substance: V_2O_5
property: phonon wavenumbers

wavenumbers of lattice vibration modes

(in cm^{-1}).The following data are taken from: A [72R], B [73G], C [73B], D [76C], Kramers-Kronig analysis, E [76C], classical oscillator dispersion, F [76C], 4-parameter oscillator dispersion, G [76C] single crystal transmission, H [76C] powder transmission. First column $(\nu/c)_{TO}$, second column: $(\nu/c)_{LO}$.

$(\nu/c)_1$	74		B	$E \parallel a$,	the lattice vibrations of crystals
	73.5	78.5	C	b_{3u}-type	with space group D_{2h}^{13} – Pmnm can
	71.9	78.1	D		be classified by
	72.0	77.0	F		
	72.4	76.2	F		$\Gamma = 7a_g + 7b_{1g} + 3b_{2g} + 4b_{3g} + 3a_u$
$(\nu/c)_2$	255.3	266	A		$+ 3b_{1u} + 6b_{2u} + 6b_{3u}$
	265		B		
	261	269	C		for E and F the paper cited [76C]
	259.1	267.0	D		also contains data on other fitting
	260.0	267.8	E		parameters
	261.0	265.5	F		
	262		H		
$(\nu/c)_3$	308.8	389	A		
	386		B		
	305	392	C		
	301.6	389.4	D		
	303.0	387.9	E		
	303.0	390.5	F		
	370		H		
$(\nu/c)_4$	408.5	582	A		
	520		B		
	412	602	C		
	410.5	585.0	D		
	410.5	582.7	E		
	411.0	586.0	F		
	472		H		
$(\nu/c)_5$	778.0	957	A		
	880		B		
	796	975	C		
	765.5	965.0	D		
	765.0	952.4	E		
	767.5	959.0	F		
	813		H		
$(\nu/c)_6$	995		B		
	980.7	987.0	D		
	981.0	986.4	E		
	980.5	982.0	F		
	982		G		
		982	H		

$(\nu/c)_1$	144		B	$E \parallel b$,
$(\nu/c)_2$	481		B	b_{2u}-type
	476.5	494	C	
	472.2	492.0	D	
	473.5	494.2	E	
	473.0	490.0	F	
	1038		G	
$(\nu/c)_3$	1035		B	
	974.1	1039.5	D	
	975.0	1037.7	E	
	975.5	1038.0	F	
	1023		H	
$(\nu/c)_1$	213.4	225	A	$E \parallel c$,
	220		B	b_{1u}-type
	214	226	C	
	212.6	226.2	D	
	212.6	226.0	E	
	212.0	225.0	F	
	217		H	
$(\nu/c)_2$	284.2	312	A	
	308		B	
	287	315	C	
	285.4	314.3	D	
	283.5	314.4	E	
	284.0	312.5	F	
	294		H	
$(\nu/c)_3$	515.0	850	A	
	700		B	
	532	865	C	
	506.0	844.0	D	
	505.7	842.4	E	
	506.5	842.5	F	
	605H			

wavenumbers of Raman active lattice vibrations

$(\nu/c)_R$ [cm^{-1}]	104, 198, 306, 406, 482, 530, 995	a_g-type	73G
	201, 310, 355, 502?, 954?, 995	b_{1g}-type	
	144, 284, 701	b_{2g}-type	
	147, 230, 287, 701	b_{3g}-type	

wavenumbers of additional far IR peaks

(All values for T = 4...78 K, except (ν/c) = 14 cm^{-1}) Such peaks have been found for doping with monovalent ions.

(ν/c)	29.5 cm^{-1}		doping with Li	77B
	56.5 cm^{-1}			
	14 cm^{-1}	$T \approx 4$ K		
	94 cm^{-1}			
	29.5 cm^{-1}		doping with Na	
	53.0 cm^{-1}			
	28.5 cm^{-1}		doping with Cu	
	53.0 cm^{-1}			

The EPR evidence suggests that the e^- from these ions is delocalized over four vanadium ions in the *b*-planes. The 4-centre MO is split into components by the local field, and the FIR absorption has been ascribed to transitions between these components [77B].

References:

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77B Broeskx, J., Clauws, P., Vennik, J.: Solid State Commun. 22 (1977) 577.