Table 39A-6-001. K_2CoCl_4. Crystal structure of phase III [91Mas]. Fractional coordinates [$\cdot 10^{-4}$] and equivalent isotropic temperature parameters [$\cdot 10^{-2}$]. T = 298 K. Fixed parameter is denoted by (*). B_{eq} is given by $4/3\Sigma b_{ij}a_i a_j$, where b_{ij} is defined by Eq. (b) in Introduction.

Atom	x	y	z	B_{eq} [Å^2]
K(1a)	2861(*)	799(2)	442(1)	561(7)
K(1b)	2623(4)	843(3)	3800(1)	570(7)
K(1c)	2210(3)	828(2)	7108(1)	427(5)
K(2a)	2401(3)	8129(2)	1663(1)	338(4)
K(2b)	2945(3)	8117(1)	4991(1)	276(3)
K(2c)	2224(3)	8116(2)	8323(1)	320(4)
Co(a)	2521(2)	4199(1)	720(1)	212(2)
Cl(1a)	1744(3)	4443(2)	–83(1)	325(4)
Cl(2a)	3169(4)	5759(2)	1129(1)	389(5)
Cl(3a)	–67(3)	3558(2)	1106(1)	393(5)
Cl(4a)	4821(3)	3022(2)	841(1)	413(5)
Co(b)	2817(1)	4181(1)	4049(1)	207(2)
Cl(1b)	3172(5)	4383(2)	3230(1)	469(6)
Cl(2b)	3140(7)	5777(2)	4448(1)	621(9)
Cl(3b)	121(4)	3484(3)	4298(1)	661(8)
Cl(4b)	5006(4)	3071(3)	4346(1)	618(7)
Co(c)	2369(1)	4178(1)	7403(1)	211(2)
Cl(1c)	3078(5)	4353(2)	6593(1)	454(6)
Cl(2c)	1686(4)	5752(2)	7799(1)	356(5)
Cl(3c)	158(3)	2936(2)	7553(1)	396(5)
Cl(4c)	5002(3)	3599(2)	7777(1)	383(5)

Table 39A-6-002. K_2CoCl_4. Crystal structure of phase III [91Mas]. Bond distances [Å] and angles [°] of $CoCl_4$. T = 298 K. The mean values are 2.252(18) Å and 109.4(38)°, respectively.

Co(a)–Cl(1a)	2.246(3)	Co(a)–Cl(2a)	2.268(3)
Co(a)–Cl(3a)	2.283(3)	Co(a)–Cl(4a)	2.237(3)
Co(b)–Cl(1b)	2.223(3)	Co(b)–Cl(2b)	2.257(3)
Co(b)–Cl(3b)	2.236(3)	Co(b)–Cl(4b)	2.243(3)
Co(c)–Cl(1c)	2.239(3)	Co(c)–Cl(2c)	2.271(3)
Co(c)–Cl(3c)	2.256(3)	Co(c)–Cl(4c)	2.269(3)
Cl(1a)–Co(a)–Cl(2a)	113.6(1)	Cl(1a)–Co(a)–Cl(3a)	105.9(1)
Cl(1a)–Co(a)–Cl(4a)	114.4(1)	Cl(2a)–Co(a)–Cl(3a)	104.3(1)
Cl(2a)–Co(a)–Cl(4a)	109.3(1)	Cl(3a)–Co(a)–Cl(4a)	108.7(1)
Cl(1b)–Co(b)–Cl(2b)	110.9(1)	Cl(1b)–Co(b)–Cl(3b)	115.9(1)
Cl(1b)–Co(b)–Cl(4b)	109.6(1)	Cl(2b)–Co(b)–Cl(3b)	106.7(1)
Cl(2b)–Co(b)–Cl(4b)	107.2(1)	Cl(3b)–Co(b)–Cl(4b)	106.0(1)
Cl(1c)–Co(c)–Cl(2c)	114.7(1)	Cl(1c)–Co(c)–Cl(3c)	113.6(1)
Cl(1c)–Co(c)–Cl(4c)	105.3(1)	Cl(2c)–Co(c)–Cl(3c)	110.3(1)
Cl(2c)–Co(c)–Cl(4c)	104.4(1)	Cl(3c)–Co(c)–Cl(4c)	107.7(1)

Table 39A-6-003. K_2CoCl_4. Crystal structure of phase IV [91Mas]. Fractional coordinates [$\cdot 10^{-4}$] and equivalent isotropic temperature parameters [$\cdot 10^{-2}$]. T = 134 K. Fixed parameter is denoted by (*). B_{eq} is given by $4/3\Sigma b_{ij}a_i a_j$, where b_{ij} is defined by Eq. (b) in Introduction.

