53 $N(CH_3)_4HgCl_3$ family

53A Pure compounds

No. 53A-1 $N(CH_3)_4CdBr_3$, Tetramethylammonium-tribromo-cadomate

(M = 426.26)

1a Ferroelectric activity in $N(CH_3)_4CdBr_3$ was found by Gesi. 90Ges

b

phase	III	II	
state	F		
crystal system	hexagonal [a])	hexagonal [b])	[a]) 90Agu
space group	$P6_1 - C_6^2$, $P6_5 - C_6^{3}$ [a])	$P6_3/m - C_{6h}^{2}$ [b])	[b]) 76Dao
Θ [K]	156		90Ges

$\rho = 2.62 \cdot 10^3$ kg m^{-3} at RT. 76Dao

2a Crystal growth: slow evaporation from an aqueous solution containing $[N(CH_3)_4]Br$ and $CdBr_2$ in the ratio 1 : 1. 90Ges

Crystal form: hexagonal prisms having pyramidal ends. 90Ges

3a Unit cell parameters: a = 9.388(2) Å, c = 6.991(5) Å at T = 295 K and a = 9.219(4) Å, c = 20.86(1) Å at T = 85 K. 93Agu

b Z = 2 in phase II. 76Dao

Crystal structure: Table 53A-1-001, Table 53A-1-002, Table 53A-1-003; Fig. 53A-1-001, Fig. 53A-1-002, Fig. 53A-1-003, Fig. 53A-1-004.

For the crystal structures at 133 K in phase III, see 91Asa

5a Dielectric constant: Fig. 53A-1-005.

c Spontaneous polarization and coercive field: Fig. 53A-1-006.

Table 53A-1-001. $N(CH_3)_4CdBr_3$. Fractional coordinates and anisotropic temperature parameters [$Å^2$] of phase II at T = 295 K [93Agu]. $N(CH_3)_4$ groups are assumed to take three orientations with equal probability. Fractional coordinates of C(1) atom represent the average position of the two neighboring sites on the mirror plane. PP is the population parameter. U_{ij} is defined by Eq. (d) in Introduction.

	x	y	z	PP	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Cd	0	0	0	1	0.0437	0.0437	0.0165(7)	0.0219(3)	0	0
Br	0.2651(2)	0.1581(2)	0.25	1	0.0351(6)	0.0472(7)	0.0298(6)	0.0150(5)	0	0
N	0.3333	0.6666	0.25	1	0.0308	0.0308	0.033(9)	0.015(2)	0	0
C(1)	0.150(4)	0.522(5)	0.25	2/3	0.04(2)	0.10(3)	0.22(5)	–0.01(2)	0	0
C(2)	0.223(7)	0.580(8)	0.094(5)	1/3	0.17(6)	0.17(7)	0.03(2)	0.06(4)	–0.06(3)	–0.04(3)

Table 53A-1-002. $N(CH_3)_4CdBr_3$. Fractional coordinates and anisotropic temperature parameters [$Å^2$] of phase III at T = 85 K [93Agu]. U_{ij} is defined by Eq. (d) in Introduction. The coordinates of H atoms were refined using soft restrictions for the C–H bond lengths. Mean square displacements of H atoms were fixed to 0.04 $Å^2$.

	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Cd	0.00211(6)	0.02445(5)	–0.0009(1)	0.0112(2)	0.0122(2)	0.0036(2)	0.0056(2)	–0.0008(1)	–0.0004(2)
Br(1)	0.28003(7)	0.19652(7)	0.0759(1)	0.0099(2)	0.0114(2)	0.0057(3)	0.0045(2)	–0.0002(2)	0.0002(2)
Br(2)	–0.13849(7)	0.14069(7)	0.0900(1)	0.0130(3)	0.0145(2)	0.0063(3)	0.0086(2)	–0.0006(2)	0.0000(2)
Br(3)	–0.08507(7)	–0.24476(6)	0.0815(1)	0.0124(3)	0.0111(2)	0.0067(2)	0.0062(2)	–0.0001(2)	0.0000(2)
N	0.3483(6)	0.6903(5)	0.0814(3)	0.010(2)	0.010(2)	0.011(2)	0.005(2)	0.001(2)	0.004(2)
C(1)	0.5066(7)	0.6807(7)	0.0878(3)	0.013(3)	0.016(2)	0.029(4)	0.009(2)	–0.001(3)	0.002(3)
C(2)	0.3927(8)	0.8726(7)	0.0822(4)	0.024(3)	0.009(2)	0.035(4)	0.011(2)	0.006(3)	0.005(3)
C(3)	0.2630(9)	0.610(1)	0.0196(3)	0.025(3)	0.034(4)	0.016(4)	0.015(3)	–0.014(3)	–0.013(3)
C(4)	0.2319(9)	0.6012(9)	0.1360(3)	0.028(3)	0.023(3)	0.017(3)	0.012(3)	0.011(3)	0.008(3)
H(11)	0.55(1)	0.71(1)	0.048(2)						
H(12)	0.56(1)	0.73(1)	0.124(3)						
H(13)	0.47(1)	0.566(3)	0.087(5)						
H(21)	0.44(1)	0.91(1)	0.044(3)						
H(22)	0.45(1)	0.92(1)	0.118(3)						
H(23)	0.32(1)	0.87(1)	0.109(4)						
H(31)	0.327(9)	0.68(1)	–0.014(4)						
H(32)	0.24(1)	0.509(5)	0.038(5)						
H(33)	0.173(9)	0.62(1)	0.026(5)						
H(41)	0.20(1)	0.492(4)	0.136(5)						
H(42)	0.29(1)	0.68(1)	0.168(3)						
H(43)	0.140(8)	0.61(1)	0.127(5)						

Table 53A-1-003. $N(CH_3)_4CdBr_3$. Interatomic distances [Å] and angles [°] of phase III at $T = 85$ K [93Agu].

