Table 39A-10-001. Rb_2ZnCl_4. Fractional coordinates and anisotropic temperature parameters at 50 °C (phase I) [83Ito]. U_{ij} [$\cdot 10^{-2}$ Å^2] is defined by Eq. (d) in Introduction. (′) on Cl denotes one of the disordered arrangements. See Fig. 39A-10-001.

Atom	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Rb(1)	0.25	0.6808(1)	0.5151(1)	6.08(6)	3.43(5)	2.94(4)	0.0	0.0	−0.12(4)
Rb(2)	0.25	0.4066(1)	0.8680(1)	6.81(8)	10.59(10)	3.08(5)	0.0	0.0	0.57(6)
Zn	0.25	0.4225(1)	0.2752(1)	3.78(6)	3.51(6)	2.90(6)	0.0	0.0	0.00(5)
Cl(1)′	0.2826(14)	0.4176(3)	0.5159(3)	6.0(8)	5.7(2)	1.9(1)	1.6(3)	0.3(2)	0.8(1)
Cl(2)′	0.2205(29)	0.5857(3)	0.1821(3)	7.9(13)	3.1(1)	3.2(1)	0.7(3)	−0.2(2)	1.1(1)
Cl(3)′	0.0173(6)	0.3405(5)	0.1866(5)	3.5(2)	13.3(4)	6.6(3)	−4.8(3)	1.0(2)	−4.3(3)
Cl(4)′	0.5128(5)	0.3435(4)	0.1825(4)	2.8(2)	9.5(3)	4.9(2)	3.2(2)	−0.4(2)	−2.3(2)

Table 39A-10-002. Rb_2ZnCl_4. Interatomic distances [Å] around Rb at 50 °C (phase I) [83Ito]. (′) on Cl denotes one of the disordered arrangements. See Fig. 39A-10-001.

Rb(1)–Cl(1)′	3.355(4)	Rb(1)–Cl(3^{iv})′	3.388(5)
–Cl(2)′	3.318(4)	–Cl(4^{v})′	3.257(4)
–Cl(2^{ii})′	3.354(4)	–Cl(4^{vi})′	3.303(4)
–Cl(3^{iii})′	3.376(5)		
Rb(2)–Cl(1)′	3.271(3)	Rb(2)–Cl(3^{vii})′	3.503(5)
–Cl(2^{iv})′	3.46(2)	–Cl(4^{vii})′	3.574(4)

Symmetry code: (i) x, y, z; (ii) $x, 1.5-y, 0.5+z$; (iii) $0.5+x, 0.5+y, 0.5-z$; (iv) $0.5+x, 1-y, 1-z$; (v) $-0.5+x, 0.5+y, 0.5-z$; (vi) $-0.5+x, 1-y, 1-z$; (vii) $x, y, 1+z$. For simplicity the code (i) is omitted in the table.

Table 39A-10-003. Rb_2ZnCl_4. Bond lengths [Å] and angles [°] of $ZnCl_4$ at 50 °C (phase I) [83Ito]. (′) on Cl denotes one of the disordered arrangements. See Fig. 39A-10-001.

Zn–Cl(1)′	2.241(3)	Zn–Cl(3)′	2.151(5)
Zn–Cl(2)′	2.258(4)	Zn–Cl(4)′	2.324(4)
Cl(1)′–Zn–Cl(2)′	114.5(1)	Cl(2)′–Zn–Cl(3)′	103.0(5)
Cl(1)′–Zn–Cl(3)′	116.7(3)	Cl(2)′–Zn–Cl(4)′	109.5(5)
Cl(1)′–Zn–Cl(4)′	105.6(3)	Cl(3)′–Zn–Cl(4)′	107.3(2)

Table 39A-10-004. Rb_2ZnCl_4. Fractional coordinates and anisotropic temperature parameters at 18 °C (phase II) [81Har]. The temperature parameter b_{ij} is defined by Eq. (b) in Introduction.