Atom	x	y	z	B_{eq} [Å^2]
K(1a)	1130(3)	804(2)	2092(2)	175(9)
K(1b)	1290(4)	811(2)	5431(2)	240(11)
K(1c)	1398(3)	772(2)	8803(2)	176(9)
K(1d)	1542(4)	4144(2)	441(2)	205(10)
K(1e)	1314(3)	4133(2)	3799(2)	237(11)
K(1f)	1117(4)	4114(2)	7100(2)	195(10)
K(1g)	3628(3)	3333(2)	2885(2)	182(9)
K(1h)	3878(3)	3413(2)	6184(2)	178(9)
K(1i)	4023(4)	3322(2)	9556(2)	233(11)
K(1j)	3765(4)	1692(2)	1193(2)	245(12)
K(1k)	3776(4)	1588(2)	4559(2)	240(11)
K(1l)	3494(3)	1649(2)	7900(2)	166(9)
K(2a)	1106(3)	2820(2)	1679(2)	159(9)
K(2b)	1512(3)	2798(2)	4989(2)	122(8)
K(2c)	1087(3)	2806(2)	8352(2)	142(8)
K(2d)	1490(3)	2202(2)	9(2)	150(9)
K(2e)	1078(3)	2196(2)	3307(2)	156(9)
K(2f)	1265(3)	2165(2)	6647(2)	156(9)
K(2g)	4008(3)	285(2)	12(2)	111(8)
K(2h)	3690(3)	335(2)	3325(2)	134(8)
K(2i)	3634(3)	297(2)	6668(2)	128(8)
K(2j)	3561(3)	4688(2)	1691(2)	130(8)
K(2k)	3936(3)	4671(2)	4999(2)	104(7)
K(2l)	3647(3)	4701(2)	8334(2)	117(8)
Co(a)	1276(*)	820(1)	704(*)	87(5)
Cl(1a)	831(3)	990(2)	–94(2)	128(9)
Cl(2a)	1568(3)	1590(2)	1141(2)	138(9)
Cl(3a)	–7(3)	453(2)	1084(2)	140(9)
Cl(4a)	2426(4)	202(2)	784(2)	227(11)
Co(b)	1365(2)	846(1)	4037(1)	80(5)
Cl(1b)	1621(4)	944(2)	3206(2)	206(11)
Cl(2b)	1427(4)	1653(2)	4438(2)	198(11)
Cl(3b)	28(4)	453(3)	4271(2)	270(12)
Cl(4b)	2512(3)	316(2)	4366(2)	218(11)
Co(c)	1166(2)	830(1)	7400(1)	81(5)
Cl(1c)	1565(4)	904(2)	6583(2)	153(9)
Cl(2c)	877(4)	1627(2)	7807(2)	171(10)
Cl(3c)	56(3)	214(2)	7548(2)	159(10)
Cl(4c)	2488(3)	514(2)	7775(2)	165(10)
Co(d)	1146(2)	4162(1)	2413(1)	89(5)
Cl(1d)	1565(4)	4064(2)	1595(2)	155(9)
Cl(2d)	744(3)	3376(2)	2804(2)	131(9)
Cl(3d)	93(4)	4822(2)	2533(2)	186(11)
Cl(4d)	2493(3)	4417(2)	2800(2)	191(11)
Co(e)	1255(2)	4125(1)	5725(1)	82(5)

(continued)

Table 39A-6-003 (continued)

