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2-Aminopyridinium (2-aminopyridine)trichloridonickelate(II)

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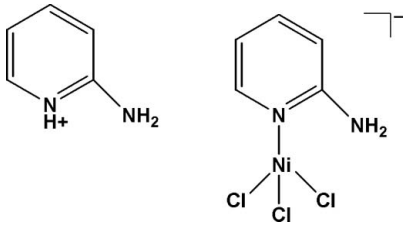
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.003 Å; R factor = 0.035; wR factor = 0.080; data-to-parameter ratio = 38.5.

In the title compound, $(C_5H_7N_2)[NiCl_3(C_5H_6N_2)]$, the Ni^{II} atom is four-coordinated by three chloride anions and one N atom of a 2-aminopyridine ligand, forming a distorted tetrahedral coordination. In the crystal structure, cations and complex anions are linked into chains along the *a*, *b* and *c* axes by N—H···Cl hydrogen bonds, leading to the formation of a three-dimensional framework.

Related literature

For related literature, see: Batsanov & Howard (2001); Bis & Zaworotko (2005); Chao *et al.* (1975); Corain *et al.* (1985); Jebas *et al.* (2006); Valdés-Martínez *et al.* (2001); Sletten & Kovacs (1993); Smith *et al.* (2000, 2001); Stibrany *et al.* (2004); Wei & Willett (1995); Windholz (1976).



Experimental

Crystal data

$(C_5H_7N_2)[NiCl_3(C_5H_6N_2)]$
M_r = 354.3
Monoclinic, *Cc*
a = 12.9265 (1) Å
b = 8.0644 (1) Å
c = 13.9893 (1) Å
β = 106.163 (1)°
V = 1400.67 (2) Å^3
Z = 4
Mo *K*α radiation
μ = 1.94 mm^{-1}
T = 100.0 (1) K
0.37 × 0.08 × 0.07 mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer with Oxford Cryosystems Cobra low-temperature attachment
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.533, T_{max} = 0.876
19539 measured reflections
6427 independent reflections
5088 reflections with $I > 2\sigma(I)$
R_{int} = 0.031

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.079
S = 1.05
6427 reflections
167 parameters
2 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.52 e Å^{-3}
$\Delta\rho_{min}$ = −0.64 e Å^{-3}
Absolute structure: Flack (1983), 1953 Friedel pairs
Flack parameter: 0.065 (9)

Table 1
Selected geometric parameters (Å, °).

Ni1—N1	2.0287 (17)	Ni1—Cl1	2.2665 (5)
Ni1—Cl2	2.2625 (6)	Ni1—Cl3	2.2722 (6)
N1—Ni1—Cl2	114.10 (5)	N1—Ni1—Cl3	104.63 (5)
N1—Ni1—Cl1	109.21 (5)	Cl2—Ni1—Cl3	108.62 (2)
Cl2—Ni1—Cl1	107.77 (2)	Cl1—Ni1—Cl3	112.60 (2)

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H1*N*3···Cl2^{i}	0.82 (3)	2.81 (3)	3.380 (2)	128 (2)
N2—H2*B*···Cl2	0.86	2.53	3.3475 (19)	159
N2—H2*C*···Cl1^{ii}	0.86	2.63	3.4866 (19)	172
N4—H4*B*···Cl3^{i}	0.86	2.36	3.197 (2)	165
N4—H4*C*···Cl1^{iii}	0.86	2.54	3.344 (2)	156

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

Data collection: *APEX2* (Bruker, 2005); cell refinement: *APEX2*; data reduction: *SAINT* (Bruker, 2005); program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2003).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2566).

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