Atom	x	y	z
Rb(1)	0.25	0.4053(5)	0.6315(3)
Rb(2)	0.25	0.8203(4)	0.4849
Zn	0.25	0.4217(5)	0.2246(3)
Cl(1)	0.25	0.4144(12)	−0.0172(7)
Cl(2)	0.25	0.5897(12)	0.3192(7)
Cl(3)	−0.0001(7)	0.3413(8)	0.3140(6)

Atom	b_{11}	b_{22}	b_{33}	b_{12}	b_{23}	b_{13}
Rb(1)	0.0261(7)	0.0154(8)	0.0073(3)	0.0	−0.0006(3)	0.0
Rb(2)	0.0244(6)	0.0059(7)	0.0072(2)	0.0	0.0001(3)	0.0
Zn	0.0160(6)	0.0077(9)	0.0063(3)	0.0	−0.0002(3)	0.0
Cl(1)	0.0493(31)	0.0079(21)	0.0056(7)	0.0	−0.0012(8)	0.0
Cl(2)	0.0563(36)	0.0060(22)	0.0073(7)	0.0	−0.0030(8)	0.0
Cl(3)	0.0162(10)	0.0184(15)	0.0149(7)	−0.0086(10)	0.0070(8)	0.0021(7)

Table 39A-10-005. Rb_2ZnCl_4. Bond lengths [Å] and angles [°] of $ZnCl_4$ at 18 °C (phase II) [81Har].

Zn–Cl(1)	2.241(7)	Cl(1)–Zn–Cl(2)	114.7(4)
Zn–Cl(2)	2.311(15)	Cl(1)–Zn–Cl(3)	110.4(4)
Zn–Cl(3)	2.247(7)	Cl(2)–Zn–Cl(3)	106.4(3)
Cl(1)–Cl(2)	3.832(15)	Cl(3)–Zn–Cl(3)	108.3(3)
Cl(1)–Cl(3)	3.686(9)		
Cl(2)–Cl(3)	3.649(16)		
Cl(3)–Cl(3)	3.641(7)		

Table 39A-10-006. Rb_2ZnCl_4. r.m.s amplitudes [Å] of thermal vibrations along the principal axes at 18 °C (phase II) [81Har].

Rb(1)	0.27	0.36	0.18
Rb(2)	0.26	0.22	0.18
Zn	0.21	0.25	0.17
Cl(1)	0.37	0.25	0.16
Cl(2)	0.39	0.22	0.18
Cl(3)	0.19	0.49	0.17

Table 39A-10-007. Rb_2ZnCl_4. Fractional coordinates and anisotropic temperature parameters at 146 K (phase III) [89Ito]. U_{ij} [$\cdot 10^{-2}$ Å^2] is defined by Eq. (d) in Introduction.

