Table 39A-18-001. $(NH_4)_2ZnBr_4$. Unit cell parameters and Z in phases I, III, IV [93Shi].

Phase	I	III	IV
T [°C]	175	25	–130
Z	4	16	12
a [Å]	7.649(2)	7.587(1)	7.531(2)
b [Å]	13.353(5)	13.220(5)	13.134(7)
c [Å]	9.727(3)	38.728(9)	28.976(7)
Angle [°]		$\alpha = 90.00(3)$	

Table 39A-18-002. $(NH_4)_2ZnBr_4$. Fractional coordinates [$\cdot 10^{-4}$] and equivalent isotropic temperature parameters [$\cdot 10^{-2}$ Å^2] in phase I at 175 °C [93Shi]. Fixed parameters are denoted by (*). $B_{eq} = 4\Sigma b_{ij}\boldsymbol{a}_i \cdot \boldsymbol{a}_j/3$, b_{ij} is defined by Eq. (b) in Introduction.

Atom	x	y	z	B_{eq}
Zn	2500(*)	4248(3)	2272(4)	478(10)
Br1	2159(13)	4164(4)	–147(4)	851(20)
Br2	2911(13)	5907(4)	3111(4)	937(27)
Br3	–120(8)	3643(5)	3331(6)	737(17)
Br4	4841(10)	3215(5)	3051(7)	885(20)
N1	2500(*)	1035(32)	1431(35)	938(130)
N2	2500(*)	8240(23)	4806(33)	746(108)

Table 39A-18-003. $(NH_4)_2ZnBr_4$. Fractional coordinates [$\cdot 10^{-4}$] and equivalent isotropic temperature parameters [$\cdot 10^{-2}$ Å^2] in phase III at 25 °C [93Shi]. $B_{eq} = 4\Sigma b_{ij}\boldsymbol{a}_i \cdot \boldsymbol{a}_j/3$, b_{ij} is defined by Eq. (b) in Introduction.

Atom	*x*	*y*	*z*	B_{eq}
Zn1	2425(9)	4246(5)	574(2)	307(14)
Zn2	2637(9)	771(5)	1789(2)	320(15)
Zn3	2413(8)	4239(5)	3074(2)	309(13)
Zn4	2475(8)	772(5)	4315(2)	315(14)
Br11	2568(14)	4204(6)	–49(1)	725(26)
Br12	1802(12)	5867(5)	796(2)	638(21)
Br13	241(8)	3059(5)	762(2)	509(18)
Br14	5182(8)	3744(6)	821(2)	516(18)
Br21	2823(11)	845(6)	1201(2)	590(21)
Br22	3107(13)	–889(5)	2037(1)	590(21)
Br23	–108(9)	1437(6)	2030(2)	590(20)
Br24	4837(11)	1853(6)	2057(2)	564(19)
Br31	1912(10)	4302(5)	2448(2)	476(17)
Br32	2979(12)	5887(5)	3297(2)	547(20)
Br33	–212(7)	3654(5)	3345(2)	401(15)
Br34	4814(10)	3157(6)	3204(2)	627(21)
Br41	2665(11)	866(6)	3728(2)	565(21)
Br42	1864(9)	–899(5)	4555(2)	462(17)
Br43	186(14)	1856(6)	4498(2)	679(24)
Br44	5249(12)	1337(5)	4569(2)	591(20)
N11	2470(72)	1115(40)	321(10)	503(159)
N12	2465(76)	8223(37)	1196(13)	528(158)
N21	2759(82)	4231(49)	1564(13)	689(192)
N22	2792(72)	6785(46)	2473(13)	582(167)
N31	2623(61)	1121(35)	2814(10)	392(131)
N32	2413(65)	8184(33)	3717(12)	378(123)
N41	2314(61)	4092(42)	4133(12)	457(143)
N42	2650(71)	6678(36)	4956(10)	392(127)

Table 39A-18-004. $(NH_4)_2ZnBr_4$. Fractional coordinates [$\cdot 10^{-4}$] and equivalent isotropic temperature parameters [$\cdot 10^{-2}$ Å^2] in phase IV at –130 °C [93Shi]. Fixed parameter is denoted by (*). $B_{eq} = 4\Sigma b_{ij}\boldsymbol{a}_i \cdot \boldsymbol{a}_j/3$, b_{ij} is defined by Eq. (b) in Introduction.

