Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.033$
$wR(F^2) = 0.095$
$S = 1.115$
1004 reflections
33 parameters
$w = 1/[\sigma^2(F_o^2) + (0.0524P)^2 + 1.7690P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 1.27$ e Å^{-3}
$\Delta\rho_{\min} = -0.94$ e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.026 (2)
Scattering factors from *International Tables for Crystallography* (Vol. C)
Absolute structure: Flack (1983)
Flack parameter = 0.010 (16)

Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters (Å^2)*

$$U_{\rm eq} = (1/3)\Sigma_i\Sigma_j U^{ij}a^i a^j \mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	$U_{\rm eq}$
Hg1	0	0	0	0.0329 (2)
Zn1	−1/2	0	1/4	0.0322 (3)
C1	−0.2730 (6)	−0.0789 (6)	−0.1170 (16)	0.0262 (11)
N1	−0.3609 (5)	−0.0490 (6)	0.012 (4)	0.0389 (13)
S1	−0.15323 (17)	−0.12430 (19)	−0.3005 (5)	0.0362 (4)

Table 2. *Selected geometric parameters (Å, °)*

Hg1—S1	2.5631 (19)	C1—N1	1.180 (12)
Zn1—N1	1.947 (11)	C1—S1	1.637 (7)
S1—Hg1—S1$^{\rm i}$	105.73 (5)	N1—C1—S1	178.1 (7)
S1—Hg1—S1$^{\rm ii}$	117.25 (10)	C1—N1—Zn1	176.2 (11)
N1—Zn1—N1$^{\rm iii}$	107.1 (4)	C1—S1—Hg1	96.5 (3)
N1—Zn1—N1$^{\rm iv}$	114.3 (8)		

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

The largest peak in the difference map (1.27 e Å^{-3}) is at (0.0917, 0.9756, 0.0025), 1.05 Å from Hg1, and the largest hole (−0.94 e Å^{-3}) is at (0.0324, 0.8843, 0.0126), 1.33 Å from Hg1.

Data collection: *XSCANS* (Siemens, 1996). Cell refinement: *XSCANS*. Data reduction: *SHELXTL* (Bruker, 1997). Program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*). Program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*b*). Molecular graphics: *SHELXTL*. Software used to prepare material for publication: *SHELXTL*.

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: TA1243). Services for accessing these data are described at the back of the journal.

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Pentaamminenitrocobalt(III) hexafluorosilicate(IV) at 293 and 150 K

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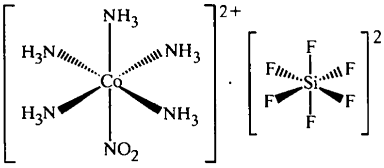
Abstract

The crystal structure of $[Co(NO_2)(NH_3)_5](SiF_6)$ has been determined at 293 and 150 K. The complex cations in the structure are linked by N—H···F hydrogen bonds to the $(SiF_6)^{2-}$ anions and by N—H···O hydrogen bonds to other cations. The role of these hydrogen bonds and of the repulsive O···F interactions in the anisotropy of the structural distortion on cooling is discussed.

Comment

Hydrogen bonds (N—H···O, N—H···Cl, N—H···Br and N—H···I) were shown to be important both for the formation of the crystal structures of a series of Co$^{\rm III}$–nitropentaammines and for the anisotropy of their structural distortion on cooling (Boertin, 1968; Boldyreva, 1996; Boldyreva & Podberezskaya, 1995; Boldyreva *et al.*, 1997*a*,*b*; Cotton & Edwards, 1968; Kubota & Ohba, 1992). The title compound, (I), was expected to have strong N—H···F hydrogen bonds in the crystal structure. Our aim was to study the effect of these hydrogen bonds on the structure and on the anisotropy of its distortion on cooling.