Atom	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Rb(11)	0.2730(1)	0.68062(7)	0.17097(3)	2.86(5)	1.71(4)	1.31(4)	0.04(4)	–0.10(3)	–0.12(3)
Rb(12)	0.2449(1)	0.68110(6)	0.50434(3)	2.64(5)	1.65(4)	1.33(3)	–0.40(4)	0.23(3)	–0.02(3)
Rb(13)	0.2770(1)	0.68106(7)	0.83716(3)	2.84(5)	1.68(4)	1.38(4)	0.18(4)	–0.18(3)	–0.07(3)
Rb(21)	0.2788(1)	0.40432(9)	0.29067(3)	3.27(5)	4.74(4)	1.41(4)	–0.15(5)	–0.30(4)	0.03(4)
Rb(22)	0.2609(1)	0.40348(9)	0.62302(3)	3.64(6)	5.67(7)	1.35(4)	0.86(5)	0.36(4)	0.23(4)
Rb(23)	0.2444(1)	0.40937(8)	0.95724(3)	3.62(6)	4.51(6)	1.23(4)	0.16(5)	0.03(4)	0.07(4)
Zn(1)	0.25	0.42132(9)	0.09265(4)	2.20(6)	1.93(5)	1.65(5)	0.19(5)	–0.32(5)	0.00(4)
Zn(2)	0.2703(1)	0.42202(9)	0.42581(4)	2.08(6)	2.02(5)	1.63(5)	0.37(5)	–0.15(4)	–0.02(4)
Zn(3)	0.2653(1)	0.42149(9)	0.75852(4)	2.09(6)	2.20(5)	1.50(5)	0.26(5)	–0.21(4)	0.12(4)
Cl(11)	0.2329(4)	0.4187(2)	0.17348(7)	5.1(2)	2.7(1)	0.5(1)	–0.8(1)	–0.6(1)	0.3(1)
Cl(12)	0.3125(4)	0.4235(2)	0.50635(8)	3.7(1)	2.6(1)	0.8(1)	1.5(1)	–0.1(1)	0.2(1)
Cl(13)	0.2437(4)	0.4199(2)	0.83940(8)	5.5(2)	2.4(1)	0.6(1)	–1.0(1)	–0.1(1)	0.3(1)
Cl(21)	0.2230(4)	0.5842(2)	0.05946(7)	5.1(1)	1.4(1)	1.2(1)	0.4(1)	–0.3(1)	0.5(1)
Cl(22)	0.2244(4)	0.5834(2)	0.39204(7)	3.8(1)	1.3(1)	0.9(1)	0.5(1)	0.0(1)	0.5(1)
Cl(23)	0.3189(4)	0.5832(2)	0.72532(8)	4.3(1)	1.3(1)	1.3(1)	–0.6(1)	0.0(1)	0.5(1)
Cl(31)	0.0231(4)	0.3210(2)	0.06127(8)	2.6(1)	5.3(2)	2.0(1)	–2.5(1)	0.4(1)	–1.7(1)
Cl(32)	0.0379(3)	0.3155(2)	0.40387(8)	2.2(1)	3.3(1)	2.8(1)	–1.1(1)	0.3(1)	–1.2(1)
Cl(33)	–0.0012(3)	0.3644(2)	0.72531(8)	1.8(1)	3.7(1)	1.7(1)	–0.7(1)	–0.3(1)	–0.5(1)
Cl(41)	0.5197(3)	0.3549(2)	0.06421(9)	1.5(1)	4.0(1)	2.9(1)	1.5(1)	–0.5(1)	–1.7(1)
Cl(42)	0.5344(3)	0.3609(2)	0.39009(7)	1.0(1)	3.4(1)	1.1(1)	1.1(1)	–0.1(1)	–0.4(1)
Cl(43)	0.4921(3)	0.3114(2)	0.73401(9)	1.8(1)	3.9(1)	2.8(1)	1.6(1)	–0.2(1)	–1.0(1)

Table 39A-10-008. Rb_2ZnCl_4. Interatomic distances [Å] around Rb at 146 K (phase III) [89Ito].

Rb(11)–Cl(11)	3.318(3)	Rb(11)–Cl(33^{iv})	3.344(2)
–Cl(21)	3.328(2)	–Cl(42^{v})	3.316(2)
–Cl(23^{ii})	3.352(2)	–Cl(43^{vi})	3.319(3)
–Cl(32^{iii})	3.292(3)		
Rb(12)–Cl(12)	3.287(3)	Rb(12)–Cl(31^{iii})	3.232(3)
–Cl(12^{vi})	3.408(3)	–Cl(32^{iv})	3.303(2)
–Cl(21^{vii})	3.332(2)	–Cl(41^{v})	3.323(3)
–Cl(22)	3.338(2)	–Cl(42^{vi})	3.330(2)
Rb(13)–Cl(11^{iv})	3.543(3)	Rb(13)–Cl(31^{iv})	3.321(2)
–Cl(13)	3.305(3)	–Cl(33^{viii})	3.301(3)
–Cl(22^{vii})	3.357(2)	–Cl(41^{vi})	3.328(3)
–Cl(23)	3.337(2)	–Cl(43^{ix})	3.288(3)
Rb(21)–Cl(11)	3.256(2)	Rb(21)–Cl(42)	3.353(2)
–Cl(23^{vi})	3.361(3)	–Cl(43^{x})	3.498(3)
–Cl(33^{iv})	3.353(3)		
Rb(22)–Cl(12)	3.251(2)	Rb(22)–Cl(33)	3.436(2)
–Cl(22^{iv})	3.383(3)	–Cl(42^{vi})	3.414(3)
Rb(23)–Cl(13)	3.254(2)	Rb(23)–Cl(31^{xi})	3.471(3)
–Cl(21^{xi})	3.584(2)	–Cl(32^{xii})	3.529(3)
–Cl(21^{iv})	3.495(3)	–Cl(41^{vi})	3.441(3)

