Table 39A-12-001. $[N(CH_3)_4]_2ZnCl_4$. Pressure coefficients of phase transition temperatures [80Shi, 96Shi].

Transition	$d\Theta/dp$ [$\cdot 10^2$ K GPa^{-1}]	
I–II	1.2(1)	1.36(3)
II–III	2.0(1)	2.4(1)
III–VII	2.6(2)	3.8(1)
II–VII	2.0(1)	
III–IV, VII–IV	1.6(1)	1.60(1)
IV–V	5.0(3)	4.38(7)
V–VI	–5.4(3)	
Ref.	[80Shi]	[96Shi]

Table 39A-12-002. $[N(CH_3)_4]_2ZnCl_4$. Unit cell parameters [87Has, 87Mad, 92Kas]. The values at 286.4 K are those for average structure.

T [K]	a [Å]	b [Å]	c [Å]	Monoclinic angle [°]	Ref.
363	9.033(2)	15.618(3)	12.302(1)		87Has
333	9.013(3)	15.577(5)	12.285(2)		87Has
303	8.998(2)	15.545(3)	12.275(2)		87Has
286.4	8.987(2)	15.503(2)	12.258(2)		87Mad
278.7	8.983(2)	15.491(3)	61.265(7)		87Has
223	8.963(1)	15.325(2)	36.612(3)	$\gamma = 90.42(1)$	92Kas
161	8.937(1)	15.204(2)	12.174(1)	$\beta = 90.00(1)$	92Kas
149	8.934(1)	15.170(3)	36.586(4)		92Kas

Table 39A-12-003. $[N(CH_3)_4]_2ZnCl_4$. Fractional coordinates and anisotropic temperature parameters [$\cdot 10^{-2}$ Å^2] in phase I at $T = 30$ °C [87Has]. U_{ij} is defined by Eq. (d) in Introduction.

Atom	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Zn	0.25	0.4070(1)	0.2459(1)	5.89(6)	5.09(5)	5.29(6)	0.00	0.00	0.15(7)
Cl(1)	0.2313(46)	0.4064(3)	0.0629(3)	9.27(185)	13.25(32)	5.07(16)	–0.29(50)	–0.13(34)	0.56(20)
Cl(2)	0.2818(13)	0.5412(3)	0.3138(4)	10.80(105)	5.86(20)	11.91(32)	–0.61(29)	–1.04(37)	–2.48(21)
Cl(3)	0.0315(5)	0.3526(3)	0.3056(4)	6.75(29)	9.83(33)	11.00(35)	–1.13(26)	1.87(27)	0.67(30)
Cl(4)	0.4419(5)	0.3250(3)	0.3066(4)	8.07(29)	8.00(28)	10.44(33)	1.76(25)	–2.61(28)	1.47(26)
N(1)	0.25	0.0956(6)	0.1493(7)	6.52(56)	7.19(57)	5.94(50)	0.00	0.00	0.08(51)
C(1)	0.2269(140)	0.0996(14)	0.2670(13)	25.40(737)	16.45(176)	5.96(105)	1.09(409)	6.55(403)	–0.40(115)
C(2)	0.2110(72)	0.0081(12)	0.1093(17)	19.57(705)	7.66(109)	13.84(168)	–3.86(224)	2.03(203)	–3.68(110)
C(3)	0.4041(24)	0.1185(19)	0.1141(22)	6.52(134)	23.28(294)	17.41(244)	–4.86(174)	3.57(157)	0.91(225)
C(4)	0.1601(31)	0.1650(16)	0.0972(21)	20.88(318)	13.63(193)	15.25(219)	7.73(202)	–4.31(207)	2.13(175)
N(2)	0.25	0.8244(6)	0.4920(7)	5.59(24)	6.47(55)	6.56(56)	0.00	0.00	–1.08(47)
C(5)	0.2861(74)	0.7384(14)	0.4428(24)	39.09(1049)	8.67(139)	23.17(277)	–2.05(267)	4.21(386)	–8.89(169)
C(6)	0.1930(45)	0.8862(17)	0.4166(19)	27.45(667)	17.39(220)	12.87(178)	11.35(314)	–8.26(271)	0.46(173)
C(7)	0.4045(19)	0.8547(13)	0.5193(18)	5.21(101)	10.60(142)	14.23(175)	–2.30(105)	–2.79(116)	0.70(133)
C(8)	0.1506(32)	0.8830(17)	0.5862(20)	23.19(325)	16.38(222)	13.22(189)	–5.88(222)	12.15(207)	–2.17(174)

Table 39A-12-004. $[N(CH_3)_4]_2ZnCl_4$. Positional [$\cdot 10^{-4}$] and temperature parameters in phase II at T = 286.4 K [87Mad]. R_0: fractional coordinates of the basic structure obtained from the structure analysis of phase I. U_n: Fourier amplitudes of shifted modulation functions; Re and Im indicate real and imaginary parts. Position of atom in basic cell $\boldsymbol{T}$ is given by $\boldsymbol{r}_b + \boldsymbol{T} + 1/2\Sigma U_n \exp\{2\pi i n \boldsymbol{q} \cdot (\boldsymbol{T} + \boldsymbol{r}_b)\}$, where $\boldsymbol{r}_b$ is the position in the basic structure and modulation wave vector $\boldsymbol{q}$ = 0.413 $\boldsymbol{c}^*$. $U_{eq} = (U_{11} + U_{22} + U_{33})/3$; U_{ij} is defined by Eq. (d) in Introduction.

