Table 39A-11-001. $(NH_4)_2ZnCl_4$. Unit cell parameters, Z and density [82Mat1]. T = 223 K, 298 K and 418 K.

T [K]	223 (V)	298 (III)	418 (I)
Z	12	16	4
a [Å]	7.184(1)	7.2129(3)	7.275(1)
b [Å]	12.568(2)	12.629(1)	12.745(2)
c [Å]	27.838(3)	37.118(2)	9.2950(8)
α [°]		89.992(6)	
ρ_X [10^3 kg m^{-3}]	1.929	1.912	1.875

Table 39A-11-002. $(NH_4)_2ZnCl_4$. Crystal structure of phase I [82Mat1]. Fractional coordinates and anisotropic temperature parameters. T = 418 K. The temperature parameter U_{ij} [$\cdot 10^{-3}$ Å^2] is defined by Eq. (d) in Introduction. See also Fig. 39A-11-001.

	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
N(1)	0.75	0.3191(6)	0.4796(9)	89(6)	56(5)	49(5)	0	0	−4(4)
N(2)	0.75	0.5948(10)	0.1380(10)	96(8)	152(10)	50(5)	0	0	8(6)
Zn	0.25	0.42463(9)	0.2725(1)	53.9(6)	58.6(6)	46.4(6)	0	0	0.4(5)
Cl(1)	0.25	0.4155(3)	0.5112(3)	170(4)	102(2)	36(1)	0	0	16(2)
Cl(2)	0.25	0.5889(2)	0.1895(3)	215(5)	56(2)	60(2)	0	0	18(1)
Cl(3)	0.0018(3)	0.3451(3)	0.1789(3)	69(1)	181(3)	89(1)	−63(2)	8(1)	−46(2)

Table 39A-11-003. $(NH_4)_2ZnCl_4$. Crystal structure of phase V [82Mat2]. Fractional coordinates [$\cdot 10^{-4}$] and mean square displacements $\overline{u^2}$ [$\cdot 10^{-2}$ Å^2]. T = 223 K. See also Fig. 39A-11-002.

Atom	x	y	z	$\overline{u^2}$
N(1)	2724(13)	6811(6)	1723(2)	3.00(29)
N(2)	2307(13)	6854(5)	5043(2)	2.89(24)
N(3)	2803(12)	6771(6)	8385(2)	2.89(27)
N(4)	2869(13)	4020(7)	2887(3)	3.91(31)
N(5)	2480(16)	4051(7)	6206(3)	4.27(40)
N(6)	2330(17)	3942(7)	9548(3)	4.46(33)
Zn(1)	2500	4225(1)	925.4(3)	2.79(3)
Zn(2)	2565(2)	4271(1)	4255.9(4)	2.77(3)
Zn(3)	2651(2)	4213(1)	7573.6(4)	2.90(3)
Cl(1)	2336(5)	4181(2)	1726(1)	3.27(11)
Cl(2)	1896(4)	5861(2)	629(1)	3.02(10)
Cl(3)	428(4)	3059(2)	608(1)	3.29(9)
Cl(4)	5322(4)	3734(2)	635(1)	3.73(9)
Cl(5)	3122(4)	4288(2)	5049(1)	2.80(8)
Cl(6)	2038(4)	5889(2)	3932(1)	2.72(8)
Cl(7)	231(4)	3175(2)	4051(1)	3.58(9)
Cl(8)	5201(3)	3632(2)	3887(1)	2.85(7)
Cl(9)	2348(5)	4158(2)	8371(1)	3.22(11)
Cl(10)	3272(4)	5847(2)	7268(1)	2.76(8)
Cl(11)	–25(4)	3671(2)	7220(1)	3.12(8)
Cl(12)	4919(4)	3076(2)	7333(1)	3.81(9)

Table 39A-11-004. $(NH_4)_2ZnCl_4$. Crystal structure of phase I [82Mat1]. Bond distances [Å] and angles [°] of $ZnCl_4$ groups. T = 418 K. The second line for each bond distance is the corrected value for the librational motion of $ZnCl_4$.

	418 K
Zn–Cl(1)	2.222(3)
	2.251
–Cl(2)	2.231(3)
	2.282
–Cl(3)	2.246(3)
	2.292
–Cl(4)	2.246(3)
	2.292
(mean)	2.236
	2.279
Cl(1)–Zn–Cl(2)	113.2(1)
Cl(1)–Zn–Cl(3)	111.3(1)
Cl(1)–Zn–Cl(4)	111.3(1)
Cl(2)–Zn–Cl(3)	106.8(1)
Cl(2)–Zn–Cl(4)	106.8(1)
Cl(3)–Zn–Cl(4)	107.0(1)

Table 39A-11-005. $(NH_4)_2ZnCl_4$. Crystal structure of phase V [82Mat2]. Bond distances [Å] and angles [°] of $ZnCl_4$ groups and N-Cl distances within 3.7 Å. $T = 223$ K. See also Fig. 39A-11-002.

