

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

**property:** crystal structure, physical properties

**α-Gd<sub>2</sub>S<sub>3</sub>**

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

**lattice parameters**

<i>a</i>	7.339 Å	color: red	68P
<i>b</i>	15.273 Å		
<i>c</i>	3.932 Å		
<i>a</i>	7.338(2) Å		68S
<i>b</i>	15.273(3) Å		
<i>c</i>	3.932(2) Å		

**electrical conductivity**

$\sigma$	25 Ω <sup>-1</sup> cm <sup>-1</sup>	(E <sub>A</sub> = 0.007 eV)	68S
	2·10 <sup>-3</sup> Ω <sup>-1</sup> cm <sup>-1</sup>	n-type	70P

**Seebeck coefficient**

<i>S</i>	– 360 μV K <sup>-1</sup>	(referred to lead)	68S
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*Figures and further references for α-Gd<sub>2</sub>S<sub>3</sub>:*

**work function** [67B]

**absorption and luminescence spectra** of Nd<sup>3+</sup>-doped samples[80L], see also Figs. 1, 2

**γ-Gd<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> –  $\bar{1}4\bar{3}d$ )

**lattice parameters**

<i>a</i>	8.387 Å	57F
	8.385 Å	81K
	8.3723(5) Å	73W

**melting point**

<i>T<sub>m</sub></i>	1885°C	57F
	1850°C	81K

**energy gap and other energy parameters**

<i>E<sub>g</sub></i>	3.4 eV	optical gap		82B
	1.4 eV			83S
<i>E<sub>b</sub></i>	5.8 eV	S 3p-level	MgKα XPS, Fig. 3 (E <sub>b</sub> rel. to E <sub>F</sub> )	91K
	9.5 eV	Gd 4f-level		
	23.0 eV	Gd 5p <sub>3/2</sub> -level		
	27.0 eV	Gd 5p <sub>1/2</sub> -level		
	44.5 eV	Gd 5s-level		
	143 eV	Gd 4d <sub>5/2</sub> -level		
	149 eV	Gd 4d <sub>3/2</sub> -level		
	273 eV	Gd (4p <sub>3/2</sub> , 4p <sub>5/2</sub> )-lev.		
<i>E<sub>b</sub></i>	1188 eV	Gd 3d <sub>5/2</sub> -level	AlKα XPS, Fig. 5	
	1220 eV	Gd 3d <sub>3/2</sub> -level	AlKα XPS, Fig. 5	
<i>E</i>	8.2 eV	S 3p-E <sub>F</sub>	ELS, Fig. 6	91K
	12.1 eV	S 3p-cond. band, surface plasmon	ELS, Fig. 6	
	17.3 eV	bulk plasmon	ELS, Fig. 6	
	24.9 eV	Gd 5p-E <sub>F</sub>	ELS, Fig. 6	

34 eV	Gd 5p-5d	ELS, Fig. 6
$\approx 50$ eV	Gd 5s- $E_F$	ELS, Fig. 6
149 eV	Gd 4d-4f	ELS, Fig. 7

**electrical conductivity**

$\sigma$	250 $\Omega^{-1} \text{ cm}^{-1}$	n-type	74T
	$10^{-8} \Omega^{-1} \text{ cm}^{-1}$		82B

**activation energy for conductivity**

$E_A$	1.6...1.9 meV	77T
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*Further figures and references:*

