No. 1A-6 $AgTaO_3$, Silver tantalate

(M = 336.81)

1a Structure changes, associated with phase transitions, were observed in $AgTaO_3$ by Francombe et al. in 1958. 58Fra

b

phase	III	II	I
crystal system	rhombohedral [b])	tetragonal [a])	cubic [a])
Θ [°C]	370	485	

[a]) 58Frau
[b]) 86Wol

Space group of phase III is considered to be $R3c - C_{3v}^6$ or $R\bar{3}c - D_{3d}^6$. 86Wol

ρ = $9.24 \cdot 10^3$ kg m^{-3}. 86Wol

3a Unit cell parameters at 295 K: Table 1A-6-001; Fig. 1A-6-001.

b Crystal structure of phase III: Fig. 1A-6-002.
Fractional coordinates and thermal parameters of atoms: Table 1A-6-002.
Interatomic distances: Table 1A-6-003.

4 Unit cell parameters vs. T: Fig. 1A-6-003.

5a Dielectric constant: Fig. 1A-6-004; see also Fig. 2 in 1C-a100.

10a Raman scattering: Fig. 1A-6-005, Fig. 1A-6-006.
Raman scattering spectra of Nb doped $AgTaO_3$: see 90Kan

Table 1A-6-001. $AgTaO_3$. Unit cell parameters in phase III [86Wol]. T= 295 K. The relation between the pseudocubic cell, the primitive rhombohedral cell and the hexagonal cell is shown in Fig. 1A-6-001.

Pseudocubic	Rhombohedral	Hexagonal
a_p = 3.926 Å	a_r = 5.5758 Å	a_h = 5.5281(1) Å
α_p =89.50°	α_r =59.434°	c_h = 13.7159(5) Å
		γ_h = 120°
V = 60.5 Å^3	V = 121.00 Å^3	V = 363.00 Å^3
Z = 1	Z = 2	Z = 6

Table 1A-6-002. $AgTaO_3$. Crystal structure in phase III [86Wol]. Fractional coordinates in the hexagonal cell (in Å) and anisotropic temperature parameters (in units of 10^{-4} Å^2) at 295 K. U_{ij} is defined by Eq. (d) in Introduction. R3c and $R\bar{3}c$ are the possible space groups for phase III.

Atom	Ag 6(a) [a])	Ta 6(a) [a])	O 18(b) [a])	Ag 6(a) [b])	Ta 6(b) [b])	O 18(e) [b])
x	0	0	0.5598(9)	0	0	0.5546(5)
y	0	0	0.0097(14)	0	0	0
z	0.2492(2)	0	0.2510(6)	0.2500	0	0.2500
U_{11}	0.0112(1)	0.0049(1)	0.0094(13)	0.0112(1)	0.0049(1)	0.0088(5)
U_{22}	0.0112(1)	0.0049(1)	0.0048(10)	0.0112(1)	0.0049(1)	0.0073(8)
U_{33}	0.0144(0)	0.0047(1)	0.0094(8)	0.0146(2)	0.0047(1)	0.0094(8)
U_{12}	0.0056(0)	0.0024(0)	0.0032(13)	0.0056(0)	0.0025(0)	0.0037(4)
U_{13}	0	0	–0.0005(15)	0	0	–0.0025(3)
U_{23}	0	0	–0.0053(7)	0	0	–0.0050(6)

[a]) R3c . [b]) $R\bar{3}c$.

Table 1A-6-003. $AgTaO_3$. Interatomic distances (in Å) in phase III [86Wol]. T = 295 K. R3c and $R\bar{3}c$ are the possible space groups for phase III.

