

**substance:** ZrSe<sub>3</sub>  
**property:** crystal structure, physical properties

(S: structure (space group), CG: crystal growth, C: colour).

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

**lattice parameters**

<i>a</i>	5.411 Å	S: ZrSe <sub>3</sub> type, C <sub>2h</sub> <sup>2</sup> – P2 <sub>1</sub> /m	61G,
<i>b</i>	3.749 Å	CG: from crystalline mass	65K,
<i>c</i>	9.444 Å	C: dark grey	75F,
<i>β</i>	97.45°		79B

**resistivity**

<i>ρ<sub>b</sub></i>	10 <sup>3</sup> Ω cm	n-type, synthetic single crystal
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**Seebeck coefficient**

<i>S<sub>b</sub></i>	– 10 <sup>3</sup> μV K <sup>–1</sup>	n-type, synthetic single crystal
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**energy gap**

<i>E<sub>g</sub></i>	1.25 eV	optical gap
	1.6 eV	direct gap, calculated
	1.5 eV	indirect gap, calculated

**Figures to this document:**

**electrical conductivity:** Fig. 1

## References:

- 61G Grimmeiss, H. G., Rabenau, A., Hahn, H., Ness, P.: Z. Elektrochem. 65 (1961) 776.
- 65K Kronert, V. W., Plieth, K.: Z. Anorg. Allg. Chem. 336 (1965) 207.
- 75F Furuseth, S., Brattas, L., Kjekshus, A.: Acta Chem. Scand. 29A (1975) 623.
- 79B Bullett, D. W.: J. Phys. C 12 (1979) 277.

**Fig. 1.**

ZrS<sub>3</sub>, ZrSe<sub>3</sub>. Conductivity vs. reciprocal temperature[61G].  $\sigma$  in  $\Omega^{-1} \text{ cm}^{-1}$ ,  $\sigma \parallel b$ .

