No. 1A-13 $SrZrO_3$, Strontium zirconate
(M = 226.84)

1a In 1957 Roth reported that the RT structure of $SrZrO_3$ is not of the ideal cubic perovskite type but orthorhombic. Swanson recomfirmed it in 1960. 57Rot 60Swa

b

phase	IV	III	II	I	
state					[a] 60Swa
crystal system	orthorhombic [a]	tetragonal [b]	tetragonal [b]	cubic [b]	[b] 67Car
Θ [°C]		700 [a]	830 [b]	1170 [b]	

3a Unit cell parameters. 67Car
phase I *): a_0 = 4.152(2) Å at 1200 °C.
phase II: a = 4.141(2) Å, c = 4.150(3) Å at 1000 °C.
phase III: a = 4.138(2) Å, c = 4.131(3) Å at 820 °C.
phase IV: a = 5.8106 Å $\cong \sqrt{2}a_0$, b = 8.1940 Å $\cong 2a_0$, c = 5.739 Å $\cong \sqrt{2}a_0$ at RT.
*) In phase I, a few lines were observed in X-ray Debye-Scherrer pattern, implying a doubling of the unit cell edges of pseudocubic cell [67Car].

4 Thermal expansion: Fig. 1A-13-001.

5a Dielectric constant: κ = 26.5 at RT (f = 1 MHz). 61Ste

6a DTA: Fig. 1A-13-002.

9a Infrared absorption: Fig. 1A-13-003, Fig. 1A-13-004; Table 1A-13-001.

16 Proton conductivity: see 92Hib
Defect structure: see 93Lab

Table 1A-13-001. $SrZrO_3$. Frequencies in 1012 Hz and symmetry of infrared modes of lattice vibration obtained from Kramers-Kronig analysis of the reflectance data at RT [65Per].

ν_1 (Zr–O stretch)	ν_2 (Zr–O_3 torsion)	ν_3 (O–Zr–O bend)	ν_4 (cation–ZrO_3 lattice mode)
15.6 (B_1, B_2, A_1)	9.75 (B_1, B_2, A_2) (10.7) (11.4)	7.20 (B_1, B_2, A_1)	4.29 (B_1, B_2, A_1)

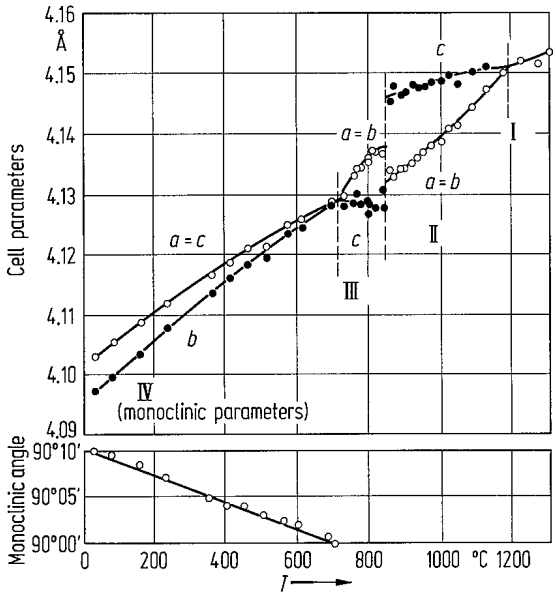

Fig. 1A-13-001. $SrZrO_3$. Lattice parameters vs. *T* [67Car].

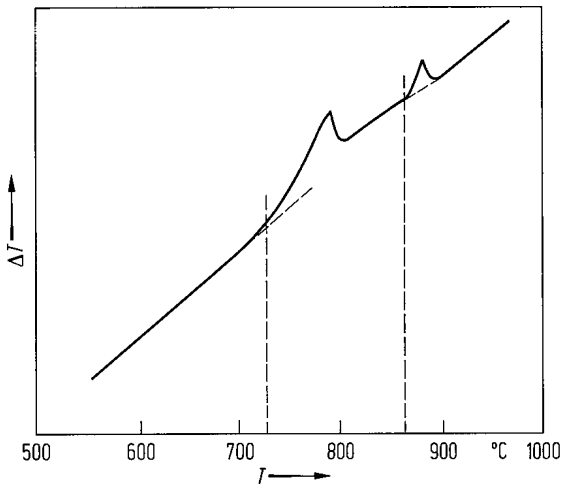

Fig. 1A-13-002. $SrZrO_3$. Differential thermal analysis curve [67Car]. Endothermic peaks represent phase transitions. The dashed lines indicate the points where the curve begins to deviate from its previous inclination: 730 °C and 860 °C.

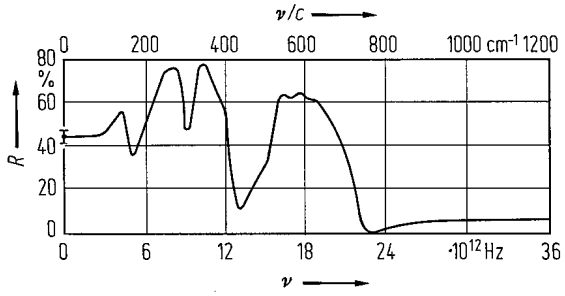

Fig. 1A-13-003. $SrZrO_3$. R vs. ν [65Per]. R: reflectance.

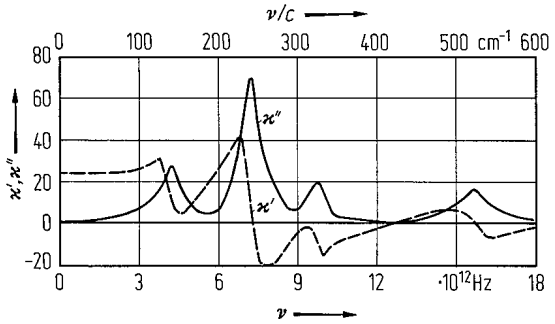

Fig. 1A-13-004. $SrZrO_3$. κ' and κ'' vs. ν [65Per]. The curves were obtained from reflectivity data using Kramers-Kronig relation.

References

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