Zn(1)–Cl(1)	2.233(2)	N(1)–Cl(1)	3.318(8)
–Cl(2)	2.257(2)	–Cl(2)	3.324(7)
–Cl(3)	2.268(3)	–Cl(7^{iii})	3.290(8)
–Cl(4)	2.268(3)	–Cl(8^{iii-a})	3.377(8)
Zn(2)–Cl(5)	2.245(2)	–Cl(9^{ii+b+c})	3.548(10)
–Cl(6)	2.257(2)	–Cl(10^{iv+b-c})	3.334(8)
–Cl(7)	2.244(3)	–Cl(11^{ii+b+c})	3.413(8)
–Cl(8)	2.299(3)	–Cl($12^{ii-a+b+c}$)	3.314(8)
Zn(3)–Cl(9)	2.230(2)	N(2)–Cl(2^{iv+b})	3.317(7)
–Cl(10)	2.267(2)	–Cl(3^{iii})	3.256(8)
–Cl(11)	2.265(3)	–Cl(4^{iii-a})	3.343(8)
–Cl(12)	2.268(3)	–Cl(5)	3.278(7)
		–Cl($5^{ii-a+b+c}$)	3.341(9)
		–Cl(6)	3.327(7)
		–Cl(7^{ii+b+c})	3.284(8)
Cl(1)–Zn(1)–Cl(2)	112.1(1)	–Cl($8^{ii-a+b+c}$)	3.396(8)
Cl(1)–Zn(1)–Cl(3)	109.8(1)	N(3)–Cl(1^{ii+b+c})	3.483(9)
Cl(1)–Zn(1)–Cl(4)	113.4(1)	–Cl(3^{ii+b+c})	3.388(8)
Cl(2)–Zn(1)–Cl(3)	108.6(1)	–Cl($4^{ii-a+b+c}$)	3.322(8)
Cl(2)–Zn(1)–Cl(4)	106.8(1)	–Cl(6^{iv+b})	3.358(7)
Cl(3)–Zn(1)–Cl(4)	105.8(1)	–Cl(9)	3.300(7)
Cl(5)–Zn(2)–Cl(6)	114.5(1)	–Cl(10)	3.334(7)
Cl(5)–Zn(2)–Cl(7)	112.9(1)	–Cl(11^{iii+c})	3.312(8)
Cl(5)–Zn(2)–Cl(8)	107.2(1)	–Cl($12^{iii-a+c}$)	3.313(8)
Cl(6)–Zn(2)–Cl(7)	109.0(1)	N(4)–Cl(1)	3.261(8)
Cl(6)–Zn(2)–Cl(8)	106.0(1)	–Cl(8)	3.286(8)
Cl(7)–Zn(2)–Cl(8)	106.7(1)	–Cl($10^{ii-a+b+c}$)	3.335(10)
Cl(9)–Zn(3)–Cl(10)	114.8(1)	–Cl(11^{ii+b+c})	3.286(10)
Cl(9)–Zn(3)–Cl(11)	109.9(1)	–Cl(12^{iv-c})	3.389(9)
Cl(9)–Zn(3)–Cl(12)	110.1(1)	N(5)–Cl(3^{iv})	3.461(10)
Cl(10)–Zn(3)–Cl(11)	106.1(1)	–Cl(5)	3.267(8)
Cl(10)–Zn(3)–Cl(12)	108.6(1)	–Cl(6^{ii+b+c})	3.298(12)
Cl(11)–Zn(3)–Cl(12)	107.0(1)	–Cl($8^{ii-a+b+c}$)	3.351(10)
		–Cl(11)	3.380(9)
		N(6)–Cl(2^{ii+b+c})	3.326(12)
		–Cl(3^{i+c})	3.435(9)
		–Cl($4^{ii-a+b+c}$)	3.297(10)
		–Cl(7^{iv})	3.357(10)
		–Cl(9)	3.289(8)

Symmetry code: (i+c) $x, y, 1+z$; (ii+b+c) $\frac{1}{2}+x, 1-y, 1-z$; (ii−a+b+c) $-\frac{1}{2}+x, 1-y, 1-z$; (iii) $\frac{1}{2}+x, \frac{1}{2}+y, \frac{1}{2}-z$; (iii−a) $-\frac{1}{2}+x, \frac{1}{2}+y, \frac{1}{2}-z$; (iii+c) $\frac{1}{2}+x, \frac{1}{2}+y, \frac{3}{2}-z$; (iii−a+c) $-\frac{1}{2}+x, \frac{1}{2}+y, \frac{3}{2}-z$; (iv) $x, \frac{1}{2}-y, \frac{1}{2}+z$; (iv+b) $x, \frac{3}{2}-y, \frac{1}{2}+z$; (iv−c) $x, \frac{1}{2}-y, -\frac{1}{2}+z$; (iv+b−c) $x, \frac{3}{2}-y, -\frac{1}{2}+z$.