		R_0	U_0	Re U_1	Im U_1	Re U_2	Im U_2	U_{eq} [Å^2]
Zn	x	2500	0	–101(7)	–153(7)	0	0	0.048(4)
	y	4070	–6(3)	0	0	5(3)	–2(4)	
	z	2454	–14(5)	0	0	–4(4)	1(5)	
Cl(1)	x	2500	0	88(14)	–199(13)	0	0	0.084(6)
	y	4063	–12(5)	0	0	8(8)	–7(7)	
	z	650	5(8)	0	0	8(9)	–9(8)	
Cl(2)	x	2500	0	–168(15)	–434(15)	0	0	0.100(7)
	y	5420	–4(6)	0	0	1(6)	4(7)	
	z	3136	21(6)	0	0	10(9)	2(9)	
Cl(3)	x	442	–7(10)	–111(10)	26(10)	5(10)	12(11)	0.093(5)
	y	3391	10(4)	–16(6)	–149(5)	11(5)	–1(5)	
	z	3059	–9(4)	–41(6)	29(6)	–4(5)	–3(6)	
N(1)	x	2500	0	96(58)	–148(58)	0	0	0.160(9)
	y	950	–119(23)	0	0	13(30)	10(27)	
	z	1484	–97(25)	0	0	–2(34)	5(32)	
C(1)	x	2500	0	–78(46)	31(46)	0	0	0.070(3)
	y	977	21(15)	0	0	1(21)	6(23)	
	z	2725	–107(25)	0	0	8(32)	9(33)	
C(2)	x	2500	0	–23(79)	319(79)	0	0	0.260(6)
	y	62	–107(31)	0	0	5(41)	4(40)	
	z	1059	62(35)	0	0	–7(48)	–15(46)	
C(5)	x	3706	24(30)	260(55)	–380(50)	–27(39)	–43(43)	0.170(5)
	y	1464	–65(12)	–43(26)	207(25)	24(18)	8(17)	
	z	967	115(18)	60(28)	–102(28)	–20(26)	–14(25)	
N(2)	x	2500	0	–138(50)	–187(50)	0	0	0.090(7)
	y	8250	–58(21)	0	0	31(29)	41(27)	
	z	4933	2(21)	0	0	10(30)	–51(31)	
C(3)	x	2500	0	496(52)	132(51)	0	0	0.080(5)
	y	8896	–50(19)	0	0	–7(26)	47(27)	
	z	4235	18(24)	0	0	63(33)	1(34)	
C(4)	x	2500	0	–136(46)	25(45)	0	0	0.090(5)
	y	7410	–66(20)	0	0	73(29)	–56(27)	
	z	4377	106(25)	0	0	–54(35)	74(35)	
C(6)	x	3940	–138(25)	–325(42)	–170(43)	3(38)	–32(34)	0.140(4)
	y	8467	–15(13)	–149(20)	–8(21)	36(20)	8(19)	
	z	5374	71(18)	208(30)	25(30)	–1(25)	–31(24)	

Table 39A-12-005. $[N(CH_3)_4]_2ZnCl_4$. Fractional coordinates and temperature parameters [$\cdot 10^{-2}$ Å^2] in phase III at T = 5.5 °C [87Has]. U_{ij} is defined by Eq. (d) in Introduction. $\overline{u^2}$: the mean square displacement of the atom. The parameters corresponding to the configuration with smaller occupancy are not listed; they are nearly at positions which are related with those for large occupancies by hypothetical mirror reflection at x = 1/4 or 3/4.

Atom	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Zn(1)	0.2750	0.4060(1)	0.0496(1)	6.00(30)	5.34(27)	4.42(18)	–0.05(29)	0.01(28)	–0.04(25)
Cl(11)	0.2612(46)	0.3981(3)	0.0125(3)	10.71(111)	12.01(117)	4.60(73)	–1.25(115)	–1.07(86)	0.53(77)
Cl(12)	0.3097(13)	0.5385(3)	0.0639(4)	8.67(87)	4.11(60)	8.46(86)	–0.46(63)	–1.31(74)	–2.06(57)
Cl(13)	0.0590(5)	0.3451(3)	0.0620(4)	5.85(79)	8.58(101)	10.82(104)	–1.73(72)	1.88(68)	2.47(84)
Cl(14)	0.4592(5)	0.3169(3)	0.0590(4)	6.90(121)	6.48(74)	8.92(84)	2.33(68)	–1.50(71)	–0.04(68)
Zn(2)	0.2380(5)	0.4055(1)	0.2488(1)	5.77(26)	5.18(26)	5.19(29)	0.08(25)	0.30(16)	–0.17(23)
Cl(21)	0.2173(46)	0.4042(3)	0.2123(3)	8.60(78)	7.99(82)	4.11(49)	–0.57(71)	0.28(55)	–0.63(54)
Cl(22)	0.1938(13)	0.5397(3)	0.2621(4)	9.71(96)	4.48(64)	10.71(101)	–0.10(63)	–1.86(79)	–1.87(68)
Cl(23)	0.0415(5)	0.3217(3)	0.2624(4)	7.28(80)	7.19(77)	9.49(82)	–1.24(68)	2.60(71)	1.60(73)
Cl(24)	0.4599(5)	0.3590(3)	0.2596(4)	5.89(70)	8.72(81)	8.82(84)	2.65(64)	0.20(66)	1.56(73)
Zn(3)	0.2655(7)	0.4063(1)	0.4491(1)	4.52(27)	5.03(26)	5.34(15)	–0.17(32)	–0.59(26)	–0.23(23)
Cl(31)	0.2697(46)	0.4028(3)	0.4121(3)	7.17(93)	11.31(108)	3.92(48)	0.78(104)	1.20(68)	0.59(68)
Cl(32)	0.2953(13)	0.5396(3)	0.4632(4)	4.77(70)	5.59(69)	8.10(82)	–0.73(60)	–0.62(60)	–2.07(59)
Cl(33)	0.0313(5)	0.3598(3)	0.4585(4)	4.65(70)	8.70(101)	7.72(82)	0.49(71)	–0.25(66)	0.79(73)
Cl(34)	0.4337(5)	0.3137(3)	0.4625(4)	7.50(92)	5.64(80)	9.36(101)	3.12(73)	–1.85(79)	0.38(73)
Zn(4)	0.2609(9)	0.4075(1)	0.6494(1)	5.51(31)	6.26(29)	5.74(29)	0.08(47)	–0.01(32)	0.36(23)
Cl(41)	0.2266(46)	0.4077(3)	0.6126(3)	5.50(88)	9.97(98)	3.92(66)	–0.55(90)	0.26(68)	1.57(68)
Cl(42)	0.2701(13)	0.5430(3)	0.6630(4)	17.58(200)	4.84(74)	12.77(137)	–0.76(147)	–3.57(179)	–3.59(86)
Cl(43)	0.0679(5)	0.3292(3)	0.6649(4)	9.35(123)	8.97(116)	8.41(102)	–1.91(100)	0.34(95)	1.56(91)
Cl(44)	0.4716(5)	0.3428(3)	0.6599(4)	5.63(88)	9.97(123)	9.64(119)	2.20(88)	–0.09(84)	–0.22(95)
Zn(5)	0.2340(8)	0.4071(1)	0.8488(1)	5.53(35)	5.61(29)	6.54(27)	0.33(36)	0.13(34)	0.50(27)
Cl(51)	0.2310(46)	0.4183(3)	0.8127(3)	7.57(83)	7.16(75)	4.37(48)	0.56(83)	0.46(68)	0.60(54)
Cl(52)	0.2455(13)	0.5436(3)	0.8626(4)	12.93(119)	6.11(78)	9.87(101)	–1.26(129)	–0.19(139)	–0.94(73)
Cl(53)	0.0271(5)	0.3380(3)	0.8603(4)	6.92(95)	11.70(137)	10.23(119)	–2.86(96)	3.11(92)	1.78(99)
Cl(54)	0.4394(5)	0.3511(3)	0.8636(4)	3.90(64)	10.03(109)	9.39(101)	3.21(71)	–1.21(66)	1.53(84)

