substance: WS_2
property: crystal structure, physical properties

3R-WS_2

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

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

lattice parameters

a	3.162 Å		S: trigonal, C_{3v}^5 – R3m	64W,
c	18.50 Å		(hexagonal $P6_3/mmc$ also exists with a = 3.155 Å, c = 12.35 Å)	70W, 72B
			CG: (i) Na_2CO_3 flux at 900°C, (ii) halogen transport	

resistivity

$\rho_\perp$	0.04 Ω cm	synthetic single crystal
	0.1 Ω cm	natural crystal

energy gap

E_g	2.1 eV	direct gap, calculated
	2.07 eV	optical gap

Figures to this document:

band structure: Fig. 1

Brillouin zone: Fig. 2

References:

64W Wildervanck, J. C., Jellinek, F.: Z. Anorg. Allg. Chem. 328 (1964) 309,
70W Wieting, T. J.: J. Phys. Chem. Solids 31 (1970) 2148.
72B Bromley, R. A., Murray, R. B., Yoffe, A. D.: J. Phys. C5 (1972) 759.

Fig. 1.

WS_2. Band structure [72B]; see Fig. 2 for Brillouin zone and for the meaning of P and Q.

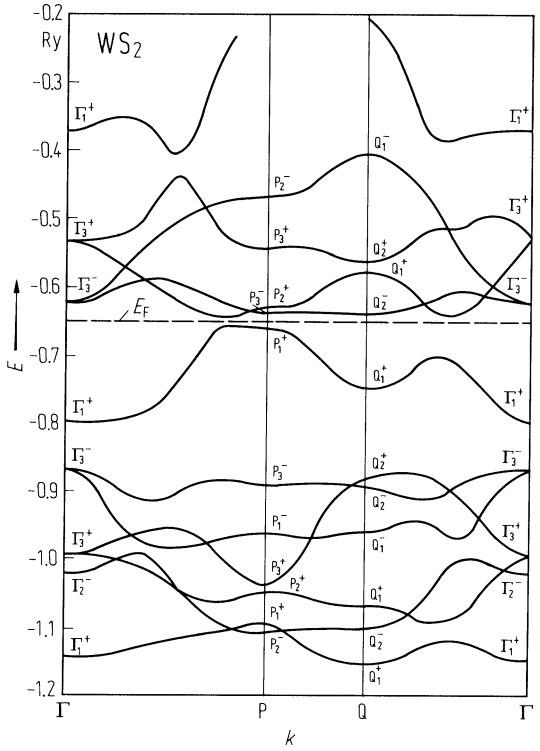

Fig. 2.

$MoSe_2$. (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.