

**substance:** WSe<sub>2</sub>

**property:** crystal structure, physical properties

## 2H-WSe<sub>2</sub>

(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

$a$	3.282 Å	S: hexagonal, $D_{6h}^4 - P6_3/mmc$	62B,
$c$	12.937 Å	CG: (i) from polycrystalline mass, (ii) halogen transport (800/720)	67F, 69W,
		C: black	72A,

### resistivity, Seebeck coefficient, hole concentration

$\rho_{\perp}$	0.167 Ω cm	p-type,	$\sigma_{\perp}/\sigma_{\parallel} \approx 200$ ( $\rho_{\perp} = 1.3$ Ω cm [70W])	72B,
$S_{\parallel}$	990 μV K <sup>-1</sup>	synthetic		72D,
$p$	$2.35 \cdot 10^{17}$ cm <sup>-3</sup>	single crystal		77E, 78E,

### energy gap

$E_g$	1.78 eV		optical gap	79A
	1.73 eV		direct gap, calculated	
$E_{g,th}$	0.17 eV	$T < 300$ K		
	1.33 eV	$T > 890$ K		

### effective hole mass

$m_p$	0.01 $m_0$	optical effective hole mass
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### Hall mobility, Hall coefficient

$\mu_{H\perp}$	100 cm <sup>2</sup> /V s	n-type
$R_{H\perp}$	- 80 cm <sup>3</sup> /C	

### electron concentration

$n$	$1.25 \cdot 10^{16}$ cm <sup>-3</sup>
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### Figures to this document:

**band structure:** Fig. 1

**Brillouin zone:** Fig. 2

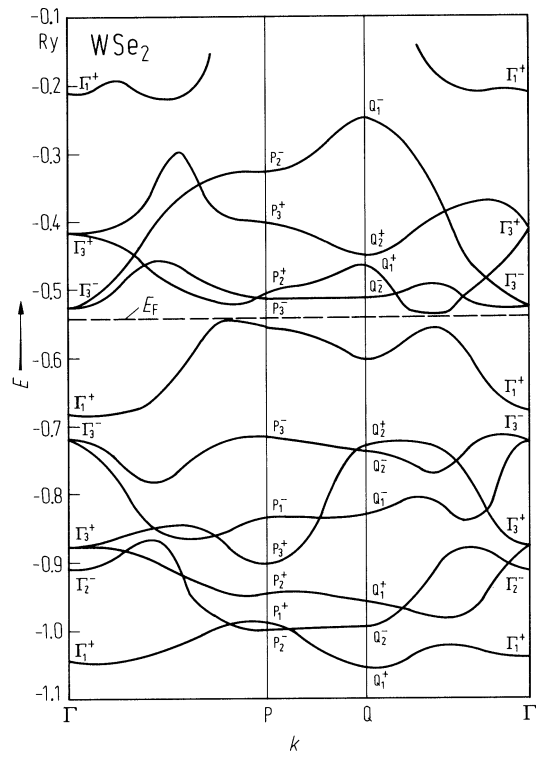
**carrier concentration:** Fig. 3

**electrical conductivity:** Fig. 4

## References:

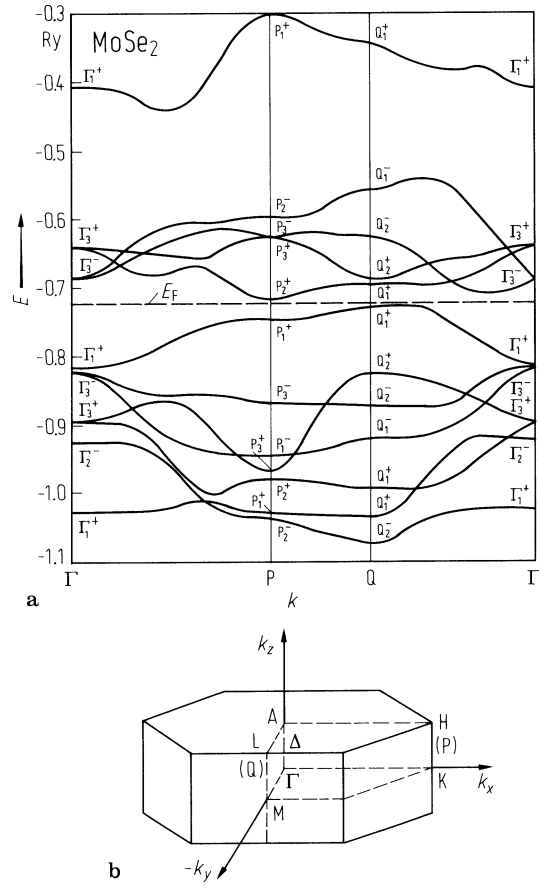
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WSe<sub>2</sub>. Band structure for 2H-modificaion [72B]; See Fig. 2 for Brillouin zone and for the meaning of P and Q.



