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Hexaamminechromium(III) diaquatetrachlorosodium(I)

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Key indicators

Single-crystal X-ray study
T = 173 K
Mean σ(Cr–N) = 0.004 Å
R factor = 0.037
wR factor = 0.073
Data-to-parameter ratio = 15.2

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

The title compound, hexaamminechromium(III) diaquatetrachlorosodium(I), $[Cr(NH_3)_6][NaCl_4(H_2O)_2]$, is composed of discrete $[Cr(NH_3)_6]^{3+}$ cations and $[NaCl_4(H_2O)_2]^{3-}$ anions. The Cr and Na ions are octahedrally coordinated. The crystal packing is characterized by an alternating arrangement of anions and cations and is stabilized by numerous hydrogen bonds.

Comment

The title compound, (I), is composed of discrete $[Cr(NH_3)_6]^{3+}$ cations and $[NaCl_4(H_2O)_2]^{3-}$ anions. Both the Cr and the Na atoms are octahedrally coordinated. The Cr^{3+} ion is bonded to six NH_3 groups. The Na^+ ion is coordinated by four Cl^- ions in a square equatorial plane. Two water molecules occupying the axial positions complete its coordination sphere. The crystal packing is characterized by an alternating arrangement of anions and cations and is stabilized by numerous hydrogen bonds.

Experimental

0.5 g Na was dissolved in 300 ml of liquid NH_3. To the blue solution was added 0.2 g of anhydrous $FeCl_2$. After obtaining a colourless solution, small portions of a total of 3.0 g $CrCl_3$ were added while stirring at 241 K. After heating to room temperature very slowly and evaporation, crystals of (I) were obtained.

Crystal data

$H_{18}CrN_6^{3+}\cdot H_4Cl_4NaO_2^{3-}$
M_r = 355.03
Orthorhombic, $P2_12_12_1$
a = 7.0596 (3) Å
b = 9.1575 (4) Å
c = 22.6310 (10) Å
V = 1463.06 (11) Å^3
Z = 4
D_x = 1.612 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 5893 reflections
θ = 1–25°
μ = 1.53 mm^{-1}
T = 173 (2) K
Plate, orange
0.34 × 0.12 × 0.06 mm

Data collection

Siemens SMART CCD three-circle diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.624, T_{max} = 0.914
14937 measured reflections
2941 independent reflections
2340 reflections with $I > 2\sigma(I)$
R_{int} = 0.062
θ_{max} = 27.1°
$h = -9 \rightarrow 8$
$k = -10 \rightarrow 10$
$l = -27 \rightarrow 27$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.073
S = 1.06
2941 reflections
194 parameters
Only coordinates of H atoms refined
$w = 1/[\sigma^2(F_o^2) + (0.0304P)^2 + 0.4093P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.41 e Å^{-3}
$\Delta\rho_{min}$ = −0.43 e Å^{-3}
Absolute structure: Flack (1983), 1188 Friedel pairs
Flack parameter = 0.18 (3)

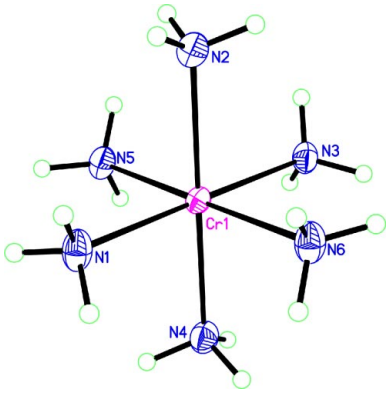

Figure 1
Perspective view of the cation of the title compound with the atom numbering. Displacement ellipsoids are drawn at the 50% probability level.

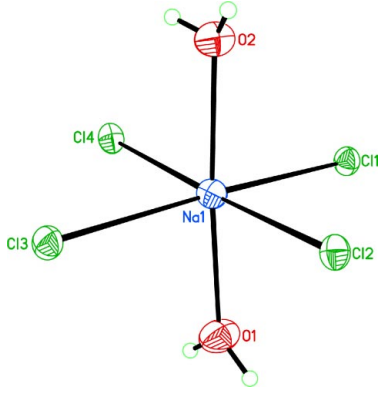

Figure 2
Perspective view of the anion of the title compound with the atom numbering. Displacement ellipsoids are drawn at the 50% probability level.