Atom	*x*	*y*	*z*	B_{eq}
Zn1	2500(*)	4269(3)	731(2)	143(8)
Zn2	2599(6)	4223(3)	4060(1)	148(8)
Zn3	2355(6)	4197(4)	7423(2)	157(9)
Br11	1883(6)	4357(3)	–72(1)	205(8)
Br12	3105(7)	5882(3)	1099(1)	212(8)
Br13	–163(6)	3607(3)	1102(1)	215(8)
Br14	4859(6)	3121(3)	905(1)	233(9)
Br21	2826(7)	4211(3)	3244(1)	250(10)
Br22	3265(7)	5853(3)	4388(1)	263(10)
Br23	–309(7)	3726(4)	4337(1)	254(9)
Br24	4623(6)	2994(3)	4381(1)	206(9)
Br31	2763(7)	4150(4)	6616(1)	267(10)
Br32	1719(7)	5833(3)	7756(1)	215(8)
Br33	63(6)	3017(4)	7642(1)	266(10)
Br34	5080(5)	3654(3)	7787(1)	210(9)
N11	2826(53)	1120(38)	454(15)	464(115)
N12	2331(45)	8303(30)	1636(13)	251(86)
N21	2764(49)	990(29)	3786(11)	250(83)
N22	2898(42)	8134(23)	4987(11)	169(68)
N31	2296(53)	951(32)	7100(11)	352(99)
N32	2317(48)	8218(22)	8283(10)	163(75)

Table 39A-18-005. $(NH_4)_2ZnBr_4$. Interatomic distances [Å] and angles [°] in phase I at 175 °C [93Shi].

Zn–Br1	2.370(6)
Zn–Br2	2.382(7)
Zn–Br3	2.394(7)
Zn–Br4	2.384(8)
(mean)	2.383
Br1–Zn–Br2	113.5(2)
Br1–Zn–Br3	108.6(3)
Br1–Zn–Br4	111.8(2)
Br2–Zn–Br3	106.0(2)
Br2–Zn–Br4	109.3(3)
Br3–Zn–Br4	107.3(2)
(mean)	109.4

Table 39A-18-006. $(NH_4)_2ZnBr_4$. Interatomic distances [Å] and angles [°] in phase III at 25 °C [93Shi].

ν	1	2	3	4
Znν–Brν1	2.419(8)	2.284(9)	2.458(8)	2.280(9)
Znν–Brν2	2.357(10)	2.424(9)	2.832(9)	2.443(10)
Znν–Brν3	2.395(9)	2.446(10)	2.380(8)	2.360(11)
Znν–Brν4	2.393(9)	2.431(10)	2.370(10)	2.441(11)
(mean)	2.391	2.396	2.398	2.381
Brν1–Znν–Brν2	113.2(1)	115.2(1)	110.7(1)	116.1(1)
Brν1–Znν–Brν3	108.6(2)	114.7(3)	108.4(3)	108.2(2)
Brν1–Znν–Brν4	110.7(3)	111.0(3)	110.4(2)	109.3(3)
Brν2–Znν–Brν3	110.2(3)	107.5(2)	106.8(2)	107.2(3)
Brν2–Znν–Brν4	106.4(2)	105.2(3)	109.7(3)	106.7(2)
Brν3–Znν–Brν4	107.6(1)	102.1(2)	110.7(2)	109.1(2)
(mean)	109.5	109.3	109.5	109.4

Table 39A-18-007. $(NH_4)_2ZnBr_4$. Interatomic distances [Å] and angles [°] in phase IV at –130 °C [93Shi].

ν	1	2	3
Znν–Brν1	2.377(6)	2.369(5)	2.361(6)
Znν–Brν2	2.415(6)	2.395(6)	2.402(6)
Znν–Brν3	2.436(5)	2.422(7)	2.405(7)
Znν–Brν4	2.384(5)	2.407(6)	2.414(6)
(mean)	2.403	2.398	2.396
Brν1–Znν–Brν2	115.3(1)	112.7(1)	116.5(1)
Brν1–Znν–Brν3	106.8(1)	113.2(2)	109.7(1)
Brν1–Znν–Brν4	112.6(1)	109.6(2)	108.3(2)
Brν2–Znν–Brν3	105.9(1)	107.4(1)	109.1(2)
Brν2–Znν–Brν4	108.7(2)	108.2(2)	105.0(1)
Brν3–Znν–Brν4	107.1(1)	105.3(1)	107.7(1)
(mean)	109.4	109.4	109.4