(continued)

Table 39A-12-005 (continued)

Atom	x	y	z	$\overline{u^2}$	Atom	x	y	z	$\overline{u^2}$
N(11)	0.2571(48)	0.0909(30)	0.0297(8)	6.86(132)	N(12)	0.2594(54)	0.8224(31)	0.0992(8)	6.98(136)
C(11)	0.2216(67)	0.1124(40)	0.0537(10)	7.48(175)	C(15)	0.2690(57)	0.7503(34)	0.0814(9)	5.28(134)
C(12)	0.1962(91)	0.0152(54)	0.0164(14)	11.16(277)	C(16)	0.2277(65)	0.8953(38)	0.0795(9)	6.55(156)
C(13)	0.4126(87)	0.1099(53)	0.0172(13)	10.60(253)	C(17)	0.3951(56)	0.8703(32)	0.1072(8)	4.95(129)
C(14)	0.2029(76)	0.1820(44)	0.0198(12)	9.11(214)	C(18)	0.1545(80)	0.8151(47)	0.1151(13)	9.17(222)
N(21)	0.2265(45)	0.0822(26)	0.2291(7)	6.45(108)	N(22)	0.2437(45)	0.8209(26)	0.2997(7)	5.60(110)
C(21)	0.2165(102)	0.0756(59)	0.2548(16)	15.50(342)	C(25)	0.2006(79)	0.7383(46)	0.2881(12)	9.44(231)
C(22)	0.2941(56)	0.0038(31)	0.2246(8)	5.88(128)	C(26)	0.3416(93)	0.8680(53)	0.2854(15)	12.22(292)
C(23)	0.3314(60)	0.1571(35)	0.2157(10)	7.26(160)	C(27)	0.3166(100)	0.7960(59)	0.3182(16)	13.41(319)
C(24)	0.0786(50)	0.0957(31)	0.2258(8)	5.52(123)	C(28)	0.0757(65)	0.8475(39)	0.3017(10)	7.42(171)
N(31)	0.2472(48)	0.1027(28)	0.4296(7)	5.56(113)	N(32)	0.2719(36)	0.8245(21)	0.4982(5)	3.90(81)
C(31)	0.2191(60)	0.1066(36)	0.4540(9)	5.73(139)	C(35)	0.2610(69)	0.7245(38)	0.4951(10)	8.17(187)
C(32)	0.2203(70)	0.0032(42)	0.4228(11)	7.04(179)	C(36)	0.2946(104)	0.8810(62)	0.4826(16)	15.46(338)
C(33)	0.4226(87)	0.1303(50)	0.4237(13)	9.64(242)	C(37)	0.3691(69)	0.8264(40)	0.5158(11)	8.45(189)
C(34)	0.1674(98)	0.1741(55)	0.4230(15)	10.88(284)	C(38)	0.1382(55)	0.8536(33)	0.5151(9)	6.02(136)
N(41)	0.2292(38)	0.0990(21)	0.6302(6)	4.37(81)	N(42)	0.2504(50)	0.8308(31)	0.6978(8)	4.55(126)
C(41)	0.2366(65)	0.0950(38)	0.6535(10)	8.34(174)	C(45)	0.2523(86)	0.7312(51)	0.6938(14)	7.92(239)
C(42)	0.2305(58)	0.0043(35)	0.6225(9)	7.16(149)	C(46)	0.3209(118)	0.9008(72)	0.6843(19)	12.37(361)
C(43)	0.3471(69)	0.1517(41)	0.6154(11)	9.60(208)	C(47)	0.3823(121)	0.8329(66)	0.7111(19)	11.99(362)
C(44)	0.1036(113)	0.1385(70)	0.6216(18)	18.22(432)	C(48)	0.0880(75)	0.8457(45)	0.7048(12)	6.24(188)
N(51)	0.2522(35)	0.0966(21)	0.8295(5)	3.77(78)	N(52)	0.2513(49)	0.8271(28)	0.8971(7)	4.79(113)
C(51)	0.2236(93)	0.0859(55)	0.8542(14)	12.61(295)	C(55)	0.2235(80)	0.7397(45)	0.8886(12)	7.12(193)
C(52)	0.2401(78)	0.0090(48)	0.8176(13)	10.45(237)	C(56)	0.3192(77)	0.8976(47)	0.8824(12)	7.94(203)
C(53)	0.3803(70)	0.1536(40)	0.8210(11)	8.40(193)	C(57)	0.3002(65)	0.8216(37)	0.9229(9)	5.28(144)
C(54)	0.1027(76)	0.1312(45)	0.8247(12)	9.37(213)	C(58)	0.0955(64)	0.8582(39)	0.9003(10)	5.19(151)

Table 39A-12-006. $[N(CH_3)_4]_2ZnCl_4$. Occupation probability of each ion in phase III at T = 5.5 °C [87Has]. The values for the larger occupancy site are listed.