(I)

The packing of the [Co(NO$_2$)(NH$_3$)$_5$]$^{2+}$ complex cations and (SiF$_6$)$^{2-}$ anions in the crystal structure of the title compound can be described as a distorted NaCl type (Frlec *et al.*, 1980; Stanko & Paul, 1967), with chains of alternating cations and anions elongated along [001]. Within the chain, cations and anions are linked by N—H···F hydrogen bonds [N···F distances are in the range 2.936 (2)–3.201 (2) Å at 293 K]. Different chains are linked to each other by N—H···O hydrogen bonds between complex cations [N···O distances are in the range 2.983 (3)–3.295 (3) Å at 293 K]. As a result of such structural organization, the distance between the centroids of the nitro groups is noticeably shorter (4.435 Å at 293 K) than that in [Co(NO$_2$)(NH$_3$)$_5$]Cl$_2$ (5.461 Å at 293 K) and [Co(NO$_2$)(NH$_3$)$_5$]Br$_2$ (5.574 Å at 293 K) (Boldyreva *et al.*, 1997*c*). Selected anion–cation hydrogen bonds are shown in Fig. 1.

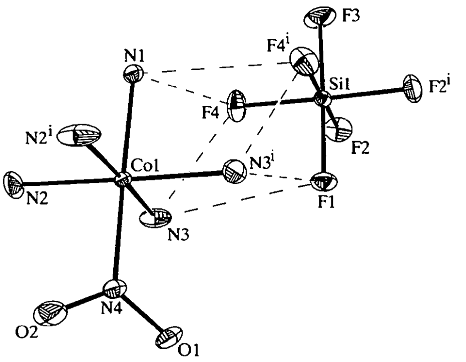


Fig. 1. The molecular structure of [Co(NO$_2$)(NH$_3$)$_5$](SiF$_6$) at 150 K. Displacement ellipsoids are plotted at the 50% probability level.

On cooling to 150 K, the structure of (I) contracted anisotropically in the three axial directions, the direction of minimum contraction [−0.275 (5)%] coinciding with the monoclinic *b* axis. The direction of minimum contraction can be correlated with the repulsive O···F interactions. The direction of maximum contraction [−0.471 (3)%] can be correlated with high compressibility of the shortest N—H···O hydrogen bonds.

The ellipsoids characterizing the anisotropic atomic displacements of one of the O atoms of the nitro ligand (O2) and of one of the F atoms of the (SiF$_6$)$^{2-}$ anion (F3) are strongly elongated along the *b* axis in comparison with that of the O1 atom, which can be explained by the existence of attractive N—H···O hydrogen bonding and repulsive F···O interactions.

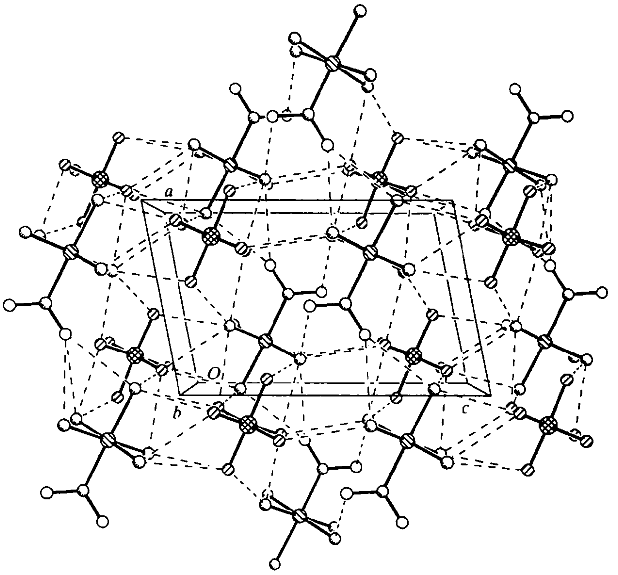


Fig. 2. A packing diagram of the structure of [Co(NO$_2$)(NH$_3$)$_5$](SiF$_6$) viewed along [010].

Experimental

Crystals of [Co(NO$_2$)(NH$_3$)$_5$](SiF$_6$) were grown in a closed silicon-glass vessel from a saturated aqueous solution of [Co(NO$_2$)(NH$_3$)$_5$](BF$_4$)$_2$ by slow infusion of (SiF$_6$)$^{2-}$ anions resulting from the interaction of the initial [Co(NO$_2$)(NH$_3$)$_5$](BF$_4$)$_2$ solution with glass. [Co(NO$_2$)(NH$_3$)$_5$](BF$_4$)$_2$ was synthesized by mixing stoichiometric solutions of AgBF$_4$ and [Co(NO$_2$)(NH$_3$)$_5$]Br$_2$.

