Table 39A-22-001. $[N(CH_3)_4]_2ZnI_4$. Fractional coordinates [$\cdot 10^{-4}$] and equivalent isotropic temperature parameters [$\cdot 10^{-4}$ Å^2] of phase I at 293 K and phase III at 150 K [90Wer]. $U_{eq} = \Sigma U_{ii}/3$, where U_{ii} is defined by Eq. (d) in Introduction. The origin of the z coordinate in phase III was fixed using the method of Flack and Schwarzenbach [88Fla]. Parameters of H: see [90Wer].

Atom	x	y	z	U_{eq}
(a) Phase I				
Zn	2500	4073.8(7)	2541.3(8)	674(7)
I(1)	2500	3989(5)	580.8(5)	970(6)
I(2)	2500	5538.7(5)	3183(7)	1173(7)
I(3)	284.1(8)	3363.3(5)	3225.6(5)	1214(6)
N(1)	2500	1005(6)	1516(6)	76(3)
C(11)	1910(30)	910(20)	2520(10)	1600(100)
C(12)	3320(50)	1660(20)	1320(40)	1900(200)
C(13)	3020(20)	210(10)	1080(20)	1500(100)
C(14)	1220(40)	1250(30)	1000(30)	2400(300)
N(2)	2500	8341(5)	4749(6)	710(30)
C(21)	2500	7543(9)	4380(10)	1570(900)
C(22)	1040(30)	8530(10)	5030(30)	1700(200)
C(23)	3220(30)	8340(20)	5680(20)	1600(200)
C(24)	3010(20)	8920(10)	4000(10)	1100(100)
(b) Phase III				
Zn(1)	2044(2)	2031.9(6)	2176(2)	280(9)
I(11)	2448(1)	1973.8(4)	199.6(9)	342(7)
I(12)	1633(1)	2773.8(3)	2773(1)	404(7)
I(13)	–166(1)	1593.4(3)	2642(1)	382(7)
I(14)	4264(1)	1749.0(4)	3104(1)	412(7)
Zn(2)	7385(2)	2984.0(6)	7069(2)	293(9)
I(21)	7246(1)	2994.0(4)	9071.9(8)	332(7)
I(22)	7204(1)	2245.3(3)	6389(1)	465(7)
I(23)	5320(1)	3408.5(4)	6321(1)	442(7)
I(24)	9780(1)	3301.1(4)	6499(1)	405(7)
N(1)	7950(10)	4500(4)	8090(10)	330(40)
C(11)	7530(20)	4900(6)	8520(20)	900(100)
C(12)	9470(20)	4450(6)	8240(20)	800(100)
C(13)	7220(20)	4177(7)	8600(20)	900(100)
C(14)	7570(20)	4484(7)	6960(10)	640(90)
N(2)	2170(20)	487(4)	1140(10)	390(50)
C(21)	3250(20)	813(6)	1250(20)	730(90)
C(22)	2870(20)	103(6)	780(20)	620(90)
C(23)	1080(30)	623(9)	390(20)	1100(100)
C(24)	1510(20)	423(6)	2140(10)	670(90)
N(3)	2490(10)	4210(4)	4380(10)	310(40)
C(31)	1670(20)	4252(6)	5330(10)	540(80)
C(32)	2380(20)	3790(6)	4000(10)	560(80)
C(33)	1880(20)	4499(5)	3600(10)	420(70)
C(34)	3960(20)	4318(6)	4540(10)	450(60)
N(4)	7200(10)	821(4)	4840(10)	320(40)
C(41)	7220(20)	1260(6)	5150(10)	490(60)
C(42)	6630(20)	570(5)	5670(10)	390(60)
C(43)	6330(20)	778(5)	3890(10)	490(70)
C(44)	8660(20)	690(5)	4640(10)	440(60)

Symmetry transformations: $x, y, z; -x+\frac{1}{2}, -y-\frac{1}{4}, \frac{1}{2}+z; -x+\frac{1}{2}, y+\frac{1}{2}, z; x, \frac{1}{4}-y, z+\frac{1}{2}$.

Table 39A-22-002. $[N(CH_3)_4]_2ZnI_4$. Fractional coordinates and equivalent isotropic temperature parameters [$\cdot 10^{-4}$ Å^2] in phase II at 250 K [90Has]. U_{eq} = (trace U)/3, where U_{ij} defined by Eq. (d) in Introduction is orthogonalized.

Atom	x	y	z	U_{eq}
Zn	0.2593(4)	0.4068(1)	0.2550(2)	5.0
I(1)	0.2386(3)	0.3992(1)	0.0583(1)	7.1
I(2)	0.2693(4)	0.5537(1)	0.3195(1)	9.5
I(3)	0.0421(2)	0.3373(1)	0.3326(2)	9.7
I(4)	0.4859(2)	0.3323(1)	0.3136(1)	9.0
N(1)	0.241(2)	0.100(1)	0.151(1)	6.4
C(1)	0.309(3)	0.094(2)	0.258(2)	12.9
C(2)	0.233(10)	0.027(2)	0.096(3)	21.4
C(3)	0.326(4)	0.162(3)	0.097(4)	20.3
C(4)	0.119(4)	0.137(3)	0.145(3)	20.8
N(2)	0.251(3)	0.836(1)	0,474(1)	5.5
C(5)	0.264(5)	0.752(1)	0.439(2)	11.5
C(6)	0.195(4)	0.894(2)	0.394(2)	10.9
C(7)	0.378(3)	0.863(2)	0.516(4)	16.3
C(8)	0.156(4)	0.837(2)	0.566(3)	13.9

Table 39A-22-003. $[N(CH_3)_4]_2ZnI_4$. Interatomic distances [Å] and angles [°] in phase I at 293 K and phase III at 150 K [90Wer]. For phase I, interatomic distances after thermal motion correction are given in the second column.

