Table 39A-17-001. Rb_2ZnBr_4. Fractional coordinates in phase I at 368(3) K [95Nov]. Used crystallographic axes are (***a′***, ***b′***, ***c′***), the case 2 in 3a.

Parameter	Zn	Br(1)	Br(2)	Br(3)	Rb(1)	Rb(2)
x	0.0772(2)	0.0838(3)	0.0879(3)	0.1586(3)	0.0964(3)	0.1766(2)
y	0.7500	0.7500	0.2500	0.4992(7)	0.7500	0.2500
z	0.2742(3)	0.5170(3)	0.8186(4)	0.1827(3)	0.8711(4)	0.4838(3)

Table 39A-17-002. Rb_2ZnBr_4. Temperature parameters in phase I at 368(3) K [95Nov]. b_{ij} is defined by Eq. (b) in Introduction. c_{ijk}, d_{ijkl}: the third and fourth-rank tensor of the Gram-Charlier expansion in 10^{-3} and in 10^{-4}, respectively. Anharmonicity was introduced only for Br atoms. Only those anharmonic terms whose values exceeded standard deviations were refined. Used crystallographic axes are (***a′***, ***b′***, ***c′***), the case 2 in 3a.

Parameter	Zn	Br(1)	Br(2)	Br(3)	Rb(1)	Rb(2)
*b*11	0.0039(2)	0.0085(4)	0.0056(4)	0.0158(4)	0.0161(4)	0.0051(2)
*b*22	0.0177(8)	0.0618(2)	0.075(2)	0.0209(7)	0.033(1)	0.032(1)
*b*33	0.0093(4)	0.0126(2)	0.0199(5)	0.0315(5)	0.0122(4)	0.0110(4)
*b*12	0	0	0	0.0086(6)	0	0
*b*13	–0.0003(2)	–0.0022(3)	–0.0035(6)	0.0082(6)	–0.0013(4)	0.0006(3)
*b*23	0	0	0	0.0021(6)	0	0
*c*111	0	0	0	0	0	0
*c*222	0	0	0	0	0	0
*c*333	0	0	0	0	0	0
*c*112	0	0	0	0.002(1)	0	0
*c*122	0	–0.016(4)	–0.009(4)	0.003(2)	0	0
*c*113	0	0	0.0018(8)	0.002(1)	0	0
*c*133	0	0	0	0.004(1)	0	0
*c*123	0	0	0	0.002(1)	0	0
*c*223	0	0	0	0	0	0
*c*233	0	0	0	0	0	0
*d*1111	0	0.0014(7)	–0.0011(3)	–0.0039(7)	0	0
*d*2222	0	0	0	–0.008(2)	0	0
*d*3333	0	0.008(1)	0.017(4)	0.047(2)	0	0
*d*1112	0	0	0	–0.001(1)	0	0
*d*1122	0	0	0.0028(8)	–0.0025(9)	0	0
*d*1222	0	0	0	–0.003(2)	0	0
*d*1113	0	0	0	0	0	0
*d*1133	0	0	0.0022(8)	0.0020(9)	0	0
*d*1333	0	0	–0.004(2)	0	0	0
*d*1223	0	0	0	0	0	0
*d*1233	0	0	0	0	0	0
*d*2223	0	0	0	0	0	0
*d*2233	0	0	0.014(4)	0	0	0
*d*2333	0	0	0	0	0	0
*d*2311	0	0	0	–0.0012(9)	0	0

Table 39A-17-003. Rb_2ZnBr_4. Fractional coordinates [$\cdot 10^{-4}$] and Fourier coefficients of the modulation functions [$\cdot 10^{-4}$] in phase II at 293 K and phase III at 140 K [88Hog]. Displacive modulation functions are defined as $d_i(t) = d_{ic} \cos 2\pi t + d_{is} \sin 2\pi t$, in which $t = (\boldsymbol{n} + \boldsymbol{x}_0) \cdot \boldsymbol{q}$, $\boldsymbol{n}$ is the position of the subcell, $\boldsymbol{x}_0$ is the basic structure position of the atom, $\boldsymbol{q}$ is the modulation wavevector. $\boldsymbol{q} = 0.293\boldsymbol{c}^*$ at 293 K [83Iiz] and $\boldsymbol{q} = 1/3\boldsymbol{c}^*$ in phase III. Used crystallographic axes are ($\boldsymbol{a}'$, $\boldsymbol{b}'$, $\boldsymbol{c}'$), the case 2 in 3a.