Table 39A-11-006. $(NH_4)_2ZnCl_4$. Crystal structure of phase I [82Mat3]. Fractional coordinates and anisotropic temperature parameters of the split atom model for the Cl atoms. T = 418 K. The temperature parameter U_{ij} [$\cdot 10^{-3}$ Å^2] is defined by Eq. (d) in Introduction. See also Fig. 39A-11-004.

Atom	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
N 1	0.75	0.3194(5)	0.4788(7)	89(5)	59(4)	48(4)	0	0	–4(3)
N 2	0.75	0.5955(8)	0.1383(8)	94(6)	149(8)	55(4)	0	0	13(5)
Zn	0.25	0.42459(7)	0.27245(9)	53.2(5)	58.3(5)	46.1(5)	0	0	0.6(4)
Cl 1′	0.2877(8)	0.4166(2)	0.5116(2)	78(5)	105(2)	36(1)	23(2)	3(1)	17(1)
Cl 2′	0.2086(7)	0.5884(2)	0.1894(3)	96(5)	56(1)	61(1)	10(2)	0(2)	18(1)
Cl 3′	0.0179(5)	0.3242(3)	0.1912(4)	66(2)	108(2)	99(2)	–39(2)	–2(2)	–23(2)
Cl 4′	0.5106(4)	0.3633(3)	0.1697(3)	49(1)	105(2)	62(2)	23(2)	6(1)	–12(2)

Table 39A-11-007. $(NH_4)_2ZnCl_4$. Crystal structure of phase I [82Mat3]. Bond distances [Å] and angles [°] of $ZnCl_4$ groups. T = 418 K. The second column for each bond distance is the corrected value for the librational motion of $ZnCl_4$. Primed symbols for Cl, see Fig. 39A-11-004.

Zn–Cl 1′	2.242(3)	2.259	Cl 1′–Zn–Cl 2′	113.5(1)
–Cl 2′	2.246(3)	2.269	Cl 1′–Zn–Cl 3′	113.5(2)
–Cl 3′	2.249(4)	2.275	Cl 1′–Zn–Cl 4′	107.5(2)
–Cl 4′	2.262(3)	2.279	Cl 2′–Zn–Cl 3′	108.2(2)
mean	2.250	2.271	Cl 2′–Zn–Cl 4′	106.7(2)
			Cl 3′–Zn–Cl 4′	106.9(1)

Table 39A-11-008. $(NH_4)_2ZnCl_4$. EFG tensor parameters at ^{14}N sites from NQR data in phase I [91Mic]. T = 137 °C. eq: maximum component of principal values of EFG tensor. η: asymmetry parameter.

Sites	$3eQ\phi_{xx}/2\,h$ [kHz]	$3eQ\phi_{yy}/2\,h$ [kHz]	$3eQ\phi_{zz}/2\,h$ [kHz]	$3eQ\phi_{yz}/2\,h$ [kHz]	eq [kHz]	η
N(1)	105.5	–5.6	–99.9	±18.5	105.5	0.97
N(2)	–26.2	48.1	–21.9	±2.1	48.2	0.087

Table 39A-11-009. $(NH_4)_2ZnCl_4$. EFG tensor at ^{14}N sites from NQR data in phase III [91Mic]. $T \approx 5$ °C. The superscripts 1, 2, 3, 4 indicate the four nonequivalent sites belonging to N defined according to phase I.

Sites	$3eQ\phi_{xx}/2\,h$ [kHz]	$3eQ\phi_{yy}/2\,h$ [kHz]	$3eQ\phi_{zz}/2\,h$ [kHz]	$3eQ\phi_{yz}/2\,h$ [kHz]	$3eQ\phi_{zx}/2\,h$ [kHz]	$3eQ\phi_{xy}/2\,h$ [kHz]
N^1(1)	114.2	–32.9	–81.2	15.3	±25.1	±3.2
N^2(1)	102.1	–10.8	–91.2	–19.7	±23.8	±4.3
N^3(1)	97.3	–26.0	–71.0	–5.1	±20.7	±13.0
N^4(1)	61.7	–5.9	–55.8	6.9	±35.3	±51.2
N^1(2)	70.5	–29.9	–40.9	–26.2	±27.8	±38.9
N^2(2)	59.0	–21.6	–37.8	32.5	±31.5	±27.3
N^3(3)	58.6	–14.4	–44.4	–25.9	±34.7	±22.2
N^4(4)	–14.7	–30.2	45.2	16.6	±12.0	±31.4