Cd–Br(1)	2.754(2)	Br(1)–Cd–Br(2)	81.99(7)
Cd–Br(2)	2.795(2)	Br(1)–Cd–Br(3)	85.69(8)
Cd–Br(3)	2.787(2)	Br(2)–Cd–Br(3)	86.58(8)
N–C(1)	1.51(1)	C(1)–N–C(2)	109.3(4)
N–C(2)	1.518(8)	C(1)–N–C(3)	109.2(6)
N–C(3)	1.50(1)	C(1)–N–C(4)	110.4(6)
N–C(4)	1.498(9)	C(2)–N–C(3)	110.1(6)
C(1)–H(11)	0.91(6)	C(2)–N–C(4)	108.7(6)
C(1)–H(12)	0.91(6)	C(3)–N–C(4)	109.2(4)
C(1)–H(13)	0.93(3)		
C(2)–H(21)	0.90(6)		
C(2)–H(22)	0.90(7)		
C(2)–H(23)	0.9(1)		
C(3)–H(31)	0.92(8)		
C(3)–H(32)	0.91(7)		
C(3)–H(33)	0.9(1)		
C(4)–H(41)	0.90(5)		
C(4)–H(42)	0.91(7)		
C(4)–H(43)	0.9(1)		

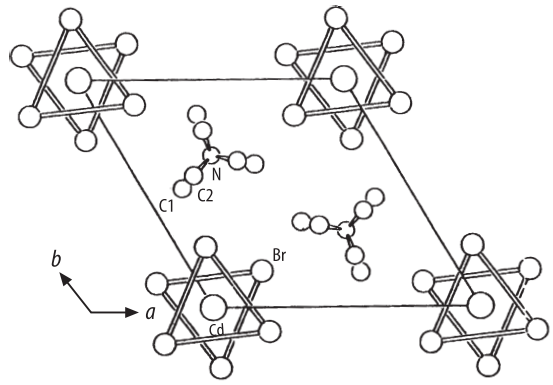

Fig. 53A-1-001. $N(CH_3)_4CdBr_3$. Crystal structure of phase II at T = 295 K [93Agu]. Projection along [001].

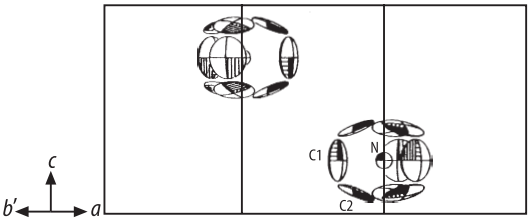

Fig. 53A-1-002. $N(CH_3)_4CdBr_3$. Crystal structure of phase II at T = 295 K [93Agu]. Projection along [120] of the disordered $N(CH_3)_4$ groups with thermal ellipsoids.

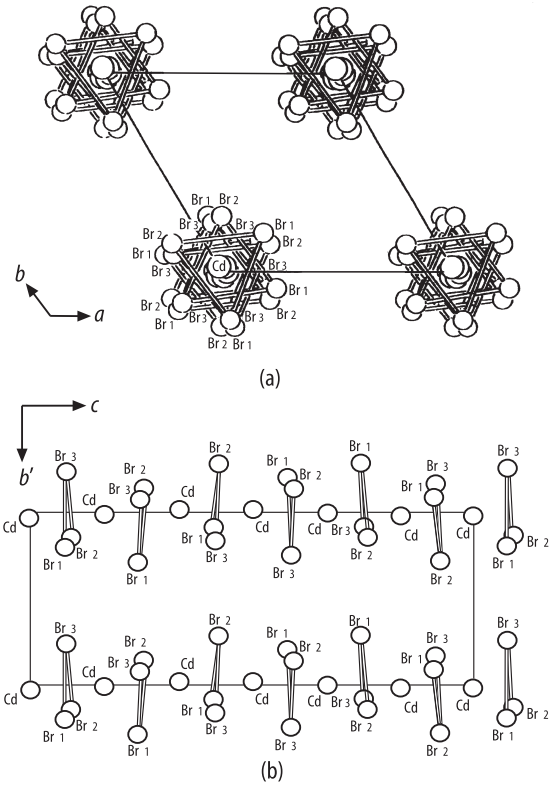

Fig. 53A-1-003. $N(CH_3)_4CdBr_3$. Crystal structure of phase III [93Agu]. (**a**) Projection along [001]. (**b**) Projection along [100]. $N(CH_3)_4$ groups are not drawn.

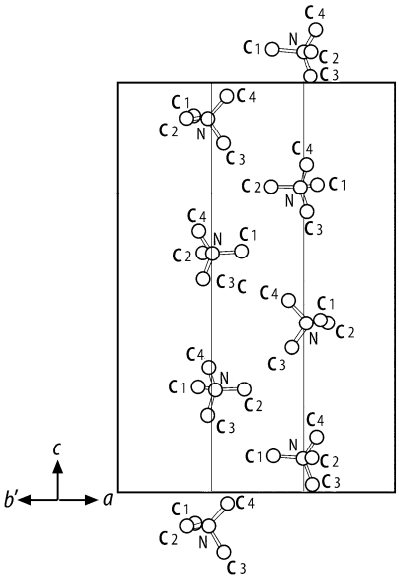

Fig. 53A-1-004. $N(CH_3)_4CdBr_3$. Crystal structure of phase III [93Agu]. Projection along [120] of the ordered $N(CH_3)_4$ groups.

