No. 1A-9 $CdTiO_3$, Cadmium titanate

(M = 208.31)

1a	$CdTiO_3$ was reported by Smolenskii in 1950 to be ferroelectric below 50...60 K. In 1950 Hulm et al. denied its ferroelectricity but Hegenbarth supported Smolenskii's findings.			50Smo 50Hul 59Heg
b	phase	II	I	
	state	(F) [a])		[a]) 50Smo
	crystal system		orthorhombic [b])	[b]) 57Kay
	space group		$Pc2_1n - C_{2v}^9$ [b])	
	Θ [°C]	–223...–213		50Smo
2a	Crystal growth: flux method (1.4 $CdTiO_3$: 6.9 KF : 2.5 KVO_3); reaction at high temperature ($CdF_2 + TiO_2 + 1/2O_2 \rightarrow CdTiO_3 + F_2$).			85Uli 79Sug
3a	a = 5.348 Å, b = 7.615 Å, c = 5.417 Å at RT. The relation between the orthorhombic unit cell and the pseudocubic monoclinic cell is the same as in the case of $NaTaO_3$; see Fig. 1A-4-001.			57Kay
b	Z = 4 in phase I. Crystal structure in phase I: Fig. 1A-9-001. Crystal structure in orthorhombically distorted perovskite and ilmenite: Fig. 1A-9-002, Table 1A-9-001.			57Kay
5a	Dielectric constant: Fig. 1A-9-003, Fig. 1A-9-004, Fig. 1A-9-005.			
b	Effect of E_{bias} on κ: Fig. 1A-9-006.			
d	Electrocaloric effect, see			61Heg
9a	Optical absorption coefficient: Fig. 1A-9-007.			
b	Electrooptic effect: Fig. 1A-9-008.			
13a	NMR: Perturbation function: see			90Cat
b	ESR: Spin Hamiltonian parameters for Mn^{2+} center at 300K: $g_{\parallel}$ = 2.008(2), $g_{\perp}$ = 2.003(2), $b_{20} = -120(2)\cdot10^{-2}\,m^{-1}$, $b_{22} = -26(3)\cdot10^{-2}\,m^{-1}$ and $A = -82.7(2)\cdot10^{-2}\,m^{-1}$.			83Gei
c	Mössbauer parameters: see			81Sho
15a	Domain structure: see			85Uli

Table 1A-9-001. $CdTiO_3$. Fractional coordinates of atoms in the unit cell of phase I [57Kay].

Positions						Estimated error
Cd	*x*:	0+0.006	0–0.006	1/2+0.006	1/2–0.006	(2)
	y:	3/4	1/4	1/4	3/4	
	z:	0+0.016	0–0.016	1/2–0.016	1/2+0.016	(2)
Ti	*x*:	1/2+0.005	1/2–0.005	0+0.005	0–0.005	(5)
	y:	0	1/2	1/2	0	
	z:	0–0.065	0+0.065	1/2+0.065	1/2–0.065	(10)
O(1)	*x*:	0–0.030	0+0.030	1/2+0.030	1/2–0.030	(15)
	y:	3/4	1/4	3/4	1/4	
	z:	1/2+0.050	1/2–0.050	0+0.050	0–0.050	(15)
O(2)	*x*:	1/4+0.050	1/4–0.050	3/4–0.050	3/4+0.050	(5)
	y:	0–0.030	0–0.030	1/2–0.030	1/2–0.030	(15)
	z:	1/4+0.060	3/4+0.060	3/4–0.060	1/4–0.060	(15)
O(3)	*x*:	1/4+0.050	1/4–0.050	3/4–0.050	3/4+0.050	(5)
	y:	1/2+0.070	1/2+0.070	0+0.070	0+0.070	(15)
	z:	1/4+0.060	3/4+0.060	3/4–0.060	1/4–0.060	(15)

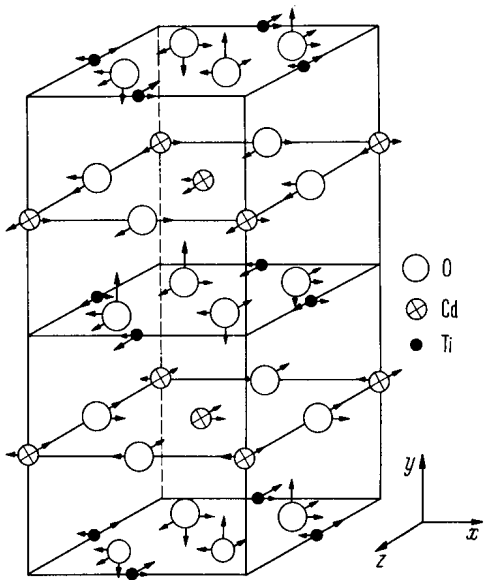

Fig. 1A-9-001. $CdTiO_3$. A sketch of the structure in phase I [57Kay]. The displacements of the atoms from the positions in the ideal cubic structure are indicated by arrows (exaggerated). See Table 1A-9-001.