Symmetry code: (i) x, y, z; (ii) $x, -y + 1.5, z - 0.5$;
(iii) $x + 0.5, y + 0.5, -z + 0.5$; (iv) $x + 0.5, -y + 1, -z + 1$;
(v) $x - 0.5, y + 0.5, -z + 0.5$; (vi) $x - 0.5, -y + 1, -z + 1$;
(vii) $x, -y + 1.5, z + 0.5$; (viii) $x + 0.5, y + 0.5, -z + 1.5$;
(ix) $x - 0.5, y + 0.5, -z + 1.5$; (x) $x, -y + 0.5, z - 0.5$;
(xi) $x, y, z + 1$; (xii) $x, -y + 0.5, z + 0.5$.
For simplicity the code (i) is omitted in the table.

Table 39A-10-009. Rb_2ZnCl_4. Interatomic distances [Å] and angles [°] of $ZnCl_4$ groups at 146 K (phase III) [89Ito].

Zn(1)–Cl(11)	2.234(2)	Zn(2)–Cl(32)	2.236(3)
–Cl(21)	2.259(2)	–Cl(42)	2.284(2)
–Cl(31)	2.247(3)	Zn(3)–Cl(13)	2.237(2)
–Cl(41)	2.264(3)	–Cl(23)	2.270(2)
Zn(2)–Cl(12)	2.243(2)	–Cl(33)	2.253(3)
–Cl(22)	2.263(2)	–Cl(43)	2.254(3)
Cl(11)–Zn(1)–Cl(21)	114.4(1)	Cl(22)–Zn(2)–Cl(32)	108.6(1)
Cl(11)–Zn(1)–Cl(31)	109.6(1)	Cl(22)–Zn(2)–Cl(42)	104.4(1)
Cl(11)–Zn(1)–Cl(41)	112.9(1)	Cl(32)–Zn(2)–Cl(42)	108.0(1)
Cl(21)–Zn(1)–Cl(31)	107.1(1)	Cl(13)–Zn(3)–Cl(23)	115.0(1)
Cl(21)–Zn(1)–Cl(41)	105.7(1)	Cl(13)–Zn(3)–Cl(33)	110.1(1)
Cl(31)–Zn(1)–Cl(41)	106.7(1)	Cl(13)–Zn(3)–Cl(43)	110.2(1)
Cl(12)–Zn(2)–Cl(22)	114.8(1)	Cl(23)–Zn(3)–Cl(33)	105.6(1)
Cl(12)–Zn(2)–Cl(32)	112.1(1)	Cl(23)–Zn(3)–Cl(43)	108.0(1)
Cl(12)–Zn(2)–Cl(42)	108.4(1)	Cl(33)–Zn(3)–Cl(43)	107.7(1)

Table 39A-10-010. Rb_2ZnCl_4. Elastic stiffness constants [89Hor]. T = 300 K. Brillouin 90° scattering. λ = 514.5 nm.

c_{11}	c_{22}	c_{33}	c_{44}	c_{55}	c_{66}	c_{12}	c_{13}	c_{23}
[$\cdot 10^9$ N m^{-2}]								
19.27(19)	20.96(19)	28.2(5)	6.10(5)	6.22(5)	3.67(8)	8.53(14)	9.2(6)	9.4(2)

Table 39A-10-011. Rb_2ZnCl_4. n vs. λ at RT [82Gun].

λ [nm]	n_a	n_b	n_c
488	1.576	1.571	1.585
514.5	1.573	1.568	1.581
547	1.568	1.564	1.578
588	1.565	1.561	1.575
632.8	1.564	1.559	1.572

Table 39A-10-012. Rb_2ZnCl_4. Electrooptic properties [84San]. V_π: half-wave voltage. $r_{\lambda i}$: constant for $\boldsymbol{E}$, $\rho_{\lambda i}$: constant for $\boldsymbol{P}$. $r_a = r_{31} - (n_2/n_3)^3 r_{21}$, $r_b = r_{11} - (n_3/n_1)^3 r_{31}$, $r_c = r_{11} - (n_2/n_1)^3 r_{21}$. $\rho_a = \rho_{31} - (n_2/n_3)^3 \rho_{21}$, $\rho_b = \rho_{11} - (n_3/n_1)^3 \rho_{31}$, $\rho_c = \rho_{11} - (n_2/n_1)^3 \rho_{21}$. λ = 633 nm. T = 186.6 K.