$ZnCl_4$(1)	$ZnCl_4$(2)	$ZnCl_4$(3)	$ZnCl_4$(4)	$ZnCl_4$(5)
0.93(1)	1.00(1)	0.84(1)	0.78(1)	0.84(2)
TMA-11	TMA-12	TMA-13	TMA-14	TMA-15
0.86(5)	0.94(4)	0.82(5)	1.00(7)	0.97(10)
TMA-21	TMA-22	TMA-23	TMA-24	TMA-25
0.77(5)	0.91(5)	0.97(5)	0.65(7)	0.95(4)

Table 39A-12-007. $[N(CH_3)_4]_2ZnCl_4$. Fractional coordinates [$\cdot 10^{-4}$] and equivalent isotropic temperature parameters [$\cdot 10^{-2}$ Å^2] in phase IV at T = 223 K [92Kas]. $B_{eq} = 4\Sigma b_{ij}\boldsymbol{a}_i \cdot \boldsymbol{a}_j/3$, b_{ij} is defined by Eq. (b) in Introduction.

Atom	x	y	z	B_{eq}
Zn(a)	2579(1)	4073(1)	813(1)	281(3)
Zn(b)	2930(1)	4078(1)	4157(1)	276(3)
Zn(c)	2118(1)	4008(1)	7488(1)	289(3)
Cl(1a)	2840(3)	4036(2)	198(1)	396(7)
Cl(2a)	2915(3)	5444(2)	1035(1)	453(7)
Cl(3a)	261(3)	3577(2)	972(1)	468(8)
Cl(4a)	4328(3)	3210(2)	1071(1)	452(7)
Cl(1b)	2681(3)	4104(2)	3543(1)	479(8)
Cl(2b)	3377(3)	5438(2)	4378(1)	458(7)
Cl(3b)	782(3)	3559(2)	4406(1)	454(7)
Cl(4b)	4874(3)	3206(2)	4312(1)	447(7)
Cl(1c)	1937(3)	4096(2)	6875(1)	459(7)
Cl(2c)	1751(3)	5317(2)	7767(1)	472(8)
Cl(3c)	331(3)	3082(2)	7697(1)	497(8)
Cl(4c)	4416(3)	3505(2)	7642(1)	464(7)
N(1a)	2841(9)	924(6)	501(2)	355(21)
N(1b)	2572(9)	981(5)	3831(2)	321(20)
N(1c)	2200(9)	888(5)	7155(2)	337(20)
N(2a)	2722(9)	8260(5)	1665(3)	376(22)
N(2b)	2632(8)	8279(5)	4963(2)	303(20)
N(2c)	2144(9)	8225(5)	8321(2)	356(21)
C(1a)	2521(16)	909(10)	909(4)	650(41)
C(2a)	2498(14)	50(8)	334(4)	542(35)
C(3a)	4467(12)	1142(10)	442(4)	604(38)
C(4a)	1903(14)	1594(8)	318(4)	567(37)
C(1b)	2475(15)	1054(8)	4243(3)	540(35)
C(2b)	2058(15)	82(8)	3715(3)	531(34)
C(3b)	4151(14)	1123(11)	3710(4)	731(46)
C(4b)	1614(18)	1653(9)	3667(4)	753(44)
C(1c)	2462(15)	939(9)	7562(3)	571(37)
C(2c)	2629(14)	–12(8)	7023(4)	544(36)
C(3c)	3165(15)	1550(8)	6971(4)	570(37)
C(4c)	599(13)	1070(10)	7078(4)	621(40)
C(5a)	2521(15)	7315(8)	1557(4)	700(41)
C(6a)	3756(21)	8680(11)	1426(6)	1491(60)
C(7a)	3361(24)	8285(11)	2035(5)	1419(59)
C(8a)	1252(16)	8662(9)	1683(6)	888(59)
C(5b)	3046(14)	7407(7)	4802(4)	529(34)
C(6b)	1944(13)	8836(8)	4676(3)	513(33)
C(7b)	4038(12)	8703(7)	5107(4)	501(34)
C(8b)	1544(14)	8137(9)	5267(4)	606(36)
C(5c)	2121(16)	7313(8)	8177(5)	800(46)
C(6c)	2766(17)	8844(10)	8034(4)	722(44)
C(7c)	3102(17)	8267(11)	8646(4)	914(45)
C(8c)	587(13)	8517(8)	8403(4)	585(38)

Table 39A-12-008. $[N(CH_3)_4]_2ZnCl_4$. Fractional coordinates [$\cdot 10^{-4}$] and equivalent isotropic temperature parameters [$\cdot 10^{-2}$ Å^2] in phase V at T = 161 K [92Kas]. $B_{eq} = 4\Sigma b_{ij}\boldsymbol{a}_i \cdot \boldsymbol{a}_j/3$, b_{ij} is defined by Eq. (b) in Introduction.

Atom	x	y	z	B_{eq}
Zn	2262(1)	4050(1)	2467(1)	155(1)
Cl(1)	2730(2)	4069(1)	631(1)	227(3)
Cl(2)	1906(2)	5419(1)	3156(1)	283(3)
Cl(3)	157(2)	3245(1)	2827(1)	244(3)
Cl(4)	4278(2)	3427(1)	3291(1)	300(3)
N(1)	2646(6)	969(3)	1493(4)	195(9)
N(2)	2470(5)	8291(3)	4966(4)	182(10)
C(1)	2220(9)	1027(5)	2690(5)	344(15)
C(2)	2510(13)	32(5)	1120(6)	454(23)
C(3)	4188(9)	1303(8)	1328(8)	559(26)
C(4)	1582(9)	1522(5)	806(6)	349(17)
C(5)	2280(9)	7339(4)	4651(6)	336(15)
C(6)	3171(9)	8789(5)	4031(6)	349(17)
C(7)	3469(9)	8363(6)	5957(6)	394(18)
C(8)	972(7)	8662(5)	5230(7)	294(15)

Table 39A-12-009. $[N(CH_3)_4]_2ZnCl_4$. Fractional coordinates [$\cdot 10^{-4}$] and equivalent isotropic temperature parameters [$\cdot 10^{-2}$ Å^2] in phase VI at T = 149 K [92Kas]. $B_{eq} = 4\Sigma b_{ij}\boldsymbol{a}_i \cdot \boldsymbol{a}_j/3$, b_{ij} is defined by Eq. (b) in Introduction.