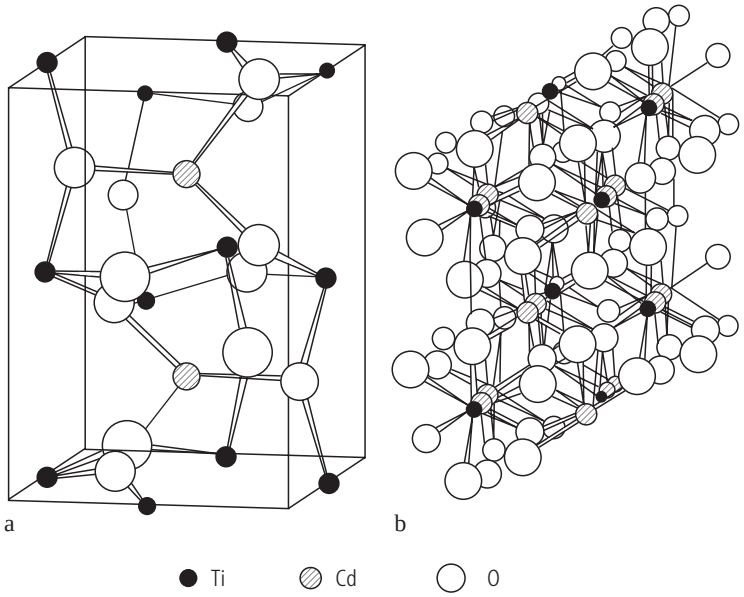

Fig. 1A-9-002. $CdTiO_3$ [90Cat]. Sketches of (**a**) orthorhombically distorted perovskite and (**b**) ilmenite structures.

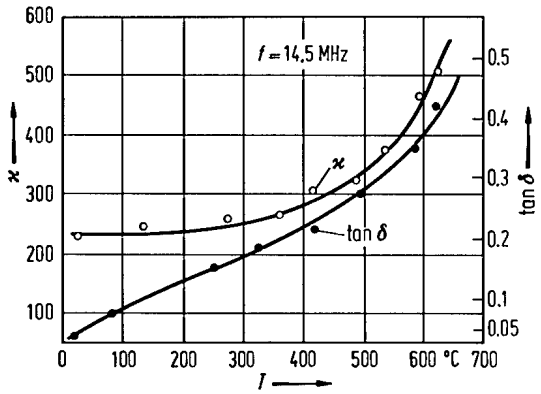

Fig. 1A-9-003. $CdTiO_3$. κ, $\tan\delta$ vs. T [68Sho].

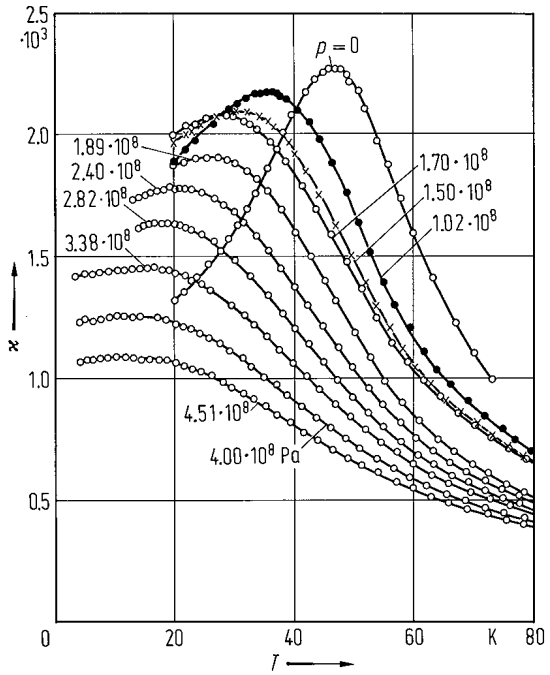

Fig. 1A-9-004. $CdTiO_3$ (ceramics). κ vs. T [73Mar]. Parameter: p.

