

**substance:** Ce<sub>2</sub>S<sub>3</sub>

**property:** crystal structure, physical properties

**α-Ce<sub>2</sub>S<sub>3</sub>**

**crystal structure** orthorhombic (D<sub>2h</sub><sup>16</sup> – Pnma)

**lattice parameters**

<i>a</i>	7.55 Å	71B
<i>b</i>	15.79 Å	
<i>c</i>	4.14 Å	

**β-Ce<sub>2</sub>S<sub>3</sub>**

<b>crystal structure</b>	tetragonal (D <sub>4h</sub> <sup>20</sup> – I4 <sub>1</sub> /acd)	transition α-phase to β-phase at 1410°C	66M
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**lattice parameters**

<i>a</i>	15.30 Å	71B
<i>c</i>	20.29 Å	

**melting point**

<i>T<sub>m</sub></i>	1700°C	60P
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**γ-Ce<sub>2</sub>S<sub>3</sub>**

**crystal structure** cubic (Th<sub>3</sub>P<sub>4</sub>-defect structure, T<sub>d</sub><sup>6</sup> – I 4̄ 3d)

**lattice parameters**

<i>a</i>	8.634 Å	85Z
	8.631 Å	81K
	8.630 Å	65F
	8.6084 Å	71A
		from neutron diffraction

**melting point**

<i>T<sub>m</sub></i>	2060°C	65F
	1870°C	81K
	2296°C	72G

**density**

<i>d</i>	5.31 g cm <sup>-3</sup>	81K
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**linear thermal expansion coefficient**

<i>α</i>	13.2·10 <sup>-6</sup> K <sup>-1</sup>	66D
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**thermal conductivity**

<i>κ</i>	3.52·10 <sup>-2</sup> Wcm <sup>-1</sup> K <sup>-1</sup>	72C
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**energy gap and other energy parameters**

<i>E<sub>g</sub></i>	2.06 eV	optical energy gap	64K	
	2.0 eV	optical energy gap	67H	
	2.7 ± 0.25 eV	thermodynamic	85Z	
	1.8 eV	X-ray spectra	83S	
<i>E<sub>b</sub></i>	5.3 eV	S 3p-level	MgKα XPS, Fig. 4 ( <i>E<sub>b</sub></i> rel. to <i>E<sub>F</sub></i> )	91K
	2.5 eV	Ce 4f-level	MgKα XPS, Fig. 4	
	13.3 eV	S 3s-level	MgKα XPS, Fig. 4	
	19.6 eV	Ce 5p <sub>3/2</sub> -level	MgKα XPS, Fig. 4	
	22.6 eV	Ce 5p <sub>1/2</sub> -level	MgKα XPS, Fig. 4	
	38 eV	Ce 5s-level	MgKα XPS, Fig. 4	
	108 eV	Ce 4d <sub>5/2</sub> -level	MgKα XPS, Fig. 5	

$E$	112 eV	Ce 4d <sub>3/2</sub> -level	MgK $\alpha$ XPS, Fig. 5	91K
	8.3 eV	S 3p- $E_F$	ELS, Fig. 6	
	11.3 eV	S 3p-cond. band, surface plasmon	ELS, Fig. 6	
	16.4 eV	bulk plasmon	ELS, Fig. 6	
	21.4 eV	Ce 5p- $E_F$	ELS, Fig. 6	
	30.4 eV	Ce 5p-5d	ELS, Fig. 6	
	$\approx 39$ eV	Ce 5s- $E_F$	ELS, Fig. 6	

**electrical conductivity**

$\sigma$	$10^{-10} \Omega^{-1} \text{ cm}^{-1}$		71A
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**activation energy**

$E_A$	2.23 eV	from electrical conductivity	67M
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*Further figures and references:*

**coordination polyhedra:** Fig. 1

**heat capacity:** Fig. 2

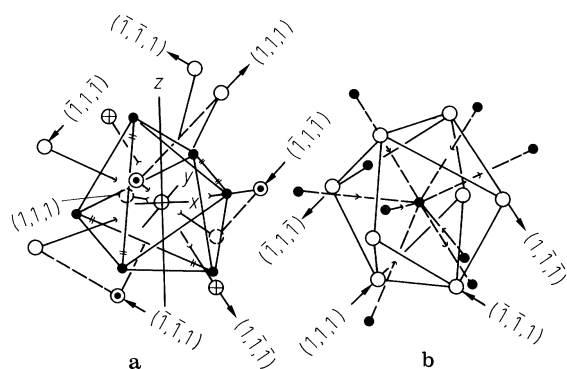
temperature dependence of **resistivity:** Fig. 3