Atom	x	y	z	B_{eq}
Zn(a)	2013(1)	3993(1)	852(1)	218(2)
Zn(b)	2762(1)	3987(1)	4157(1)	213(2)
Zn(c)	2756(1)	4157(1)	7498(1)	219(2)
Cl(1a)	2161(3)	4210(2)	241(1)	280(5)
Cl(2a)	1586(3)	5279(2)	1151(1)	275(5)
Cl(3a)	76(3)	3062(2)	984(1)	288(5)
Cl(4a)	4218(3)	3421(2)	1057(1)	313(6)
Cl(1b)	3039(3)	3967(2)	3543(1)	283(5)
Cl(2b)	3189(3)	5346(2)	4398(1)	299(6)
Cl(3b)	379(3)	3570(2)	4302(1)	319(6)
Cl(4b)	4393(3)	3022(2)	4417(1)	324(6)
Cl(1c)	2291(3)	4105(2)	6887(1)	289(5)
Cl(2c)	3090(3)	5565(2)	7686(1)	338(6)
Cl(3c)	767(3)	3540(2)	7789(1)	312(6)
Cl(4c)	4873(3)	3379(2)	7634(1)	303(6)
N(1a)	2278(9)	923(5)	499(2)	232(17)
N(1b)	2876(10)	750(5)	3848(2)	261(18)
N(1c)	2272(9)	1131(5)	7173(2)	225(17)
N(2a)	2264(9)	8212(5)	1633(2)	230(17)
N(2b)	2799(10)	8161(5)	5043(2)	255(18)
N(2c)	2508(9)	8403(5)	8293(2)	218(17)
C(1a)	2434(12)	973(8)	913(3)	334(25)
C(2a)	2808(14)	22(7)	367(3)	356(26)
C(3a)	3184(14)	1647(8)	326(3)	382(28)
C(4a)	643(11)	1046(9)	397(3)	362(27)
C(1b)	2463(17)	666(11)	4251(3)	577(41)
C(2b)	2519(13)	–73(8)	3649(4)	416(31)
C(3b)	4538(11)	945(9)	3816(3)	415(30)
C(4b)	1988(15)	1530(8)	3680(3)	434(31)
C(1c)	2627(14)	1204(8)	7579(3)	384(29)
C(2c)	2260(18)	154(7)	7071(3)	460(33)
C(3c)	3445(15)	1603(8)	6948(3)	403(29)
C(4c)	760(13)	1548(10)	7098(3)	447(32)
C(5a)	1989(16)	7291(7)	1483(3)	415(30)
C(6a)	2947(12)	8782(8)	1337(3)	337(24)
C(7a)	3351(14)	8183(8)	1950(3)	369(28)
C(8a)	814(11)	8599(7)	1757(3)	307(24)
C(5b)	2727(13)	7193(6)	4950(3)	307(24)
C(6b)	1409(14)	8605(9)	4913(3)	438(31)
C(7b)	4205(15)	8548(8)	4881(4)	487(32)
C(8b)	2891(15)	8252(8)	5454(3)	365(27)
C(5c)	2883(14)	7480(7)	8162(3)	345(26)
C(6c)	1837(12)	8935(8)	7988(3)	341(25)
C(7c)	3948(12)	8835(7)	8419(3)	368(27)
C(8c)	1416(13)	8343(8)	8611(3)	375(27)

Table 39A-12-010. $[N(CH_3)_4]_2ZnCl_4$. Interatomic distances [Å] and angles [°] in phase I at T = 30 °C and in phase III at T = 5.5 °C [87Has]. Roman numerals specify five independent ions along the c direction. Values are not corrected for the librational motions.

	30 °C	5.5 °C				
		I	II	III	IV	V
Zn–Cl(1)	2.250(47)	2.282(19)	2.247(14)	2.265(18)	2.275(19)	2.218(18)
–Cl(2)	2.262(13)	2.253(16)	2.267(17)	2.254(16)	2.261(35)	2.278(27)
–Cl(3)	2.262(6)	2.286(17)	2.342(15)	2.299(17)	2.320(21)	2.259(19)
–Cl(4)	2.269(6)	2.230(15)	2.220(15)	2.240(16)	2.237(19)	2.230(18)
N(1)–C(1)	1.46(13)	1.54(8)	1.58(11)	1.52(7)	1.43(7)	1.55(9)
–C(2)	1.49(7)	1.53(9)	1.39(6)	1.61(8)	1.54(7)	1.54(8)
–C(3)	1.49(3)	1.62(9)	1.71(7)	1.67(9)	1.62(8)	1.54(8)
–C(4)	1.49(3)	1.61(9)	1.36(6)	1.39(10)	1.39(12)	1.48(8)
N(2)–C(5)	1.50(7)	1.56(7)	1.51(9)	1.56(7)	1.56(9)	1.47(9)
–C(6)	1.43(4)	1.68(8)	1.44(10)	1.31(10)	1.50(12)	1.54(9)
–C(7)	1.50(2)	1.51(7)	1.37(10)	1.38(7)	1.44(12)	1.64(7)
–C(8)	1.46(3)	1.36(9)	1.57(8)	1.65(6)	1.54(8)	1.49(8)
Cl(1)–Zn-Cl(2)	112.3(10)	116.3(6)	110.5(6)	113.7(6)	111.7(10)	107.3(8)
Cl(1)–Zn-Cl(3)	104.9(11)	105.2(6)	106.6(5)	105.1(6)	107.8(7)	109.7(7)
Cl(1)–Zn-Cl(4)	112.5(11)	105.3(6)	111.6(5)	110.0(6)	113.7(7)	116.4(7)
Cl(2)–Zn–Cl(3)	109.5(3)	111.4(6)	104.4(6)	107.4(6)	111.2(10)	111.2(9)
Cl(2)–Zn–Cl(4)	107.4(3)	111.2(6)	110.4(6)	111.5(6)	106.2(10)	100.0(8)
Cl(3)–Zn–Cl(4)	110.2(2)	106.8(6)	113.1(6)	108.9(6)	106.2(7)	111.7(7)
C(1)–N(1)–C(2)	109.4(56)	126.9(51)	99.6(46)	105.6(41)	105.3(38)	110.8(47)
C(1)–N(1)–C(3)	114.1(51)	126.3(49)	123.7(46)	111.2(44)	123.5(42)	121.0(46)
C(1)–N(1)–C(4)	108.4(51)	96.2(44)	95.9(46)	99.9(51)	115.8(57)	94.9(46)
C(2)–N(1)–C(3)	109.9(28)	101.2(52)	105.0(37)	109.2(44)	107.7(38)	113.4(43)
C(2)–N(1)–C(4)	113.0(28)	111.2(51)	122.2(42)	127.7(53)	108.1(55)	99.2(44)
C(3)–N(1)–C(4)	102.0(17)	85.5(46)	111.3(38)	102.8(53)	95.6(56)	113.9(43)
C(5)–N(2)–C(6)	114.5(31)	89.3(37)	107.3(53)	125.4(54)	128.4(62)	120.8(49)
C(5)–N(2)–C(7)	99.7(27)	122.2(42)	105.9(56)	99.0(41)	95.9(57)	109.7(44)
C(5)–N(2)–C(8)	115.9(29)	118.6(51)	90.7(43)	107.7(35)	101.7(47)	100.5(46)
C(6)–N(2)–C(7)	105.4(19)	92.3(38)	110.9(61)	117.0(56)	87.0(65)	119.6(44)
C(6)–N(2)–C(8)	107.7(21)	116.9(50)	120.0(51)	112.8(51)	116.4(57)	102.6(45)
C(7)–N(2)–C(8)	113.1(15)	111.7(50)	118.2(54)	88.1(37)	128.3(63)	98.3(40)