Atom	*x*	*y*	*z*	B_{eq} [Å^2]
Cl(1e)	830(3)	3991(2)	4921(2)	148(9)
Cl(2e)	1677(4)	3343(2)	6136(2)	174(10)
Cl(3e)	–44(3)	4425(2)	6121(2)	149(9)
Cl(4e)	2378(4)	4739(2)	5835(2)	189(11)
Co(f)	1441(2)	4175(1)	9054(1)	89(5)
Cl(1f)	1654(4)	4038(2)	8218(2)	166(10)
Cl(2f)	1793(4)	3390(2)	9474(2)	200(11)
Cl(3f)	22(4)	4451(2)	9274(2)	230(12)
Cl(4f)	2407(3)	4830(2)	9314(2)	158(9)
Co(g)	3880(2)	3329(1)	970(1)	100(5)
Cl(1g)	4161(4)	3471(2)	1770(2)	183(11)
Cl(2g)	3972(4)	4126(2)	529(2)	178(10)
Cl(3g)	2496(3)	2947(2)	778(2)	184(10)
Cl(4g)	4967(4)	2767(3)	640(2)	271(12)
Co(h)	3796(2)	3320(1)	4282(1)	116(5)
Cl(1h)	3355(3)	3464(2)	5079(2)	128(9)
Cl(2h)	4179(3)	4086(2)	3854(2)	155(10)
Cl(3h)	2477(4)	3011(2)	3879(2)	199(11)
Cl(4h)	4897(3)	2678(2)	4222(2)	156(9)
Co(i)	3668(2)	3355(1)	7607(1)	99(5)
Cl(1i)	4056(4)	3460(2)	8409(2)	204(11)
Cl(2i)	3302(4)	4140(2)	7179(2)	177(10)
Cl(3i)	2546(3)	2713(2)	7467(2)	157(10)
Cl(4i)	5005(3)	3088(2)	7212(2)	144(9)
Co(j)	3659(2)	1689(1)	2582(1)	99(5)
Cl(1j)	4001(4)	1603(2)	3398(2)	193(11)
Cl(2j)	3313(4)	899(2)	2175(2)	154(10)
Cl(3j)	2538(3)	2322(2)	2429(2)	150(9)
Cl(4j)	4994(3)	1967(2)	2202(2)	157(10)
Co(k)	3909(2)	1661(1)	5949(1)	101(5)
Cl(1k)	3996(4)	1567(2)	6779(2)	170(10)
Cl(2k)	4326(4)	862(2)	5568(2)	215(11)
Cl(3k)	2502(3)	1897(2)	5633(2)	192(10)
Cl(4k)	4898(4)	2328(3)	5705(2)	263(13)
Co(l)	3738(2)	1618(1)	9285(1)	92(5)
Cl(1l)	3341(3)	1506(2)	10095(2)	137(9)
Cl(2l)	4050(4)	826(2)	8871(2)	163(10)
Cl(3l)	2415(4)	1944(2)	8907(2)	185(11)
Cl(4l)	4926(3)	2215(2)	9151(2)	142(9)

Table 39A-6-004. K_2CoCl_4. Crystal structure of phase IV [91Mas]. Bond distances [Å] and angles [°] of $CoCl_4$ groups. Here, for example, Co(a) – Cl(1a) and Cl(1a) – Co(a) – Cl(2a) are abbreviated by (a – 1) and (1 – a – 2), respectively. For atom numbering, see Table 39A-6-003. The mean values are 2.267(22) Å and 109.4(41)°, respectively. T = 134 K.

(a-1)	2.263(31)	(a-2)	2.264(53)	(a-3)	2.295(45)	(a-4)	2.258(38)
(b-1)	2.262(20)	(b-2)	2.256(49)	(b-3)	2.244(37)	(b-4)	2.279(48)
(c-1)	2.264(24)	(c-2)	2.278(51)	(c-3)	2.237(40)	(c-4)	2.288(42)
(d-1)	2.280(26)	(d-2)	2.270(50)	(d-3)	2.245(39)	(d-4)	2.286(41)
(e-1)	2.254(28)	(e-2)	2.295(52)	(e-3)	2.274(43)	(e-4)	2.233(39)
(f-1)	2.276(22)	(f-2)	2.289(52)	(f-3)	2.234(31)	(f-4)	2.239(45)
(g-1)	2.200(24)	(g-2)	2.288(53)	(g-3)	2.264(35)	(g-4)	2.269(49)
(h-1)	2.247(29)	(h-2)	2.271(53)	(h-3)	2.313(44)	(h-4)	2.246(38)
(i-1)	2.227(25)	(i-2)	2.302(53)	(i-3)	2.289(41)	(i-4)	2.293(42)
(j-1)	2.242(22)	(j-2)	2.281(51)	(j-3)	2.280(41)	(j-4)	2.280(41)
(k-1)	2.231(14)	(k-2)	2.291(50)	(k-3)	2.271(36)	(k-4)	2.267(45)
(l-1)	2.252(26)	(l-2)	2.282(52)	(l-3)	2.302(43)	(l-4)	2.284(40)