**phase diagram:** Fig. 8

**coordination polyhedra:** Fig. 9

**thermal conductivity:** Fig. 11

**Raman and IR spectra:** Fig. 10

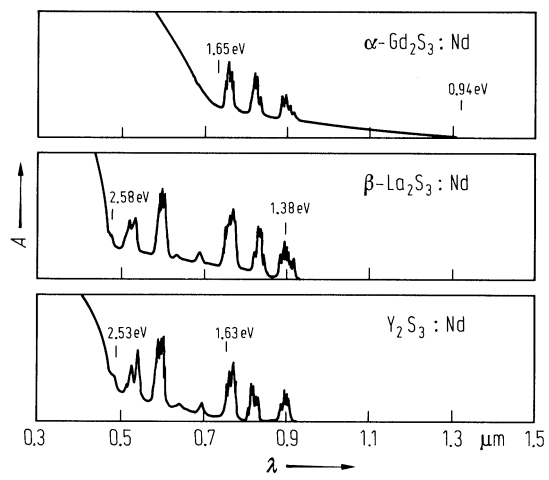
temperature dependence of **resistivity, Hall coefficient, Seebeck coefficient:** Figs. 12...14

## References:

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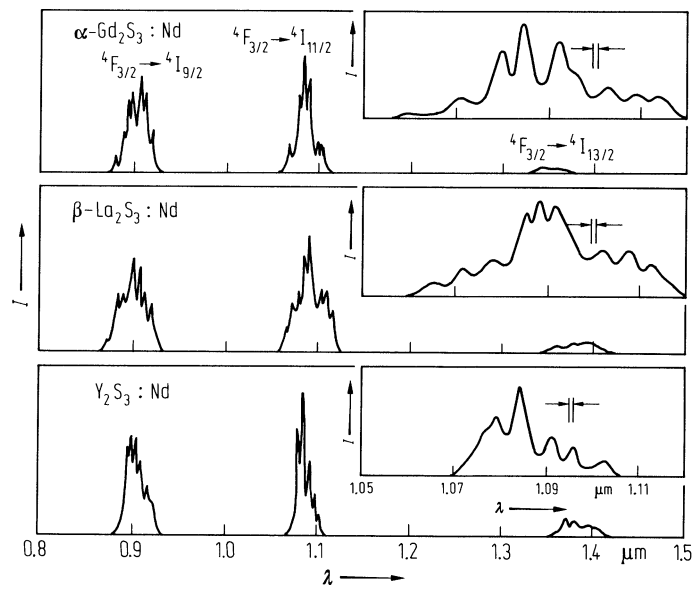
**Fig. 1.**

$\alpha$ -Gd<sub>2</sub>S<sub>3</sub>:Nd,  $\beta$ -La<sub>2</sub>S<sub>3</sub>:Nd, Y<sub>2</sub>S<sub>3</sub>:Nd. Absorbance  $A$  vs. wavelength [80L].



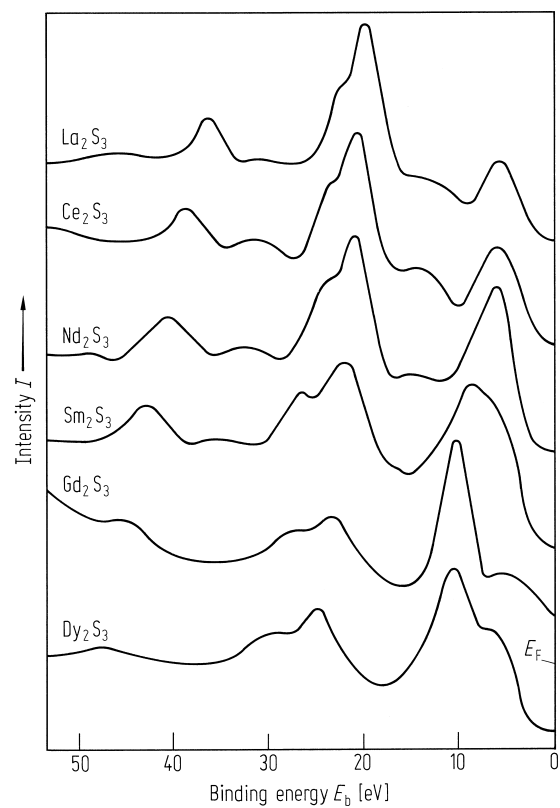
**Fig. 2.**

$\alpha$ -Gd<sub>2</sub>S<sub>3</sub>:Nd,  $\beta$ -La<sub>2</sub>S<sub>3</sub>:Nd, Y<sub>2</sub>S<sub>3</sub>:Nd. Photoluminescence intensity vs. wavelength for  $\alpha$ -Gd<sub>2</sub>S<sub>3</sub>:Nd excited at 752.5 nm,  $\beta$ -La<sub>2</sub>S<sub>3</sub>:Nd and Y<sub>2</sub>S<sub>3</sub>:Nd excited at 600 nm [80L].