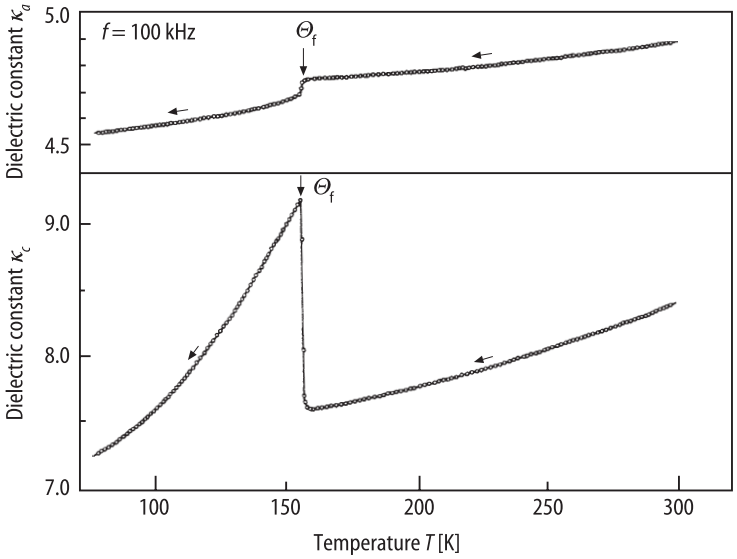

Fig. 53A-1-005. $N(CH_3)_4CdBr_3$. κ_a, κ_c vs. T [90Ges].

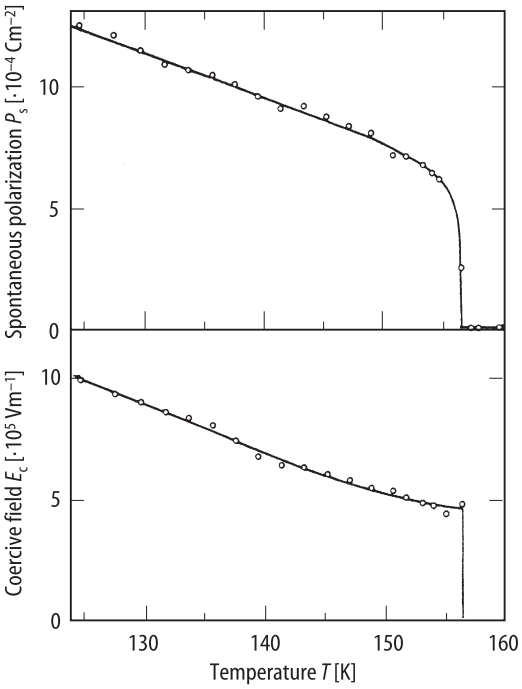

Fig. 53A-1-006. $N(CH_3)_4CdBr_3$. P_s, E_c vs. T [90Ges].

References

76Dao Daoud, A.: Bull. Soc. Chim. France, Part I (1976) 751.
90Agu Aguirre-Zamalloa, G., Couzi, M., Chank, N.B., Gallois, B.: J. Phys. (Paris) **51** (1990) 2135.
90Ges Gesi, K.: J. Phys. Soc. Jpn. **59** (1990) 432.
91Asa Asahi, T., Hasebe, K., Gesi, K.: Acta Crystallogr. Sect. C **47** (1991) 1208.
93Agu Aguirre-Zamalloa, G., Madriage, G., Couzi, M., Breczewski, T.: Acta Crystallogr. Sect. B **49** (1993) 691.

No. 53A-2 $N(CH_3)_4HgCl_3$, Tetramethylammonium-trichloro-mercurate

(M = 381.09)

1a	Ferroelectricity in $N(CH_3)_4HgCl_3$ was discovered by Fatuzzo and Nitsche in 1960.		60Fat
b	state	F	
	crystal system	monoclinic [a])	[a]) 63Whi
	space group	$P2_1 - C_2^{2}$ [a])	
	Temperature of decomposition ≈ 200 °C.		60Fat
	$\rho = 2.45 \cdot 10^3$ kg m^{-3}.		82Moh
	Colorless.		60Fat
2a	Crystal growth: slow evaporation from an aqueous solution containing $[N(CH_3)_4]Cl$ and $HgCl_2$ in the molar ratio 2 : 1.		60Fat
b	Crystal form: needle shape.		60Fat
3a	Unit cell parameters: a = 8.70(1) Å, b = 16.02(2) Å, c = 7.47(1) Å, β = 93.5(5)° at RT.		82Moh
b	Z = 4.		82Moh
	Crystal structure: Table 53A-2-001, Table 53A-2-002, Table 53A-2-003; Fig. 53A-2-001.		
5a	$\kappa \approx 60$ at RT; almost independence of T.		60Fat
c	$P_s \approx 1.2 \cdot 10^{-2}$ C m^{-2} at RT; only slightly T dependent.		60Fat
	$E_c \approx 3 \cdot 10^5$ V m^{-1} at RT.		60Fat
10a	Raman scattering: Table 53A-2-004.		
15b	Switching: Fig. 53A-2-002, Fig. 53A-2-003.		

Table 53A-2-001. $N(CH_3)_4HgCl_3$. Crystal structure [82Moh]. Fractional coordinates and isotropic temperature parameters. *B* is defined by Eq. (e) in Introduction.