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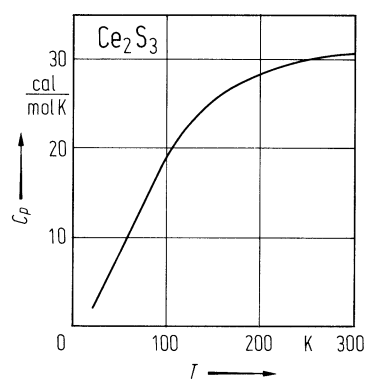
**Fig. 1.**

Th<sub>3</sub>P<sub>4</sub>-type compounds. The coordination polyhedra of the cations and the anions. Full circles: Th- atoms, other circles: P-atoms [66H].



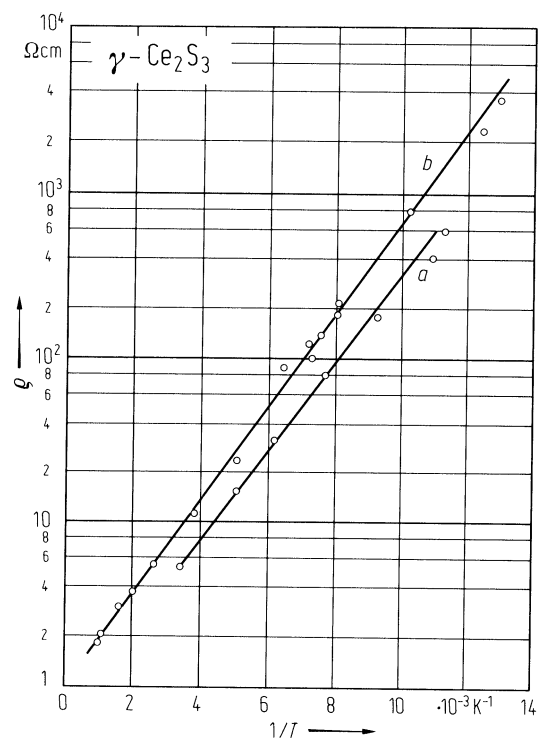
**Fig. 2.**

$\gamma$ -Ce<sub>2</sub>S<sub>3</sub>. Temperature dependence of the molar heat capacity [72S].



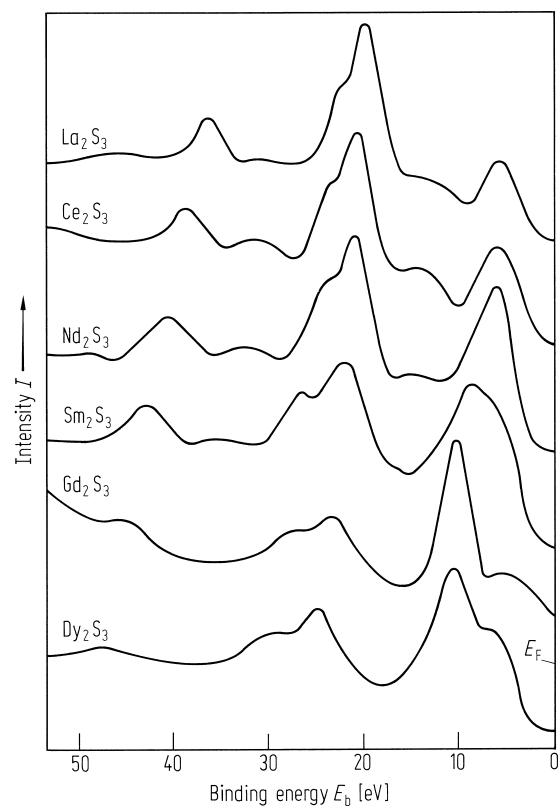
**Fig. 3.**

$\gamma\text{-Ce}_2\text{S}_3$ . Low temperature resistivity vs. reciprocal temperature. For curves a and b the electron concentrations are  $8.7 \cdot 10^{17} \text{ cm}^{-3}$  and  $5 \cdot 10^{17} \text{ cm}^{-3}$ , respectively [64C].