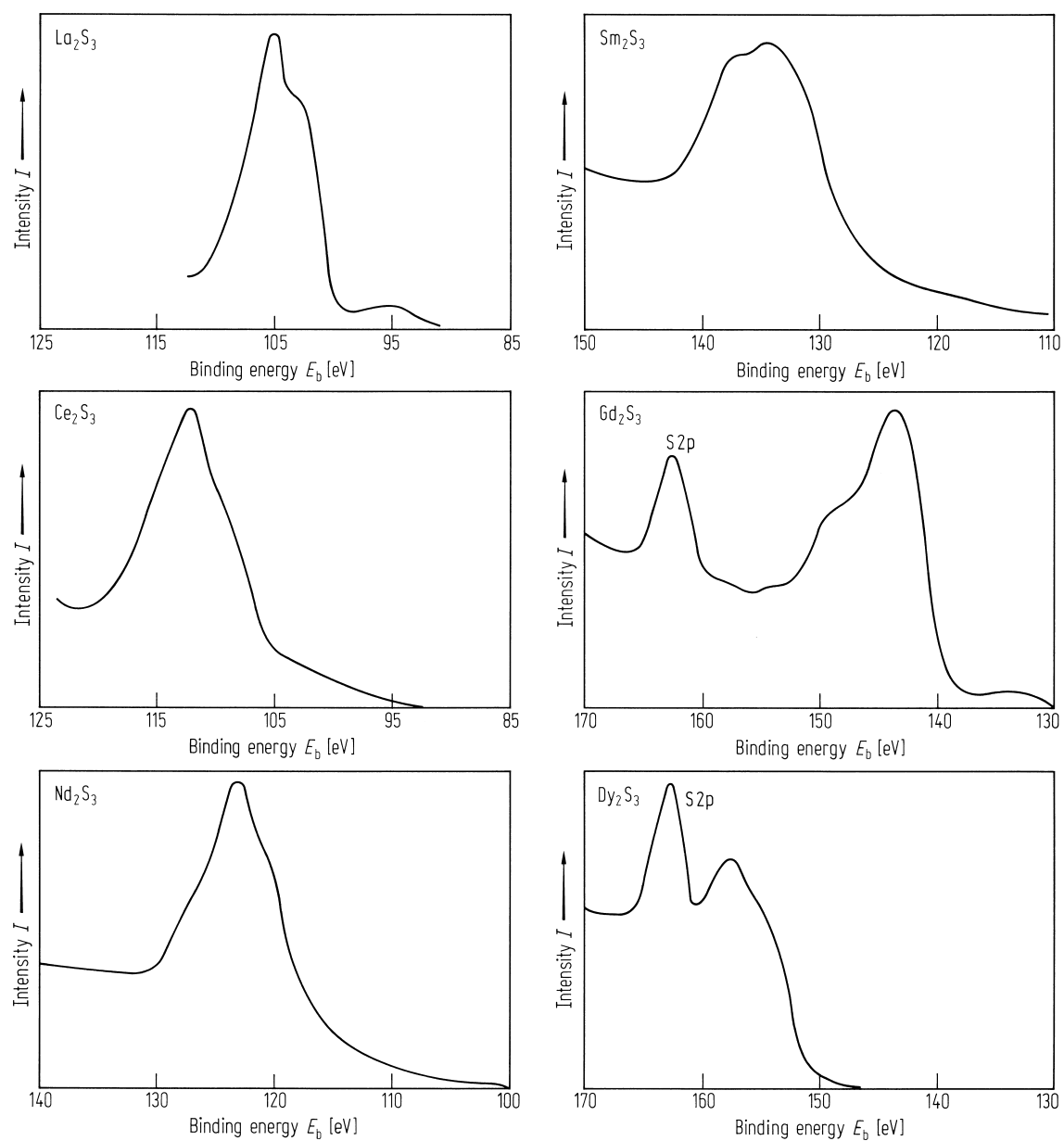
**Fig. 3.**

$\gamma$ - $\text{Ln}_2\text{S}_3$ .  $\text{MgK}\alpha$  X-ray photoelectron spectra of the rare-earth sesquisulfides ( $\text{Ln} = \text{La, Ce, Nd, Sm, Gd, Dy}$ ) in the energy region below Fermi level down to Ln 5s core level [91K].