Atom	*x*	*y*	*z*	*B* [Å^2]
Hg(1)	0.1710(4)	0.0	0.0398(6)	*
Hg(2)	0.2855(4)	0.0450(4)	0.5520(6)	*
Cl(1)	0.411(2)	0.964(2)	0.927(4)	*
Cl(2)	0.957(2)	0.906(2)	–0.006(4)	*
Cl(3)	0.156(3)	0.126(2)	0.226(3)	*
Cl(4)	0.264(3)	0.909(2)	0.423(4)	*
Cl(5)	0.516(2)	0.128(2)	0.546(4)	*
Cl(6)	0.093(2)	0.104(2)	0.726(4)	*
N(1)	0.694(5)	0.204(6)	0.035(4)	3(1)
N(2)	0.239(6)	0.379(3)	0.517(9)	2(1)
C(11)	0.763(13)	0.229(9)	0.213(22)	8(3)
C(12)	0.728(7)	0.114(4)	0.021(11)	2(1)
C(13)	0.531(6)	0.230(4)	0.004(10)	2(1)
C(14)	0.806(15)	0.235(9)	–0.091(10)	8(3)
C(21)	0.287(11)	0.351(7)	0.701(18)	6(3)
C(22)	0.190(12)	0.468(8)	0.506(19)	6(3)
C(23)	0.087(14)	0.341(8)	0.467(22)	7(3)
C(24)	0.331(11)	0.347(6)	0.371(16)	5(2)

* Anisotropic temperature parameters shown in Table 53A-2-002.

Table 53A-2-002. $N(CH_3)_4HgCl_3$. Crystal structure [82Moh]. Anisotropic temperature parameters. B_{ij} is defined by Eq. (a) in Introduction.

Atom	B_{11}	B_{22}	B_{33}	B_{12}	B_{13}	B_{23}
Hg(1)	0.0163(6)	0.0057(2)	0.0145(12)	–0.0005(6)	0.0037(12)	–0.0045(9)
Hg(2)	0.0165(6)	0.0054(2)	0.0142(11)	–0.0001(6)	0.0034(12)	–0.0037(8)
Cl(1)	0.005(2)	0.007(1)	0.033(9)	–0.007(3)	0.008(7)	0.007(5)
Cl(2)	0.016(3)	0.007(1)	0.007(6)	–0.005(3)	0.007(7)	0.002(4)
Cl(3)	0.019(4)	0.007(1)	0.002(7)	0.005(4)	–0.013(7)	–0.000(4)
Cl(4)	0.013(3)	0.005(1)	0.029(8)	–0.007(3)	–0.003(8)	–0.008(5)
Cl(5)	0.009(3)	0.009(2)	0.011(7)	–0.007(3)	–0.005(6)	–0.008(5)
Cl(6)	0.011(3)	0.008(1)	0.015(7)	0.001(3)	0.005(6)	0.008(5)

Table 53A-2-003. $N(CH_3)_4HgCl_3$. Crystal structure [82Moh]. Interatomic distances and angles.

Interatomic distances [Å]			
Hg(1)–Cl(1)	2.37(3)	Hg(2)–Cl(4)	2.38(2)
Hg(1)–Cl(2)	2.40(3)	Hg(2)–Cl(5)	2.41(2)
Hg(1)–Cl(3)	2.46(2)	Hg(2)–Cl(6)	2.38(2)
Hg(1)–Cl(4)	3.27(3)	Hg(2)–Cl(1) [2])	3.22(3)
Hg(1)–Cl(6) [1])	2.93(3)	Hg(2)–Cl(3)	2.92(2)
Angles [°]			
Cl(1)–Hg(1)–Cl(2)	119.2(9)	Cl(4)–Hg(2)–Cl(5)	122.8(9)
Cl(1)–Hg(1)–Cl(3)	118.6(9)	Cl(4)–Hg(2)–Cl(6)	123.0(9)
Cl(2)–Hg(1)–Cl(3)	121.9(8)	Cl(5)–Hg(2)–Cl(6)	113.9(9)
Cl(1)–Hg(1)–Cl(4)	91.6(8)	Cl(4)–Hg(2)–Cl(3)	93.1(8)
Cl(2)–Hg(1)–Cl(4)	89.8(8)	Cl(5)–Hg(2)–Cl(3)	91.1(8)
Cl(3)–Hg(1)–Cl(4)	83.6(8)	Cl(6)–Hg(2)–Cl(3)	91.7(8)
Cl(1)–Hg(1)–Cl(6) [1])	91.2(8)	Cl(4)–Hg(2)–Cl(1) [2])	89.8(8)
Cl(2)–Hg(1)–Cl(6) [1])	95.8(8)	Cl(5)–Hg(2)–Cl(1) [2])	89.9(8)
Cl(3)–Hg(1)–Cl(6) [1])	92.0(8)	Cl(6)–Hg(2)–Cl(1) [2])	84.2(8)

[1]) Position is at (x, y, z–1).
[2]) Position is at (x, y–1, z).

Table 53A-2-004. $N(CH_3)_4HgCl_3$. Frequencies and assignments of lattice vibrational modes obtained from Raman scattering spectra [75Her]. Scattering intensities are represented by vs (very strong), s (strong) and w (weak). br indicates that the mode gives a broad spectrum. In the column of assignment following abbreviations are used, ν_s: symmetric stretch, ν_{as}: asymmetric stretch, δ_s: symmetric bend, δ_{as}: asymmetric bend. Frequencies are given in the unit of cm^{-1}. 1 $cm^{-1} = 3 \cdot 10^{10}$ Hz.

