substance: VO_2
property: phonon wavenumbers, Debye temperature, heat capacity

wavenumbers of phonon modes

infrared-active modes

ν/c	189 cm^{-1}	$E \perp a_m$	low-temperature phase	66B
	270 cm^{-1}		(no IR modes seen in high-	
	310 cm^{-1}		temperature phase)	
	340 cm^{-1}		Vibrational absorption peaks at	
	505 cm^{-1}		435, 535 and 680 cm^{-1} reported	
	600 cm^{-1}		by [80R]; on 18.7 at % ^{18}O doping	
	710 cm^{-1}		these decrease to 428, 530 and	
	227.5 cm^{-1}	$E \parallel a_m$	667 cm^{-1}, respectively [80R].	
	285 cm^{-1}			
	324 cm^{-1}			
	355 cm^{-1}			
	392.5 cm^{-1}			
	478 cm^{-1}			
	530 cm^{-1}			
	700 cm^{-1}			

Raman-active modes

$(\nu/c)_R$	149 cm^{-1}	low-	assignment: –	71S,
	200 cm^{-1}	temperature	A_g	77A
	226 cm^{-1}	phase	A_g	
	259 cm^{-1}		A_g	
	313 cm^{-1}		A_g	
	340 cm^{-1}		A_g	
	392 cm^{-1}		A_g	
	501 cm^{-1}		A_g	
	594 cm^{-1}		B_g	
	620 cm^{-1}		A_g	
	550 cm^{-1}	high-	broad band	
	300 cm^{-1}	temperature	weak band	
		phase	at $T \rightarrow T_{tr}$ the bands are broadened considerably (Fig. 1). This suggests a considerable role for the lattice in the transition	

Debye temperature

Θ_D	750(20) K	heat capacity data 150...300 K	73C

heat capacity

C_p	$0.068(4)\cdot10^{-4}\ T^3$ cal K^{-1} mol^{-1}	$T \le 25$ K	for VO_2	73M
	$80(5)\ T + (0.127(10)\cdot10^{-4})\ T^3$ cal K^{-1} mol^{-1}	$T \le 25$ K	for $W_{0.14}V_{0.86}O_2$	73M

References:

66B Barker, A. S., Verleur, H. W., Guggenheim, H. J.: Phys. Rev. Lett. 17 (1966) 1286.

71S Srivastava, R., Chase, L. L.: Phys. Rev. Lett. 27 (1971) 727.

73C Chandrashekhar, G. V., Barros, H. L. C., Honig, J. M.: Mater. Res. Bull. 8 (1973) 369.

73M McWhan, D. B., Remeika, J. P., Maita, J. P., Okinaka, H., Kosuge, K., Kachi, S.: Phys. Rev. B7 (1973) 326.

77A Aronov, A. G., Mirlin, D. N., Reshina, I. I., Chudnovskii, F. A.: Fiz. Tverd. Tela 19 (1977) 193.

80R Reichelt, W., Oppermann, H., Wagner, H., Terukov, E. I., Wolf, E.: Z. Anorg. Allg. Chem. 463 (1980) 193.

Fig. 1.

VO_2:Nb. Line widths Γ of lattice modes: (a) 223 cm^{-1} line, (b) 389 cm^{-1} line, (c) temperature dependence of the same lines in polycrystalline samples [77A]. Curves *1, 2. 3* refer to VO_2, $V_{0.983}Nb_{0.017}O_2$ and $V_{0.976}Nb_{0.024}O_2$.