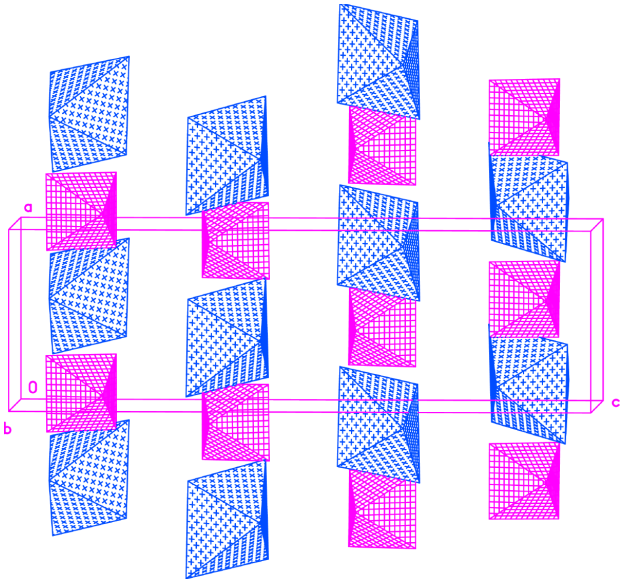

Figure 3
Packing diagram of the title compound, projected onto the *ac* plane. The cations are drawn as magenta and the anions as blue octahedra.

Table 1
Selected geometric parameters (Å).

Cr1—N1	2.069 (4)	Na1—O1	2.316 (4)
Cr1—N3	2.072 (4)	Na1—O2	2.345 (4)
Cr1—N4	2.072 (4)	Na1—Cl4	2.797 (2)
Cr1—N2	2.079 (4)	Na1—Cl2	2.824 (2)
Cr1—N6	2.082 (3)	Na1—Cl3	2.8690 (17)
Cr1—N5	2.087 (3)	Na1—Cl1	2.9318 (17)

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*A*···Cl1^{i}	0.881 (10)	2.467 (15)	3.325 (4)	165 (4)
N1—H1*B*···Cl4^{ii}	0.874 (10)	2.71 (3)	3.415 (4)	139 (3)
N1—H1*C*···O1^{iii}	0.878 (10)	2.66 (3)	3.326 (6)	133 (3)
N1—H1*C*···Cl1^{iii}	0.878 (10)	2.79 (3)	3.525 (4)	142 (3)
N2—H2*A*···Cl1^{iii}	0.878 (10)	2.92 (3)	3.586 (4)	134 (3)
N2—H2*A*···Cl4^{iii}	0.878 (10)	2.77 (3)	3.434 (4)	134 (4)
N2—H2*B*···Cl1^{iv}	0.873 (10)	2.426 (14)	3.282 (4)	167 (4)
N2—H2*C*···Cl3^{v}	0.875 (10)	2.79 (3)	3.486 (4)	138 (3)
N2—H2*C*···O1^{v}	0.875 (10)	2.58 (3)	3.278 (5)	137 (3)
N3—H3*A*···Cl3^{v}	0.877 (10)	2.53 (2)	3.329 (4)	151 (4)
N3—H3*B*···Cl2^{vi}	0.873 (10)	2.487 (14)	3.344 (4)	167 (4)
N3—H3*C*···Cl2^{iv}	0.872 (10)	2.471 (17)	3.306 (3)	161 (4)
N4—H4*A*···Cl3^{ii}	0.875 (10)	2.443 (16)	3.291 (4)	164 (4)
N4—H4*B*···Cl2^{vi}	0.877 (10)	2.74 (3)	3.450 (4)	139 (4)
N4—H4*C*···O2^{i}	0.876 (10)	2.26 (2)	3.064 (5)	153 (4)
N5—H5*B*···Cl3^{v}	0.880 (10)	2.69 (2)	3.513 (4)	156 (4)
N5—H5*A*···Cl2^{vi}	0.875 (10)	2.589 (19)	3.406 (3)	156 (4)
N5—H5*C*···Cl4^{ii}	0.877 (10)	2.575 (19)	3.392 (3)	156 (3)
N6—H6*A*···Cl1^{iii}	0.883 (10)	2.573 (16)	3.424 (3)	162 (3)
N6—H6*B*···Cl1^{i}	0.876 (10)	2.74 (2)	3.558 (4)	156 (4)
N6—H6*C*···Cl2^{iv}	0.874 (10)	2.84 (3)	3.539 (3)	138 (3)
O1—H1*D*···Cl4^{vii}	0.836 (10)	2.360 (11)	3.195 (3)	177 (6)
O1—H1*E*···Cl4^{viii}	0.837 (10)	2.312 (17)	3.131 (4)	167 (5)
O2—H2*D*···Cl3^{ix}	0.840 (10)	2.354 (15)	3.179 (3)	167 (4)
O2—H2*E*···Cl2^{x}	0.836 (10)	2.51 (3)	3.269 (4)	151 (4)

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

H atoms were located in a difference map and refined with fixed individual displacement parameters [U_{iso}(H) = 1.5U_{eq}(N,O)]. The O—H bond lengths were restrained to 0.84 (1) Å and the N—H bond lengths to 0.88 (1) Å.

Data collection: *SMART* (Siemens, 1995); cell refinement: *SMART*; data reduction: *SAINT* (Siemens, 1995); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1990); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *XP* in *SHELXTL-Plus* (Sheldrick, 1991); software used to prepare material for publication: *SHELXL*97.

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