

substance: chromium sesquioxide (Cr₂O₃)

property: optical properties, dielectric constants

The visible spectrum is dominated by ligand-field transitions (Fig. 2). The UV-spectrum from Kramers-Kronig analysis is shown in Fig. 3. The wavelength modulated reflectance spectrum shows structure at 2.1 eV ($^4A_{2g} \rightarrow ^4T_{2g}$) 2.4...2.5eV ($^4A_{2g} \rightarrow ^2T_{2g}$) and 2.6 eV ($^4A_{2g} \rightarrow ^4T_{1g}$) [72B]. At higher energies, both spectra show the energy gap to be at 3.3 eV. The transition has been assigned to a charge transfer process; O 2p – Cr 3d. This assignment again suggests that the cluster calculation of Fig. 1 greatly overestimates the 3d – 2p energy separation.

dielectric constants

(see also Fig. 4)

$\epsilon(0)$	10.33	RT, $E \perp c$	from ir active E_u -modes	65R,
$\epsilon(\infty)$	5.73			77L
$\epsilon(0)$	10.93	RT, $E \parallel c$	from ir active A_{2u} -modes	
$\epsilon(\infty)$	5.97			
$\epsilon(0)$	13.0	$T = 303$ K	from ac measurement at $\nu \geq 106$ Hz on single crystals with electric field along the a axis	77R

References:

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Fig. 1.

Cr_2O_3 . SCF-X α scattered wave valence MO diagrams for (a) a CrO_6^{9-} cluster, (b) CrO_6^{8-} 2p hole state, (c) Cr_6^{8-} 2t_{2g} valence hole state [76T]. Arrows indicate spin direction.

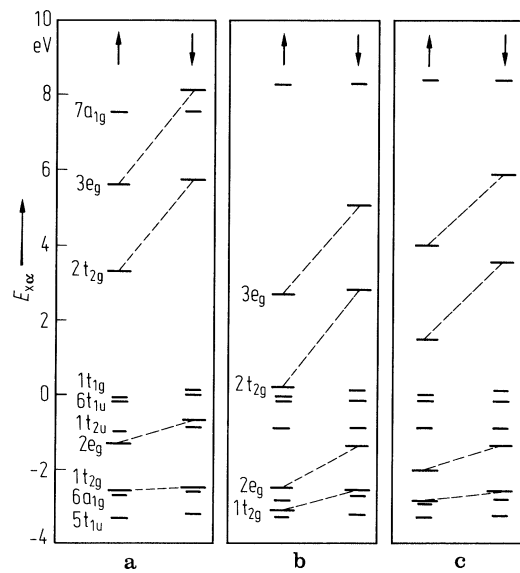


Fig. 2.

Cr_2O_3 . Absorbance vs. wavenumber in the visible region; I Cr_2O_3 , II $\text{Cr}_{0.1}\text{Al}_{1.9}\text{O}_3$; Solid line: $T = 4\text{ K}$, dashed line: $T = 300\text{ K}$ [74G].

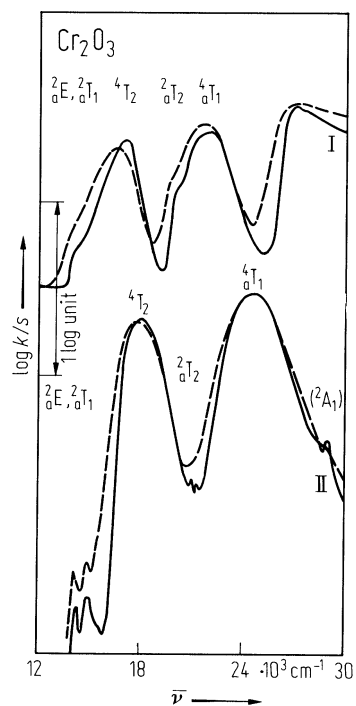


Fig. 3.

Cr_2O_3 . Imaginary part of the dielectric constant vs. photon energy for two different samples [77A].

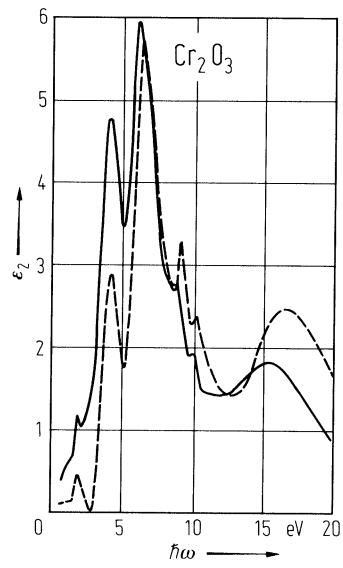


Fig. 4.

Cr_2O_3 . Real part of the dielectric constant vs. temperature for a single crystal with and without impressed magnetic fields; (a) without magnetic fields, (b) $H = 3.5$ kOe, (c) $H = 9$ kOe [67L].