Phase I at T = 293 K						
Zn–I(1)	2.602(2)	2.623	I(1)–Zn–I(2)			112.28(5)
I(2)	2.593(2)	2.622	I(1)	I(3)		108.82(4)
I(3)	2.607(2)	2.639	I(2)	I(3)		108.44(4)
N(1)–C(11)	1.45(2)	1.55	C(11)–N(1)–C(12)			119(2)
C(12)	1.38(4)	1.48	C(11)	C(13)		112(1)
C(13)	1.53(2)	1.63	C(11)	C(14)		97(2)
C(14)	1.46(4)	1.59	C(12)	C(13)		115(2)
			C(12)	C(14)		100(3)
			C(13)	C(14)		110(2)
N(2)–C(21)	1.42(2)	1.49	C(21)–N(2)–C(22)			107(1)
C(22)	1.49(3)	1.58	C(21)	C(23)		107(1)
C(23)	1.42(3)	1.51	C(21)	C(24)		113(1)
C(24)	1.48(2)	1.51	C(22)	C(23)		104(2)
			C(22)	C(24)		110(1)
			C(23)	C(24)		115(1)
Phase III at T = 150 K						
Zn(1)–I(11)	2.626(3)		I(11)–Zn(1)–I(12)			112.80(9)
I(12)	2.601(2)		I(11)	I(13)		107.86(9)
I(13)	2.635(2)		I(11)	I(14)		108.17(8)
I(14)	2.621(3)		I(11)	I(13)		109.05(8)
			I(12)	I(14)		108.61(9)
			I(13)	I(14)		110.35(9)
Zn(2)–I(21)	2.628(3)		I(21)–Zn(2)–I(22)			110.51(8)
I(22)	2.602(2)		I(21)	I(23)		109.25(9)
I(23)	2.615(3)		I(21)	I(24)		108.85(9)
I(24)	2.629(3)		I(22)	I(23)		108.88(9)
			I(22)	I(24)		109.51(9)
			I(23)	I(24)		109.83(8)
N(1)–C(11)	1.46(2)		C(11)–N(1)–C(12)			108(1)
C(12)	1.49(2)		C(11)	C(13)		111(1)
C(13)	1.51(2)		C(11)	C(14)		109(1)
C(14)	1.51(3)		C(12)	C(13)		109(1)
			C(12)	C(14)		109(1)
			C(13)	C(14)		110(1)
N(2)–C(21)	1.47(2)		C(21)–N(2)–C(22)			110(1)
C(22)	1.48(2)		C(21)	C(23)		109(1)
C(23)	1.48(2)		C(21)	C(24)		110(1)
C(24)	1.51(2)		C(22)	C(23)		111(1)
			C(22)	C(24)		108(1)
			C(23)	C(24)		108(1)
N(3)–C(31)	1.50(2)		C(31)–N(3)–C(32)			110(1)
C(32)	1.47(2)		C(31)	C(33)		108(1)
C(33)	1.51(2)		C(31)	C(34)		109(1)
C(34)	1.48(2)		C(32)	C(33)		110(1)
			C(32)	C(34)		108(1)
			C(33)	C(34)		110(1)
N(4)–C(41)	1.49(2)		C(41)–N(4)–C(42)			108(1)
C(42)	1.48(2)		C(41)	C(43)		111(1)
C(43)	1.44(3)		C(41)	C(44)		109(1)
C(44)	1.52(2)		C(42)	C(43)		110(1)
			C(42)	C(44)		111(1)
			C(43)	C(44)		108(1)

Table 39A-22-004. $[N(CH_3)_4]_2ZnI_4$. Interatomic distances [Å] and angles [°] in phase II at 250 K [90Has].

Zn–I(1)	2.611(5)	N(1)–C(3)	1.49(5)
Zn–I(2)	2.592(5)	N(1)–C(4)	1.34(6)
Zn–I(3)	2.601(4)	N(2)–C(5)	1.49(6)
Zn–I(4)	2.622(4)	N(2)–C(6)	1.53(4)
N(1)–C(1)	1.56(4)	N(2)–C(7)	1.41(6)
N(1)–C(2)	1.42(10)	N(2)–C(8)	1.52(5)
I(1)–Zn–I(2)	112.1(2)	I(2)–Zn–I(3)	108.6(2)
I(1)–Zn–I(3)	108.2(2)	I(2)–Zn–I(4)	108.6(2)
I(1)–Zn–I(4)	109.4(4)	I(3)–Zn–I(4)	109.9(2)
C(1)–N(1)–C(2)	116(4)	C(5)–N(2)–C(6)	114(3)
C(1)–N(1)–C(3)	104(3)	C(5)–N(2)–C(7)	110(3)
C(1)–N(1)–C(4)	117(3)	C(5)–N(2)–C(8)	108(3)
C(2)–N(1)–C(3)	112(5)	C(6)–N(2)–C(7)	112(3)
C(2)–N(1)–C(4)	108(5)	C(6)–N(2)–C(8)	110(2)
C(3)–N(1)–C(4)	97(3)	C(7)–N(2)–C(8)	102(3)

Table 39A-22-005. $[N(CH_3)_4]_2ZnI_4$. Displacements of the tetrahedra from the ideal structure with symmetry Pmcn for phase III at 150 K [90Wer]. T_x: translation along the *a* axis in relative units. R_y, R_z: rotation [°] about the axis parallel to the *b* and *c* axes, respectively.

	Zn(1)	Zn(2)	N(1)	N(2)	N(3)	N(4)
T_x	–0.046	–0.012	–0.033	–0.001	–0.030	–0.045
R_y	7	3	25	28	22	15
R_z	6	6	13	3	5	18