	R3c [Å]	$R\bar{3}c$ [Å]		R3c [Å]	$R\bar{3}c$ [Å]
Ag-Ta	3.440(3)	3.429(0)	Ta-O	2.032(6)	1.986(3)
	3.418(2)	3.390(2)		1.941(4)	
	3.394(3)		O-O	2.894(11)	2.813(1)
	3.387(4)			2.814(23)	2.804(0)
Ag-O	2.811(3)	2.804(3)		2.797(1)	
	2.799(3)	2.462(3)		2.734(11)	
	2.461(3)				

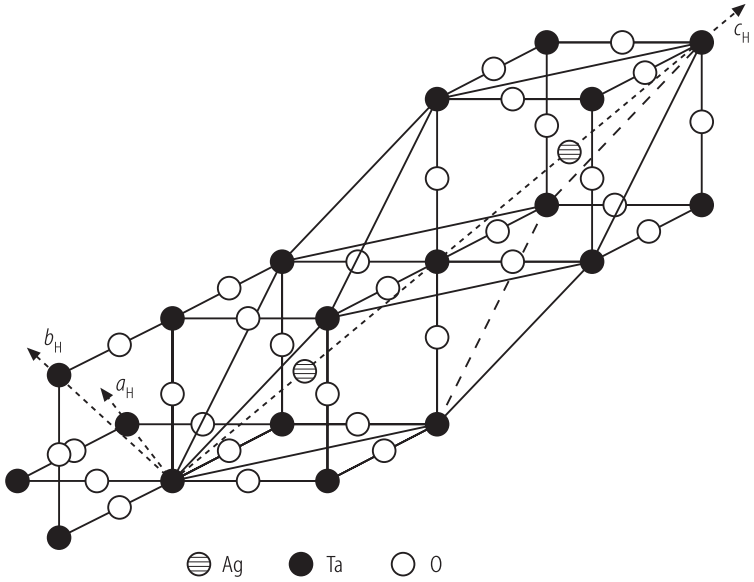

Fig. 1A-6-001. $AgTaO_3$. Structure of rhombohedral phase III [86Wol]. The relation of the primitive rhombohedral cell to the pseudocubic cell is shown. a_H, b_H, c_H: crystallographic axes of hexagonal cell.

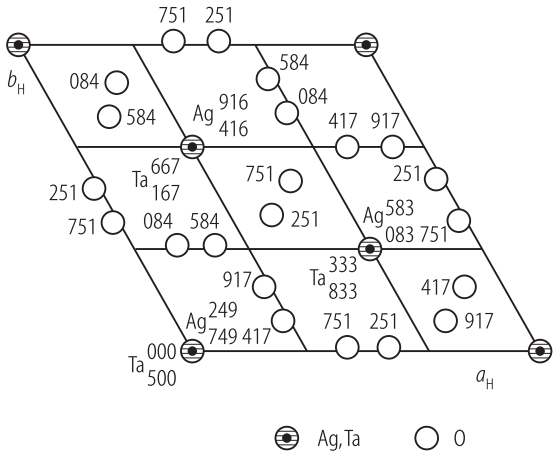

Fig. 1A-6-002. $AgTaO_3$. Structure of rhombohedral phase III [86Wol]. T = 295 K. Projection on a_H-b_H plane. The numbers denote the fractional c_H-coordinates multiplied by 10^3.

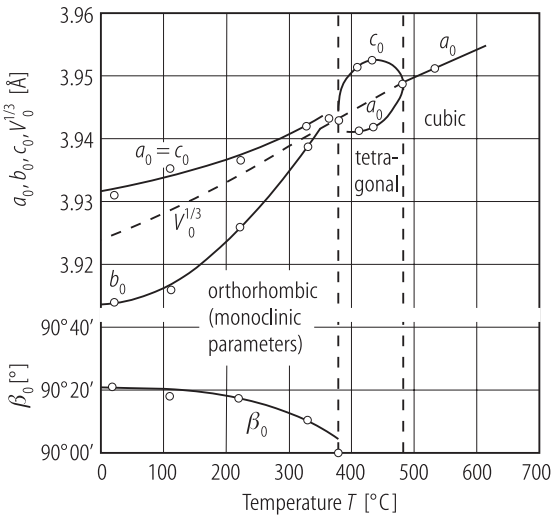

Fig. 1A-6-003. $AgTaO_3$. Lattice parameters of pseudo-cubic cell vs. T [58Fra].

