substance: $HfSe_2$
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	3.733 Å		S: C6, $D_{3d}^3 - P\bar{3}m1$	65G,
c	6.146 Å		CG: halogen transport (900/800)	73B,
			C: dark-red metallic	78B

energy gap

E_g	1.05 eV	synthetic	$dE_g/dT = -6.8 \cdot 10^{-4}$ eV/K
		single crystal	(E_g: optical gap)
	1.1 eV		indirect gap, calculated

Figures to this document:

band structure, density of states: Fig. 3

Brillouin zone: Fig. 1b

reflectivity: Fig. 2

References:

65G Greenaway, D. L., Nitsche, R.: J. Phys. Chem. Solids 26 (1965) 1445.
73B Brattas, L., Kjekshus, A.: Acta Chem. Scand. 27 (1973) 1290.
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].

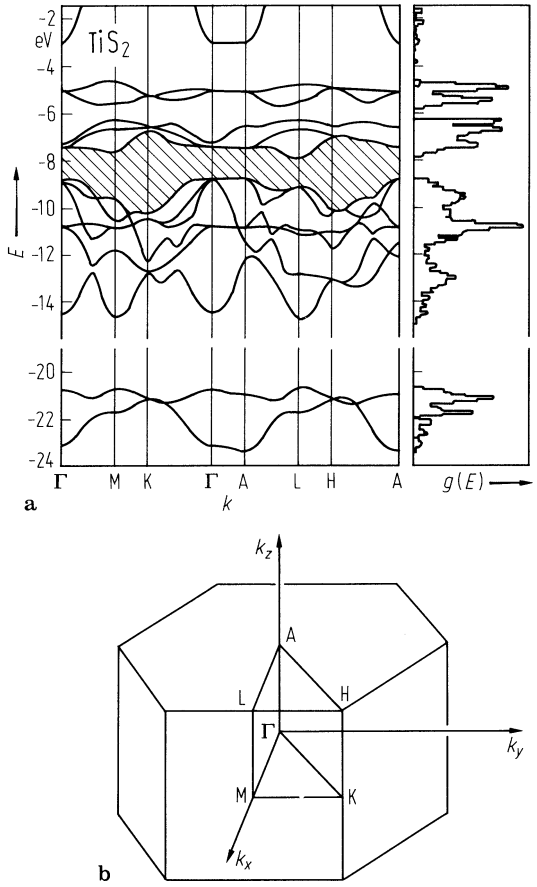

Fig. 2.

$HfSe_2$. Reflectivity vs. photon energy in the fundamental region at room temperature [65G].

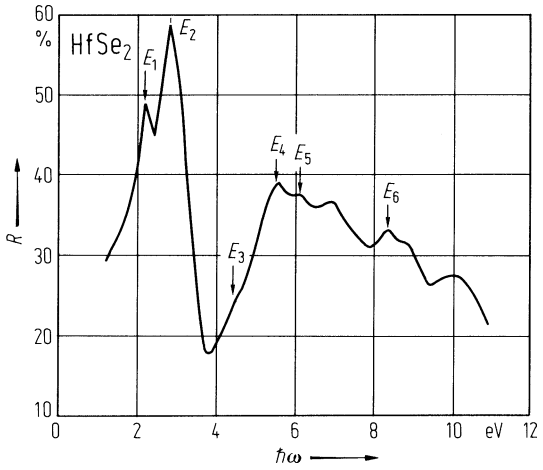

Fig. 3.

$HfSe_2$. Band structure and density of states [78B]. See Fig. 1b for Brillouin zone.