substance: WO_3
property: band structure, energy gap

band structure: No calculation of monoclinic or triclinic WO_3 has been reported but a calculation of cubic $NaWO_3$ and idealized cubic WO_3 [77K]) gives the band structure of Fig. 1. The $NaWO_3$ density of states is shown in Fig. 2. Strong covalent interaction is evident.

energy gap

(due to O(2p) – W(5d) transitions)

E_g	2.585 eV	T = 300 K, $E \parallel [0\,0\,1]$	absorption, see Fig. 3 for absorption coefficient, Fig. 4	74S, 76H
	3.1 eV	T = 0 K	for temperature shift (extrapolated)	
dE_g/dT	$-9.0\cdot10^{-4}$ eV K^{-1}	*a*-polarized light	in the temperature range 0...700°C	60I
	$-6.5\cdot10^{-4}$ eV K^{-1}	*c*-polarized light		

References:

60I Iwai, T.: J. Phys. Soc. Jpn. 15 (1960) 1596.
72S Schröder, F. A., Felser, H.: Z. Kristallogr. 135 (1972) 391.
74S Salje, E.: J. Appl. Crystallogr. 7 (1974) 615.
76H Hollinger, G., Tranh Minh Duc, Deneuville, A.: Phys. Rev. Lett. 37 (1976) 1564.
77K Kopp, L., Harmon, H. N., Liu, S. H.: Solid State Commun. 22 (1977) 677.

Fig. 1.

WO_3. Energy bands of ideal cubic WO_3 along the major symmetry axes [77K].

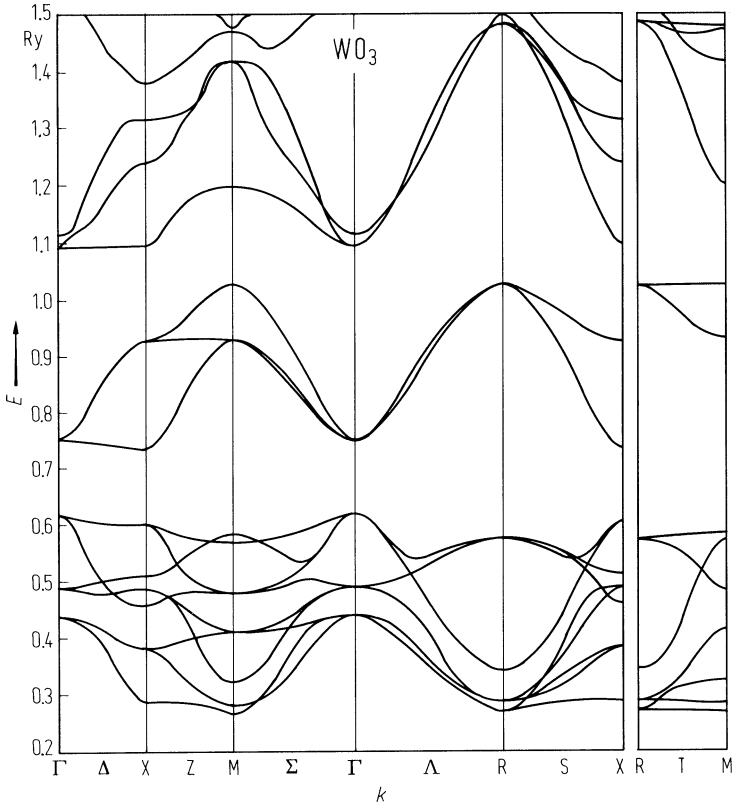

Fig. 2.

$NaWO_3$. Orbital density of states together with their sum (a) and total density of state (b) [77K].

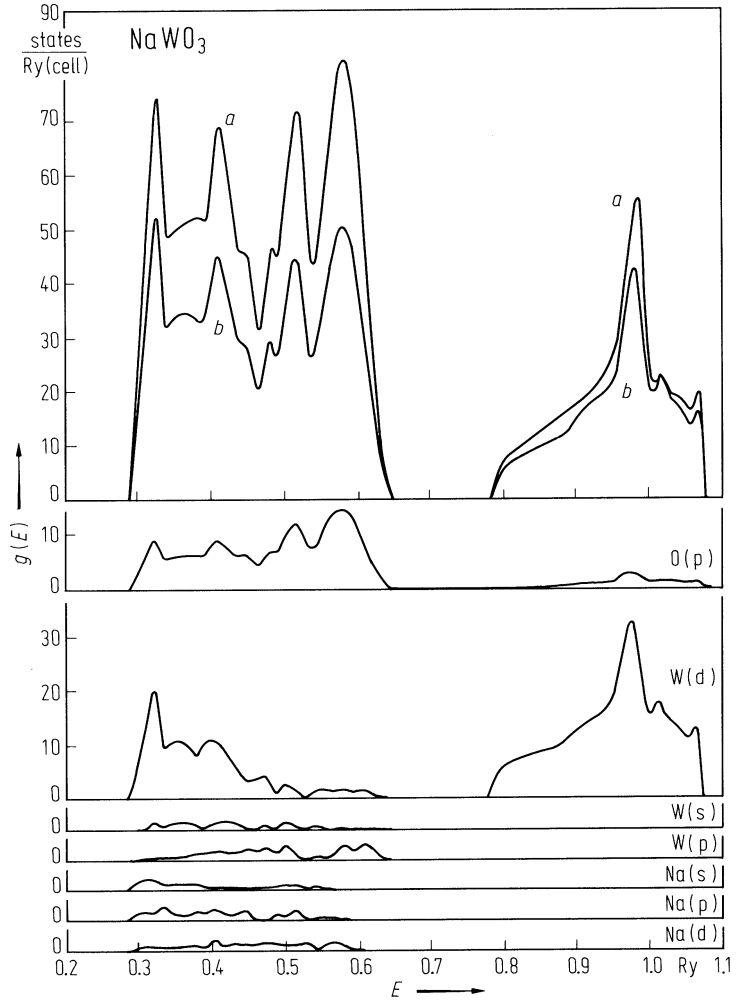

Fig. 3.

WO_3. Transmission vs. wavelength in [001]-direction at RT [72S].

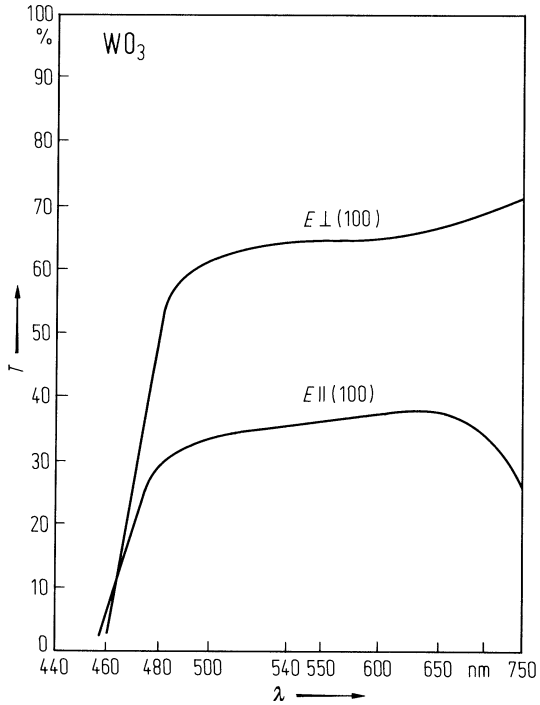

Fig. 4.

WO_3. Optical absorption edge vs. temperature in the *b* plane (a), in the *c* plane (b), in the *c* plane (c) at low temperature [60I].