substance: Fe_3O_4
property: phonon dispersion, phonon wavenumbers

phonon dispersion spectrum: Fig. 1.

In the cubic phase the symmetries of lattice modes at Γ are given by

$\Gamma = a_{1g} + e_g + t_{1g} + 3t_{2g} + 2a_{2u} + 2e_u + 4t_{1u} + 2t_{2u}$.

wavenumbers of IR and Raman active modes

IR-active modes (in cm^{-1}) (see Figs. 2, 3)

$(\nu/c)_1(t_{1u})$	565	$T > T_V$	Fe – O stretch at both (tetrahedral) A and (octahedral) B sites	72I
	570			72G
	570			77K
	615,585	$T < T_V$		77K
$(\nu/c)_2(t_{1u})$	360	$T > T_V$		72I
	390			72G
	380			77K
	420, 405, 375	$T < T_V$		77K
$(\nu/c)_3(t_{1u})$	268	$T > T_V$	motion of $Fe_{tetr.}$ vs. $Fe_{oct.}$	72G
$(\nu/c)_4(t_{1u})$	178	$T > T_V$	O–Fe–O bending mode	72G

Raman active modes (see Fig. 4)

$(\nu/c)_R(a_{1g})$	680	T = 77 K	see also Fig. 2. Five Raman active modes are expected in the cubic phase and 15 in the orthorhombic phase (T < 119 K) but only five are observed in both phases. No dramatic changes are noted in passing through the Verwey transitions. All lines are anomalously broad (30 cm^{-1}) even at low temperatures.	74V
$(\nu/c)_R(t_{2g})$	560			
	320			
	300			
$(\nu/c)_R(e_g)$	420			

No soft mode observed at T_V.

References:

72G Grimes, N. W.: Philos. Mag. 26 (1972) 1217.
72I Ishii, M., Nakahiri, M.: Solid State Commun. 11 (1972) 209.
74S Sarmelson, E. J., Steinsvoll, O.: Phys. Status Solidi (b) 61 (1974) 615.
74V Verble, J. L.: Phys. Rev. B9 (1974) 5236.
77K Kuipers, A. J. M., Brabers, V. A. M.: Phys. Rev. Lett. 39 (1977) 488.

Fig. 1.

Fe_3O_4. Phonon dispersion curves at 300 K for the principal symmetry directions [74S]. Squares: longitudinal modes; circles: transverse modes; open symbols: observations in [110] zone, filled symbols: observations in [100] zone; small symbols: observations with 13.8 meV incident energy neutrons, large symbols: observations with 38 meV incident energy neutrons. Circles with crosses: observations with time of flight. Solid lines: confidently assigned, dotted and dashed lines: tentatively assigned, dot-dash lines near the Γ point: ultrasonic measurements, IR: measured by [72G].

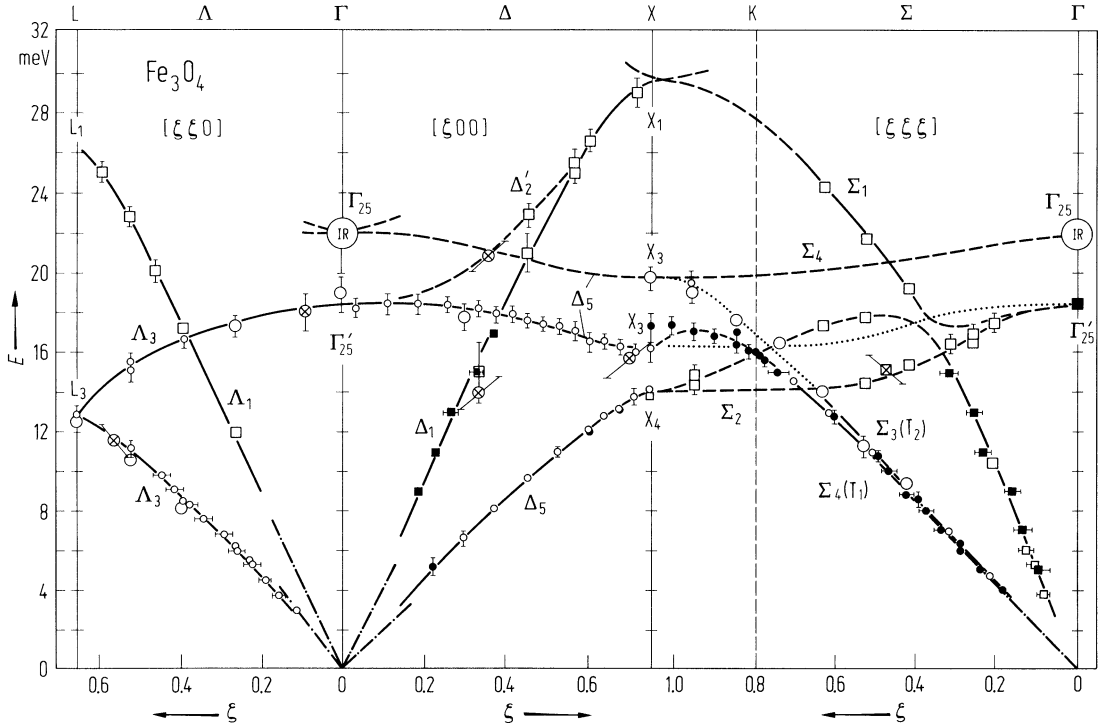

Fig. 2.