Compound (I) at 293 K

Crystal data

[Co(NO$_2$)(NH$_3$)$_5$](SiF$_6$)
$M_r = 332.20$
Monoclinic
$P2_1/m$
$a = 6.5333$ (2) Å
$b = 7.9424$ (4) Å
$c = 10.2197$ (4) Å
$\beta = 100.966$ (2)°
$V = 520.62$ (4) Å^3
$Z = 2$
$D_x = 2.119$ Mg m^{-3}
D_m not measured

Mo $K\alpha$ radiation
$\lambda = 0.71073$ Å
Cell parameters from 1441 reflections
$\theta = 2.03$–29.82°
$\mu = 1.852$ mm^{-1}
$T = 293$ (2) K
Prism
0.16 × 0.13 × 0.08 mm
Brown

Data collection

Siemens SMART diffractometer
ω scans
Absorption correction: analytical (*XPREP*; Siemens, 1995)
$T_{\min} = 0.773$, $T_{\max} = 0.871$

1280 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.036$
$\theta_{\max} = 29.82°$
$h = -8 \rightarrow 9$
$k = -11 \rightarrow 11$
$l = -12 \rightarrow 13$

3703 measured reflections
1441 independent reflections
Intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.044$
$wR(F^2) = 0.077$
$S = 1.144$
1441 reflections
92 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0055P)^2 + 0.9782P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.374$ e Å^{-3}
$\Delta\rho_{\min} = -0.516$ e Å^{-3}
Extinction correction: *SHELXL*97 (Sheldrick, 1997*a*)
Extinction coefficient: 0.0026 (14)
Scattering factors from *International Tables for Crystallography* (Vol. C)

Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters (Å^2) for (I) at 293 K*

$$U_{\rm eq} = (1/3)\Sigma_i\Sigma_j U^{ij}a^i a^j \mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	$U_{\rm eq}$
Co1	0.25814 (8)	1/4	0.28791 (5)	0.01550 (15)
N1	−0.0174 (5)	1/4	0.1645 (3)	0.0225 (7)
N2	0.1622 (4)	0.0802 (4)	0.4023 (2)	0.0319 (6)
N3	0.3502 (4)	0.0713 (3)	0.1795 (2)	0.0299 (6)
N4	0.5264 (5)	1/4	0.4040 (3)	0.0235 (7)
O1	0.6895 (4)	1/4	0.3592 (3)	0.0331 (7)
O2	0.5381 (5)	1/4	0.5255 (3)	0.0566 (12)
Si1	0.17336 (16)	1/4	−0.18949 (10)	0.0183 (2)
F1	0.4116 (4)	1/4	−0.0933 (3)	0.0369 (6)
F2	0.2420 (3)	0.0987 (2)	−0.28803 (18)	0.0391 (5)
F3	−0.0697 (4)	1/4	−0.2820 (3)	0.0419 (7)
F4	0.0979 (3)	0.1006 (2)	−0.09150 (18)	0.0411 (5)

Table 2. *Selected geometric parameters (Å, °) for (I) at 293 K*

Co1—N1	1.992 (3)	N4—O2	1.229 (5)
Co1—N2	1.964 (2)	Si1—F1	1.675 (3)
Co1—N3	1.964 (2)	Si1—F2	1.6827 (18)
Co1—N4	1.920 (3)	Si1—F3	1.687 (3)
N4—O1	1.237 (4)	Si1—F4	1.6859 (19)
Co1—N4—O1	121.4 (3)	O1—N4—O2	118.7 (3)
Co1—N4—O2	119.9 (3)	F1—Si1—F2	91.57 (11)
N1—Co1—N2	91.40 (10)	F1—Si1—F3	178.22 (16)
N1—Co1—N3	88.84 (10)	F1—Si1—F4	89.75 (10)
N1—Co1—N4	178.92 (15)	F2—Si1—F2$^{\rm i}$	91.16 (15)
N2—Co1—N2$^{\rm i}$	86.76 (17)	F2—Si1—F3	89.67 (10)
N2—Co1—N3	90.35 (11)	F2—Si1—F4	89.67 (10)
N2—Co1—N3$^{\rm i}$	177.10 (12)	F2—Si1—F4$^{\rm i}$	178.42 (12)
N2—Co1—N4	89.38 (11)	F3—Si1—F4	88.98 (11)
N3—Co1—N3$^{\rm i}$	92.55 (16)	F4—Si1—F4$^{\rm i}$	89.47 (15)
N3—Co1—N4	90.41 (10)		

Symmetry code: (i) $x, \frac{1}{2} - y, z$.