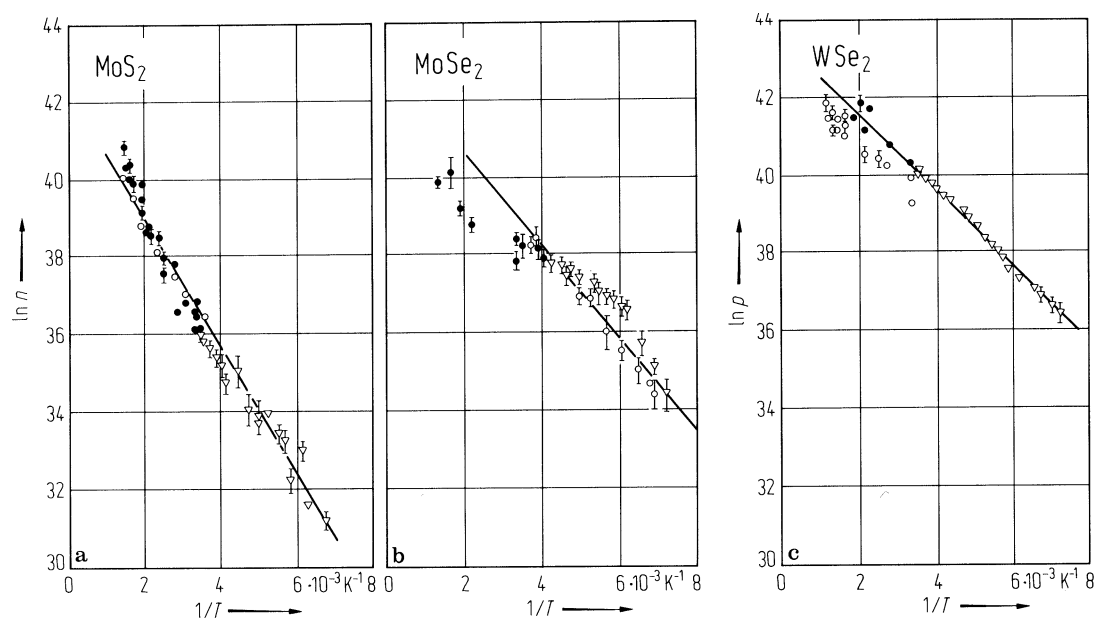
**Fig. 2.**

MoSe<sub>2</sub>. (a) Band structure and (b) Brillouin zone for 2H-MoSe<sub>2</sub> [72B]. Q and P are the middle of each edge and the vertex of the hexagon in the two-dimensional approximation used for the calculations.



**Fig. 3.**

MoS<sub>2</sub>, MoSe<sub>2</sub>, WSe<sub>2</sub>. Carrier concentration (in cm<sup>-3</sup>) vs. reciprocal temperature for (a) three different single crystal samples of n-type 2H-MoS<sub>2</sub>, (b) three different single crystal samples of n-type 2H-MoSe<sub>2</sub>, (c) three different single crystal samples of p-type 2H-WSe<sub>2</sub>. A line of representative slope is shown. Unless otherwise marked, the experimental errors are within the symbol representing each measurement [77E].



**Fig. 4.**

WSe<sub>2</sub>. Electrical conductivity vs. pressure at room temperature for 2H-modification [75F].  $\sigma$  in  $\Omega^{-1} \text{ cm}^{-1}$ .

