

substance: V₂O₃

property: phonon wavenumbers, elastic moduli, Debye temperature

phonon wavenumbers

$\nu/)$	203 cm ⁻¹	$T = 300$ K	assignment: E _g	77K
	209 cm ⁻¹			77M
	231 cm ⁻¹		A _{1g}	77K
	238 cm ⁻¹			77M
	290 cm ⁻¹		E _g	77K
	290 cm ⁻¹			77M
	500 cm ⁻¹		A _{1g}	77K
	500 cm ⁻¹			77M
	590 cm ⁻¹		E _g	77K

Raman spectrum in the temperature range 4...300 K: Fig. 1. A peak at 450 cm⁻¹ in the antiferromagnetic phase disappears at T_{tr} and is ascribed to a magnon [77K].

elastic moduli

(in dyn cm⁻²)

c_{11}	$25.6(6) \cdot 10^{11}(1-7.1(3) \cdot 10^{-4}(T-273))$	$T = 150...273$ K	76A
c_{12}	$6.7(8) \cdot 10^{11}(1-2.2(1) \cdot 10^{-4}(T-273))$		
c_{14}	$1.7(3) \cdot 10^{11}(1-13.6(4) \cdot 10^{-4}(T-273))$		
c_{13}	$15.0(2) \cdot 10^{11}(1-8.8(3) \cdot 10^{-4}(T-273))$		
c_{33}	$33.6(3) \cdot 10^{11}(1-1.9(2) \cdot 10^{-4}(T-273))$		
c_{44}	$8.0(3) \cdot 10^{11}(1+5.3(2) \cdot 10^{-4}(T-273))$		
c_{11}	$26.5 \cdot 10^{11}$	RT	79Y
c_{12}	$7.15 \cdot 10^{11}$		
c_{33}	$31.6 \cdot 10^{11}$		
c_{44}	$8.55 \cdot 10^{11}$		

Debye temperature

Θ_D	643 K	from elastic constants, $T = 150...273$ K	76A
	610 K	from heat capacity, $T = 150...273$ K	66G
	585 K	from heat capacity, $T = 0.4...30$ K	75W
	575 K	from heat capacity, $T = 0.3...30$ K under pressure	73M

References:

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Fig. 1.

V_2O_3 . Stokes shift $\Delta(\nu/c)$ of Raman wavenumber vs. temperature [77K]. T was estimated by a thermosensor, if needed a better estimate was obtained from the intensity ratios of the Stokes/anti-Stokes scatterings.