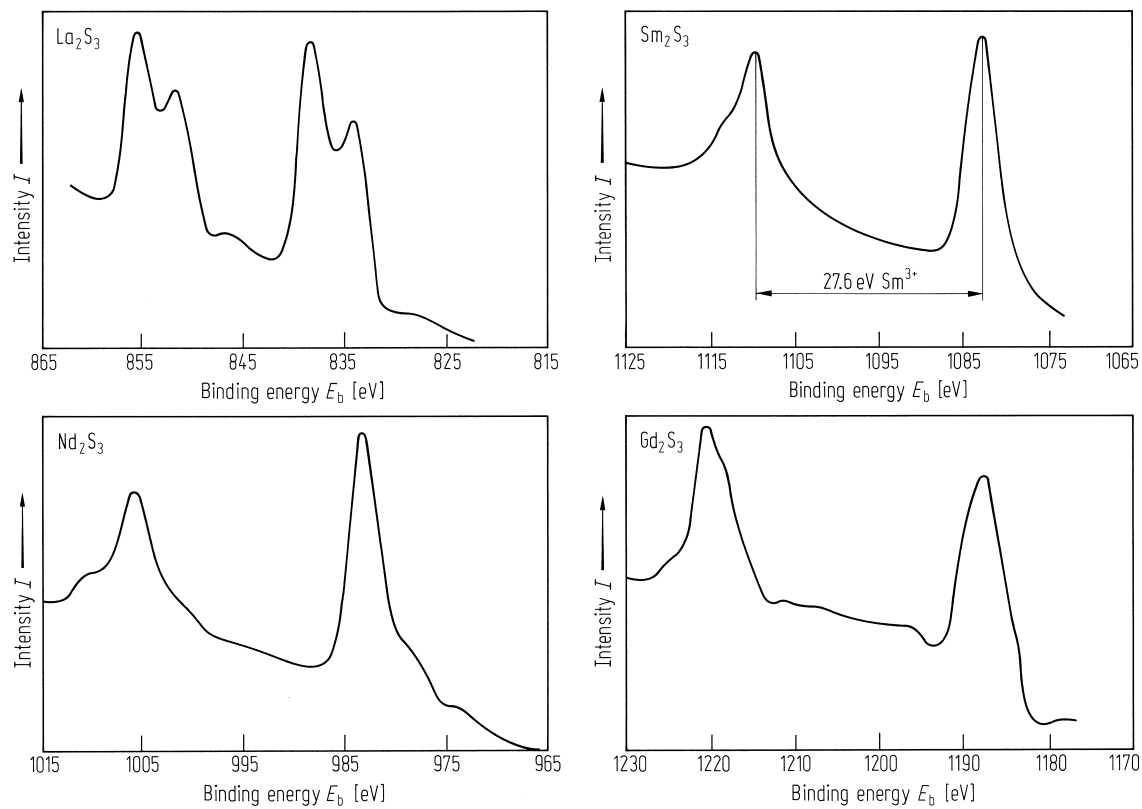
**Fig. 4.**

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



**Fig. 5.**

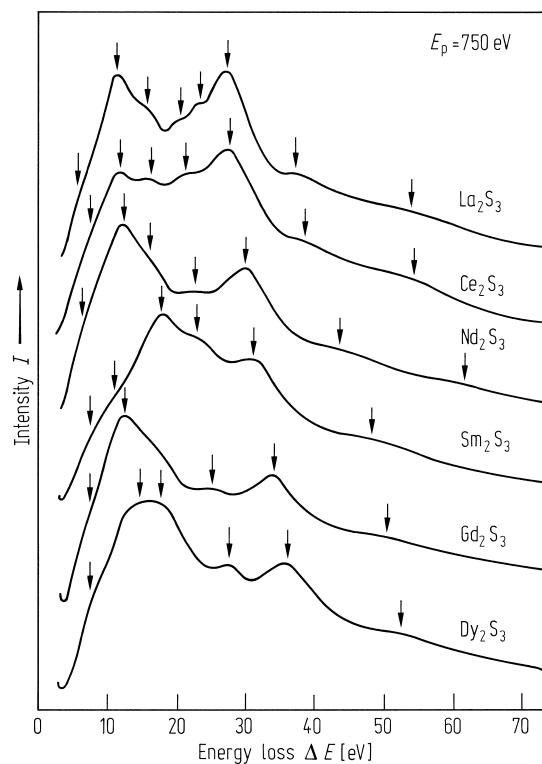
$\gamma$ - $\text{Ln}_2\text{S}_3$ .  $\text{AlK}_\alpha$  X-ray photoelectron spectra of the rare-earth sesquisulfides ( $\text{Ln} = \text{La, Nd, Sm, Gd}$ ) in the 3d core level region [91K]. The trivalence of Sm is testified by the value of the Sm 3d doublet line spin-orbit splitting ( $= 27.6 \text{ eV}$ ).  $E_b$  relative to  $E_F$ .





