Table 39A-15-001. $[N(CH_3)_4]_2CuBr_4$. Crystal structure of phase I [85Has1]. Fractional coordinates and isotropic temperature parameters. T = 25 °C. B [Å^2] is defined by Eq. (e) in Introduction. All the ions are in disorder with respect to mirror operation.

Atom	x	y	z	B
Cu	0.244(1)	0.4073(2)	0.2377(3)	5.5(1)
Br(1)	0.247(2)	0.3809(3)	0.0527(3)	9.6(2)
Br(2)	0.276(3)	0.5409(3)	0.3204(4)	8.8(2)
Br(3)	0.0191(5)	0.3662(3)	0.2880(5)	9.5(3)
Br(4)	0.4630(5)	0.3349(3)	0.2927(4)	9.0(2)
N(1)	0.244	0.097(1)	0.140(2)	6.2(5)
C(1)	0.290(7)	0.150(3)	0.253(4)	11.7(17)
C(2)	0.204(5)	0.008(2)	0.113(3)	9.5(14)
C(3)	0.365(5)	0.135(3)	0.072(4)	9.7(13)
C(4)	0.117(6)	0.149(3)	0.123(4)	11.5(16)
N(2)	0.258	0.829(1)	0.509(2)	6.3(5)
C(5)	0.280(8)	0.754(3)	0.439(3)	10.5(15)
C(6)	0.203(6)	0.905(3)	0.439(4)	12.8(18)
C(7)	0.392(4)	0.856(2)	0.550(3)	7.7(10)
C(8)	0.152(6)	0.806(3)	0.591(4)	12.4(17)

Table 39A-15-002. $[N(CH_3)_4]_2CuBr_4$. Crystal structure of phase II [90Mad]. Fractional coordinates of the average structure. T = 248 K. The average structure was obtained by taking into account only those reflections that are also present in phase I. Equivalent temperature parameters U [$\cdot 10^{-2}$ Å^2] are defined by $U = (1/3)\Sigma\Sigma U_{ij} a_i^* a_j^* \boldsymbol{a}_i \cdot \boldsymbol{a}_j$. U_{ij} is defined by Eq. (d) in Introduction.

Atom	x	y	z	U
Cu	0.2559(8)	0.4060(2)	0.2377(3)	6.2(1)
Br(1)	0.2682(9)	0.3755(3)	0.0540(3)	8.8(1)
Br(2)	0.0190(6)	0.3616(5)	0.2804(5)	11.8(2)
Br(3)	0.2719(9)	0.5409(2)	0.3216(3)	10.0(2)
Br(4)	0.4690(6)	0.3419(4)	0.2976(5)	10.0(2)
N(1)	0.237(4)	0.098(1)	0.135(1)	6.4(5)
C(11)	0.291(4)	0.112(2)	0.243(2)	9(1)
C(12)	0.115(4)	0.149(2)	0.109(3)	8(2)
C(13)	0.217(4)	0.008(1)	0.122(3)	8(1)
C(14)	0.357(4)	0.119(2)	0.061(3)	7(1)
N(2)	0.249(5)	0.667(1)	0.005(1)	6.3(5)
C(21)	0.279(4)	0.743(1)	–0.062(2)	6.5(9)
C(22)	0.147(3)	0.671(2)	0.089(3)	6(1)
C(23)	0.214(4)	0.595(1)	–0.063(2)	7(1)
C(24)	0.390(4)	0.645(2)	0.051(3)	9(1)

Table 39A-15-003. $[N(CH_3)_4]_2CuBr_4$. Crystal structure of phase II [90Mad]. T = 248 K. Moduli [$\cdot 10^{-4}$] and phases of the displacive modulation function for each atom: $u_\alpha(t) = A_\alpha \cos [2\pi(t + \phi_\alpha)]$; α: x, y, z; t: internal coordinate.

Atom	A_x	ϕ_x	A_y	ϕ_y	A_z	ϕ_z
Cu	145(7)	0.371(7)	42(5)	0.91(4)	89(7)	–0.05(2)
Br(1)	270(9)	0.285(5)	16(7)	0.52(9)	104(6)	–0.02(1)
Br(2)	127(7)	0.404(9)	66(8)	0.78(2)	162(8)	0.875(9)
Br(3)	160(10)	0.44(1)	72(5)	–0.17(2)	30(13)	0.04(4)
Br(4)	112(8)	0.43(1)	86(6)	0.01(1)	143(8)	0.100(9)
N(1)	35(35)	0.2(2)	51(40)	–0.3(1)	47(46)	0.0(2)
C(11)	285(66)	0.62(4)	203(32)	0.32(4)	120(37)	0.00(5)
C(12)	228(49)	0.44(3)	245(30)	0.54(3)	234(48)	0.75(3)
C(13)	443(60)	0.05(2)	83(29)	0.70(6)	323(38)	0.35(3)
C(14)	202(48)	0.19(4)	294(29)	0.86(2)	238(40)	0.04(3)
N(2)	65(37)	0.07(9)	72(34)	–0.07(9)	68(47)	0.3(1)
C(21)	55(50)	–0.1(2)	89(25)	0.32(6)	303(32)	0.33(3)
C(22)	346(50)	0.10(2)	321(28)	0.94(2)	214(37)	0.16(3)
C(23)	368(65)	0.66(3)	122(28)	0.32(4)	236(36)	0.98(3)
C(24)	172(47)	0.12(4)	195(36)	0.76(3)	236(45)	0.62(3)

Table 39A-15-004. $[N(CH_3)_4]_2CuBr_4$. Crystal structure of phase II [90Mad]. T = 248 K. Moduli [$\cdot 10^{-3}$] and phases ($1/(2\pi)$) of the occupation modulation function for each tetrahedron: $P_\mu(t) = P_{c.a.} \cos [2\pi (t + \phi_\mu)]$; $\phi_\mu = \phi_{c.a} + \boldsymbol{q} \cdot (\boldsymbol{r}_{c.a.av} - \boldsymbol{r}_{\mu av})$; index c.a. refers to the parameters of the central atoms of the tetrahedron to which the atom μ belongs. av: average structure. t: internal coordinate.

