Table 39A-8-001. $[N(CH_3)_4]_2CoCl_4$. Crystal structure of phase III [85Fja1]. Fractional coordinates [$\cdot 10^{-4}$] of the basic structure. The basic structure was obtained by taking into account only those reflections that are also present in phase I.

	Co	N(a)	N(b)
x	2500 *)	2500 *)	2500 *)
y	4065(1)	945(6)	8246(6)
z	2454(1)	1483(7)	4928(8)
	Cl(1)	C(1a)	C(1b)
x	2500 *)	2500 *)	2500 *)
y	4064(3)	996(13)	7365(11)
z	622(3)	2690(11)	4496(20)
	Cl(2)	C(2a)	C(2b)
x	2500 *)	2500 *)	2500 *)
y	5411(2)	51(9)	8904(17)
z	3148(4)	1090(15)	4087(19)
	Cl(3)	C(3a)	C(3b)
x	447(3)	1200(21)	1185(20)
y	3374(2)	1402(14)	8430(11)
z	3051(2)	1053(13)	5500(18)

*) Value required by symmetry.

Table 39A-8-002. $[N(CH_3)_4]_2CoCl_4$. Crystal structure of phase III [85Fja1]. Temperature parameters U_{ij} [$\cdot 10^{-4}$ Å] for the basic structure. U_{ii} is defined by Eq. (d) in Introduction.

	Co	N(a)	N(b)
U_{11}	649(9)	691(60)	602(54)
U_{22}	419(7)	660(56)	500(49)
U_{33}	440(8)	489(51)	614(56)
U_{12}	*)	*)	*)
U_{13}	*)	*)	*)
U_{23}	2(5)	3(43)	−118(45)
	Cl(1)	C(1a)	C(1b)
U_{11}	1303(34)	2236(238)	1883(207)
U_{22}	1126(30)	1501(168)	723(109)
U_{33}	442(30)	445(77)	2238(241)
U_{12}	*)	*)	*)
U_{13}	*)	*)	*)
U_{23}	62(18)	−59(97)	−835(139)
	Cl(2)	C(2a)	C(2b)
U_{11}	3211(85)	2729(271)	5104(608)
U_{22}	479(18)	567(81)	1468(213)
U_{33}	1053(32)	1151(141)	1037(165)
U_{12}	*)	*)	*)
U_{13}	*)	*)	*)
U_{23}	−225(21)	−344(91)	23(163)
	Cl(3)	C(3a)	C(3b)
U_{11}	787(17)	2453(198)	2039(171)
U_{22}	1521(27)	3473(257)	1737(151)
U_{33}	998(19)	1549(140)	3641(274)
U_{12}	−325(18)	2169(194)	−810(136)
U_{13}	272(16)	−840(140)	2031(188)
U_{23}	43(19)	−413(158)	−1162(172)

*) Required to be zero by symmetry.

Table 39A-8-003. $[N(CH_3)_4]_2CoCl_4$. Crystal structure of phase III [85Fja1]. Bond lengths [Å] and angles [°] for the basic structure. Primed atoms are related to unprimed ones by reflection in the mirror plane at $x = 1/4$.

Co–Cl(1)	2.245(3)	C(1a)–N(a)–C(2a)	112(2)
Co–Cl(2)	2.251(4)	C(1a)–N(a)–C(3a)	110(2)
Co–Cl(3)	2.253(3)	C(2a)–N(a)–C(3a)	110(2)
		C(3a)–N(a)–C(3a′)	106(2)
Cl(1)–Co–Cl(2)	112.2(3)		
Cl(1)–Co–Cl(3)	108.9(2)	N(b)–C(1b)	1.46(2)
Cl(2)–Co–Cl(3)	108.5(3)	N(b)–C(2b)	1.45(3)
Cl(3)–Co–Cl(3′)	109.7(2)	N(b)–C(3b)	1.40(2)
N(a)–C(1a)	1.48(2)	C(1b)–N(b)–C(2b)	113(3)
N(a)–C(2a)	1.47(2)	C(1b)–N(b)–C(3b)	112(2)
N(a)–C(3a)	1.46(2)	C(2b)–N(b)–C(3b)	102(2)
		C(3b)–N(b)–C(3b′)	115(3)

Table 39A-8-004. $[N(CH_3)_4]_2CoCl_4$. Pressure coefficients of the transition temperatures [80Shi].

Transition	$d\Theta/dp$ [$\cdot 10^2$ K GPa^{-1}]
II–I	1.3(1)
III–II	2.0(1)
IV–III	2.6(2)
IV–II	2.0(1)
V–IV	1.6(1)

Table 39A-8-005. $[N(CH_3)_4]_2CoCl_4$. Transition heat (ΔQ) and transition entropy (ΔS) [81Gom]. R: gas constant.

Transition	Θ [K]	$\Delta Q/R$ [K]	$\Delta S/R$
VII–VI	115.90(5)	21.02(50)	0.18(5)
VI–V	191.90(5)	58.00(50)	0.295(4)
IV–III	277.65(10)	10.20(50)	0.367(20)
III–II	282.35(10)	3.49(100)	0.012(4)
II–I	294.00(20)	285(15)	1.06(5)

Table 39A-8-006. $[N(CH_3)_4]_2CoCl_4$. **D** tensor and its principal axes for Mn^{2+} center [81Tsu]. T = 21 °C. θ, ϕ: azimuthal and polar angles with respect to the crystalline frame.

	Principal values	Principal axis [°]	
	[$\cdot 10^2$ A m^{-1}]	θ	ϕ
D_A	–40(2)	90	0
D_B	–31(2)	108	90
D_C	–71(2)	18	90