atom donor. Surprisingly, the structural elucidation of anhydrous sodium nicotinate has not been reported until now. In the present report, the structural determination and analysis of (I) is described.

(I)
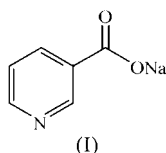
Compound (I) (Fig. 1) has two distinct Na–nicotinate units, with one disposed about a twofold axis, with the unique position refined as 50% N2 and 50% C10. The extended structure (Fig. 2) consists of infinite two-dimensional chains of Na and O atoms, lying parallel to the c axis, each surrounded by the pyridyl groups of the pendant nicotinate ligands. The individual chains are periodically linked by Na—N bonds from the pyridyl groups of neighbouring chains. Each Na atom is six-coordinate, with Na1 bound to six O atoms and Na2 bound

to five O and one N atom. The coordination geometry of both Na1 and Na2 is approximately trigonal prismatic, distorted from a regular polyhedron by the acute bite angles [48.12 (3) and 53.62 (4)°] of the nicotinate ligands, which each lie along one of the edges between the trigonal planes. The two-dimensional chains are built up from repeat units of three edge-shared trigonal prisms derived from Na2/Na1/Na2, which are subsequently inverted and translated to form successive components of each two-dimensional chain (Fig. 3).

The two unique nicotinate ligands display differing coordination modes (see scheme at end of Comment). Ligand 1 (O1/O2/N1/C1–C6) chelates to Na1 and is μ_5-bridging to four other Na atoms. Thus, atom O1 is bound to Na1, Na2 and Na2^{ii} [symmetry code: (ii) x, $-y$, $z + \frac{1}{2}$], whilst atom O2 bridges between Na2 and its symmetry equivalent Na2^v [symmetry code: (v) x, $-y$, $z - \frac{1}{2}$] (Table 1). Pyridyl atom N1 also binds to an Na atom, Na2^{iii} [symmetry code: (iii) $-x - \frac{1}{2}$, $y + \frac{1}{2}$, $-z - \frac{1}{2}$]. The second nicotinate ligand (O3/N2/C7–C10) lies on the twofold axis and thus has a symmetrical environment, with O3 bridging Na1, Na2 and Na1^i [symmetry code: (i) $-x$, $-y$, $-z$]
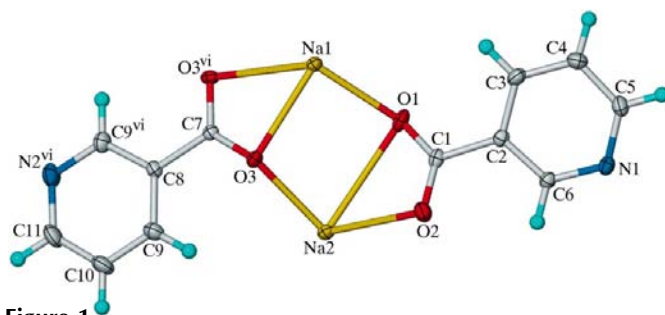

Figure 1
The unique component and some symmetry-related atoms of [Na(nicotinate)]$_\infty$, shown with 50% probability displacement ellipsoids and H atoms as spheres of arbitrary size. The second nicotinate group is shown with symmetry-equivalent atoms [symmetry code: (vi) $-x$, y, $\frac{1}{2} - z$] to complete the ligand, and only one component of the disordered N2/C10 position.
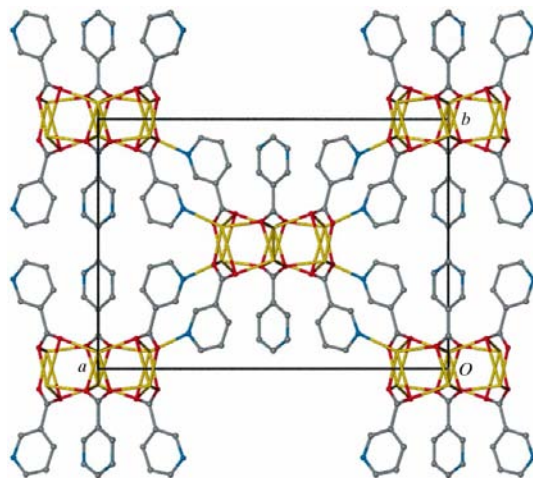