Table 3. *Hydrogen-bonding geometry (Å, °) for (I) at 293 K*

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
N1—H1$A\cdots$F4	0.89	2.59	3.094 (4)	176
N1—H1$A\cdots$F4$^{\rm i}$	0.89	2.22	3.094 (4)	168
N1—H1$C\cdots$F4$^{\rm ii}$	0.89	2.04	2.905 (2)	165
N2—H2$B\cdots$F2$^{\rm ii}$	0.85	2.38	3.030 (3)	134
N2—H2$C\cdots$F2$^{\rm iii}$	0.85	2.31	3.111 (3)	157
N2—H2$A\cdots$F3$^{\rm ii}$	0.85	2.20	2.910 (3)	141
N3—H3$B\cdots$F1	0.86	2.37	3.221 (4)	171
N3—H3$A\cdots$F2$^{\rm iv}$	0.86	2.16	3.005 (3)	168
N3—H3$B\cdots$F4	0.86	2.35	2.950 (3)	128
N3—H3$C\cdots$F4$^{\rm ii}$	0.86	2.45	3.200 (3)	146
N1—H1$B\cdots$O1$^{\rm v}$	0.89	2.32	3.012 (4)	135
N2—H2$B\cdots$O1$^{\rm v}$	0.85	2.56	3.322 (4)	151
N2—H2$A\cdots$O2$^{\rm vi}$	0.85	2.58	3.272 (3)	140

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

Compound (I) at 150 K

Crystal data

[Co(NO$_2$)(NH$_3$)$_5$](SiF$_6$)
$M_r = 332.20$
Monoclinic
$P2_1/m$
$a = 6.5034$ (2) Å
$b = 7.9206$ (3) Å
$c = 10.1816$ (4) Å
$\beta = 100.911$ (2)°
$V = 514.98$ (3) Å^3
$Z = 2$
$D_x = 2.142$ Mg m^{-3}
D_m not measured
Mo $K\alpha$ radiation
$\lambda = 0.71073$ Å
Cell parameters from 1988 reflections
$\theta = 2.04$–29.91°
$\mu = 1.872$ mm^{-1}
$T = 150$ (2) K
Prism
0.16 × 0.13 × 0.08 mm
Brown

Data collection

Siemens SMART diffractometer
ω scans
Absorption correction: analytical (*XPREP*; Siemens, 1995)
$T_{\min} = 0.771$, $T_{\max} = 0.869$
3841 measured reflections
1441 independent reflections
1340 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.028$
$\theta_{\max} = 29.91°$
$h = -8 \rightarrow 9$
$k = -11 \rightarrow 11$
$l = -12 \rightarrow 13$
Intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.031$
$wR(F^2) = 0.063$
$S = 1.135$
1441 reflections
92 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0103P)^2 + 0.7537P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.413$ e Å^{-3}
$\Delta\rho_{\min} = -0.379$ e Å^{-3}
Extinction correction: *SHELXL*97 (Sheldrick, 1997*a*)
Extinction coefficient: 0.0046 (13)
Scattering factors from *International Tables for Crystallography* (Vol. C)

Table 4. *Fractional atomic coordinates and equivalent isotropic displacement parameters (Å^2) for (I) at 150 K*

$$U_{\rm eq} = (1/3)\Sigma_i\Sigma_j U^{ij}a^i a^j \mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	$U_{\rm eq}$
Co1	0.25830 (5)	1/4	0.28798 (4)	0.00866 (11)
N1	−0.0181 (3)	1/4	0.1644 (2)	0.0120 (4)
N2	0.1622 (3)	0.0800 (3)	0.40297 (19)	0.0288 (5)
N3	0.3500 (3)	0.0708 (2)	0.17893 (18)	0.0204 (4)
N4	0.5277 (4)	1/4	0.4042 (2)	0.0139 (5)
O1	0.6917 (3)	1/4	0.3588 (2)	0.0188 (4)
O2	0.5394 (4)	1/4	0.5267 (2)	0.0434 (8)
Si1	0.17301 (11)	1/4	−0.18937 (7)	0.01028 (16)
F1	0.4123 (3)	1/4	−0.09258 (17)	0.0205 (4)
F2	0.2434 (2)	0.09832 (16)	−0.28858 (12)	0.0235 (3)
F3	−0.0709 (3)	1/4	−0.28305 (19)	0.0323 (5)
F4	0.0959 (2)	0.09990 (17)	−0.09110 (12)	0.0247 (3)