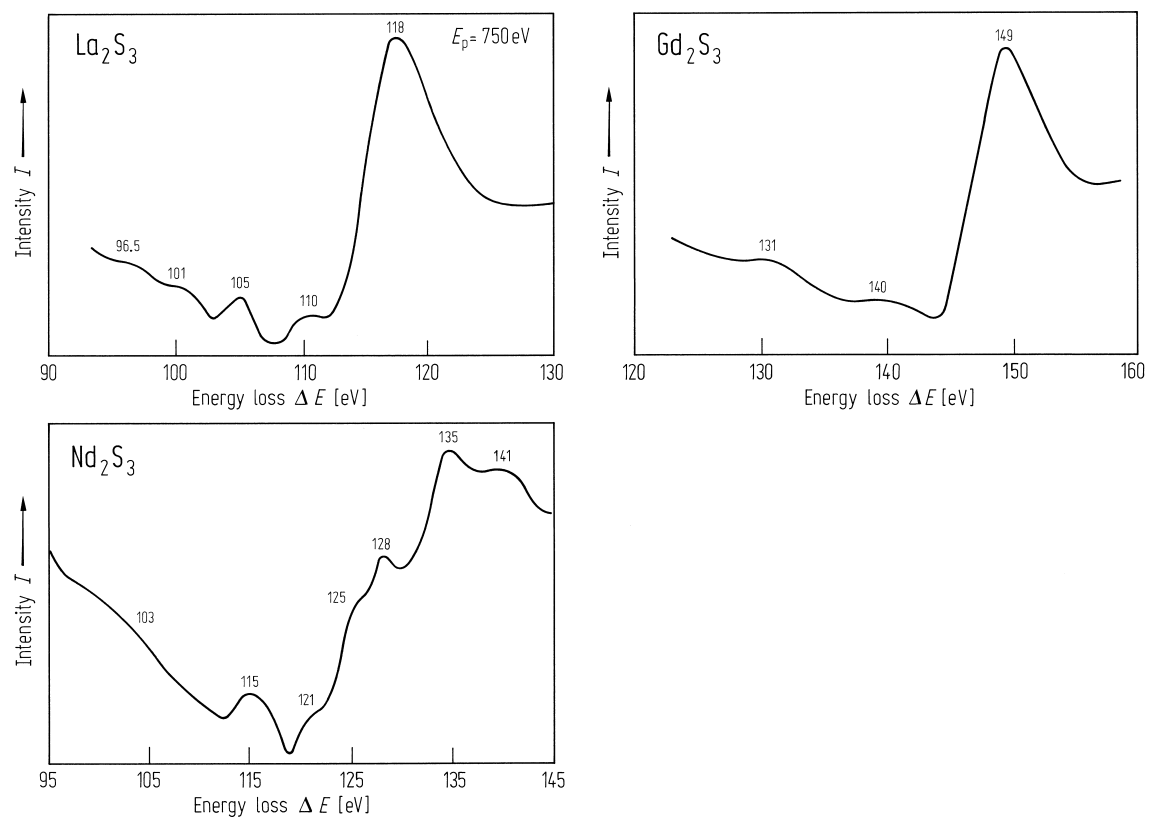
**Fig. 6.**

$\gamma$ - $\text{Ln}_2\text{S}_3$ . 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].



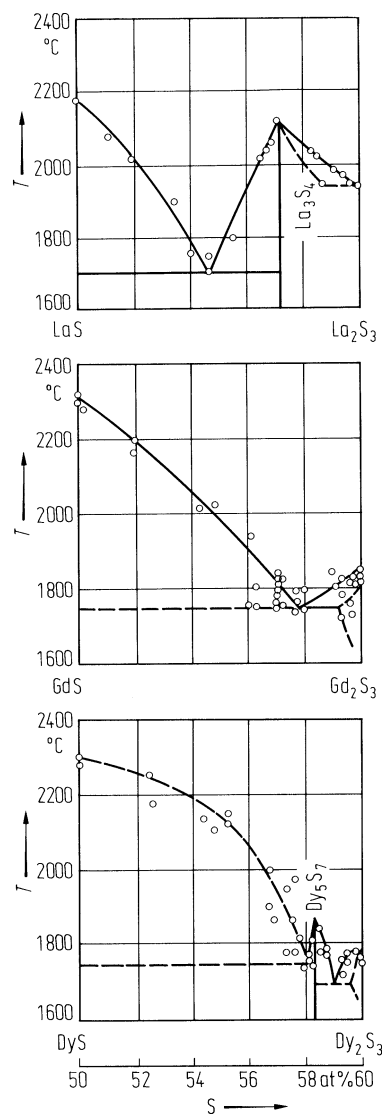
**Fig. 7.**

$\gamma$ - $\text{Ln}_2\text{S}_3$ ,  $\text{Ln} = \text{La, Nd, Gd}$ . 4f-4f giant resonance in energy loss spectra at primary electron energy  $E_p = 750$  eV after Shirley background subtraction [91K].



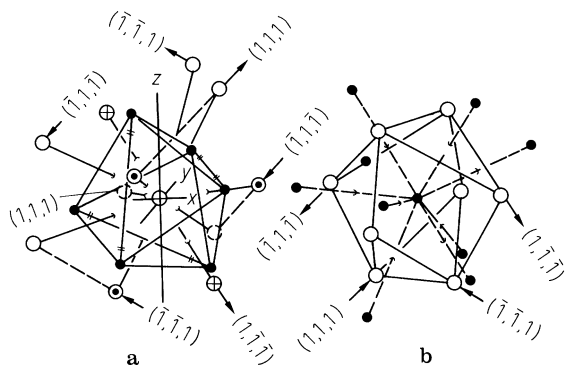
**Fig. 8.**

LnS–Ln<sub>2</sub>S<sub>3</sub> system, Ln = La, Gd, Dy. Phase diagrams [81K].



