substance: HfS_2
property: crystal structure, physical properties

(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	3.622 Å		S: C6, $D_{3d}^3 - P\bar{3}m1$	65G,
c	5.88 Å		CG: halogen transport (900/800)	68C,
			C: dark-red metallic	70W,
				78B

resistivity

$\rho_\perp$	$3.3 \cdot 10^7$ ...10^8 Ω cm	n-type, synthetic single crystal

energy gap

E_g	1.96 eV		optical gap, $dE_g/dT = -4.3 \cdot 10^{-4}$ eV/K
	1.9 eV		indirect gap, calculated
$E_{g,th}$	2.1 eV	$T > 500$ K	

Figures to this document:

band structure, density of states: Fig. 4

Brillouin zone : Fig. 1b

electrical conductivity : Fig. 2

reflectivity : Fig. 3

References:

65G Greenaway, D. L., Nitsche, R.: J. Phys. Chem. Solids 26 (1965) 1445.
68C Conroy, L. E., Park, K. C.: Inorg. Chem. 7 (1968) 459.
70W Wieting, T. J.: J. Phys. Chem. Solids 31 (1970) 2148.
78B Bullett, D. W.: J. Phys. C 11 (1978) 4501.

Fig. 1.

TiS_2. (a) Band structure and density of states. (b) Brillouin zone [78B].

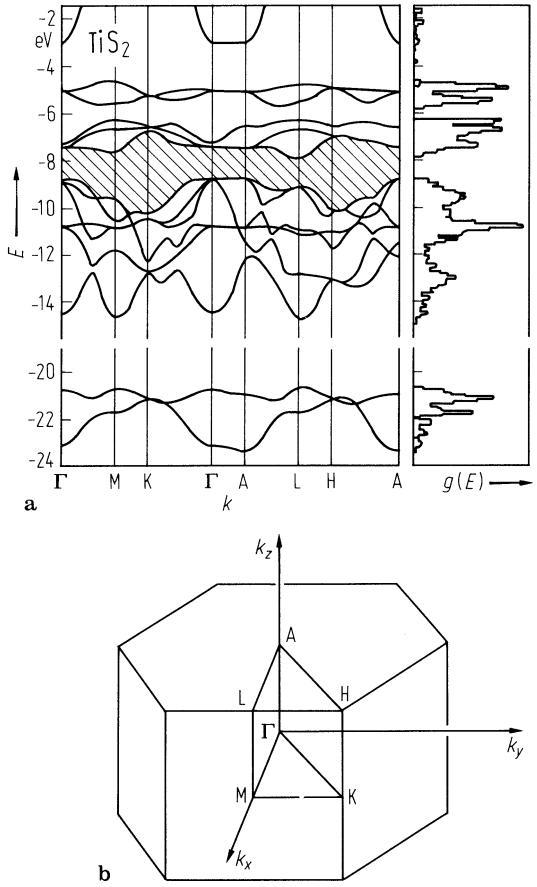

Fig. 2.

HfS_2. Electrical conductivity ($\sigma \perp c$) vs. reciprocal temperature for a single crystal [68C].

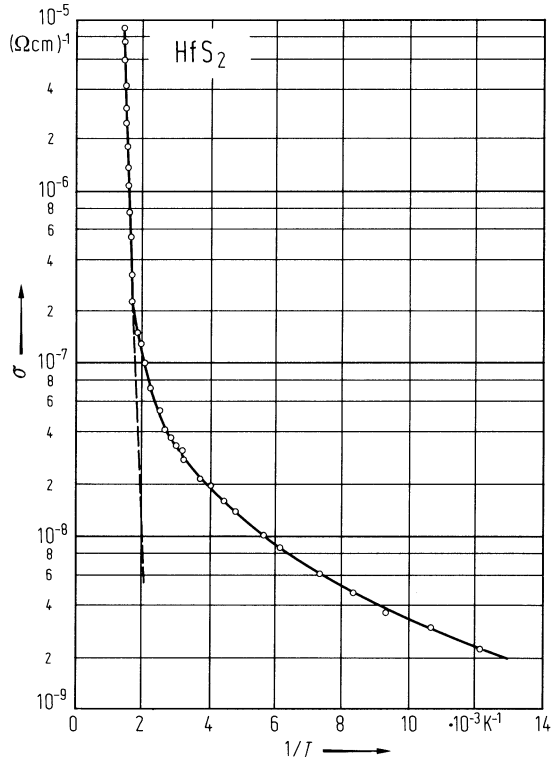

Fig. 3.

HfS_2. Reflectivity vs. photon energy in the fundamental region at room temperature [65G].

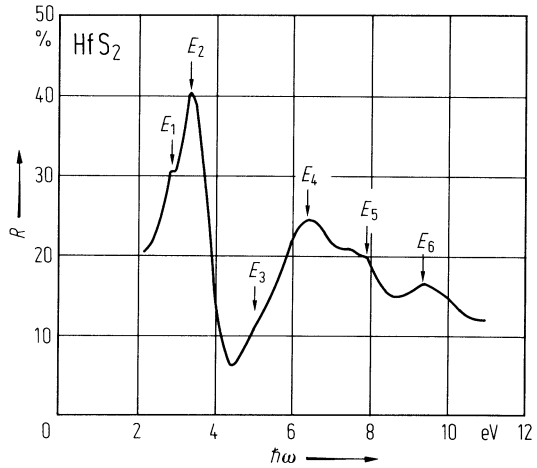

Fig. 4.

HfS_2. Band structure and density of states [78B]. See Fig. 1b for Brillouin zone.