		293 K			140 K		
	i	x_{0i}	d_{ic}	d_{is}	x_{0i}	d_{ic}	d_{is}
Rb(1)	1	3234(1)	0	0	3229(1)	23(3)	–24(3)
	2	2500	–11(5)	–147(4)	2476(8)	149(3)	167(3)
	3	5153(1)	0	0	5127(1)	0(4)	–14(5)
Rb(2)	1	5968(1)	0	0	5970(2)	20(5)	53(4)
	2	2500	110(5)	91(5)	2530(9)	–195(4)	–34(4)
	3	8730(1)	0	0	8759(2)	16(5)	–28(5)
Zn	1	5777(1)	0	0	5785(1)	–6(3)	10(4)
	2	2500	–30(4)	93(4)	2491	–17(3)	–137(3)
	3	2746(1)	0	0	2766(1)	1(5)	–11(5)
Br(1)	1	5831(1)	0	0	5803(1)	–27(3)	–46(3)
	2	2500	–60(6)	349(5)	2479(8)	–169(5)	–508(4)
	3	5184(1)	0	0	5224(1)	40(4)	7(4)
Br(2)	1	4126(1)	0	0	4146(1)	–1(3)	13(3)
	2	2500	–516(5)	59(7)	2603(8)	545(5)	–438(5)
	3	1802(1)	0	0	1756(2)	4(5)	–23(4)
Br(3)	1	6593(1)	–252(2)	1(3)	6687(2)	291(3)	–178(3)
	2	5012(1)	183(3)	62(4)	4966(6)	–243(5)	62(4)
	3	1839(1)	–118(3)	–92(3)	1910(3)	240(4)	58(4)
Br(4)	1				6569(2)	–297(3)	182(3)
	2				–47(6)	–278(5)	85(5)
	3				1858(3)	–184(4)	–9(3)

Table 39A-17-004. Rb_2ZnBr_4. Amplitudes A_i [$\cdot 10^{-4}$] and phases ϕ_i of the modulation functions in phase II at 293 K and phase III at 140 K [88Hog]. A_i and ϕ_i are defined as $d_i(t) = A_i \cos 2\pi(t - \phi_i)$; see caption of Table. 39A-17-003 for the definition of $d_i(t)$. 5/12 has been added to the phases at 293 K in order to make them comparable with those at 140 K. Used crystallographic axes are (***a′***, ***b′***, ***c′***), the case 2 in 3a.

		293 K		140 K	
	i	A_i	ϕ_i	A_i	ϕ_i
Rb(1)	1	0		33(3)	0.87(1)
	2	147(4)	0.155(4)	223(3)	0.134(2)
	3	0		14(5)	0.75(5)
Rb(2)	1	0		56(4)	0.19(1)
	2	143(5)	0.527(5)	198(4)	0.527(3)
	3	0		32(5)	0.84(2)
Zn	1	0		12(4)	0.33(5)
	2	98(4)	0.716(6)	138(3)	0.730(4)
	3	0		11(5)	0.76(7)
Br(1)	1	0		53(3)	0.67(1)
	2	354(5)	0.694(2)	535(4)	0.699(1)
	3	0		41(4)	0.03(1)
Br(2)	1	0		13(3)	0.27(4)
	2	520(5)	0.899(2)	699(5)	0.892(1)
	3	0		23(4)	0.77(3)
Br(3)	1	252(2)	0.916(1)	341(3)	0.913(1)
	2	193(3)	0.468(2)	251(5)	0.460(3)
	3	150(3)	0.022(3)	247(4)	0.038(2)
Br(4)	1			348(3)	0.413(1)
	2			291(5)	0.453(3)
	3			184(4)	0.508(3)

Table 39A-17-005. Rb_2ZnBr_4. Anisotropic temperature parameters [$\cdot 10^{-4}$ Å^2] in phase II at 293(2) K and phase III at 140(3) K [88Hog]. U_{ij} is defined by Eq. (d) in Introduction.