Table 39A-12-011. $[N(CH_3)_4]_2ZnCl_4$. Interatomic distances [Å] in phase II at T = 286.4 K [87Mad]. D_{av}, D_{max} and D_{min} are the average, maximum and minimum distances, respectively.

	D_{av}	D_{max}	D_{min}
Zn–Cl(1)	2.19(1)	2.20(2)	2.17(2)
–Cl(2)	2.28(1)	2.30(2)	2.27(2)
–Cl(3)	2.26(1)	2.28(2)	2.22(2)
N(1)–C(1)	1.54(6)	1.54(8)	1.54(8)
–C(2)	1.43(7)	1.4(1)	1.4(1)
–C(5)	1.49(5)	1.57(9)	1.37(9)
N(2)–C(3)	1.39(7)	1.41(9)	1.36(9)
–C(4)	1.44(6)	1.55(9)	1.35(9)
–C(6)	1.41(4)	1.52(8)	1.35(8)

Table 39A-12-012. $[N(CH_3)_4]_2ZnCl_4$. Interatomic distances [Å] and angles [°] in phase IV at T = 223 K [92Kas].

Zn(a)–Cl(1a)	2.263(3)	Zn(a)–Cl(2a)	2.271(4)
Zn(a)–Cl(3a)	2.283(8)	Zn(a)–Cl(4a)	2.264(10)
Zn(b)–Cl(1b)	2.261(3)	Zn(b)–Cl(2b)	2.268(5)
Zn(b)–Cl(3b)	2.268(7)	Zn(b)–Cl(4b)	2.276(11)
Zn(c)–Cl(1c)	2.255(3)	Zn(c)–Cl(2c)	2.278(4)
Zn(c)–Cl(3c)	2.265(11)	Zn(c)–Cl(4c)	2.275(8)
N(1a)–C(1a)	1.520(16)	N(1a)–C(2a)	1.502(15)
N(1a)–C(3a)	1.509(14)	N(1a)–C(4a)	1.492(17)
N(1b)–C(1b)	1.514(14)	N(1b)–C(2b)	1.511(15)
N(1b)–C(3b)	1.498(15)	N(1b)–C(4b)	1.474(18)
N(1c)–C(1c)	1.511(15)	N(1c)–C(2c)	1.515(15)
N(1c)–C(3c)	1.489(16)	N(1c)–C(4c)	1.490(14)
N(2a)–C(5a)	1.512(15)	N(2a)–C(6a)	1.424(21)
N(2a)–C(7a)	1.472(21)	N(2a)–C(8a)	1.459(18)
N(2b)–C(5b)	1.510(14)	N(2b)–C(6b)	1.492(15)
N(2b)–C(7b)	1.508(14)	N(2b)–C(8b)	1.495(15)
N(2c)–C(5c)	1.493(16)	N(2c)–C(6c)	1.518(18)
N(2c)–C(7c)	1.467(18)	N(2c)–C(8c)	1.499(15)
Cl(1a)–Zn(a)–Cl(2a)	111.5(1)	Cl(1a)–Zn(a)–Cl(3a)	109.9(1)
Cl(1a)–Zn(a)–Cl(4a)	109.1(2)	Cl(2a)–Zn(a)–Cl(3a)	109.3(5)
Cl(2a)–Zn(a)–Cl(4a)	107.6(3)	Cl(3a)–Zn(a)–Cl(4a)	109.3(2)
Cl(1b)–Zn(b)–Cl(2b)	110.8(1)	Cl(1b)–Zn(b)–Cl(3b)	108.8(1)
Cl(1b)–Zn(b)–Cl(4b)	109.5(1)	Cl(2b)–Zn(b)–Cl(3b)	108.9(4)
Cl(2b)–Zn(b)–Cl(4b)	108.7(3)	Cl(3b)–Zn(b)–Cl(4b)	110.2(1)
Cl(1c)–Zn(c)–Cl(2c)	112.5(1)	Cl(1c)–Zn(c)–Cl(3c)	108.8(1)
Cl(1c)–Zn(c)–Cl(4c)	109.4(1)	Cl(2c)–Zn(c)–Cl(3c)	107.1(3)
Cl(2c)–Zn(c)–Cl(4c)	109.0(4)	Cl(3c)–Zn(c)–Cl(4c)	110.0(2)
C(1a)–N(1a)–C(2a)	110.5(4)	C(1a)–N(1a)–C(3a)	109.1(7)
C(1a)–N(1a)–C(4a)	110.2(6)	C(2a)–N(1a)–C(3a)	109.3(7)
C(2a)–N(1a)–C(4a)	108.5(6)	C(3a)–N(1a)–C(4a)	109.3(6)
C(1b)–N(1b)–C(2b)	109.3(3)	C(1b)–N(1b)–C(3b)	109.8(6)
C(1b)–N(1b)–C(4b)	108.7(5)	C(2b)–N(1b)–C(3b)	109.3(7)
C(2b)–N(1b)–C(4b)	110.4(7)	C(3b)–N(1b)–C(4b)	109.5(7)
C(1c)–N(1c)–C(2c)	108.7(4)	C(1c)–N(1c)–C(3c)	108.8(6)
C(1c)–N(1c)–C(4c)	109.0(6)	C(2c)–N(1c)–C(3c)	109.1(6)
C(2c)–N(1c)–C(4c)	111.2(7)	C(3c)–N(1c)–C(4c)	110.1(5)
C(5a)–N(2a)–C(6a)	110.1(6)	C(5a)–N(2a)–C(7a)	108.0(4)
C(5a)–N(2a)–C(8a)	108.3(9)	C(6a)–N(2a)–C(7a)	107.6(10)
C(6a)–N(2a)–C(8a)	115.1(5)	C(7a)–N(2a)–C(8a)	107.5(6)
C(5b)–N(2b)–C(6b)	109.6(3)	C(5b)–N(2b)–C(7b)	108.0(8)
C(5b)–N(2b)–C(8b)	109.0(5)	C(6b)–N(2b)–C(7b)	110.3(4)
C(6b)–N(2b)–C(8b)	109.7(8)	C(7b)–N(2b)–C(8b)	110.2(4)
C(5c)–N(2c)–C(6c)	110.1(4)	C(5c)–N(2c)–C(7c)	109.3(6)
C(5c)–N(2c)–C(8c)	110.1(9)	C(6c)–N(2c)–C(7c)	108.7(8)
C(6c)–N(2c)–C(8c)	106.9(6)	C(7c)–N(2c)–C(8c)	111.7(4)