Table 5. *Selected geometric parameters (Å, °) for (I) at 150 K*

Co1—N1	1.990 (2)	N4—O2	1.235 (3)
Co1—N2	1.9623 (19)	Si1—F1	1.6769 (18)
Co1—N3	1.9629 (17)	Si1—F2	1.6877 (13)
Co1—N4	1.920 (2)	Si1—F3	1.6890 (19)
N4—O1	1.240 (3)	Si1—F4	1.6899 (13)
Co1—N4—O1	121.29 (19)	O1—N4—O2	118.9 (2)
Co1—N4—O2	119.81 (19)	F1—Si1—F2	91.43 (7)
N1—Co1—N2	91.47 (7)	F1—Si1—F3	178.43 (10)
N1—Co1—N3	88.68 (7)	F1—Si1—F4	89.90 (7)
N1—Co1—N4	178.86 (10)	F2—Si1—F2^{i}	90.77 (10)
N2—Co1—N2^{i}	86.63 (14)	F2—Si1—F3	89.67 (7)
N2—Co1—N3	90.38 (9)	F2—Si1—F4	89.89 (7)
N2—Co1—N3^{i}	177.01 (9)	F2—Si1—F4^{i}	178.50 (8)
N2—Co1—N4	89.36 (8)	F3—Si1—F4	88.98 (7)
N3—Co1—N3^{i}	92.60 (12)	F4^{i}—Si1—F4	89.42 (10)
N3—Co1—N4	90.53 (7)		

Symmetry code: (i) $x, \frac{1}{2} - y, z$.

Table 6. *Hydrogen-bonding geometry (Å, °) for (I) at 150 K*

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*A*···F4	0.89	2.54	3.076 (2)	120
N1—H1*A*···F4^{i}	0.89	2.19	3.076 (2)	169
N1—H1*C*···F4^{ii}	0.89	2.03	2.8897 (14)	161
N2—H2*B*···F2^{ii}	0.86	2.36	3.024 (2)	134
N2—H2*C*···F2^{iii}	0.86	2.28	3.088 (2)	158
N2—H2*A*···F3^{ii}	0.86	2.19	2.899 (2)	140
N3—H3*B*···F1	0.87	2.34	3.201 (2)	172
N3—H3*A*···F2^{iv}	0.87	2.13	2.986 (2)	169
N3—H3*B*···F4	0.87	2.34	2.936 (2)	126
N3—H3*C*···F4^{ii}	0.87	2.41	3.171 (2)	148
N1—H1*B*···O1^{v}	0.89	2.32	2.983 (3)	131
N2—H2*B*···O1^{v}	0.86	2.52	3.295 (3)	1450
N2—H2*A*···O2^{vi}	0.86	2.54	3.254 (3)	141

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

H atoms were located from a difference electron-density map. The positions of the H atoms were refined as rotating ammine groups with fixed Co—N—H angles and free N—H bond lengths.

For both compounds, data collection: *SMART* (Siemens, 1994*a*); cell refinement: *SAINT* (Siemens, 1994*b*); data reduction: *SAINT*; program(s) used to solve structures: *SHELXS*97 (Sheldrick, 1997*b*); program(s) used to refine structures: *SHELXL*97 (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Siemens, 1994*c*); software used to prepare material for publication: *SHELXL*97.

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: AV1028). Services for accessing these data are described at the back of the journal.

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Dirubidium *catena*-poly[dichloroargentate(I)-μ-chloro]

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Abstract

The crystal structure of the title compound, Rb_2AgCl_3, consists of polymeric $[AgCl_3]^{2-}$ anions composed of corner-sharing slightly distorted $AgCl_4$ tetrahedra, with Rb^+ ions situated between the chains.

Comment

Compounds of the type R_2MX_3 (R is a monovalent cation), such as K_2AgI_3 (Brink & Kroese, 1952), K_2CuCl_3 (Brink & MacGillavry, 1949) and $(NH_4)_2CuX_3$ (X = Cl, Br; Brink & van Arkel, 1952), have been studied previously and found to be of three closely related structural types (Brink Shoemaker,