Frequencies [cm^{-1}]	Scattering intensities	Assignments	Symmetries
274	vs	ν_s (Hg-Cl)	A_1
244	w, br	ν_{as} (Hg-Cl)	E
90	s, br	δ_s (ClHgCl)	A_1
74	s	δ_{as} (ClHgCl)	E
56	s	external vibrations	
37	w		
33	w		

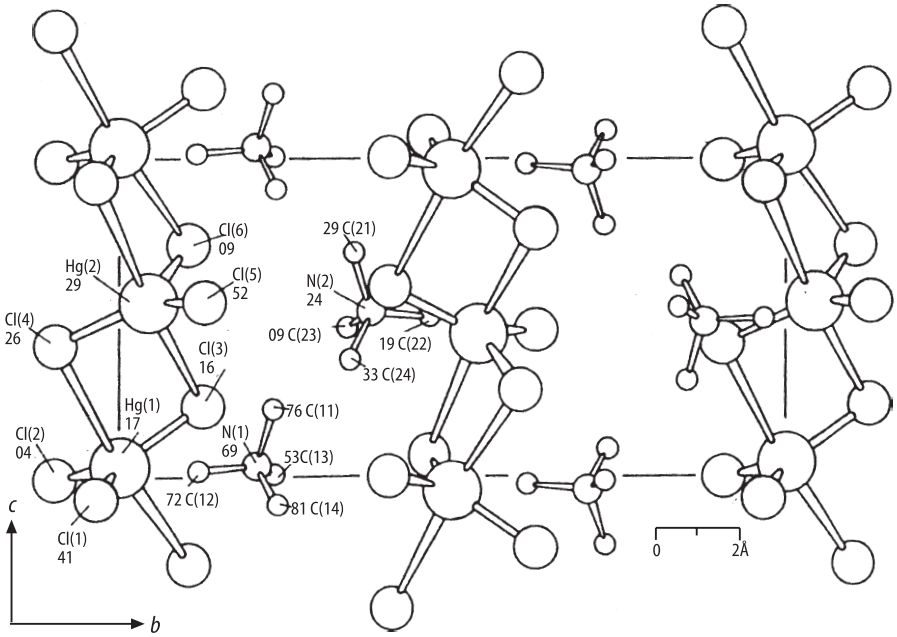

Fig. 53A-2-001. $N(CH_3)_4HgCl_3$. Crystal structure [82Moh]. Projection along [100]. The number indicates x coordinate [$\cdot 10^{-2}$].

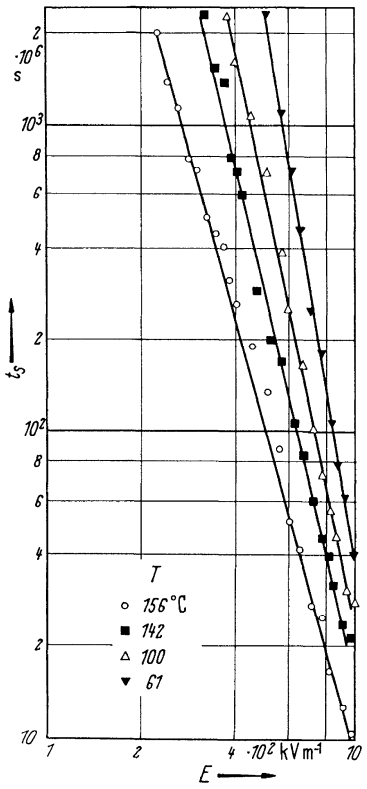

Fig. 53A-2-002. $N(CH_3)_4HgCl_3$. t_s vs. E [60Fat]. Parameter: T. t_s: switching time.

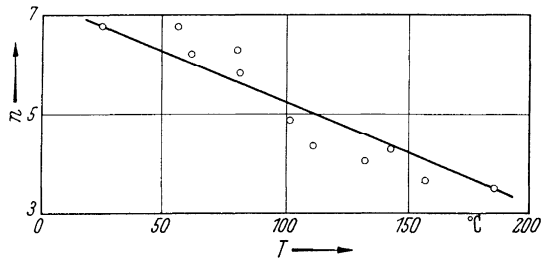

Fig. 53A-2-003. $N(CH_3)_4HgCl_3$. n vs. T [60Fat]. n: exponent of equation $t_s \propto E^{-n}$.

References

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63Whi White, J.G.: Acta Crystallogr. **16** (1963) 397.
75Her Herlinger, A.W.: Spectrosc. Lett. **8** (1975) 787.
82Moh Mohana Rao, J.K., Rajaram, R.K.: Z. Kristallogr. **160** (1982) 219.

No. 53A-3 $N(CH_3)_4HgBr_3$, Tetramethylammonium-tribromo-mercurate

(M = 514.45)

1a	Ferroelectricity in $N(CH_3)_4HgBr_3$ was discovered by Fatuzzo et al. in 1962.		62Fat
b	state	F	
	crystal system	monoclinic [a])	[a]) 63Whi
	space group	$P2_1 - C_2^{2\,a}$)	
	Temperature of decomposition ≈ 170 °C.		62Fat
	$\rho = 2.96 \cdot 10^3$ kg m^{-3}.		63Whi
	Color: white.		62Fat
2a	Crystal growth: slow cooling from a saturated solution containing $[N(CH_3)_4]Br$ and $HgBr_2$ in 1.3 normal HBr.		62Fat
b	Crystal form: needle shape.		62Fat
3a	Unit cell parameters: a = 9.05(2) Å, b = 15.90(5) Å, c = 7.94(2) Å, β = 93.6(2)° at RT.		63Whi
b	Z = 4.		63Whi
	Crystal structure: Table 53A-3-001, Table 53A-3-002, Table 53A-3-003; Fig. 53A-3-001.		
5a	$\kappa \approx 10$; almost independence of T (–40 °C < T < 160 °C).		62Fat
b	$P_s \approx 1 \cdot 10^{-2}$ C m^{-2}; almost independence of T (–40 °C < T < 160 °C).		62Fat
	$E_c \approx 10^6$ V m^{-1} at 50 °C.		62Fat