	293 K			140 K		
	U_{11} U_{23}	U_{22} U_{13}	U_{33} U_{12}	U_{11} U_{23}	U_{22} U_{13}	U_{33} U_{12}
Rb(1)	354(6) 0	593(9) 29(5)	367(6) 0	254(6) –22(18)	369(8) 9(5)	172(6) –1(13)
Rb(2)	1170(14) 0	696(11) –55(8)	369(8) 0	654(12) –8(19)	450(11) –6(7)	176(7) 90(21)
Zn	296(7) 0	279(7) –4(5)	292(7) 0	217(6) 4(18)	210(7) 0(5)	140(6) –2(16)
Br(1)	602(9) 0	1152(18) –74(6)	240(6) 0	376(8) –23(15)	540(13) –36(6)	119(6) –81(16)
Br(2)	338(7) 0	1165(22) –121(6)	414(8) 0	258(7) –10(17)	581(12) –54(6)	200(7) 53(15)
Br(3)	982(11) –46(6)	378(7) 250(9)	631(8) –316(8)	604(16) –25(12)	237(13) 133(13)	291(13) –165(12)
Br(4)				549(15) 10(12)	266(14) 71(13)	306(14) 90(12)

Table 39A-17-006. Rb_2ZnBr_4. Interatomic distances [$\cdot 10^{-3}$ Å] in $ZnBr_4$ tetrahedra in phase II at 293 K and phase III at 140 K [88Hog]. The estimated standard deviations are 0.004 and 0.008 Å for the distances at 293 and 140 K, respectively. Used crystallographic axes are (***a′***, ***b′***, ***c′***), the case 2 in 3a.

	293 K	140 K		
Zn–Br(1)	2360—2370	2417	2337	2373
Zn–Br(2)	2378—2409	2404	2411	2381
Zn–Br(3)	2361—2414	2382	2416	2418
Zn–Br(4)	2361—2414	2403	2360	2396
Br(1)–Br(2)	3982—4019	4043	4026	4010
Br(1)–Br(3)	3876—3937	3959	3876	3889
Br(1)–Br(4)	3876—3937	3904	3858	3984
Br(2)–Br(3)	3795—3874	3885	3824	3862
Br(2)–Br(4)	3795—3874	3814	3868	3812
Br(3)–Br(4)	3838—3900	3914	3857	3855

Table 39A-17-007. Rb_2ZnBr_4. Transition temperatures, transition heats (ΔQ) and transition entropies (ΔS) [83Nom].

$\Theta_{III–II}$ [K]	193.6(3)
$\Delta Q_{III–II}$ [J mol^{-1}]	9.3
$\Delta S_{III–II}$ [J K^{-1} mol^{-1}]	0.048
$\Theta_{IV–III}$ [K]	111.7(2)
$\Delta Q_{IV–III}$ [J mol^{-1}]	47
$\Delta S_{IV–III}$ [J K^{-1} mol^{-1}]	0.45
$\Theta_{V–IV}$ [K]	76.5(1)
$\Delta Q_{V–IV}$ [J mol^{-1}]	2.0
$\Delta S_{V–IV}$ [J K^{-1} mol^{-1}]	0.027

Table 39A-17-008. Rb_2ZnBr_4. $c_{\lambda\mu}$ at 300 K [89Hor]. Brillouin scattering. $\lambda = 5145$ Å.

c_{11}	c_{22}	c_{33}	c_{44}	c_{55}	c_{66}	c_{12}	c_{13}	c_{23}
[$\cdot 10^9$ Nm^{-2}]								
17.07(16)	17.54(16)	22.63(19)	4.73(4)	5.13(7)	3.41(7)	7.85(13)	8.70(16)	8.30(15)

Table 39A-17-009. Rb_2ZnBr_4. ^{87}Rb quadrupole coupling tensors [MHz] in the crystallographic *a*, *b*, *c* frame in phase I near $\Theta_{II–I}$ [87Wal]. Accuracy is better than ±0.010 MHz.

Rb(1)	–4.330	0	0
		–0.180	±0.225
			4.510
Rb(2)	0.765	0	0
		–3.115	±0.080
			2.350