substance: ZrS_{3-x}
property: crystal structure, physical properties

ZrS_{3-x} ($0 \leq x \leq 0.05$)

(S: structure (space group), CG: crystal growth (the numbers in parentheses correspond to T_1 and T_2, the temperatures (in °C) of the hot and cold end of the crystal growth tube, respectively), C: colour).

(The references in the last column refer to all data of this document)

lattice parameters

a	5.123 Å	S: $ZrSe_3$-type, $C_{2h}^2 - P2_1/m$	61G,
b	3.627 Å	CG: halogen transport	63H,
c	8.986 Å	(750...900/550....600)	73S,
β	97.15°	C: dark orange	75F

resistivity

ρ_b	10^4 Ω cm	n-type, synthetic single crystal

Seebeck coefficient

S_b	– 500 µV K^{-1}	n-type, synthetic single crystal

energy gap

E_g	2.8 eV	optical gap

Figures to this document:

electrical conductivity: Fig. 1

References:

61G Grimmeiss, H. G., Rabenau, A., Hahn, H., Ness, P.: Z. Elektrochem. 65 (1961) 776.
63H Haraldsen, H., Kjekshus, A., Rost, E., Steffensen, A.: Acta Chem. Scand. 17 (1963) 1283.
73S Schairer, W., Shafer, M. W.: Phys. Status. Solidi 17A (1973) 181.
75F Furuseth, S., Brattas, L., Kjekshus, A.: Acta Chem. Scand. 29A (1975) 623.

Fig. 1.

ZrS_3, $ZrSe_3$. Conductivity vs. reciprocal temperature[61G]. σ in Ω^{-1} cm^{-1}, $\sigma \parallel b$.