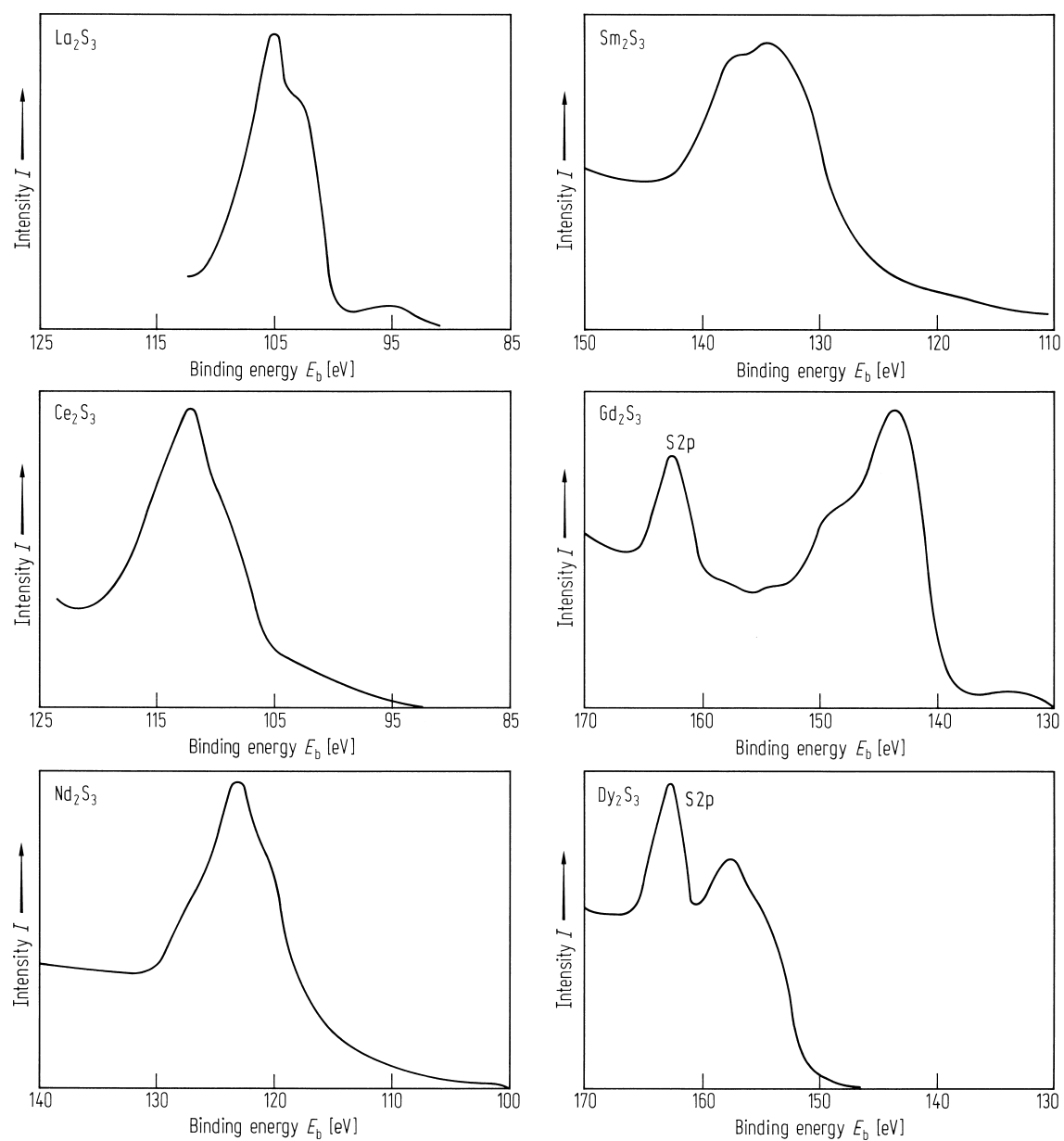
**Fig. 4.**

$\gamma$ -Ln<sub>2</sub>S<sub>3</sub>. MgK<sub>α</sub> X-ray photoelectron spectra of the rare-earth sesquisulfides (Ln = La, Ce, Nd, Sm, Gd, Dy) in the energy region below Fermi level down to Ln 5s core level [91K].



**Fig. 5.**

$\gamma$ - $\text{Ln}_2\text{S}_3$ .  $\text{MgK}_{\alpha}$  X-ray photoelectron spectra of the rare-earth sesquisulfides ( $\text{Ln} = \text{La}, \text{Ce}, \text{Nd}, \text{Sm}, \text{Gd}, \text{Dy}$ ) in the 4d core level region [91K].  $E_b$  relative to  $E_F$ .





**Fig. 6.**

$\gamma$ - $\text{Ln}_2\text{S}_3$ . Electron loss spectra of the rare-earth sesquisulfides ( $\text{Ln} = \text{La, Ce, Nd, Sm, Gd, Dy}$ ) for primary electron beam energy  $E_p = 750 \text{ eV}$ . All the peaks, revealed from the second derivative  $d^2N/dE^2$  are indicated by arrows [91K].