Figure 2
A ball-and-stick representation of the unit-cell contents of [Na(nicotinate)]$_\infty$, as viewed down the c axis.
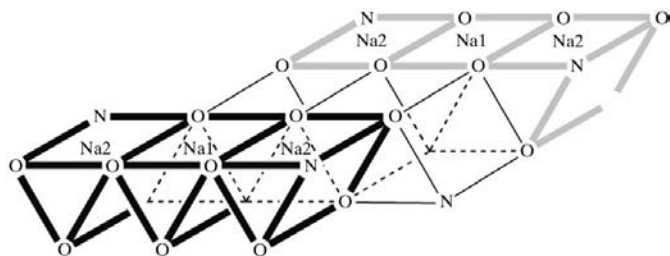
metal-organic compounds

Figure 3
Schematic representation of the arrangement of the Na trigonal prisms within the infinite two-dimensional chains in [Na(nicotinate)]$_\infty$.

(Table 1). The Na—O bond distances are generally in the range 2.3352 (8)–2.4416 (9) Å. However, one longer distance [Na2—O1 = 2.9577 (10) Å] occurs, indicating unsymmetrical chelation of ligand 2 to Na2. This is typical of NaO$_2$CR structures, in particular when the RCO$_2^-$ group is bridging. The Na2—N1^{iv} [symmetry code: (iv) $-x - \frac{1}{2}, y - \frac{1}{2}, -z - \frac{1}{2}$] (Table 1) distance is marginally longer than those for Na—O, as expected for a neutral donor interaction.
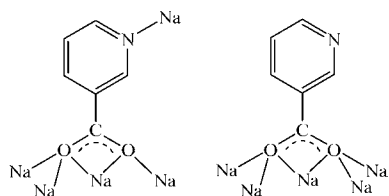
Experimental

The title compound was obtained from the recrystallization of its impure industrial product. The crystal used for data collection was obtained by slow evaporation of an acetonitrile solution, at 298 K, over a period of seven days.

Crystal data

Na$^+$·C$_6$H$_4$NO$_2^-$	$V = 1778.34$ (13) Å^3
$M_r = 145.09$	$Z = 12$
Monoclinic, $C2/c$	Mo $K\alpha$ radiation
$a = 20.1983$ (7) Å	$\mu = 0.18$ mm^{-1}
$b = 14.1880$ (5) Å	$T = 123$ (2) K
$c = 6.3000$ (2) Å	$0.20 \times 0.20 \times 0.15$ mm
$\beta = 99.935$ (13)°	

Data collection

Bruker X8 APEX KappaCCD diffractometer	18325 measured reflections
	2040 independent reflections
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)	1954 reflections with $I > 2/\sigma(I)$
$T_{min} = 0.957$, $T_{max} = 0.973$	$R_{int} = 0.025$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.029$	138 parameters
$wR(F^2) = 0.084$	H-atom parameters constrained
$S = 1.07$	$\Delta\rho_{max} = 0.42$ e Å^{-3}
2040 reflections	$\Delta\rho_{min} = -0.23$ e Å^{-3}

Table 1
Selected bond lengths (Å).

Na1—O1	2.3352 (8)	Na2—O3	2.3283 (9)
Na1—O3^i	2.3898 (8)	Na2—O2	2.3559 (9)
Na1—O3	2.4636 (9)	Na2—N1^{iv}	2.5450 (10)
O1—Na2^{ii}	2.4416 (9)	O2—Na2^v	2.3637 (9)
O1—Na2	2.9577 (10)	O3—Na1^i	2.3898 (8)
N1—Na2^{iii}	2.5450 (10)		

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

The *meta* position within the O3/N2/C7–C10 nicotinate ligand was refined as 50% C10 and 50% N2. Disordered atoms were treated with varying U_{iso} values. All H atoms were observed in difference syntheses, and were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H distances of 0.95 Å and U_{iso}(H) values of 1.2U_{eq}(C).

Data collection: *APEXII* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003) and *POV-RAY* (Cason, 2002); software used to prepare material for publication: *SHELXL97*.

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