substance: $MoSe_2$
property: crystal structure, physical properties

2H-$MoSe_2$

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

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

lattice parameters

a	3.288 Å	S: hexagonal, D_{6h}^4 – $P6_3/mmc$	62B,
c	12.92 Å	(3R-$MoSe_2$ also exists with	69W,
		a = 3.292 Å, c = 19.392 Å)	71E
		CG: from polycrystalline mass	72A,
		at 1000°C	72B
		C: black	75G
			77E

resistivity, Seebeck coefficient, electron concentration

$\rho_\perp$	≈ 1...5 Ω cm	n-type,	$\sigma_\perp/\sigma_\parallel \approx 200$
$S_\perp$	– 900 µV K^{-1}	synthetic	
n	0.35...1.6·10^{17} cm^{-3}	single crystal	

energy gap

E_g	1.6 eV		optical gap,
			dE_g/dp = 1.2 meV/kbar
	1.6 eV		direct gap, calculated
$E_{g,th}$	0.28 eV	T < 300 K	
	0.95 eV	T > 760 K	

Figures to this document:

carrier concentration: Fig. 1

band structure, Brillouin zone: Figs. 2

References:

62B Brixner, L. H.: J. Inorg. Nucl. Chem. 24 (1962) 257.
69W Wilson, J. A., Yoffee, A. D.: Adv. Phys. 18 (1969) 193.
71E Evans, B. L., Hazelwood, R. A.: Phys. Status. Solidi (a) 4 (1971) 181.
72A AlHilli, A. A., Evans, B. L.: J. Cryst. Growth 15 (1972) 93.
72B Bromley, R. A., Murray, R. B., Yoffe, A. D.: J. Phys. C5 (1972) 759.
75G Grant, A. J., Griffiths, T. M., Pitt, G. D., Yoffe, A. D.: J. Phys. C 8 (1975) L17.
77E El-Mahalawy, S. H., Evans, B. L.: Phys. Status. Solidi (b) 79 (1977) 713.

Fig. 1.

MoS_2, $MoSe_2$, WSe_2. Carrier concentration (in cm^{-3}) vs. reciprocal temperature for (a) three different single crystal samples of n-type 2H–MoS_2, (b) three different single crystal samples of n-type 2H– $MoSe_2$, (c) three different single crystal samples of p-type 2H–WSe_2. A line of representative slope is shown. Unless otherwise marked, the experimental errors are within the symbol representing each measurement [77E].

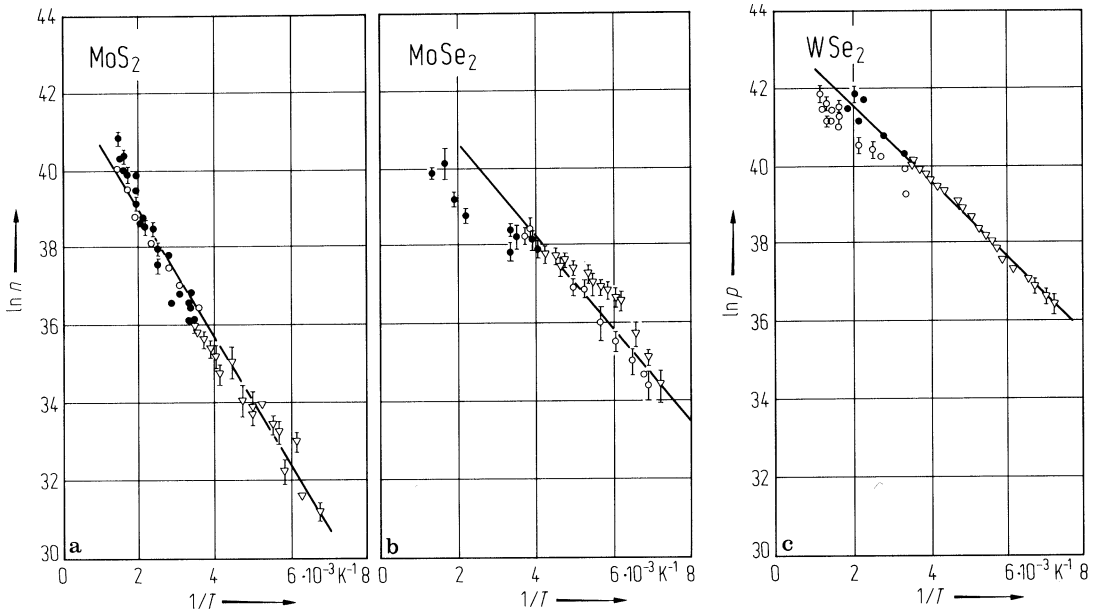

Fig. 2.

$MoSe_2$. (a) Band structure and (b) Brillouin zone for 2H-$MoSe_2$ [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.