Table 39A-12-013. $[N(CH_3)_4]_2ZnCl_4$. Interatomic distances [Å] and angles [°] in phase V at T = 161 K [92Kas].

Zn–Cl(1)	2.274(4)	Zn–Cl(2)	2.267(2)
Zn–Cl(3)	2.286(4)	Zn–Cl(4)	2.271(7)
N(1)–C(1)	1.509(8)	N(1)–C(2)	1.502(9)
N(1)–C(3)	1.482(10)	N(1)–C(4)	1.520(10)
N(2)–C(5)	1.508(8)	N(2)–C(6)	1.504(10)
N(2)–C(7)	1.505(11)	N(2)–C(8)	1.487(8)
Cl(1)–Zn–Cl(2)	112.2(1)	Cl(1)–Zn–Cl(3)	110.3(4)
Cl(1)–Zn–Cl(4)	107.1(4)	Cl(2)–Zn–Cl(3)	107.8(2)
Cl(2)–Zn–Cl(4)	109.3(2)	Cl(3)–Zn–Cl(4)	110.2(1)
C(1)–N(1)–C(2)	109.1(3)	C(1)–N(1)–C(3)	110.3(6)
C(1)–N(1)–C(4)	110.0(5)	C(2)–N(1)–C(3)	111.1(6)
C(2)–N(1)–C(4)	107.9(5)	C(3)–N(1)–C(4)	108.5(4)
C(5)–N(2)–C(6)	109.8(3)	C(5)–N(2)–C(7)	109.9(3)
C(5)–N(2)–C(8)	108.5(4)	C(6)–N(2)–C(7)	108.8(4)
C(6)–N(2)–C(8)	110.4(4)	C(7)–N(2)–C(8)	109.5(4)

Table 39A-12-014. $[N(CH_3)_4]_2ZnCl_4$. Interatomic distances [Å] and angles [°] in phase VI at T = 149 K [92Kas].