Fe_3O_4. Normal modes of a cubic spinel [72I, 74V]. (a) IR active modes; (b) Raman active modes.

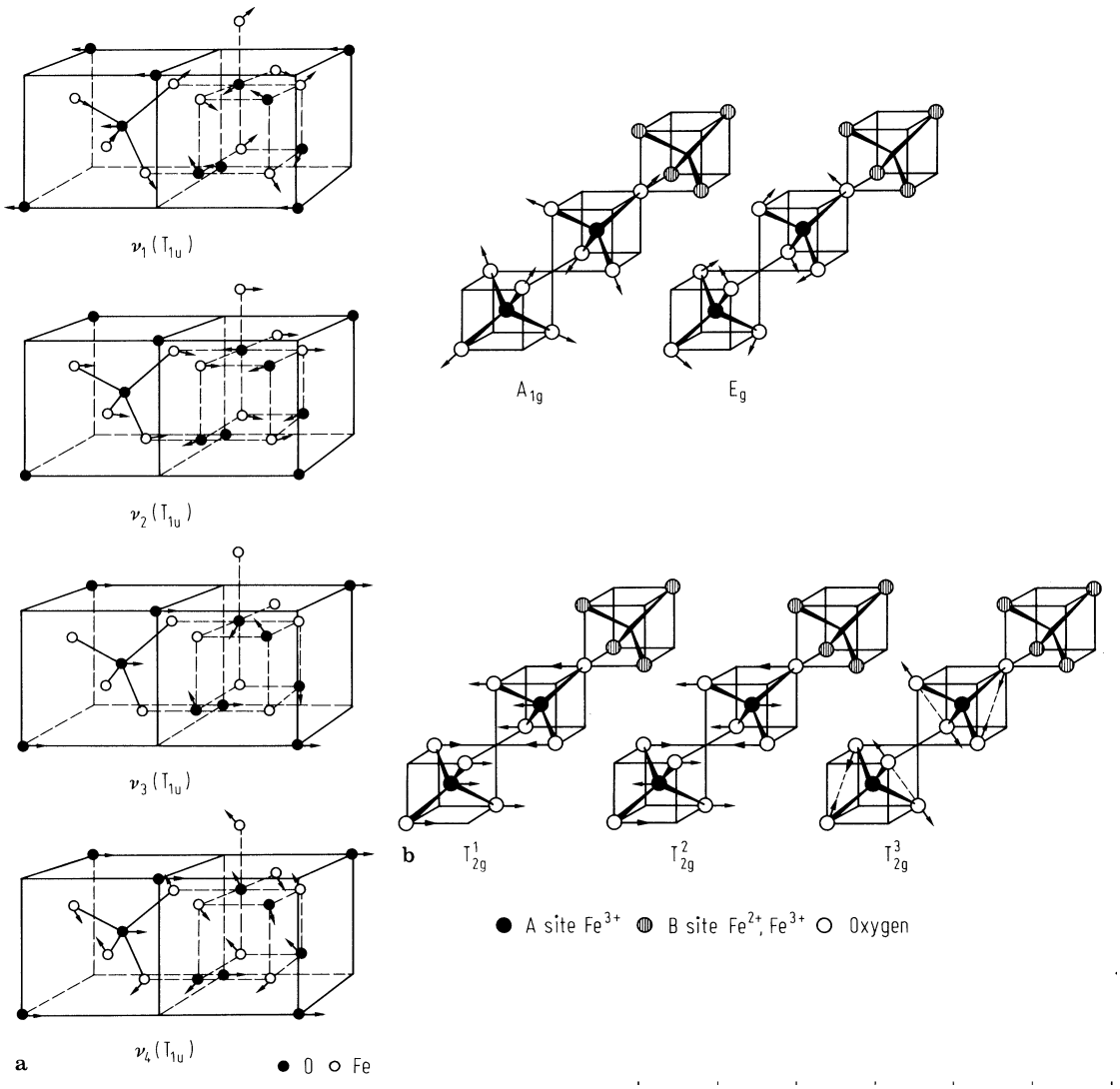

Fig. 3.

Fe_3O_4, $Fe_{2.8}Ti_{0.2}O_4$. Transmission vs. wavenumber at 77 K [77K].

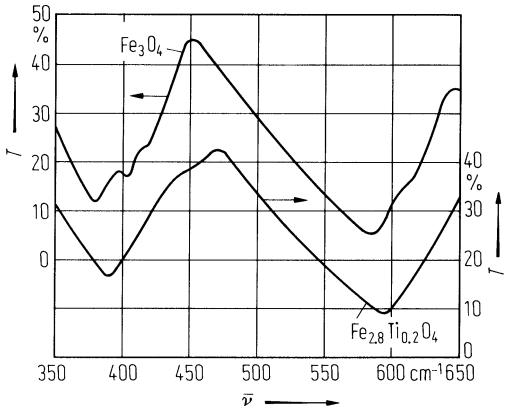

Fig. 4.

Fe_3O_4. Wavenumber and linewidth of the highest frequency mode vs. temperature [74V]. This phonon has A_{1g} symmetry in the cubic phase and A_g symmetry in the low-temperature (orthorhombic) phase.