Table 53A-3-001. $N(CH_3)_4HgBr_3$. Crystal structure [63Whi]. Fractional coordinates. e.s.d.: estimated standard deviation.

	x	*y*	*z*	e.s.d. [Å]
Hg(1)	0.165	0.000	0.025	0.009
Br(1)	0.421	–0.045	–0.023	
Br(2)	–0.052	–0.101	–0.007	0.022
Br(3)	0.148	0.127	0.223	
Hg(2)	0.278	0.046	0.528	0.009
Br(4)	0.250	–0.106	0.430	
Br(5)	0.514	0.126	0.550	0.022
Br(6)	0.089	0.100	0.720	
N(1)	0.67	–0.13	0.42	
C(1)	0.57	–0.18	0.35	
C(2)	0.59	–0.08	0.51	
C(3)	0.74	–0.08	0.30	
C(4)	0.77	–0.17	0.50	
N(2)	0.64	0.19	0.07	
C(5)	0.56	0.25	–0.01	
C(6)	0.56	0.13	0.14	
C(7)	0.73	0.23	0.19	
C(8)	0.73	0.15	–0.05	

Table 53A-3-002. $N(CH_3)_4HgBr_3$. Crystal structure [63Whi]. Interatomic distances and bond angles. e.s.d.: estimated standard deviation.

Hg–Br distances			Br–Hg–Br bond angles		
Atoms	Intra-anion distance [Å]	e.s.d. [Å]	Atoms	Angle [°]	e.s.d. [°]
Hg(1)–Br(1)	2.48		Br(1)–Hg(1)–Br(2)	121.8	
Hg(1)–Br(2)	2.53		Br(2)–Hg(1)–Br(3)	119.1	
Hg(1)–Br(3)	2.56		Br(1)–Hg(1)–Br(3)	114.4	
Hg(2)–Br(4)	2.55		Br(4)–Hg(2)–Br(5)	125.3	0.8
Hg(2)–Br(5)	2.49	0.025	Br(5)–Hg(2)–Br(6)	113.3	
Hg(2)–Br(6)	2.52		Br(4)–Hg(2)–Br(6)	116.9	
Hg(1)–Br(6)	2.94				
Hg(2)–Br(3)	2.92				

Table 53A-3-003. $N(CH_3)_4HgBr_3$. Crystal structure [63Whi]. C–Br distances less than 4 Å. Br atoms related by the screw axis to those of Table 53A-3-001 are represented by attaching a prime, and atoms with coordinates related by a translation along *a*, *b* or *c* to those of Table 53A-3-001 are indicated by the corresponding symbols in parentheses.

Atom	Distance [Å]
C(1)–Br(1)	3.88
C(1)–Br(4)	3.28
C(1)–Br(5)' (+*a* –*b* +*c*)	3.25
C(2)–Br(4)	3.14
C(2)–Br(5)	3.43
C(3)–Br(1)	3.80
C(3)–Br(2) (+*a*)	3.18
C(5)–Br(1)' (+*a*)	3.27
C(6)–Br(1)	3.25
C(6)–Br(3)	3.78
C(6)–Br(5)	3.28
C(7)–Br(5)	3.91
C(8)–Br(5) (–*c*)	3.65

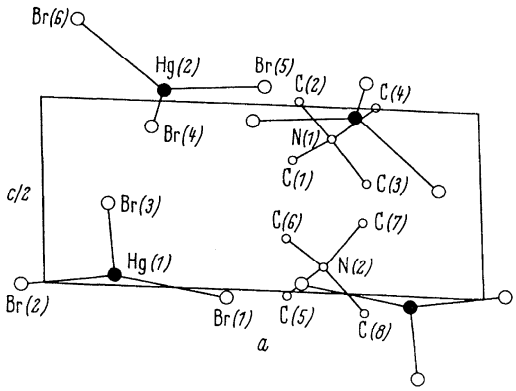

Fig. 53A-3-001. $N(CH_3)_4HgBr_3$. Crystal structure [63Whi]. Projection on (010).

References

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No. 53A-4 $N(CH_3)_4HgBrI_2$, Tetramethylammonium-diiodo-bromo-mercurate

(M = 608.45)

1a Dielectric anomalies associated with phase transitions in $N(CH_3)_4HgBrI_2$ were reported by Arend et al. in 1982. 82Are

b

phase	II	I	
crystal system	orthorhombic	monoclinic	82Are
space group	$Pb2_1m-C_{2v}^2$	$P2_1/n-C_{2h}^5$	82Are
Θ [K]	375		

$\rho = 3.11 \cdot 10^3$ kg m^{-3}. 82Are

3a Unit cell parameters: a = 9.35(1) Å, b = 16.79(3) Å, c = 8.28(1) Å, β = 96.40(8)° in phase I and a = 9.417(3) Å, b = 16.104(5) Å, c = 8.339(3) Å in phase II. 82Are
Crystal structure: Z = 4 in phase II. 82Are

5a Dielectric constant: Fig. 53A-4-001.