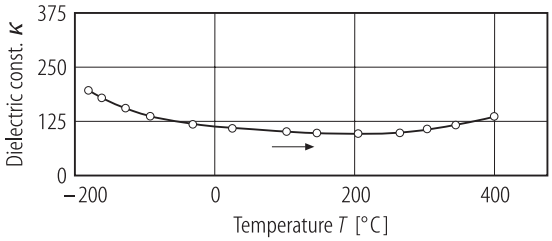

Fig. 1A-6-004. $AgTaO_3$ (ceramics). κ vs. T [80Rae]. f = 16 kHz.

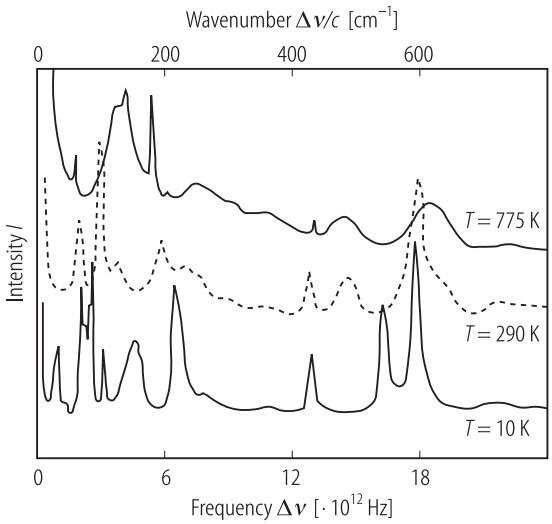

Fig. 1A-6-005. $AgTaO_3$. I vs. $\Delta\nu$ [88Kan]. I: Raman scattering intensity. Parameter: T.

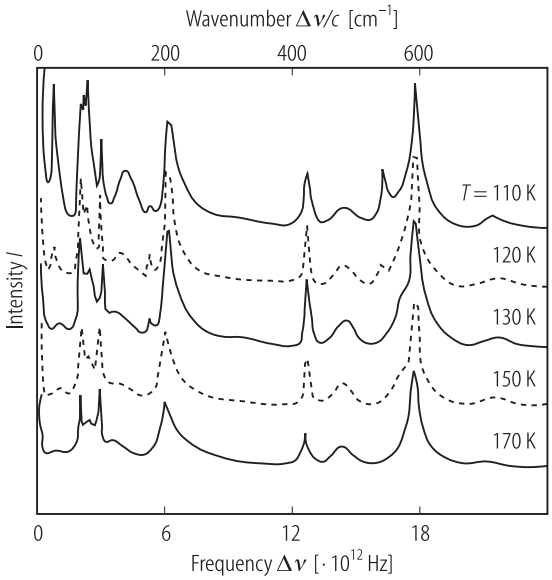

Fig. 1A-6-006. $AgTaO_3$. I vs. $\Delta\nu$ [88Kan]. I: Raman scattering intensity. Parameter: T.

References

58Fra Francombe, M.H., Lewis, B.: Acta Crystallogr. **11** (1958) 175.
80Rae Raevskii, I.P., Malitskaya, M.A., Reznichenko, L.A., Prokopalo, O.I.: Izv. Akad. Nauk SSSR, Neorg. Mater. **16** (1980) 1618; Inorg. Mater. (English Transl.) **16** (1980) 1108.
86Wol Wolcyrz, M., Lukaszewski, M.: Z. Kristallogr. **177** (1986) 53.
88Kan Kania, A., Kugel, G.E., Roleder, K., Pawelczyk, M., Hafid, M., Fontana, M.D., Carabatos, C.: Ferroelectrics **80** (1988) 137.
90Kan Kania, A., Kugel, G.E., Roleder, K., Fontana, M.D.: Ferroelectrics **107** (1990) 109.