λi	V_π [kV]	$r_{\lambda i}$ [$\cdot 10^{-12}$ m V^{-1}]	$\varrho_{\lambda i}$ [$\cdot 10^{-2}$ m^2 C^{-1}]
11	–	0.3(1)	0.14(5)
21	–	1.5(1)	0.68(6)
31	–	1.0(5)	0.5(2)
a	313(6)	0.52(1)	0.24(1)
b	247(11)	0.67(3)	0.31(2)
c	141(2)	1.17(2)	0.53(2)

Table 39A-10-013. Rb_2ZnCl_4. Nonlinear optical properties [85San1]. l_{ij}: coherence length. λ = 1.06 μm.

T [K]	d_{11} [$\cdot 10^{-12}$ m V^{-1}]	d_{12} [$\cdot 10^{-12}$ m V^{-1}]	d_{26} [$\cdot 10^{-12}$ m V^{-1}]	l_{11} [μm]	l_{12} [μm]	l_{26} [μm]
100	0.085(15)	0.075(15)	0.069(15)	14.5(2)	13.5(2)	15.5(2)
190	0.045(10)	0.041(10)	0.037(10)	14.5(2)	12.5(2)	15.5(2)

Table 39A-10-014. Rb_2ZnCl_4. Principal values and direction cosines of ^{87}Rb quadrupole coupling tensors [80Nak]. T = 35.0 °C.

	$\lvert eQ\phi_{ii}/h\rvert$	Direction cosines		
	[kHz]	*a*	*b*	*c*
Rb(1)	5487	1	0	0
	89	0	0.9888	∓0.1491
	5398	0	±0.1491	0.9888
Rb(2)	510	1	0	0
	3755	0	0.9987	∓0.0513
	3246	0	±0.0513	0.9987

Table 39A-10-015. Rb_2ZnCl_4. ^{87}Rb quadrupole coupling tensors [MHz] in the crystallographic *a*, *b*, *c* frame [81Rut]. For 27 °C, only those tensors which correspond to the extreme incommensurate wave are listed.

	$T = 35\,°C > \Theta_{II-I}$				$T = 27\,°C < \Theta_{II-I}$			
Rb(1):		−5.48	0.0	0		−5.48	±0.65	∓0.30
	$\frac{eQ\phi_{ij}}{h} =$		0.24	∓0.8	$\frac{eQ\phi_{ij}}{h} =$		0.24	∓0.80
				5.24				5.24
Rb(2):		0.48	0.0	0.0		0.48	∓0.4	∓0.7
	$\frac{eQ\phi_{ij}}{h} =$		−3.75	∓0.15	$\frac{eQ\phi_{ij}}{h} =$		−3.75	∓0.2
				3.27				3.27

Table 39A-10-016. Rb_2ZnCl_4. ESR of Mn^{2+} [84Boc]. Spin Hamiltonian parameters of Mn^{2+}. T = 318 K. Spin Hamiltonian is given by Eq. (7) in Introduction.

g	*D*	*E*	*a*	*A*
	$[\cdot 10^{-2}\ m^{-1}]$			
2.0038	449	–85.1	–4.8	73

Table 39A-10-017. Rb_2ZnCl_4, $(Rb_{0.995}K_{0.005})_2ZnCl_4$. Critical exponents β, γ and ν determined by X-ray scattering [83And].

		β	γ	ν
Experiment	Rb_2ZnCl_4	0.345(5) [a]	$1.26(^{+4}_{-2})$	0.693(15)
	$(Rb_{0.995}K_{0.005})_2ZnCl_4$	0.350(5) [b]	1.31(5)	0.683(15)

[a]) [81Mas], [b]) [83Mas].