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catena-Poly[[[bis(2-pyridone-κO)sodium]-di-μ-2-pyridone-$\kappa^4 O$:O] tetrafluoroborate]

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Key indicators

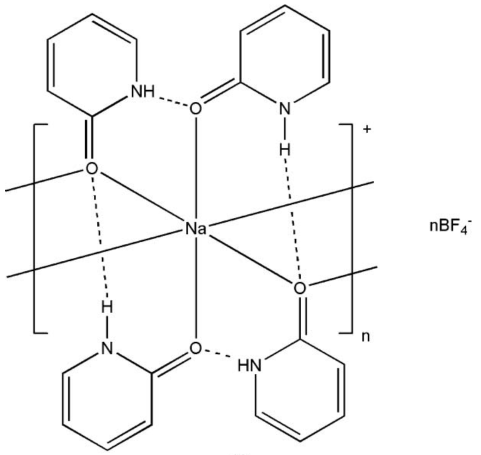
Single-crystal X-ray study
T = 173 K
Mean σ(C–C) = 0.004 Å
R factor = 0.065
wR factor = 0.147
Data-to-parameter ratio = 15.5

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

In the title compound, $[Na(C_5H_5NO)_4]BF_4$, each Na^+ ion, lying on an inversion centre, is octahedrally coordinated by four bridging and two terminal pyridone ligands, creating a cationic coordination polymer chain with tetrafluoroborate anions occupying the spaces between the chains.

Comment

The title compound, (I), was prepared during the course of our investigations on the tautomerization of 2-pyridone and 2-mercaptopyridine rings in the preparation of new scorpionate ligands. We are currently investigating the effect of tautomerization on ligand coordination properties.



(I)

The compound forms a coordination polymer chain with two independent $Na(pyridone)_4^+$ units, each sodium sitting on an inversion centre. Each Na^+ ion is connected to the sodium on either side by two bridging pyridone groups and is also coordinated by two terminal pyridone ligands, making each sodium octahedrally coordinated (Fig. 1 and Table 1). The pyridone ligands are arranged such that the amide H atom on each pyridone is hydrogen bonded to the oxygen of an adjacent pyridone ligand (Table 2), and these $Na(pyridone)_4^+$ groups stack together to form the coordination polymer (Fig. 2), with the BF_4^- anions occupying the spaces between the chains (Fig. 3). Some π stacking occurs between the 2-pyridone rings with minimum distances between the atoms in the rings of 3.125 (3) (C11–C16) and 3.284 (4) Å [C16–N1^{ii}; symmetry code: (ii) $2 - x, 1 - y, 1 - z$].

Experimental

A round-bottomed flask was charged with $NaBF_4$ (0.05 g, 0.45 mmol) and methanol (40 ml). The mixture was stirred until the salt had

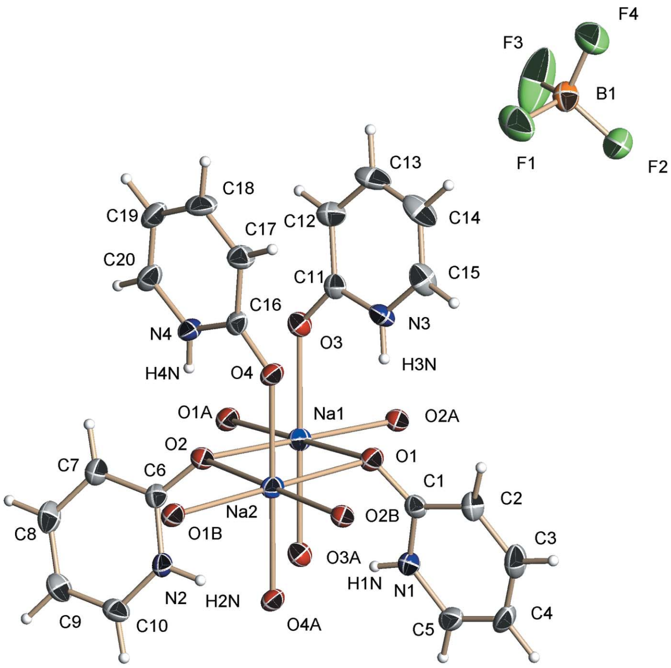


Figure 1
The Na(pyridone)$_4^+$ and BF$_4^-$ ions with the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level with H atoms represented as spheres of arbitrary size. [Symmetry codes: (A) $1 - x, 1 - y, 1 - z$; (B) $2 - x, 1 - y, 1 - z$.