9a Refractive indices and birefringence: Fig. 53A-4-002, Fig. 53A-4-003.
n_a = 1.761, n_b = 1.802, n_c = 1.755 at 22 °C (λ = 633 nm). 86Zhu

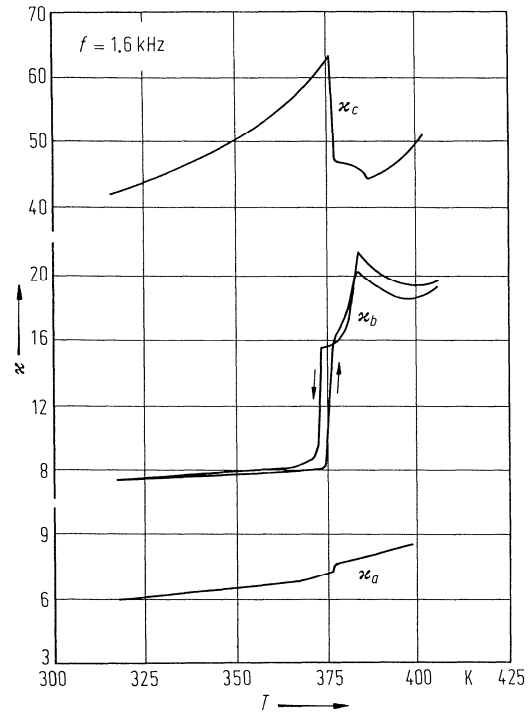

Fig. 53A-4-001. $N(CH_3)_4HgBrI_2$. κ_a, κ_b, κ_c vs. T [82Are].

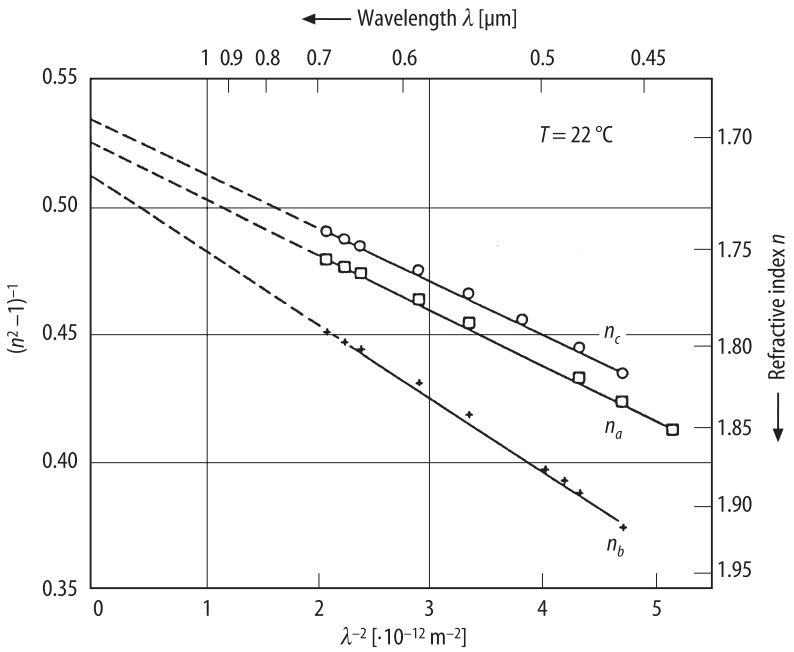

Fig. 53A-4-002. $N(CH_3)_4HgBrI_2$. $(n^2 - 1)^{-1}$ vs. λ^{-2} [86Zhu].

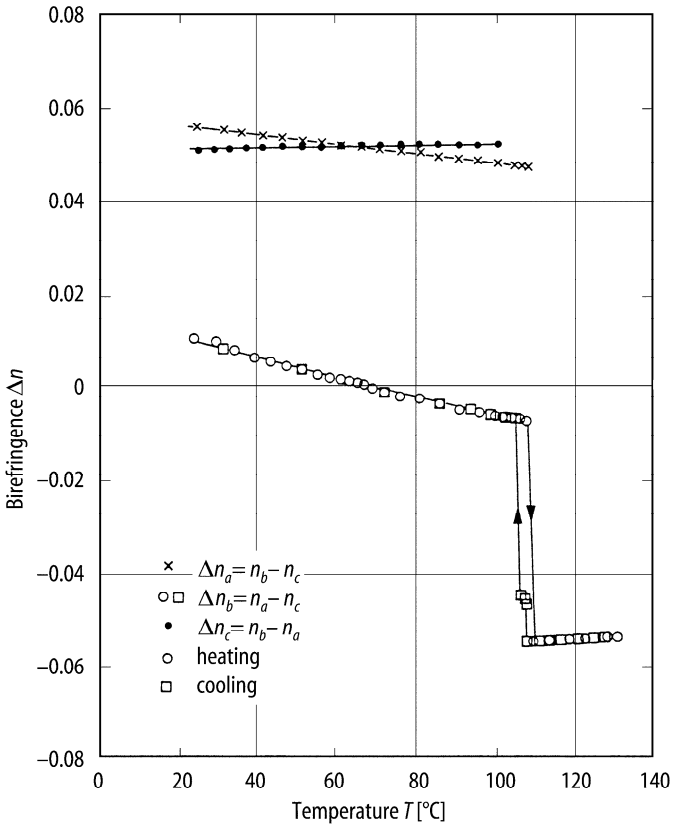

Fig. 53A-4-003. $N(CH_3)_4HgBrI_2$. Δn vs. T [86Zhu].

References

82Are Arend, H., Ehrensperger, M., Muralt, P., Chapuis, G., Zuniga, J.F.: Ferroelectrics Lett. **44** (1982) 147.

86Zhu Zhu, Y., Arend, H., Guenter, P.: Ferroelectrics Lett. **5** (1986) 107.