Tetrahedron	P	ϕ
$CuBr_4$	397(11)	0.392(6)
$(NC_4)_1$	216(42)	–0.047(33)
$(NC_4)_2$	208(48)	0.132(27)

Table 39A-15-005. $[N(CH_3)_4]_2CuBr_4$. Crystal structure of phase III [85Has1]. Fractional coordinates and isotropic temperature parameters. B [Å^2] is defined by Eq. (e) in Introduction. T = –33.5 °C. Symmetry codes: x, y, z; 1/2 – x, 1/2 + y, z; x, 1/4 – y, 1/2 + z; 1/2 – x, 3/4 – y, 1/2 + z.

Atom	x	y	z	B	Atom	x	y	z	B
Cu(1)	0.2439(9)	0.2011(3)	0.2378(7)	6.2(3)	N(2)	0.259(7)	0.417(2)	0.509(5)	8.1(16)
Br(11)	0.2200(8)	0.1879(2)	0.0491(6)	6.1(2)	C(21)	0.266(7)	0.375(2)	0.457(6)	5.3(14)
Br(12)	0.2753(11)	0.2686(7)	0.3186(7)	8.5(3)	C(22)	0.191(7)	0.448(2)	0.451(6)	6.5(16)
Br(13)	0.0246(8)	0.1749(3)	0.2993(8)	8.8(3)	C(23)	0.397(6)	0.430(2)	0.571(5)	4.5(13)
Br(14)	0.4711(7)	0.1688(3)	0.2764(6)	6.6(2)	C(24)	0.154(8)	0.403(2)	0.607(6)	6.5(17)
Cu(2)	0.7297(6)	0.2978(2)	0.7692(5)	2.9(1)	N(3)	0.755(4)	0.452(1)	0.863(3)	3.2(8)
Br(21)	0.7114(7)	0.3132(2)	0.9517(5)	5.6(2)	C(31)	0.730(10)	0.444(3)	0.757(8)	12.1(29)
Br(22)	0.7105(8)	0.2315(2)	0.6761(6)	6.1(2)	C(32)	0.772(8)	0.497(2)	0.895(6)	6.9(18)
Br(23)	0.9679(8)	0.3157(3)	0.7340(7)	7.3(3)	C(33)	0.617(10)	0.450(3)	0.913(8)	10.4(28)
Br(24)	0.5132(8)	0.3330(3)	0.7077(7)	6.9(3)	C(34)	0.889(10)	0.435(3)	0.906(6)	7.2(19)
N(1)	0.244(6)	0.050(2)	0.135(4)	6.2(12)	N(4)	0.740(4)	0.083(1)	0.496(3)	1.7(7)
C(11)	0.258(9)	0.055(3)	0.252(7)	9.5(23)	C(41)	0.740(9)	0.124(3)	0.575(7)	10.4(24)
C(12)	0.252(12)	0.001(3)	0.135(9)	12.5(31)	C(42)	0.779(8)	0.042(2)	0.576(6)	7.6(19)
C(13)	0.349(4)	0.073(1)	0.073(4)	2.2(9)	C(43)	0.585(6)	0.070(2)	0.480(5)	4.5(13)
C(14)	0.117(11)	0.077(3)	0.106(8)	11.6(30)	C(44)	0.848(9)	0.087(3)	0.416(7)	8.1(21)

Table 39A-15-006. $[N(CH_3)_4]_2CuBr_4$. Pressure coefficients of the phase boundaries [82Ges2].

Transition	$d\Theta/dp$ [$\cdot 10^2$ K GPa^{-1}]
II-I	0.97(5)
III-II	1.2(3)
IV-III	3.7(5)
IV-I	2.3(1)
IV-II	2.7(1)

Table 39A-15-007. $[N(CH_3)_4]_2CuBr_4$. The pressures and temperatures at the triple points (p_{triple}, Θ_{triple}) [82Ges2].

Triple point	p_{triple} [GPa]	Θ_{triple} [°C]
IV-II-I	0.191(5)	16.0(2)
IV-III-II	0.016(5)	–31.3(2)

Table 39A-15-008. $[N(CH_3)_4]_2CuBr_4$. Transition heat (ΔQ) and transition entropy (ΔS) [89Lop]. R: gas constant.

Transition	Θ [K] on heating	Θ [K] on cooling	$\Delta Q/R$ [K]	$\Delta S/R$
I–II	270.70(5)	270.7(1)	185(15)	0.70(5)
II–III	249.35(5)	241.7(1)	1.15(5)	0.0040(2)
III–IV	242.80(5)	234 to 237	450(50)	1.9(2)