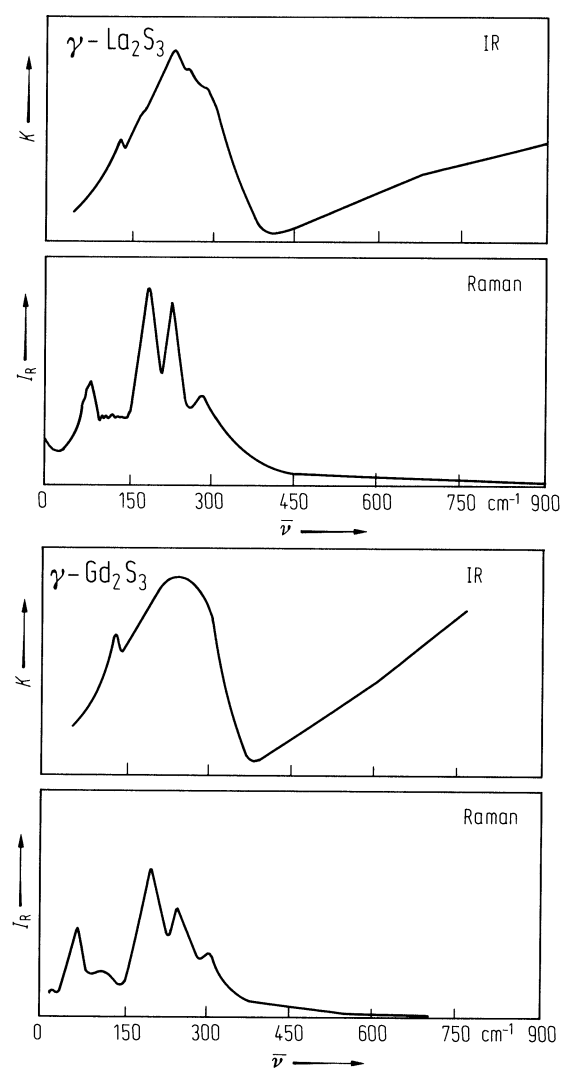
**Fig. 9.**

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].



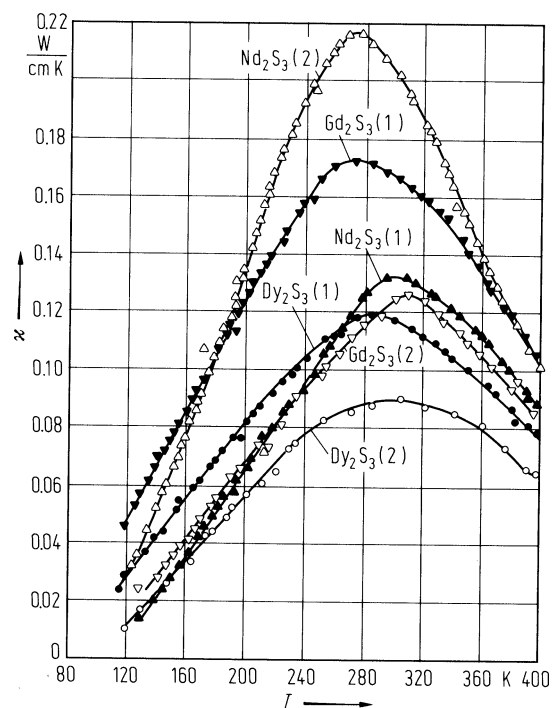
**Fig. 10.**

$\gamma$ - $\text{La}_2\text{S}_3$ ,  $\gamma$ - $\text{Gd}_2\text{S}_3$ . Infrared absorption and Raman intensity vs. wavenumber at 300 K [67B].