No. 53A-5 $P(CH_3)_4HgBr_3$, Tetramethylphosphonium-tribromo-mercurate

(M = 531.41)

1a	Ferroelectricity in $P(CH_3)_4HgBr_3$ was discovered by Fatuzzo et al. in 1962.	62Fat
b	State: F.	62Fat
	Temperature of decomposition ≈170 °C.	62Fat
	Color: white.	62Fat
2a	Crystal growth: vacuum evaporation of the solution containing $[P(CH_3)_4]$ Br and $HgBr_2$.	62Fat
b	Crystal form: flat plate.	62Fat
5a	$\kappa \approx 10$; independence of T (–40 °C < T < 160 °C).	62Fat
c	$P_s \approx 3 \cdot 10^{-2}$ C m^{-2}; independence of T (–40 °C < T < 160 °C).	62Fat
	$E_c \approx 23 \cdot 10^5$ V m^{-1} at 50 °C.	62Fat

Reference

62Fat Fatuzzo, E., Nitsche, R., Roetschi, H., Zingg, S.: Phys. Rev. **125** (1962) 514.

No. 53A-6 $N(CH_3)_4HgI_3$, Tetramethylammonium-triiodo-mercurate

(M = 655.45)

1a	Ferroelectricity in $N(CH_3)_4HgI_3$ was discovered by Fatuzzo et al. in 1962.	62Fat
b	state: F; crystal system: orthorhombic [a]); space group: $Pb2_1m - C_{2v}^2$ [a])	[a]) 65Pak
	Temperature decomposition ≈170 °C.	62Fat
	$\rho = 3.15 \cdot 10^3$ kg m^{-3}.	67Ger
	Color: pale-yellow.	62Fat
	Cleavage plane: (100).	67Ger
2a	Crystal growth: slow evaporation from an equimolar mixture of $[N(CH_3)_4I]$ and HgI_2 in cyclohexanone.	62Fat
b	Crystal form: polyhedral shape.	62Fat
3a	Unit cell parameters: a = 9.46 Å, b = 16.48 Å, c = 8.56 Å at RT.	67Ger
b	Z = 4.	65Pak
	Crystal structure: Table 53A-6-001; Fig. 53A-6-001.	
	For approximate positions of light atoms, see	65Pak
5a	$\kappa \approx 10$; independence of T (–40 °C < T < 100 °C).	62Fat
c	$P_s = 1.2 \cdot 10^{-2}$ C m^{-2} at –40 °C; $1.7 \cdot 10^{-2}$ C m^{-2} at RT; $2.3 \cdot 10^{-2}$ C m^{-2} at 80 °C.	62Fat
	$E_c \approx 8 \cdot 10^5$ V m^{-1} at RT.	62Fat
9a	Birefringence: Fig. 53A-6-002, Fig. 53A-6-003.	

Table 53A-6-001. $N(CH_3)_4HgI_3$. Crystal structure [67Ger]. Fractional coordinates of Hg and I. For the notations of atoms, see Fig. 53A-6-001.

Atom	*x*	*y*	*z*
Hg(1)	0.154	0.000	0.000
Hg(2)	0.278	0.045	0.500
I(1)	0.427	–0.039	0.000
I(2)	–0.068	–0.106	0.000
I(3)	0.109	0.115	0.258
I(4)	0.246	–0.114	0.500
I(5)	0.503	0.131	0.500
I(6)	0.109	0.115	0.742

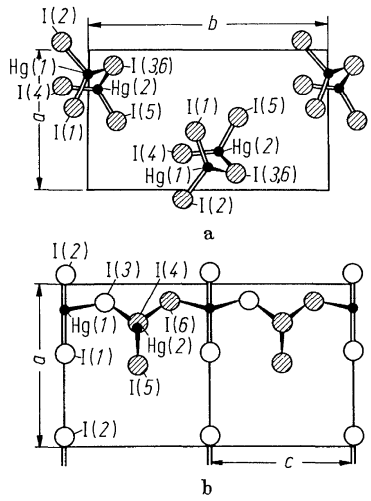

Fig. 53A-6-001. $N(CH_3)_4HgI_3$. Crystal structure [67Ger]. (**a**) projection on (001), (**b**) projection on (010).

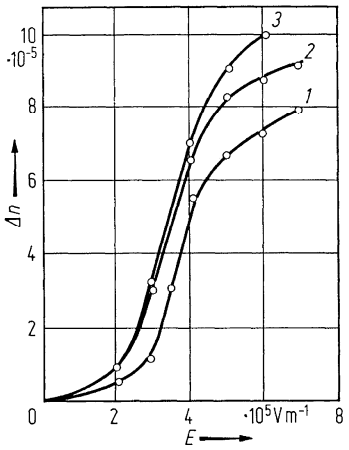

Fig. 53A-6-002. $N(CH_3)_4HgI_3$. Δn vs. E at RT [69Son]. $\Delta n = (n_1^3 r_{13} - n_3^3 r_{33})\, E/2$. Parameter: λ; curve *1*: $\lambda = 585$ nm, *2*: 535 nm, *3*: 465 nm.

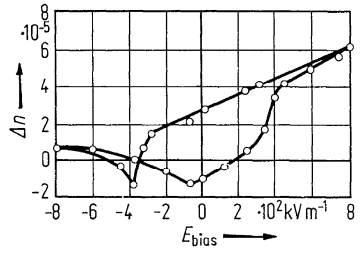

Fig. 53A-6-003. $N(CH_3)_4HgI_3$. Δn vs. E_{bias} at RT [69Son]. $\Delta n = (n_1^3 r_{13} - n_3^3 r_{33})\, E/2$. $\lambda = 535$ nm.

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69Son Sonin, A.S., Vasilevskaya, A.S., Kalitina, M.P., Marchenko, E.I.: Kristallografiya **14** (1969) 343; Sov. Phys. Crystallogr. (English Transl.) **14** (1969) 275.