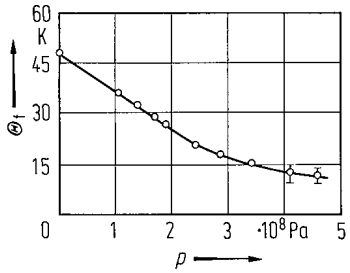

Fig. 1A-9-005. $CdTiO_3$. Θ_f vs. p [73Mar].

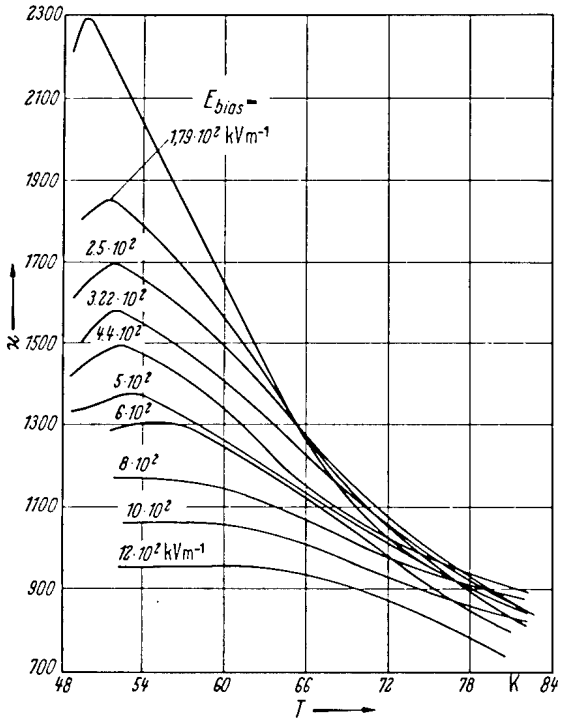

Fig. 1A-9-006. $CdTiO_3$. κ vs. T [59Heg]. Parameter: E_{bias}. f = 800 Hz.

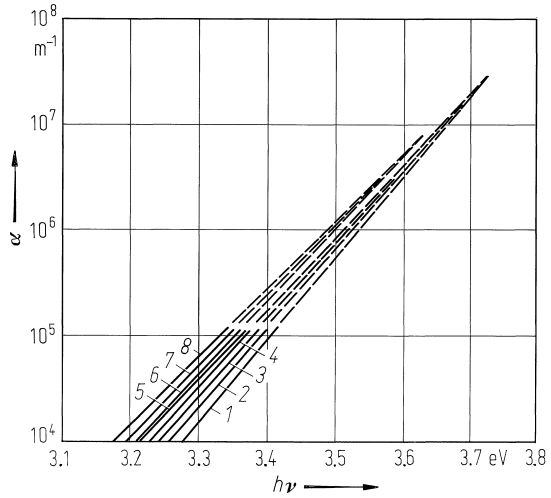

Fig. 1A-9-007. $CdTiO_3$. α vs. $h\nu$ [84Zam]. α: optical absorption coefficient. Parameter: *T*. Curve *1*: 300 K; *2*: 327 K; *3*: 350 K; *4*: 364 K; *5*: 379 K; *6*: 391 K; *7*: 403 K; *8*: 416 K.

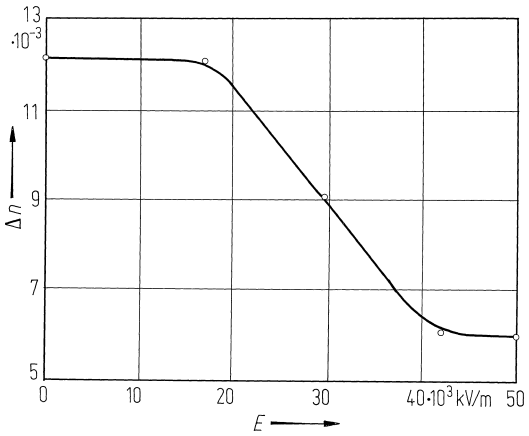

Fig. 1A-9-008. $CdTiO_3$. Δn vs. E [86Fes]. $E \parallel [010]$, $T = 293$ K.

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