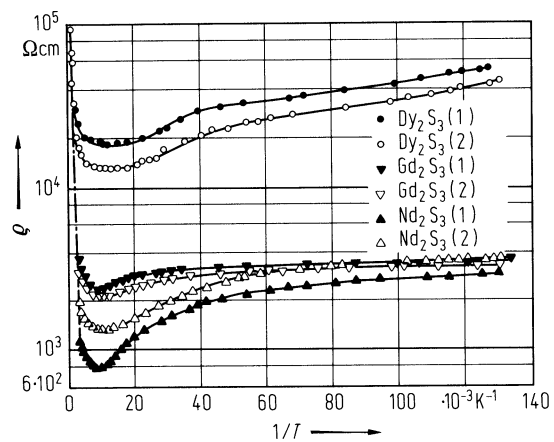
**Fig. 11.**

$\gamma$ -Nd<sub>2</sub>S<sub>3</sub>,  $\gamma$ -Gd<sub>2</sub>S<sub>3</sub>,  $\gamma$ -Dy<sub>2</sub>S<sub>3</sub>. Thermal conductivity vs. temperature of several single crystals. The samples show the following excess metal content: Nd<sub>2</sub>S<sub>3</sub> (1): 0.7% Nd, Nd<sub>2</sub>S<sub>3</sub> (2): 0.6% Nd, Gd<sub>2</sub>S<sub>3</sub> (1): 0.4% Gd, Gd<sub>2</sub>S<sub>3</sub> (2): 0.5% Gd, Dy<sub>2</sub>S<sub>3</sub> (1): 0.1% Dy, Dy<sub>2</sub>S<sub>3</sub> (2): 0.2% Dy [77T].



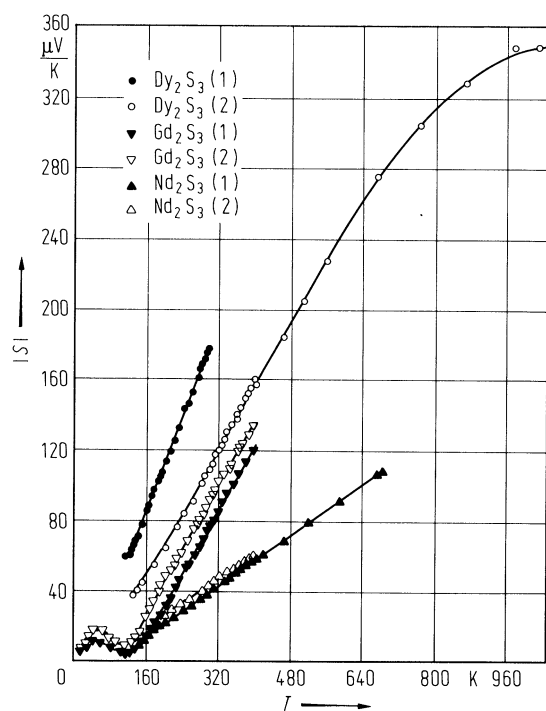
**Fig. 12.**

$\gamma$ -Nd<sub>2</sub>S<sub>3</sub>,  $\gamma$ -Gd<sub>2</sub>S<sub>3</sub>,  $\gamma$ -Dy<sub>2</sub>S<sub>3</sub>. Temperature dependence of the electrical conductivity. The sample compositions are given in Fig. 11 [77T].



**Fig. 13.**

$\gamma$ -Nd<sub>2</sub>S<sub>3</sub>,  $\gamma$ -Gd<sub>2</sub>S<sub>3</sub>,  $\gamma$ -Dy<sub>2</sub>S<sub>3</sub>. Thermoelectric power vs. temperature. The sample compositions are given in Fig. 11 [77T].





**Fig. 14.**

$\gamma$ -Nd<sub>2</sub>S<sub>3</sub>,  $\gamma$ -Gd<sub>2</sub>S<sub>3</sub>. Absolute value of the Hall coefficient vs. temperature. The excess metal content is as follows: Nd<sub>2</sub>S<sub>3</sub> (1): 0.7% Nd, Nd<sub>2</sub>S<sub>3</sub> (2): 0.65% Nd, Gd<sub>2</sub>S<sub>3</sub> (1): 0.6% Gd, Gd<sub>2</sub>S<sub>3</sub> (2): 0.6% Gd [74T].

