substance: NbO_2
property: phonon wavenumbers

The following data are best fit oscillator parameters for IR reflectance (Fig. 1) at room temperature. When the mode is very weak and the TO–LO splitting very small only the TO wavenumber is indicated. First column: $(\nu/c)_{TO,LO}$ (in cm^{-1}), second column: contribution of this mode to $\varepsilon(0) - \varepsilon(\infty)$, third column: damping parameter γ of the oscillator equation (in cm^{-1}).

$(\nu/c)_{TO}$ ($E \parallel c$)	255	0.78	20	with these parameters the	79G
$(\nu/c)_{LO}$	257		20	dielectric constants become	
$(\nu/c)_{TO}$	318	8.23	35	$\varepsilon(\infty) = 7.4$, $\varepsilon(0) = 17.5$	
$(\nu/c)_{LO}$	366		8		
$(\nu/c)_{TO}$	368	0.18	8		
$(\nu/c)_{LO}$	415		16		
$(\nu/c)_{TO}$	434	0.38	16		
$(\nu/c)_{LO}$	480		11		
$(\nu/c)_{(TO,LO)}$	550	0.02	(20)		
$(\nu/c)_{TO}$	613	0.16	20		
$(\nu/c)_{LO}$	621		20		
$(\nu/c)_{TO}$	689	0.42	25		
$(\nu/c)_{LO}$	720		25		
$(\nu/c)_{TO}$ ($E \perp c$)	164	2.1	2.4	with these parameters the	79G
$(\nu/c)_{LO}$	168		2.4	dielectric constants become	
$(\nu/c)_{TO}$	222	10.9	8	$\varepsilon(\infty) = 7.2$, $\varepsilon(0) = 28$	
$(\nu/c)_{LO}$	243		12		
$(\nu/c)_{TO}$	245	0.73	12		
$(\nu/c)_{LO}$	264		5		
$(\nu/c)_{TO}$	275.5	1.37	5		
$(\nu/c)_{(TO,LO)}$	291	0.13	(12)		
$(\nu/c)_{LO}$	302.5		6		
$(\nu/c)_{TO}$	306	0.19	6		
$(\nu/c)_{LO}$	329		7		
$(\nu/c)_{(TO,LO)}$	350	0.03	(10)		
$(\nu/c)_{(TO,LO)}$	370	0.02	(10)		
$(\nu/c)_{TO}$	397	0.15	18		
$(\nu/c)_{LO}$	400		18		
$(\nu/c)_{TO}$	464	0.22	30		
$(\nu/c)_{LO}$	467		30		
$(\nu/c)_{TO}$	499	0.25	30		
$(\nu/c)_{LO}$	502		30		
$(\nu/c)_{TO}$	572	4.24	29		
$(\nu/c)_{LO}$	677		16		
$(\nu/c)_{TO}$	696	0.31	15		
$(\nu/c)_{(TO,LO)}$	770	0.01	(30)		
$(\nu/c)_{LO}$	800.5		20		

References:

79G Gervais, F., Baumard, J. F.: J. Phys. C12 (1979) 1977.

Fig. 1.

NbO_2. Reflectivity vs. wavenumber for $E \parallel c$ and $E \perp c$. -o-o-: experimental, —— model calculation using parameters in the text [79G].