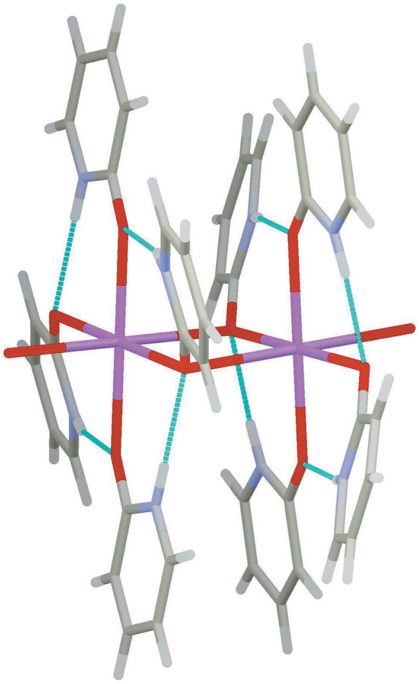


Figure 2
Hydrogen-bonded (dashed lines) units are stacked to form a coordination polymer structure.

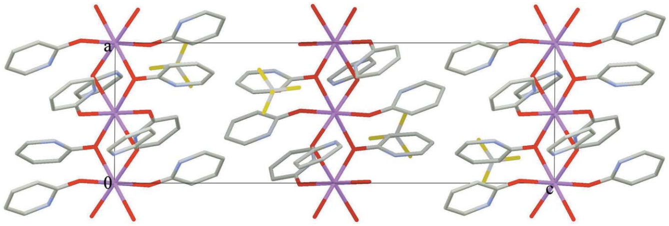


Figure 3
Packing diagram, viewed along the *b* axis. H atoms have been omitted.

dissolved. 2-Hydroxypyridine (0.17 g, 1.80 mmol) was subsequently added to the mixture, which was left to stir overnight. The solvent was removed under reduced pressure and the residue was dissolved in the minimum amount of THF. The resulting solution was left to stand at 273 K for 48 h, resulting in the formation of colourless needles (0.21 g, 0.43 mmol, 95%). Calcd for $C_{20}H_{20}N_4O_4F_4BNa$: C, 49.00; H, 4.11; N, 11.43. Found: C, 49.00; H, 4.14; N, 11.77.

Crystal data

$[Na(C_5H_5NO)_4]BF_4$
$M_r = 490.20$
Monoclinic, $P2_1/n$
$a = 7.2259$ (12) Å
$b = 13.521$ (2) Å
$c = 22.655$ (4) Å
$\beta = 90.322$ (4)°
$V = 2213.5$ (6) Å^3
$Z = 4$
$D_x = 1.471$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.14$ mm^{-1}
$T = 173$ (2) K
Needle, colourless
0.42 × 0.06 × 0.06 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.849$, $T_{max} = 0.992$
22997 measured reflections
5053 independent reflections
3175 reflections with $I > 2\sigma(I)$
$R_{int} = 0.076$
$\theta_{max} = 27.5°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.065$
$wR(F^2) = 0.147$
$S = 1.03$
5053 reflections
326 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0576P)^2 + 1.6958P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.31$ e Å^{-3}
$\Delta\rho_{min} = -0.26$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Na1—O1	2.4099 (18)	Na2—O1	2.5422 (19)
Na1—O2	2.4940 (19)	Na2—O2	2.4043 (18)
Na1—O3	2.3122 (19)	Na2—O4	2.3172 (19)
Na1—O1—Na2	93.66 (6)	Na1—O2—Na2	95.04 (6)

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*N*···O3^{i}	0.82 (3)	1.97 (3)	2.772 (3)	168 (3)
N2—H2*N*···O4^{ii}	0.88 (3)	1.92 (3)	2.776 (3)	163 (3)
N3—H3*N*···O1	0.85 (3)	2.00 (3)	2.838 (3)	169 (3)
N4—H4*N*···O2	0.87 (3)	1.96 (3)	2.827 (3)	169 (3)

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

H atoms were treated as riding, with C—H = 0.95 Å and $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(C) for aromatic H atoms. Amine protons were refined isotropically.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2001); software used to prepare material for publication: *SHELXTL*.

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