(1-a-2)	112.5(20)	(1-a-3)	105.1(18)	(1-a-4)	114.9(23)
(2-a-3)	104.5(17)	(2-a-4)	112.1(14)	(3-a-4)	106.6(14)
(1-b-2)	111.4(23)	(1-b-3)	117.4(21)	(1-b-4)	108.7(21)
(2-b-3)	106.2(17)	(2-b-4)	106.9(15)	(3-b-4)	105.7(14)
(1-c-2)	115.9(22)	(1-c-3)	114.0(24)	(1-c-4)	103.7(18)
(2-c-3)	111.5(13)	(2-c-4)	103.7(18)	(3-c-4)	106.7(15)
(1-d-2)	114.7(22)	(1-d-3)	113.1(24)	(1-d-4)	103.6(17)
(2-d-3)	112.2(12)	(2-d-4)	104.1(18)	(3-d-4)	108.1(16)
(1-e-2)	113.8(21)	(1-e-3)	105.5(17)	(1-e-4)	114.9(23)
(2-e-3)	105.6(18)	(2-e-4)	108.1(13)	(3-e-4)	108.5(15)
(1-f-2)	108.9(22)	(1-f-3)	115.3(20)	(1-f-4)	109.1(24)
(2-f-3)	109.3(18)	(2-f-4)	108.5(12)	(3-f-4)	105.6(14)
(1-g-2)	110.7(21)	(1-g-3)	116.6(21)	(1-g-4)	110.3(21)
(2-g-3)	106.8(17)	(2-g-4)	106.3(14)	(3-g-4)	105.5(13)
(1-h-2)	114.5(20)	(1-h-3)	105.0(17)	(1-h-4)	112.3(24)
(2-h-3)	103.8(17)	(2-h-4)	112.0(13)	(3-h-4)	108.5(15)
(1-i-2)	115.9(21)	(1-i-3)	114.4(24)	(1-i-4)	105.3(17)
(2-i-3)	109.6(13)	(2-i-4)	101.8(18)	(3-i-4)	108.7(15)
(1-j-2)	115.5(22)	(1-j-3)	113.2(24)	(1-j-4)	106.0(18)
(2-j-3)	109.9(13)	(2-j-4)	103.1(18)	(3-j-4)	108.3(15)
(1-k-2)	109.7(23)	(1-k-3)	116.3(19)	(1-k-4)	108.9(24)
(2-k-3)	106.8(18)	(2-k-4)	109.1(12)	(3-k-4)	105.7(16)
(1-l-2)	114.2(21)	(1-l-3)	104.6(18)	(1-l-4)	114.8(23)
(2-1-3)	104.4(18)	(2-1-4)	108.9(14)	(3-1-4)	109.2(14

Table 39A-6-005. K_2CoCl_4. Static displacement and rotation of $CoCl_4$(b) [91Mas]. $A(X)$: translation of the center of mass along the *a* axis, $A(\Phi_y)$: rotation about the *b* axis, $A(\Phi_z)$: rotation about the *c* axis. $CoCl_4$(b)'s in phase III split into 4 groups (b), (g), (f) and (k) in phase IV. For atom numbering, see Table 39A-6-001 and Table 39A-6-003.

	$A(X)$ [Å]	$A(\Phi_y)$ [°]	$A(\Phi_z)$ [°]
298 K			
(b)	0.18	–6.7	6.7
134 K			
(b)	0.14	–9.4	2.4
(g)	0.14	10.9	4.1
(f)	0.23	–7.7	–14.9
(k)	0.21	3.3	–16.9