Zn(a)–Cl(1a)	2.265(3)	Zn(a)–Cl(2a)	2.269(3)
Zn(a)–Cl(3a)	2.285(3)	Zn(a)–Cl(4a)	2.279(3)
Zn(b)–Cl(1b)	2.261(3)	Zn(b)–Cl(2b)	2.274(3)
Zn(b)–Cl(3b)	2.283(3)	Zn(b)–Cl(4b)	2.275(3)
Zn(c)–Cl(1c)	2.277(3)	Zn(c)–Cl(2c)	2.265(3)
Zn(c)–Cl(3c)	2.273(3)	Zn(c)–Cl(4c)	2.283(3)
N(1a)–C(1a)	1.523(12)	N(1a)–C(2a)	1.527(13)
N(1a)–C(3a)	1.504(14)	N(1a)–C(4a)	1.520(12)
N(1b)–C(1b)	1.525(14)	N(1b)–C(2b)	1.480(14)
N(1b)–C(3b)	1.518(13)	N(1b)–C(4b)	1.552(15)
N(1c)–C(1c)	1.523(12)	N(1c)–C(2c)	1.530(13)
N(1c)–C(3c)	1.514(15)	N(1c)–C(4c)	1.517(15)
N(2a)–C(5a)	1.521(13)	N(2a)–C(6a)	1.515(13)
N(2a)–C(7a)	1.513(14)	N(2a)–C(8a)	1.493(13)
N(2b)–C(5b)	1.509(13)	N(2b)–C(6b)	1.490(16)
N(2b)–C(7b)	1.508(16)	N(2b)–C(8b)	1.513(12)
N(2c)–C(5c)	1.518(13)	N(2c)–C(6c)	1.502(13)
N(2c)–C(7c)	1.516(13)	N(2c)–C(8c)	1.519(14)
Cl(1a)–Zn(a)–Cl(2a)	111.2(1)	Cl(1a)–Zn(a)–Cl(3a)	110.0(1)
Cl(1a)–Zn(a)–Cl(4a)	109.2(1)	Cl(2a)–Zn(a)–Cl(3a)	107.6(1)
Cl(2a)–Zn(a)–Cl(4a)	108.3(1)	Cl(3a)–Zn(a)–Cl(4a)	110.5(1)
Cl(1b)–Zn(b)–Cl(2b)	112.3(1)	Cl(1b)–Zn(b)–Cl(3b)	109.2(1)
Cl(1b)–Zn(b)–Cl(4b)	109.7(1)	Cl(2b)–Zn(b)–Cl(3b)	108.5(1)
Cl(2b)–Zn(b)–Cl(4b)	108.3(1)	Cl(3b)–Zn(b)–Cl(4b)	108.8(1)
Cl(1c)–Zn(c)–Cl(2c)	110.8(1)	Cl(1c)–Zn(c)–Cl(3c)	107.6(1)
Cl(1c)–Zn(c)–Cl(4c)	110.3(1)	Cl(2c)–Zn(c)–Cl(3c)	110.4(1)
Cl(2c)–Zn(c)–Cl(4c)	108.2(1)	Cl(3c)–Zn(c)–Cl(4c)	109.5(1)
C(1a)–N(1a)–C(2a)	109.4(3)	C(1a)–N(1a)–C(3a)	109.5(4)
C(1a)–N(1a)–C(4a)	109.1(5)	C(2a)–N(1a)–C(3a)	110.7(6)
C(2a)–N(1a)–C(4a)	109.2(5)	C(3a)–N(1a)–C(4a)	108.9(4)
C(1b)–N(1b)–C(2b)	110.6(5)	C(1b)–N(1b)–C(3b)	109.2(6)
C(1b)–N(1b)–C(4b)	108.8(6)	C(2b)–N(1b)–C(3b)	109.7(6)
C(2b)–N(1b)–C(4b)	109.9(5)	C(3b)–N(1b)–C(4b)	108.7(5)
C(1c)–N(1c)–C(2c)	108.2(3)	C(1c)–N(1c)–C(3c)	110.7(7)
C(1c)–N(1c)–C(4c)	109.4(5)	C(2c)–N(1c)–C(3c)	109.3(6)
C(2c)–N(1c)–C(4c)	110.7(7)	C(3c)–N(1c)–C(4c)	108.7(4)
C(5a)–N(2a)–C(6a)	109.4(2)	C(5a)–N(2a)–C(7a)	110.7(4)
C(5a)–N(2a)–C(8a)	109.3(8)	C(6a)–N(2a)–C(7a)	107.9(7)
C(6a)–N(2a)–C(8a)	110.0(4)	C(7a)–N(2a)–C(8a)	109.6(3)
C(5b)–N(2b)–C(6b)	109.4(6)	C(5b)–N(2b)–C(7b)	109.0(6)
C(5b)–N(2b)–C(8b)	108.4(2)	C(6b)–N(2b)–C(7b)	113.1(4)
C(6b)–N(2b)–C(8b)	108.7(7)	C(7b)–N(2b)–C(8b)	108.2(7)
C(5c)–N(2c)–C(6c)	110.3(2)	C(5c)–N(2c)–C(7c)	107.9(7)
C(5c)–N(2c)–C(8c)	109.2(4)	C(6c)–N(2c)–C(7c)	109.4(4)
C(6c)–N(2c)–C(8c)	110.1(7)	C(7c)–N(2c)–C(8c)	109.9(3)

Table 39A-12-015. $N(CH_3)_4]_2ZnCl_4$. $c_{\lambda\mu}$ [84Ber]. T = RT. Brillouin scattering.

c_{11}	c_{22}	c_{33}	c_{44}	c_{55}	c_{66}	c_{23}	c_{31}	c_{12}
$[\cdot 10^9\ N^{-2}]$								
13.90	11.14	11.63	2.94	3.52	1.93	6.8	5.03	6.76

Table 39A-12-016. $[N(CH_3)_4]_2ZnCl_4$. ^{14}N nuclear quadrupole coupling tensors in phase I at T = 26 °C in the crystal fixed frame [87Dol].

$\frac{3}{2} eQ\phi_{ij}(1,2)/h$ [kHz] =	19.5	0	0	
	0	42.5	±4	; $(e^2qQ/h)_{1,2}$ = 41.4 kHz
	0	±4	–62	$\eta_{1,2}$ = 0.373
$\frac{3}{2} eQ\phi_{ij}(3,4)/h$ [kHz] =	–78	0	0	
	0	89	±48.5	; $(e^2qQ/h)_{3,4}$ = 72.4 kHz
	0	±48.5	–11	$\eta_{3,4}$ = 0.436

Table 39A-12-017. $[N(CH_3)_4]_2ZnCl_4$. Spin-Hamiltonian parameters and principal axes (in the *a*, *b*, *c* axis systems) of the **D**-tensor for Mn^{2+} ions [83Mac]. T = 27 °C (phase I) and –105 °C (phase V).

$T = 27\,°C$

	Principal values	Principal axes by direction cosines
D_x	$47 \cdot 10^{-2}\,m^{-1}$	1, 0, 0
D_y	$37 \cdot 10^{-2}\,m^{-1}$	0, 0.9455, −0.3256
D_z	$-84 \cdot 10^{-2}\,m^{-1}$	0, 0.3256, 0.9455
A_x	$-74 \cdot 10^{-2}\,m^{-1}$	
A_y	$-74 \cdot 10^{-2}\,m^{-1}$	
A_z	$-77 \cdot 10^{-2}\,m^{-1}$	
g_x	2.001	
g_y	1.997	
g_z	2.000	

$T = -105\,°C$

	Principal values
D_x	$69 \cdot 10^{-2}\,m^{-1}$
D_y	$18 \cdot 10^{-2}\,m^{-1}$
D_z	$-87 \cdot 10^{-2}\,m^{-1}$
A_x	$-73 \cdot 10^{-2}\,m^{-1}$
A_y	$-75 \cdot 10^{-2}\,m^{-1}$
A_z	$-78 \cdot 10^{-2}\,m^{-1}$
g_x	2.002
g_y	2.001
g_z	2.001